



## Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 11:44 AM UTC

PDB ID : 6ZP4 / pdb\_00006zp4  
EMDB ID : EMD-11335  
Title : SARS-CoV-2 Nsp1 bound to a human 43S preinitiation ribosome complex - state 2  
Authors : Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.  
Deposited on : 2020-07-08  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

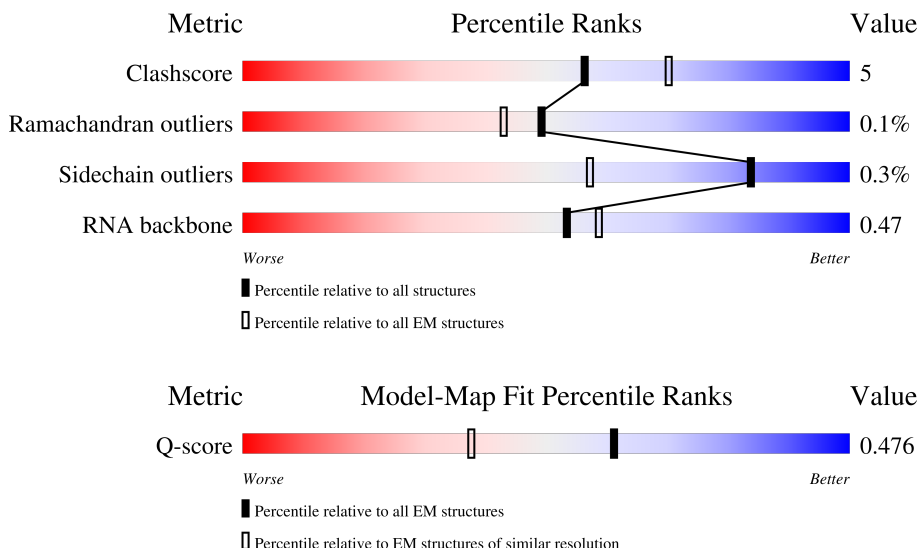
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



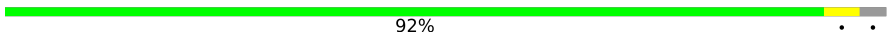
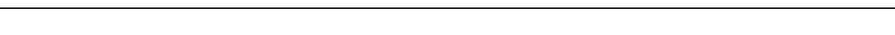
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | a     | 295    |                  |
| 2   | p     | 264    |                  |
| 3   | d     | 293    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | Q     | 115    |    |
| 5   | q     | 263    |    |
| 6   | W     | 25     |    |
| 7   | r     | 249    |    |
| 8   | s     | 194    |    |
| 9   | t     | 208    |    |
| 10  | c     | 194    |    |
| 11  | n     | 158    |    |
| 12  | m     | 151    |    |
| 13  | y     | 83     |    |
| 14  | D     | 130    |    |
| 15  | z     | 133    |    |
| 16  | R     | 84     |  |
| 17  | T     | 59     |  |
| 18  | 2     | 1868   |  |
| 19  | w     | 135    |  |
| 20  | b     | 243    |  |
| 21  | e     | 204    |  |
| 22  | u     | 165    |  |
| 23  | v     | 132    |  |
| 24  | o     | 145    |  |
| 25  | g     | 146    |  |
| 26  | k     | 152    |  |
| 27  | x     | 145    |  |
| 28  | h     | 119    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | P     | 125    |                  |
| 30  | S     | 69     |                  |
| 31  | l     | 56     |                  |
| 32  | U     | 156    |                  |
| 33  | V     | 317    |                  |
| 34  | i     | 151    |                  |
| 35  | j     | 143    |                  |
| 36  | G     | 144    |                  |
| 37  | I     | 325    |                  |
| 38  | B     | 814    |                  |
| 39  | A     | 1382   |                  |
| 40  | C     | 913    |                  |
| 41  | E     | 445    |                  |
| 42  | F     | 357    |                  |
| 43  | H     | 352    |                  |
| 44  | K     | 218    |                  |
| 45  | L     | 564    |                  |
| 46  | M     | 374    |                  |
| 47  | N     | 548    |                  |
| 48  | X     | 78     |                  |
| 49  | 1     | 75     |                  |
| 50  | 4     | 333    |                  |
| 51  | O     | 315    |                  |
| 52  | Y     | 472    |                  |
| 53  | Z     | 113    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 54  | J     | 180    |  |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 117784 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 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | a     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1705  | 1083 | 299 | 315 | 8 |         |       |
|     |       |          |       |      |     |     |   |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | p     | 211      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1715  | 1088 | 307 | 306 | 14 |         |       |
|     |       |          |       |      |     |     |    |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | d     | 216      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1674  | 1085 | 287 | 292 | 10 |         |       |
|     |       |          |       |      |     |     |    |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | Q     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 814   | 507 | 170 | 132 | 5 |         |       |
|     |       |          |       |     |     |     |   |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | q     | 255      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2031  | 1299 | 377 | 347 | 8 |         |       |
|     |       |          |       |      |     |     |   |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | W     | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |
|     |       |          |       |     |    |    |   |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | r     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1794  | 1123 | 357 | 308 | 6 |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | s     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1399  | 898 | 256 | 244 | 1 |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | t     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1638  | 1027 | 322 | 284 | 5 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | c     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1499  | 955 | 300 | 242 | 2 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | n     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1119  | 715 | 211 | 187 | 6 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | m     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1202  | 770 | 228 | 203 | 1 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | y     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 384 | 116 | 120 | 5 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | D     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | z     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 999   | 633 | 196 | 165 | 5 |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | R     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 640   | 402 | 118 | 113 | 7 |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | T     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 354   | 216 | 81 | 56 | 1 |         |       |

- Molecule 18 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 18  | 2     | 1721     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36718 | 16400 | 6603 | 12004 | 1711 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference |
|-------|---------|----------|--------|----------|-----------|
| 2     | 1772    | C        | G      | conflict | GB 337376 |

- Molecule 19 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | w     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 641 | 182 | 184 | 4 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | b     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1745  | 1112 | 314 | 312 | 7 |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | e     | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 934 | 284 | 270 | 7 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | u     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 524 | 139 | 130 | 6 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | v     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 861   | 544 | 151 | 159 | 7 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | o     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 980   | 623 | 183 | 167 | 7 |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | g     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1100  | 699 | 208 | 190 | 3 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | k     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 731 | 234 | 196 | 1 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | x     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1094  | 685 | 210 | 196 | 3 |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | h     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 780   | 489 | 148 | 139 | 4 |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 29  | P     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 557   | 358 | 101 | 97 | 1 |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30  | S     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 479   | 292 | 95 | 90 | 2 |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | l     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 450   | 282 | 93 | 70 | 5 |         |       |

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | U     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 295 | 89 | 74 | 7 |         |       |

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 33  | V     | 296      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2314  | 1464 | 404 | 434 | 12 |         |       |

- Molecule 34 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | i     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 939   | 574 | 187 | 172 | 6 |         |       |

- Molecule 35 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | j     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 682 | 214 | 181 | 3 |         |       |

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | G     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 712   | 451 | 129 | 128 | 4 |         |       |

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit I.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | I     | 305      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1497  | 887 | 305 | 305 |   |         |       |

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit B.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | B     | 536      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2966  | 1801 | 580 | 580 | 5 |         |       |

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit A.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 39  | A     | 692      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5380  | 3375 | 980 | 1003 | 22 |         |       |

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit C.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40  | C     | 633      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5110  | 3228 | 906 | 941 | 35 |         |       |

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit E.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41  | E     | 416      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3437  | 2202 | 585 | 630 | 20 |         |       |

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit F.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42  | F     | 269      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2090  | 1317 | 356 | 405 | 12 |         |       |

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit H.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43  | H     | 295      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2413  | 1532 | 417 | 449 | 15 |         |       |

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit K.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | K     | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1750  | 1116 | 288 | 334 | 12 |         |       |

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit L.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 45  | L     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3111  | 2011 | 520 | 563 | 17 |         |       |

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit M.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 46  | M     | 338      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2705  | 1727 | 457 | 504 | 17 |         |       |

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit D.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47  | N     | 447      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3617  | 2279 | 625 | 691 | 22 |         |       |

- Molecule 48 is a protein called Unknown factor.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 48  | X     | 78       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 390   | 234 | 78 | 78 |         |       |

- Molecule 49 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 49  | 1     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1603  | 717 | 298 | 514 | 74 |         |       |

- Molecule 50 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | 4     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 679 | 202 | 192 | 7 |         |       |

- Molecule 51 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51  | O     | 296      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2138  | 1342 | 384 | 404 | 8 |         |       |

- Molecule 52 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 52  | Y     | 414      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2156  | 1296 | 433 | 427 |         |       |

- Molecule 53 is a protein called Eukaryotic translation initiation factor 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | Z     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 524 | 150 | 154 | 2 |         |       |

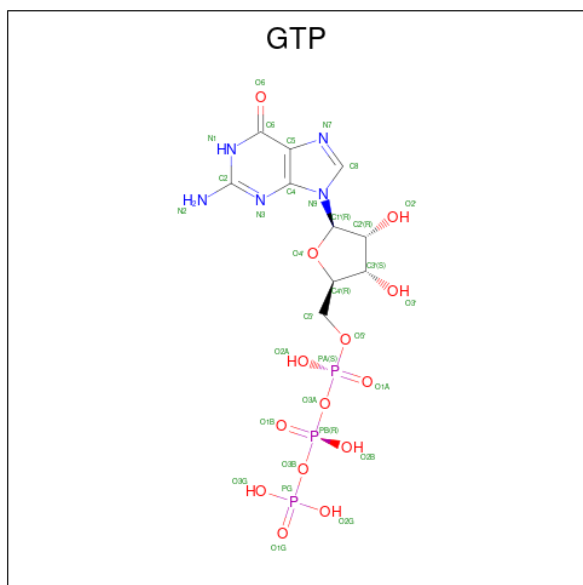
- Molecule 54 is a protein called Non-structural protein 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | J     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 261   | 159 | 47 | 54 | 1 |         |       |

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 55  | Q     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 55  | 1     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 55  | U     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 55  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

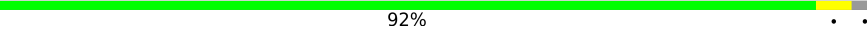




Chain Q:  80% 7% 12%

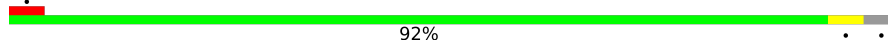


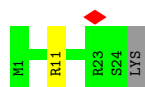
- Molecule 5: 40S ribosomal protein S4, X isoform

Chain q:  92% . .



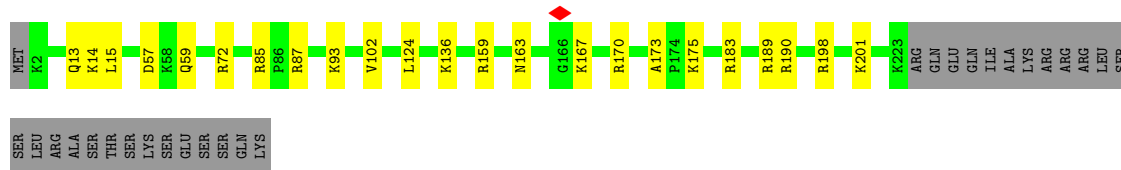
- Molecule 6: 60S ribosomal protein L41

Chain W:  92% . .



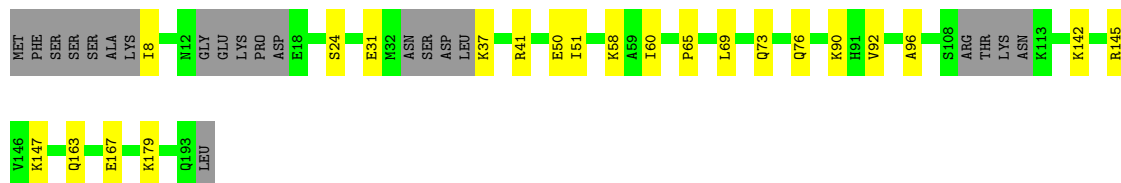
- Molecule 7: 40S ribosomal protein S6

Chain r:  80% 9% 11%



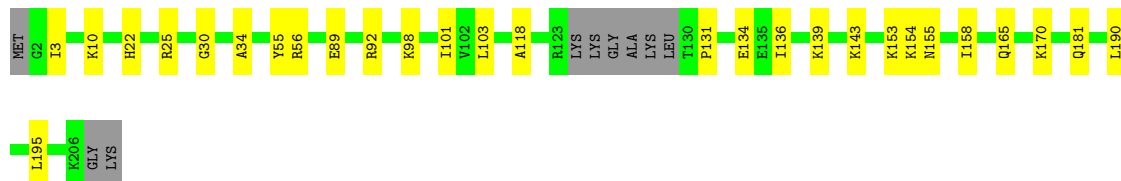
- Molecule 8: 40S ribosomal protein S7

Chain s:  78% 11% 11%



- Molecule 9: 40S ribosomal protein S8

Chain t:  82% 13% .



- Molecule 10: 40S ribosomal protein S9

Chain c:  87% 6% 7%

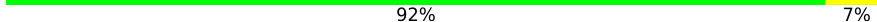


- Molecule 11: 40S ribosomal protein S11

Chain n:  81% 15%

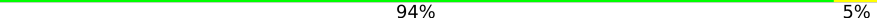


- Molecule 12: 40S ribosomal protein S13

Chain m:  92% 7%



- Molecule 13: 40S ribosomal protein S21

Chain y:  94% 5%



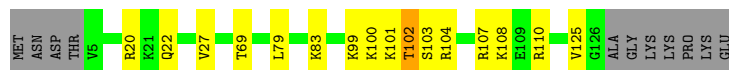
- Molecule 14: 40S ribosomal protein S15a

Chain D:  88% 11%



- Molecule 15: 40S ribosomal protein S24

Chain z:  80% 11% 8%



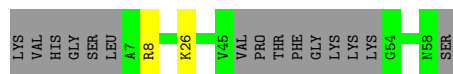
- Molecule 16: 40S ribosomal protein S27

Chain R:  88% 10%



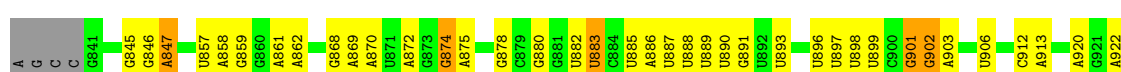
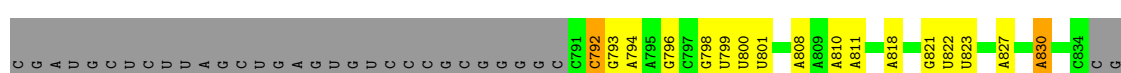
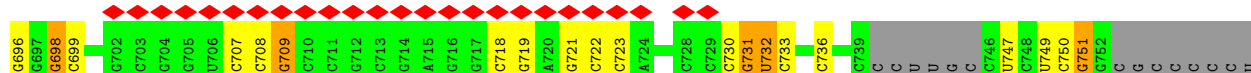
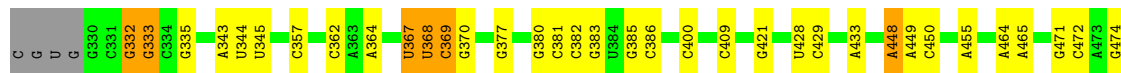
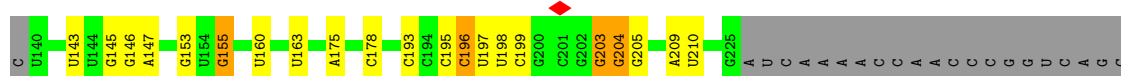
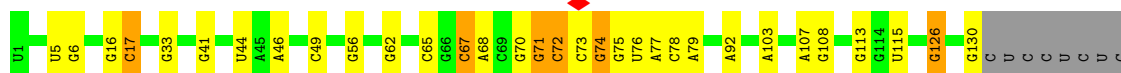
• Molecule 17: 40S ribosomal protein S30

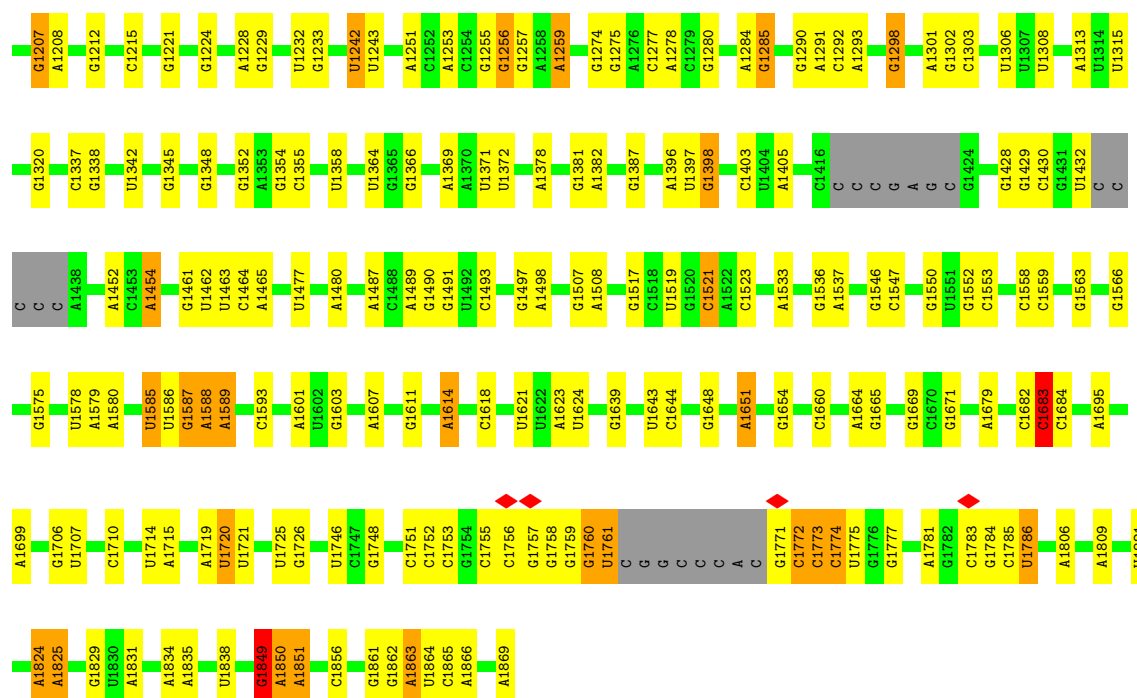
Chain T:  71% 25%



• Molecule 18: 18S ribosomal RNA

Chain 2:  65% 23% 8%





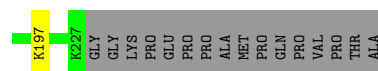
• Molecule 19: 40S ribosomal protein S17

Chain w: 84% 10% 5%



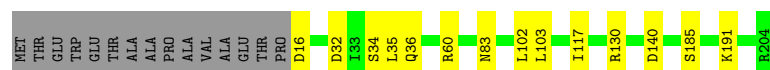
• Molecule 20: 40S ribosomal protein S3

Chain b: 79% 13% 8%



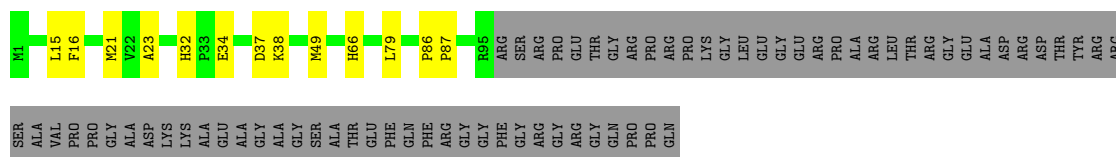
• Molecule 21: 40S ribosomal protein S5

Chain e: 86% 7% 7%

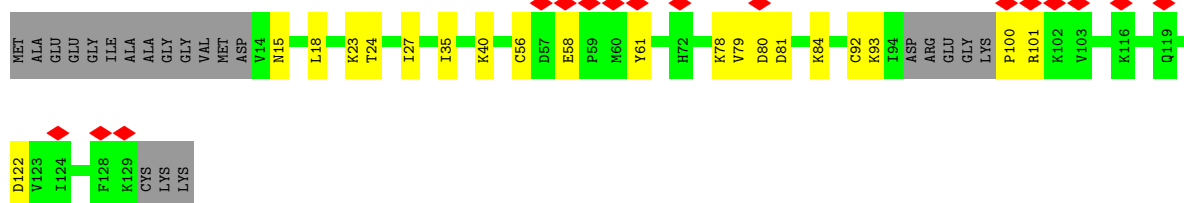


• Molecule 22: 40S ribosomal protein S10

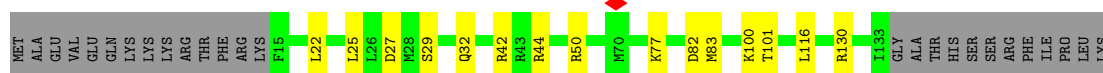
Chain u: 50% 8% 42%



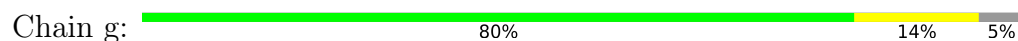
- Molecule 23: 40S ribosomal protein S12



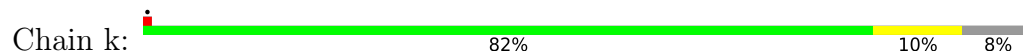
- Molecule 24: 40S ribosomal protein S15



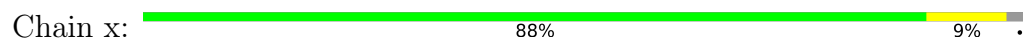
- Molecule 25: 40S ribosomal protein S16



- Molecule 26: 40S ribosomal protein S18



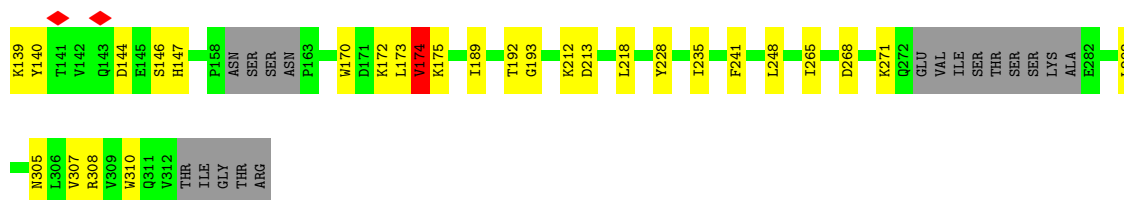
- Molecule 27: 40S ribosomal protein S19



- Molecule 28: 40S ribosomal protein S20







- Molecule 34: 40S ribosomal protein S14

Chain i: 70% 13% 17%



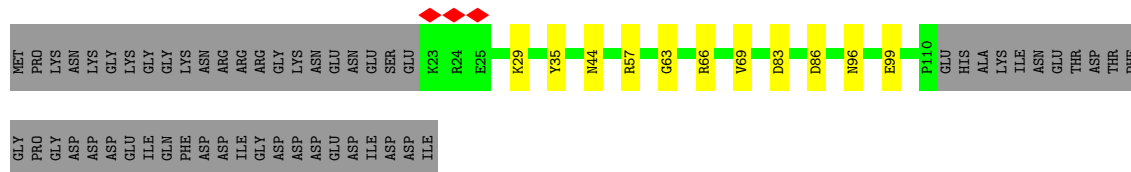
- Molecule 35: 40S ribosomal protein S23

Chain j: 88% 8% ..



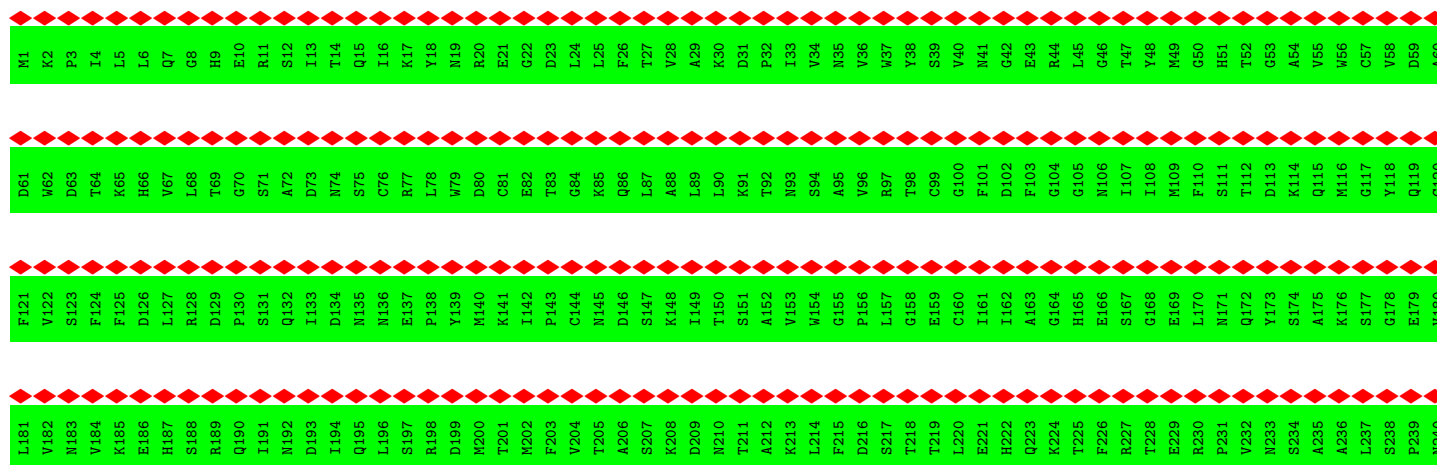
- Molecule 36: Eukaryotic translation initiation factor 1A, X-chromosomal

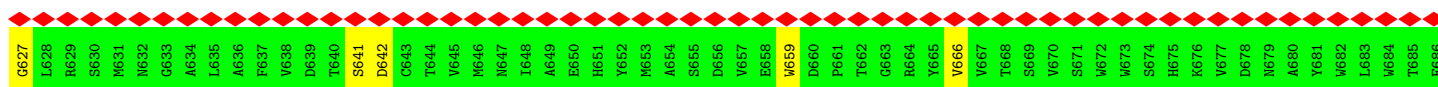
Chain G: 53% 8% 39%



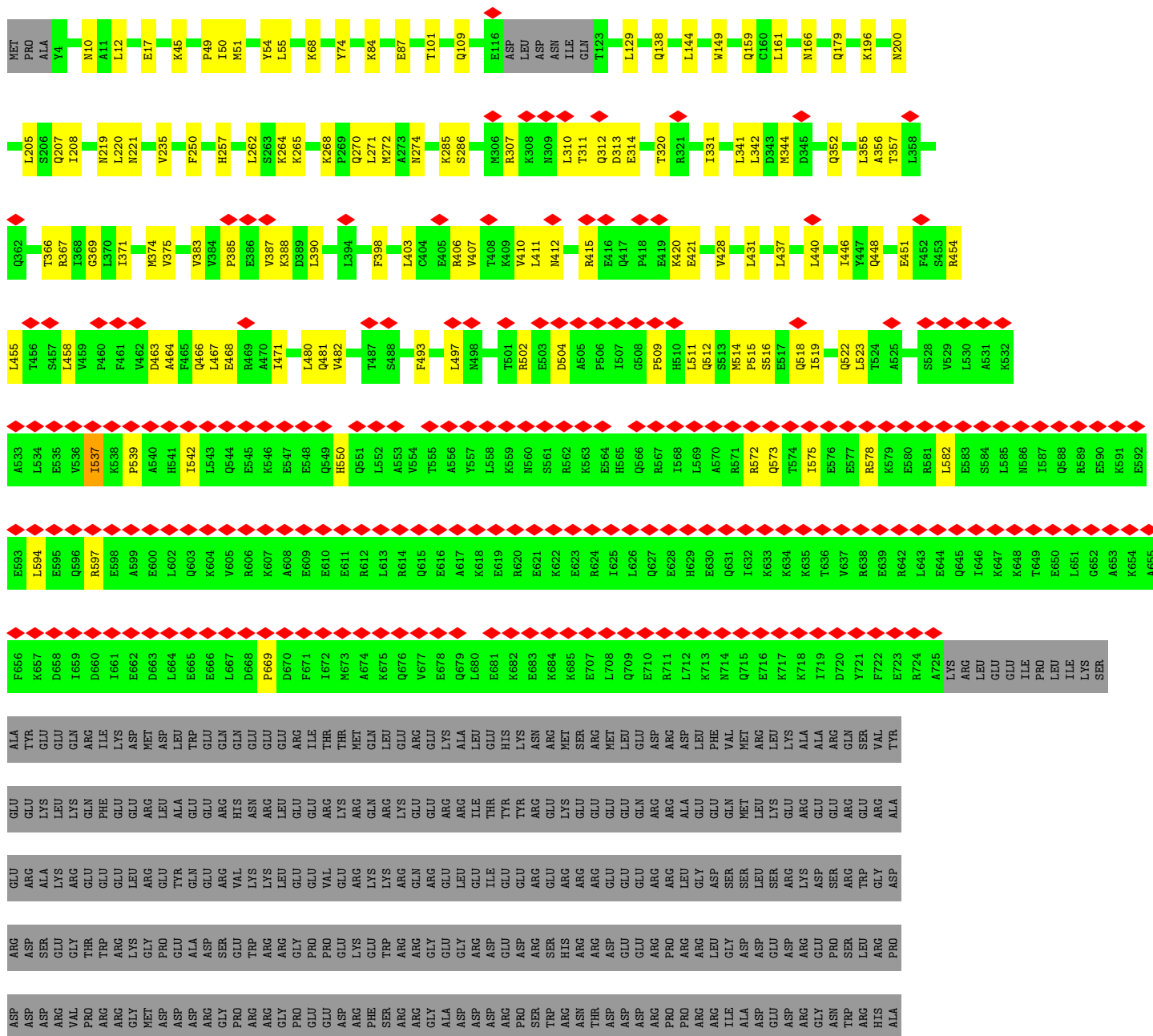
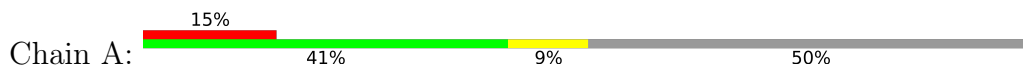
- Molecule 37: Eukaryotic translation initiation factor 3 subunit I

