



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 07:11 AM UTC

PDB ID : 8AGZ / pdb\_00008agz  
EMDB ID : EMD-15428  
Title : Yeast RQC complex in state with the RING domain of Ltn1 in the OUT position  
Authors : Tesina, P.; Buschauer, R.; Beckmann, R.  
Deposited on : 2022-07-20  
Resolution : 2.60 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  
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

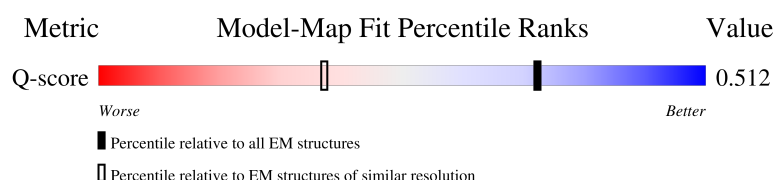
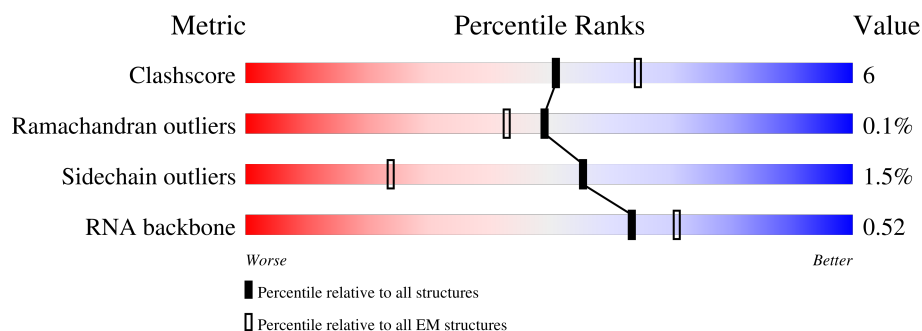
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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.



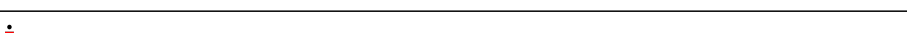
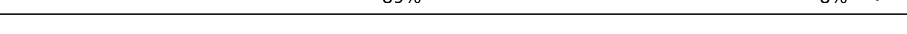
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 8728 ( 2.10 - 3.10 )                                     |

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     | 204    |                  |
| 2   | B     | 199    |                  |
| 3   | C     | 184    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 186    |    |
| 5   | E     | 189    |    |
| 6   | F     | 172    |    |
| 7   | G     | 160    |    |
| 8   | H     | 121    |    |
| 9   | I     | 137    |    |
| 10  | J     | 155    |    |
| 11  | K     | 142    |    |
| 12  | L     | 127    |    |
| 13  | M     | 136    |    |
| 14  | N     | 149    |    |
| 15  | O     | 59     |    |
| 16  | P     | 105    |  |
| 17  | Q     | 113    |  |
| 18  | R     | 130    |  |
| 19  | S     | 107    |  |
| 20  | T     | 121    |  |
| 21  | U     | 120    |  |
| 22  | V     | 100    |  |
| 23  | W     | 88     |  |
| 24  | X     | 78     |  |
| 25  | Y     | 51     |  |
| 26  | Z     | 128    |  |
| 27  | b     | 106    |  |
| 28  | c     | 92     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | d     | 25     |                  |
| 30  | f     | 3395   |                  |
| 31  | h     | 121    |                  |
| 32  | i     | 158    |                  |
| 33  | j     | 254    |                  |
| 34  | k     | 387    |                  |
| 35  | l     | 362    |                  |
| 36  | m     | 297    |                  |
| 37  | n     | 176    |                  |
| 38  | o     | 244    |                  |
| 39  | p     | 256    |                  |
| 40  | q     | 191    |                  |
| 41  | r     | 221    |                  |
| 42  | s     | 174    |                  |
| 43  | t     | 199    |                  |
| 44  | u     | 138    |                  |
| 45  | a     | 1038   |                  |
| 46  | e     | 1562   |                  |
| 47  | g     | 245    |                  |
| 48  | v     | 157    |                  |
| 49  | w     | 217    |                  |
| 50  | x     | 76     |                  |
| 50  | y     | 76     |                  |
| 51  | z     | 165    |                  |
| 52  | 0     | 312    |                  |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 53  | 1     | 18     | <br>61% 39% |

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 151339 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 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |       |

- Molecule 2 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | B     | 197      | Total | C    | N   | O   | S | 197     | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |       |

- Molecule 3 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 3   | C     | 183      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1416  | 879 | 284 | 253 |  |         |       |

- Molecule 4 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 5   | E     | 156      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1258  | 781 | 265 | 212 |  |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1437  | 925 | 266 | 243 | 3 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1272  | 802 | 245 | 221 | 4 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 796   | 516 | 131 | 149 |   |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | I     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 10  | J     | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 518   | 333 | 102 | 82 | 1 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 620 | 169 | 173 | 2 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 984   | 620 | 191 | 173 |   |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 701 | 199 | 180 |   |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1169  | 747 | 231 | 188 | 3 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 15  | O     | 58       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |   |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | P     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 737   | 476 | 123 | 137 | 1 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 556 | 167 | 152 | 1 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1013  | 642 | 205 | 165 | 1 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L35-A.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | U     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | V     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 766   | 478 | 154 | 132 | 2 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | W     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 645   | 393 | 141 | 106 | 5 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 24  | X     | 77       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |  |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25  | Y     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |       |

- Molecule 26 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | Z     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 410   | 254 | 86 | 65 | 5 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | b     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 824   | 517 | 167 | 135 | 5 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | c     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | d     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 207   | 127 | 56 | 23 | 1 |         |       |

- Molecule 30 is a RNA chain called 25S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 30  | f     | 3216     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 68782 | 30723 | 12389 | 22454 | 3216 |         |       |

- Molecule 31 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 31  | h     | 121      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |       |

- Molecule 32 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 32  | i     | 158      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 33  | j     | 246      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1874  | 1168 | 380 | 325 | 1 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | k     | 386      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | l     | 361      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | m     | 294      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2351  | 1484 | 410 | 455 | 2 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L6-B.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 37  | n     | 167      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1307  | 843 | 234 | 230 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | o     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1784  | 1151 | 324 | 308 | 1 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | p     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1804  | 1151 | 323 | 327 | 3 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | q     | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 957 | 274 | 273 | 4 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | r     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1764  | 1117 | 334 | 306 | 7 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | s     | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 843 | 252 | 247 | 4 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | t     | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1543  | 962 | 315 | 266 |   |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | u     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 | 2 |         |       |

- Molecule 45 is a protein called RQC2 isoform 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 45  | a     | 848      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6579  | 4194 | 1142 | 1226 | 17 |         |       |

- Molecule 46 is a protein called E3 ubiquitin-protein ligase listerin.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 46  | e     | 1527     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11506 | 7350 | 1937 | 2181 | 38 |         |       |

- Molecule 47 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | g     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1651  | 1030 | 282 | 332 | 7 |         |       |

- Molecule 48 is a protein called Eukaryotic translation initiation factor 5A-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | v     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1085  | 676 | 183 | 217 | 9 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | w     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1709  | 1092 | 298 | 310 | 9 |         |       |

- Molecule 50 is a RNA chain called Ala tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 50  | x     | 74       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1579  | 702 | 277 | 526 | 74 |         |       |
| 50  | y     | 73       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1556  | 692 | 272 | 519 | 73 |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L12-B.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 51  | z     | 148      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 728   | 432 | 148 | 148 |         |       |

- Molecule 52 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | 0     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 961   | 618 | 167 | 173 | 3 |         |       |

- Molecule 53 is a protein called CAT-tailed nascent chain.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 53  | 1     | 18       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 90    | 54 | 18 | 18 |         |       |

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 54  | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 54  | C     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 54  | E     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 54  | I     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 54  | R     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

*Continued on next page...*

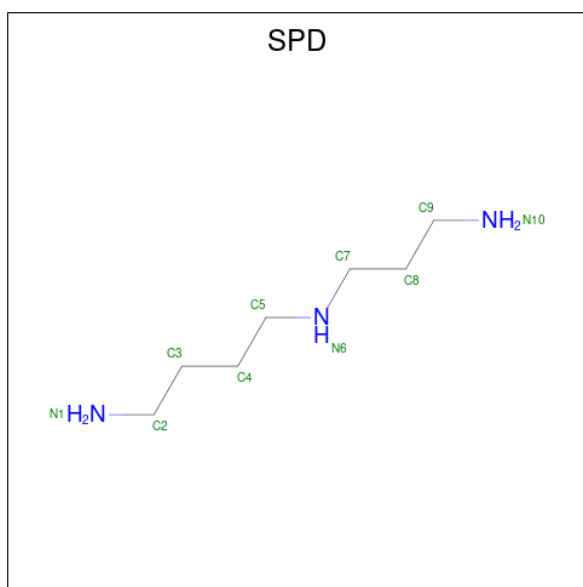
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 54  | T     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 54  | f     | 3        | Total<br>3 | Mg<br>3 | 0       |
| 54  | h     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 54  | j     | 2        | Total<br>2 | Mg<br>2 | 0       |
| 54  | k     | 1        | Total<br>1 | Mg<br>1 | 0       |

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

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 55  | T     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 55  | W     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 55  | Z     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 55  | b     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 55  | c     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 55  | e     | 2        | Total<br>2 | Zn<br>2 | 0       |

- Molecule 56 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).

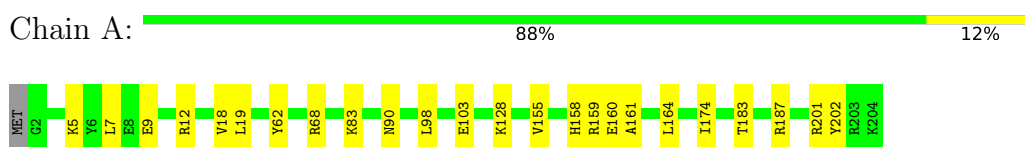


| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 56  | f     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

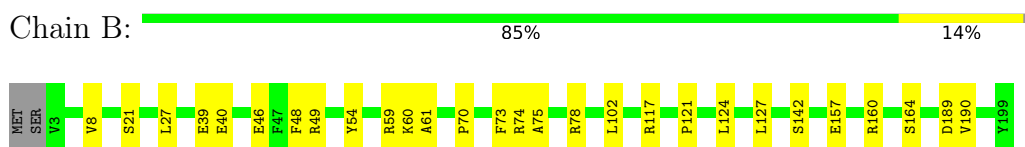
### 3 Residue-property plots

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

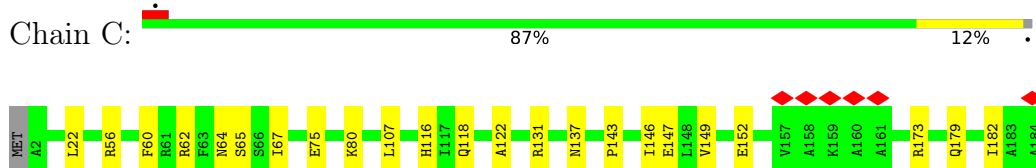
- Molecule 1: 60S ribosomal protein L15-A



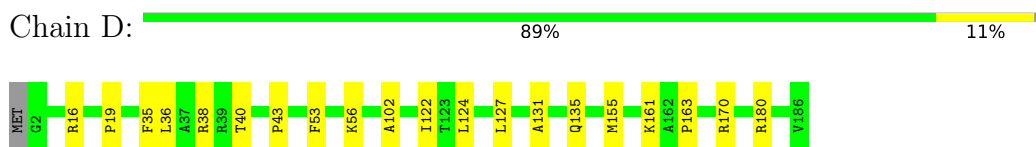
- Molecule 2: 60S ribosomal protein L16-A



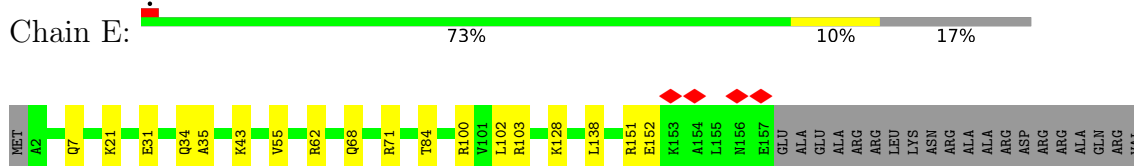
- Molecule 3: 60S ribosomal protein L17-A



- Molecule 4: 60S ribosomal protein L18-A



- Molecule 5: 60S ribosomal protein L19-A





ALA  
GLU  
LYS  
ARG  
ASP  
ALA  
LEU  
LEU  
LYS  
GLU  
ASP  
ALA

• Molecule 6: 60S ribosomal protein L20-A

Chain F:  85% 15% .

MET A2 Q8 P22 S32 I36 Y43 I64 T70 V77 R80 T87 M90 E93 I94 R95 D96 V97 L106 M110 H122 I123 L124 R125 V126 R137 V140 R155 V156 Y172

• Molecule 7: 60S ribosomal protein L21-A

Chain G:  87% 12% .

MET G2 R17 H22 T68 K69 G73 Y84 R88 L89 S99 K100 C101 R102 R108 M112 R116 A133 R136 R139 M146 P155 T168 F169 I160

• Molecule 8: 60S ribosomal protein L22-A

Chain H:  69% 14% 17%

MET ALA PRO ASN THR SER ARG LYS D9 V19 S20 T23 I41 K42 V43 E44 N49 L50 G51 V54 T55 V56 V65 K81 R90 D91 L105 A106 F107 Y108 GLN VAL THR PRO GLU GLU ASP GLU GLU ASP GLU

• Molecule 9: 60S ribosomal protein L23-A

Chain I:  88% 11% .

MET S2 R12 I13 S14 P18 A38 A51 M59 R80 Q81 Y94 A99 P117 R128 V129 S133 G134 V135 V136 V137

• Molecule 10: 60S ribosomal protein L24-A

Chain J:  35% 5% 59%

M1 D6 G16 Q32 R33 S34 K41 K44 R47 H58 I63 THR GLU GLU VAL ALA LYS LYS ARG SER THR VAL ALA GLN ARG PRO ILE THR GLY ALA SER LEU ASP LEU ILE LYS LYS GLU ARG SER LEU LYS PRO GLU VAL ARG LYS ALA ASN  
ARG GLU LYS LYS LYS ALA ASN GLU LYS LYS LYS ALA GLU LYS LYS ALA THR VAL VAL GLY THR ASN GLY LYS K22 A50 I142

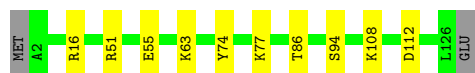
• Molecule 11: 60S ribosomal protein L25

Chain K:  85% 15%

MET ALA PRO SER LYS LYS LYS LYS LYS LYS VAL VAL LYS LYS THR ASN LYS K22 A50 I142

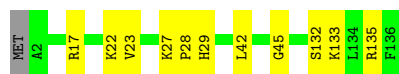
• Molecule 12: 60S ribosomal protein L26-A

Chain L:  91% 8% .



- Molecule 13: 60S ribosomal protein L27-A

Chain M:  91% 8% .



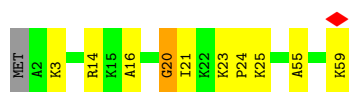
- Molecule 14: 60S ribosomal protein L28

Chain N:  87% 13% .



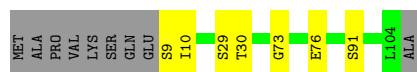
- Molecule 15: 60S ribosomal protein L29

Chain O:  81% 15% . .



- Molecule 16: 60S ribosomal protein L30

Chain P:  85% 7% 9%



- Molecule 17: 60S ribosomal protein L31-A

Chain Q:  80% 17% .

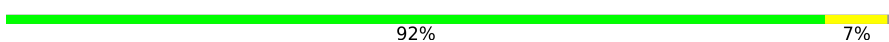


- Molecule 18: 60S ribosomal protein L32

Chain R:  89% 8% .



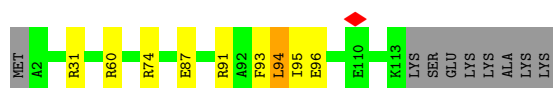
- Molecule 19: 60S ribosomal protein L33-A

Chain S:  92% 7%

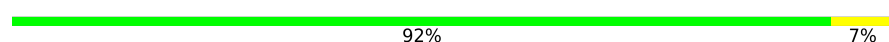


- Molecule 20: 60S ribosomal protein L34-A

Chain T:  85% 7% 7%

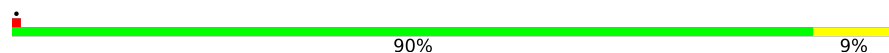


- Molecule 21: 60S ribosomal protein L35-A

Chain U:  92% 7%



- Molecule 22: 60S ribosomal protein L36-A

Chain V:  90% 9%

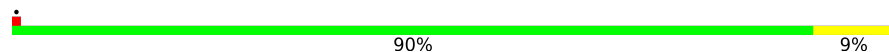


- Molecule 23: 60S ribosomal protein L37-A

Chain W:  76% 16% 8%

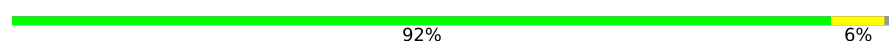


- Molecule 24: 60S ribosomal protein L38

Chain X:  90% 9%

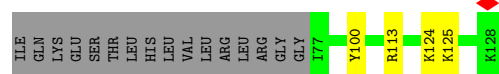


- Molecule 25: 60S ribosomal protein L39

Chain Y:  92% 6%



- Molecule 26: Ubiquitin-60S ribosomal protein L40



- [illegible]

- 

- Chain d: 

Diagram illustrating the 20 amino acids in the genetic code, categorized by color and labeled with their corresponding amino acid abbreviations:

- Orange:** M4
- Yellow:** R20, R21
- Green:** K22, V23
- Red:** R24, A25
- Grey:** ARG, SER, LYS

- |   |   |   |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |     |
|---|---|---|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|-----|
| G | U | U | A6 | A13 | U14 | U19 | A20 | G21 | A26 | C36 | A40 | A43 | A49 | G58 | G59 | A60 | A63 | G64 | A65 | A66 | A67 | G68 | G76 | U77 | U78 | G86 | G92 | G93 | G94 | A95 | G98 | A99 | A109 | G110 | C111 | A116 | G120 | A121 | A122 | A123 | ... |
|---|---|---|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|-----|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A130 | U133 | U134 | C135 | G136 | G139 | G156 | A157 | G158 | A159 | A165 | C166 | G172 | G173 | U182 | G183 | A187 | U190 | U191 | C200 | G206 | U210 | A211 | G212 | A213 | G216 | U217 | G218 | A219 | G234 | U240 | G241 | C242 | G243 | G244 | U245 | U249 | U252 | G269 | G282 | G283 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