Chain I: 94% 94% 6%



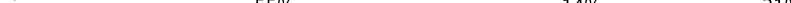


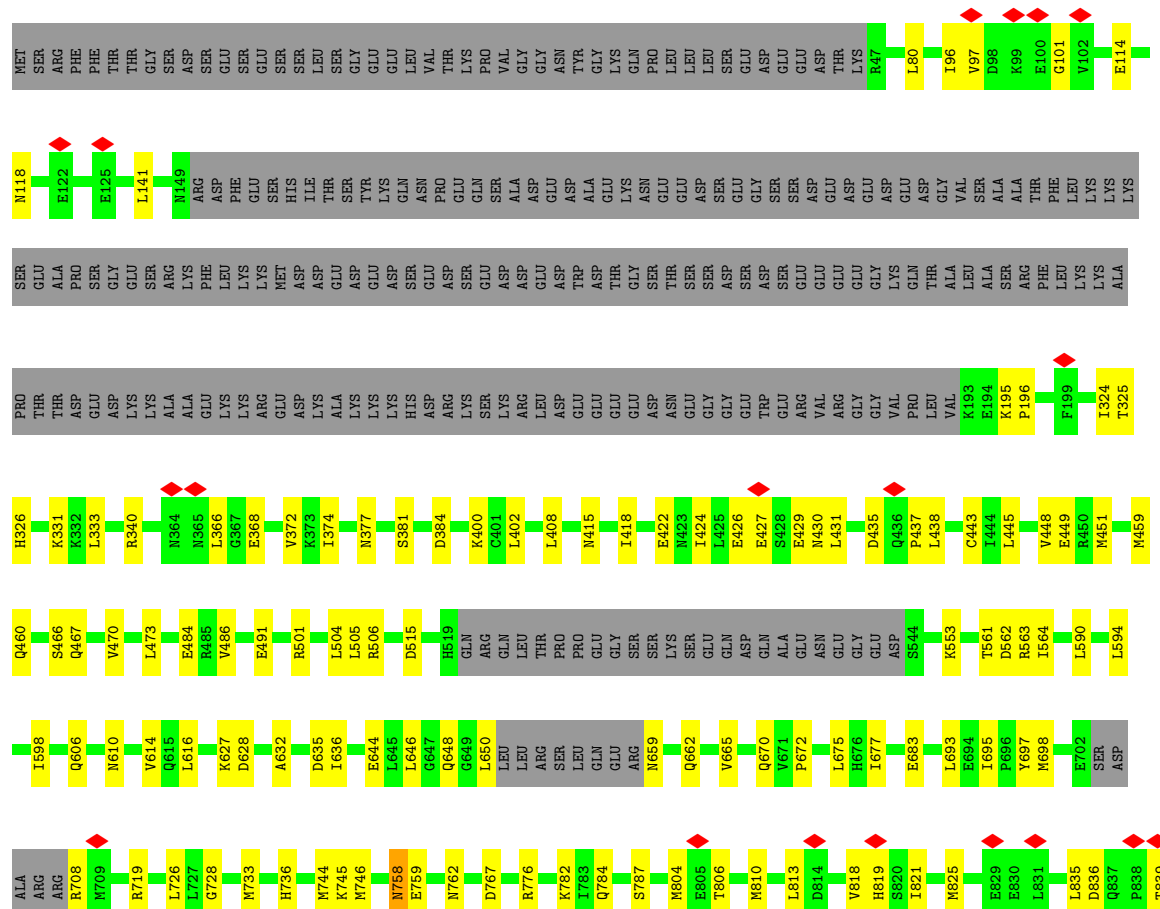
- Molecule 39: Eukaryotic translation initiation factor 3 subunit A



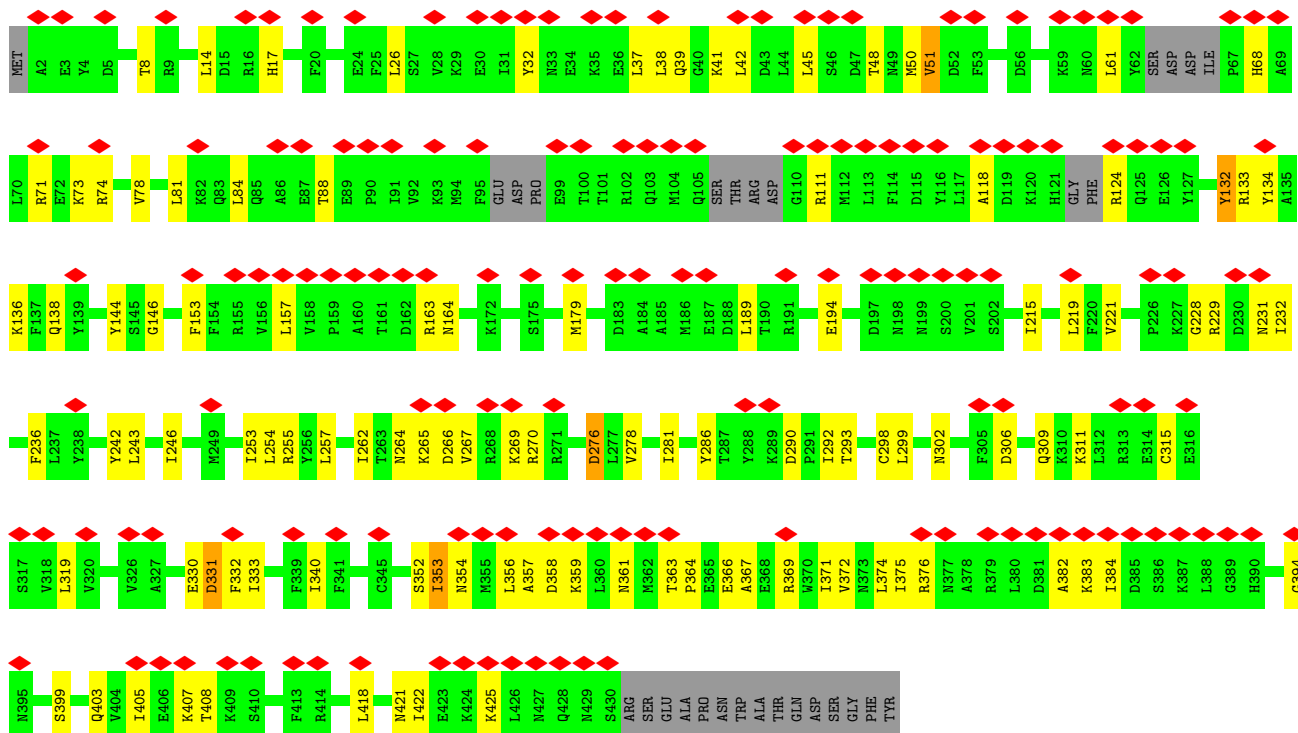
|     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASP | GLU | ASP | GLU | ALA | ARG | ALA | ASP | LEU | ASP |
| GLU | ASP | GLU | GLU | GLU | GLU | GLU | ASP | ASP | ASP |
| GLY | ASP | GLU | GLU | GLU | GLU | GLU | ASP | ASP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

- Molecule 40: Eukaryotic translation initiation factor 3 subunit C

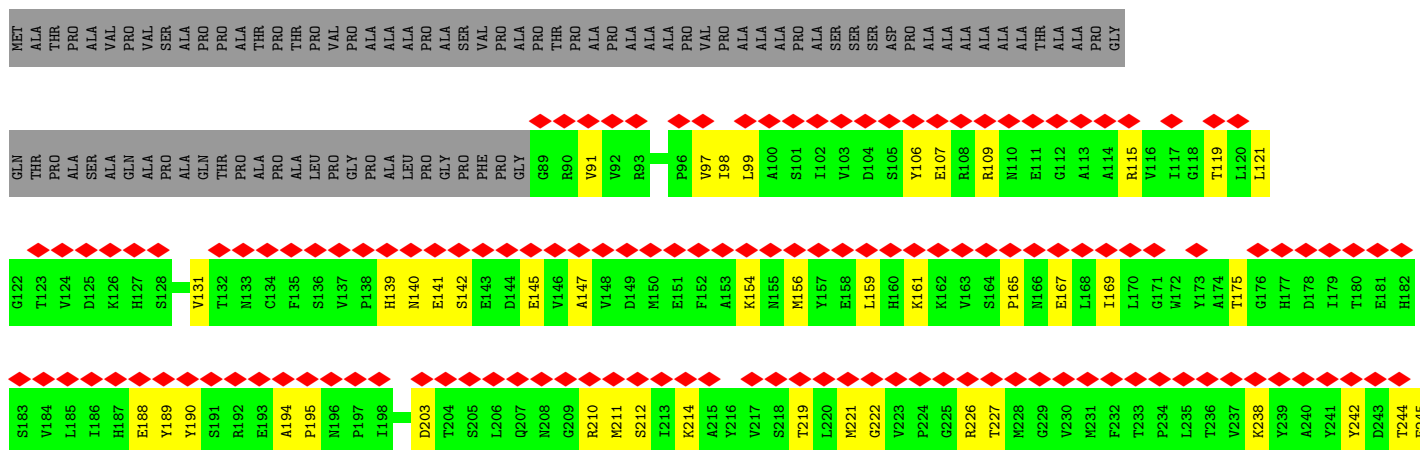
Chain C: 

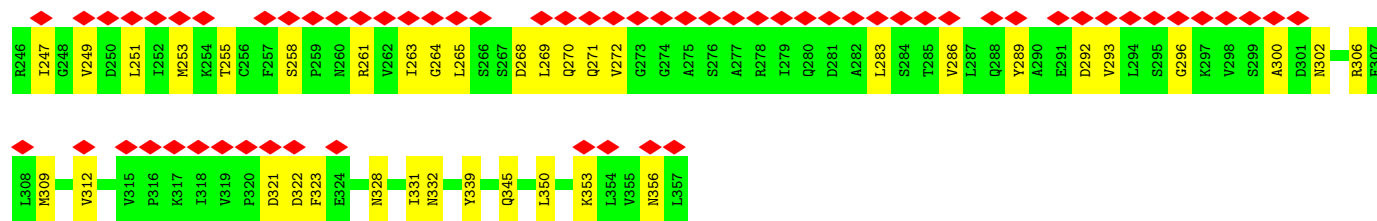


- Molecule 41: Eukaryotic translation initiation factor 3 subunit E



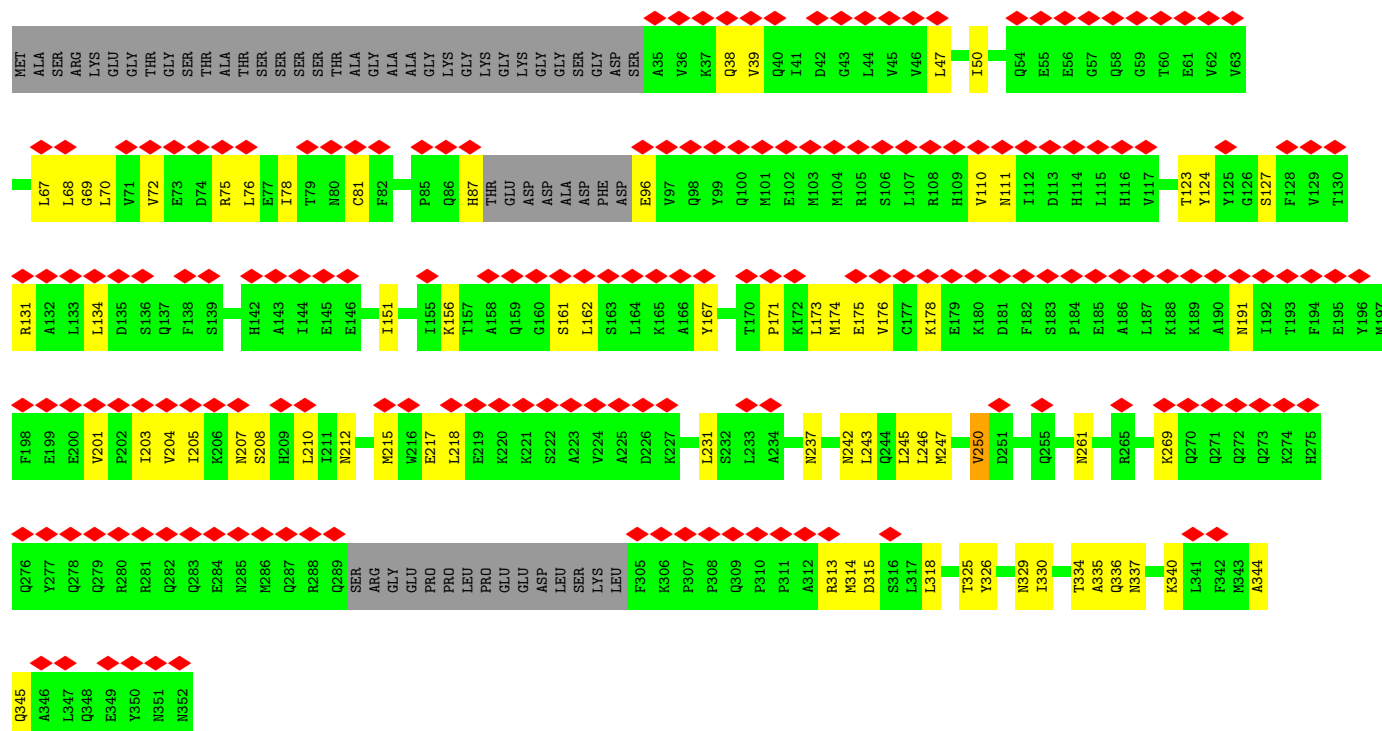
- Molecule 42: Eukaryotic translation initiation factor 3 subunit F





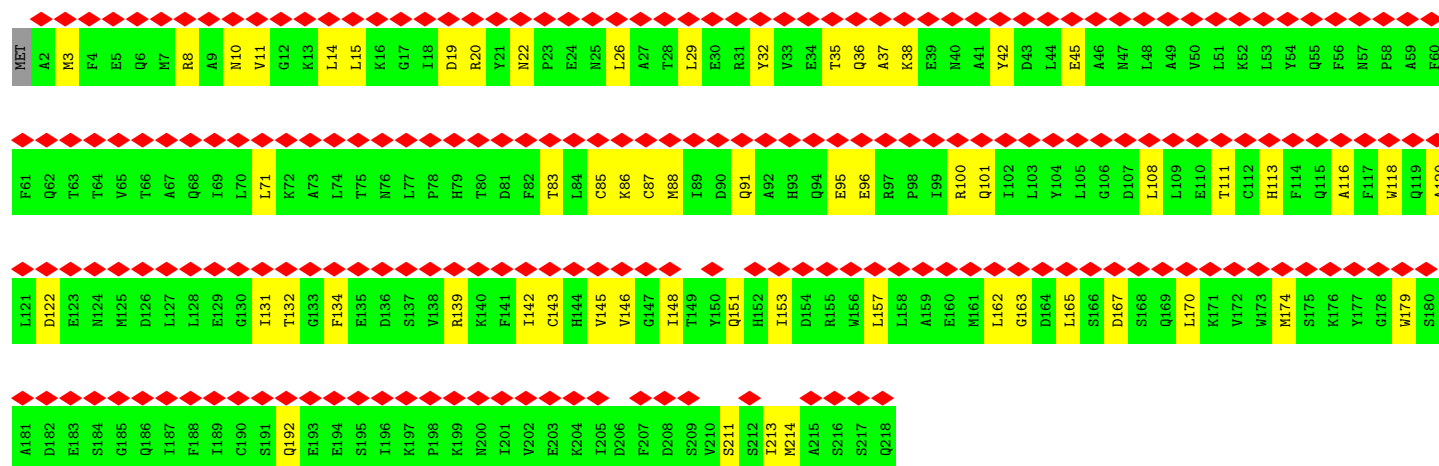
• Molecule 43: Eukaryotic translation initiation factor 3 subunit H

Chain H: 51% 64% 20% 16%

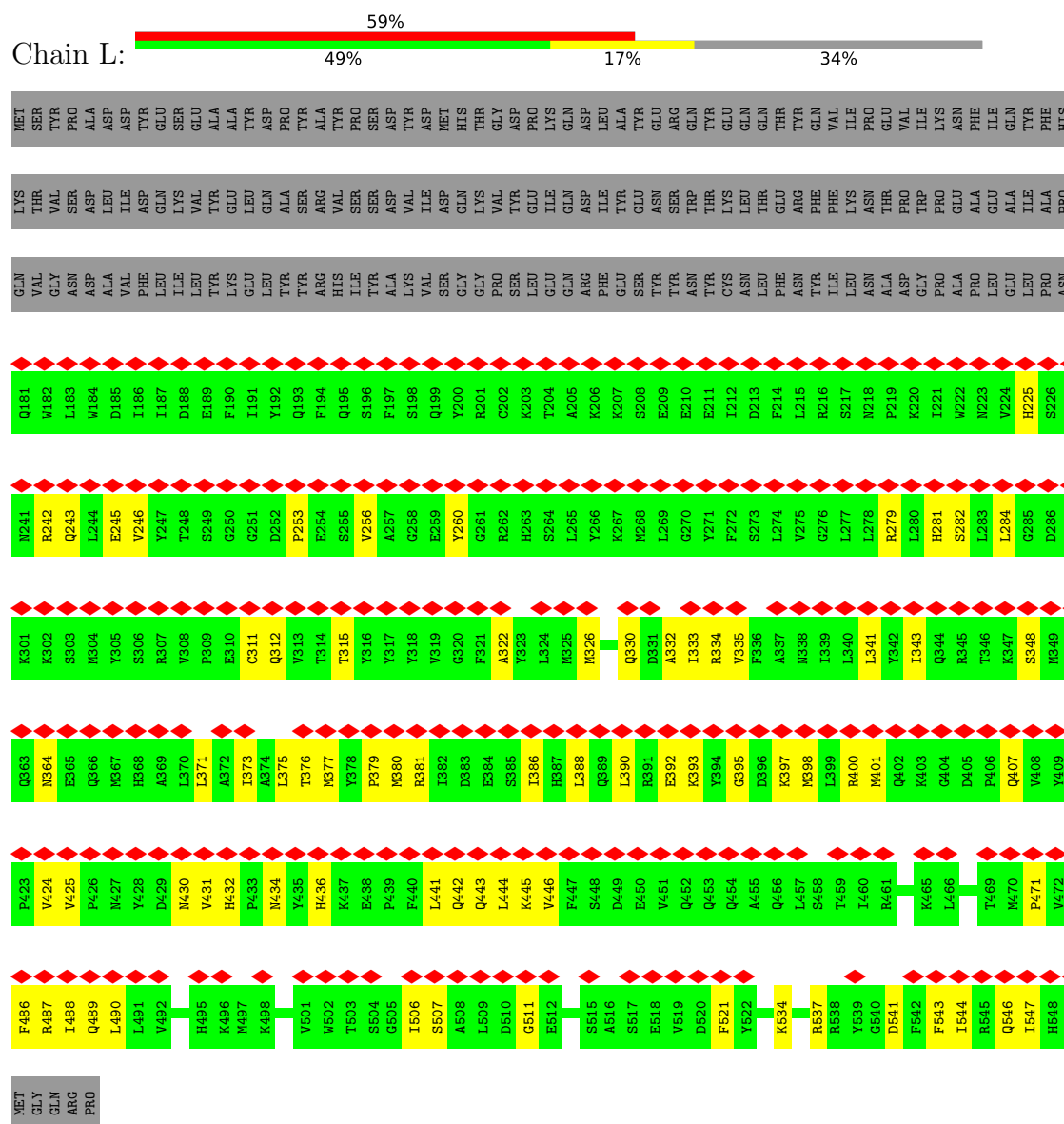


• Molecule 44: Eukaryotic translation initiation factor 3 subunit K

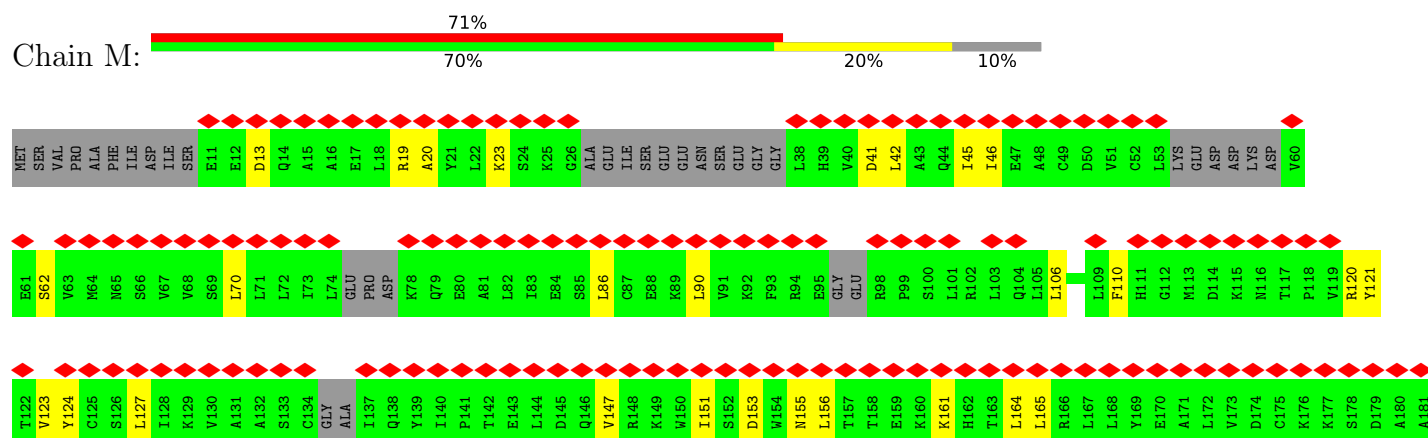
Chain K: 96% 72% 27%



• Molecule 45: Eukaryotic translation initiation factor 3 subunit L



• Molecule 46: Eukaryotic translation initiation factor 3 subunit M





WORLD WIDE  
PDB  
PROTEIN DATA BANK





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 53769                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 44.8                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.332                                   | Depositor |
| Minimum map value                    | -0.083                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.011                                   | Depositor |
| Recommended contour level            | 0.03                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 381.24, 381.24, 381.24                  | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.059, 1.059, 1.059                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.35         | 0/1742         | 0.46        | 0/2367          |
| 2   | p     | 0.33         | 0/1742         | 0.49        | 0/2330          |
| 3   | d     | 0.38         | 0/1710         | 0.51        | 0/2310          |
| 4   | Q     | 0.36         | 0/828          | 0.54        | 0/1109          |
| 5   | q     | 0.32         | 0/2073         | 0.50        | 2/2791 (0.1%)   |
| 6   | W     | 0.35         | 0/231          | 0.64        | 0/294           |
| 7   | r     | 0.26         | 0/1817         | 0.45        | 0/2421          |
| 8   | s     | 0.27         | 0/1418         | 0.50        | 0/1895          |
| 9   | t     | 0.31         | 0/1666         | 0.47        | 0/2223          |
| 10  | c     | 0.32         | 0/1524         | 0.49        | 0/2035          |
| 11  | n     | 0.35         | 0/1139         | 0.45        | 0/1524          |
| 12  | m     | 0.31         | 0/1226         | 0.45        | 0/1649          |
| 13  | y     | 0.32         | 0/631          | 0.44        | 0/844           |
| 14  | D     | 0.38         | 0/1051         | 0.54        | 0/1406          |
| 15  | z     | 0.31         | 0/1016         | 0.55        | 2/1349 (0.1%)   |
| 16  | R     | 0.34         | 0/653          | 0.55        | 0/876           |
| 17  | T     | 0.32         | 0/356          | 0.46        | 0/466           |
| 18  | 2     | 0.40         | 1/41061 (0.0%) | 0.45        | 14/64001 (0.0%) |
| 19  | w     | 0.33         | 0/1024         | 0.61        | 2/1377 (0.1%)   |
| 20  | b     | 0.32         | 0/1773         | 0.50        | 0/2387          |
| 21  | e     | 0.32         | 0/1516         | 0.53        | 0/2037          |
| 22  | u     | 0.29         | 0/823          | 0.50        | 0/1111          |
| 23  | v     | 0.21         | 0/870          | 0.60        | 0/1168          |
| 24  | o     | 0.30         | 0/999          | 0.44        | 0/1336          |
| 25  | g     | 0.36         | 0/1117         | 0.53        | 0/1494          |
| 26  | k     | 0.33         | 0/1180         | 0.56        | 0/1581          |
| 27  | x     | 0.33         | 0/1113         | 0.45        | 0/1493          |
| 28  | h     | 0.33         | 0/789          | 0.55        | 0/1059          |
| 29  | P     | 0.28         | 0/563          | 0.46        | 0/758           |
| 30  | S     | 0.31         | 0/481          | 0.47        | 0/643           |
| 31  | l     | 0.41         | 0/461          | 0.61        | 0/612           |
| 32  | U     | 0.20         | 0/474          | 0.52        | 0/626           |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 33  | V     | 0.28         | 0/2369          | 0.56        | 2/3221 (0.1%)    |
| 34  | i     | 0.33         | 0/951           | 0.51        | 0/1275           |
| 35  | j     | 0.35         | 0/1097          | 0.50        | 0/1464           |
| 36  | G     | 0.19         | 0/721           | 0.39        | 0/963            |
| 37  | I     | 0.11         | 0/1495          | 0.31        | 0/2073           |
| 38  | B     | 0.16         | 0/2981          | 0.42        | 0/4115           |
| 39  | A     | 0.21         | 0/5464          | 0.55        | 1/7396 (0.0%)    |
| 40  | C     | 0.23         | 0/5193          | 0.56        | 3/6995 (0.0%)    |
| 41  | E     | 0.23         | 0/3503          | 0.62        | 0/4728           |
| 42  | F     | 0.23         | 0/2126          | 0.62        | 0/2890           |
| 43  | H     | 0.22         | 0/2458          | 0.57        | 0/3313           |
| 44  | K     | 0.22         | 0/1785          | 0.61        | 2/2414 (0.1%)    |
| 45  | L     | 0.27         | 0/3187          | 0.68        | 6/4299 (0.1%)    |
| 46  | M     | 0.25         | 0/2743          | 0.66        | 0/3697           |
| 47  | N     | 0.20         | 0/3699          | 0.48        | 0/5001           |
| 48  | X     | 0.15         | 0/389           | 0.40        | 0/543            |
| 49  | 1     | 0.27         | 0/1794          | 0.34        | 0/2796           |
| 50  | 4     | 0.24         | 0/1095          | 0.58        | 0/1477           |
| 51  | O     | 0.22         | 0/2167          | 0.50        | 0/2943           |
| 52  | Y     | 0.17         | 0/2161          | 0.49        | 2/2985 (0.1%)    |
| 53  | Z     | 0.29         | 0/843           | 0.55        | 0/1134           |
| 54  | J     | 0.35         | 0/266           | 0.45        | 0/358            |
| All | All   | 0.32         | 1/123554 (0.0%) | 0.50        | 36/175652 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | a     | 0                   | 1                   |
| 14  | D     | 0                   | 1                   |
| 19  | w     | 0                   | 2                   |
| 21  | e     | 0                   | 1                   |
| 25  | g     | 0                   | 1                   |
| 33  | V     | 0                   | 1                   |
| 40  | C     | 0                   | 1                   |
| 42  | F     | 0                   | 1                   |
| 45  | L     | 0                   | 2                   |
| 50  | 4     | 0                   | 2                   |
| 51  | O     | 0                   | 1                   |
| 52  | Y     | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 53  | Z     | 0                   | 2                   |
| All | All   | 0                   | 19                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 18  | 2     | 367 | U    | O3'-P | -6.20 | 1.51        | 1.61     |

All (36) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 18  | 2     | 1850 | A    | C1'-C2'-O2' | -13.38 | 88.33       | 108.40   |
| 18  | 2     | 1849 | G    | C1'-C2'-O2' | -10.73 | 92.31       | 108.40   |
| 18  | 2     | 1683 | C    | C1'-C2'-O2' | -10.32 | 92.92       | 108.40   |
| 18  | 2     | 1208 | A    | C1'-C2'-O2' | -7.95  | 96.48       | 108.40   |
| 18  | 2     | 1208 | A    | C4'-C3'-O3' | 7.63   | 124.44      | 113.00   |
| 40  | C     | 196  | PRO  | N-CA-CB     | 7.30   | 109.84      | 102.17   |
| 18  | 2     | 1850 | A    | C4'-C3'-O3' | 6.93   | 123.39      | 113.00   |
| 18  | 2     | 1849 | G    | C4'-C3'-O3' | 6.91   | 123.36      | 113.00   |
| 45  | L     | 348  | SER  | CA-C-N      | 6.81   | 133.96      | 121.70   |
| 45  | L     | 348  | SER  | C-N-CA      | 6.81   | 133.96      | 121.70   |
| 45  | L     | 379  | PRO  | CA-C-N      | 6.63   | 133.63      | 121.70   |
| 45  | L     | 379  | PRO  | C-N-CA      | 6.63   | 133.63      | 121.70   |
| 18  | 2     | 1682 | C    | C4'-C3'-O3' | -6.63  | 99.46       | 109.40   |
| 18  | 2     | 369  | C    | C2'-C3'-O3' | -6.50  | 99.75       | 109.50   |
| 39  | A     | 669  | PRO  | N-CA-CB     | 6.39   | 110.29      | 103.52   |
| 33  | V     | 174  | VAL  | CA-C-N      | 5.99   | 132.98      | 121.54   |
| 33  | V     | 174  | VAL  | C-N-CA      | 5.99   | 132.98      | 121.54   |
| 18  | 2     | 1850 | A    | N9-C1'-C2'  | -5.98  | 103.03      | 112.00   |
| 45  | L     | 353  | THR  | CA-C-N      | 5.77   | 132.09      | 121.70   |
| 45  | L     | 353  | THR  | C-N-CA      | 5.77   | 132.09      | 121.70   |
| 15  | z     | 102  | THR  | CA-C-N      | 5.59   | 131.77      | 121.70   |
| 15  | z     | 102  | THR  | C-N-CA      | 5.59   | 131.77      | 121.70   |
| 5   | q     | 86   | PHE  | CA-C-N      | 5.51   | 132.06      | 121.54   |
| 5   | q     | 86   | PHE  | C-N-CA      | 5.51   | 132.06      | 121.54   |
| 19  | w     | 43   | SER  | CA-C-N      | 5.47   | 128.37      | 120.38   |
| 19  | w     | 43   | SER  | C-N-CA      | 5.47   | 128.37      | 120.38   |
| 40  | C     | 758  | ASN  | CA-C-N      | 5.44   | 131.94      | 121.54   |
| 40  | C     | 758  | ASN  | C-N-CA      | 5.44   | 131.94      | 121.54   |
| 18  | 2     | 369  | C    | C3'-C2'-O2' | 5.37   | 122.66      | 114.60   |
| 18  | 2     | 1683 | C    | C4'-C3'-O3' | 5.33   | 120.99      | 113.00   |
| 18  | 2     | 1207 | G    | C1'-C2'-O2' | -5.33  | 100.41      | 108.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | 2     | 1682 | C    | C2'-C3'-O3' | -5.09 | 101.86      | 109.50   |
| 44  | K     | 96   | GLU  | CA-C-N      | 5.04  | 138.40      | 121.27   |
| 44  | K     | 96   | GLU  | C-N-CA      | 5.04  | 138.40      | 121.27   |
| 52  | Y     | 51   | ALA  | CA-C-N      | 5.04  | 131.16      | 121.54   |
| 52  | Y     | 51   | ALA  | C-N-CA      | 5.04  | 131.16      | 121.54   |

There are no chirality outliers.

All (19) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 50  | 4     | 321 | VAL  | Peptide |
| 50  | 4     | 324 | LYS  | Peptide |
| 40  | C     | 424 | ILE  | Peptide |
| 14  | D     | 54  | ASP  | Peptide |
| 42  | F     | 194 | ALA  | Peptide |
| 45  | L     | 401 | MET  | Peptide |
| 45  | L     | 432 | HIS  | Peptide |
| 51  | O     | 184 | THR  | Peptide |
| 33  | V     | 174 | VAL  | Peptide |
| 52  | Y     | 50  | VAL  | Peptide |
| 52  | Y     | 51  | ALA  | Peptide |
| 52  | Y     | 52  | HIS  | Peptide |
| 53  | Z     | 55  | ASP  | Peptide |
| 53  | Z     | 58  | LYS  | Peptide |
| 1   | a     | 73  | ASP  | Peptide |
| 21  | e     | 130 | ARG  | Peptide |
| 25  | g     | 42  | ILE  | Peptide |
| 19  | w     | 42  | PRO  | Peptide |
| 19  | w     | 71  | ILE  | Peptide |

## 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     | 1705  | 0        | 1706     | 11      | 0            |
| 2   | p     | 1715  | 0        | 1785     | 15      | 0            |
| 3   | d     | 1674  | 0        | 1764     | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | Q     | 814   | 0        | 863      | 8       | 0            |
| 5   | q     | 2031  | 0        | 2133     | 8       | 0            |
| 6   | W     | 230   | 0        | 276      | 1       | 0            |
| 7   | r     | 1794  | 0        | 1942     | 20      | 0            |
| 8   | s     | 1399  | 0        | 1492     | 15      | 0            |
| 9   | t     | 1638  | 0        | 1710     | 19      | 0            |
| 10  | c     | 1499  | 0        | 1618     | 8       | 0            |
| 11  | n     | 1119  | 0        | 1186     | 4       | 0            |
| 12  | m     | 1202  | 0        | 1289     | 6       | 0            |
| 13  | y     | 625   | 0        | 628      | 4       | 0            |
| 14  | D     | 1034  | 0        | 1080     | 12      | 0            |
| 15  | z     | 999   | 0        | 1071     | 10      | 0            |
| 16  | R     | 640   | 0        | 665      | 7       | 0            |
| 17  | T     | 354   | 0        | 388      | 2       | 0            |
| 18  | 2     | 36718 | 0        | 18569    | 170     | 0            |
| 19  | w     | 1011  | 0        | 1053     | 8       | 0            |
| 20  | b     | 1745  | 0        | 1839     | 18      | 0            |
| 21  | e     | 1495  | 0        | 1549     | 10      | 0            |
| 22  | u     | 799   | 0        | 823      | 7       | 0            |
| 23  | v     | 861   | 0        | 895      | 15      | 0            |
| 24  | o     | 980   | 0        | 1025     | 11      | 0            |
| 25  | g     | 1100  | 0        | 1166     | 13      | 0            |
| 26  | k     | 1162  | 0        | 1221     | 8       | 0            |
| 27  | x     | 1094  | 0        | 1120     | 8       | 0            |
| 28  | h     | 780   | 0        | 850      | 8       | 0            |
| 29  | P     | 557   | 0        | 610      | 11      | 0            |
| 30  | S     | 479   | 0        | 507      | 5       | 0            |
| 31  | l     | 450   | 0        | 448      | 1       | 0            |
| 32  | U     | 465   | 0        | 481      | 11      | 0            |
| 33  | V     | 2314  | 0        | 2273     | 34      | 0            |
| 34  | i     | 939   | 0        | 965      | 13      | 0            |
| 35  | j     | 1080  | 0        | 1147     | 7       | 0            |
| 36  | G     | 712   | 0        | 736      | 7       | 0            |
| 37  | I     | 1497  | 0        | 676      | 0       | 0            |
| 38  | B     | 2966  | 0        | 1764     | 33      | 0            |
| 39  | A     | 5380  | 0        | 5160     | 82      | 0            |
| 40  | C     | 5110  | 0        | 5127     | 88      | 0            |
| 41  | E     | 3437  | 0        | 3433     | 73      | 0            |
| 42  | F     | 2090  | 0        | 2092     | 62      | 0            |
| 43  | H     | 2413  | 0        | 2411     | 53      | 0            |
| 44  | K     | 1750  | 0        | 1717     | 32      | 0            |
| 45  | L     | 3111  | 0        | 3085     | 60      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 46  | M     | 2705   | 0        | 2759     | 46      | 0            |
| 47  | N     | 3617   | 0        | 3495     | 63      | 0            |
| 48  | X     | 390    | 0        | 392      | 1       | 0            |
| 49  | 1     | 1603   | 0        | 816      | 0       | 0            |
| 50  | 4     | 1080   | 0        | 1045     | 16      | 0            |
| 51  | O     | 2138   | 0        | 1930     | 21      | 0            |
| 52  | Y     | 2156   | 0        | 1160     | 15      | 0            |
| 53  | Z     | 830    | 0        | 793      | 8       | 0            |
| 54  | J     | 261    | 0        | 229      | 4       | 0            |
| 55  | 4     | 1      | 0        | 0        | 0       | 0            |
| 55  | Q     | 1      | 0        | 0        | 0       | 0            |
| 55  | U     | 1      | 0        | 0        | 0       | 0            |
| 55  | l     | 1      | 0        | 0        | 0       | 0            |
| 56  | Y     | 32     | 0        | 12       | 0       | 0            |
| 57  | Y     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 117784 | 0        | 96969    | 1028    | 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 5.