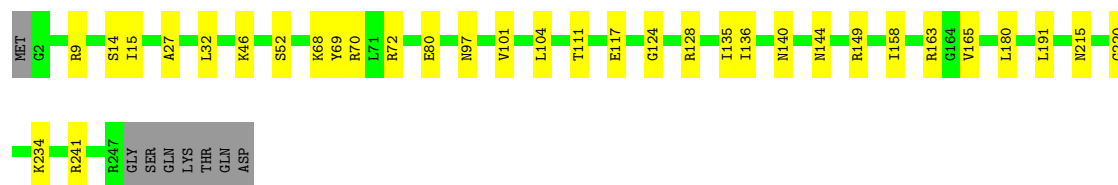
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A285 | U286 | A295 | A296 | G297 | U298 | G299 | G300 | G301 | U305 | A306 | A307 | A308 | A323 | U329 | G339 | A348 | A349 | G350 | A351 | A352 | G358 | A361 | A365 | A374 | A375 | G376 | G394 | A397 | A398 | A399 | G400 | U401 | A402 | C403 | U411 | G412 | A417 | A418 | G421 | A422 | C439 | A440 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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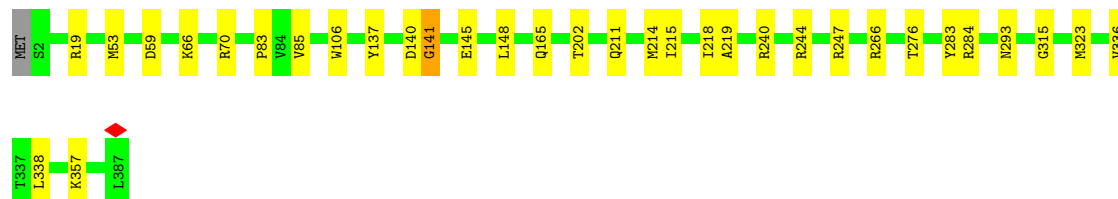
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| U528 | A529 | G530 | G531 | A532 | G535 | U536 | G542 | G543 | G544 | U545 | G546 | G547 | G548 | U549 | A550 | G552 | U555 | A556 | A557 | U558 | A559 | U571 | A572 | A578 | G579 | A585 | A589 | G590 | G591 | G595 | G596 | G597 | A598 | C599 | G604 | A608 | G609 | G610 | A611 | G618 | A619 | U620 | A621 | A622 | U623 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A2397 | A2402 | G2403 | A2404 | U2411 | G2412 | A2413 | G2414 | A2419 | A2424 | G2437 | G2442 | A2443 | U2446 | A2447 | G2450 | G2451 | G2452 | U2453 | G2454 | U2455 | A2458 | A2459 | U2460 | A2461 | A2462 | G2463 | U2464 | G2465 | G2466 | G2467 | A2468 | G2469 | C2470 | U2471 | U2472 | C2473 | G2474 | G2475 | G2476 | U2479 | A2480 | A2484 | A2485 |       |       |       |       |       |       |       |       |       |       |
| A2224 | U2225 | A2228 | G2239 | C2245 | G2249 | U2254 | U     | A     | A     | C     | U     | A     | U2268 | G2272 | G2273 | U2274 | A2281 | U2282 | G2283 | C2284 | G2288 | G2307 | C2308 | A2309 | U2310 | A2313 | U2314 | G2315 | U2334 | U2335 | U2336 | A2357 | A2358 | A2373 | C2374 | G2375 | G2385 | U2388 | C2392 | G2393 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U2112 | A2113 | C2114 | G2115 | A2116 | G2117 | C2118 | G2121 | G2122 | U2129 | G2130 | A2131 | G2134 | U2137 | A2138 | G2139 | U2140 | U2141 | A2142 | A2143 | A2144 | G2155 | A2158 | U2159 | G2160 | G2161 | U2162 | G2169 | U2176 | G2177 | G2185 | U2193 | G2194 | G2201 | U2205 | G2206 | A2207 | A2208 | U2209 | A2213 | A2214 | G2218 | A2219 | A2222 | A2223 |       |       |       |       |       |       |       |       |       |
| G     | U     | U     | G     | U     | U     | C     | U     | U     | C     | G     | G     | A     | C     | U     | C     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     |       |       |       |       |       |       |       |       |       |
| A1850 | A1864 | G1865 | C1866 | A1867 | U1871 | U1880 | U1881 | U1888 | A1893 | G1899 | G1906 | C1907 | A1915 | G1940 | C1943 | G1949 | U1952 | G1953 | G1954 | U1955 | U     | A     | G     | U     | G     | A     | C     | U     | U     | A     | C     | C     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     | U     |       |       |       |       |       |       |       |       |
| G1736 | A1741 | G1747 | A1750 | G1751 | A1760 | C1761 | U1764 | U1765 | G1766 | G1770 | C1771 | U1772 | G1775 | G1778 | C1779 | G1780 | G1786 | A1787 | C1793 | A1797 | C1802 | C1805 | A1806 | G1807 | G1808 | A1813 | A1814 | U1815 | A1816 | U1819 | U1820 | U1716 | U1717 | G1718 | U1721 | U1722 | A1723 | U1724 | A1841 | A1842 | C1846 | C1849 |       |       |       |       |       |       |       |       |       |       |       |
| A1589 | G1590 | A1593 | C1596 | C1597 | A1605 | U1606 | U1607 | A1613 | U1620 | U1629 | G1634 | C1639 | A1642 | A1643 | C1644 | U1645 | C1657 | C1660 | G1661 | G1662 | G1666 | A1667 | G1675 | A1676 | A1683 | U1686 | C1693 | U1716 | U1717 | G1718 | U1721 | U1722 | A1723 | U1724 | C1725 | G1726 | G1727 | G1730 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G1421 | G1422 | G1434 | C1437 | A1446 | G1447 | G1450 | A1477 | G1480 | A1481 | A1482 | G1483 | G1487 | G1488 | C1497 | A1498 | C1502 | C1508 | C1513 | A1530 | U1539 | U1555 | C1556 | A1557 | G1560 | G1561 | C1562 | C1563 | U1566 | U1567 | U1568 | U1569 | A1571 | U1572 | C1574 | A1575 | G1576 | G1577 | C1578 | U1579 | A1580 | C1581 | C1582 | A1583 |       |       |       |       |       |       |       |       |       |       |
| U1265 | G1268 | U1269 | C1272 | A1273 | C1277 | A1278 | C1279 | A1280 | G1281 | G1282 | G1285 | A1286 | A1287 | U1288 | G1289 | G1295 | G1307 | A1308 | U1309 | G1313 | A1330 | U1348 | G1349 | A1350 | U1351 | A1352 | U1353 | G1354 | A1355 | U1356 | G1357 | A1369 | G1383 | A1386 | G1387 | U1388 | G1389 | A1390 | G1391 | G1392 | A1399 | G1400 | A1418 | A1419 | C1420 |       |       |       |       |       |       |       |       |
| U1191 | C1192 | G1193 | A1047 | A1048 | C1049 | G1063 | A1064 | A1065 | G1072 | U1081 | U1082 | G1083 | A1084 | G1087 | A1093 | U1094 | U1095 | U1096 | G1097 | A1098 | A1103 | G1104 | A1105 | C1106 | C1107 | U1108 | U1109 | G1117 | C1118 | A836  | A837  | G838  | A846  | U1008 | A1009 | G1010 | U1015 | C1016 | C1017 | G1018 | G1019 | G1020 | G1021 | G1024 | A1025 | A1026 | A1027 | U1028 | U1033 | U1034 | G1035 | A1036 | U1041 |
| G763  | U764  | C765  | G637  | C638  | G639  | U640  | A649  | G770  | U776  | U777  | C655  | A656  | A660  | U664  | A665  | U673  | G674  | C675  | G676  | G805  | A677  | G678  | U679  | G680  | U681  | G684  | U829  | G831  | G835  | A836  | A837  | G838  | A846  | C849  | U850  | A710  | A711  | G712  | A715  | A716  | U719  | A720  | G728  | A895  | A896  | A746  | C752  | G907  | G908  | C911  |       |       |       |

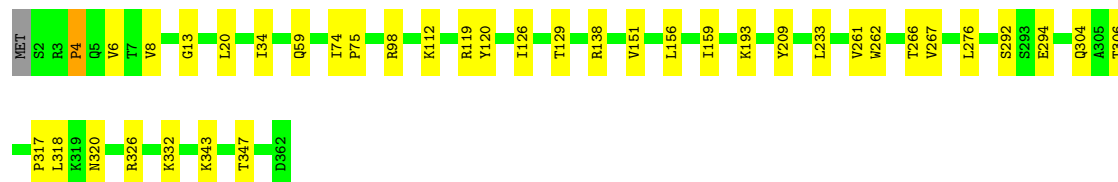
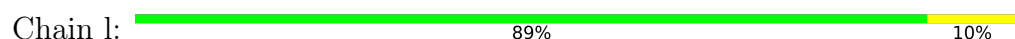




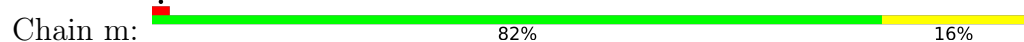
- Molecule 34: 60S ribosomal protein L3



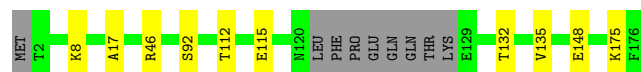
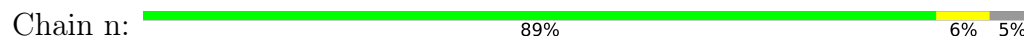
- Molecule 35: 60S ribosomal protein L4-A



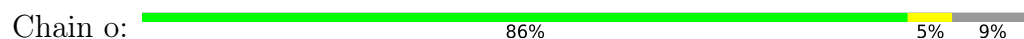
- Molecule 36: 60S ribosomal protein L5

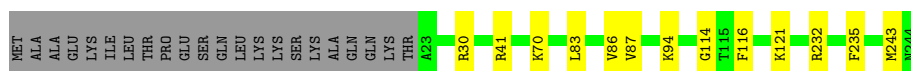


- Molecule 37: 60S ribosomal protein L6-B

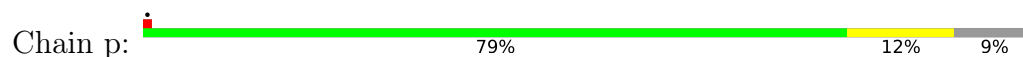


- Molecule 38: 60S ribosomal protein L7-A

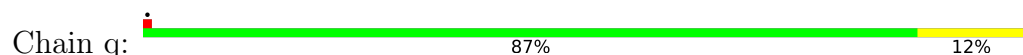




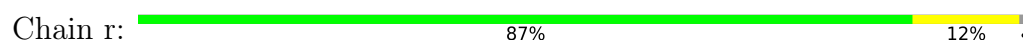
- Molecule 39: 60S ribosomal protein L8-A



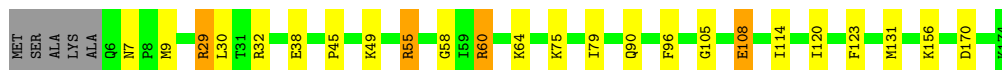
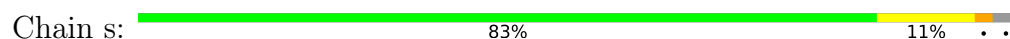
- Molecule 40: 60S ribosomal protein L9-A



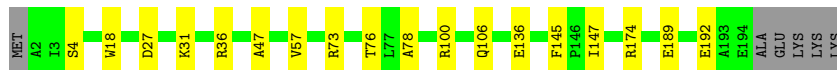
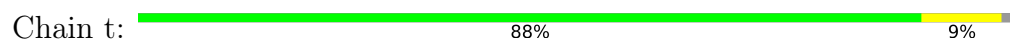
- Molecule 41: 60S ribosomal protein L10



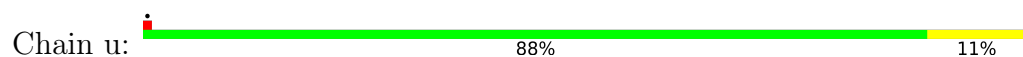
- Molecule 42: 60S ribosomal protein L11-A



- Molecule 43: 60S ribosomal protein L13-A

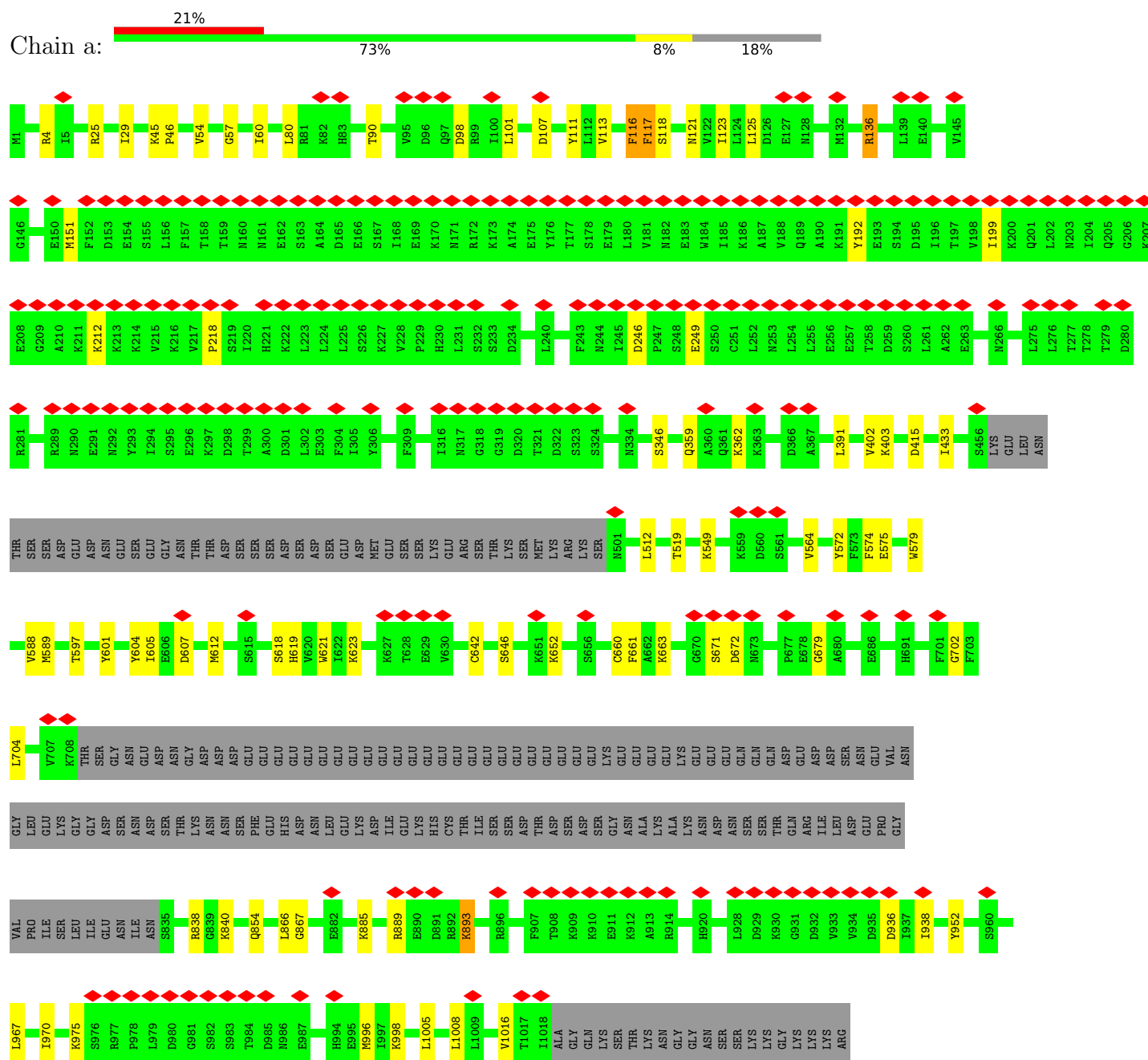


- Molecule 44: 60S ribosomal protein L14-A

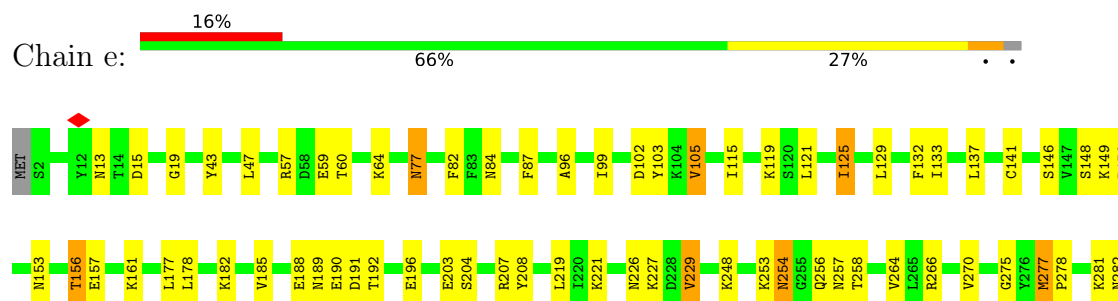




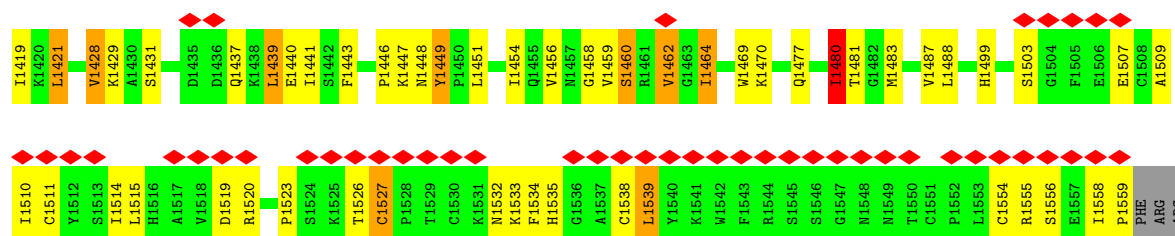
• Molecule 45: RQC2 isoform 1



• Molecule 46: E3 ubiquitin-protein ligase listerin

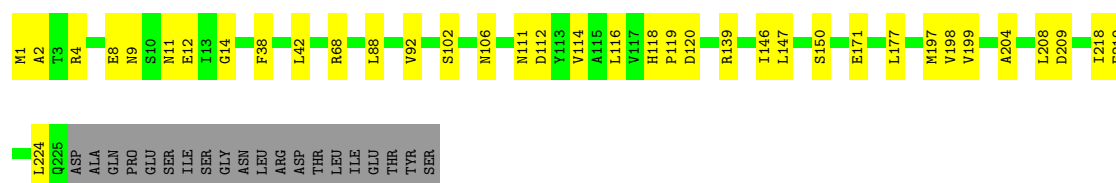






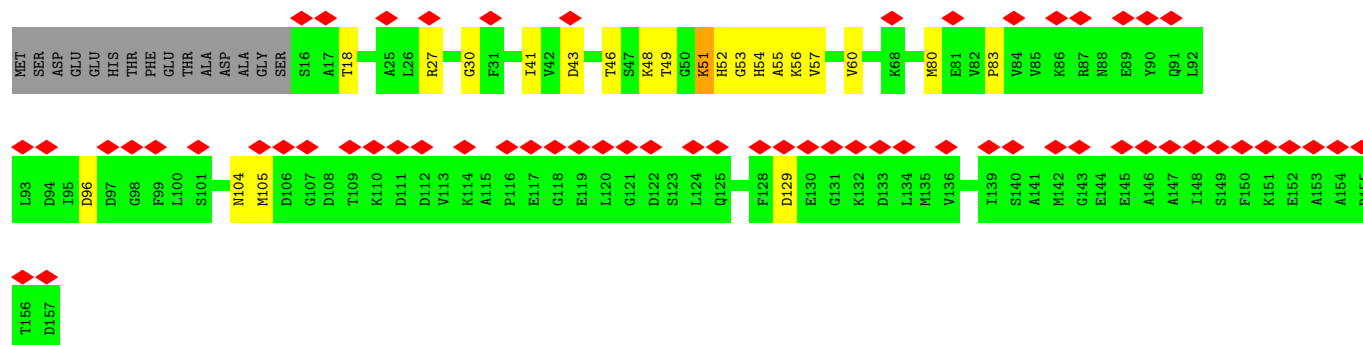
• Molecule 47: Eukaryotic translation initiation factor 6

Chain g: 77% 15% 8%



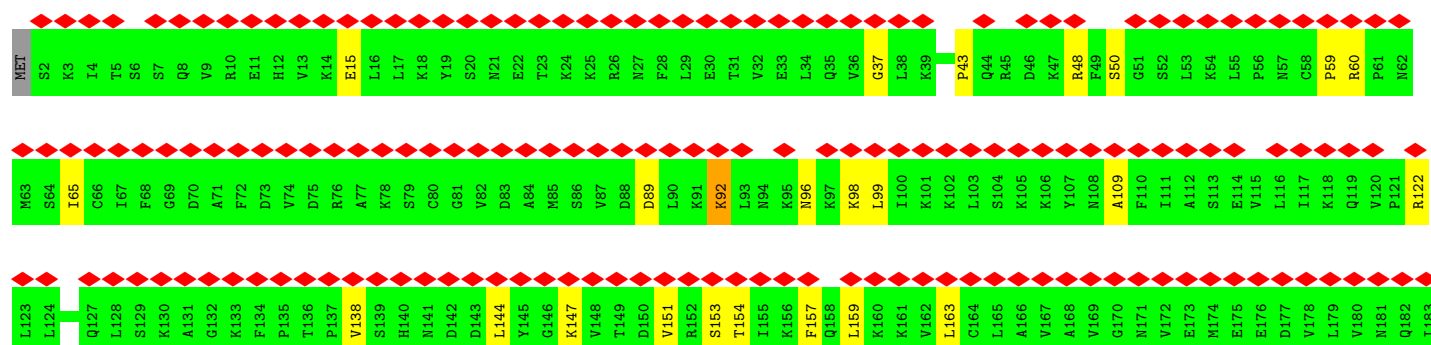
• Molecule 48: Eukaryotic translation initiation factor 5A-1