All (1028) 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) |
|------------------|------------------|--------------------------|-------------------|
| 8:s:8:ILE:N      | 8:s:24:SER:HG    | 1.64                     | 0.95              |
| 18:2:698:G:H1    | 18:2:732:U:H3    | 0.97                     | 0.91              |
| 40:C:697:TYR:HH  | 40:C:708:ARG:N   | 1.76                     | 0.84              |
| 18:2:928:G:H1    | 18:2:1013:U:H3   | 1.32                     | 0.76              |
| 40:C:872:ARG:O   | 40:C:876:HIS:HB2 | 1.85                     | 0.76              |
| 27:x:11:GLN:HE21 | 27:x:62:ARG:HH11 | 1.36                     | 0.74              |
| 18:2:925:G:H1    | 18:2:1017:U:H3   | 1.38                     | 0.72              |
| 45:L:322:ALA:O   | 45:L:326:MET:HB3 | 1.90                     | 0.71              |
| 18:2:1366:G:H21  | 18:2:1465:A:H8   | 1.36                     | 0.70              |
| 33:V:87:LEU:HB2  | 33:V:101:PHE:HB2 | 1.74                     | 0.69              |
| 18:2:537:C:N3    | 18:2:545:A:N1    | 2.40                     | 0.69              |
| 40:C:594:LEU:O   | 40:C:598:ILE:HB  | 1.93                     | 0.68              |
| 42:F:249:VAL:O   | 42:F:253:MET:HB2 | 1.94                     | 0.68              |
| 18:2:1192:U:HO2' | 18:2:1821:U:HO2' | 1.43                     | 0.67              |
| 9:t:34:ALA:HB2   | 9:t:56:ARG:HD3   | 1.76                     | 0.66              |
| 14:D:2:VAL:N     | 18:2:1091:C:HO2' | 1.94                     | 0.66              |
| 18:2:1618:C:H4'  | 24:o:50:ARG:HH12 | 1.62                     | 0.65              |
| 15:z:20:ARG:HE   | 15:z:22:GLN:HE21 | 1.42                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:E:331:ASP:N    | 41:E:331:ASP:OD1  | 2.30                     | 0.64              |
| 45:L:424:VAL:HG23 | 45:L:425:VAL:HG12 | 1.79                     | 0.64              |
| 39:A:311:THR:HG21 | 39:A:314:GLU:HB3  | 1.79                     | 0.64              |
| 47:N:169:GLU:HB2  | 47:N:521:SER:HB2  | 1.79                     | 0.64              |
| 24:o:44:ARG:NH1   | 24:o:82:ASP:O     | 2.31                     | 0.63              |
| 47:N:171:LYS:HB2  | 47:N:519:VAL:HG13 | 1.80                     | 0.63              |
| 41:E:144:TYR:HB2  | 41:E:179:MET:HG2  | 1.80                     | 0.63              |
| 39:A:341:LEU:HD21 | 40:C:698:MET:HB3  | 1.80                     | 0.63              |
| 18:2:1293:A:H61   | 18:2:1306:U:H3    | 1.47                     | 0.63              |
| 46:M:124:TYR:HA   | 46:M:127:LEU:HD12 | 1.81                     | 0.63              |
| 44:K:139:ARG:HH21 | 44:K:165:LEU:HD13 | 1.63                     | 0.62              |
| 45:L:232:HIS:O    | 45:L:236:ASP:HB2  | 1.99                     | 0.62              |
| 39:A:463:ASP:H    | 39:A:466:GLN:HE21 | 1.45                     | 0.62              |
| 43:H:69:GLY:HA3   | 43:H:78:ILE:HA    | 1.79                     | 0.62              |
| 41:E:372:VAL:O    | 41:E:376:ARG:HB2  | 2.00                     | 0.62              |
| 41:E:26:LEU:HG    | 41:E:37:LEU:HD21  | 1.82                     | 0.62              |
| 46:M:120:ARG:HA   | 46:M:123:VAL:HG12 | 1.81                     | 0.61              |
| 41:E:422:ILE:HA   | 41:E:425:LYS:HG2  | 1.81                     | 0.61              |
| 20:b:54:ARG:HE    | 20:b:57:ASN:HD22  | 1.48                     | 0.61              |
| 44:K:10:ASN:O     | 44:K:14:LEU:HB3   | 2.00                     | 0.61              |
| 45:L:284:LEU:HD11 | 45:L:299:LEU:HD22 | 1.82                     | 0.61              |
| 52:Y:52:HIS:HD2   | 52:Y:160:ALA:H    | 1.47                     | 0.61              |
| 40:C:806:THR:O    | 40:C:810:MET:HB2  | 2.01                     | 0.61              |
| 42:F:97:VAL:HG12  | 43:H:47:LEU:HB3   | 1.82                     | 0.61              |
| 18:2:1725:U:H3    | 18:2:1809:A:H61   | 1.49                     | 0.60              |
| 40:C:372:VAL:HG23 | 40:C:408:LEU:HD11 | 1.83                     | 0.60              |
| 10:c:18:ARG:O     | 10:c:24:ARG:NH1   | 2.34                     | 0.60              |
| 33:V:124:SER:OG   | 33:V:126:ASP:OD1  | 2.19                     | 0.60              |
| 39:A:268:LYS:HB3  | 39:A:271:LEU:HD13 | 1.83                     | 0.60              |
| 39:A:342:LEU:HG   | 39:A:344:MET:HG2  | 1.84                     | 0.60              |
| 3:d:108:LYS:HE2   | 3:d:110:MET:HB3   | 1.84                     | 0.60              |
| 42:F:142:SER:HB2  | 42:F:145:GLU:HB3  | 1.83                     | 0.60              |
| 18:2:1566:G:N7    | 27:x:101:ARG:NH2  | 2.50                     | 0.60              |
| 3:d:113:GLN:NE2   | 3:d:120:GLN:OE1   | 2.34                     | 0.60              |
| 42:F:261:ARG:HE   | 43:H:208:SER:HA   | 1.66                     | 0.60              |
| 18:2:952:G:H1     | 18:2:974:C:H5     | 1.47                     | 0.60              |
| 18:2:1290:G:N7    | 32:U:95:ARG:NH2   | 2.49                     | 0.60              |
| 20:b:175:VAL:HG13 | 20:b:182:LEU:HB3  | 1.83                     | 0.60              |
| 33:V:31:ILE:HG12  | 33:V:45:LEU:HD21  | 1.83                     | 0.59              |
| 40:C:418:ILE:HG12 | 40:C:438:LEU:HD23 | 1.83                     | 0.59              |
| 39:A:310:LEU:HG   | 39:A:311:THR:HG22 | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:H:207:ASN:ND2  | 43:H:215:MET:SD   | 2.76                     | 0.59              |
| 40:C:484:GLU:OE2  | 40:C:506:ARG:NH1  | 2.35                     | 0.59              |
| 40:C:869:ASN:OD1  | 43:H:261:ASN:ND2  | 2.36                     | 0.59              |
| 10:c:39:ASN:ND2   | 18:2:643:A:OP1    | 2.35                     | 0.59              |
| 38:B:565:ILE:HA   | 38:B:581:HIS:HA   | 1.84                     | 0.59              |
| 43:H:39:VAL:HA    | 43:H:76:LEU:HB2   | 1.85                     | 0.59              |
| 18:2:594:A:H61    | 18:2:643:A:H5''   | 1.68                     | 0.59              |
| 39:A:371:ILE:HA   | 39:A:374:MET:HE3  | 1.85                     | 0.59              |
| 33:V:35:SER:OG    | 33:V:37:ASP:OD1   | 2.21                     | 0.59              |
| 41:E:39:GLN:HA    | 41:E:42:LEU:HD12  | 1.84                     | 0.59              |
| 33:V:64:HIS:CD2   | 33:V:65:PHE:H     | 2.21                     | 0.58              |
| 9:t:143:LYS:NZ    | 18:2:203:G:N7     | 2.48                     | 0.58              |
| 47:N:357:ALA:HB3  | 47:N:377:HIS:HB2  | 1.86                     | 0.58              |
| 43:H:173:LEU:HA   | 43:H:176:VAL:HG22 | 1.85                     | 0.58              |
| 40:C:636:ILE:HD13 | 47:N:42:VAL:HG12  | 1.84                     | 0.58              |
| 47:N:245:VAL:HG12 | 47:N:276:LEU:HB3  | 1.86                     | 0.58              |
| 42:F:353:LYS:HG3  | 45:L:544:ILE:HG21 | 1.86                     | 0.58              |
| 47:N:375:CYS:HB3  | 47:N:442:ALA:HA   | 1.86                     | 0.58              |
| 47:N:242:GLN:HB2  | 47:N:362:ARG:HH12 | 1.69                     | 0.58              |
| 18:2:698:G:O6     | 18:2:732:U:O4     | 2.21                     | 0.57              |
| 38:B:548:ARG:HB2  | 38:B:555:PRO:HD2  | 1.84                     | 0.57              |
| 39:A:270:GLN:HE21 | 39:A:274:ASN:HD22 | 1.52                     | 0.57              |
| 18:2:1521:C:OP1   | 26:k:124:ARG:NH1  | 2.37                     | 0.57              |
| 41:E:219:LEU:HD11 | 41:E:253:ILE:HG23 | 1.87                     | 0.57              |
| 39:A:366:THR:HG23 | 39:A:369:GLY:H    | 1.69                     | 0.57              |
| 41:E:243:LEU:HA   | 41:E:246:ILE:HD12 | 1.87                     | 0.57              |
| 41:E:299:LEU:HD13 | 41:E:340:ILE:HG22 | 1.86                     | 0.57              |
| 33:V:4:GLN:N      | 33:V:268:ASP:OD2  | 2.37                     | 0.57              |
| 18:2:1491:G:H1'   | 28:h:72:GLU:HG2   | 1.85                     | 0.57              |
| 39:A:166:ASN:HD21 | 39:A:207:GLN:HB3  | 1.69                     | 0.57              |
| 41:E:309:GLN:HB2  | 41:E:359:LYS:HE3  | 1.85                     | 0.57              |
| 45:L:486:PHE:HA   | 45:L:489:GLN:HB2  | 1.87                     | 0.57              |
| 44:K:8:ARG:NH2    | 44:K:42:TYR:O     | 2.37                     | 0.57              |
| 47:N:251:ILE:HD12 | 47:N:278:PHE:HB2  | 1.87                     | 0.57              |
| 41:E:382:ALA:HA   | 41:E:394:GLY:H    | 1.70                     | 0.57              |
| 43:H:131:ARG:HD2  | 43:H:314:MET:HE1  | 1.87                     | 0.57              |
| 43:H:325:THR:O    | 43:H:329:ASN:ND2  | 2.38                     | 0.57              |
| 46:M:196:ASN:HB2  | 46:M:199:GLN:HE21 | 1.70                     | 0.57              |
| 8:s:58:LYS:HB2    | 8:s:90:LYS:HD2    | 1.87                     | 0.56              |
| 40:C:448:VAL:HG11 | 40:C:486:VAL:HG21 | 1.85                     | 0.56              |
| 47:N:73:HIS:HB3   | 47:N:76:ASP:HB3   | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:A:109:GLN:HE22 | 39:A:138:GLN:HE22 | 1.53                     | 0.56              |
| 39:A:572:ARG:HH11 | 39:A:573:GLN:HE22 | 1.53                     | 0.56              |
| 5:q:106:LYS:NZ    | 18:2:847:A:O2'    | 2.37                     | 0.56              |
| 18:2:952:G:O2'    | 18:2:953:C:O2     | 2.22                     | 0.56              |
| 39:A:270:GLN:O    | 39:A:274:ASN:ND2  | 2.39                     | 0.56              |
| 41:E:88:THR:HG21  | 41:E:134:TYR:HB2  | 1.87                     | 0.56              |
| 45:L:373:ILE:HG22 | 45:L:398:MET:HB3  | 1.87                     | 0.56              |
| 47:N:445:GLU:OE2  | 47:N:472:LYS:NZ   | 2.39                     | 0.56              |
| 40:C:445:LEU:HD21 | 40:C:501:ARG:HG3  | 1.88                     | 0.56              |
| 42:F:345:GLN:OE1  | 45:L:537:ARG:NH1  | 2.39                     | 0.56              |
| 42:F:356:ASN:ND2  | 43:H:191:ASN:OD1  | 2.39                     | 0.56              |
| 51:O:71:VAL:HG23  | 51:O:89:VAL:HG22  | 1.87                     | 0.56              |
| 9:t:98:LYS:HB3    | 18:2:377:G:H5'    | 1.86                     | 0.56              |
| 20:b:143:ARG:NH2  | 54:J:156:ASP:OD1  | 2.35                     | 0.56              |
| 45:L:341:LEU:HD12 | 45:L:343:ILE:H    | 1.70                     | 0.56              |
| 18:2:1614:A:OP2   | 24:o:42:ARG:NH1   | 2.38                     | 0.56              |
| 45:L:430:ASN:H    | 45:L:436:HIS:HE1  | 1.54                     | 0.56              |
| 2:p:26:SER:O      | 2:p:51:ARG:NH2    | 2.39                     | 0.56              |
| 43:H:134:LEU:HD11 | 43:H:318:LEU:HD11 | 1.88                     | 0.56              |
| 17:T:8:ARG:NH2    | 18:2:616:A:OP1    | 2.38                     | 0.56              |
| 38:B:497:GLN:HE22 | 38:B:504:ILE:HG23 | 1.70                     | 0.56              |
| 40:C:333:LEU:HD11 | 40:C:377:ASN:HD22 | 1.70                     | 0.56              |
| 42:F:115:ARG:O    | 42:F:139:HIS:NE2  | 2.38                     | 0.56              |
| 12:m:87:ASP:OD1   | 12:m:87:ASP:N     | 2.39                     | 0.56              |
| 41:E:14:LEU:O     | 47:N:10:GLN:NE2   | 2.39                     | 0.56              |
| 7:r:59:GLN:HE21   | 7:r:72:ARG:HH12   | 1.54                     | 0.56              |
| 8:s:69:LEU:HD22   | 8:s:96:ALA:HB2    | 1.87                     | 0.56              |
| 20:b:18:LYS:HE2   | 20:b:39:VAL:HB    | 1.87                     | 0.56              |
| 45:L:373:ILE:HD13 | 45:L:397:LYS:HD2  | 1.86                     | 0.56              |
| 18:2:830:A:OP2    | 18:2:846:G:N2     | 2.39                     | 0.55              |
| 24:o:29:SER:H     | 24:o:32:GLN:HE21  | 1.52                     | 0.55              |
| 44:K:95:GLU:HA    | 44:K:100:ARG:HE   | 1.71                     | 0.55              |
| 46:M:121:TYR:HE1  | 46:M:164:LEU:HB2  | 1.70                     | 0.55              |
| 47:N:292:SER:OG   | 47:N:404:CYS:SG   | 2.65                     | 0.55              |
| 39:A:481:GLN:NE2  | 39:A:514:MET:SD   | 2.80                     | 0.55              |
| 41:E:276:ASP:OD1  | 41:E:276:ASP:N    | 2.31                     | 0.55              |
| 42:F:242:TYR:H    | 42:F:245:GLU:HB2  | 1.70                     | 0.55              |
| 34:i:139:SER:OG   | 34:i:140:THR:N    | 2.37                     | 0.55              |
| 45:L:240:ILE:HG13 | 45:L:253:PRO:HB2  | 1.88                     | 0.55              |
| 3:d:146:GLU:OE2   | 54:J:158:GLN:NE2  | 2.38                     | 0.55              |
| 14:D:4:MET:HG3    | 18:2:683:G:H4'    | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:G:57:ARG:NH1   | 36:G:86:ASP:O     | 2.39                     | 0.55              |
| 11:n:13:GLN:HE22  | 11:n:36:TYR:H     | 1.54                     | 0.55              |
| 18:2:559:G:O2'    | 38:B:487:LYS:NZ   | 2.39                     | 0.55              |
| 18:2:573:U:H1'    | 18:2:576:A:H2     | 1.72                     | 0.55              |
| 42:F:211:MET:HE2  | 43:H:217:GLU:HB3  | 1.89                     | 0.55              |
| 16:R:34:ASP:OD2   | 16:R:80:ARG:NH2   | 2.40                     | 0.55              |
| 18:2:1825:A:N6    | 36:G:69:VAL:O     | 2.39                     | 0.55              |
| 21:e:36:GLN:OE1   | 47:N:479:GLN:NE2  | 2.40                     | 0.55              |
| 38:B:514:ASP:OD2  | 38:B:516:LYS:NZ   | 2.39                     | 0.55              |
| 39:A:12:LEU:HG    | 39:A:50:ILE:HG22  | 1.89                     | 0.55              |
| 39:A:68:LYS:HD3   | 39:A:159:GLN:HG2  | 1.87                     | 0.55              |
| 40:C:460:GLN:NE2  | 40:C:670:GLN:O    | 2.40                     | 0.55              |
| 41:E:266:ASP:HB3  | 41:E:269:LYS:HE2  | 1.88                     | 0.55              |
| 7:r:85:ARG:O      | 7:r:87:ARG:NH1    | 2.40                     | 0.55              |
| 9:t:22:HIS:HB3    | 18:2:433:A:H5''   | 1.89                     | 0.55              |
| 43:H:72:VAL:HB    | 43:H:75:ARG:HG3   | 1.89                     | 0.55              |
| 46:M:153:ASP:O    | 46:M:155:ASN:ND2  | 2.40                     | 0.55              |
| 47:N:363:TRP:HB2  | 47:N:371:LEU:HB3  | 1.88                     | 0.55              |
| 5:q:100:ARG:HH21  | 5:q:118:GLU:HG2   | 1.72                     | 0.55              |
| 16:R:78:SER:HB3   | 47:N:80:PHE:HB3   | 1.89                     | 0.55              |
| 39:A:286:SER:HA   | 40:C:728:GLY:HA2  | 1.89                     | 0.55              |
| 41:E:298:CYS:HA   | 41:E:302:ASN:HD22 | 1.71                     | 0.55              |
| 43:H:67:LEU:HD23  | 43:H:78:ILE:HG21  | 1.88                     | 0.55              |
| 45:L:544:ILE:HA   | 45:L:547:ILE:HG12 | 1.88                     | 0.55              |
| 45:L:281:HIS:HD2  | 45:L:311:CYS:HB3  | 1.72                     | 0.54              |
| 18:2:1298:G:H5'   | 24:o:77:LYS:HB2   | 1.88                     | 0.54              |
| 18:2:1856:C:H5''  | 34:i:141:ARG:HH12 | 1.72                     | 0.54              |
| 40:C:449:GLU:OE1  | 40:C:501:ARG:NH1  | 2.40                     | 0.54              |
| 41:E:363:THR:HG23 | 41:E:366:GLU:H    | 1.71                     | 0.54              |
| 9:t:131:PRO:HA    | 9:t:134:GLU:HB2   | 1.88                     | 0.54              |
| 50:4:251:ASP:HB2  | 50:4:254:ASN:HB2  | 1.89                     | 0.54              |
| 50:4:281:CYS:SG   | 50:4:282:HIS:N    | 2.80                     | 0.54              |
| 16:R:40:CYS:SG    | 16:R:41:TYR:N     | 2.78                     | 0.54              |
| 18:2:1850:A:H2'   | 18:2:1851:A:C8    | 2.43                     | 0.54              |
| 26:k:22:GLY:HA2   | 26:k:56:ALA:HB3   | 1.89                     | 0.54              |
| 33:V:241:PHE:HA   | 33:V:248:LEU:HA   | 1.90                     | 0.54              |
| 41:E:51:VAL:HG22  | 41:E:73:LYS:HZ2   | 1.71                     | 0.54              |
| 42:F:289:TYR:OH   | 42:F:300:ALA:O    | 2.26                     | 0.54              |
| 2:p:29:ASP:OD1    | 2:p:51:ARG:NH1    | 2.41                     | 0.54              |
| 10:c:80:ARG:NH2   | 18:2:818:A:OP1    | 2.39                     | 0.54              |
| 15:z:107:ARG:NH2  | 18:2:492:C:OP2    | 2.39                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:F:356:ASN:OD1  | 43:H:313:ARG:NH2  | 2.36                     | 0.54              |
| 8:s:60:ILE:HB     | 8:s:92:VAL:HG12   | 1.89                     | 0.54              |
| 20:b:136:VAL:HG23 | 20:b:186:VAL:HG12 | 1.90                     | 0.54              |
| 46:M:294:PHE:HB2  | 46:M:330:ARG:HB3  | 1.89                     | 0.54              |
| 15:z:108:LYS:NZ   | 18:2:507:G:OP1    | 2.40                     | 0.54              |
| 38:B:403:ALA:H    | 38:B:419:HIS:HA   | 1.73                     | 0.54              |
| 40:C:97:VAL:O     | 40:C:101:GLY:N    | 2.38                     | 0.54              |
| 40:C:854:ASN:HA   | 40:C:857:LEU:HD12 | 1.89                     | 0.54              |
| 46:M:20:ALA:HA    | 46:M:23:LYS:HD2   | 1.88                     | 0.54              |
| 51:O:176:ILE:HA   | 51:O:179:ILE:HG22 | 1.90                     | 0.54              |
| 22:u:16:PHE:HB2   | 22:u:79:LEU:HD23  | 1.89                     | 0.54              |
| 28:h:35:VAL:HG13  | 28:h:105:SER:HB2  | 1.90                     | 0.54              |
| 40:C:859:LEU:HD13 | 43:H:247:MET:HG2  | 1.90                     | 0.54              |
| 42:F:203:ASP:HB3  | 42:F:212:SER:H    | 1.73                     | 0.54              |
| 43:H:215:MET:HA   | 43:H:218:LEU:HB2  | 1.90                     | 0.54              |
| 45:L:441:LEU:HA   | 45:L:445:LYS:HG2  | 1.90                     | 0.54              |
| 46:M:312:VAL:HG21 | 46:M:325:ILE:HD11 | 1.90                     | 0.54              |
| 7:r:57:ASP:OD2    | 7:r:72:ARG:NH1    | 2.42                     | 0.53              |
| 18:2:587:A:H5'    | 18:2:592:C:H41    | 1.73                     | 0.53              |
| 18:2:1507:G:N2    | 32:U:88:PRO:O     | 2.41                     | 0.53              |
| 24:o:83:MET:HB3   | 24:o:116:LEU:HD12 | 1.90                     | 0.53              |
| 33:V:172:LYS:HD3  | 33:V:193:GLY:H    | 1.72                     | 0.53              |
| 41:E:278:VAL:HA   | 41:E:281:ILE:HG22 | 1.91                     | 0.53              |
| 45:L:400:ARG:O    | 45:L:407:GLN:NE2  | 2.40                     | 0.53              |
| 18:2:1396:A:O2'   | 18:2:1398:G:N7    | 2.34                     | 0.53              |
| 35:j:123:VAL:HG12 | 35:j:124:LYS:HG3  | 1.90                     | 0.53              |
| 40:C:606:GLN:O    | 40:C:610:ASN:ND2  | 2.41                     | 0.53              |
| 44:K:118:TRP:HB3  | 44:K:163:GLY:HA2  | 1.89                     | 0.53              |
| 18:2:695:C:H2'    | 18:2:696:G:H8     | 1.74                     | 0.53              |
| 40:C:632:ALA:HA   | 47:N:40:GLY:HA3   | 1.90                     | 0.53              |
| 40:C:695:ILE:HG21 | 40:C:744:MET:HG3  | 1.90                     | 0.53              |
| 41:E:215:ILE:HD11 | 41:E:242:TYR:HB3  | 1.90                     | 0.53              |
| 4:Q:4:LYS:NZ      | 18:2:1863:A:OP2   | 2.41                     | 0.53              |
| 39:A:502:ARG:HG3  | 39:A:504:ASP:H    | 1.73                     | 0.53              |
| 40:C:863:LEU:HD13 | 40:C:866:LEU:HD12 | 1.91                     | 0.53              |
| 47:N:318:TYR:O    | 47:N:322:ASN:ND2  | 2.41                     | 0.53              |
| 53:Z:27:THR:OG1   | 53:Z:28:GLU:N     | 2.42                     | 0.53              |
| 15:z:99:LYS:O     | 15:z:101:LYS:NZ   | 2.42                     | 0.53              |
| 20:b:172:VAL:HG12 | 20:b:185:LYS:HG2  | 1.91                     | 0.53              |
| 21:e:35:LEU:HD12  | 21:e:117:ILE:HD13 | 1.91                     | 0.53              |
| 41:E:78:VAL:HA    | 41:E:81:LEU:HD12  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:H:246:LEU:O    | 43:H:250:VAL:HB   | 2.09                     | 0.53              |
| 3:d:200:ARG:O     | 10:c:54:ARG:NH2   | 2.39                     | 0.53              |
| 40:C:866:LEU:HD21 | 43:H:250:VAL:HG22 | 1.90                     | 0.53              |
| 41:E:330:GLU:HA   | 41:E:333:ILE:HD12 | 1.90                     | 0.53              |
| 47:N:234:VAL:HA   | 47:N:237:LYS:HD2  | 1.91                     | 0.53              |
| 2:p:179:ASN:ND2   | 2:p:183:GLU:OE1   | 2.39                     | 0.53              |
| 5:q:62:LYS:HE3    | 18:2:502:C:H4'    | 1.91                     | 0.53              |
| 39:A:448:GLN:NE2  | 39:A:493:PHE:O    | 2.41                     | 0.53              |
| 39:A:464:ALA:HA   | 39:A:467:LEU:HD12 | 1.90                     | 0.53              |
| 39:A:594:LEU:HD22 | 39:A:597:ARG:HH21 | 1.74                     | 0.53              |
| 42:F:306:ARG:HH21 | 46:M:219:LEU:HD11 | 1.74                     | 0.53              |
| 9:t:136:ILE:HA    | 9:t:139:LYS:HD2   | 1.90                     | 0.53              |
| 20:b:172:VAL:O    | 20:b:173:ARG:NH1  | 2.42                     | 0.53              |
| 38:B:520:GLN:NE2  | 38:B:571:GLU:O    | 2.42                     | 0.53              |
| 46:M:165:LEU:HB3  | 46:M:188:LEU:HD12 | 1.90                     | 0.53              |
| 1:a:128:ARG:NH2   | 1:a:151:ASP:O     | 2.42                     | 0.53              |
| 25:g:62:ARG:NH2   | 25:g:107:GLU:OE2  | 2.42                     | 0.53              |
| 41:E:353:ILE:O    | 41:E:357:ALA:HB2  | 2.09                     | 0.53              |
| 44:K:3:MET:HE2    | 44:K:35:THR:HG21  | 1.91                     | 0.53              |
| 40:C:659:ASN:OD1  | 40:C:662:GLN:NE2  | 2.42                     | 0.52              |
| 41:E:369:ARG:NH1  | 45:L:480:ASP:OD1  | 2.42                     | 0.52              |
| 43:H:123:THR:OG1  | 43:H:124:TYR:N    | 2.41                     | 0.52              |
| 44:K:32:TYR:O     | 44:K:36:GLN:HB2   | 2.09                     | 0.52              |
| 53:Z:51:ALA:HB3   | 53:Z:54:TYR:HB2   | 1.91                     | 0.52              |
| 7:r:15:LEU:HD13   | 18:2:155:G:H4'    | 1.91                     | 0.52              |
| 18:2:1550:G:H3'   | 18:2:1579:A:H61   | 1.74                     | 0.52              |
| 40:C:449:GLU:HG2  | 40:C:505:LEU:HD11 | 1.90                     | 0.52              |
| 8:s:147:LYS:HA    | 14:D:49:GLU:HG2   | 1.91                     | 0.52              |
| 15:z:104:ARG:NH2  | 18:2:507:G:OP2    | 2.41                     | 0.52              |
| 35:j:41:PHE:O     | 35:j:76:LYS:NZ    | 2.43                     | 0.52              |
| 47:N:226:THR:OG1  | 47:N:280:LYS:NZ   | 2.43                     | 0.52              |
| 39:A:129:LEU:HD13 | 40:C:470:VAL:HG12 | 1.92                     | 0.52              |
| 39:A:179:GLN:HG2  | 39:A:235:VAL:HG11 | 1.91                     | 0.52              |
| 39:A:398:PHE:HD2  | 39:A:509:PRO:HB2  | 1.74                     | 0.52              |
| 41:E:254:LEU:HA   | 41:E:257:LEU:HB2  | 1.92                     | 0.52              |
| 21:e:16:ASP:OD1   | 21:e:16:ASP:N     | 2.43                     | 0.52              |
| 38:B:612:ASN:H    | 38:B:627:GLY:HA2  | 1.73                     | 0.52              |
| 45:L:253:PRO:HA   | 45:L:256:VAL:HG12 | 1.91                     | 0.52              |
| 8:s:8:ILE:N       | 8:s:24:SER:OG     | 2.37                     | 0.52              |
| 18:2:1280:G:H5''  | 23:v:100:PRO:HA   | 1.92                     | 0.52              |
| 41:E:372:VAL:HA   | 41:E:375:ILE:HG12 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:F:270:GLN:NE2  | 46:M:372:SER:OG   | 2.42                     | 0.52              |
| 25:g:28:GLY:HA3   | 25:g:67:ASP:HB2   | 1.91                     | 0.52              |
| 38:B:389:VAL:HA   | 38:B:406:ILE:HA   | 1.92                     | 0.52              |
| 44:K:26:LEU:HA    | 44:K:29:LEU:HB2   | 1.92                     | 0.52              |
| 47:N:345:GLU:HG2  | 47:N:348:MET:HB2  | 1.91                     | 0.52              |
| 52:Y:256:LEU:HA   | 52:Y:283:ILE:HA   | 1.92                     | 0.52              |
| 3:d:94:ILE:HG21   | 3:d:162:ILE:HD12  | 1.92                     | 0.52              |
| 10:c:166:GLY:O    | 38:B:492:ARG:NH1  | 2.43                     | 0.52              |
| 18:2:1771:G:O2'   | 18:2:1774:C:N4    | 2.42                     | 0.52              |
| 40:C:628:ASP:N    | 40:C:628:ASP:OD1  | 2.39                     | 0.52              |
| 45:L:386:ILE:HG13 | 45:L:390:LEU:HD21 | 1.91                     | 0.52              |
| 47:N:359:ARG:O    | 47:N:375:CYS:N    | 2.42                     | 0.52              |
| 16:R:34:ASP:OD1   | 16:R:34:ASP:N     | 2.40                     | 0.52              |
| 33:V:146:SER:OG   | 33:V:147:HIS:N    | 2.43                     | 0.52              |
| 39:A:428:VAL:HA   | 39:A:431:LEU:HD12 | 1.92                     | 0.52              |
| 41:E:84:LEU:HD21  | 41:E:134:TYR:HA   | 1.92                     | 0.52              |
| 18:2:72:C:OP2     | 18:2:74:G:N2      | 2.43                     | 0.52              |
| 20:b:135:GLU:HG2  | 20:b:153:VAL:HG12 | 1.92                     | 0.52              |
| 34:i:34:PHE:HB3   | 34:i:41:PHE:HB2   | 1.91                     | 0.52              |
| 35:j:68:LYS:HB3   | 35:j:91:LEU:HD22  | 1.92                     | 0.52              |
| 38:B:306:TYR:HA   | 38:B:704:TRP:HA   | 1.91                     | 0.52              |
| 38:B:510:PHE:O    | 38:B:532:ARG:NH2  | 2.43                     | 0.52              |
| 43:H:47:LEU:HD13  | 43:H:50:ILE:HD11  | 1.92                     | 0.52              |
| 7:r:183:ARG:NH2   | 18:2:317:C:OP2    | 2.42                     | 0.51              |
| 9:t:101:ILE:HD12  | 9:t:190:LEU:HD11  | 1.92                     | 0.51              |
| 18:2:640:A:H2'    | 18:2:641:A:C8     | 2.45                     | 0.51              |
| 21:e:140:ASP:HB2  | 30:S:46:VAL:HG12  | 1.92                     | 0.51              |
| 38:B:500:THR:OG1  | 38:B:502:GLN:NE2  | 2.44                     | 0.51              |
| 39:A:196:LYS:O    | 39:A:200:ASN:ND2  | 2.43                     | 0.51              |
| 41:E:315:CYS:O    | 41:E:319:LEU:HB2  | 2.11                     | 0.51              |
| 43:H:207:ASN:ND2  | 43:H:212:ASN:OD1  | 2.42                     | 0.51              |
| 45:L:333:ILE:HB   | 45:L:381:ARG:HG3  | 1.90                     | 0.51              |
| 47:N:200:GLU:OE2  | 47:N:334:ARG:NH2  | 2.42                     | 0.51              |
| 51:O:190:ILE:HA   | 51:O:276:VAL:HA   | 1.92                     | 0.51              |
| 16:R:67:THR:OG1   | 16:R:70:LYS:O     | 2.27                     | 0.51              |
| 18:2:940:U:H3     | 18:2:1002:U:H3    | 1.56                     | 0.51              |
| 38:B:407:TRP:HA   | 38:B:415:LYS:H    | 1.74                     | 0.51              |
| 43:H:175:GLU:HA   | 43:H:178:LYS:HG2  | 1.91                     | 0.51              |
| 44:K:19:ASP:HA    | 44:K:22:ASN:HD21  | 1.75                     | 0.51              |
| 18:2:1255:G:OP1   | 18:2:1256:G:O2'   | 2.25                     | 0.51              |
| 39:A:515:PRO:HA   | 39:A:518:GLN:HB2  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:C:515:ASP:OD1  | 40:C:515:ASP:N    | 2.43                     | 0.51              |
| 41:E:41:LYS:O     | 41:E:45:LEU:HB2   | 2.10                     | 0.51              |
| 1:a:37:TYR:OH     | 1:a:57:LYS:NZ     | 2.44                     | 0.51              |
| 18:2:949:G:H1     | 18:2:977:C:H5     | 1.57                     | 0.51              |
| 20:b:114:ALA:HB3  | 20:b:117:ARG:HG3  | 1.92                     | 0.51              |
| 33:V:10:THR:HG22  | 33:V:308:ARG:HG2  | 1.91                     | 0.51              |
| 23:v:122:ASP:OD1  | 23:v:122:ASP:N    | 2.43                     | 0.51              |
| 36:G:96:ASN:ND2   | 36:G:99:GLU:OE1   | 2.43                     | 0.51              |
| 40:C:594:LEU:HD22 | 40:C:598:ILE:HD13 | 1.92                     | 0.51              |
| 40:C:857:LEU:O    | 41:E:407:LYS:NZ   | 2.43                     | 0.51              |
| 41:E:306:ASP:N    | 41:E:306:ASP:OD1  | 2.43                     | 0.51              |
| 41:E:408:THR:HG21 | 42:F:339:TYR:HE2  | 1.75                     | 0.51              |
| 41:E:418:LEU:HA   | 41:E:421:ASN:HD22 | 1.76                     | 0.51              |
| 46:M:205:HIS:HE1  | 46:M:236:LEU:HD21 | 1.73                     | 0.51              |
| 47:N:346:ASP:OD1  | 47:N:346:ASP:N    | 2.44                     | 0.51              |
| 38:B:576:LYS:HA   | 38:B:593:HIS:HA   | 1.92                     | 0.51              |
| 41:E:38:LEU:HD21  | 41:E:61:LEU:HB2   | 1.92                     | 0.51              |
| 41:E:267:VAL:HG23 | 41:E:270:ARG:HE   | 1.75                     | 0.51              |
| 47:N:398:GLU:OE2  | 47:N:401:SER:OG   | 2.29                     | 0.51              |
| 9:t:181:GLN:NE2   | 18:2:380:G:OP2    | 2.44                     | 0.51              |
| 41:E:153:PHE:O    | 41:E:157:LEU:HB3  | 2.11                     | 0.51              |
| 41:E:163:ARG:HD3  | 41:E:164:ASN:HB2  | 1.93                     | 0.51              |
| 46:M:156:LEU:HB2  | 46:M:161:LYS:HE2  | 1.92                     | 0.51              |
| 46:M:327:GLN:O    | 46:M:330:ARG:NH2  | 2.42                     | 0.51              |
| 38:B:548:ARG:HD2  | 38:B:555:PRO:HB2  | 1.93                     | 0.51              |
| 39:A:342:LEU:HD11 | 40:C:719:ARG:HB3  | 1.93                     | 0.51              |
| 51:O:23:VAL:HA    | 51:O:33:VAL:HG12  | 1.92                     | 0.51              |
| 52:Y:81:LEU:O     | 52:Y:260:ARG:NH1  | 2.43                     | 0.51              |
| 1:a:106:GLY:N     | 1:a:136:GLU:OE2   | 2.43                     | 0.50              |
| 11:n:126:VAL:HG12 | 11:n:145:VAL:HG22 | 1.93                     | 0.50              |
| 18:2:1387:G:H21   | 19:w:8:THR:HG21   | 1.76                     | 0.50              |
| 39:A:12:LEU:HD11  | 39:A:49:PRO:HB2   | 1.92                     | 0.50              |
| 41:E:118:ALA:HA   | 41:E:124:ARG:HH11 | 1.76                     | 0.50              |
| 9:t:165:GLN:HE22  | 9:t:195:LEU:HD11  | 1.75                     | 0.50              |
| 40:C:114:GLU:O    | 40:C:118:ASN:ND2  | 2.44                     | 0.50              |
| 45:L:256:VAL:HA   | 45:L:260:TYR:HB2  | 1.93                     | 0.50              |
| 18:2:1748:G:H1    | 18:2:1786:U:H3    | 1.58                     | 0.50              |
| 24:o:100:LYS:HG3  | 24:o:101:THR:HG23 | 1.93                     | 0.50              |
| 33:V:116:ASP:N    | 33:V:116:ASP:OD1  | 2.43                     | 0.50              |
| 33:V:298:LEU:HB3  | 33:V:310:TRP:HB2  | 1.93                     | 0.50              |
| 39:A:407:VAL:HA   | 39:A:410:VAL:HG12 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:A:420:LYS:HD2  | 39:A:421:GLU:HG2  | 1.93                     | 0.50              |
| 42:F:212:SER:O    | 42:F:214:LYS:NZ   | 2.39                     | 0.50              |
| 42:F:251:LEU:HD21 | 42:F:271:GLN:HE22 | 1.76                     | 0.50              |
| 42:F:302:ASN:OD1  | 42:F:306:ARG:NH1  | 2.40                     | 0.50              |
| 43:H:242:ASN:HD22 | 43:H:330:ILE:HG22 | 1.74                     | 0.50              |
| 1:a:80:ARG:NH2    | 1:a:165:ASN:O     | 2.41                     | 0.50              |
| 18:2:1760:G:H21   | 18:2:1773:C:H41   | 1.58                     | 0.50              |
| 27:x:76:THR:OG1   | 27:x:95:GLY:O     | 2.30                     | 0.50              |
| 46:M:193:THR:OG1  | 46:M:195:ASP:OD1  | 2.27                     | 0.50              |
| 51:O:26:ILE:HD11  | 51:O:62:ILE:HG21  | 1.93                     | 0.50              |
| 12:m:54:LEU:HD23  | 12:m:58:HIS:HD2   | 1.77                     | 0.50              |
| 26:k:13:LEU:HB2   | 26:k:20:ILE:HB    | 1.94                     | 0.50              |
| 43:H:38:GLN:HA    | 43:H:201:VAL:HB   | 1.92                     | 0.50              |
| 43:H:171:PRO:HA   | 43:H:174:MET:HB2  | 1.94                     | 0.50              |
| 44:K:143:CYS:HA   | 44:K:146:VAL:HG12 | 1.92                     | 0.50              |
| 44:K:167:ASP:HA   | 44:K:170:LEU:HB2  | 1.94                     | 0.50              |
| 25:g:62:ARG:HH12  | 25:g:111:ILE:HD12 | 1.76                     | 0.50              |
| 42:F:292:ASP:O    | 42:F:296:GLY:N    | 2.43                     | 0.50              |
| 45:L:322:ALA:O    | 45:L:326:MET:CB   | 2.57                     | 0.50              |
| 45:L:380:MET:HE2  | 45:L:521:PHE:HB3  | 1.92                     | 0.50              |
| 47:N:271:ARG:HH12 | 47:N:274:SER:HA   | 1.77                     | 0.50              |
| 18:2:880:G:N2     | 18:2:906:U:O2     | 2.45                     | 0.50              |
| 30:S:29:GLN:HA    | 30:S:45:ASN:HA    | 1.93                     | 0.50              |
| 41:E:153:PHE:O    | 41:E:157:LEU:CB   | 2.59                     | 0.50              |
| 45:L:360:ILE:O    | 45:L:364:ASN:ND2  | 2.44                     | 0.50              |
| 47:N:248:THR:H    | 47:N:251:ILE:HD11 | 1.77                     | 0.50              |
| 52:Y:54:LYS:NZ    | 52:Y:133:VAL:O    | 2.44                     | 0.50              |
| 23:v:24:THR:HA    | 23:v:27:ILE:HG12  | 1.92                     | 0.50              |
| 23:v:80:ASP:OD1   | 23:v:80:ASP:N     | 2.44                     | 0.50              |
| 39:A:220:LEU:HD23 | 39:A:262:LEU:HD22 | 1.93                     | 0.50              |
| 44:K:85:CYS:HA    | 44:K:88:MET:HG2   | 1.94                     | 0.50              |
| 46:M:249:LEU:HD23 | 46:M:281:THR:HG21 | 1.94                     | 0.50              |
| 51:O:156:VAL:HG12 | 51:O:180:ASN:HD22 | 1.75                     | 0.50              |
| 3:d:116:THR:OG1   | 3:d:119:GLY:O     | 2.28                     | 0.50              |
| 7:r:163:ASN:HA    | 18:2:67:C:H41     | 1.76                     | 0.50              |
| 18:2:874:G:H2'    | 18:2:875:A:H8     | 1.77                     | 0.50              |
| 18:2:1536:G:H2'   | 18:2:1537:A:C8    | 2.46                     | 0.50              |
| 23:v:92:CYS:SG    | 23:v:93:LYS:N     | 2.83                     | 0.50              |
| 33:V:74:ASP:N     | 33:V:74:ASP:OD1   | 2.45                     | 0.50              |
| 51:O:23:VAL:HB    | 51:O:64:ILE:HA    | 1.93                     | 0.50              |
| 18:2:883:U:O4     | 18:2:902:G:N1     | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:B:516:LYS:HE2  | 38:B:529:LYS:HG3  | 1.94                     | 0.49              |
| 39:A:412:ASN:HA   | 39:A:415:ARG:HB2  | 1.94                     | 0.49              |
| 42:F:169:ILE:HG13 | 42:F:195:PRO:HG3  | 1.94                     | 0.49              |
| 46:M:212:LEU:O    | 46:M:273:ASN:ND2  | 2.45                     | 0.49              |
| 8:s:50:GLU:OE1    | 8:s:58:LYS:NZ     | 2.44                     | 0.49              |
| 14:D:86:LEU:HD21  | 14:D:113:HIS:HB2  | 1.94                     | 0.49              |
| 18:2:195:C:H2'    | 18:2:196:C:H4'    | 1.93                     | 0.49              |
| 23:v:93:LYS:O     | 23:v:101:ARG:NH2  | 2.45                     | 0.49              |
| 39:A:84:LYS:HA    | 39:A:87:GLU:HG2   | 1.93                     | 0.49              |
| 40:C:325:THR:OG1  | 40:C:326:HIS:N    | 2.45                     | 0.49              |
| 47:N:165:ARG:NH1  | 47:N:167:ASP:OD1  | 2.45                     | 0.49              |
| 18:2:1228:A:H2'   | 18:2:1229:G:C8    | 2.47                     | 0.49              |
| 22:u:37:ASP:OD2   | 22:u:38:LYS:NZ    | 2.44                     | 0.49              |
| 39:A:518:GLN:O    | 39:A:522:GLN:NE2  | 2.40                     | 0.49              |
| 47:N:238:LEU:HD23 | 47:N:242:GLN:HE21 | 1.77                     | 0.49              |
| 18:2:1651:A:H1'   | 21:e:83:ASN:HD22  | 1.78                     | 0.49              |
| 22:u:23:ALA:O     | 22:u:66:HIS:ND1   | 2.45                     | 0.49              |
| 44:K:116:ALA:HA   | 44:K:120:ALA:HB3  | 1.94                     | 0.49              |
| 47:N:268:VAL:O    | 47:N:279:ASP:N    | 2.45                     | 0.49              |
| 38:B:523:GLY:O    | 38:B:550:ARG:NH2  | 2.46                     | 0.49              |
| 51:O:117:VAL:HG21 | 51:O:174:VAL:HG21 | 1.95                     | 0.49              |
| 2:p:123:ALA:HB2   | 2:p:165:ARG:HG3   | 1.95                     | 0.49              |
| 18:2:1771:G:N2    | 18:2:1775:U:OP1   | 2.46                     | 0.49              |
| 20:b:137:VAL:HG22 | 20:b:151:LYS:HG3  | 1.94                     | 0.49              |
| 44:K:20:ARG:NH2   | 44:K:45:GLU:OE1   | 2.39                     | 0.49              |
| 51:O:124:GLU:HA   | 51:O:127:GLU:HB3  | 1.94                     | 0.49              |
| 18:2:681:U:H4'    | 35:j:9:THR:HG22   | 1.93                     | 0.49              |
| 18:2:1683:C:H2'   | 18:2:1684:C:H6    | 1.77                     | 0.49              |
| 39:A:311:THR:OG1  | 39:A:312:GLN:N    | 2.44                     | 0.49              |
| 40:C:868:GLU:OE1  | 40:C:872:ARG:NH1  | 2.46                     | 0.49              |
| 45:L:483:GLU:OE2  | 45:L:489:GLN:NE2  | 2.45                     | 0.49              |
| 4:Q:2:THR:N       | 18:2:1199:A:OP1   | 2.46                     | 0.49              |
| 7:r:14:LYS:HE3    | 7:r:124:LEU:HG    | 1.94                     | 0.49              |
| 18:2:641:A:O2'    | 18:2:645:C:OP1    | 2.30                     | 0.49              |
| 39:A:101:THR:HG22 | 39:A:149:TRP:HB3  | 1.95                     | 0.49              |
| 41:E:136:LYS:NZ   | 47:N:15:GLY:O     | 2.46                     | 0.49              |
| 43:H:68:LEU:HD23  | 43:H:81:CYS:HA    | 1.95                     | 0.49              |
| 42:F:115:ARG:NH1  | 42:F:141:GLU:OE2  | 2.45                     | 0.49              |
| 44:K:151:GLN:OE1  | 44:K:192:GLN:NE2  | 2.46                     | 0.49              |
| 46:M:337:SER:OG   | 46:M:338:THR:N    | 2.46                     | 0.49              |
| 5:q:171:ASP:OD1   | 5:q:171:ASP:N     | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:2:145:G:H2'    | 18:2:146:G:C8     | 2.48                     | 0.49              |
| 18:2:1119:A:H2'   | 18:2:1120:U:C2    | 2.48                     | 0.49              |
| 24:o:22:LEU:HA    | 24:o:25:LEU:HD12  | 1.95                     | 0.49              |
| 38:B:358:ALA:HA   | 38:B:370:ARG:HA   | 1.94                     | 0.49              |
| 41:E:68:HIS:HA    | 41:E:71:ARG:HD2   | 1.94                     | 0.49              |
| 41:E:111:ARG:O    | 41:E:111:ARG:NH1  | 2.46                     | 0.49              |
| 42:F:91:VAL:HG22  | 42:F:238:LYS:HZ2  | 1.76                     | 0.49              |
| 42:F:264:GLY:HA2  | 43:H:204:VAL:HA   | 1.95                     | 0.49              |
| 8:s:65:PRO:O      | 8:s:69:LEU:N      | 2.46                     | 0.48              |
| 44:K:37:ALA:HB1   | 44:K:131:ILE:HG12 | 1.94                     | 0.48              |
| 16:R:41:TYR:OH    | 40:C:563:ARG:NH2  | 2.46                     | 0.48              |
| 24:o:27:ASP:OD1   | 24:o:27:ASP:N     | 2.47                     | 0.48              |
| 29:P:103:HIS:HD2  | 29:P:105:ALA:H    | 1.61                     | 0.48              |
| 40:C:504:LEU:HD22 | 40:C:564:ILE:HG23 | 1.95                     | 0.48              |
| 40:C:697:TYR:OH   | 40:C:708:ARG:N    | 2.42                     | 0.48              |
| 40:C:835:LEU:HA   | 40:C:842:VAL:HA   | 1.94                     | 0.48              |
| 42:F:283:LEU:HA   | 42:F:286:VAL:HG22 | 1.94                     | 0.48              |
| 43:H:334:THR:HA   | 43:H:337:ASN:HD22 | 1.78                     | 0.48              |
| 41:E:255:ARG:HB2  | 41:E:292:ILE:HD11 | 1.96                     | 0.48              |
| 50:4:231:ARG:HH21 | 50:4:279:VAL:HA   | 1.78                     | 0.48              |
| 53:Z:76:HIS:ND1   | 53:Z:77:PRO:O     | 2.46                     | 0.48              |
| 2:p:78:GLU:OE1    | 39:A:10:ASN:ND2   | 2.47                     | 0.48              |
| 39:A:390:LEU:HD11 | 39:A:410:VAL:HG11 | 1.96                     | 0.48              |
| 42:F:323:PHE:HZ   | 43:H:345:GLN:HA   | 1.79                     | 0.48              |
| 45:L:477:GLY:O    | 45:L:481:LEU:HB2  | 2.13                     | 0.48              |
| 34:i:57:THR:H     | 34:i:60:MET:HE3   | 1.77                     | 0.48              |
| 41:E:32:TYR:HB2   | 47:N:2:ALA:HA     | 1.96                     | 0.48              |
| 44:K:71:LEU:HB3   | 44:K:134:PHE:HE2  | 1.78                     | 0.48              |
| 48:X:5:ALA:HA     | 48:X:47:ALA:HA    | 1.96                     | 0.48              |
| 2:p:190:PRO:HB3   | 39:A:17:GLU:HG3   | 1.94                     | 0.48              |
| 2:p:214:LYS:NZ    | 18:2:943:U:OP1    | 2.46                     | 0.48              |
| 8:s:31:GLU:O      | 8:s:37:LYS:N      | 2.45                     | 0.48              |
| 18:2:1536:G:H2'   | 18:2:1537:A:H8    | 1.79                     | 0.48              |
| 18:2:1849:G:H2'   | 18:2:1850:A:C8    | 2.49                     | 0.48              |
| 35:j:28:LYS:HE2   | 35:j:32:LEU:HD22  | 1.95                     | 0.48              |
| 39:A:331:ILE:HD13 | 39:A:437:LEU:HD11 | 1.95                     | 0.48              |
| 40:C:818:VAL:HA   | 40:C:821:ILE:HG22 | 1.95                     | 0.48              |
| 41:E:399:SER:O    | 41:E:403:GLN:NE2  | 2.47                     | 0.48              |
| 42:F:265:LEU:HB2  | 43:H:203:ILE:HB   | 1.95                     | 0.48              |
| 52:Y:191:LYS:H    | 52:Y:226:ALA:H    | 1.62                     | 0.48              |
| 18:2:1563:G:OP1   | 27:x:121:ARG:NH1  | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:B:526:LEU:HB3  | 38:B:547:PHE:HB2  | 1.96                     | 0.48              |
| 39:A:144:LEU:HD22 | 40:C:467:GLN:HB3  | 1.95                     | 0.48              |
| 41:E:132:TYR:CD2  | 41:E:132:TYR:C    | 2.92                     | 0.48              |
| 18:2:1285:G:H1    | 23:v:56:CYS:HA    | 1.79                     | 0.48              |
| 39:A:497:LEU:HD12 | 39:A:519:ILE:HD13 | 1.95                     | 0.48              |
| 2:p:209:ASP:N     | 2:p:209:ASP:OD1   | 2.46                     | 0.48              |
| 18:2:1773:C:OP2   | 18:2:1774:C:N4    | 2.42                     | 0.48              |
| 30:S:31:ARG:NH1   | 30:S:41:SER:OG    | 2.47                     | 0.48              |
| 44:K:153:ILE:HB   | 44:K:157:LEU:HD11 | 1.96                     | 0.48              |
| 50:4:284:CYS:SG   | 50:4:304:THR:OG1  | 2.69                     | 0.48              |
| 3:d:187:ARG:NH2   | 18:2:1154:U:OP2   | 2.47                     | 0.48              |
| 18:2:540:U:H1'    | 18:2:544:G:H22    | 1.78                     | 0.48              |
| 18:2:1292:C:O2    | 32:U:138:ARG:NE   | 2.47                     | 0.48              |
| 45:L:330:GLN:O    | 45:L:334:ARG:NH1  | 2.44                     | 0.48              |
| 45:L:388:LEU:O    | 45:L:392:GLU:N    | 2.47                     | 0.48              |
| 2:p:173:THR:O     | 2:p:177:GLN:HB2   | 2.14                     | 0.47              |
| 7:r:190:ARG:NH1   | 18:2:333:G:OP2    | 2.46                     | 0.47              |
| 9:t:118:ALA:HB3   | 9:t:153:LYS:HD2   | 1.96                     | 0.47              |
| 10:c:177:ASN:HA   | 10:c:180:LYS:HE2  | 1.95                     | 0.47              |
| 18:2:938:A:H62    | 18:2:1004:U:H3    | 1.60                     | 0.47              |
| 39:A:578:ARG:HE   | 39:A:582:LEU:HD21 | 1.79                     | 0.47              |
| 40:C:415:ASN:N    | 40:C:415:ASN:OD1  | 2.47                     | 0.47              |
| 50:4:209:VAL:HG11 | 50:4:267:ILE:HG13 | 1.94                     | 0.47              |
| 9:t:3:ILE:O       | 9:t:30:GLY:N      | 2.44                     | 0.47              |
| 18:2:1521:C:OP2   | 26:k:136:THR:OG1  | 2.23                     | 0.47              |
| 32:U:137:ASP:OD1  | 32:U:137:ASP:N    | 2.46                     | 0.47              |
| 42:F:226:ARG:NH1  | 46:M:13:ASP:OD2   | 2.47                     | 0.47              |
| 47:N:76:ASP:OD1   | 47:N:76:ASP:N     | 2.45                     | 0.47              |
| 47:N:247:ALA:HA   | 47:N:251:ILE:HD11 | 1.96                     | 0.47              |
| 1:a:122:LEU:HD23  | 1:a:144:THR:HG23  | 1.96                     | 0.47              |
| 8:s:31:GLU:OE2    | 8:s:41:ARG:NH1    | 2.45                     | 0.47              |
| 18:2:691:G:H2'    | 18:2:692:G:C8     | 2.49                     | 0.47              |
| 18:2:751:G:H22    | 18:2:792:C:H1'    | 1.79                     | 0.47              |
| 38:B:306:TYR:N    | 38:B:319:PHE:O    | 2.45                     | 0.47              |
| 40:C:430:ASN:ND2  | 40:C:437:PRO:O    | 2.45                     | 0.47              |
| 47:N:526:THR:HG23 | 47:N:527:PHE:HD1  | 1.79                     | 0.47              |
| 7:r:189:ARG:NH2   | 18:2:332:G:O6     | 2.47                     | 0.47              |
| 18:2:1643:U:O2'   | 25:g:142:GLN:O    | 2.31                     | 0.47              |
| 39:A:523:LEU:HD11 | 43:H:344:ALA:HB2  | 1.96                     | 0.47              |
| 45:L:245:GLU:HB3  | 45:L:436:HIS:HD2  | 1.79                     | 0.47              |
| 52:Y:375:TYR:H    | 52:Y:424:LEU:HA   | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:r:175:LYS:HG3   | 18:2:77:A:H2      | 1.80                     | 0.47              |
| 18:2:511:U:O2'    | 18:2:576:A:N6     | 2.47                     | 0.47              |
| 23:v:79:VAL:HG12  | 23:v:81:ASP:H     | 1.79                     | 0.47              |
| 40:C:804:MET:HG3  | 40:C:819:HIS:HE1  | 1.79                     | 0.47              |
| 41:E:189:LEU:HD21 | 41:E:221:VAL:HG11 | 1.97                     | 0.47              |
| 41:E:358:ASP:O    | 41:E:361:ASN:ND2  | 2.47                     | 0.47              |
| 41:E:418:LEU:HD11 | 42:F:350:LEU:HD13 | 1.96                     | 0.47              |
| 42:F:98:ILE:HG13  | 42:F:131:VAL:HG13 | 1.96                     | 0.47              |
| 46:M:292:ILE:HB   | 46:M:332:VAL:HB   | 1.96                     | 0.47              |
| 47:N:184:TYR:OH   | 47:N:492:ARG:NH1  | 2.47                     | 0.47              |
| 47:N:393:ILE:HD13 | 47:N:448:LYS:HB2  | 1.95                     | 0.47              |
| 4:Q:52:ASP:OD2    | 34:i:117:ARG:NH1  | 2.48                     | 0.47              |
| 39:A:311:THR:OG1  | 39:A:313:ASP:OD1  | 2.32                     | 0.47              |
| 42:F:263:ILE:O    | 43:H:205:ILE:N    | 2.45                     | 0.47              |
| 1:a:3:GLY:N       | 13:y:78:ILE:O     | 2.48                     | 0.47              |
| 2:p:48:LEU:HB3    | 34:i:51:GLU:HG2   | 1.96                     | 0.47              |
| 18:2:1242:U:O2    | 18:2:1517:G:O2'   | 2.30                     | 0.47              |
| 45:L:281:HIS:HA   | 45:L:284:LEU:HB2  | 1.96                     | 0.47              |
| 3:d:205:VAL:O     | 3:d:224:THR:OG1   | 2.30                     | 0.47              |
| 18:2:1285:G:H5'   | 23:v:35:ILE:HG22  | 1.97                     | 0.47              |
| 20:b:41:VAL:HG23  | 20:b:46:THR:HG22  | 1.97                     | 0.47              |
| 40:C:80:LEU:HA    | 40:C:141:LEU:HD13 | 1.96                     | 0.47              |
| 40:C:784:GLN:HB3  | 40:C:813:LEU:HD11 | 1.97                     | 0.47              |
| 41:E:138:GLN:HE22 | 41:E:146:GLY:HA3  | 1.80                     | 0.47              |
| 45:L:471:PRO:O    | 45:L:475:LEU:N    | 2.47                     | 0.47              |
| 46:M:189:LEU:HB3  | 46:M:226:LEU:HG   | 1.95                     | 0.47              |
| 46:M:345:GLN:HA   | 46:M:348:GLN:HG3  | 1.97                     | 0.47              |
| 8:s:163:GLN:O     | 8:s:167:GLU:HB2   | 2.15                     | 0.47              |
| 18:2:1719:A:N6    | 18:2:1720:U:O2    | 2.48                     | 0.47              |
| 25:g:89:SER:OG    | 25:g:119:LEU:O    | 2.33                     | 0.47              |
| 36:G:63:GLY:HA2   | 36:G:66:ARG:HB2   | 1.97                     | 0.47              |
| 41:E:45:LEU:HD22  | 41:E:50:MET:HB3   | 1.96                     | 0.47              |
| 45:L:295:GLU:HB2  | 45:L:298:GLU:HB2  | 1.96                     | 0.47              |
| 45:L:332:ALA:HA   | 45:L:335:VAL:HG12 | 1.97                     | 0.47              |
| 47:N:303:GLY:O    | 47:N:311:ASN:ND2  | 2.48                     | 0.47              |
| 7:r:198:ARG:NH1   | 18:2:126:G:OP2    | 2.48                     | 0.47              |
| 14:D:90:GLN:HB2   | 14:D:94:LEU:HD12  | 1.97                     | 0.47              |
| 38:B:337:GLU:N    | 38:B:352:PHE:O    | 2.47                     | 0.47              |
| 46:M:110:PHE:CG   | 46:M:127:LEU:HD11 | 2.50                     | 0.47              |
| 47:N:301:ASP:OD2  | 47:N:305:SER:OG   | 2.28                     | 0.47              |
| 1:a:54:THR:OG1    | 1:a:162:PRO:O     | 2.33                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:c:125:HIS:O    | 10:c:129:LEU:HB2  | 2.16                     | 0.46              |
| 18:2:885:U:H2'    | 18:2:901:G:H1     | 1.79                     | 0.46              |
| 21:e:185:SER:O    | 21:e:191:LYS:NZ   | 2.47                     | 0.46              |
| 22:u:21:MET:HG2   | 22:u:49:MET:HE3   | 1.98                     | 0.46              |
| 29:P:101:SER:HB3  | 29:P:108:ILE:HD12 | 1.97                     | 0.46              |
| 42:F:293:VAL:O    | 46:M:344:LYS:NZ   | 2.48                     | 0.46              |
| 45:L:442:GLN:OE1  | 45:L:443:GLN:NE2  | 2.44                     | 0.46              |
| 45:L:480:ASP:HB3  | 45:L:486:PHE:HB3  | 1.96                     | 0.46              |
| 46:M:253:VAL:HB   | 46:M:257:GLN:HE22 | 1.78                     | 0.46              |
| 18:2:751:G:H1     | 18:2:792:C:H1'    | 1.79                     | 0.46              |
| 26:k:109:GLU:HA   | 26:k:112:GLU:HG2  | 1.96                     | 0.46              |
| 33:V:11:LEU:HB2   | 33:V:307:VAL:HB   | 1.98                     | 0.46              |
| 33:V:30:MET:HE2   | 33:V:30:MET:HB3   | 1.86                     | 0.46              |
| 41:E:229:ARG:HB2  | 41:E:265:LYS:HZ1  | 1.80                     | 0.46              |
| 7:r:93:LYS:HE2    | 7:r:93:LYS:HB2    | 1.84                     | 0.46              |
| 9:t:103:LEU:HD22  | 9:t:170:LYS:HB3   | 1.98                     | 0.46              |
| 11:n:111:VAL:HG11 | 11:n:128:VAL:HG11 | 1.96                     | 0.46              |
| 18:2:718:C:N4     | 18:2:719:G:O6     | 2.49                     | 0.46              |
| 33:V:64:HIS:HD2   | 33:V:65:PHE:H     | 1.62                     | 0.46              |
| 41:E:8:THR:HG22   | 47:N:7:PRO:HB3    | 1.96                     | 0.46              |
| 46:M:46:ILE:HD11  | 46:M:86:LEU:HD13  | 1.98                     | 0.46              |
| 29:P:73:VAL:O     | 29:P:77:LEU:HB2   | 2.14                     | 0.46              |
| 40:C:553:LYS:HE3  | 47:N:28:MET:HB2   | 1.96                     | 0.46              |
| 42:F:328:ASN:HA   | 42:F:331:ILE:HG12 | 1.96                     | 0.46              |
| 44:K:174:MET:HB3  | 44:K:179:TRP:HB2  | 1.96                     | 0.46              |
| 42:F:169:ILE:HG23 | 42:F:195:PRO:HB3  | 1.97                     | 0.46              |
| 44:K:11:VAL:HG13  | 44:K:15:LEU:HD12  | 1.97                     | 0.46              |
| 50:4:266:GLN:HB2  | 53:Z:113:PHE:HB2  | 1.98                     | 0.46              |
| 7:r:136:LYS:NZ    | 7:r:175:LYS:O     | 2.40                     | 0.46              |
| 9:t:25:ARG:HA     | 18:2:448:A:H5''   | 1.98                     | 0.46              |
| 18:2:1585:U:O2'   | 18:2:1587:G:OP2   | 2.33                     | 0.46              |
| 23:v:15:ASN:HA    | 23:v:18:LEU:HD13  | 1.98                     | 0.46              |
| 40:C:759:GLU:HA   | 40:C:762:ASN:HD22 | 1.80                     | 0.46              |
| 46:M:42:LEU:HD13  | 46:M:70:LEU:HD11  | 1.98                     | 0.46              |
| 51:O:158:ASP:OD1  | 51:O:158:ASP:N    | 2.49                     | 0.46              |
| 15:z:110:ARG:NH2  | 15:z:125:VAL:O    | 2.40                     | 0.46              |
| 18:2:196:C:O2'    | 18:2:204:G:N2     | 2.49                     | 0.46              |
| 18:2:528:A:H2'    | 18:2:529:A:H8     | 1.80                     | 0.46              |
| 21:e:102:LEU:HD11 | 29:P:100:VAL:HG21 | 1.98                     | 0.46              |
| 29:P:47:LEU:HB2   | 29:P:79:ILE:HG22  | 1.97                     | 0.46              |
| 40:C:821:ILE:HG12 | 40:C:825:MET:HE3  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:D:71:LYS:NZ    | 18:2:1156:U:OP1   | 2.45                     | 0.46              |
| 18:2:546:G:O2'    | 18:2:549:C:OP1    | 2.34                     | 0.46              |
| 18:2:1454:A:H5''  | 19:w:3:ARG:HD2    | 1.97                     | 0.46              |
| 28:h:56:MET:HE3   | 28:h:88:LEU:HD21  | 1.97                     | 0.46              |
| 32:U:91:ASN:OD1   | 32:U:91:ASN:N     | 2.46                     | 0.46              |
| 39:A:250:PHE:HB2  | 40:C:726:LEU:HD22 | 1.97                     | 0.46              |
| 40:C:368:GLU:HG3  | 40:C:415:ASN:HD21 | 1.81                     | 0.46              |
| 40:C:614:VAL:HG11 | 40:C:646:LEU:HD21 | 1.97                     | 0.46              |
| 42:F:322:ASP:N    | 42:F:322:ASP:OD1  | 2.49                     | 0.46              |
| 51:O:284:GLU:O    | 51:O:288:GLN:N    | 2.47                     | 0.46              |
| 25:g:53:GLU:OE1   | 25:g:85:ARG:NH2   | 2.43                     | 0.46              |
| 33:V:213:ASP:OD1  | 33:V:213:ASP:N    | 2.45                     | 0.46              |
| 38:B:507:ARG:HB2  | 38:B:547:PHE:HZ   | 1.80                     | 0.46              |
| 39:A:272:MET:HE2  | 39:A:272:MET:HB3  | 1.88                     | 0.46              |
| 40:C:767:ASP:OD1  | 40:C:776:ARG:NH2  | 2.49                     | 0.46              |
| 8:s:73:GLN:HA     | 8:s:76:GLN:HB2    | 1.97                     | 0.46              |
| 39:A:54:TYR:HD2   | 39:A:55:LEU:HD22  | 1.81                     | 0.46              |
| 39:A:407:VAL:O    | 39:A:411:LEU:HB2  | 2.16                     | 0.46              |
| 39:A:572:ARG:NH2  | 43:H:111:ASN:OD1  | 2.49                     | 0.46              |
| 41:E:232:ILE:O    | 41:E:236:PHE:HB2  | 2.16                     | 0.46              |
| 41:E:286:TYR:OH   | 47:N:35:LYS:NZ    | 2.40                     | 0.46              |
| 42:F:309:MET:HA   | 42:F:312:VAL:HG22 | 1.97                     | 0.46              |
| 46:M:121:TYR:HD1  | 46:M:164:LEU:HD22 | 1.79                     | 0.46              |
| 47:N:222:ARG:HH11 | 47:N:352:GLU:HA   | 1.81                     | 0.46              |
| 51:O:70:VAL:HG21  | 51:O:84:LEU:HD13  | 1.97                     | 0.46              |
| 7:r:159:ARG:NH2   | 18:2:78:C:OP1     | 2.49                     | 0.45              |
| 39:A:307:ARG:HB3  | 39:A:310:LEU:HB3  | 1.98                     | 0.45              |
| 44:K:213:ILE:HG12 | 45:L:534:LYS:HZ1  | 1.80                     | 0.45              |
| 18:2:1761:U:O2'   | 18:2:1772:C:N4    | 2.45                     | 0.45              |
| 39:A:468:GLU:HA   | 39:A:471:ILE:HG12 | 1.98                     | 0.45              |
| 40:C:451:MET:HE3  | 40:C:451:MET:HB3  | 1.74                     | 0.45              |
| 51:O:122:LYS:HE2  | 51:O:125:GLN:HB2  | 1.97                     | 0.45              |
| 52:Y:295:GLU:HA   | 52:Y:315:PHE:HA   | 1.98                     | 0.45              |
| 4:Q:79:ILE:HD13   | 18:2:1863:A:H1'   | 1.98                     | 0.45              |
| 27:x:25:SER:O     | 27:x:27:LYS:NZ    | 2.50                     | 0.45              |
| 18:2:1546:G:H5'   | 25:g:18:THR:HG21  | 1.99                     | 0.45              |
| 33:V:39:THR:HG22  | 33:V:60:ARG:HB3   | 1.99                     | 0.45              |
| 41:E:264:ASN:OD1  | 41:E:270:ARG:NH1  | 2.49                     | 0.45              |
| 41:E:383:LYS:NZ   | 41:E:384:ILE:O    | 2.50                     | 0.45              |
| 42:F:99:LEU:HD22  | 43:H:218:LEU:HD21 | 1.98                     | 0.45              |
| 42:F:253:MET:HE1  | 43:H:215:MET:HG3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:t:55:TYR:OH     | 18:2:309:G:OP2    | 2.34                     | 0.45              |
| 14:D:14:ILE:HG13  | 14:D:27:ILE:HD11  | 1.99                     | 0.45              |
| 14:D:102:ILE:H    | 14:D:113:HIS:CD2  | 2.35                     | 0.45              |
| 18:2:1588:A:H2'   | 18:2:1589:A:C8    | 2.51                     | 0.45              |
| 18:2:1679:A:H2'   | 21:e:60:ARG:HD2   | 1.97                     | 0.45              |
| 18:2:1706:G:H2'   | 18:2:1707:U:H6    | 1.80                     | 0.45              |
| 21:e:32:ASP:OD1   | 21:e:34:SER:OG    | 2.34                     | 0.45              |
| 28:h:80:PHE:HB3   | 31:l:52:PHE:HB3   | 1.99                     | 0.45              |
| 41:E:353:ILE:O    | 41:E:357:ALA:CB   | 2.65                     | 0.45              |
| 42:F:119:THR:HG1  | 42:F:190:TYR:HH   | 1.57                     | 0.45              |
| 42:F:270:GLN:NE2  | 46:M:372:SER:O    | 2.50                     | 0.45              |
| 42:F:328:ASN:O    | 42:F:332:ASN:HB2  | 2.16                     | 0.45              |
| 34:i:101:GLY:HA3  | 34:i:134:PRO:HG2  | 1.98                     | 0.45              |
| 39:A:285:LYS:HA   | 39:A:285:LYS:HD3  | 1.81                     | 0.45              |
| 39:A:550:HIS:CE1  | 42:F:210:ARG:HG2  | 2.52                     | 0.45              |
| 42:F:244:THR:HA   | 42:F:247:ILE:HG22 | 1.97                     | 0.45              |
| 44:K:145:VAL:HA   | 44:K:148:ILE:HG22 | 1.98                     | 0.45              |
| 1:a:157:VAL:O     | 13:y:65:SER:OG    | 2.35                     | 0.45              |
| 23:v:23:LYS:HE2   | 23:v:23:LYS:HB2   | 1.75                     | 0.45              |
| 39:A:385:PRO:HA   | 39:A:388:LYS:HB2  | 1.97                     | 0.45              |
| 42:F:251:LEU:HD22 | 43:H:162:LEU:HD23 | 1.98                     | 0.45              |
| 52:Y:297:ARG:N    | 52:Y:357:VAL:O    | 2.50                     | 0.45              |
| 54:J:162:ASN:OD1  | 54:J:162:ASN:N    | 2.50                     | 0.45              |
| 3:d:75:ILE:HG21   | 3:d:81:ILE:HD11   | 1.99                     | 0.45              |
| 17:T:26:LYS:NZ    | 18:2:525:A:OP2    | 2.38                     | 0.45              |
| 19:w:98:VAL:HG13  | 19:w:102:THR:HB   | 1.97                     | 0.45              |
| 33:V:129:ILE:O    | 33:V:140:TYR:OH   | 2.26                     | 0.45              |
| 39:A:403:LEU:HA   | 39:A:406:ARG:HD2  | 1.99                     | 0.45              |
| 39:A:451:GLU:HG3  | 39:A:454:ARG:H    | 1.81                     | 0.45              |
| 39:A:514:MET:O    | 39:A:518:GLN:N    | 2.50                     | 0.45              |
| 40:C:635:ASP:OD1  | 40:C:635:ASP:N    | 2.48                     | 0.45              |
| 42:F:115:ARG:HA   | 42:F:175:THR:HB   | 1.99                     | 0.45              |
| 2:p:150:ILE:HG12  | 18:2:1124:C:H5''  | 1.98                     | 0.45              |
| 18:2:536:A:H2'    | 18:2:537:C:H4'    | 1.98                     | 0.45              |
| 39:A:575:ILE:HD13 | 43:H:70:LEU:HB2   | 1.98                     | 0.45              |
| 42:F:221:MET:HG2  | 46:M:62:SER:HB2   | 1.99                     | 0.45              |
| 42:F:286:VAL:HG23 | 46:M:354:LEU:HD21 | 1.99                     | 0.45              |
| 7:r:167:LYS:NZ    | 18:2:70:G:OP2     | 2.50                     | 0.45              |
| 18:2:981:A:H2'    | 18:2:982:G:C8     | 2.52                     | 0.45              |
| 18:2:1120:U:H2'   | 18:2:1121:G:H8    | 1.82                     | 0.45              |
| 18:2:1683:C:H2'   | 18:2:1684:C:C6    | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:C:648:GLN:HE22 | 40:C:677:ILE:H    | 1.64                     | 0.45              |
| 46:M:183:LYS:HA   | 46:M:186:VAL:HG22 | 1.99                     | 0.45              |
| 47:N:244:ASN:HD21 | 47:N:370:ASP:H    | 1.65                     | 0.45              |
| 41:E:352:SER:OG   | 41:E:354:ASN:OD1  | 2.35                     | 0.44              |
| 43:H:151:ILE:HD13 | 43:H:167:TYR:HD2  | 1.82                     | 0.44              |
| 30:S:38:THR:OG1   | 30:S:39:SER:N     | 2.50                     | 0.44              |
| 33:V:120:ILE:HB   | 33:V:132:TRP:HB2  | 2.00                     | 0.44              |
| 12:m:53:ILE:O     | 12:m:57:SER:OG    | 2.35                     | 0.44              |
| 29:P:79:ILE:HB    | 29:P:83:LEU:HD23  | 2.00                     | 0.44              |
| 33:V:212:LYS:HA   | 33:V:235:ILE:HG23 | 1.98                     | 0.44              |
| 38:B:507:ARG:HD2  | 38:B:507:ARG:HA   | 1.84                     | 0.44              |
| 39:A:264:LYS:HB3  | 39:A:265:LYS:HZ2  | 1.82                     | 0.44              |
| 39:A:440:LEU:HD21 | 39:A:480:LEU:HG   | 1.99                     | 0.44              |
| 40:C:333:LEU:HD13 | 40:C:374:ILE:HG22 | 1.99                     | 0.44              |
| 42:F:222:GLY:HA2  | 42:F:227:THR:HG21 | 1.98                     | 0.44              |
| 47:N:271:ARG:HD2  | 47:N:276:LEU:HD13 | 1.99                     | 0.44              |
| 50:4:289:THR:HG23 | 50:4:302:CYS:HA   | 1.99                     | 0.44              |
| 3:d:196:ILE:HB    | 3:d:223:TYR:HB2   | 1.98                     | 0.44              |
| 15:z:102:THR:H    | 15:z:103:SER:HA   | 1.83                     | 0.44              |
| 18:2:1259:A:N6    | 18:2:1519:U:OP1   | 2.47                     | 0.44              |
| 22:u:15:LEU:HD22  | 22:u:49:MET:HE1   | 2.00                     | 0.44              |
| 32:U:100:LEU:HG   | 32:U:103:LEU:HD13 | 2.00                     | 0.44              |
| 42:F:269:LEU:HD21 | 43:H:335:ALA:HB1  | 1.99                     | 0.44              |
| 27:x:112:MET:HG2  | 27:x:127:GLY:HA2  | 1.99                     | 0.44              |
| 40:C:759:GLU:HA   | 40:C:762:ASN:HB2  | 1.99                     | 0.44              |
| 44:K:211:SER:HA   | 44:K:214:MET:HB3  | 2.00                     | 0.44              |
| 46:M:19:ARG:HG3   | 46:M:23:LYS:HE3   | 2.00                     | 0.44              |
| 38:B:513:VAL:HG22 | 38:B:532:ARG:HA   | 1.98                     | 0.44              |
| 38:B:659:TRP:HA   | 38:B:666:VAL:HA   | 1.99                     | 0.44              |
| 39:A:374:MET:HG3  | 39:A:375:VAL:HG13 | 2.00                     | 0.44              |
| 43:H:156:LYS:NZ   | 43:H:329:ASN:O    | 2.47                     | 0.44              |
| 11:n:120:VAL:HG12 | 11:n:145:VAL:HG11 | 1.99                     | 0.44              |
| 18:2:1189:A:H4'   | 35:j:34:THR:HG21  | 1.99                     | 0.44              |
| 38:B:327:VAL:HA   | 38:B:328:SER:HA   | 1.64                     | 0.44              |
| 42:F:121:LEU:HB3  | 42:F:167:GLU:HG2  | 2.00                     | 0.44              |
| 45:L:397:LYS:HD3  | 45:L:415:TYR:HE2  | 1.83                     | 0.44              |
| 46:M:343:GLY:N    | 46:M:346:GLN:OE1  | 2.48                     | 0.44              |
| 47:N:5:MET:SD     | 47:N:5:MET:N      | 2.86                     | 0.44              |
| 39:A:511:LEU:HD23 | 39:A:512:GLN:HG3  | 1.99                     | 0.44              |
| 42:F:154:LYS:NZ   | 42:F:189:TYR:OH   | 2.45                     | 0.44              |
| 43:H:245:LEU:HB3  | 43:H:326:TYR:CZ   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:L:479:LEU:HD13 | 45:L:489:GLN:HB3  | 2.00                     | 0.44              |
| 50:4:284:CYS:SG   | 50:4:286:SER:OG   | 2.72                     | 0.44              |
| 50:4:302:CYS:SG   | 50:4:304:THR:OG1  | 2.76                     | 0.44              |
| 7:r:159:ARG:HD3   | 7:r:173:ALA:HB2   | 2.00                     | 0.44              |
| 41:E:17:HIS:NE2   | 41:E:48:THR:OG1   | 2.48                     | 0.44              |
| 41:E:371:ILE:HA   | 41:E:374:LEU:HG   | 2.00                     | 0.44              |
| 44:K:139:ARG:HA   | 44:K:142:ILE:HG22 | 2.00                     | 0.44              |
| 44:K:162:LEU:HG   | 44:K:170:LEU:HD11 | 2.00                     | 0.44              |
| 47:N:383:GLY:N    | 47:N:387:GLU:O    | 2.43                     | 0.44              |
| 15:z:27:VAL:HB    | 15:z:69:THR:HB    | 2.00                     | 0.43              |
| 18:2:880:G:H1     | 18:2:906:U:H3     | 1.65                     | 0.43              |
| 45:L:371:LEU:O    | 45:L:375:LEU:N    | 2.51                     | 0.43              |
| 47:N:271:ARG:HB3  | 47:N:504:GLY:H    | 1.83                     | 0.43              |
| 51:O:156:VAL:HG21 | 51:O:185:PRO:HG3  | 2.00                     | 0.43              |
| 51:O:285:LEU:O    | 51:O:289:MET:N    | 2.50                     | 0.43              |
| 18:2:1669:G:OP1   | 28:h:79:ARG:NH1   | 2.51                     | 0.43              |
| 33:V:218:LEU:HB2  | 33:V:228:TYR:HB2  | 2.00                     | 0.43              |
| 40:C:340:ARG:NE   | 40:C:384:ASP:OD2  | 2.50                     | 0.43              |
| 40:C:745:LYS:HB3  | 40:C:746:MET:HE2  | 1.99                     | 0.43              |
| 47:N:289:LEU:HD22 | 47:N:435:TRP:HZ2  | 1.83                     | 0.43              |
| 2:p:227:LYS:HA    | 2:p:230:GLU:HG2   | 2.00                     | 0.43              |
| 18:2:367:U:O2'    | 18:2:368:U:OP2    | 2.31                     | 0.43              |
| 19:w:72:LYS:HE3   | 19:w:72:LYS:HB3   | 1.76                     | 0.43              |
| 28:h:46:LYS:HD3   | 28:h:97:ILE:HD11  | 2.00                     | 0.43              |
| 33:V:20:GLN:NE2   | 33:V:68:ASP:OD1   | 2.40                     | 0.43              |
| 39:A:352:GLN:HA   | 39:A:355:LEU:HB3  | 2.00                     | 0.43              |
| 42:F:156:MET:HA   | 42:F:159:LEU:HG   | 2.00                     | 0.43              |
| 3:d:221:ASP:OD1   | 3:d:221:ASP:N     | 2.50                     | 0.43              |
| 9:t:89:GLU:OE1    | 9:t:92:ARG:NH1    | 2.44                     | 0.43              |
| 15:z:79:LEU:HG    | 15:z:83:LYS:HE2   | 2.00                     | 0.43              |
| 18:2:1611:G:OP2   | 26:k:121:ARG:NH2  | 2.51                     | 0.43              |
| 28:h:20:ILE:HG21  | 28:h:98:VAL:HG11  | 2.00                     | 0.43              |
| 39:A:366:THR:OG1  | 39:A:367:ARG:N    | 2.52                     | 0.43              |
| 40:C:96:ILE:HG13  | 40:C:97:VAL:H     | 1.82                     | 0.43              |
| 40:C:644:GLU:HG2  | 40:C:650:LEU:HA   | 1.99                     | 0.43              |
| 41:E:51:VAL:HG11  | 41:E:74:ARG:HB2   | 2.00                     | 0.43              |
| 43:H:231:LEU:HA   | 43:H:340:LYS:HG2  | 1.99                     | 0.43              |
| 45:L:356:LYS:HD2  | 45:L:356:LYS:HA   | 1.82                     | 0.43              |
| 51:O:168:ASN:HD21 | 51:O:170:ASP:HB2  | 1.83                     | 0.43              |
| 53:Z:58:LYS:HA    | 53:Z:60:VAL:HG12  | 2.01                     | 0.43              |
| 7:r:13:GLN:HE22   | 18:2:153:G:H21    | 1.66                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:P:68:ILE:HB    | 29:P:109:TYR:HB2  | 1.99                     | 0.43              |
| 32:U:96:LYS:HA    | 32:U:96:LYS:HD3   | 1.82                     | 0.43              |
| 39:A:455:LEU:HD13 | 39:A:458:LEU:HD23 | 2.01                     | 0.43              |
| 47:N:350:LYS:HE3  | 47:N:350:LYS:HB3  | 1.90                     | 0.43              |
| 18:2:1824:A:O4'   | 36:G:44:ASN:ND2   | 2.51                     | 0.43              |
| 25:g:101:ASP:OD1  | 25:g:101:ASP:N    | 2.51                     | 0.43              |
| 39:A:161:LEU:HD23 | 39:A:161:LEU:HA   | 1.91                     | 0.43              |
| 39:A:539:PRO:HG2  | 39:A:542:ILE:HD11 | 2.01                     | 0.43              |
| 41:E:405:ILE:HA   | 41:E:408:THR:HG22 | 2.00                     | 0.43              |
| 46:M:361:LEU:HA   | 46:M:364:VAL:HG12 | 2.00                     | 0.43              |
| 47:N:215:LYS:HE2  | 47:N:215:LYS:HB3  | 1.75                     | 0.43              |
| 34:i:61:LYS:NZ    | 34:i:80:ASP:OD2   | 2.45                     | 0.43              |
| 47:N:248:THR:HA   | 47:N:374:ARG:HB3  | 2.01                     | 0.43              |
| 47:N:251:ILE:HB   | 47:N:267:ILE:HD11 | 2.00                     | 0.43              |
| 53:Z:58:LYS:HB3   | 53:Z:61:LYS:HE2   | 2.00                     | 0.43              |
| 8:s:145:ARG:HH21  | 14:D:51:GLU:HG3   | 1.84                     | 0.43              |
| 18:2:107:A:H2'    | 18:2:108:G:C8     | 2.53                     | 0.43              |
| 29:P:103:HIS:CD2  | 29:P:105:ALA:H    | 2.37                     | 0.43              |
| 33:V:144:ASP:OD1  | 33:V:144:ASP:N    | 2.50                     | 0.43              |
| 33:V:192:THR:O    | 33:V:192:THR:OG1  | 2.35                     | 0.43              |
| 40:C:466:SER:OG   | 40:C:467:GLN:N    | 2.51                     | 0.43              |
| 47:N:264:SER:HB3  | 47:N:512:PRO:HB3  | 2.00                     | 0.43              |
| 41:E:311:LYS:HA   | 41:E:311:LYS:HD3  | 1.83                     | 0.43              |
| 42:F:161:LYS:HE2  | 42:F:165:PRO:HA   | 2.01                     | 0.43              |
| 43:H:237:ASN:OD1  | 43:H:237:ASN:N    | 2.52                     | 0.43              |
| 46:M:296:THR:HA   | 46:M:299:GLN:HG3  | 2.01                     | 0.43              |
| 1:a:33:GLN:HG3    | 1:a:154:LEU:HD12  | 2.01                     | 0.43              |
| 5:q:133:THR:H     | 18:2:297:A:H5''   | 1.84                     | 0.43              |
| 9:t:10:LYS:NZ     | 18:2:370:G:O2'    | 2.50                     | 0.43              |
| 14:D:27:ILE:HB    | 14:D:61:ILE:HB    | 2.00                     | 0.43              |
| 21:e:103:LEU:HD23 | 21:e:103:LEU:HA   | 1.91                     | 0.43              |
| 30:S:22:GLY:HA2   | 30:S:68:LEU:HB2   | 2.00                     | 0.43              |
| 33:V:32:LEU:HD22  | 33:V:71:ILE:HG12  | 2.00                     | 0.43              |
| 33:V:91:ASP:OD1   | 33:V:93:THR:OG1   | 2.34                     | 0.43              |
| 38:B:516:LYS:HB2  | 38:B:529:LYS:HG3  | 1.99                     | 0.43              |
| 40:C:381:SER:HA   | 40:C:384:ASP:HB2  | 2.01                     | 0.43              |
| 40:C:627:LYS:HA   | 40:C:693:LEU:HD21 | 2.00                     | 0.43              |
| 40:C:736:HIS:CE1  | 40:C:758:ASN:HD22 | 2.37                     | 0.43              |
| 45:L:507:SER:HB2  | 45:L:511:GLY:H    | 1.84                     | 0.43              |
| 52:Y:373:ILE:O    | 52:Y:425:GLY:N    | 2.50                     | 0.43              |
| 18:2:948:C:H2'    | 18:2:949:G:H8     | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:2:1461:G:H21   | 18:2:1465:A:H2    | 1.66                     | 0.42              |
| 40:C:422:GLU:HG2  | 40:C:443:CYS:HB2  | 2.01                     | 0.42              |
| 40:C:744:MET:HE1  | 40:C:787:SER:HB3  | 2.01                     | 0.42              |
| 44:K:101:GLN:NE2  | 44:K:122:ASP:OD1  | 2.52                     | 0.42              |
| 45:L:413:PHE:HZ   | 45:L:444:LEU:HB3  | 1.84                     | 0.42              |
| 45:L:541:ASP:HA   | 45:L:544:ILE:HG12 | 2.01                     | 0.42              |
| 47:N:285:ASP:OD1  | 47:N:285:ASP:N    | 2.48                     | 0.42              |
| 12:m:104:ARG:HE   | 12:m:104:ARG:HB2  | 1.64                     | 0.42              |
| 39:A:205:LEU:HD12 | 39:A:208:ILE:HD12 | 2.00                     | 0.42              |
| 50:4:246:THR:OG1  | 50:4:247:SER:N    | 2.52                     | 0.42              |
| 3:d:64:THR:OG1    | 3:d:90:GLU:OE2    | 2.34                     | 0.42              |
| 18:2:730:C:H2'    | 18:2:731:G:C8     | 2.53                     | 0.42              |
| 40:C:430:ASN:HD21 | 40:C:435:ASP:HB2  | 1.84                     | 0.42              |
| 40:C:616:LEU:HD23 | 40:C:616:LEU:HA   | 1.89                     | 0.42              |
| 41:E:315:CYS:O    | 41:E:319:LEU:CB   | 2.67                     | 0.42              |
| 45:L:312:GLN:HA   | 45:L:315:THR:HG22 | 2.02                     | 0.42              |
| 46:M:365:LYS:HA   | 46:M:368:LEU:HG   | 2.01                     | 0.42              |
| 50:4:302:CYS:SG   | 50:4:303:GLU:N    | 2.93                     | 0.42              |
| 7:r:14:LYS:HG2    | 7:r:124:LEU:HD21  | 2.00                     | 0.42              |
| 12:m:66:VAL:HG23  | 12:m:67:THR:HG23  | 2.02                     | 0.42              |
| 18:2:549:C:O2'    | 38:B:538:GLN:OE1  | 2.37                     | 0.42              |
| 40:C:672:PRO:HD2  | 40:C:675:LEU:HD12 | 2.02                     | 0.42              |
| 42:F:321:ASP:N    | 42:F:321:ASP:OD1  | 2.52                     | 0.42              |
| 44:K:38:LYS:O     | 44:K:132:THR:OG1  | 2.37                     | 0.42              |
| 1:a:12:GLU:HG2    | 19:w:114:LEU:HD21 | 2.01                     | 0.42              |
| 18:2:861:A:H1'    | 18:2:862:A:H2     | 1.85                     | 0.42              |
| 18:2:1760:G:N1    | 18:2:1774:C:N3    | 2.68                     | 0.42              |
| 20:b:80:PRO:O     | 20:b:83:SER:OG    | 2.34                     | 0.42              |
| 33:V:271:LYS:HE3  | 33:V:271:LYS:HB3  | 1.83                     | 0.42              |
| 38:B:482:TRP:CE2  | 38:B:515:CYS:HB3  | 2.55                     | 0.42              |
| 41:E:228:GLY:HA2  | 41:E:231:ASN:HD22 | 1.83                     | 0.42              |
| 41:E:262:ILE:HG21 | 41:E:332:PHE:HD1  | 1.84                     | 0.42              |
| 42:F:106:TYR:O    | 42:F:109:ARG:NH1  | 2.47                     | 0.42              |
| 18:2:5:U:H2'      | 18:2:6:G:H8       | 1.84                     | 0.42              |
| 18:2:901:G:H2'    | 18:2:902:G:H4'    | 2.00                     | 0.42              |
| 18:2:1644:C:H4'   | 25:g:140:ARG:HB2  | 2.02                     | 0.42              |
| 34:i:98:ARG:NH1   | 34:i:99:ALA:O     | 2.49                     | 0.42              |
| 40:C:836:ASP:OD2  | 40:C:839:THR:OG1  | 2.31                     | 0.42              |
| 41:E:290:ASP:HB3  | 41:E:293:THR:HG23 | 2.02                     | 0.42              |
| 5:q:87:MET:HE1    | 5:q:236:ILE:HD13  | 2.00                     | 0.42              |
| 9:t:154:LYS:HB2   | 9:t:154:LYS:HE3   | 1.76                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:w:45:LYS:HE3   | 19:w:45:LYS:HB2   | 1.71                     | 0.42              |
| 40:C:553:LYS:HD2  | 40:C:553:LYS:HA   | 1.86                     | 0.42              |
| 45:L:239:ASN:HA   | 45:L:242:ARG:HB2  | 2.01                     | 0.42              |
| 45:L:243:GLN:HA   | 45:L:246:VAL:HG22 | 2.00                     | 0.42              |
| 52:Y:266:LYS:NZ   | 52:Y:267:PRO:O    | 2.52                     | 0.42              |
| 18:2:857:U:H2'    | 18:2:858:A:C8     | 2.55                     | 0.42              |
| 18:2:944:A:H1'    | 34:i:139:SER:HB2  | 2.02                     | 0.42              |
| 43:H:123:THR:OG1  | 43:H:127:SER:O    | 2.37                     | 0.42              |
| 52:Y:280:GLY:HA3  | 52:Y:338:GLY:HA2  | 2.01                     | 0.42              |
| 52:Y:293:GLU:HA   | 52:Y:317:LYS:HA   | 2.02                     | 0.42              |
| 2:p:107:ARG:NH2   | 34:i:133:THR:O    | 2.53                     | 0.42              |
| 18:2:562:U:H2'    | 18:2:563:G:C8     | 2.55                     | 0.42              |
| 25:g:97:GLN:HE22  | 33:V:60:ARG:NE    | 2.18                     | 0.42              |
| 40:C:426:GLU:HG3  | 40:C:427:GLU:H    | 1.85                     | 0.42              |
| 42:F:268:ASP:OD1  | 43:H:161:SER:OG   | 2.36                     | 0.42              |
| 2:p:217:MET:HE2   | 2:p:217:MET:HB2   | 1.86                     | 0.42              |
| 4:Q:70:LYS:HB3    | 4:Q:70:LYS:HE3    | 1.89                     | 0.42              |
| 18:2:1232:U:H2'   | 18:2:1233:G:C8    | 2.54                     | 0.42              |
| 29:P:78:LYS:HE2   | 29:P:78:LYS:HB2   | 1.92                     | 0.42              |
| 33:V:133:ASN:HD22 | 33:V:139:LYS:HD3  | 1.85                     | 0.42              |
| 33:V:173:LEU:HD22 | 33:V:189:ILE:HG12 | 2.02                     | 0.42              |
| 39:A:537:ILE:HG23 | 39:A:539:PRO:HD3  | 2.02                     | 0.42              |
| 40:C:864:GLY:HA2  | 40:C:867:VAL:HG12 | 2.02                     | 0.42              |
| 41:E:364:PRO:HA   | 41:E:367:ALA:HB3  | 2.01                     | 0.42              |
| 42:F:272:VAL:HG11 | 43:H:336:GLN:HE22 | 1.84                     | 0.42              |
| 43:H:87:HIS:NE2   | 43:H:96:GLU:OE2   | 2.53                     | 0.42              |
| 47:N:261:SER:HB2  | 47:N:510:LYS:HE3  | 2.01                     | 0.42              |
| 5:q:27:PHE:O      | 18:2:495:U:O2'    | 2.33                     | 0.41              |
| 13:y:69:ILE:HD13  | 13:y:69:ILE:HA    | 1.93                     | 0.41              |
| 18:2:943:U:O2'    | 34:i:135:ILE:O    | 2.37                     | 0.41              |
| 18:2:1714:U:H2'   | 18:2:1715:A:C8    | 2.55                     | 0.41              |
| 32:U:121:CYS:HA   | 32:U:132:MET:HE3  | 2.02                     | 0.41              |
| 39:A:482:VAL:HG22 | 39:A:493:PHE:HD1  | 1.84                     | 0.41              |
| 45:L:376:THR:HA   | 45:L:377:MET:HA   | 1.71                     | 0.41              |
| 46:M:220:PHE:HB2  | 46:M:245:VAL:HG22 | 2.01                     | 0.41              |
| 50:4:283:THR:OG1  | 50:4:284:CYS:N    | 2.53                     | 0.41              |
| 5:q:115:THR:OG1   | 5:q:117:GLU:OE1   | 2.36                     | 0.41              |
| 16:R:17:ARG:HE    | 16:R:17:ARG:HB2   | 1.71                     | 0.41              |
| 18:2:708:C:H2'    | 18:2:709:G:C8     | 2.55                     | 0.41              |
| 25:g:19:ALA:HB2   | 25:g:75:GLY:HA3   | 2.02                     | 0.41              |
| 36:G:83:ASP:OD1   | 36:G:83:ASP:N     | 2.48                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:A:320:THR:HG22 | 39:A:383:VAL:HG13 | 2.02                     | 0.41              |
| 40:C:561:THR:OG1  | 40:C:562:ASP:N    | 2.53                     | 0.41              |
| 44:K:10:ASN:O     | 44:K:14:LEU:CB    | 2.65                     | 0.41              |
| 50:4:208:GLN:HG3  | 50:4:220:VAL:HB   | 2.02                     | 0.41              |
| 9:t:155:ASN:OD1   | 9:t:155:ASN:N     | 2.48                     | 0.41              |
| 18:2:541:U:OP1    | 18:2:543:C:N4     | 2.53                     | 0.41              |
| 22:u:86:PRO:HA    | 22:u:87:PRO:HD3   | 1.90                     | 0.41              |
| 40:C:590:LEU:HD13 | 47:N:35:LYS:HA    | 2.01                     | 0.41              |
| 44:K:83:THR:HA    | 44:K:86:LYS:HG2   | 2.03                     | 0.41              |
| 39:A:51:MET:HE2   | 39:A:74:TYR:HB2   | 2.02                     | 0.41              |
| 39:A:514:MET:HG3  | 39:A:516:SER:H    | 1.85                     | 0.41              |
| 40:C:459:MET:HE1  | 40:C:473:LEU:HD13 | 2.02                     | 0.41              |
| 43:H:243:LEU:HD23 | 43:H:247:MET:HG3  | 2.02                     | 0.41              |
| 45:L:225:HIS:O    | 45:L:229:ASN:ND2  | 2.54                     | 0.41              |
| 45:L:395:GLY:HA2  | 45:L:398:MET:HG2  | 2.01                     | 0.41              |
| 47:N:514:LYS:HA   | 47:N:514:LYS:HD3  | 1.88                     | 0.41              |
| 52:Y:380:ARG:HA   | 52:Y:393:ALA:HA   | 2.02                     | 0.41              |
| 1:a:38:ILE:HD13   | 1:a:38:ILE:HA     | 1.88                     | 0.41              |
| 3:d:169:TYR:OH    | 3:d:175:GLY:O     | 2.37                     | 0.41              |
| 18:2:1337:C:H2'   | 18:2:1338:G:H8    | 1.85                     | 0.41              |
| 19:w:23:ARG:HB3   | 33:V:170:TRP:HZ3  | 1.85                     | 0.41              |
| 20:b:163:PRO:O    | 20:b:167:TYR:HB2  | 2.19                     | 0.41              |
| 33:V:107:ASP:OD2  | 33:V:125:ARG:NH1  | 2.45                     | 0.41              |
| 39:A:352:GLN:O    | 39:A:356:ALA:N    | 2.54                     | 0.41              |
| 39:A:387:VAL:HA   | 39:A:390:LEU:HD23 | 2.03                     | 0.41              |
| 44:K:108:LEU:HB2  | 44:K:113:HIS:HB2  | 2.02                     | 0.41              |
| 46:M:210:ARG:HE   | 46:M:210:ARG:HB3  | 1.72                     | 0.41              |
| 47:N:199:LEU:O    | 47:N:335:TYR:N    | 2.51                     | 0.41              |
| 51:O:55:ILE:HG21  | 51:O:58:ILE:HG13  | 2.01                     | 0.41              |
| 51:O:141:TYR:HE2  | 51:O:151:ALA:HB2  | 1.85                     | 0.41              |
| 6:W:11:ARG:NH2    | 18:2:1184:G:OP1   | 2.53                     | 0.41              |
| 18:2:382:C:H2'    | 18:2:383:G:H8     | 1.86                     | 0.41              |
| 23:v:84:LYS:HA    | 23:v:84:LYS:HD2   | 1.83                     | 0.41              |
| 34:i:97:LEU:HD11  | 34:i:112:ALA:HB1  | 2.02                     | 0.41              |
| 41:E:376:ARG:HH22 | 45:L:482:THR:HG22 | 1.86                     | 0.41              |
| 51:O:190:ILE:O    | 51:O:238:THR:N    | 2.52                     | 0.41              |
| 4:Q:60:ASP:OD1    | 4:Q:60:ASP:N      | 2.53                     | 0.41              |
| 18:2:16:G:H2'     | 18:2:17:C:C6      | 2.56                     | 0.41              |
| 18:2:996:A:H2'    | 18:2:997:A:C8     | 2.56                     | 0.41              |
| 18:2:1337:C:H2'   | 18:2:1338:G:C8    | 2.55                     | 0.41              |
| 38:B:569:ALA:HB3  | 38:B:578:ALA:HB3  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:A:219:ASN:HD21 | 39:A:221:ASN:HB2  | 1.85                     | 0.41              |
| 39:A:446:ILE:HA   | 39:A:512:GLN:HE21 | 1.86                     | 0.41              |
| 40:C:662:GLN:HA   | 40:C:665:VAL:HG12 | 2.03                     | 0.41              |
| 42:F:119:THR:OG1  | 42:F:190:TYR:OH   | 2.31                     | 0.41              |
| 46:M:250:ALA:HA   | 46:M:253:VAL:HG22 | 2.01                     | 0.41              |
| 47:N:430:TYR:CZ   | 47:N:434:ARG:HD2  | 2.56                     | 0.41              |
| 9:t:158:ILE:HD13  | 9:t:158:ILE:HA    | 1.90                     | 0.41              |
| 10:c:133:ARG:NH2  | 18:2:581:U:OP1    | 2.38                     | 0.41              |
| 18:2:1277:C:H2'   | 18:2:1278:A:H8    | 1.86                     | 0.41              |
| 20:b:173:ARG:HA   | 20:b:173:ARG:HD3  | 1.78                     | 0.41              |
| 40:C:324:ILE:HG22 | 40:C:325:THR:H    | 1.85                     | 0.41              |
| 40:C:782:LYS:HA   | 40:C:782:LYS:HD3  | 1.93                     | 0.41              |
| 42:F:140:ASN:HD22 | 42:F:147:ALA:HB3  | 1.86                     | 0.41              |
| 42:F:219:THR:O    | 42:F:219:THR:OG1  | 2.36                     | 0.41              |
| 3:d:257:LYS:O     | 13:y:16:LYS:NZ    | 2.44                     | 0.41              |
| 7:r:170:ARG:NH2   | 18:2:71:G:N7      | 2.52                     | 0.41              |
| 7:r:201:LYS:HE3   | 7:r:201:LYS:HB3   | 1.92                     | 0.41              |
| 15:z:100:LYS:HA   | 15:z:100:LYS:HD3  | 1.93                     | 0.41              |
| 18:2:1285:G:H4'   | 32:U:100:LEU:HD13 | 2.02                     | 0.41              |
| 20:b:7:LYS:NZ     | 28:h:113:GLU:OE2  | 2.54                     | 0.41              |
| 20:b:22:ASN:O     | 20:b:26:THR:OG1   | 2.27                     | 0.41              |
| 23:v:78:LYS:HB3   | 23:v:78:LYS:HE3   | 1.81                     | 0.41              |
| 24:o:50:ARG:HA    | 24:o:50:ARG:HD3   | 1.91                     | 0.41              |
| 36:G:29:LYS:HB2   | 36:G:35:TYR:CZ    | 2.56                     | 0.41              |
| 38:B:641:SER:HA   | 38:B:642:ASP:HA   | 1.91                     | 0.41              |
| 39:A:45:LYS:HE3   | 39:A:45:LYS:HB3   | 1.93                     | 0.41              |
| 40:C:758:ASN:O    | 40:C:759:GLU:HG3  | 2.21                     | 0.41              |
| 45:L:390:LEU:HA   | 45:L:393:LYS:HG2  | 2.03                     | 0.41              |
| 45:L:431:VAL:HA   | 45:L:434:ASN:HA   | 2.02                     | 0.41              |
| 46:M:290:LYS:HE3  | 46:M:336:HIS:HA   | 2.03                     | 0.41              |
| 2:p:179:ASN:HB3   | 2:p:183:GLU:HB2   | 2.04                     | 0.41              |
| 18:2:1025:U:OP1   | 18:2:1090:C:O2'   | 2.38                     | 0.41              |
| 20:b:193:ASP:OD2  | 20:b:197:LYS:N    | 2.43                     | 0.41              |
| 33:V:54:ILE:HD13  | 33:V:54:ILE:HA    | 1.89                     | 0.41              |
| 40:C:331:LYS:HA   | 40:C:331:LYS:HD2  | 1.94                     | 0.41              |
| 45:L:279:ARG:HA   | 45:L:282:SER:HB2  | 2.03                     | 0.41              |
| 52:Y:374:SER:HA   | 52:Y:424:LEU:HA   | 2.03                     | 0.41              |
| 3:d:137:VAL:HG11  | 3:d:244:ILE:HD12  | 2.03                     | 0.40              |
| 4:Q:46:GLU:HG3    | 4:Q:48:ALA:H      | 1.86                     | 0.40              |
| 4:Q:84:VAL:HG22   | 18:2:1866:A:N6    | 2.36                     | 0.40              |
| 8:s:142:LYS:HB3   | 14:D:54:ASP:HB3   | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:2:928:G:H2'    | 18:2:929:G:C8     | 2.56                     | 0.40              |
| 18:2:948:C:H2'    | 18:2:949:G:C8     | 2.56                     | 0.40              |
| 19:w:51:ALA:HA    | 19:w:54:VAL:HG22  | 2.03                     | 0.40              |
| 23:v:40:LYS:NZ    | 32:U:129:GLY:O    | 2.39                     | 0.40              |
| 40:C:400:LYS:HB2  | 40:C:400:LYS:HE3  | 1.76                     | 0.40              |
| 41:E:356:LEU:HD23 | 41:E:367:ALA:HB1  | 2.02                     | 0.40              |
| 43:H:315:ASP:OD1  | 43:H:315:ASP:N    | 2.53                     | 0.40              |
| 45:L:487:ARG:HA   | 45:L:488:ILE:HA   | 1.69                     | 0.40              |
| 45:L:490:LEU:HD23 | 45:L:490:LEU:HA   | 1.95                     | 0.40              |
| 46:M:90:LEU:HD23  | 46:M:106:LEU:HD22 | 2.03                     | 0.40              |
| 54:J:171:ARG:NH1  | 54:J:172:GLU:OE2  | 2.53                     | 0.40              |
| 8:s:51:ILE:HG21   | 8:s:179:LYS:HG2   | 2.02                     | 0.40              |
| 18:2:1291:A:O2'   | 32:U:145:CYS:SG   | 2.70                     | 0.40              |
| 26:k:34:LYS:HD3   | 26:k:103:LEU:HD23 | 2.04                     | 0.40              |
| 38:B:429:PHE:N    | 38:B:439:ALA:O    | 2.55                     | 0.40              |
| 39:A:257:HIS:NE2  | 39:A:357:THR:O    | 2.54                     | 0.40              |
| 40:C:402:LEU:HD23 | 40:C:402:LEU:HA   | 1.92                     | 0.40              |
| 40:C:806:THR:O    | 40:C:810:MET:CB   | 2.69                     | 0.40              |
| 41:E:132:TYR:CD2  | 41:E:133:ARG:N    | 2.89                     | 0.40              |
| 44:K:87:CYS:HA    | 45:L:446:VAL:HG22 | 2.04                     | 0.40              |
| 45:L:359:MET:N    | 45:L:359:MET:SD   | 2.94                     | 0.40              |
| 45:L:543:PHE:HA   | 45:L:546:GLN:HG3  | 2.02                     | 0.40              |
| 47:N:365:LEU:HD12 | 47:N:369:ILE:HG21 | 2.03                     | 0.40              |
| 47:N:492:ARG:HA   | 47:N:492:ARG:HD2  | 1.84                     | 0.40              |
| 47:N:501:LEU:HD23 | 47:N:501:LEU:HA   | 1.90                     | 0.40              |
| 50:4:263:GLN:H    | 50:4:266:GLN:HE21 | 1.69                     | 0.40              |
| 12:m:36:GLN:HA    | 12:m:39:LYS:HG2   | 2.04                     | 0.40              |
| 18:2:551:U:H2'    | 18:2:552:G:C8     | 2.57                     | 0.40              |
| 18:2:634:A:H2'    | 18:2:635:G:C8     | 2.56                     | 0.40              |
| 18:2:691:G:H2'    | 18:2:692:G:H8     | 1.86                     | 0.40              |
| 18:2:1593:C:O2    | 27:x:12:GLN:NE2   | 2.51                     | 0.40              |
| 20:b:141:LYS:HE2  | 20:b:179:GLN:HB3  | 2.02                     | 0.40              |
| 22:u:32:HIS:HD2   | 22:u:34:GLU:H     | 1.69                     | 0.40              |
| 23:v:58:GLU:HG2   | 23:v:61:TYR:H     | 1.86                     | 0.40              |
| 26:k:28:PHE:HE1   | 26:k:38:ARG:HD3   | 1.85                     | 0.40              |
| 29:P:69:THR:H     | 29:P:72:VAL:HG22  | 1.86                     | 0.40              |
| 39:A:575:ILE:HA   | 39:A:578:ARG:HB3  | 2.03                     | 0.40              |
| 43:H:313:ARG:HE   | 43:H:313:ARG:HB3  | 1.66                     | 0.40              |
| 46:M:41:ASP:O     | 46:M:45:ILE:HG12  | 2.21                     | 0.40              |
| 46:M:218:PHE:HB3  | 46:M:283:MET:HE1  | 2.02                     | 0.40              |
| 50:4:259:LYS:HE2  | 50:4:259:LYS:HB3  | 1.90                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:Y:444:SER:HA   | 52:Y:453:LEU:HA   | 2.02                     | 0.40              |
| 3:d:110:MET:HA    | 3:d:111:PRO:HD3   | 1.95                     | 0.40              |
| 3:d:238:LYS:NZ    | 18:2:1355:C:O3'   | 2.54                     | 0.40              |
| 14:D:16:ASN:OD1   | 18:2:1152:U:O2'   | 2.33                     | 0.40              |
| 24:o:130:ARG:NH2  | 50:4:254:ASN:OD1  | 2.54                     | 0.40              |
| 25:g:21:ALA:HB2   | 25:g:72:VAL:HG13  | 2.04                     | 0.40              |
| 25:g:116:ASP:OD1  | 25:g:118:THR:OG1  | 2.38                     | 0.40              |
| 29:P:91:LEU:HD22  | 29:P:96:LEU:HD12  | 2.03                     | 0.40              |
| 35:j:112:VAL:HG12 | 35:j:113:GLY:H    | 1.85                     | 0.40              |
| 41:E:111:ARG:HA   | 41:E:111:ARG:HD2  | 1.89                     | 0.40              |
| 45:L:238:SER:OG   | 45:L:239:ASN:OD1  | 2.36                     | 0.40              |
| 53:Z:28:GLU:CD    | 53:Z:29:ASP:H     | 2.29                     | 0.40              |
| 53:Z:47:VAL:HG13  | 53:Z:83:ILE:HB    | 2.03                     | 0.40              |
| 18:2:537:C:N3     | 18:2:545:A:C6     | 2.90                     | 0.40              |
| 27:x:56:ARG:HG3   | 27:x:103:VAL:HG21 | 2.04                     | 0.40              |
| 40:C:429:GLU:HB2  | 40:C:431:LEU:HD22 | 2.03                     | 0.40              |
| 40:C:683:GLU:HG2  | 40:C:733:MET:HE1  | 2.04                     | 0.40              |
| 42:F:107:GLU:HB2  | 43:H:210:LEU:HD11 | 2.02                     | 0.40              |
| 42:F:255:THR:O    | 42:F:258:SER:OG   | 2.29                     | 0.40              |
| 43:H:269:LYS:HD3  | 43:H:269:LYS:HA   | 1.83                     | 0.40              |
| 44:K:91:GLN:HG2   | 45:L:445:LYS:HB2  | 2.02                     | 0.40              |
| 46:M:147:VAL:O    | 46:M:151:ILE:HG12 | 2.21                     | 0.40              |
| 46:M:264:ASP:N    | 46:M:264:ASP:OD1  | 2.52                     | 0.40              |
| 47:N:12:ASN:OD1   | 47:N:12:ASN:N     | 2.51                     | 0.40              |
| 51:O:189:LYS:O    | 51:O:277:VAL:N    | 2.54                     | 0.40              |
| 51:O:228:LEU:HA   | 51:O:234:TYR:HA   | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | a     | 214/295 (72%) | 212 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 2   | p     | 209/264 (79%) | 199 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 3   | d     | 214/293 (73%) | 202 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 4   | Q     | 99/115 (86%)  | 98 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 5   | q     | 253/263 (96%) | 243 (96%) | 9 (4%)   | 1 (0%)   | 30          | 59  |
| 6   | W     | 22/25 (88%)   | 22 (100%) | 0        | 0        | 100         | 100 |
| 7   | r     | 220/249 (88%) | 215 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 8   | s     | 165/194 (85%) | 162 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 9   | t     | 195/208 (94%) | 187 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 10  | c     | 178/194 (92%) | 172 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 11  | n     | 131/158 (83%) | 129 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 12  | m     | 147/151 (97%) | 146 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 13  | y     | 80/83 (96%)   | 80 (100%) | 0        | 0        | 100         | 100 |
| 14  | D     | 127/130 (98%) | 124 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 15  | z     | 120/133 (90%) | 111 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 16  | R     | 80/84 (95%)   | 74 (92%)  | 6 (8%)   | 0        | 100         | 100 |
| 17  | T     | 40/59 (68%)   | 40 (100%) | 0        | 0        | 100         | 100 |
| 19  | w     | 124/135 (92%) | 115 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 20  | b     | 222/243 (91%) | 217 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 21  | e     | 187/204 (92%) | 175 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 22  | u     | 93/165 (56%)  | 87 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 23  | v     | 107/132 (81%) | 104 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 24  | o     | 117/145 (81%) | 115 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 25  | g     | 136/146 (93%) | 130 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 26  | k     | 138/152 (91%) | 131 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 27  | x     | 139/145 (96%) | 136 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 28  | h     | 96/119 (81%)  | 92 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 29  | P     | 68/125 (54%)  | 67 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | S     | 59/69 (86%)   | 54 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 31  | l     | 52/56 (93%)   | 48 (92%)  | 4 (8%)   | 0        | 100         | 100 |
| 32  | U     | 53/156 (34%)  | 47 (89%)  | 6 (11%)  | 0        | 100         | 100 |
| 33  | V     | 290/317 (92%) | 260 (90%) | 28 (10%) | 2 (1%)   | 18          | 48  |

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| Mol | Chain | Analysed          | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|----------|----------|-------------|-----|
| 34  | i     | 123/151 (82%)     | 115 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 35  | j     | 137/143 (96%)     | 133 (97%)  | 3 (2%)   | 1 (1%)   | 18          | 48  |
| 36  | G     | 86/144 (60%)      | 84 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 37  | I     | 301/325 (93%)     | 293 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 38  | B     | 528/814 (65%)     | 503 (95%)  | 25 (5%)  | 0        | 100         | 100 |
| 39  | A     | 682/1382 (49%)    | 665 (98%)  | 17 (2%)  | 0        | 100         | 100 |
| 40  | C     | 621/913 (68%)     | 586 (94%)  | 34 (6%)  | 1 (0%)   | 43          | 72  |
| 41  | E     | 406/445 (91%)     | 394 (97%)  | 12 (3%)  | 0        | 100         | 100 |
| 42  | F     | 267/357 (75%)     | 251 (94%)  | 16 (6%)  | 0        | 100         | 100 |
| 43  | H     | 289/352 (82%)     | 275 (95%)  | 14 (5%)  | 0        | 100         | 100 |
| 44  | K     | 215/218 (99%)     | 197 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 45  | L     | 370/564 (66%)     | 336 (91%)  | 34 (9%)  | 0        | 100         | 100 |
| 46  | M     | 326/374 (87%)     | 315 (97%)  | 11 (3%)  | 0        | 100         | 100 |
| 47  | N     | 441/548 (80%)     | 412 (93%)  | 29 (7%)  | 0        | 100         | 100 |
| 48  | X     | 76/78 (97%)       | 75 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 50  | 4     | 140/333 (42%)     | 115 (82%)  | 25 (18%) | 0        | 100         | 100 |
| 51  | O     | 294/315 (93%)     | 278 (95%)  | 16 (5%)  | 0        | 100         | 100 |
| 52  | Y     | 408/472 (86%)     | 334 (82%)  | 71 (17%) | 3 (1%)   | 18          | 48  |
| 53  | Z     | 108/113 (96%)     | 95 (88%)   | 13 (12%) | 0        | 100         | 100 |
| 54  | J     | 31/180 (17%)      | 29 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| All | All   | 10224/13428 (76%) | 9679 (95%) | 537 (5%) | 8 (0%)   | 49          | 77  |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | V     | 175 | LYS  |
| 52  | Y     | 56  | THR  |
| 5   | q     | 86  | PHE  |
| 52  | Y     | 51  | ALA  |
| 33  | V     | 174 | VAL  |
| 35  | j     | 86  | PRO  |
| 40  | C     | 195 | LYS  |
| 52  | Y     | 224 | ILE  |