Chain v: 39% 76% 13% 10%



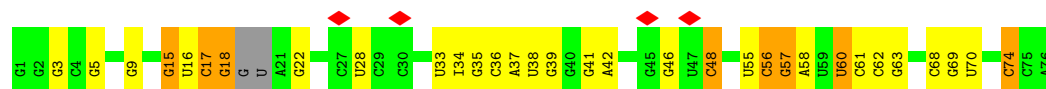
• Molecule 49: 60S ribosomal protein L1-A

Chain w: 88% 86% 13%

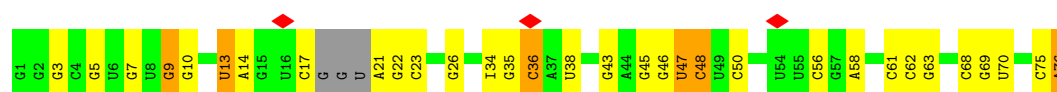




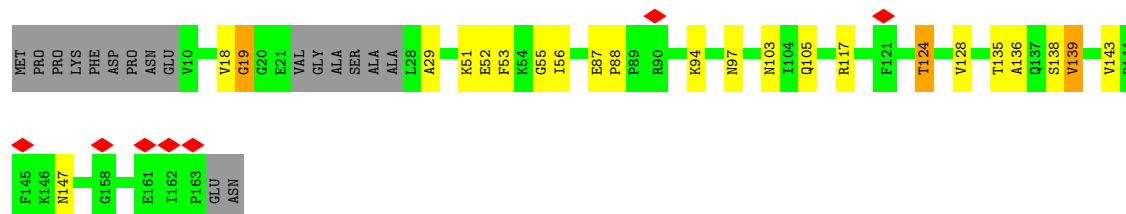
• Molecule 50: Ala tRNA



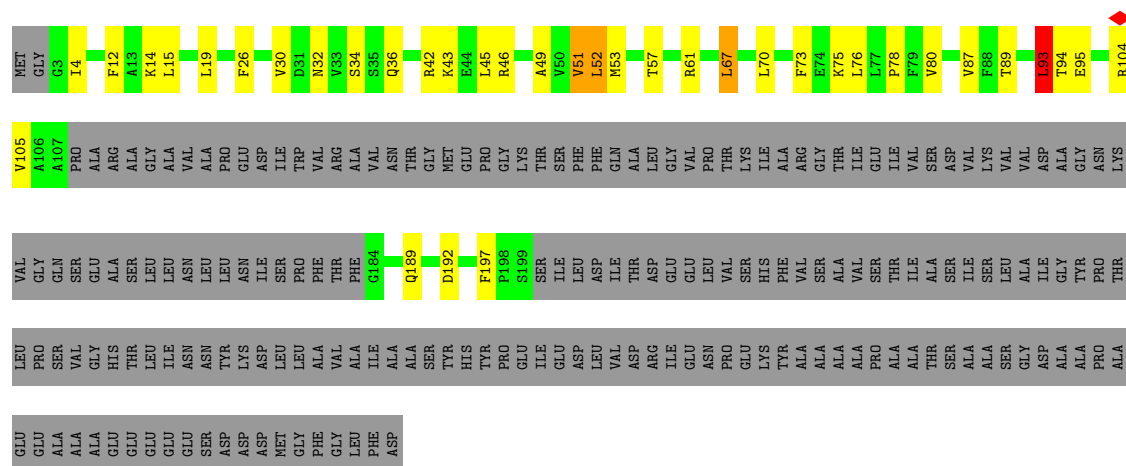
• Molecule 50: Ala tRNA



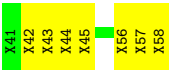
• Molecule 51: 60S ribosomal protein L12-B



• Molecule 52: 60S acidic ribosomal protein P0



• Molecule 53: CAT-tailed nascent chain



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 79267                                   | 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 ( $e^-/\text{\AA}^2$ ) | 46                                      | Depositor |
| Minimum defocus (nm)                 | 400                                     | Depositor |
| Maximum defocus (nm)                 | 4000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.680                                   | Depositor |
| Minimum map value                    | -0.672                                  | Depositor |
| Average map value                    | 0.021                                   | Depositor |
| Map value standard deviation         | 0.131                                   | Depositor |
| Recommended contour level            | 0.4                                     | Depositor |
| Map size ( $\text{\AA}$ )            | 476.55002, 476.55002, 476.55002         | wwPDB     |
| Map dimensions                       | 450, 450, 450                           | 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: SPD, ZN, 5CT, MG

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.31         | 0/1757      | 0.54        | 0/2354          |
| 2   | B     | 0.32         | 0/1585      | 0.54        | 0/2128          |
| 3   | C     | 0.30         | 0/1439      | 0.61        | 0/1938          |
| 4   | D     | 0.28         | 0/1465      | 0.57        | 0/1965          |
| 5   | E     | 0.29         | 0/1275      | 0.56        | 0/1702          |
| 6   | F     | 0.31         | 0/1473      | 0.56        | 0/1980          |
| 7   | G     | 0.27         | 0/1296      | 0.56        | 0/1739          |
| 8   | H     | 0.37         | 0/812       | 0.77        | 2/1099 (0.2%)   |
| 9   | I     | 0.27         | 0/1018      | 0.50        | 0/1369          |
| 10  | J     | 0.27         | 0/530       | 0.52        | 0/703           |
| 11  | K     | 0.31         | 0/979       | 0.57        | 0/1321          |
| 12  | L     | 0.27         | 0/995       | 0.53        | 0/1329          |
| 13  | M     | 0.27         | 0/1106      | 0.56        | 0/1485          |
| 14  | N     | 0.32         | 0/1200      | 0.56        | 1/1607 (0.1%)   |
| 15  | O     | 0.25         | 0/473       | 0.62        | 0/629           |
| 16  | P     | 0.26         | 0/745       | 0.60        | 0/1001          |
| 17  | Q     | 0.31         | 0/890       | 0.68        | 2/1196 (0.2%)   |
| 18  | R     | 0.26         | 0/1034      | 0.47        | 0/1385          |
| 19  | S     | 0.30         | 0/868       | 0.47        | 0/1168          |
| 20  | T     | 0.29         | 0/890       | 0.58        | 2/1189 (0.2%)   |
| 21  | U     | 0.27         | 0/978       | 0.53        | 0/1301          |
| 22  | V     | 0.28         | 0/772       | 0.57        | 0/1026          |
| 23  | W     | 0.32         | 0/660       | 0.60        | 0/875           |
| 24  | X     | 0.28         | 0/618       | 0.65        | 1/826 (0.1%)    |
| 25  | Y     | 0.29         | 0/443       | 0.46        | 0/588           |
| 26  | Z     | 0.28         | 0/416       | 0.60        | 0/553           |
| 27  | b     | 0.28         | 0/836       | 0.53        | 0/1104          |
| 28  | c     | 0.27         | 0/701       | 0.56        | 0/934           |
| 29  | d     | 0.22         | 0/208       | 0.81        | 2/267 (0.7%)    |
| 30  | f     | 0.30         | 0/76989     | 0.39        | 6/120031 (0.0%) |
| 31  | h     | 0.26         | 0/2883      | 0.32        | 0/4491          |
| 32  | i     | 0.30         | 0/3746      | 0.36        | 0/5832          |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 33  | j     | 0.31         | 0/1908          | 0.53        | 0/2564            |
| 34  | k     | 0.29         | 0/3146          | 0.53        | 0/4228            |
| 35  | l     | 0.29         | 0/2800          | 0.57        | 4/3790 (0.1%)     |
| 36  | m     | 0.27         | 0/2400          | 0.57        | 0/3239            |
| 37  | n     | 0.28         | 0/1329          | 0.60        | 0/1794            |
| 38  | o     | 0.31         | 0/1821          | 0.58        | 0/2451            |
| 39  | p     | 0.27         | 0/1836          | 0.58        | 1/2481 (0.0%)     |
| 40  | q     | 0.30         | 0/1529          | 0.64        | 2/2060 (0.1%)     |
| 41  | r     | 0.25         | 0/1801          | 0.49        | 0/2416            |
| 42  | s     | 0.33         | 0/1367          | 0.73        | 4/1834 (0.2%)     |
| 43  | t     | 0.29         | 0/1568          | 0.62        | 1/2106 (0.0%)     |
| 44  | u     | 0.30         | 0/1068          | 0.53        | 0/1438            |
| 45  | a     | 0.26         | 0/6689          | 0.56        | 2/9023 (0.0%)     |
| 46  | e     | 0.60         | 0/11705         | 0.96        | 65/15895 (0.4%)   |
| 47  | g     | 0.24         | 0/1672          | 0.59        | 1/2281 (0.0%)     |
| 48  | v     | 0.25         | 0/1084          | 0.61        | 1/1456 (0.1%)     |
| 49  | w     | 0.29         | 0/1736          | 0.62        | 1/2332 (0.0%)     |
| 50  | x     | 0.26         | 0/1760          | 0.41        | 0/2738            |
| 50  | y     | 0.31         | 1/1734 (0.1%)   | 0.44        | 0/2697            |
| 51  | z     | 0.66         | 0/726           | 1.24        | 13/1006 (1.3%)    |
| 52  | 0     | 0.49         | 0/976           | 0.94        | 3/1313 (0.2%)     |
| All | All   | 0.33         | 1/161735 (0.0%) | 0.52        | 114/236257 (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 |
|-----|-------|---------------------|---------------------|
| 15  | O     | 0                   | 1                   |
| 21  | U     | 0                   | 1                   |
| 34  | k     | 0                   | 1                   |
| 35  | l     | 0                   | 2                   |
| 39  | p     | 0                   | 3                   |
| 40  | q     | 0                   | 1                   |
| 44  | u     | 0                   | 1                   |
| 46  | e     | 0                   | 1                   |
| 47  | g     | 0                   | 1                   |
| All | All   | 0                   | 12                  |

All (1) bond length outliers are listed below:



| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 50  | y     | 34  | I    | O3'-P | 7.21 | 1.63        | 1.56     |

All (114) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | e     | 884  | ILE  | N-CA-C  | -9.16 | 101.28      | 110.62   |
| 46  | e     | 19   | GLY  | N-CA-C  | 9.15  | 122.07      | 111.36   |
| 46  | e     | 1182 | LYS  | N-CA-C  | 8.97  | 121.06      | 111.28   |
| 46  | e     | 1364 | GLY  | N-CA-C  | 8.39  | 122.64      | 112.49   |
| 46  | e     | 868  | LYS  | N-CA-C  | 8.32  | 120.35      | 111.28   |
| 46  | e     | 1298 | GLY  | N-CA-C  | -8.30 | 103.76      | 115.30   |
| 46  | e     | 1252 | VAL  | N-CA-C  | -8.26 | 102.42      | 109.19   |
| 46  | e     | 1460 | SER  | N-CA-C  | 8.08  | 119.86      | 111.14   |
| 8   | H     | 51   | GLY  | CA-C-N  | 7.88  | 136.59      | 121.54   |
| 8   | H     | 51   | GLY  | C-N-CA  | 7.88  | 136.59      | 121.54   |
| 45  | a     | 116  | PHE  | N-CA-C  | -7.76 | 103.87      | 112.72   |
| 46  | e     | 901  | SER  | N-CA-C  | 7.74  | 119.72      | 111.28   |
| 48  | v     | 53   | GLY  | N-CA-C  | 7.67  | 124.24      | 112.51   |
| 46  | e     | 893  | MET  | N-CA-C  | -7.51 | 103.09      | 111.28   |
| 51  | z     | 87   | GLU  | CA-C-N  | -7.42 | 112.73      | 120.38   |
| 51  | z     | 87   | GLU  | C-N-CA  | -7.42 | 112.73      | 120.38   |
| 46  | e     | 573  | PHE  | N-CA-C  | -7.36 | 103.33      | 111.36   |
| 46  | e     | 258  | THR  | N-CA-C  | -7.33 | 104.34      | 113.28   |
| 51  | z     | 138  | SER  | N-CA-C  | -7.28 | 103.28      | 111.14   |
| 46  | e     | 57   | ARG  | N-CA-C  | 7.10  | 119.01      | 111.28   |
| 45  | a     | 117  | PHE  | N-CA-CB | -7.04 | 100.29      | 110.36   |
| 46  | e     | 1447 | LYS  | N-CA-C  | -7.03 | 101.26      | 110.53   |
| 46  | e     | 793  | ASN  | N-CA-C  | -7.02 | 103.71      | 111.36   |
| 46  | e     | 1459 | VAL  | N-CA-C  | 6.78  | 116.90      | 110.53   |
| 51  | z     | 94   | LYS  | N-CA-C  | -6.76 | 103.99      | 111.36   |
| 35  | l     | 4    | PRO  | CA-C-N  | 6.74  | 134.41      | 121.54   |
| 35  | l     | 4    | PRO  | C-N-CA  | 6.74  | 134.41      | 121.54   |
| 46  | e     | 437  | LYS  | N-CA-C  | -6.55 | 96.85       | 110.80   |
| 46  | e     | 951  | ASP  | N-CA-C  | -6.47 | 104.23      | 111.28   |
| 14  | N     | 66   | ALA  | N-CA-C  | -6.41 | 106.42      | 114.56   |
| 46  | e     | 185  | VAL  | N-CA-C  | 6.41  | 116.56      | 110.53   |
| 46  | e     | 1462 | VAL  | N-CA-C  | 6.39  | 117.50      | 108.36   |
| 46  | e     | 667  | GLN  | N-CA-C  | -6.34 | 105.12      | 112.92   |
| 46  | e     | 691  | ASP  | N-CA-C  | -6.32 | 105.43      | 113.01   |
| 46  | e     | 148  | SER  | N-CA-C  | 6.30  | 118.23      | 111.36   |
| 46  | e     | 798  | LEU  | N-CA-C  | 6.28  | 117.79      | 111.07   |
| 46  | e     | 132  | PHE  | N-CA-C  | 6.27  | 118.19      | 111.36   |
| 46  | e     | 1070 | ILE  | N-CA-C  | -6.25 | 103.28      | 112.04   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 40  | q     | 138  | THR  | CA-C-N    | 6.23  | 133.44      | 121.54   |
| 40  | q     | 138  | THR  | C-N-CA    | 6.23  | 133.44      | 121.54   |
| 29  | d     | 4    | MET  | CA-C-N    | 6.20  | 133.38      | 121.54   |
| 29  | d     | 4    | MET  | C-N-CA    | 6.20  | 133.38      | 121.54   |
| 46  | e     | 699  | GLU  | N-CA-C    | -6.17 | 105.69      | 113.72   |
| 46  | e     | 666  | GLY  | N-CA-C    | -6.16 | 106.82      | 115.32   |
| 46  | e     | 553  | GLN  | N-CA-C    | -6.09 | 100.08      | 109.52   |
| 46  | e     | 892  | ALA  | N-CA-C    | -6.06 | 97.89       | 110.80   |
| 46  | e     | 436  | GLY  | N-CA-C    | 5.97  | 118.98      | 112.29   |
| 46  | e     | 1317 | GLU  | N-CA-C    | 5.96  | 117.78      | 111.28   |
| 46  | e     | 43   | TYR  | N-CA-C    | 5.93  | 117.75      | 111.28   |
| 46  | e     | 1069 | GLY  | N-CA-C    | 5.92  | 119.99      | 110.87   |
| 46  | e     | 1483 | MET  | N-CA-C    | -5.92 | 100.34      | 109.52   |
| 46  | e     | 885  | GLN  | N-CA-C    | -5.90 | 99.96       | 109.40   |
| 46  | e     | 736  | VAL  | N-CA-C    | 5.88  | 116.66      | 110.72   |
| 46  | e     | 946  | ASP  | N-CA-C    | 5.84  | 117.82      | 108.41   |
| 51  | z     | 124  | THR  | N-CA-C    | 5.83  | 117.64      | 111.28   |
| 46  | e     | 204  | SER  | N-CA-C    | -5.83 | 104.92      | 111.28   |
| 46  | e     | 479  | PHE  | N-CA-C    | -5.71 | 105.06      | 111.28   |
| 30  | f     | 2541 | U    | P-O3'-C3' | 5.69  | 128.74      | 120.20   |
| 46  | e     | 1124 | GLY  | N-CA-C    | 5.68  | 119.54      | 112.73   |
| 46  | e     | 650  | LEU  | N-CA-C    | 5.67  | 118.50      | 110.50   |
| 46  | e     | 1449 | TYR  | CA-C-N    | -5.66 | 112.77      | 119.05   |
| 46  | e     | 1449 | TYR  | C-N-CA    | -5.66 | 112.77      | 119.05   |
| 47  | g     | 171  | GLU  | N-CA-CB   | 5.66  | 119.05      | 110.28   |
| 42  | s     | 114  | ILE  | CA-C-N    | 5.64  | 132.31      | 121.54   |
| 42  | s     | 114  | ILE  | C-N-CA    | 5.64  | 132.31      | 121.54   |
| 46  | e     | 196  | GLU  | N-CA-C    | 5.61  | 117.40      | 111.28   |
| 46  | e     | 435  | CYS  | N-CA-C    | -5.59 | 105.19      | 111.28   |
| 42  | s     | 7    | ASN  | N-CA-C    | 5.55  | 117.57      | 109.30   |
| 46  | e     | 275  | GLY  | N-CA-C    | -5.55 | 107.67      | 115.32   |
| 46  | e     | 1480 | ILE  | N-CA-C    | 5.49  | 116.27      | 110.72   |
| 46  | e     | 1181 | ASP  | N-CA-C    | 5.48  | 117.33      | 111.36   |
| 46  | e     | 992  | LEU  | N-CA-C    | -5.46 | 105.32      | 111.28   |
| 43  | t     | 136  | GLU  | CA-CB-CG  | 5.46  | 125.02      | 114.10   |
| 46  | e     | 1163 | GLU  | N-CA-C    | 5.46  | 118.15      | 110.23   |
| 20  | T     | 94   | LEU  | CA-C-N    | -5.44 | 112.76      | 121.35   |
| 20  | T     | 94   | LEU  | C-N-CA    | -5.44 | 112.76      | 121.35   |
| 46  | e     | 535  | ILE  | N-CA-C    | 5.43  | 116.16      | 110.62   |
| 46  | e     | 1252 | VAL  | CA-C-N    | -5.41 | 113.76      | 120.79   |
| 46  | e     | 1252 | VAL  | C-N-CA    | -5.41 | 113.76      | 120.79   |
| 46  | e     | 326  | GLY  | N-CA-C    | -5.41 | 104.03      | 113.76   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | s     | 108  | GLU  | CA-CB-CG    | 5.39  | 124.89      | 114.10   |
| 30  | f     | 2502 | A    | P-O3'-C3'   | 5.37  | 128.25      | 120.20   |
| 51  | z     | 19   | GLY  | N-CA-C      | 5.34  | 119.37      | 112.54   |
| 30  | f     | 282  | G    | C2'-C3'-O3' | 5.34  | 121.71      | 113.70   |
| 51  | z     | 29   | ALA  | N-CA-C      | -5.33 | 105.58      | 113.16   |
| 30  | f     | 1307 | G    | P-O3'-C3'   | 5.33  | 128.19      | 120.20   |
| 46  | e     | 373  | TYR  | N-CA-C      | 5.32  | 116.77      | 111.07   |
| 30  | f     | 1815 | U    | P-O3'-C3'   | 5.31  | 128.17      | 120.20   |
| 52  | 0     | 94   | THR  | N-CA-C      | 5.31  | 117.07      | 111.28   |
| 17  | Q     | 83   | GLU  | CA-C-N      | 5.28  | 131.63      | 121.54   |
| 17  | Q     | 83   | GLU  | C-N-CA      | 5.28  | 131.63      | 121.54   |
| 46  | e     | 1283 | SER  | N-CA-C      | -5.24 | 103.11      | 110.50   |
| 39  | p     | 79   | GLN  | CA-CB-CG    | 5.20  | 124.49      | 114.10   |
| 51  | z     | 117  | ARG  | N-CA-C      | -5.20 | 105.61      | 111.28   |
| 51  | z     | 18   | VAL  | N-CA-C      | -5.19 | 102.89      | 109.58   |
| 46  | e     | 1519 | ASP  | N-CA-C      | 5.16  | 119.67      | 113.17   |
| 35  | l     | 317  | PRO  | CA-C-N      | 5.14  | 131.36      | 121.54   |
| 35  | l     | 317  | PRO  | C-N-CA      | 5.14  | 131.36      | 121.54   |
| 51  | z     | 147  | ASN  | CA-C-N      | -5.14 | 114.28      | 119.83   |
| 51  | z     | 147  | ASN  | C-N-CA      | -5.14 | 114.28      | 119.83   |
| 46  | e     | 133  | ILE  | CA-C-N      | -5.14 | 113.34      | 119.05   |
| 46  | e     | 133  | ILE  | C-N-CA      | -5.14 | 113.34      | 119.05   |
| 51  | z     | 139  | VAL  | N-CA-C      | 5.14  | 115.36      | 110.53   |
| 52  | 0     | 104  | ARG  | N-CA-C      | 5.13  | 118.51      | 111.54   |
| 51  | z     | 103  | ASN  | N-CA-C      | 5.12  | 116.97      | 109.24   |
| 46  | e     | 965  | ASN  | N-CA-C      | -5.10 | 105.72      | 111.28   |
| 52  | 0     | 89   | THR  | N-CA-C      | 5.10  | 117.73      | 109.06   |
| 46  | e     | 1487 | VAL  | N-CA-C      | -5.08 | 105.44      | 110.62   |
| 46  | e     | 257  | ASN  | N-CA-C      | 5.05  | 117.21      | 109.07   |
| 24  | X     | 67   | GLN  | N-CA-CB     | 5.05  | 118.64      | 110.40   |
| 46  | e     | 256  | GLN  | N-CA-C      | 5.05  | 116.78      | 111.28   |
| 49  | w     | 15   | GLU  | N-CA-CB     | 5.04  | 118.09      | 110.28   |
| 46  | e     | 779  | ALA  | N-CA-C      | 5.01  | 115.92      | 108.60   |
| 30  | f     | 2537 | U    | P-O3'-C3'   | 5.01  | 127.71      | 120.20   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 15  | O     | 20  | GLY  | Peptide |
| 21  | U     | 83  | LYS  | Peptide |
| 46  | e     | 392 | GLY  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 47  | g     | 8   | GLU  | Peptide |
| 34  | k     | 141 | GLY  | Peptide |
| 35  | l     | 13  | GLY  | Peptide |
| 35  | l     | 318 | LEU  | Peptide |
| 39  | p     | 158 | ASP  | Peptide |
| 39  | p     | 30  | THR  | Peptide |
| 39  | p     | 76  | ALA  | Peptide |
| 40  | q     | 21  | LYS  | Peptide |
| 44  | u     | 12  | TRP  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1720  | 0        | 1779     | 18      | 0            |
| 2   | B     | 1555  | 0        | 1659     | 18      | 0            |
| 3   | C     | 1416  | 0        | 1433     | 14      | 0            |
| 4   | D     | 1441  | 0        | 1543     | 15      | 0            |
| 5   | E     | 1258  | 0        | 1342     | 13      | 0            |
| 6   | F     | 1437  | 0        | 1475     | 19      | 0            |
| 7   | G     | 1272  | 0        | 1312     | 14      | 0            |
| 8   | H     | 796   | 0        | 812      | 9       | 0            |
| 9   | I     | 1003  | 0        | 1048     | 10      | 0            |
| 10  | J     | 518   | 0        | 542      | 6       | 0            |
| 11  | K     | 964   | 0        | 1025     | 1       | 0            |
| 12  | L     | 984   | 0        | 1075     | 7       | 0            |
| 13  | M     | 1080  | 0        | 1122     | 7       | 0            |
| 14  | N     | 1169  | 0        | 1211     | 14      | 0            |
| 15  | O     | 462   | 0        | 491      | 8       | 0            |
| 16  | P     | 737   | 0        | 792      | 4       | 0            |
| 17  | Q     | 876   | 0        | 912      | 10      | 0            |
| 18  | R     | 1013  | 0        | 1077     | 8       | 0            |
| 19  | S     | 850   | 0        | 880      | 5       | 0            |
| 20  | T     | 880   | 0        | 942      | 8       | 0            |
| 21  | U     | 969   | 0        | 1078     | 5       | 0            |
| 22  | V     | 766   | 0        | 844      | 7       | 0            |
| 23  | W     | 645   | 0        | 645      | 12      | 0            |
| 24  | X     | 612   | 0        | 682      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25  | Y     | 436   | 0        | 475      | 2       | 0            |
| 26  | Z     | 410   | 0        | 442      | 5       | 0            |
| 27  | b     | 824   | 0        | 888      | 13      | 0            |
| 28  | c     | 694   | 0        | 734      | 8       | 0            |
| 29  | d     | 207   | 0        | 250      | 3       | 0            |
| 30  | f     | 68782 | 0        | 34563    | 334     | 0            |
| 31  | h     | 2579  | 0        | 1304     | 10      | 0            |
| 32  | i     | 3353  | 0        | 1695     | 14      | 0            |
| 33  | j     | 1874  | 0        | 1943     | 25      | 0            |
| 34  | k     | 3075  | 0        | 3142     | 21      | 0            |
| 35  | l     | 2748  | 0        | 2859     | 25      | 0            |
| 36  | m     | 2351  | 0        | 2294     | 32      | 0            |
| 37  | n     | 1307  | 0        | 1377     | 7       | 0            |
| 38  | o     | 1784  | 0        | 1862     | 9       | 0            |
| 39  | p     | 1804  | 0        | 1877     | 17      | 0            |
| 40  | q     | 1508  | 0        | 1572     | 16      | 0            |
| 41  | r     | 1764  | 0        | 1804     | 18      | 0            |
| 42  | s     | 1346  | 0        | 1370     | 17      | 0            |
| 43  | t     | 1543  | 0        | 1608     | 14      | 0            |
| 44  | u     | 1053  | 0        | 1149     | 11      | 0            |
| 45  | a     | 6579  | 0        | 6482     | 62      | 0            |
| 46  | e     | 11506 | 0        | 10754    | 633     | 0            |
| 47  | g     | 1651  | 0        | 1613     | 20      | 0            |
| 48  | v     | 1085  | 0        | 1087     | 16      | 0            |
| 49  | w     | 1709  | 0        | 1799     | 21      | 0            |
| 50  | x     | 1579  | 0        | 798      | 14      | 0            |
| 50  | y     | 1556  | 0        | 788      | 16      | 0            |
| 51  | z     | 728   | 0        | 337      | 16      | 0            |
| 52  | 0     | 961   | 0        | 979      | 46      | 0            |
| 53  | 1     | 90    | 0        | 23       | 7       | 0            |
| 54  | A     | 1     | 0        | 0        | 0       | 0            |
| 54  | C     | 1     | 0        | 0        | 0       | 0            |
| 54  | E     | 1     | 0        | 0        | 0       | 0            |
| 54  | I     | 1     | 0        | 0        | 0       | 0            |
| 54  | R     | 1     | 0        | 0        | 0       | 0            |
| 54  | T     | 1     | 0        | 0        | 0       | 0            |
| 54  | f     | 3     | 0        | 0        | 0       | 0            |
| 54  | h     | 1     | 0        | 0        | 0       | 0            |
| 54  | j     | 2     | 0        | 0        | 0       | 0            |
| 54  | k     | 1     | 0        | 0        | 0       | 0            |
| 55  | T     | 1     | 0        | 0        | 0       | 0            |
| 55  | W     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 55  | Z     | 1      | 0        | 0        | 0       | 0            |
| 55  | b     | 1      | 0        | 0        | 0       | 0            |
| 55  | c     | 1      | 0        | 0        | 0       | 0            |
| 55  | e     | 2      | 0        | 0        | 0       | 0            |
| 56  | f     | 10     | 0        | 19       | 1       | 0            |
| All | All   | 151339 | 0        | 113608   | 1439    | 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 6.