### 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     | 180/243 (74%) | 180 (100%) | 0        | 100         | 100 |
| 2   | p     | 192/231 (83%) | 192 (100%) | 0        | 100         | 100 |
| 3   | d     | 182/225 (81%) | 182 (100%) | 0        | 100         | 100 |
| 4   | Q     | 88/98 (90%)   | 87 (99%)   | 1 (1%)   | 65          | 88  |
| 5   | q     | 220/225 (98%) | 220 (100%) | 0        | 100         | 100 |
| 6   | W     | 23/24 (96%)   | 23 (100%)  | 0        | 100         | 100 |
| 7   | r     | 193/218 (88%) | 192 (100%) | 1 (0%)   | 81          | 93  |
| 8   | s     | 155/174 (89%) | 155 (100%) | 0        | 100         | 100 |
| 9   | t     | 174/180 (97%) | 174 (100%) | 0        | 100         | 100 |
| 10  | c     | 160/168 (95%) | 160 (100%) | 0        | 100         | 100 |
| 11  | n     | 125/142 (88%) | 125 (100%) | 0        | 100         | 100 |
| 12  | m     | 130/131 (99%) | 130 (100%) | 0        | 100         | 100 |
| 13  | y     | 66/67 (98%)   | 66 (100%)  | 0        | 100         | 100 |
| 14  | D     | 112/113 (99%) | 112 (100%) | 0        | 100         | 100 |
| 15  | z     | 106/115 (92%) | 106 (100%) | 0        | 100         | 100 |
| 16  | R     | 74/76 (97%)   | 74 (100%)  | 0        | 100         | 100 |
| 17  | T     | 35/48 (73%)   | 35 (100%)  | 0        | 100         | 100 |
| 19  | w     | 111/122 (91%) | 110 (99%)  | 1 (1%)   | 70          | 90  |
| 20  | b     | 188/202 (93%) | 188 (100%) | 0        | 100         | 100 |
| 21  | e     | 159/170 (94%) | 159 (100%) | 0        | 100         | 100 |
| 22  | u     | 86/136 (63%)  | 86 (100%)  | 0        | 100         | 100 |
| 23  | v     | 94/108 (87%)  | 94 (100%)  | 0        | 100         | 100 |
| 24  | o     | 107/130 (82%) | 107 (100%) | 0        | 100         | 100 |
| 25  | g     | 114/121 (94%) | 114 (100%) | 0        | 100         | 100 |
| 26  | k     | 122/132 (92%) | 120 (98%)  | 2 (2%)   | 55          | 83  |
| 27  | x     | 111/115 (96%) | 111 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 28  | h     | 91/107 (85%)     | 90 (99%)    | 1 (1%)   | 65          | 88  |
| 29  | P     | 62/103 (60%)     | 62 (100%)   | 0        | 100         | 100 |
| 30  | S     | 54/62 (87%)      | 54 (100%)   | 0        | 100         | 100 |
| 31  | l     | 47/49 (96%)      | 47 (100%)   | 0        | 100         | 100 |
| 32  | U     | 51/140 (36%)     | 50 (98%)    | 1 (2%)   | 48          | 78  |
| 33  | V     | 256/275 (93%)    | 254 (99%)   | 2 (1%)   | 73          | 90  |
| 34  | i     | 98/119 (82%)     | 98 (100%)   | 0        | 100         | 100 |
| 35  | j     | 111/115 (96%)    | 110 (99%)   | 1 (1%)   | 70          | 90  |
| 36  | G     | 75/123 (61%)     | 75 (100%)   | 0        | 100         | 100 |
| 38  | B     | 90/702 (13%)     | 90 (100%)   | 0        | 100         | 100 |
| 39  | A     | 544/1259 (43%)   | 543 (100%)  | 1 (0%)   | 87          | 96  |
| 40  | C     | 553/811 (68%)    | 551 (100%)  | 2 (0%)   | 84          | 94  |
| 41  | E     | 380/406 (94%)    | 374 (98%)   | 6 (2%)   | 55          | 83  |
| 42  | F     | 237/289 (82%)    | 236 (100%)  | 1 (0%)   | 84          | 94  |
| 43  | H     | 269/310 (87%)    | 267 (99%)   | 2 (1%)   | 76          | 92  |
| 44  | K     | 192/193 (100%)   | 191 (100%)  | 1 (0%)   | 81          | 93  |
| 45  | L     | 342/515 (66%)    | 341 (100%)  | 1 (0%)   | 86          | 96  |
| 46  | M     | 304/335 (91%)    | 304 (100%)  | 0        | 100         | 100 |
| 47  | N     | 398/494 (81%)    | 397 (100%)  | 1 (0%)   | 86          | 96  |
| 50  | 4     | 109/304 (36%)    | 109 (100%)  | 0        | 100         | 100 |
| 51  | O     | 190/280 (68%)    | 190 (100%)  | 0        | 100         | 100 |
| 52  | Y     | 33/397 (8%)      | 33 (100%)   | 0        | 100         | 100 |
| 53  | Z     | 79/96 (82%)      | 78 (99%)    | 1 (1%)   | 61          | 86  |
| 54  | J     | 27/151 (18%)     | 27 (100%)   | 0        | 100         | 100 |
| All | All   | 7899/11349 (70%) | 7873 (100%) | 26 (0%)  | 84          | 96  |

All (26) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Q     | 84  | VAL  |
| 7   | r     | 102 | VAL  |
| 19  | w     | 9   | VAL  |
| 26  | k     | 15  | VAL  |
| 26  | k     | 36  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | h     | 63  | ILE  |
| 32  | U     | 103 | LEU  |
| 33  | V     | 265 | ILE  |
| 33  | V     | 305 | ASN  |
| 35  | j     | 112 | VAL  |
| 39  | A     | 537 | ILE  |
| 40  | C     | 366 | LEU  |
| 40  | C     | 491 | GLU  |
| 41  | E     | 51  | VAL  |
| 41  | E     | 132 | TYR  |
| 41  | E     | 194 | GLU  |
| 41  | E     | 276 | ASP  |
| 41  | E     | 331 | ASP  |
| 41  | E     | 353 | ILE  |
| 42  | F     | 188 | GLU  |
| 43  | H     | 110 | VAL  |
| 43  | H     | 250 | VAL  |
| 44  | K     | 111 | THR  |
| 45  | L     | 506 | ILE  |
| 47  | N     | 228 | THR  |
| 53  | Z     | 47  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (191) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 50  | ASN  |
| 1   | a     | 132 | GLN  |
| 1   | a     | 141 | ASN  |
| 2   | p     | 40  | ASN  |
| 2   | p     | 92  | GLN  |
| 2   | p     | 157 | GLN  |
| 3   | d     | 113 | GLN  |
| 3   | d     | 235 | ASN  |
| 5   | q     | 8   | HIS  |
| 5   | q     | 214 | ASN  |
| 5   | q     | 224 | ASN  |
| 7   | r     | 56  | ASN  |
| 7   | r     | 59  | GLN  |
| 7   | r     | 65  | GLN  |
| 7   | r     | 177 | GLN  |
| 8   | s     | 44  | ASN  |
| 8   | s     | 114 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | s     | 126 | HIS  |
| 8   | s     | 193 | GLN  |
| 9   | t     | 35  | ASN  |
| 9   | t     | 64  | ASN  |
| 9   | t     | 116 | HIS  |
| 9   | t     | 138 | ASN  |
| 9   | t     | 165 | GLN  |
| 10  | c     | 132 | GLN  |
| 10  | c     | 154 | GLN  |
| 10  | c     | 156 | HIS  |
| 11  | n     | 11  | GLN  |
| 11  | n     | 13  | GLN  |
| 11  | n     | 19  | ASN  |
| 11  | n     | 94  | HIS  |
| 11  | n     | 112 | HIS  |
| 12  | m     | 58  | HIS  |
| 13  | y     | 29  | HIS  |
| 13  | y     | 35  | ASN  |
| 14  | D     | 15  | ASN  |
| 15  | z     | 22  | GLN  |
| 16  | R     | 9   | HIS  |
| 16  | R     | 26  | GLN  |
| 16  | R     | 51  | GLN  |
| 16  | R     | 65  | GLN  |
| 17  | T     | 15  | GLN  |
| 17  | T     | 44  | ASN  |
| 19  | w     | 29  | HIS  |
| 19  | w     | 93  | GLN  |
| 20  | b     | 57  | ASN  |
| 20  | b     | 179 | GLN  |
| 21  | e     | 31  | ASN  |
| 21  | e     | 51  | HIS  |
| 21  | e     | 65  | GLN  |
| 21  | e     | 74  | ASN  |
| 21  | e     | 82  | ASN  |
| 21  | e     | 83  | ASN  |
| 21  | e     | 186 | ASN  |
| 21  | e     | 203 | ASN  |
| 23  | v     | 15  | ASN  |
| 23  | v     | 48  | HIS  |
| 24  | o     | 32  | GLN  |
| 24  | o     | 114 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | g     | 11  | GLN  |
| 25  | g     | 24  | HIS  |
| 25  | g     | 80  | GLN  |
| 25  | g     | 97  | GLN  |
| 26  | k     | 19  | ASN  |
| 26  | k     | 42  | HIS  |
| 26  | k     | 72  | GLN  |
| 26  | k     | 73  | ASN  |
| 26  | k     | 120 | HIS  |
| 26  | k     | 135 | HIS  |
| 27  | x     | 11  | GLN  |
| 27  | x     | 42  | HIS  |
| 27  | x     | 85  | ASN  |
| 27  | x     | 117 | GLN  |
| 27  | x     | 128 | GLN  |
| 28  | h     | 81  | GLN  |
| 28  | h     | 100 | GLN  |
| 29  | P     | 103 | HIS  |
| 31  | l     | 26  | ASN  |
| 33  | V     | 64  | HIS  |
| 33  | V     | 76  | GLN  |
| 33  | V     | 143 | GLN  |
| 33  | V     | 196 | ASN  |
| 33  | V     | 222 | ASN  |
| 34  | i     | 38  | ASN  |
| 34  | i     | 79  | GLN  |
| 34  | i     | 83  | GLN  |
| 35  | j     | 16  | HIS  |
| 36  | G     | 44  | ASN  |
| 38  | B     | 502 | GLN  |
| 38  | B     | 520 | GLN  |
| 39  | A     | 10  | ASN  |
| 39  | A     | 16  | ASN  |
| 39  | A     | 25  | GLN  |
| 39  | A     | 47  | HIS  |
| 39  | A     | 109 | GLN  |
| 39  | A     | 166 | ASN  |
| 39  | A     | 274 | ASN  |
| 39  | A     | 312 | GLN  |
| 39  | A     | 430 | GLN  |
| 39  | A     | 433 | ASN  |
| 39  | A     | 466 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | A     | 498 | ASN  |
| 39  | A     | 512 | GLN  |
| 39  | A     | 518 | GLN  |
| 39  | A     | 560 | ASN  |
| 39  | A     | 573 | GLN  |
| 40  | C     | 364 | ASN  |
| 40  | C     | 365 | ASN  |
| 40  | C     | 377 | ASN  |
| 40  | C     | 433 | ASN  |
| 40  | C     | 467 | GLN  |
| 40  | C     | 595 | GLN  |
| 40  | C     | 648 | GLN  |
| 40  | C     | 717 | GLN  |
| 40  | C     | 819 | HIS  |
| 40  | C     | 858 | GLN  |
| 40  | C     | 870 | ASN  |
| 41  | E     | 33  | ASN  |
| 41  | E     | 49  | ASN  |
| 41  | E     | 60  | ASN  |
| 41  | E     | 138 | GLN  |
| 41  | E     | 231 | ASN  |
| 41  | E     | 282 | GLN  |
| 41  | E     | 302 | ASN  |
| 41  | E     | 361 | ASN  |
| 41  | E     | 373 | ASN  |
| 41  | E     | 390 | HIS  |
| 41  | E     | 403 | GLN  |
| 41  | E     | 427 | ASN  |
| 42  | F     | 133 | ASN  |
| 42  | F     | 140 | ASN  |
| 42  | F     | 160 | HIS  |
| 42  | F     | 270 | GLN  |
| 42  | F     | 271 | GLN  |
| 42  | F     | 280 | GLN  |
| 42  | F     | 342 | ASN  |
| 42  | F     | 351 | ASN  |
| 43  | H     | 159 | GLN  |
| 43  | H     | 209 | HIS  |
| 43  | H     | 242 | ASN  |
| 43  | H     | 244 | GLN  |
| 43  | H     | 261 | ASN  |
| 43  | H     | 266 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | H     | 276 | GLN  |
| 43  | H     | 278 | GLN  |
| 43  | H     | 279 | GLN  |
| 43  | H     | 329 | ASN  |
| 43  | H     | 336 | GLN  |
| 43  | H     | 337 | ASN  |
| 44  | K     | 22  | ASN  |
| 44  | K     | 25  | ASN  |
| 44  | K     | 47  | ASN  |
| 44  | K     | 62  | GLN  |
| 44  | K     | 68  | GLN  |
| 45  | L     | 181 | GLN  |
| 45  | L     | 225 | HIS  |
| 45  | L     | 263 | HIS  |
| 45  | L     | 281 | HIS  |
| 45  | L     | 300 | ASN  |
| 45  | L     | 338 | ASN  |
| 45  | L     | 344 | GLN  |
| 45  | L     | 363 | GLN  |
| 45  | L     | 364 | ASN  |
| 45  | L     | 436 | HIS  |
| 45  | L     | 499 | ASN  |
| 46  | M     | 65  | ASN  |
| 46  | M     | 116 | ASN  |
| 46  | M     | 146 | GLN  |
| 46  | M     | 155 | ASN  |
| 46  | M     | 205 | HIS  |
| 46  | M     | 257 | GLN  |
| 46  | M     | 259 | ASN  |
| 46  | M     | 302 | GLN  |
| 46  | M     | 339 | HIS  |
| 46  | M     | 355 | ASN  |
| 46  | M     | 366 | ASN  |
| 47  | N     | 57  | ASN  |
| 47  | N     | 68  | GLN  |
| 47  | N     | 73  | HIS  |
| 47  | N     | 307 | ASN  |
| 47  | N     | 322 | ASN  |
| 47  | N     | 336 | ASN  |
| 47  | N     | 385 | ASN  |
| 47  | N     | 474 | ASN  |
| 50  | 4     | 266 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | O     | 10  | HIS  |
| 51  | O     | 131 | GLN  |
| 51  | O     | 168 | ASN  |
| 51  | O     | 180 | ASN  |
| 53  | Z     | 37  | GLN  |
| 53  | Z     | 111 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 18  | 2     | 1711/1868 (91%) | 362 (21%)         | 8 (0%)          |
| 49  | 1     | 74/75 (98%)     | 15 (20%)          | 0               |
| All | All   | 1785/1943 (91%) | 377 (21%)         | 8 (0%)          |

All (377) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | 2     | 17  | C    |
| 18  | 2     | 33  | G    |
| 18  | 2     | 41  | G    |
| 18  | 2     | 44  | U    |
| 18  | 2     | 46  | A    |
| 18  | 2     | 49  | C    |
| 18  | 2     | 56  | G    |
| 18  | 2     | 62  | G    |
| 18  | 2     | 65  | C    |
| 18  | 2     | 67  | C    |
| 18  | 2     | 68  | A    |
| 18  | 2     | 71  | G    |
| 18  | 2     | 72  | C    |
| 18  | 2     | 73  | C    |
| 18  | 2     | 74  | G    |
| 18  | 2     | 75  | G    |
| 18  | 2     | 76  | U    |
| 18  | 2     | 79  | A    |
| 18  | 2     | 92  | A    |
| 18  | 2     | 103 | A    |
| 18  | 2     | 113 | G    |
| 18  | 2     | 115 | U    |
| 18  | 2     | 126 | G    |
| 18  | 2     | 130 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | 2     | 143 | U    |
| 18  | 2     | 147 | A    |
| 18  | 2     | 155 | G    |
| 18  | 2     | 160 | U    |
| 18  | 2     | 163 | U    |
| 18  | 2     | 175 | A    |
| 18  | 2     | 178 | C    |
| 18  | 2     | 193 | C    |
| 18  | 2     | 196 | C    |
| 18  | 2     | 197 | U    |
| 18  | 2     | 198 | U    |
| 18  | 2     | 199 | C    |
| 18  | 2     | 203 | G    |
| 18  | 2     | 204 | G    |
| 18  | 2     | 205 | G    |
| 18  | 2     | 209 | A    |
| 18  | 2     | 210 | U    |
| 18  | 2     | 294 | U    |
| 18  | 2     | 308 | G    |
| 18  | 2     | 309 | G    |
| 18  | 2     | 312 | G    |
| 18  | 2     | 319 | C    |
| 18  | 2     | 320 | G    |
| 18  | 2     | 333 | G    |
| 18  | 2     | 335 | G    |
| 18  | 2     | 343 | A    |
| 18  | 2     | 344 | U    |
| 18  | 2     | 345 | U    |
| 18  | 2     | 357 | C    |
| 18  | 2     | 362 | C    |
| 18  | 2     | 364 | A    |
| 18  | 2     | 368 | U    |
| 18  | 2     | 369 | C    |
| 18  | 2     | 381 | C    |
| 18  | 2     | 385 | G    |
| 18  | 2     | 386 | C    |
| 18  | 2     | 400 | C    |
| 18  | 2     | 409 | C    |
| 18  | 2     | 421 | G    |
| 18  | 2     | 428 | U    |
| 18  | 2     | 429 | C    |
| 18  | 2     | 448 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | 2     | 449 | A    |
| 18  | 2     | 450 | C    |
| 18  | 2     | 455 | A    |
| 18  | 2     | 464 | A    |
| 18  | 2     | 465 | A    |
| 18  | 2     | 471 | G    |
| 18  | 2     | 472 | C    |
| 18  | 2     | 474 | G    |
| 18  | 2     | 482 | G    |
| 18  | 2     | 483 | C    |
| 18  | 2     | 487 | U    |
| 18  | 2     | 492 | C    |
| 18  | 2     | 493 | A    |
| 18  | 2     | 516 | A    |
| 18  | 2     | 525 | A    |
| 18  | 2     | 537 | C    |
| 18  | 2     | 538 | U    |
| 18  | 2     | 539 | C    |
| 18  | 2     | 540 | U    |
| 18  | 2     | 541 | U    |
| 18  | 2     | 543 | C    |
| 18  | 2     | 544 | G    |
| 18  | 2     | 545 | A    |
| 18  | 2     | 547 | G    |
| 18  | 2     | 548 | C    |
| 18  | 2     | 549 | C    |
| 18  | 2     | 556 | U    |
| 18  | 2     | 559 | G    |
| 18  | 2     | 563 | G    |
| 18  | 2     | 564 | A    |
| 18  | 2     | 568 | C    |
| 18  | 2     | 570 | C    |
| 18  | 2     | 574 | A    |
| 18  | 2     | 576 | A    |
| 18  | 2     | 585 | C    |
| 18  | 2     | 587 | A    |
| 18  | 2     | 588 | G    |
| 18  | 2     | 591 | U    |
| 18  | 2     | 604 | A    |
| 18  | 2     | 607 | U    |
| 18  | 2     | 608 | C    |
| 18  | 2     | 614 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | 2     | 617 | G    |
| 18  | 2     | 621 | C    |
| 18  | 2     | 623 | G    |
| 18  | 2     | 628 | A    |
| 18  | 2     | 629 | A    |
| 18  | 2     | 639 | C    |
| 18  | 2     | 640 | A    |
| 18  | 2     | 643 | A    |
| 18  | 2     | 644 | G    |
| 18  | 2     | 655 | A    |
| 18  | 2     | 660 | C    |
| 18  | 2     | 663 | C    |
| 18  | 2     | 664 | A    |
| 18  | 2     | 668 | A    |
| 18  | 2     | 669 | A    |
| 18  | 2     | 671 | A    |
| 18  | 2     | 672 | A    |
| 18  | 2     | 683 | G    |
| 18  | 2     | 691 | G    |
| 18  | 2     | 698 | G    |
| 18  | 2     | 699 | C    |
| 18  | 2     | 707 | C    |
| 18  | 2     | 709 | G    |
| 18  | 2     | 721 | G    |
| 18  | 2     | 722 | C    |
| 18  | 2     | 723 | C    |
| 18  | 2     | 731 | G    |
| 18  | 2     | 732 | U    |
| 18  | 2     | 733 | C    |
| 18  | 2     | 736 | C    |
| 18  | 2     | 747 | U    |
| 18  | 2     | 749 | U    |
| 18  | 2     | 750 | C    |
| 18  | 2     | 751 | G    |
| 18  | 2     | 792 | C    |
| 18  | 2     | 793 | G    |
| 18  | 2     | 794 | A    |
| 18  | 2     | 796 | G    |
| 18  | 2     | 798 | G    |
| 18  | 2     | 799 | U    |
| 18  | 2     | 800 | U    |
| 18  | 2     | 801 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | 2     | 808 | A    |
| 18  | 2     | 810 | A    |
| 18  | 2     | 811 | A    |
| 18  | 2     | 821 | G    |
| 18  | 2     | 822 | U    |
| 18  | 2     | 823 | U    |
| 18  | 2     | 827 | A    |
| 18  | 2     | 830 | A    |
| 18  | 2     | 845 | G    |
| 18  | 2     | 847 | A    |
| 18  | 2     | 859 | G    |
| 18  | 2     | 869 | A    |
| 18  | 2     | 870 | A    |
| 18  | 2     | 872 | A    |
| 18  | 2     | 874 | G    |
| 18  | 2     | 878 | G    |
| 18  | 2     | 882 | U    |
| 18  | 2     | 883 | U    |
| 18  | 2     | 886 | A    |
| 18  | 2     | 887 | U    |
| 18  | 2     | 888 | U    |
| 18  | 2     | 889 | U    |
| 18  | 2     | 890 | U    |
| 18  | 2     | 891 | G    |
| 18  | 2     | 893 | U    |
| 18  | 2     | 896 | U    |
| 18  | 2     | 897 | U    |
| 18  | 2     | 898 | U    |
| 18  | 2     | 899 | U    |
| 18  | 2     | 901 | G    |
| 18  | 2     | 902 | G    |
| 18  | 2     | 903 | A    |
| 18  | 2     | 913 | A    |
| 18  | 2     | 920 | A    |
| 18  | 2     | 922 | A    |
| 18  | 2     | 933 | G    |
| 18  | 2     | 938 | A    |
| 18  | 2     | 952 | G    |
| 18  | 2     | 953 | C    |
| 18  | 2     | 963 | A    |
| 18  | 2     | 971 | G    |
| 18  | 2     | 990 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | 2     | 992  | A    |
| 18  | 2     | 1001 | A    |
| 18  | 2     | 1008 | A    |
| 18  | 2     | 1017 | U    |
| 18  | 2     | 1023 | A    |
| 18  | 2     | 1026 | C    |
| 18  | 2     | 1045 | U    |
| 18  | 2     | 1049 | A    |
| 18  | 2     | 1050 | A    |
| 18  | 2     | 1055 | A    |
| 18  | 2     | 1058 | A    |
| 18  | 2     | 1059 | G    |
| 18  | 2     | 1060 | A    |
| 18  | 2     | 1061 | U    |
| 18  | 2     | 1080 | A    |
| 18  | 2     | 1083 | A    |
| 18  | 2     | 1085 | C    |
| 18  | 2     | 1087 | A    |
| 18  | 2     | 1089 | G    |
| 18  | 2     | 1096 | G    |
| 18  | 2     | 1109 | C    |
| 18  | 2     | 1113 | A    |
| 18  | 2     | 1114 | U    |
| 18  | 2     | 1116 | C    |
| 18  | 2     | 1117 | C    |
| 18  | 2     | 1118 | C    |
| 18  | 2     | 1119 | A    |
| 18  | 2     | 1120 | U    |
| 18  | 2     | 1133 | A    |
| 18  | 2     | 1138 | C    |
| 18  | 2     | 1153 | C    |
| 18  | 2     | 1154 | U    |
| 18  | 2     | 1157 | G    |
| 18  | 2     | 1171 | G    |
| 18  | 2     | 1188 | A    |
| 18  | 2     | 1195 | A    |
| 18  | 2     | 1203 | G    |
| 18  | 2     | 1207 | G    |
| 18  | 2     | 1212 | G    |
| 18  | 2     | 1215 | C    |
| 18  | 2     | 1221 | G    |
| 18  | 2     | 1224 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | 2     | 1242 | U    |
| 18  | 2     | 1243 | U    |
| 18  | 2     | 1251 | A    |
| 18  | 2     | 1253 | A    |
| 18  | 2     | 1256 | G    |
| 18  | 2     | 1257 | G    |
| 18  | 2     | 1259 | A    |
| 18  | 2     | 1274 | G    |
| 18  | 2     | 1275 | G    |
| 18  | 2     | 1284 | A    |
| 18  | 2     | 1285 | G    |
| 18  | 2     | 1298 | G    |
| 18  | 2     | 1301 | A    |
| 18  | 2     | 1302 | G    |
| 18  | 2     | 1303 | C    |
| 18  | 2     | 1308 | U    |
| 18  | 2     | 1313 | A    |
| 18  | 2     | 1315 | U    |
| 18  | 2     | 1320 | G    |
| 18  | 2     | 1342 | U    |
| 18  | 2     | 1345 | G    |
| 18  | 2     | 1348 | G    |
| 18  | 2     | 1352 | G    |
| 18  | 2     | 1354 | G    |
| 18  | 2     | 1358 | U    |
| 18  | 2     | 1364 | U    |
| 18  | 2     | 1369 | A    |
| 18  | 2     | 1371 | U    |
| 18  | 2     | 1372 | U    |
| 18  | 2     | 1378 | A    |
| 18  | 2     | 1381 | G    |
| 18  | 2     | 1382 | A    |
| 18  | 2     | 1397 | U    |
| 18  | 2     | 1398 | G    |
| 18  | 2     | 1403 | C    |
| 18  | 2     | 1405 | A    |
| 18  | 2     | 1428 | G    |
| 18  | 2     | 1429 | G    |
| 18  | 2     | 1430 | C    |
| 18  | 2     | 1432 | U    |
| 18  | 2     | 1452 | A    |
| 18  | 2     | 1454 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | 2     | 1462 | U    |
| 18  | 2     | 1463 | U    |
| 18  | 2     | 1464 | C    |
| 18  | 2     | 1477 | U    |
| 18  | 2     | 1480 | A    |
| 18  | 2     | 1487 | A    |
| 18  | 2     | 1489 | A    |
| 18  | 2     | 1490 | G    |
| 18  | 2     | 1493 | C    |
| 18  | 2     | 1497 | G    |
| 18  | 2     | 1498 | A    |
| 18  | 2     | 1508 | A    |
| 18  | 2     | 1521 | C    |
| 18  | 2     | 1523 | C    |
| 18  | 2     | 1533 | A    |
| 18  | 2     | 1547 | C    |
| 18  | 2     | 1552 | G    |
| 18  | 2     | 1553 | C    |
| 18  | 2     | 1558 | C    |
| 18  | 2     | 1559 | C    |
| 18  | 2     | 1575 | G    |
| 18  | 2     | 1578 | U    |
| 18  | 2     | 1580 | A    |
| 18  | 2     | 1585 | U    |
| 18  | 2     | 1586 | U    |
| 18  | 2     | 1587 | G    |
| 18  | 2     | 1588 | A    |
| 18  | 2     | 1589 | A    |
| 18  | 2     | 1601 | A    |
| 18  | 2     | 1603 | G    |
| 18  | 2     | 1607 | A    |
| 18  | 2     | 1614 | A    |
| 18  | 2     | 1621 | U    |
| 18  | 2     | 1623 | A    |
| 18  | 2     | 1624 | U    |
| 18  | 2     | 1639 | G    |
| 18  | 2     | 1648 | G    |
| 18  | 2     | 1651 | A    |
| 18  | 2     | 1654 | G    |
| 18  | 2     | 1660 | C    |
| 18  | 2     | 1664 | A    |
| 18  | 2     | 1665 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | 2     | 1671 | G    |
| 18  | 2     | 1683 | C    |
| 18  | 2     | 1695 | A    |
| 18  | 2     | 1699 | A    |
| 18  | 2     | 1710 | C    |
| 18  | 2     | 1720 | U    |
| 18  | 2     | 1721 | U    |
| 18  | 2     | 1726 | G    |
| 18  | 2     | 1746 | U    |
| 18  | 2     | 1751 | C    |
| 18  | 2     | 1752 | C    |
| 18  | 2     | 1753 | C    |
| 18  | 2     | 1755 | C    |
| 18  | 2     | 1756 | C    |
| 18  | 2     | 1757 | G    |
| 18  | 2     | 1758 | G    |
| 18  | 2     | 1759 | G    |
| 18  | 2     | 1760 | G    |
| 18  | 2     | 1761 | U    |
| 18  | 2     | 1772 | C    |
| 18  | 2     | 1773 | C    |
| 18  | 2     | 1774 | C    |
| 18  | 2     | 1777 | G    |
| 18  | 2     | 1781 | A    |
| 18  | 2     | 1783 | C    |
| 18  | 2     | 1784 | G    |
| 18  | 2     | 1785 | C    |
| 18  | 2     | 1786 | U    |
| 18  | 2     | 1806 | A    |
| 18  | 2     | 1824 | A    |
| 18  | 2     | 1825 | A    |
| 18  | 2     | 1829 | G    |
| 18  | 2     | 1831 | A    |
| 18  | 2     | 1834 | A    |
| 18  | 2     | 1835 | A    |
| 18  | 2     | 1838 | U    |
| 18  | 2     | 1849 | G    |
| 18  | 2     | 1851 | A    |
| 18  | 2     | 1861 | G    |
| 18  | 2     | 1862 | G    |
| 18  | 2     | 1863 | A    |
| 18  | 2     | 1864 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | 2     | 1865 | C    |
| 18  | 2     | 1869 | A    |
| 49  | 1     | 10   | G    |
| 49  | 1     | 12   | G    |
| 49  | 1     | 13   | C    |
| 49  | 1     | 16   | C    |
| 49  | 1     | 18   | G    |
| 49  | 1     | 19   | G    |
| 49  | 1     | 20   | A    |
| 49  | 1     | 21   | A    |
| 49  | 1     | 22   | G    |
| 49  | 1     | 48   | C    |
| 49  | 1     | 49   | G    |
| 49  | 1     | 58   | A    |
| 49  | 1     | 72   | U    |
| 49  | 1     | 74   | C    |
| 49  | 1     | 76   | A    |

All (8) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | 2     | 92   | A    |
| 18  | 2     | 332  | G    |
| 18  | 2     | 368  | U    |
| 18  | 2     | 369  | C    |
| 18  | 2     | 868  | G    |
| 18  | 2     | 912  | C    |
| 18  | 2     | 1058 | A    |
| 18  | 2     | 1060 | A    |

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | GTP  | Y     | 501 | 57   | 33,34,34     | 0.94 | 2 (6%)   | 50,54,54    | 1.74 | 8 (16%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 56  | GTP  | Y     | 501 | 57   | -       | 4/22/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 56  | Y     | 501 | GTP  | C2-N3 | 2.20  | 1.38        | 1.33     |
| 56  | Y     | 501 | GTP  | C5-N7 | -2.03 | 1.35        | 1.39     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 56  | Y     | 501 | GTP  | C5-C4-N3 | -6.15 | 118.61      | 128.39   |
| 56  | Y     | 501 | GTP  | C2-N3-C4 | 5.15  | 121.17      | 112.30   |
| 56  | Y     | 501 | GTP  | N9-C4-N3 | 4.31  | 134.58      | 125.95   |
| 56  | Y     | 501 | GTP  | C2-N1-C6 | -3.24 | 119.23      | 125.11   |
| 56  | Y     | 501 | GTP  | C5-C6-N1 | 2.67  | 120.04      | 113.25   |
| 56  | Y     | 501 | GTP  | O6-C6-C5 | -2.50 | 119.94      | 126.53   |
| 56  | Y     | 501 | GTP  | C8-N7-C5 | 2.39  | 108.53      | 104.26   |
| 56  | Y     | 501 | GTP  | N9-C8-N7 | -2.15 | 109.41      | 113.40   |

There are no chirality outliers.

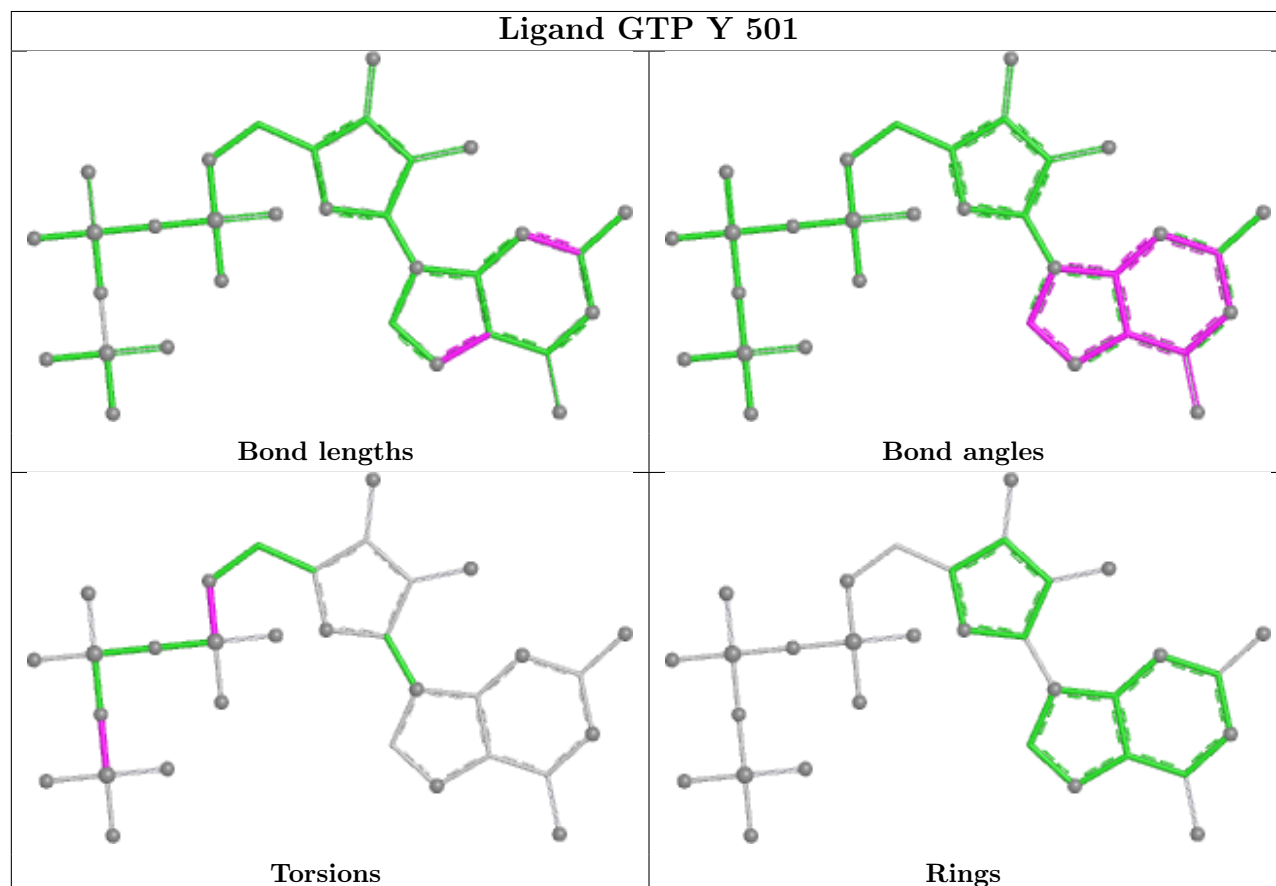
All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 56  | Y     | 501 | GTP  | C5'-O5'-PA-O1A |
| 56  | Y     | 501 | GTP  | PB-O3B-PG-O1G  |
| 56  | Y     | 501 | GTP  | PB-O3B-PG-O2G  |
| 56  | Y     | 501 | GTP  | PB-O3B-PG-O3G  |

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 39  | A     | 3                |
| 40  | C     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 200:ALA   | C      | 320:LYS   | N      | 76.80        |
| 1     | A     | 685:LYS   | C      | 707:GLU   | N      | 37.30        |
| 1     | A     | 639:GLU   | C      | 642:ARG   | N      | 9.91         |
| 1     | A     | 600:GLU   | C      | 602:LEU   | N      | 9.04         |

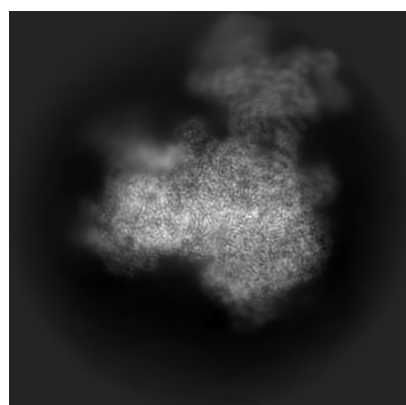
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11335. These allow visual inspection of the internal detail of the map and identification of artifacts.

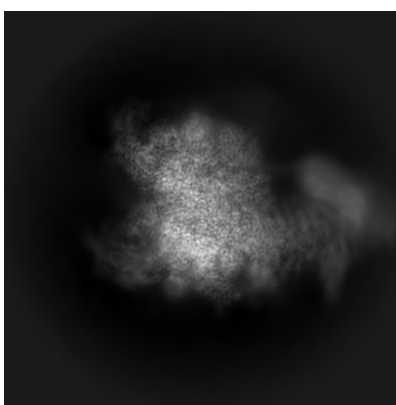
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

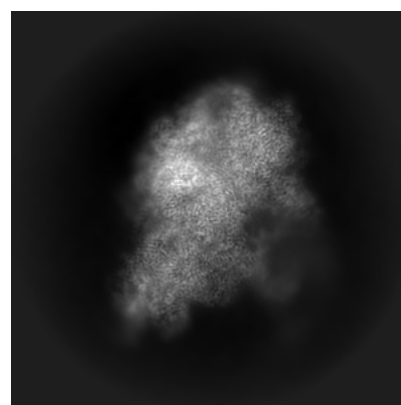
#### 6.1.1 Primary map



X



Y

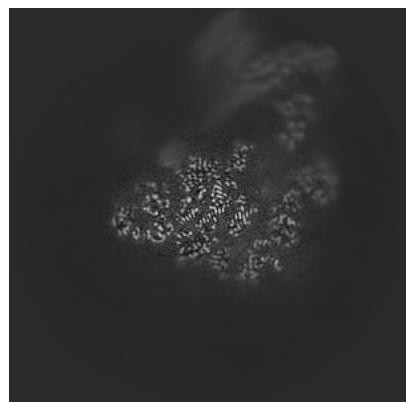


Z

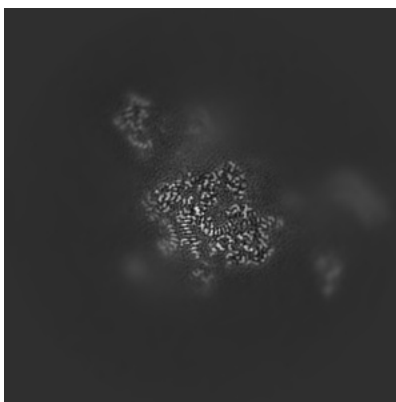
The images above show the map projected in three orthogonal directions.