All (1439) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:e:368:HIS:CE1  | 46:e:370:PHE:HB2   | 1.29                     | 1.62              |
| 46:e:989:GLU:HG2  | 46:e:1034:TRP:CA   | 1.21                     | 1.61              |
| 46:e:838:ILE:CD1  | 46:e:864:HIS:HB2   | 1.29                     | 1.60              |
| 46:e:545:ILE:CB   | 46:e:579:ALA:HB1   | 1.32                     | 1.58              |
| 46:e:972:GLU:HA   | 46:e:975:LYS:CE    | 1.18                     | 1.57              |
| 46:e:989:GLU:HG2  | 46:e:1034:TRP:CB   | 1.27                     | 1.56              |
| 46:e:841:VAL:HG11 | 46:e:862:PHE:CZ    | 1.38                     | 1.56              |
| 46:e:838:ILE:CD1  | 46:e:864:HIS:CB    | 1.83                     | 1.55              |
| 46:e:989:GLU:HG3  | 46:e:1034:TRP:CD1  | 1.43                     | 1.54              |
| 46:e:839:THR:HA   | 46:e:865:THR:CG2   | 1.31                     | 1.54              |
| 46:e:253:LYS:C    | 46:e:254:ASN:HD22  | 1.13                     | 1.51              |
| 46:e:839:THR:CB   | 46:e:865:THR:HG23  | 1.37                     | 1.50              |
| 46:e:1527:CYS:HB2 | 46:e:1558:ILE:CD1  | 1.42                     | 1.48              |
| 46:e:839:THR:CA   | 46:e:865:THR:CG2   | 1.87                     | 1.48              |
| 46:e:989:GLU:CG   | 46:e:1034:TRP:CB   | 1.92                     | 1.47              |
| 30:f:1259:A:C8    | 52:0:53:MET:HB2    | 1.51                     | 1.46              |
| 46:e:839:THR:CB   | 46:e:865:THR:CG2   | 1.91                     | 1.45              |
| 46:e:989:GLU:HB3  | 46:e:1034:TRP:CG   | 1.48                     | 1.45              |
| 46:e:1527:CYS:HB2 | 46:e:1558:ILE:CG1  | 1.48                     | 1.42              |
| 46:e:839:THR:CA   | 46:e:865:THR:HG23  | 0.94                     | 1.41              |
| 30:f:1258:U:H4'   | 52:0:42:ARG:NH1    | 1.26                     | 1.40              |
| 46:e:989:GLU:CB   | 46:e:1034:TRP:HB3  | 1.51                     | 1.40              |
| 46:e:1066:ARG:NH2 | 46:e:1111:GLN:HB2  | 1.32                     | 1.38              |
| 46:e:989:GLU:CB   | 46:e:1034:TRP:CG   | 2.04                     | 1.38              |
| 46:e:1534:PHE:CB  | 46:e:1539:LEU:HD13 | 1.52                     | 1.38              |
| 46:e:1283:SER:OG  | 46:e:1286:MET:CG   | 1.70                     | 1.37              |
| 46:e:989:GLU:CG   | 46:e:1034:TRP:CG   | 2.05                     | 1.36              |
| 46:e:989:GLU:CG   | 46:e:1034:TRP:CD1  | 2.08                     | 1.36              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:f:1258:U:C4'   | 52:0:42:ARG:HH12   | 1.36                     | 1.35              |
| 46:e:324:GLU:HB3  | 46:e:327:THR:OG1   | 1.28                     | 1.33              |
| 46:e:1534:PHE:HB3 | 46:e:1539:LEU:CD1  | 1.55                     | 1.33              |
| 46:e:972:GLU:CA   | 46:e:975:LYS:HE2   | 1.61                     | 1.30              |
| 46:e:972:GLU:CA   | 46:e:975:LYS:CE    | 2.10                     | 1.30              |
| 46:e:1066:ARG:NE  | 46:e:1111:GLN:OE1  | 1.62                     | 1.30              |
| 46:e:884:ILE:CD1  | 46:e:935:SER:HB3   | 1.61                     | 1.29              |
| 46:e:545:ILE:CB   | 46:e:579:ALA:CB    | 2.09                     | 1.29              |
| 46:e:750:ALA:O    | 46:e:754:ILE:HG22  | 1.19                     | 1.28              |
| 46:e:838:ILE:HD12 | 46:e:864:HIS:CB    | 1.46                     | 1.28              |
| 46:e:841:VAL:CG1  | 46:e:862:PHE:CE2   | 2.17                     | 1.28              |
| 46:e:990:VAL:N    | 46:e:1039:LEU:CD2  | 1.95                     | 1.28              |
| 46:e:1066:ARG:NH2 | 46:e:1111:GLN:CB   | 1.96                     | 1.28              |
| 46:e:1429:LYS:HE2 | 46:e:1440:GLU:OE2  | 1.24                     | 1.27              |
| 46:e:838:ILE:HG21 | 46:e:863:GLY:O     | 1.18                     | 1.26              |
| 46:e:989:GLU:CB   | 46:e:1034:TRP:CB   | 2.08                     | 1.26              |
| 46:e:867:PHE:O    | 46:e:871:LYS:HA    | 1.16                     | 1.26              |
| 46:e:751:VAL:HA   | 46:e:754:ILE:CG2   | 1.65                     | 1.25              |
| 46:e:754:ILE:CD1  | 46:e:829:ARG:HH11  | 1.50                     | 1.24              |
| 46:e:841:VAL:CG1  | 46:e:862:PHE:CZ    | 2.19                     | 1.24              |
| 46:e:1290:PHE:O   | 46:e:1294:LEU:HD13 | 1.37                     | 1.23              |
| 46:e:253:LYS:C    | 46:e:254:ASN:ND2   | 1.95                     | 1.23              |
| 46:e:750:ALA:CB   | 46:e:764:PHE:CZ    | 2.21                     | 1.23              |
| 46:e:1534:PHE:CG  | 46:e:1539:LEU:HD11 | 1.73                     | 1.22              |
| 46:e:1066:ARG:NE  | 46:e:1111:GLN:CD   | 1.97                     | 1.21              |
| 46:e:884:ILE:CD1  | 46:e:935:SER:CB    | 2.19                     | 1.21              |
| 46:e:1534:PHE:CB  | 46:e:1539:LEU:CD1  | 2.13                     | 1.20              |
| 46:e:839:THR:HB   | 46:e:865:THR:CG2   | 1.55                     | 1.20              |
| 46:e:989:GLU:CG   | 46:e:1034:TRP:HA   | 1.72                     | 1.19              |
| 46:e:749:HIS:O    | 46:e:753:LEU:HD23  | 1.41                     | 1.19              |
| 46:e:368:HIS:CE1  | 46:e:370:PHE:CB    | 2.25                     | 1.19              |
| 46:e:972:GLU:HA   | 46:e:975:LYS:HE3   | 1.21                     | 1.19              |
| 46:e:709:PHE:CE1  | 46:e:753:LEU:HD21  | 1.79                     | 1.18              |
| 46:e:750:ALA:HA   | 46:e:764:PHE:CZ    | 1.78                     | 1.18              |
| 30:f:1257:C:H5'   | 51:z:124:THR:CB    | 1.74                     | 1.18              |
| 46:e:754:ILE:CG1  | 46:e:829:ARG:NH1   | 2.07                     | 1.18              |
| 46:e:1527:CYS:CB  | 46:e:1558:ILE:HG12 | 1.72                     | 1.18              |
| 46:e:841:VAL:HG12 | 46:e:862:PHE:CE2   | 1.78                     | 1.18              |
| 46:e:754:ILE:HG12 | 46:e:829:ARG:NH1   | 1.58                     | 1.17              |
| 46:e:754:ILE:HD11 | 46:e:829:ARG:HH11  | 1.02                     | 1.17              |
| 46:e:324:GLU:CB   | 46:e:327:THR:OG1   | 1.77                     | 1.17              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:e:1066:ARG:CZ  | 46:e:1111:GLN:OE1  | 1.93                     | 1.17              |
| 46:e:1527:CYS:HB2 | 46:e:1558:ILE:HD11 | 1.25                     | 1.17              |
| 46:e:546:ASN:HA   | 46:e:582:SER:CB    | 1.72                     | 1.16              |
| 46:e:751:VAL:O    | 46:e:754:ILE:HG23  | 1.45                     | 1.15              |
| 46:e:838:ILE:HD13 | 46:e:864:HIS:CB    | 1.58                     | 1.15              |
| 46:e:884:ILE:HD13 | 46:e:935:SER:CB    | 1.74                     | 1.15              |
| 46:e:1527:CYS:HB2 | 46:e:1558:ILE:HG12 | 1.25                     | 1.15              |
| 46:e:253:LYS:HG2  | 46:e:254:ASN:ND2   | 1.59                     | 1.15              |
| 46:e:371:LEU:HB2  | 46:e:377:TRP:HE1   | 1.12                     | 1.15              |
| 46:e:1303:MET:HE2 | 46:e:1303:MET:CA   | 1.77                     | 1.14              |
| 46:e:1303:MET:HA  | 46:e:1303:MET:CE   | 1.75                     | 1.14              |
| 46:e:1066:ARG:NH2 | 46:e:1111:GLN:OE1  | 1.80                     | 1.14              |
| 46:e:754:ILE:HD11 | 46:e:829:ARG:CD    | 1.79                     | 1.13              |
| 46:e:990:VAL:HG13 | 46:e:1039:LEU:HD11 | 1.23                     | 1.13              |
| 46:e:989:GLU:CG   | 46:e:1034:TRP:CA   | 2.15                     | 1.13              |
| 46:e:1527:CYS:CB  | 46:e:1558:ILE:CD1  | 2.26                     | 1.12              |
| 30:f:1259:A:C8    | 52:0:53:MET:CB     | 2.32                     | 1.11              |
| 46:e:989:GLU:HB3  | 46:e:1034:TRP:CB   | 1.73                     | 1.11              |
| 46:e:709:PHE:HE1  | 46:e:753:LEU:HD21  | 1.01                     | 1.10              |
| 46:e:1283:SER:OG  | 46:e:1286:MET:HG3  | 0.93                     | 1.10              |
| 46:e:750:ALA:CA   | 46:e:764:PHE:CZ    | 2.32                     | 1.10              |
| 46:e:838:ILE:CG2  | 46:e:863:GLY:O     | 1.98                     | 1.10              |
| 46:e:753:LEU:HB3  | 46:e:760:THR:HG21  | 1.33                     | 1.09              |
| 46:e:867:PHE:O    | 46:e:871:LYS:CA    | 2.00                     | 1.09              |
| 30:f:1221:A:C2    | 52:0:12:PHE:HE2    | 1.69                     | 1.09              |
| 46:e:754:ILE:CD1  | 46:e:829:ARG:NH1   | 2.13                     | 1.09              |
| 46:e:750:ALA:HB1  | 46:e:764:PHE:CE1   | 1.87                     | 1.08              |
| 46:e:751:VAL:HA   | 46:e:754:ILE:HG21  | 1.34                     | 1.08              |
| 46:e:839:THR:HB   | 46:e:865:THR:HG22  | 1.11                     | 1.08              |
| 46:e:368:HIS:NE2  | 46:e:370:PHE:HB2   | 1.68                     | 1.08              |
| 46:e:990:VAL:CG1  | 46:e:1039:LEU:HD11 | 1.83                     | 1.07              |
| 46:e:371:LEU:HD12 | 46:e:377:TRP:CE2   | 1.88                     | 1.07              |
| 46:e:989:GLU:HG2  | 46:e:1034:TRP:HA   | 1.10                     | 1.06              |
| 46:e:1192:ARG:HG2 | 46:e:1270:TRP:CH2  | 1.91                     | 1.05              |
| 46:e:937:GLU:HG2  | 46:e:976:LEU:HG    | 1.38                     | 1.04              |
| 46:e:981:ALA:CB   | 46:e:1023:ARG:HD3  | 1.87                     | 1.04              |
| 46:e:321:ASP:CA   | 46:e:328:ILE:HD11  | 1.88                     | 1.04              |
| 46:e:751:VAL:CA   | 46:e:754:ILE:CG2   | 2.35                     | 1.04              |
| 46:e:838:ILE:CD1  | 46:e:864:HIS:HB3   | 1.66                     | 1.04              |
| 46:e:981:ALA:HB3  | 46:e:1023:ARG:HD3  | 1.38                     | 1.04              |
| 46:e:546:ASN:CA   | 46:e:582:SER:CB    | 2.37                     | 1.03              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:e:13:ASN:HD21  | 46:e:15:ASP:HB3    | 1.21                     | 1.02              |
| 46:e:972:GLU:O    | 46:e:975:LYS:HG3   | 1.60                     | 1.02              |
| 46:e:321:ASP:OD1  | 46:e:326:GLY:HA2   | 1.58                     | 1.02              |
| 46:e:754:ILE:HD11 | 46:e:829:ARG:NH1   | 1.70                     | 1.02              |
| 46:e:321:ASP:HB2  | 46:e:328:ILE:HD11  | 1.41                     | 1.02              |
| 46:e:750:ALA:HB1  | 46:e:764:PHE:CZ    | 1.88                     | 1.02              |
| 46:e:371:LEU:HB2  | 46:e:377:TRP:NE1   | 1.75                     | 1.01              |
| 46:e:253:LYS:HG2  | 46:e:254:ASN:HD21  | 0.87                     | 1.01              |
| 46:e:971:ASP:O    | 46:e:975:LYS:HG2   | 1.60                     | 1.01              |
| 46:e:1066:ARG:HE  | 46:e:1111:GLN:CD   | 1.60                     | 1.01              |
| 46:e:750:ALA:CB   | 46:e:764:PHE:CE1   | 2.42                     | 1.01              |
| 46:e:841:VAL:HG11 | 46:e:862:PHE:CE2   | 1.88                     | 1.00              |
| 46:e:812:LEU:O    | 46:e:812:LEU:HD23  | 1.61                     | 0.99              |
| 30:f:1259:A:N7    | 52:0:53:MET:CB     | 2.25                     | 0.99              |
| 46:e:709:PHE:CE1  | 46:e:753:LEU:CD2   | 2.46                     | 0.99              |
| 46:e:1087:CYS:SG  | 46:e:1099:ARG:HA   | 2.02                     | 0.99              |
| 46:e:277:MET:HG3  | 46:e:278:PRO:HD3   | 1.02                     | 0.98              |
| 46:e:989:GLU:HB3  | 46:e:1034:TRP:CD2  | 1.99                     | 0.98              |
| 46:e:321:ASP:CB   | 46:e:328:ILE:HD11  | 1.93                     | 0.98              |
| 46:e:839:THR:HA   | 46:e:865:THR:HG21  | 1.46                     | 0.97              |
| 46:e:1534:PHE:CG  | 46:e:1539:LEU:CD1  | 2.45                     | 0.97              |
| 46:e:989:GLU:HG2  | 46:e:1034:TRP:CG   | 1.87                     | 0.97              |
| 30:f:1259:A:H8    | 52:0:53:MET:HB2    | 1.29                     | 0.97              |
| 46:e:277:MET:CG   | 46:e:278:PRO:HD3   | 1.94                     | 0.97              |
| 46:e:321:ASP:OD1  | 46:e:329:TRP:CD1   | 2.17                     | 0.97              |
| 46:e:545:ILE:O    | 46:e:582:SER:CB    | 2.12                     | 0.97              |
| 46:e:1290:PHE:O   | 46:e:1294:LEU:CD1  | 2.12                     | 0.97              |
| 46:e:13:ASN:ND2   | 46:e:15:ASP:HB3    | 1.79                     | 0.96              |
| 46:e:937:GLU:HA   | 46:e:976:LEU:CD1   | 1.94                     | 0.96              |
| 46:e:1066:ARG:CZ  | 46:e:1111:GLN:CD   | 2.36                     | 0.96              |
| 46:e:1534:PHE:CD2 | 46:e:1539:LEU:HD11 | 2.00                     | 0.96              |
| 46:e:972:GLU:CA   | 46:e:975:LYS:HE3   | 1.82                     | 0.96              |
| 46:e:884:ILE:HD13 | 46:e:935:SER:HB3   | 0.97                     | 0.96              |
| 46:e:277:MET:HG3  | 46:e:278:PRO:CD    | 1.94                     | 0.96              |
| 27:b:103:ALA:HB1  | 42:s:60:ARG:NH1    | 1.80                     | 0.96              |
| 30:f:1258:U:P     | 52:0:46:ARG:HH22   | 1.89                     | 0.95              |
| 46:e:937:GLU:HA   | 46:e:976:LEU:HD11  | 1.48                     | 0.95              |
| 46:e:1192:ARG:NH2 | 46:e:1338:SER:O    | 1.99                     | 0.95              |
| 46:e:990:VAL:N    | 46:e:1039:LEU:HD23 | 1.82                     | 0.94              |
| 46:e:1192:ARG:HG2 | 46:e:1270:TRP:HH2  | 1.28                     | 0.94              |
| 50:y:3:G:H1       | 50:y:70:U:H3       | 1.00                     | 0.94              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:e:754:ILE:CD1   | 46:e:829:ARG:HD3   | 1.97                     | 0.93              |
| 50:x:3:G:H1        | 50:x:70:U:H3       | 1.17                     | 0.93              |
| 46:e:1429:LYS:CE   | 46:e:1440:GLU:OE2  | 2.15                     | 0.93              |
| 30:f:1257:C:O3'    | 52:0:46:ARG:NH2    | 2.02                     | 0.93              |
| 46:e:371:LEU:HD12  | 46:e:377:TRP:CZ2   | 2.03                     | 0.93              |
| 46:e:989:GLU:HB2   | 46:e:1034:TRP:HB3  | 1.47                     | 0.93              |
| 46:e:1429:LYS:HB3  | 46:e:1440:GLU:OE2  | 1.67                     | 0.93              |
| 42:s:29:ARG:NH2    | 42:s:123:PHE:CE1   | 2.37                     | 0.93              |
| 46:e:253:LYS:O     | 46:e:254:ASN:ND2   | 1.98                     | 0.93              |
| 46:e:371:LEU:HD12  | 46:e:377:TRP:NE1   | 1.84                     | 0.92              |
| 46:e:726:LEU:HD23  | 46:e:753:LEU:HD11  | 1.51                     | 0.92              |
| 46:e:989:GLU:CD    | 46:e:1034:TRP:HA   | 1.93                     | 0.92              |
| 46:e:751:VAL:C     | 46:e:754:ILE:HG23  | 1.93                     | 0.92              |
| 46:e:1020:ALA:HB2  | 46:e:1023:ARG:NH1  | 1.85                     | 0.92              |
| 46:e:750:ALA:O     | 46:e:754:ILE:CG2   | 2.16                     | 0.91              |
| 46:e:321:ASP:HA    | 46:e:328:ILE:HG12  | 1.53                     | 0.91              |
| 46:e:750:ALA:HA    | 46:e:764:PHE:HZ    | 1.26                     | 0.91              |
| 46:e:884:ILE:CD1   | 46:e:935:SER:HB2   | 2.01                     | 0.91              |
| 46:e:266:ARG:O     | 46:e:270:VAL:HG23  | 1.70                     | 0.91              |
| 46:e:324:GLU:HB3   | 46:e:327:THR:CB    | 1.99                     | 0.91              |
| 15:O:16:ALA:O      | 15:O:20:GLY:HA3    | 1.69                     | 0.90              |
| 46:e:254:ASN:HD22  | 46:e:254:ASN:N     | 1.68                     | 0.90              |
| 45:a:893:LYS:NZ    | 48:v:129:ASP:HB3   | 1.84                     | 0.90              |
| 46:e:839:THR:N     | 46:e:865:THR:HG23  | 1.86                     | 0.90              |
| 46:e:1066:ARG:HH22 | 46:e:1111:GLN:HB2  | 1.14                     | 0.90              |
| 46:e:937:GLU:HG2   | 46:e:976:LEU:CG    | 2.02                     | 0.90              |
| 46:e:807:LYS:HE3   | 46:e:808:ASN:OD1   | 1.71                     | 0.90              |
| 46:e:1066:ARG:CZ   | 46:e:1111:GLN:HB2  | 2.02                     | 0.90              |
| 46:e:735:GLN:HG2   | 46:e:815:TYR:HB2   | 1.53                     | 0.90              |
| 46:e:1527:CYS:CB   | 46:e:1558:ILE:HD11 | 1.94                     | 0.90              |
| 30:f:1222:G:OP2    | 52:0:57:THR:OG1    | 1.90                     | 0.89              |
| 30:f:1258:U:O5'    | 52:0:42:ARG:NH1    | 2.04                     | 0.89              |
| 46:e:841:VAL:HG11  | 46:e:862:PHE:HZ    | 1.25                     | 0.89              |
| 46:e:253:LYS:CG    | 46:e:254:ASN:HD21  | 1.82                     | 0.89              |
| 46:e:812:LEU:HD23  | 46:e:812:LEU:C     | 1.98                     | 0.89              |
| 50:y:76:A:O3'      | 53:1:57:UNK:O      | 1.90                     | 0.88              |
| 46:e:1172:LYS:HB2  | 46:e:1173:ARG:NH2  | 1.89                     | 0.88              |
| 27:b:103:ALA:HB1   | 42:s:60:ARG:HH12   | 1.34                     | 0.88              |
| 46:e:321:ASP:HA    | 46:e:328:ILE:CG1   | 2.03                     | 0.88              |
| 46:e:820:ASP:HA    | 46:e:823:LEU:HD12  | 1.53                     | 0.87              |
| 30:f:1258:U:C5'    | 52:0:42:ARG:HH12   | 1.86                     | 0.87              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:e:709:PHE:CZ   | 46:e:753:LEU:HD22  | 2.10                     | 0.87              |
| 46:e:351:SER:OG   | 46:e:354:PHE:HB2   | 1.73                     | 0.87              |
| 46:e:368:HIS:HE1  | 46:e:370:PHE:HB2   | 1.24                     | 0.86              |
| 46:e:321:ASP:CA   | 46:e:328:ILE:CD1   | 2.53                     | 0.86              |
| 46:e:709:PHE:CZ   | 46:e:753:LEU:CD2   | 2.58                     | 0.86              |
| 42:s:29:ARG:NH2   | 42:s:123:PHE:HE1   | 1.74                     | 0.85              |
| 46:e:378:LEU:HB3  | 46:e:379:PRO:HD3   | 1.58                     | 0.85              |
| 46:e:813:ILE:CG1  | 46:e:844:LEU:HD21  | 2.06                     | 0.85              |
| 46:e:749:HIS:O    | 46:e:753:LEU:CD2   | 2.24                     | 0.85              |
| 46:e:546:ASN:C    | 46:e:582:SER:CB    | 2.49                     | 0.85              |
| 51:z:19:GLY:HA3   | 51:z:55:GLY:HA2    | 1.56                     | 0.85              |
| 30:f:1221:A:C2    | 52:0:12:PHE:CE2    | 2.62                     | 0.84              |
| 46:e:380:PHE:CD2  | 46:e:381:TRP:HD1   | 1.95                     | 0.84              |
| 46:e:750:ALA:C    | 46:e:754:ILE:HG22  | 2.03                     | 0.84              |
| 46:e:1283:SER:OG  | 46:e:1286:MET:SD   | 2.35                     | 0.84              |
| 46:e:13:ASN:HD21  | 46:e:15:ASP:CB     | 1.91                     | 0.84              |
| 46:e:989:GLU:CG   | 46:e:1034:TRP:HB3  | 1.78                     | 0.84              |
| 46:e:838:ILE:HG21 | 46:e:863:GLY:C     | 2.02                     | 0.83              |
| 30:f:1259:A:N7    | 52:0:53:MET:HG3    | 1.92                     | 0.83              |
| 45:a:893:LYS:HZ3  | 48:v:129:ASP:HB3   | 1.38                     | 0.83              |
| 46:e:838:ILE:HD12 | 46:e:864:HIS:HB3   | 0.84                     | 0.83              |
| 30:f:1258:U:H4'   | 52:0:42:ARG:HH12   | 0.66                     | 0.83              |
| 46:e:884:ILE:HD11 | 46:e:935:SER:HB2   | 1.58                     | 0.82              |
| 46:e:321:ASP:HA   | 46:e:328:ILE:CD1   | 2.09                     | 0.82              |
| 46:e:350:PRO:HB3  | 46:e:355:PHE:CZ    | 2.14                     | 0.82              |
| 46:e:936:VAL:O    | 46:e:940:VAL:HG23  | 1.79                     | 0.82              |
| 46:e:972:GLU:HA   | 46:e:975:LYS:HE2   | 0.82                     | 0.82              |
| 30:f:1229:G:H4'   | 52:0:32:ASN:OD1    | 1.79                     | 0.81              |
| 46:e:571:LYS:O    | 46:e:575:MET:N     | 2.13                     | 0.81              |
| 46:e:754:ILE:HD11 | 46:e:829:ARG:HD2   | 1.61                     | 0.81              |
| 30:f:1222:G:N7    | 52:0:57:THR:HB     | 1.95                     | 0.80              |
| 46:e:943:THR:HG21 | 46:e:957:CYS:SG    | 2.21                     | 0.80              |
| 46:e:1020:ALA:CB  | 46:e:1023:ARG:NH1  | 2.44                     | 0.80              |
| 46:e:1527:CYS:CB  | 46:e:1558:ILE:CG1  | 2.31                     | 0.80              |
| 46:e:989:GLU:CB   | 46:e:1034:TRP:CD1  | 2.54                     | 0.80              |
| 46:e:1303:MET:HE2 | 46:e:1303:MET:HA   | 0.86                     | 0.80              |
| 46:e:253:LYS:CG   | 46:e:254:ASN:ND2   | 2.43                     | 0.79              |
| 46:e:321:ASP:OD1  | 46:e:326:GLY:CA    | 2.30                     | 0.79              |
| 46:e:1104:ASN:O   | 46:e:1108:THR:HG23 | 1.82                     | 0.79              |
| 46:e:738:PHE:HB3  | 46:e:814:ARG:HB3   | 1.64                     | 0.79              |
| 46:e:782:TYR:O    | 46:e:786:LEU:HG    | 1.81                     | 0.79              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:e:1283:SER:HG  | 46:e:1286:MET:HG3  | 0.96                     | 0.79              |
| 46:e:371:LEU:CB   | 46:e:377:TRP:HE1   | 1.94                     | 0.79              |
| 46:e:1440:GLU:H   | 46:e:1460:SER:HB2  | 1.46                     | 0.79              |
| 46:e:709:PHE:HZ   | 46:e:753:LEU:HD22  | 1.47                     | 0.79              |
| 46:e:546:ASN:O    | 46:e:582:SER:CB    | 2.31                     | 0.79              |
| 46:e:990:VAL:CG1  | 46:e:1039:LEU:CD1  | 2.61                     | 0.78              |
| 46:e:725:LYS:O    | 46:e:729:VAL:HG23  | 1.82                     | 0.78              |
| 46:e:864:HIS:HA   | 46:e:869:HIS:HB2   | 1.66                     | 0.78              |
| 46:e:992:LEU:HA   | 46:e:996:GLU:HB2   | 1.64                     | 0.78              |
| 30:f:1258:U:C5'   | 52:0:42:ARG:NH1    | 2.46                     | 0.77              |
| 46:e:726:LEU:O    | 46:e:730:ILE:HG12  | 1.84                     | 0.77              |
| 46:e:13:ASN:ND2   | 46:e:15:ASP:CB     | 2.47                     | 0.77              |
| 46:e:972:GLU:CB   | 46:e:975:LYS:HE3   | 2.13                     | 0.77              |
| 46:e:372:ASP:OD2  | 46:e:375:LEU:HB2   | 1.85                     | 0.77              |
| 46:e:751:VAL:C    | 46:e:754:ILE:CG2   | 2.57                     | 0.77              |
| 30:f:1259:A:N7    | 52:0:53:MET:CG     | 2.47                     | 0.77              |
| 46:e:754:ILE:CG1  | 46:e:829:ARG:CZ    | 2.63                     | 0.77              |
| 46:e:1020:ALA:HB2 | 46:e:1023:ARG:HH12 | 1.49                     | 0.77              |
| 46:e:754:ILE:HG12 | 46:e:829:ARG:HH12  | 1.49                     | 0.77              |
| 46:e:839:THR:HA   | 46:e:865:THR:CB    | 2.15                     | 0.77              |
| 46:e:839:THR:HA   | 46:e:865:THR:HG23  | 0.84                     | 0.77              |
| 46:e:380:PHE:CD2  | 46:e:381:TRP:CD1   | 2.73                     | 0.76              |
| 46:e:751:VAL:HA   | 46:e:754:ILE:HG23  | 1.66                     | 0.76              |
| 46:e:371:LEU:CD1  | 46:e:377:TRP:NE1   | 2.48                     | 0.76              |
| 46:e:324:GLU:HB3  | 46:e:327:THR:CG2   | 2.16                     | 0.76              |
| 46:e:1149:THR:HA  | 46:e:1189:ASN:HD21 | 1.51                     | 0.76              |
| 46:e:754:ILE:CD1  | 46:e:829:ARG:CD    | 2.55                     | 0.75              |
| 46:e:731:LEU:HD12 | 46:e:731:LEU:C     | 2.12                     | 0.75              |
| 46:e:750:ALA:O    | 46:e:764:PHE:CE2   | 2.40                     | 0.75              |
| 46:e:839:THR:HB   | 46:e:866:PHE:H     | 1.52                     | 0.74              |
| 30:f:1258:U:C4'   | 52:0:42:ARG:NH1    | 2.13                     | 0.74              |
| 46:e:750:ALA:HA   | 46:e:764:PHE:CE2   | 2.22                     | 0.74              |
| 46:e:937:GLU:HG3  | 46:e:972:GLU:O     | 1.88                     | 0.74              |
| 46:e:972:GLU:CB   | 46:e:975:LYS:CE    | 2.64                     | 0.74              |
| 46:e:709:PHE:HE1  | 46:e:753:LEU:CD2   | 1.86                     | 0.74              |
| 46:e:1294:LEU:N   | 46:e:1294:LEU:HD12 | 2.03                     | 0.74              |
| 15:O:16:ALA:O     | 15:O:20:GLY:CA     | 2.36                     | 0.73              |
| 46:e:989:GLU:HG3  | 46:e:1034:TRP:HD1  | 0.96                     | 0.73              |
| 23:W:2:GLY:N      | 30:f:2138:A:HO2'   | 1.85                     | 0.73              |
| 46:e:813:ILE:HG12 | 46:e:844:LEU:CD2   | 2.18                     | 0.73              |
| 46:e:371:LEU:CB   | 46:e:377:TRP:NE1   | 2.49                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:a:671:SER:O    | 49:w:98:LYS:HE2    | 1.89                     | 0.73              |
| 46:e:371:LEU:CD1  | 46:e:377:TRP:CE2   | 2.70                     | 0.73              |
| 46:e:321:ASP:N    | 46:e:328:ILE:CD1   | 2.51                     | 0.73              |
| 46:e:1066:ARG:NH2 | 46:e:1111:GLN:CD   | 2.43                     | 0.73              |
| 46:e:937:GLU:CG   | 46:e:976:LEU:HG    | 2.18                     | 0.72              |
| 51:z:105:GLN:HA   | 51:z:143:VAL:HA    | 1.71                     | 0.72              |
| 46:e:321:ASP:OD1  | 46:e:329:TRP:HD1   | 1.69                     | 0.72              |
| 46:e:1527:CYS:CA  | 46:e:1558:ILE:HG12 | 2.18                     | 0.72              |
| 46:e:750:ALA:HB2  | 46:e:764:PHE:CE1   | 2.23                     | 0.72              |
| 46:e:712:SER:O    | 46:e:716:ALA:N     | 2.23                     | 0.72              |
| 46:e:1527:CYS:HA  | 46:e:1558:ILE:HG23 | 1.72                     | 0.72              |
| 46:e:750:ALA:HB2  | 46:e:764:PHE:CZ    | 2.25                     | 0.71              |
| 46:e:782:TYR:OH   | 46:e:1141:GLN:NE2  | 2.23                     | 0.71              |
| 46:e:1335:ASN:OD1 | 46:e:1338:SER:HB2  | 1.91                     | 0.71              |
| 46:e:1526:THR:O   | 46:e:1558:ILE:CG2  | 2.38                     | 0.71              |
| 46:e:380:PHE:HD2  | 46:e:381:TRP:HD1   | 1.37                     | 0.71              |
| 46:e:731:LEU:HD12 | 46:e:732:GLN:N     | 2.05                     | 0.71              |
| 46:e:839:THR:CB   | 46:e:865:THR:HG22  | 1.83                     | 0.71              |
| 46:e:981:ALA:HB1  | 46:e:1023:ARG:HD3  | 1.69                     | 0.71              |
| 46:e:990:VAL:H    | 46:e:1039:LEU:CD2  | 2.03                     | 0.71              |
| 40:q:92:TYR:HB2   | 40:q:142:ASP:HB3   | 1.73                     | 0.71              |
| 46:e:838:ILE:HG22 | 46:e:865:THR:OG1   | 1.91                     | 0.70              |
| 46:e:1087:CYS:SG  | 46:e:1099:ARG:CA   | 2.78                     | 0.70              |
| 46:e:1441:ILE:HA  | 46:e:1458:GLY:HA2  | 1.71                     | 0.70              |
| 46:e:1534:PHE:CD2 | 46:e:1539:LEU:CD1  | 2.71                     | 0.70              |
| 46:e:141:CYS:SG   | 46:e:221:LYS:HD2   | 2.32                     | 0.69              |
| 46:e:1066:ARG:NH2 | 46:e:1111:GLN:HB3  | 2.03                     | 0.69              |
| 30:f:1018:G:H1    | 30:f:1034:U:H3     | 1.38                     | 0.69              |
| 46:e:813:ILE:HG12 | 46:e:844:LEU:HD21  | 1.73                     | 0.69              |
| 46:e:933:LEU:HD21 | 46:e:973:ILE:HG12  | 1.74                     | 0.69              |
| 46:e:105:VAL:HG22 | 47:g:1:MET:HE1     | 1.73                     | 0.69              |
| 46:e:812:LEU:C    | 46:e:812:LEU:CD2   | 2.63                     | 0.69              |
| 30:f:1219:C:OP1   | 52:0:4:ILE:HG21    | 1.92                     | 0.69              |
| 46:e:1192:ARG:CG  | 46:e:1270:TRP:HH2  | 2.05                     | 0.69              |
| 46:e:324:GLU:CB   | 46:e:327:THR:CB    | 2.67                     | 0.69              |
| 23:W:21:ARG:HE    | 23:W:39:TYR:HB2    | 1.58                     | 0.69              |
| 46:e:751:VAL:CA   | 46:e:754:ILE:HG23  | 2.14                     | 0.69              |
| 46:e:754:ILE:HG13 | 46:e:761:SER:HB2   | 1.74                     | 0.69              |
| 52:0:26:PHE:HB2   | 52:0:87:VAL:HB     | 1.73                     | 0.69              |
| 46:e:1283:SER:HG  | 46:e:1286:MET:CG   | 1.81                     | 0.69              |
| 46:e:1534:PHE:HB3 | 46:e:1539:LEU:HD13 | 0.74                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:f:2193:U:H5'    | 30:f:2194:G:H5'    | 1.75                     | 0.68              |
| 46:e:1526:THR:O    | 46:e:1558:ILE:HG23 | 1.93                     | 0.68              |
| 2:B:46[A]:GLU:HB3  | 2:B:49[A]:ARG:HG3  | 1.75                     | 0.68              |
| 46:e:1172:LYS:CB   | 46:e:1173:ARG:NH2  | 2.56                     | 0.68              |
| 30:f:1222:G:C8     | 52:0:57:THR:HB     | 2.29                     | 0.68              |
| 49:w:138:VAL:HG23  | 49:w:147:LYS:HD2   | 1.75                     | 0.68              |
| 46:e:515:VAL:O     | 46:e:519:TYR:N     | 2.22                     | 0.68              |
| 46:e:1066:ARG:HH21 | 46:e:1111:GLN:CB   | 2.06                     | 0.68              |
| 46:e:374:TYR:O     | 46:e:379:PRO:CD    | 2.42                     | 0.67              |
| 46:e:754:ILE:HD12  | 46:e:829:ARG:HD3   | 1.76                     | 0.67              |
| 46:e:813:ILE:HG13  | 46:e:844:LEU:HD21  | 1.74                     | 0.67              |
| 46:e:545:ILE:CB    | 46:e:579:ALA:HB2   | 2.22                     | 0.67              |
| 46:e:972:GLU:HA    | 46:e:975:LYS:CD    | 2.18                     | 0.67              |
| 45:a:90:THR:HG21   | 45:a:107:ASP:OD1   | 1.94                     | 0.67              |
| 46:e:1303:MET:CA   | 46:e:1303:MET:CE   | 2.52                     | 0.67              |
| 46:e:839:THR:N     | 46:e:865:THR:HA    | 2.10                     | 0.67              |
| 42:s:29:ARG:HH22   | 42:s:123:PHE:HE1   | 1.43                     | 0.67              |
| 46:e:1172:LYS:HB2  | 46:e:1173:ARG:CZ   | 2.24                     | 0.67              |
| 53:1:44:UNK:O      | 53:1:45:UNK:C      | 2.43                     | 0.67              |
| 46:e:156:THR:HG22  | 46:e:161:LYS:HA    | 1.75                     | 0.67              |
| 50:y:76:A:O3'      | 53:1:58:UNK:C      | 2.43                     | 0.67              |
| 30:f:2969:A:N7     | 33:j:215:ASN:ND2   | 2.42                     | 0.66              |
| 46:e:754:ILE:HD11  | 46:e:829:ARG:CZ    | 2.26                     | 0.66              |
| 30:f:1222:G:C8     | 52:0:57:THR:CB     | 2.79                     | 0.66              |
| 30:f:1240:A:OP1    | 51:z:97:ASN:O      | 2.14                     | 0.66              |
| 30:f:1222:G:C8     | 52:0:57:THR:HG21   | 2.31                     | 0.66              |
| 30:f:1254:C:O2     | 51:z:135:THR:CB    | 2.43                     | 0.66              |
| 46:e:972:GLU:HG3   | 46:e:975:LYS:HZ3   | 1.60                     | 0.66              |
| 46:e:1066:ARG:NH2  | 46:e:1111:GLN:CG   | 2.58                     | 0.66              |
| 30:f:1940:G:H21    | 30:f:3362:A:H8     | 1.44                     | 0.66              |
| 46:e:1294:LEU:CD1  | 46:e:1294:LEU:H    | 2.09                     | 0.66              |
| 46:e:1020:ALA:HB3  | 46:e:1023:ARG:HB3  | 1.77                     | 0.66              |
| 46:e:60:THR:O      | 46:e:64:LYS:HG3    | 1.95                     | 0.66              |
| 46:e:1279:PHE:CE1  | 46:e:1290:PHE:HB3  | 2.31                     | 0.66              |
| 30:f:1221:A:N3     | 52:0:12:PHE:HE2    | 1.94                     | 0.65              |
| 30:f:1238:C:H4'    | 51:z:139:VAL:CB    | 2.27                     | 0.65              |
| 30:f:1258:U:P      | 52:0:46:ARG:NH2    | 2.64                     | 0.65              |
| 46:e:368:HIS:NE2   | 46:e:370:PHE:CB    | 2.46                     | 0.65              |
| 46:e:866:PHE:HD1   | 46:e:893:MET:HB2   | 1.61                     | 0.65              |
| 30:f:3018:C:OP1    | 47:g:9:ASN:ND2     | 2.29                     | 0.65              |
| 30:f:687:U:OP2     | 43:t:36:ARG:NH2    | 2.30                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:e:254:ASN:ND2   | 46:e:254:ASN:N     | 2.31                     | 0.65              |
| 46:e:838:ILE:HD13  | 46:e:864:HIS:HB2   | 0.67                     | 0.65              |
| 46:e:1294:LEU:CD1  | 46:e:1294:LEU:N    | 2.60                     | 0.65              |
| 7:G:84:TYR:HB2     | 15:O:24:PRO:HD3    | 1.78                     | 0.65              |
| 46:e:289:LYS:HA    | 46:e:292:LEU:HD12  | 1.79                     | 0.65              |
| 46:e:1144:ASN:HA   | 46:e:1339:PRO:HG2  | 1.79                     | 0.65              |
| 46:e:1192:ARG:NH2  | 46:e:1339:PRO:HA   | 2.12                     | 0.65              |
| 46:e:351:SER:OG    | 46:e:354:PHE:CB    | 2.45                     | 0.64              |
| 46:e:937:GLU:HA    | 46:e:976:LEU:HD12  | 1.77                     | 0.64              |
| 46:e:372:ASP:OD1   | 46:e:372:ASP:C     | 2.39                     | 0.64              |
| 5:E:128:LYS:NZ     | 30:f:1724:U:OP2    | 2.31                     | 0.64              |
| 46:e:750:ALA:CA    | 46:e:764:PHE:CE2   | 2.79                     | 0.64              |
| 46:e:1020:ALA:CB   | 46:e:1023:ARG:HH11 | 2.10                     | 0.64              |
| 45:a:672:ASP:HA    | 49:w:98:LYS:HE3    | 1.80                     | 0.64              |
| 46:e:371:LEU:HB2   | 46:e:377:TRP:CD1   | 2.32                     | 0.64              |
| 46:e:1188:ILE:HG22 | 46:e:1192:ARG:CZ   | 2.28                     | 0.64              |
| 46:e:958:ALA:HB2   | 46:e:1002:LEU:HD22 | 1.80                     | 0.64              |
| 46:e:884:ILE:HD11  | 46:e:935:SER:CB    | 2.14                     | 0.63              |
| 46:e:753:LEU:HB2   | 46:e:764:PHE:HE2   | 1.62                     | 0.63              |
| 46:e:981:ALA:HB3   | 46:e:1023:ARG:CD   | 2.24                     | 0.63              |
| 46:e:1527:CYS:HA   | 46:e:1558:ILE:HG12 | 1.79                     | 0.63              |
| 2:B:27[A]:LEU:HD21 | 2:B:102[A]:LEU:HB2 | 1.80                     | 0.63              |
| 9:I:12:ARG:NH1     | 30:f:3041:U:OP1    | 2.32                     | 0.63              |
| 47:g:111:ASN:ND2   | 47:g:114:VAL:O     | 2.32                     | 0.63              |
| 46:e:380:PHE:CE2   | 46:e:381:TRP:CD1   | 2.86                     | 0.63              |
| 46:e:321:ASP:HA    | 46:e:328:ILE:HD11  | 1.70                     | 0.63              |
| 46:e:882:ASN:O     | 46:e:886:PRO:CA    | 2.44                     | 0.62              |
| 28:c:87:ARG:NH1    | 33:j:97:ASN:OD1    | 2.33                     | 0.62              |
| 30:f:2442:G:H1     | 30:f:2505:U:H3     | 1.46                     | 0.62              |
| 13:M:27:LYS:HB3    | 13:M:42:LEU:HB2    | 1.81                     | 0.62              |
| 29:d:4:MET:N       | 30:f:1802:C:OP1    | 2.32                     | 0.62              |
| 46:e:321:ASP:N     | 46:e:328:ILE:HD13  | 2.13                     | 0.62              |
| 30:f:1232:C:O2'    | 52:0:36:GLN:NE2    | 2.31                     | 0.62              |
| 50:y:76:A:HO3'     | 53:1:57:UNK:C      | 2.05                     | 0.62              |
| 46:e:1066:ARG:CZ   | 46:e:1111:GLN:CG   | 2.78                     | 0.62              |
| 9:I:14:SER:O       | 9:I:81:GLN:NE2     | 2.33                     | 0.62              |
| 5:E:43:LYS:NZ      | 30:f:1764:U:OP1    | 2.31                     | 0.61              |
| 23:W:21:ARG:HG2    | 32:i:103:G:H4'     | 1.82                     | 0.61              |
| 46:e:697:LEU:O     | 46:e:698:TYR:HB2   | 2.00                     | 0.61              |
| 46:e:820:ASP:CA    | 46:e:823:LEU:HD12  | 2.26                     | 0.61              |
| 30:f:1221:A:N3     | 52:0:12:PHE:CE2    | 2.67                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:e:754:ILE:HG13  | 46:e:761:SER:CB    | 2.31                     | 0.61              |
| 46:e:1187:ASN:HB3  | 46:e:1190:GLN:HB3  | 1.81                     | 0.61              |
| 30:f:3348:G:H1     | 30:f:3357:U:H3     | 1.48                     | 0.61              |
| 30:f:1235:U:O4     | 51:z:136:ALA:HA    | 2.00                     | 0.61              |
| 38:o:87:VAL:HG11   | 38:o:243:MET:HE1   | 1.83                     | 0.61              |
| 30:f:1348:U:O2     | 30:f:1349:G:N2     | 2.34                     | 0.61              |
| 36:m:50:ARG:NH1    | 36:m:147:ASP:OD2   | 2.34                     | 0.61              |
| 46:e:836:ALA:HB2   | 46:e:894:LEU:HA    | 1.82                     | 0.61              |
| 46:e:972:GLU:HG3   | 46:e:975:LYS:NZ    | 2.16                     | 0.61              |
| 45:a:403:LYS:NZ    | 45:a:512:LEU:O     | 2.28                     | 0.61              |
| 46:e:321:ASP:N     | 46:e:328:ILE:HD11  | 2.14                     | 0.60              |
| 46:e:753:LEU:HB3   | 46:e:760:THR:CG2   | 2.20                     | 0.60              |
| 36:m:294:ALA:HB1   | 41:r:217:PHE:HB3   | 1.83                     | 0.60              |
| 46:e:989:GLU:N     | 46:e:1034:TRP:CD1  | 2.70                     | 0.60              |
| 20:T:74:ARG:NH2    | 30:f:1639:C:OP2    | 2.30                     | 0.60              |
| 46:e:972:GLU:CG    | 46:e:975:LYS:CE    | 2.79                     | 0.60              |
| 3:C:173:ARG:NH2    | 30:f:618:C:OP1     | 2.35                     | 0.60              |
| 46:e:754:ILE:CD1   | 46:e:826:LEU:HD13  | 2.31                     | 0.60              |
| 46:e:1534:PHE:HB2  | 46:e:1539:LEU:CD1  | 2.26                     | 0.60              |
| 4:D:38:ARG:NH2     | 30:f:1348:U:OP2    | 2.34                     | 0.60              |
| 23:W:55:ARG:NH2    | 35:l:59:GLN:OE1    | 2.34                     | 0.60              |
| 46:e:373:TYR:HA    | 46:e:377:TRP:HB2   | 1.83                     | 0.60              |
| 1:A:201:ARG:NH2    | 30:f:692:A:OP1     | 2.35                     | 0.60              |
| 40:q:89:LYS:HG2    | 40:q:145:VAL:HG22  | 1.84                     | 0.60              |
| 52:O:192:ASP:HB2   | 52:O:197:PHE:HE2   | 1.67                     | 0.60              |
| 6:F:80:ARG:HH21    | 6:F:87:THR:HG21    | 1.66                     | 0.59              |
| 14:N:21:ARG:NH2    | 30:f:640:U:OP1     | 2.32                     | 0.59              |
| 30:f:1253:U:H5''   | 30:f:1254:C:H5'    | 1.83                     | 0.59              |
| 46:e:950:THR:O     | 46:e:954:TYR:N     | 2.30                     | 0.59              |
| 43:t:27:ASP:O      | 43:t:31:LYS:HB2    | 2.01                     | 0.59              |
| 46:e:1164:LEU:O    | 46:e:1168:GLU:HG3  | 2.02                     | 0.59              |
| 46:e:374:TYR:O     | 46:e:379:PRO:HD3   | 2.02                     | 0.59              |
| 48:v:43:ASP:HB3    | 48:v:60:VAL:HB     | 1.83                     | 0.59              |
| 6:F:8:GLN:HB3      | 6:F:64:ILE:HD11    | 1.84                     | 0.59              |
| 31:h:31:U:O2'      | 36:m:218:ARG:NH1   | 2.35                     | 0.59              |
| 36:m:277:LEU:HG    | 36:m:281:GLU:HG3   | 1.82                     | 0.59              |
| 46:e:819:LEU:O     | 46:e:823:LEU:HD12  | 2.03                     | 0.59              |
| 46:e:1177:VAL:O    | 46:e:1180:ASN:O    | 2.21                     | 0.59              |
| 45:a:975:LYS:HE2   | 45:a:998:LYS:HA    | 1.84                     | 0.59              |
| 46:e:1084:LEU:HD12 | 46:e:1127:ILE:HG23 | 1.83                     | 0.59              |
| 1:A:183:THR:HG22   | 1:A:187:ARG:HB2    | 1.85                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:a:4:ARG:NH1    | 45:a:57:GLY:O      | 2.35                     | 0.59              |
| 30:f:439:C:O2'    | 30:f:494:G:N2      | 2.34                     | 0.59              |
| 31:h:52:G:H21     | 42:s:9:MET:HE1     | 1.68                     | 0.59              |
| 33:j:27:ALA:O     | 33:j:128:ARG:NH2   | 2.36                     | 0.59              |
| 46:e:882:ASN:O    | 46:e:886:PRO:HA    | 2.03                     | 0.59              |
| 49:w:65:ILE:HG12  | 49:w:109:ALA:HB3   | 1.84                     | 0.59              |
| 46:e:669:GLU:HA   | 46:e:700:VAL:HG12  | 1.83                     | 0.59              |
| 46:e:972:GLU:CG   | 46:e:975:LYS:NZ    | 2.65                     | 0.59              |
| 21:U:5:LYS:HB2    | 21:U:8:GLU:HG2     | 1.84                     | 0.58              |
| 46:e:1527:CYS:SG  | 46:e:1558:ILE:HG12 | 2.43                     | 0.58              |
| 30:f:804:C:OP1    | 35:l:98:ARG:NH2    | 2.35                     | 0.58              |
| 30:f:1268:G:O2'   | 30:f:1273:A:N6     | 2.36                     | 0.58              |
| 45:a:619:HIS:NE2  | 45:a:679:GLY:O     | 2.36                     | 0.58              |
| 46:e:374:TYR:O    | 46:e:379:PRO:CG    | 2.51                     | 0.58              |
| 14:N:21:ARG:NH1   | 30:f:1369:A:OP1    | 2.36                     | 0.58              |
| 28:c:4:ARG:NH1    | 30:f:837:A:OP2     | 2.37                     | 0.58              |
| 30:f:2854:U:OP2   | 41:r:3:ARG:NH2     | 2.37                     | 0.58              |
| 46:e:350:PRO:HB3  | 46:e:355:PHE:CE2   | 2.37                     | 0.58              |
| 46:e:322:ASP:HA   | 46:e:367:ARG:HH22  | 1.69                     | 0.58              |
| 5:E:100:ARG:NH1   | 30:f:1722:U:OP1    | 2.36                     | 0.58              |
| 28:c:17:ARG:NH1   | 30:f:860:G:OP1     | 2.36                     | 0.58              |
| 30:f:1354:G:N3    | 37:n:8:LYS:NZ      | 2.51                     | 0.58              |
| 46:e:728:GLN:HA   | 46:e:731:LEU:HG    | 1.85                     | 0.58              |
| 46:e:857:ASP:HA   | 46:e:860:TYR:HD2   | 1.69                     | 0.58              |
| 46:e:968:ASN:HA   | 46:e:973:ILE:HG21  | 1.85                     | 0.58              |
| 6:F:77:VAL:HG22   | 6:F:126:VAL:HG23   | 1.86                     | 0.58              |
| 41:r:205:SER:OG   | 41:r:208:ASN:OD1   | 2.21                     | 0.58              |
| 46:e:1279:PHE:CE1 | 46:e:1290:PHE:CB   | 2.87                     | 0.58              |
| 46:e:902:ASN:HB3  | 46:e:905:TYR:HB2   | 1.84                     | 0.58              |
| 14:N:42:ARG:NH2   | 30:f:2800:G:O6     | 2.37                     | 0.58              |
| 46:e:324:GLU:HB2  | 46:e:327:THR:OG1   | 1.93                     | 0.58              |
| 30:f:1259:A:N7    | 52:0:53:MET:HB3    | 2.15                     | 0.58              |
| 32:i:21:C:OP1     | 35:l:193:LYS:NZ    | 2.36                     | 0.58              |
| 30:f:3187:A:OP1   | 40:q:23:ARG:NH1    | 2.37                     | 0.57              |
| 46:e:385:VAL:HB   | 46:e:405:PHE:CE1   | 2.39                     | 0.57              |
| 46:e:776:TYR:HB3  | 46:e:812:LEU:HB2   | 1.86                     | 0.57              |
| 46:e:1429:LYS:HE2 | 46:e:1440:GLU:CD   | 2.21                     | 0.57              |
| 36:m:166:ALA:HB1  | 36:m:171:LEU:HD12  | 1.86                     | 0.57              |
| 46:e:321:ASP:CG   | 46:e:329:TRP:HE1   | 2.12                     | 0.57              |
| 46:e:989:GLU:HG2  | 46:e:1034:TRP:N    | 2.11                     | 0.57              |
| 52:0:43:LYS:HA    | 52:0:46:ARG:HG2    | 1.87                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:60[A]:LYS:HE3  | 30:f:1307:G:H5'    | 1.86                     | 0.57              |
| 46:e:292:LEU:HD13  | 46:e:332:ASP:HB2   | 1.85                     | 0.57              |
| 46:e:767:ALA:HA    | 46:e:831:ASN:ND2   | 2.19                     | 0.57              |
| 11:K:50:ALA:HB1    | 21:U:66:VAL:HG11   | 1.86                     | 0.57              |
| 45:a:151:MET:HE3   | 50:x:36:C:H42      | 1.69                     | 0.57              |
| 45:a:359:GLN:HA    | 45:a:362:LYS:HD2   | 1.85                     | 0.57              |
| 46:e:972:GLU:O     | 46:e:975:LYS:CG    | 2.43                     | 0.57              |
| 46:e:1086:MET:HB2  | 46:e:1092:THR:HG21 | 1.87                     | 0.57              |
| 36:m:64:ILE:HG13   | 36:m:109:THR:HG21  | 1.87                     | 0.57              |
| 46:e:320:LEU:HB3   | 46:e:328:ILE:HG21  | 1.87                     | 0.57              |
| 26:Z:125:LYS:O     | 40:q:173:ARG:NH1   | 2.35                     | 0.57              |
| 45:a:936:ASP:HA    | 45:a:996:MET:HE1   | 1.86                     | 0.57              |
| 46:e:838:ILE:HB    | 46:e:864:HIS:C     | 2.29                     | 0.57              |
| 28:c:4:ARG:NH2     | 30:f:838:G:O6      | 2.38                     | 0.57              |
| 46:e:1340:TYR:O    | 46:e:1344:ILE:HG13 | 2.05                     | 0.57              |
| 30:f:1390:A:N6     | 30:f:1418:A:O2'    | 2.38                     | 0.57              |
| 30:f:2842:U:OP1    | 30:f:2844:C:N4     | 2.37                     | 0.57              |
| 30:f:2557:A:OP1    | 33:j:69:TYR:OH     | 2.24                     | 0.56              |
| 34:k:59:ASP:HB2    | 34:k:357:LYS:HE3   | 1.87                     | 0.56              |
| 46:e:1030:SER:O    | 46:e:1033:LYS:HG2  | 2.05                     | 0.56              |
| 51:z:51:LYS:O      | 51:z:52:GLU:C      | 2.47                     | 0.56              |
| 22:V:68:ARG:NH2    | 30:f:2219:A:OP2    | 2.38                     | 0.56              |
| 37:n:132:THR:HA    | 37:n:135:VAL:HG12  | 1.87                     | 0.56              |
| 45:a:893:LYS:CE    | 48:v:129:ASP:HB3   | 2.35                     | 0.56              |
| 50:y:13:U:H2'      | 50:y:14:A:H8       | 1.70                     | 0.56              |
| 4:D:43:PRO:HB2     | 30:f:728:G:H5''    | 1.86                     | 0.56              |
| 13:M:17:ARG:NH1    | 30:f:1634:G:N7     | 2.53                     | 0.56              |
| 46:e:314:LEU:CD1   | 46:e:358:VAL:HG22  | 2.35                     | 0.56              |
| 46:e:866:PHE:CD1   | 46:e:893:MET:HB2   | 2.40                     | 0.56              |
| 47:g:118:HIS:HD1   | 47:g:120:ASP:H     | 1.52                     | 0.56              |
| 17:Q:4:LEU:O       | 17:Q:79:ARG:NH2    | 2.38                     | 0.56              |
| 17:Q:55:LEU:HB2    | 17:Q:95:PRO:HD3    | 1.86                     | 0.56              |
| 26:Z:100:TYR:O     | 30:f:2895:G:O2'    | 2.24                     | 0.56              |
| 28:c:49:ARG:NH2    | 30:f:1793:C:OP2    | 2.38                     | 0.56              |
| 25:Y:5:LYS:HE2     | 25:Y:13:MET:HE1    | 1.87                     | 0.56              |
| 48:v:49:THR:HG22   | 48:v:56:LYS:HE3    | 1.87                     | 0.56              |
| 30:f:542:G:H1      | 30:f:549:U:H3      | 1.52                     | 0.56              |
| 30:f:1231:A:H5''   | 30:f:1232:C:H5'    | 1.86                     | 0.56              |
| 34:k:66:LYS:O      | 34:k:70:ARG:NH2    | 2.39                     | 0.56              |
| 46:e:1282:THR:HG21 | 46:e:1287:ARG:HG3  | 1.88                     | 0.56              |
| 46:e:1283:SER:CB   | 46:e:1286:MET:SD   | 2.94                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:r:143:SER:C     | 41:r:144:ASN:HD22  | 2.14                     | 0.55              |
| 46:e:751:VAL:O     | 46:e:754:ILE:CG2   | 2.35                     | 0.55              |
| 20:T:87:GLU:OE2    | 20:T:91:ARG:NH1    | 2.39                     | 0.55              |
| 30:f:831:G:O2'     | 30:f:1864:A:N3     | 2.39                     | 0.55              |
| 36:m:75:LEU:O      | 36:m:112:LYS:NZ    | 2.40                     | 0.55              |
| 45:a:90:THR:HG21   | 45:a:107:ASP:H     | 1.70                     | 0.55              |
| 46:e:972:GLU:HG3   | 46:e:975:LYS:CE    | 2.36                     | 0.55              |
| 46:e:1534:PHE:HB2  | 46:e:1539:LEU:HD13 | 1.75                     | 0.55              |
| 18:R:19:ARG:HD3    | 18:R:33:ARG:HB2    | 1.89                     | 0.55              |
| 45:a:885:LYS:O     | 45:a:889:ARG:HG3   | 2.06                     | 0.55              |
| 52:0:42:ARG:HG2    | 52:0:51:VAL:HG11   | 1.89                     | 0.55              |
| 46:e:989:GLU:C     | 46:e:1039:LEU:HD23 | 2.30                     | 0.55              |
| 8:H:19:VAL:HG12    | 8:H:105:LEU:HD22   | 1.89                     | 0.55              |
| 30:f:394:G:N1      | 30:f:397:A:OP2     | 2.39                     | 0.55              |
| 33:j:70:ARG:HD2    | 33:j:72:ARG:HE     | 1.72                     | 0.55              |
| 46:e:750:ALA:CA    | 46:e:764:PHE:HZ    | 1.94                     | 0.55              |
| 2:B:157[A]:GLU:OE2 | 2:B:160[A]:ARG:NH2 | 2.40                     | 0.55              |
| 14:N:44:ASN:ND2    | 43:t:4:SER:O       | 2.40                     | 0.55              |
| 30:f:2493:U:OP1    | 49:w:215:ARG:NH2   | 2.39                     | 0.55              |
| 33:j:111:THR:HB    | 33:j:136:ILE:HD13  | 1.87                     | 0.55              |
| 46:e:188:GLU:OE1   | 46:e:188:GLU:HA    | 2.06                     | 0.55              |
| 30:f:3045:G:OP1    | 34:k:19:ARG:NH2    | 2.39                     | 0.55              |
| 46:e:839:THR:OG1   | 46:e:865:THR:CG2   | 2.51                     | 0.55              |
| 49:w:48:ARG:HG2    | 49:w:159:LEU:HD23  | 1.88                     | 0.55              |
| 45:a:1005:LEU:HA   | 45:a:1008:LEU:HD12 | 1.89                     | 0.55              |
| 46:e:769:ALA:HB1   | 46:e:837:PHE:HB2   | 1.89                     | 0.54              |
| 46:e:1020:ALA:HB3  | 46:e:1023:ARG:CB   | 2.37                     | 0.54              |
| 53:1:43:UNK:C      | 53:1:45:UNK:H2     | 2.20                     | 0.54              |
| 30:f:3231:U:H2'    | 30:f:3232:G:H8     | 1.72                     | 0.54              |
| 41:r:61:SER:OG     | 41:r:63:GLU:OE1    | 2.25                     | 0.54              |
| 46:e:735:GLN:HG2   | 46:e:815:TYR:CB    | 2.30                     | 0.54              |
| 46:e:1534:PHE:HB2  | 46:e:1539:LEU:CD2  | 2.37                     | 0.54              |
| 30:f:3042:U:OP2    | 30:f:3092:C:N4     | 2.38                     | 0.54              |
| 40:q:57:VAL:HG12   | 40:q:68:LEU:HD22   | 1.88                     | 0.54              |
| 46:e:350:PRO:CB    | 46:e:355:PHE:CE2   | 2.91                     | 0.54              |
| 46:e:940:VAL:HB    | 46:e:976:LEU:HD11  | 1.89                     | 0.54              |
| 46:e:992:LEU:HG    | 46:e:996:GLU:HB2   | 1.90                     | 0.54              |
| 46:e:1066:ARG:NE   | 46:e:1111:GLN:NE2  | 2.51                     | 0.54              |
| 30:f:1222:G:C8     | 52:0:57:THR:CG2    | 2.91                     | 0.54              |
| 50:y:21:A:N6       | 50:y:48:C:OP2      | 2.40                     | 0.54              |
| 30:f:1256:G:O2'    | 51:z:124:THR:CB    | 2.55                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:f:2674:A:H5''  | 42:s:105:GLY:HA3   | 1.89                     | 0.54              |
| 46:e:371:LEU:CB   | 46:e:377:TRP:CD1   | 2.91                     | 0.54              |
| 30:f:68:C:OP2     | 30:f:301:G:N2      | 2.40                     | 0.54              |
| 30:f:76:G:O2'     | 43:t:100:ARG:NH1   | 2.37                     | 0.54              |
| 30:f:1352:A:H4'   | 30:f:1353:U:H5'    | 1.88                     | 0.54              |
| 30:f:2268:U:H3    | 30:f:2272:G:H22    | 1.55                     | 0.54              |
| 46:e:324:GLU:HB3  | 46:e:327:THR:HG21  | 1.90                     | 0.54              |
| 30:f:1257:C:C5'   | 51:z:124:THR:CB    | 2.68                     | 0.54              |
| 46:e:989:GLU:H    | 46:e:1034:TRP:CD1  | 2.26                     | 0.54              |
| 46:e:1534:PHE:HB2 | 46:e:1539:LEU:HD22 | 1.89                     | 0.54              |
| 46:e:1535:HIS:HB2 | 46:e:1538:CYS:HB2  | 1.90                     | 0.54              |
| 8:H:56:VAL:HG12   | 8:H:65:VAL:HG22    | 1.88                     | 0.54              |
| 17:Q:9:THR:HG23   | 17:Q:109:VAL:HG23  | 1.88                     | 0.54              |
| 34:k:140:ASP:OD1  | 34:k:141:GLY:N     | 2.36                     | 0.54              |
| 36:m:236:LEU:HA   | 36:m:239:ILE:HG12  | 1.90                     | 0.54              |
| 40:q:23:ARG:HE    | 40:q:39:LYS:HA     | 1.71                     | 0.54              |
| 46:e:149:LYS:HB3  | 46:e:150:PRO:HD3   | 1.90                     | 0.54              |
| 46:e:749:HIS:C    | 46:e:753:LEU:HD23  | 2.28                     | 0.54              |
| 46:e:839:THR:HA   | 46:e:865:THR:HG1   | 1.71                     | 0.54              |
| 36:m:270:LYS:HG2  | 36:m:273:ARG:HE    | 1.73                     | 0.54              |
| 7:G:17:ARG:HG2    | 7:G:22:HIS:HA      | 1.90                     | 0.53              |
| 30:f:1221:A:C4    | 52:0:12:PHE:CZ     | 2.95                     | 0.53              |
| 46:e:726:LEU:CD2  | 46:e:753:LEU:HD11  | 2.34                     | 0.53              |
| 46:e:884:ILE:HG23 | 46:e:939:PHE:HB2   | 1.91                     | 0.53              |
| 14:N:95:SER:OG    | 14:N:98:THR:OG1    | 2.25                     | 0.53              |
| 30:f:1221:A:C4    | 52:0:12:PHE:CE2    | 2.96                     | 0.53              |
| 30:f:2162:U:OP1   | 33:j:234:LYS:NZ    | 2.39                     | 0.53              |
| 46:e:1527:CYS:HA  | 46:e:1558:ILE:CG1  | 2.38                     | 0.53              |
| 30:f:1242:G:H1    | 45:a:519:THR:HG22  | 1.73                     | 0.53              |
| 30:f:3115:C:OP1   | 40:q:62:ARG:NH2    | 2.41                     | 0.53              |
| 46:e:1437:GLN:HB3 | 46:e:1462:VAL:HG11 | 1.90                     | 0.53              |
| 10:J:6:ASP:OD1    | 10:J:32:GLN:N      | 2.40                     | 0.53              |
| 10:J:44:LYS:HD2   | 30:f:2111:G:H1'    | 1.90                     | 0.53              |
| 30:f:1256:G:H4'   | 51:z:128:VAL:CB    | 2.39                     | 0.53              |
| 30:f:3268:A:OP1   | 37:n:46:ARG:NH2    | 2.35                     | 0.53              |
| 46:e:321:ASP:CG   | 46:e:329:TRP:NE1   | 2.66                     | 0.53              |
| 46:e:781:ASP:HB3  | 46:e:804:ILE:HG23  | 1.91                     | 0.53              |
| 46:e:1515:LEU:HB3 | 46:e:1520:ARG:HA   | 1.91                     | 0.53              |
| 2:B:75[A]:ALA:HB3 | 2:B:78[A]:ARG:HG2  | 1.90                     | 0.53              |
| 30:f:3375:A:O2'   | 30:f:3378:C:OP2    | 2.26                     | 0.53              |
| 34:k:284:ARG:NH1  | 34:k:293:ASN:O     | 2.42                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:e:388:LEU:HB3   | 46:e:402:LEU:HD13  | 1.89                     | 0.53              |
| 46:e:1441:ILE:O    | 46:e:1441:ILE:CG2  | 2.57                     | 0.53              |
| 50:y:3:G:O6        | 50:y:70:U:O4       | 2.27                     | 0.53              |
| 30:f:1156:C:OP2    | 38:o:94:LYS:NZ     | 2.40                     | 0.53              |
| 30:f:2245:C:O2'    | 33:j:220:GLY:O     | 2.26                     | 0.53              |
| 46:e:817:LEU:HD11  | 46:e:859:TYR:HA    | 1.90                     | 0.53              |
| 46:e:838:ILE:CG2   | 46:e:865:THR:N     | 2.72                     | 0.53              |
| 46:e:1527:CYS:CB   | 46:e:1558:ILE:HD13 | 2.33                     | 0.53              |
| 20:T:31:ARG:NH2    | 30:f:1598:G:OP2    | 2.42                     | 0.53              |
| 23:W:52:LYS:NZ     | 35:l:59:GLN:O      | 2.39                     | 0.53              |
| 36:m:120:LYS:O     | 36:m:248:ARG:NH2   | 2.42                     | 0.53              |
| 42:s:32:ARG:HD2    | 42:s:120:ILE:HA    | 1.91                     | 0.53              |
| 48:v:46:THR:HG22   | 48:v:57:VAL:HG22   | 1.90                     | 0.53              |
| 45:a:607:ASP:HB3   | 45:a:663:LYS:HB3   | 1.90                     | 0.53              |
| 46:e:773:PHE:HZ    | 46:e:908:TYR:HD2   | 1.57                     | 0.53              |
| 2:B:21[A]:SER:OG   | 30:f:1181:U:O4     | 2.27                     | 0.53              |
| 6:F:96:ASP:OD1     | 6:F:97:VAL:N       | 2.38                     | 0.53              |
| 46:e:754:ILE:HG13  | 46:e:829:ARG:CZ    | 2.38                     | 0.53              |
| 46:e:1024:LEU:HD11 | 46:e:1059:LEU:HD21 | 1.91                     | 0.53              |
| 10:J:47:ARG:HH21   | 10:J:58:HIS:HB2    | 1.73                     | 0.52              |
| 45:a:604:TYR:O     | 45:a:623:LYS:NZ    | 2.39                     | 0.52              |
| 46:e:867:PHE:O     | 46:e:871:LYS:N     | 2.41                     | 0.52              |
| 46:e:1282:THR:HG23 | 46:e:1287:ARG:HB2  | 1.89                     | 0.52              |
| 50:x:55:U:H2'      | 50:x:56:C:H2'      | 1.91                     | 0.52              |
| 50:y:13:U:H3       | 50:y:22:G:H1       | 1.56                     | 0.52              |
| 8:H:44:GLU:OE2     | 8:H:49:ASN:ND2     | 2.41                     | 0.52              |
| 46:e:1456:VAL:HG23 | 46:e:1480:ILE:HD11 | 1.92                     | 0.52              |
| 30:f:1288:U:H2'    | 30:f:1289:G:H8     | 1.74                     | 0.52              |
| 46:e:787:VAL:HG11  | 46:e:847:ASP:HA    | 1.91                     | 0.52              |
| 46:e:1192:ARG:HH21 | 46:e:1339:PRO:HA   | 1.73                     | 0.52              |
| 7:G:158:THR:OG1    | 41:r:169:LYS:NZ    | 2.42                     | 0.52              |
| 30:f:3230:G:H4'    | 44:u:132:LYS:HD3   | 1.92                     | 0.52              |
| 46:e:985:ILE:CB    | 46:e:1027:ILE:CB   | 2.87                     | 0.52              |
| 46:e:1421:LEU:HB3  | 46:e:1428:VAL:HG13 | 1.92                     | 0.52              |
| 46:e:1480:ILE:HD12 | 46:e:1481:THR:HG23 | 1.91                     | 0.52              |
| 2:B:61[A]:ALA:HA   | 2:B:70[A]:PRO:HD2  | 1.90                     | 0.52              |
| 45:a:612:MET:HE1   | 45:a:642:CYS:HB2   | 1.92                     | 0.52              |
| 46:e:371:LEU:HD12  | 46:e:377:TRP:HE1   | 1.73                     | 0.52              |
| 6:F:77:VAL:HG11    | 6:F:106:LEU:HD22   | 1.92                     | 0.52              |
| 27:b:2:VAL:N       | 27:b:90:HIS:O      | 2.42                     | 0.52              |
| 46:e:1080:LEU:HD21 | 46:e:1106:TYR:HD1  | 1.72                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:e:832:ASN:HD22  | 46:e:895:THR:HG23  | 1.74                     | 0.52              |
| 6:F:80:ARG:HB2     | 6:F:122:HIS:HB2    | 1.91                     | 0.52              |
| 30:f:2177:G:OP2    | 33:j:128:ARG:NH1   | 2.43                     | 0.52              |
| 45:a:111:TYR:HB2   | 45:a:125:LEU:HB2   | 1.91                     | 0.52              |
| 46:e:1167:LEU:HB2  | 46:e:1201:LEU:HD21 | 1.90                     | 0.52              |
| 3:C:118:GLN:NE2    | 3:C:147:GLU:OE2    | 2.39                     | 0.52              |
| 10:J:16:GLY:O      | 30:f:3050:U:O2'    | 2.27                     | 0.52              |
| 46:e:1400:PHE:HE1  | 46:e:1428:VAL:HG22 | 1.74                     | 0.52              |
| 9:I:94:TYR:OH      | 10:J:41:LYS:NZ     | 2.39                     | 0.52              |
| 24:X:44:LYS:NZ     | 30:f:1750:A:OP1    | 2.38                     | 0.52              |
| 45:a:618:SER:OG    | 45:a:646:SER:OG    | 2.26                     | 0.52              |
| 46:e:838:ILE:HD13  | 46:e:863:GLY:O     | 2.10                     | 0.52              |
| 46:e:839:THR:HB    | 46:e:866:PHE:N     | 2.22                     | 0.52              |
| 46:e:977:ARG:HG2   | 46:e:1006:LEU:HD13 | 1.92                     | 0.52              |
| 14:N:100:PRO:HG2   | 14:N:123:VAL:HG23  | 1.93                     | 0.51              |
| 17:Q:102:LYS:NZ    | 30:f:3373:U:OP2    | 2.38                     | 0.51              |
| 30:f:3160:U:H3     | 30:f:3290:G:H1     | 1.59                     | 0.51              |
| 7:G:136:ARG:HD2    | 7:G:139:ARG:HH12   | 1.74                     | 0.51              |
| 46:e:813:ILE:CG1   | 46:e:844:LEU:CD2   | 2.78                     | 0.51              |
| 46:e:972:GLU:N     | 46:e:975:LYS:HE2   | 2.22                     | 0.51              |
| 46:e:984:LEU:HD13  | 46:e:1000:LEU:HD23 | 1.91                     | 0.51              |
| 46:e:1282:THR:CG2  | 46:e:1287:ARG:HB2  | 2.40                     | 0.51              |
| 46:e:1464:ILE:HD12 | 46:e:1469:TRP:HE3  | 1.75                     | 0.51              |
| 29:d:20:ARG:HA     | 29:d:23:VAL:HG12   | 1.92                     | 0.51              |
| 36:m:54:ARG:NH1    | 36:m:147:ASP:O     | 2.42                     | 0.51              |
| 42:s:49:LYS:HG3    | 42:s:64:LYS:HD3    | 1.92                     | 0.51              |
| 46:e:731:LEU:C     | 46:e:731:LEU:CD1   | 2.84                     | 0.51              |
| 46:e:754:ILE:HD11  | 46:e:829:ARG:NE    | 2.25                     | 0.51              |
| 46:e:937:GLU:HG2   | 46:e:976:LEU:CD1   | 2.40                     | 0.51              |
| 27:b:75:VAL:HG23   | 27:b:76:LYS:HD2    | 1.92                     | 0.51              |
| 30:f:1778:G:O2'    | 30:f:1780:G:OP2    | 2.28                     | 0.51              |
| 36:m:50:ARG:NH2    | 36:m:72:ASP:OD2    | 2.43                     | 0.51              |
| 30:f:2540:A:N3     | 30:f:2541:U:N3     | 2.59                     | 0.51              |
| 30:f:3027:A:O2'    | 45:a:415:ASP:OD1   | 2.29                     | 0.51              |
| 46:e:793:ASN:HB3   | 46:e:955:LEU:HD13  | 1.93                     | 0.51              |
| 46:e:1019:ILE:HD12 | 46:e:1024:LEU:HD13 | 1.92                     | 0.51              |
| 46:e:1509:ALA:HB2  | 46:e:1532:ASN:HB3  | 1.92                     | 0.51              |
| 47:g:68:ARG:NH2    | 47:g:112:ASP:O     | 2.44                     | 0.51              |
| 19:S:70:LYS:HD2    | 30:f:585:A:H5''    | 1.91                     | 0.51              |
| 20:T:96:GLU:OE2    | 30:f:2555:G:N1     | 2.42                     | 0.51              |
| 21:U:67:ARG:NH2    | 32:i:97:A:OP1      | 2.44                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:b:41:ARG:NH1   | 30:f:284:A:OP2     | 2.40                     | 0.51              |
| 30:f:1234:G:N2    | 51:z:135:THR:CB    | 2.73                     | 0.51              |
| 33:j:241:ARG:HD3  | 45:a:866:LEU:HD21  | 1.91                     | 0.51              |
| 35:l:266:THR:HG23 | 35:l:267:VAL:HG13  | 1.92                     | 0.51              |
| 39:p:207:ASP:OD1  | 39:p:207:ASP:N     | 2.44                     | 0.51              |
| 40:q:22:SER:OG    | 40:q:39:LYS:NZ     | 2.44                     | 0.51              |
| 30:f:591:G:O2'    | 37:n:17:ALA:O      | 2.28                     | 0.51              |
| 30:f:1256:G:O3'   | 51:z:124:THR:CB    | 2.59                     | 0.51              |
| 45:a:704:LEU:HB3  | 45:a:938:ILE:HG13  | 1.91                     | 0.51              |
| 30:f:1661:G:H2'   | 30:f:1662:G:C8     | 2.46                     | 0.51              |
| 21:U:118:ILE:HD11 | 43:t:145:PHE:HE2   | 1.76                     | 0.51              |
| 30:f:2489:C:O2'   | 49:w:210:MET:SD    | 2.69                     | 0.51              |
| 30:f:2948:C:OP1   | 34:k:244:ARG:NH2   | 2.36                     | 0.51              |
| 32:i:29:U:H5''    | 43:t:27:ASP:HB3    | 1.92                     | 0.51              |
| 35:l:156:LEU:HD12 | 35:l:159:ILE:HD12  | 1.93                     | 0.51              |
| 45:a:579:TRP:HA   | 45:a:588:VAL:O     | 2.11                     | 0.51              |
| 46:e:1168:GLU:O   | 46:e:1171:TYR:HB3  | 2.11                     | 0.51              |
| 30:f:123:A:OP1    | 39:p:105:LYS:NZ    | 2.37                     | 0.50              |
| 30:f:544:C:H2'    | 30:f:547:G:H1      | 1.76                     | 0.50              |
| 39:p:52:TRP:O     | 39:p:57:ARG:NH1    | 2.44                     | 0.50              |
| 46:e:1020:ALA:HB3 | 46:e:1023:ARG:NH1  | 2.26                     | 0.50              |
| 46:e:1084:LEU:HB3 | 46:e:1130:ASN:HD22 | 1.75                     | 0.50              |
| 46:e:1527:CYS:CA  | 46:e:1558:ILE:CD1  | 2.87                     | 0.50              |
| 1:A:103:GLU:HG3   | 1:A:160:GLU:HB2    | 1.93                     | 0.50              |
| 30:f:2307:G:O2'   | 30:f:2310:U:OP2    | 2.28                     | 0.50              |
| 30:f:2828:G:OP2   | 41:r:7:ARG:NH2     | 2.44                     | 0.50              |
| 36:m:206:GLN:NE2  | 36:m:210:GLU:OE2   | 2.44                     | 0.50              |
| 46:e:1188:ILE:CG2 | 46:e:1192:ARG:NH2  | 2.74                     | 0.50              |
| 48:v:18:THR:HG22  | 48:v:83:PRO:HA     | 1.93                     | 0.50              |
| 30:f:655:C:H2'    | 30:f:656:A:H8      | 1.76                     | 0.50              |
| 35:l:126:ILE:O    | 35:l:129:THR:OG1   | 2.30                     | 0.50              |
| 46:e:816:ALA:HB1  | 46:e:841:VAL:HG21  | 1.93                     | 0.50              |
| 46:e:1192:ARG:HB2 | 46:e:1337:PHE:HD1  | 1.77                     | 0.50              |
| 3:C:107:LEU:HD12  | 3:C:152:GLU:HG3    | 1.92                     | 0.50              |
| 15:O:23:LYS:HG3   | 15:O:24:PRO:HD2    | 1.93                     | 0.50              |
| 30:f:110:G:OP2    | 43:t:73:ARG:NH2    | 2.42                     | 0.50              |
| 39:p:161:GLU:HA   | 39:p:164:VAL:HG22  | 1.93                     | 0.50              |
| 5:E:62:ARG:HH22   | 30:f:3067:C:H3'    | 1.77                     | 0.50              |
| 30:f:664:U:H2'    | 30:f:665:A:C8      | 2.47                     | 0.50              |
| 30:f:2897:A:H2'   | 30:f:2899:C:H5''   | 1.93                     | 0.50              |
| 46:e:1083:SER:HA  | 46:e:1086:MET:HE2  | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:N:26:ARG:NH1    | 30:f:938:C:OP2     | 2.44                     | 0.50              |
| 46:e:1149:THR:HG22 | 46:e:1339:PRO:HD3  | 1.94                     | 0.50              |
| 49:w:59:PRO:HD2    | 49:w:153:SER:HA    | 1.93                     | 0.50              |
| 2:B:74[A]:ARG:O    | 2:B:142[A]:SER:OG  | 2.23                     | 0.50              |
| 3:C:65:SER:OG      | 30:f:1447:G:OP1    | 2.28                     | 0.50              |
| 28:c:18:TYR:HB3    | 33:j:180:LEU:HD22  | 1.93                     | 0.50              |
| 30:f:3214:U:OP2    | 44:u:128:ARG:NH1   | 2.34                     | 0.50              |
| 46:e:546:ASN:N     | 46:e:579:ALA:HA    | 2.27                     | 0.50              |
| 46:e:1558:ILE:O    | 46:e:1559:PRO:C    | 2.54                     | 0.50              |
| 50:y:9:G:O2'       | 50:y:10:G:N7       | 2.42                     | 0.50              |
| 45:a:192:TYR:HE1   | 45:a:218:PRO:HD2   | 1.76                     | 0.50              |
| 46:e:841:VAL:HG12  | 46:e:862:PHE:CD2   | 2.40                     | 0.50              |
| 49:w:50:SER:HA     | 49:w:157:PHE:O     | 2.11                     | 0.50              |
| 31:h:44:C:H4'      | 36:m:152:ARG:HG3   | 1.93                     | 0.49              |
| 36:m:90:HIS:NE2    | 36:m:229:ASP:OD2   | 2.41                     | 0.49              |
| 45:a:29:ILE:HD12   | 45:a:80:LEU:HB3    | 1.94                     | 0.49              |
| 3:C:60:PHE:HB3     | 3:C:64:ASN:HB3     | 1.93                     | 0.49              |
| 30:f:2137:U:OP2    | 30:f:2142:A:N6     | 2.40                     | 0.49              |
| 47:g:116:LEU:HG    | 47:g:177:LEU:HD21  | 1.94                     | 0.49              |
| 24:X:2:ALA:N       | 30:f:1613:A:OP1    | 2.46                     | 0.49              |
| 46:e:831:ASN:HB2   | 46:e:834:ILE:HG13  | 1.94                     | 0.49              |
| 17:Q:77:ARG:HD2    | 17:Q:89:LEU:HD13   | 1.94                     | 0.49              |
| 46:e:839:THR:CA    | 46:e:865:THR:CB    | 2.82                     | 0.49              |
| 46:e:1527:CYS:CA   | 46:e:1558:ILE:HD13 | 2.42                     | 0.49              |
| 46:e:1527:CYS:HB3  | 46:e:1558:ILE:HD11 | 1.91                     | 0.49              |
| 18:R:104:ASN:ND2   | 30:f:1389:G:OP1    | 2.42                     | 0.49              |
| 27:b:7:THR:OG1     | 27:b:22:GLN:NE2    | 2.36                     | 0.49              |
| 30:f:1019:G:H1     | 30:f:1033:U:H3     | 1.59                     | 0.49              |
| 42:s:29:ARG:NH2    | 42:s:123:PHE:CZ    | 2.80                     | 0.49              |
| 2:B:46[A]:GLU:HG3  | 2:B:48[A]:PHE:H    | 1.77                     | 0.49              |
| 30:f:1569:U:H5'    | 30:f:1570:U:H5''   | 1.94                     | 0.49              |
| 32:i:156:U:OP2     | 39:p:84:ARG:NH2    | 2.45                     | 0.49              |
| 46:e:84:ASN:H      | 46:e:87:PHE:HB3    | 1.77                     | 0.49              |
| 46:e:1076:SER:HB2  | 46:e:1105:LEU:HD11 | 1.93                     | 0.49              |
| 7:G:99:SER:HG      | 7:G:101:CYS:HG     | 1.59                     | 0.49              |
| 46:e:59:GLU:HG2    | 46:e:103:TYR:CD1   | 2.47                     | 0.49              |
| 46:e:354:PHE:CE1   | 46:e:358:VAL:CG2   | 2.95                     | 0.49              |
| 46:e:1033:LYS:HG3  | 46:e:1034:TRP:N    | 2.26                     | 0.49              |
| 16:P:30:THR:HG23   | 16:P:91:SER:HB2    | 1.95                     | 0.49              |
| 30:f:348:A:N3      | 30:f:352:A:O2'     | 2.46                     | 0.49              |
| 42:s:90:GLN:NE2    | 42:s:170:ASP:OD1   | 2.45                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:e:819:LEU:O    | 46:e:823:LEU:CD1   | 2.60                     | 0.49              |
| 46:e:845:VAL:HG11 | 46:e:860:TYR:HA    | 1.93                     | 0.49              |
| 46:e:1527:CYS:HA  | 46:e:1558:ILE:CG2  | 2.40                     | 0.49              |
| 6:F:155:ARG:HB2   | 6:F:172:TYR:HD1    | 1.77                     | 0.49              |
| 17:Q:80:ASN:OD1   | 17:Q:81:GLU:N      | 2.45                     | 0.49              |
| 30:f:2185:G:O2'   | 30:f:2314:U:OP2    | 2.28                     | 0.49              |
| 30:f:2901:G:O2'   | 30:f:3024:A:N1     | 2.44                     | 0.49              |
| 35:l:292:SER:OG   | 35:l:294:GLU:OE1   | 2.31                     | 0.49              |
| 45:a:107:ASP:OD2  | 50:y:36:C:OP1      | 2.30                     | 0.49              |
| 45:a:970:ILE:HD11 | 45:a:1016:VAL:HG11 | 1.95                     | 0.49              |
| 49:w:138:VAL:HG21 | 49:w:144:LEU:HD23  | 1.94                     | 0.49              |
| 1:A:83:LYS:NZ     | 30:f:36:C:OP2      | 2.42                     | 0.49              |
| 4:D:56:LYS:NZ     | 30:f:674:G:O6      | 2.46                     | 0.49              |
| 14:N:94:ALA:HA    | 14:N:121:VAL:HG23  | 1.95                     | 0.49              |
| 16:P:9:SER:OG     | 16:P:10:ILE:N      | 2.38                     | 0.49              |
| 37:n:92:SER:OG    | 37:n:148:GLU:OE2   | 2.30                     | 0.49              |
| 30:f:505:G:OP1    | 35:l:320:ASN:ND2   | 2.43                     | 0.48              |
| 39:p:91:PHE:O     | 39:p:95:ASN:ND2    | 2.46                     | 0.48              |
| 4:D:131:ALA:HB1   | 4:D:135:GLN:H      | 1.78                     | 0.48              |
| 15:O:3:LYS:HD3    | 30:f:2617:U:H3'    | 1.95                     | 0.48              |
| 46:e:782:TYR:OH   | 46:e:1096:LEU:HG   | 2.13                     | 0.48              |
| 46:e:1554:CYS:SG  | 46:e:1556:SER:HB3  | 2.53                     | 0.48              |
| 7:G:108:ARG:O     | 7:G:112:ASN:HB2    | 2.12                     | 0.48              |
| 30:f:520:U:OP2    | 38:o:70:LYS:NZ     | 2.45                     | 0.48              |
| 30:f:1480:G:O2'   | 30:f:1871:U:O4     | 2.27                     | 0.48              |
| 34:k:145:GLU:HA   | 34:k:148:LEU:HB2   | 1.95                     | 0.48              |
| 19:S:49:ILE:HD11  | 19:S:71:VAL:HG22   | 1.96                     | 0.48              |
| 27:b:30:ALA:O     | 30:f:2767:U:O2'    | 2.29                     | 0.48              |
| 30:f:1814:A:H4'   | 30:f:1815:U:H5'    | 1.95                     | 0.48              |
| 30:f:2568:C:O2'   | 30:f:2569:A:O4'    | 2.27                     | 0.48              |
| 46:e:1527:CYS:CA  | 46:e:1558:ILE:CG1  | 2.84                     | 0.48              |
| 47:g:197:MET:HE3  | 47:g:218:ILE:HD12  | 1.96                     | 0.48              |
| 13:M:133:LYS:HE3  | 13:M:135:ARG:HD3   | 1.95                     | 0.48              |
| 30:f:1477:A:OP1   | 30:f:3075:G:O2'    | 2.31                     | 0.48              |
| 46:e:277:MET:SD   | 46:e:277:MET:C     | 2.95                     | 0.48              |
| 46:e:989:GLU:HB3  | 46:e:1034:TRP:HB3  | 1.44                     | 0.48              |
| 2:B:164[A]:SER:HG | 30:f:3181:C:HO2'   | 1.61                     | 0.48              |
| 40:q:18:VAL:HG12  | 40:q:27:VAL:HG22   | 1.94                     | 0.48              |
| 45:a:672:ASP:HA   | 49:w:98:LYS:CE     | 2.43                     | 0.48              |
| 45:a:893:LYS:HZ1  | 48:v:129:ASP:C     | 2.21                     | 0.48              |
| 46:e:77:ASN:OD1   | 46:e:77:ASN:N      | 2.46                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:e:865:THR:HB    | 46:e:868:LYS:HB2   | 1.94                     | 0.48              |
| 30:f:3198:U:O2     | 40:q:21:LYS:N      | 2.44                     | 0.48              |
| 32:i:9:A:H2'       | 32:i:10:A:C8       | 2.49                     | 0.48              |
| 46:e:203:GLU:O     | 46:e:207:ARG:HG3   | 2.13                     | 0.48              |
| 46:e:1080:LEU:HD13 | 46:e:1105:LEU:HB3  | 1.95                     | 0.48              |
| 4:D:102:ALA:HA     | 4:D:122:ILE:O      | 2.14                     | 0.48              |
| 27:b:45:ARG:NH1    | 30:f:283:G:OP1     | 2.46                     | 0.48              |
| 30:f:2209:U:C4     | 45:a:838:ARG:HD2   | 2.49                     | 0.48              |
| 42:s:38:GLU:HB2    | 42:s:45:PRO:HD3    | 1.95                     | 0.48              |
| 46:e:754:ILE:HD13  | 46:e:826:LEU:CD1   | 2.44                     | 0.48              |
| 3:C:62:ARG:NH1     | 30:f:412:G:OP1     | 2.45                     | 0.48              |
| 34:k:85:VAL:HG22   | 34:k:202:THR:HG22  | 1.95                     | 0.48              |
| 40:q:47:LYS:H      | 44:u:7:VAL:HG21    | 1.78                     | 0.48              |
| 46:e:719:ASN:HB3   | 46:e:722:ILE:HB    | 1.95                     | 0.48              |
| 47:g:146:ILE:HG13  | 47:g:147:LEU:HD12  | 1.96                     | 0.48              |
| 6:F:93:GLU:HG3     | 6:F:140:VAL:HG11   | 1.95                     | 0.48              |
| 30:f:2155:G:OP1    | 33:j:241:ARG:NH1   | 2.46                     | 0.48              |
| 33:j:117:GLU:HG2   | 33:j:124:GLY:H     | 1.79                     | 0.48              |
| 45:a:402:VAL:HG22  | 45:a:433:ILE:HG23  | 1.95                     | 0.48              |
| 46:e:754:ILE:HD11  | 46:e:826:LEU:HD13  | 1.95                     | 0.48              |
| 46:e:1499:HIS:O    | 46:e:1503:SER:HB2  | 2.14                     | 0.48              |
| 4:D:16:ARG:HB2     | 30:f:974:G:H5'     | 1.95                     | 0.47              |
| 30:f:1383:G:O3'    | 35:l:138:ARG:NH2   | 2.47                     | 0.47              |
| 35:l:304:GLN:NE2   | 35:l:306:THR:O     | 2.42                     | 0.47              |
| 42:s:29:ARG:O      | 42:s:30:LEU:C      | 2.57                     | 0.47              |
| 46:e:961:LEU:HB3   | 46:e:1006:LEU:HG   | 1.95                     | 0.47              |
| 46:e:1059:LEU:HB3  | 46:e:1060:MET:HE2  | 1.96                     | 0.47              |
| 46:e:1178:VAL:HG13 | 46:e:1184:ILE:HD13 | 1.94                     | 0.47              |
| 19:S:99:ARG:NH1    | 30:f:3275:U:O2'    | 2.48                     | 0.47              |
| 30:f:411:U:H2'     | 30:f:412:G:H8      | 1.79                     | 0.47              |
| 30:f:1805:C:H2'    | 30:f:1806:A:H8     | 1.79                     | 0.47              |
| 3:C:22:LEU:HD12    | 3:C:146:ILE:HD12   | 1.97                     | 0.47              |
| 17:Q:75:