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

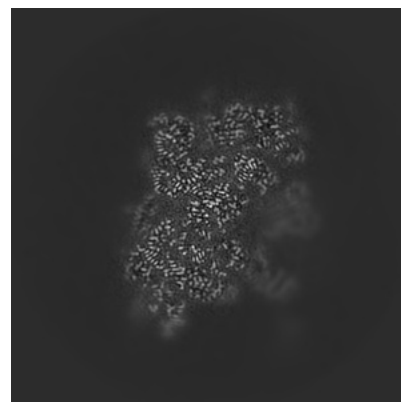
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

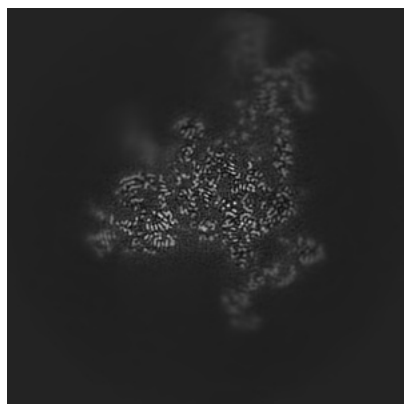


Z Index: 180

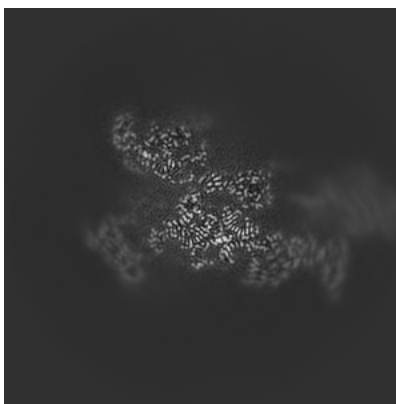
The images above show central slices of the map in three orthogonal directions.

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

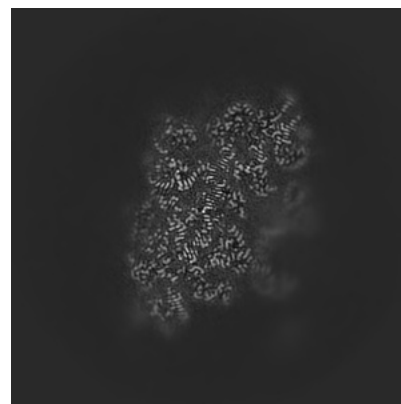
### 6.3.1 Primary map



X Index: 157



Y Index: 203

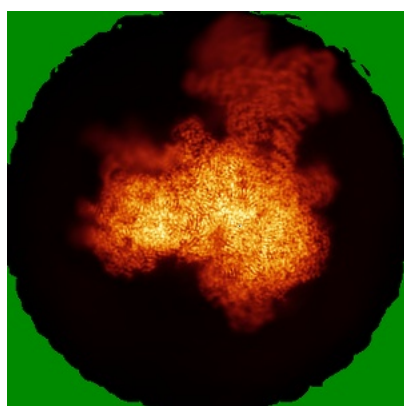


Z Index: 174

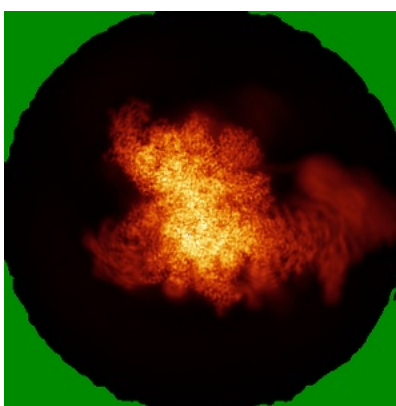
The images above show the largest variance slices of the map in three orthogonal directions.

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

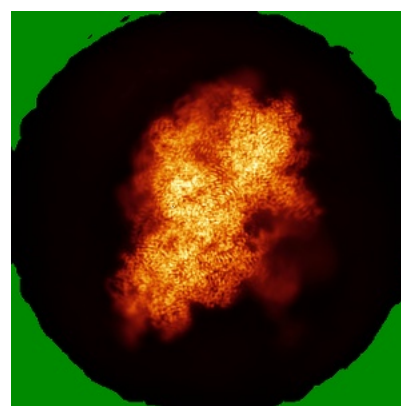
### 6.4.1 Primary map



X



Y

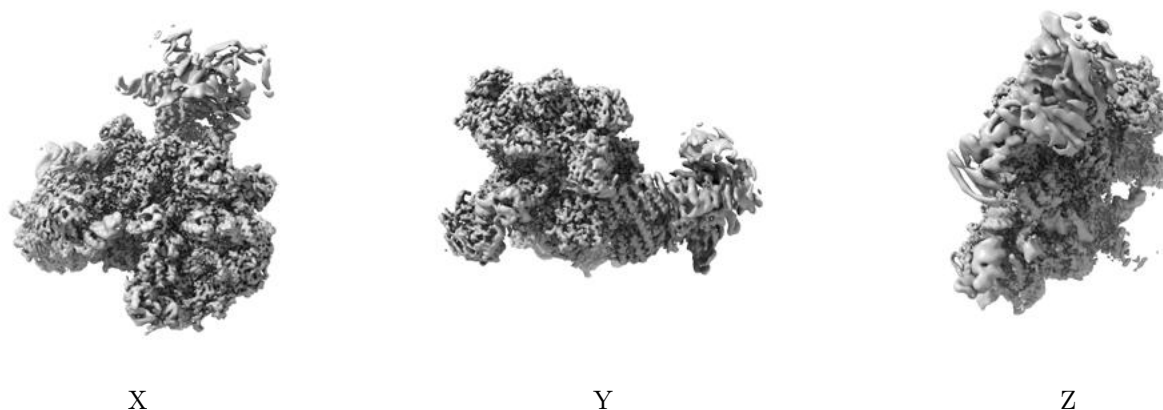


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

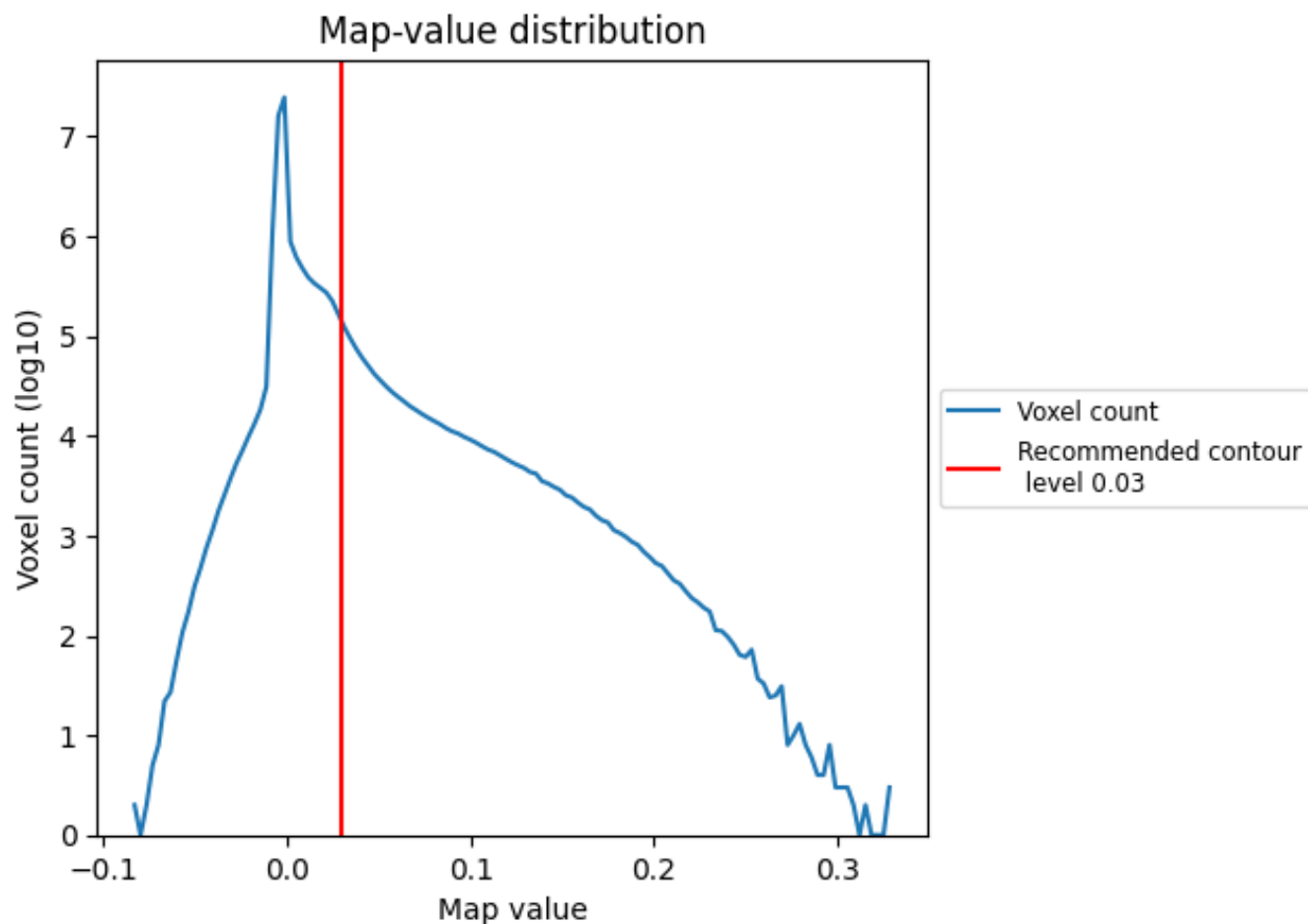
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

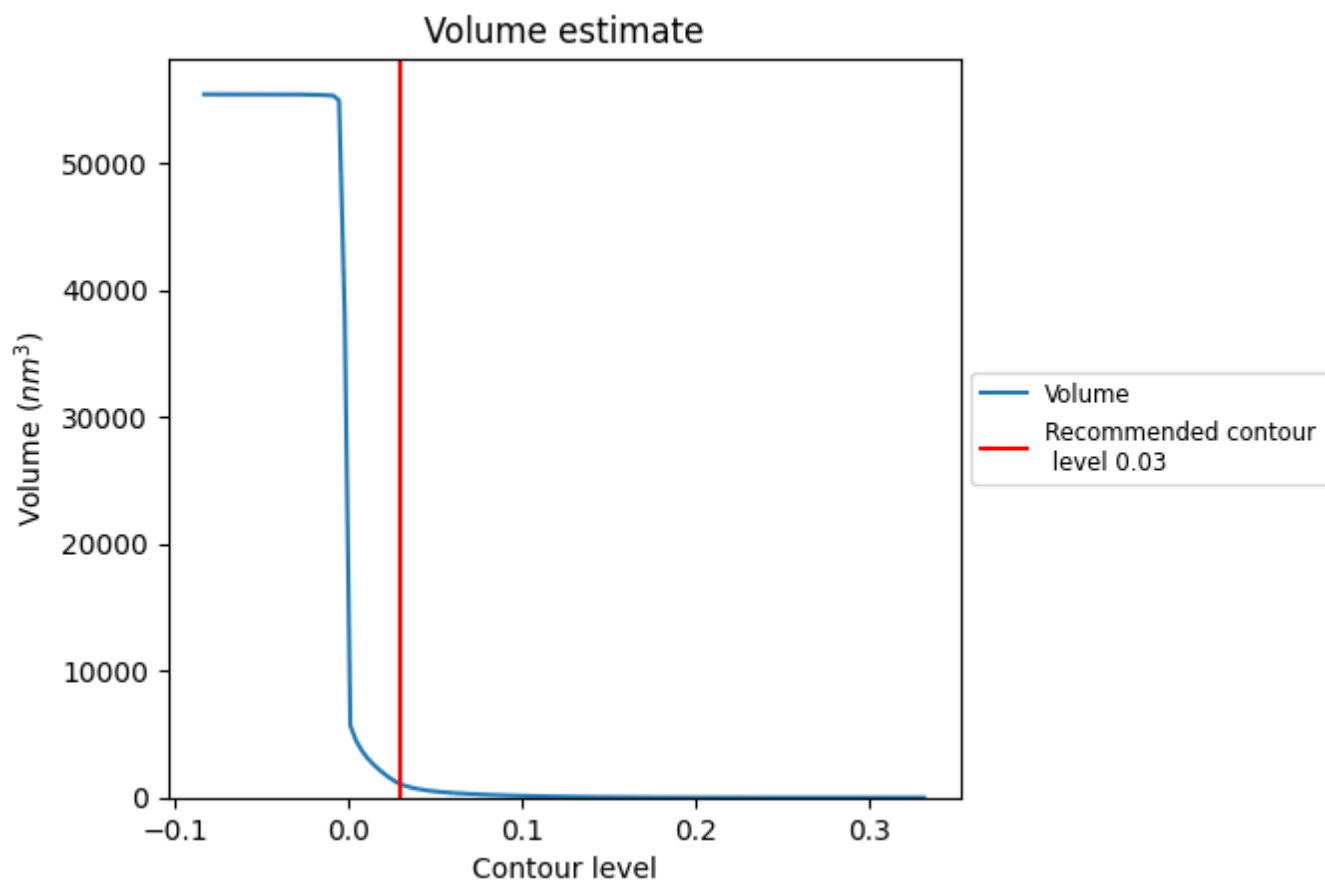
This section contains the results of statistical analysis of the map.

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



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

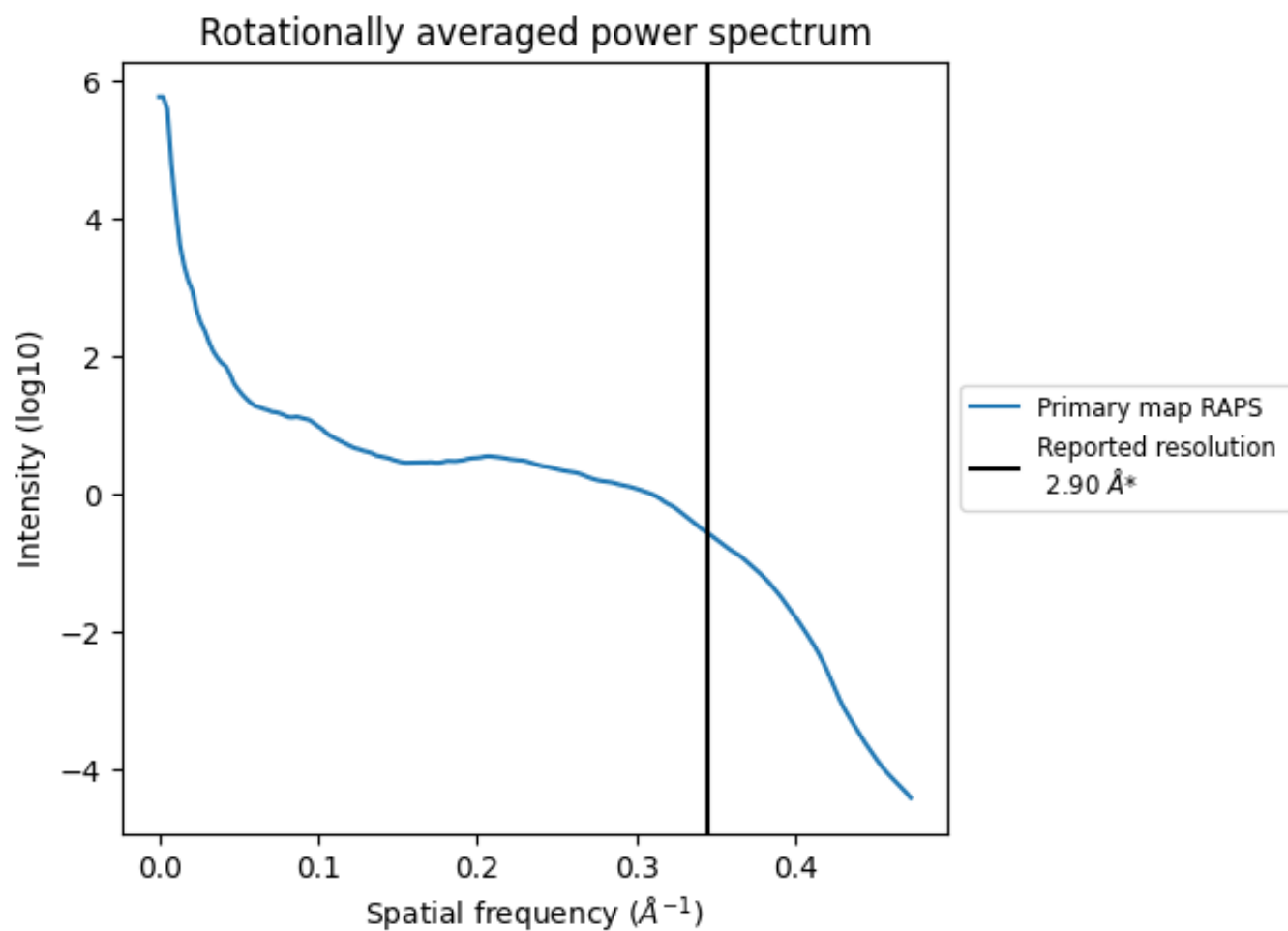
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1065 nm<sup>3</sup>; this corresponds to an approximate mass of 962 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

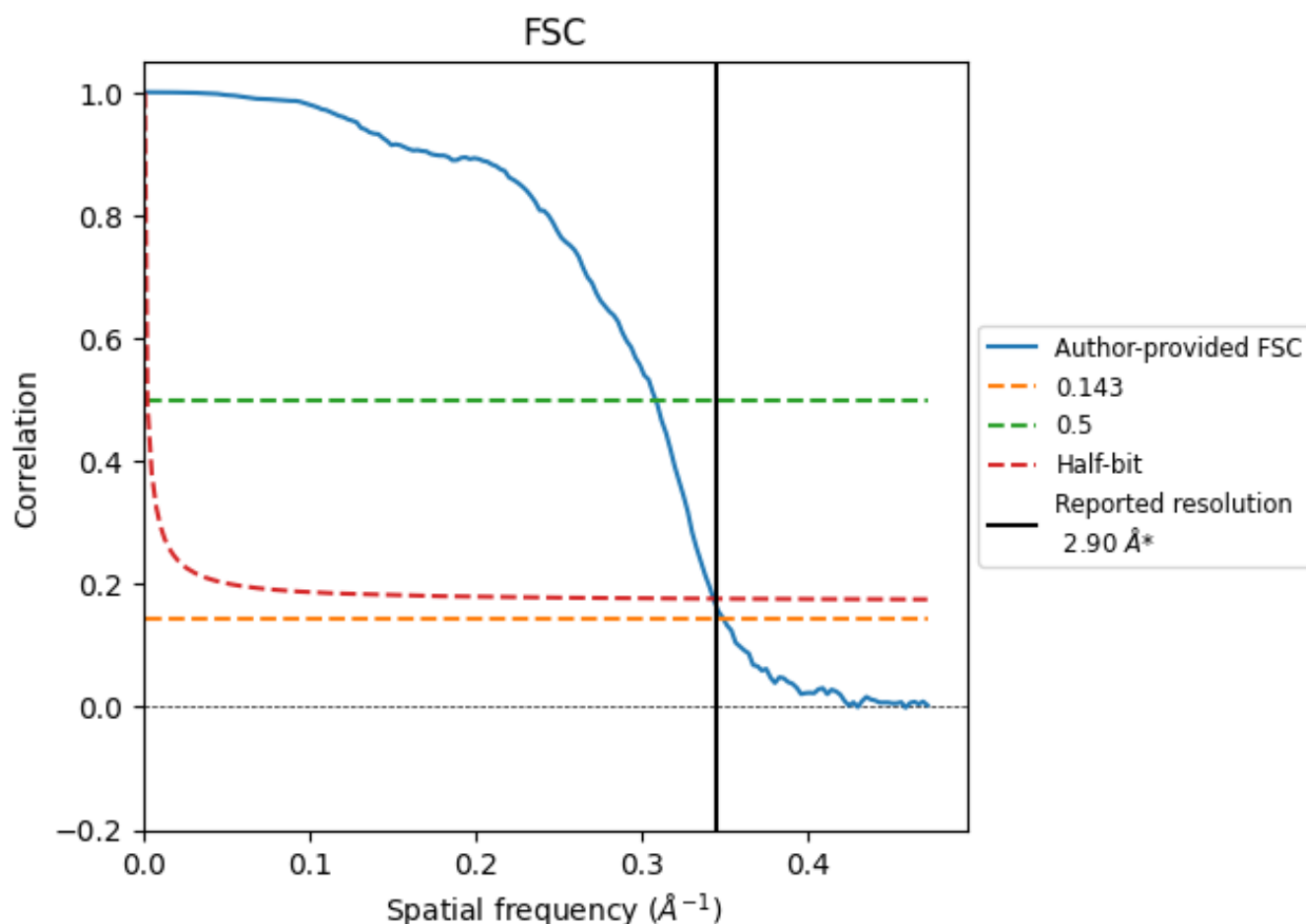


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

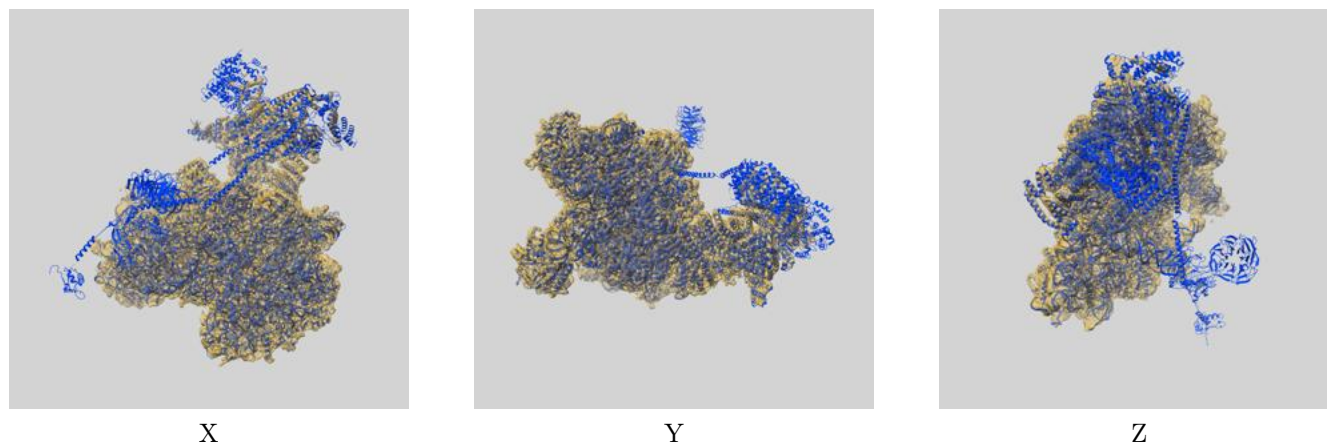
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | 2.86                               | 3.24 | 2.91     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

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

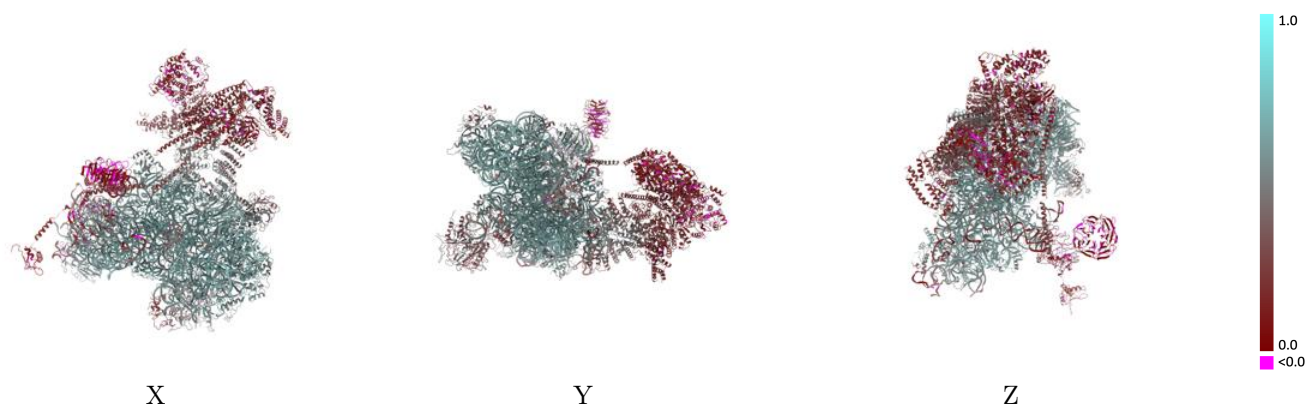
This section contains information regarding the fit between EMDB map EMD-11335 and PDB model 6ZP4. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



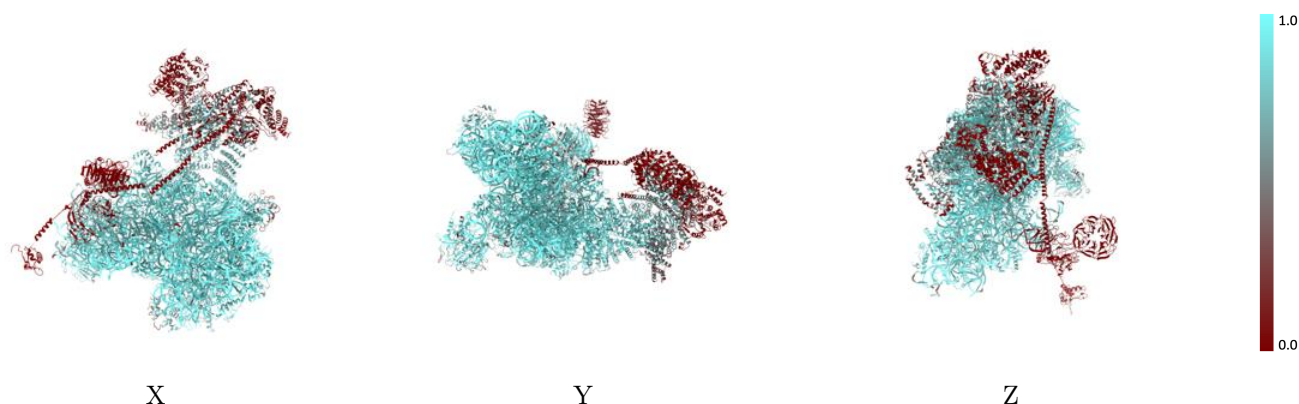
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



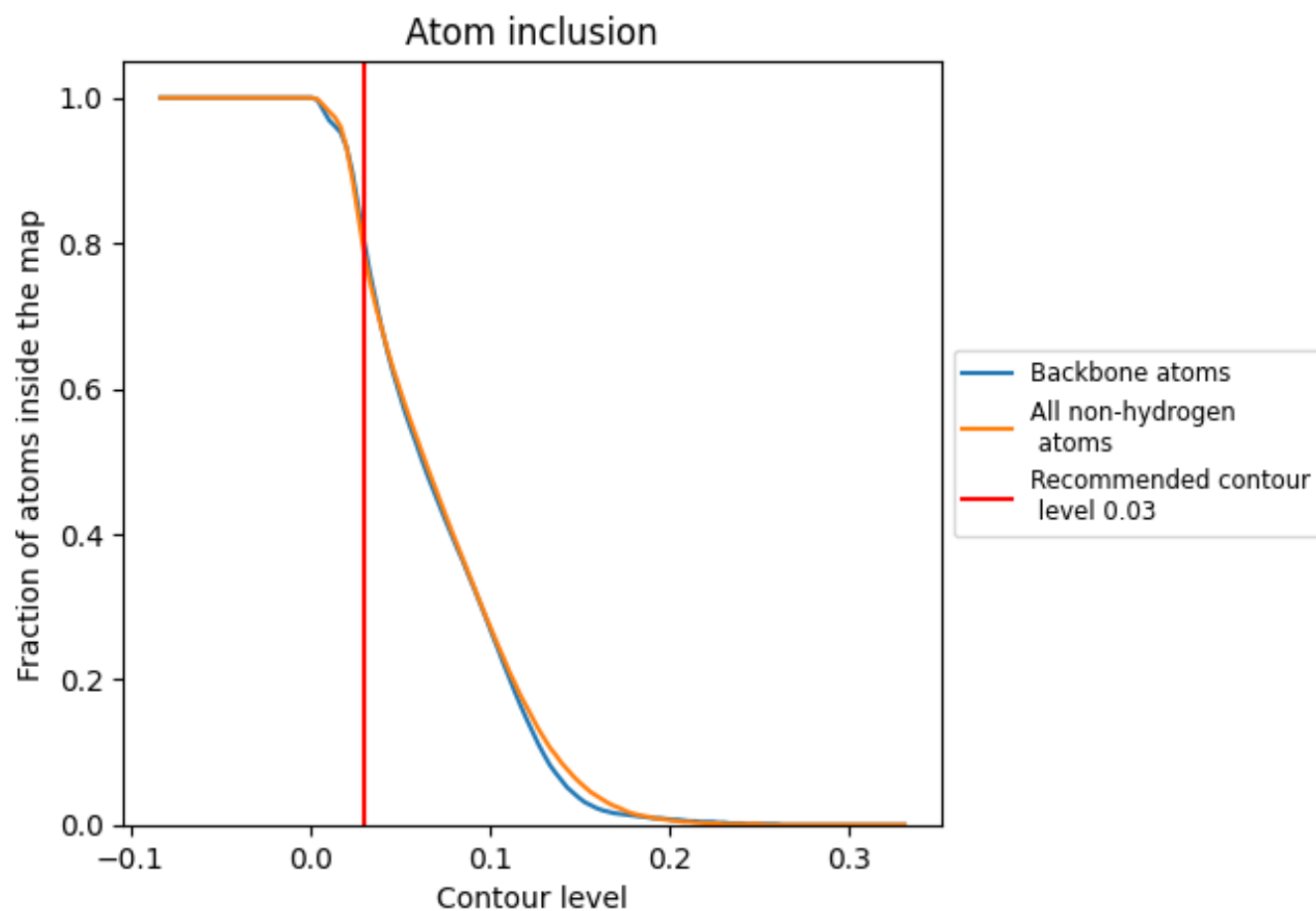
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7920   |  0.4760   |
| 1     |  0.9840   |  0.5230   |
| 2     |  0.9730   |  0.5860   |
| 4     |  0.9070   |  0.4890   |
| A     |  0.5830   |  0.3170   |
| B     |  0.1780   |  0.2080   |
| C     |  0.8010   |  0.4020   |
| D     |  0.9900   |  0.6430   |
| E     |  0.4520   |  0.1970   |
| F     |  0.2080   |  0.1340   |
| G     |  0.8440   |  0.5510   |
| H     |  0.2990   |  0.1580   |
| I     |  0.0000   |  0.0540   |
| J     |  0.9770   |  0.6310   |
| K     |  0.0280  |  0.1220  |
| L     |  0.0980 |  0.1200 |
| M     |  0.1770 |  0.1630 |
| N     |  0.7380 |  0.4130 |
| O     |  0.7960 |  0.4200 |
| P     |  0.9280 |  0.5630 |
| Q     |  0.9730 |  0.6160 |
| R     |  0.9700 |  0.5950 |
| S     |  0.9310 |  0.5630 |
| T     |  0.9790 |  0.6060 |
| U     |  0.8250 |  0.4630 |
| V     |  0.9330 |  0.5490 |
| W     |  0.9470 |  0.5850 |
| X     |  0.7820 |  0.3710 |
| Y     |  0.7850 |  0.3630 |
| Z     |  0.8820 |  0.5170 |
| a     |  0.9510 |  0.6040 |
| b     |  0.9580 |  0.5890 |
| c     |  0.9740 |  0.6160 |
| d     |  0.9820 |  0.6360 |
| e     |  0.9750 |  0.6060 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                            | Q-score                                                                                   |
|-------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| g     |  0.9680  |  0.6230  |
| h     |  0.9100  |  0.5670  |
| i     |  0.9800  |  0.6130  |
| j     |  0.9820  |  0.6300  |
| k     |  0.9060  |  0.5710  |
| l     |  0.9890  |  0.6450  |
| m     |  0.9670  |  0.6060  |
| n     |  0.9780  |  0.6160  |
| o     |  0.9100  |  0.5770  |
| p     |  0.9560  |  0.6050  |
| q     |  0.9750  |  0.6100  |
| r     |  0.9040  |  0.5250  |
| s     |  0.9220  |  0.5360  |
| t     |  0.9410  |  0.5660  |
| u     |  0.9480  |  0.5760  |
| v     |  0.6000  |  0.3280  |
| w     |  0.9440  |  0.5850  |
| x     |  0.9610  |  0.6170  |
| y     |  0.9710  |  0.6220  |
| z     |  0.9580 |  0.5790 |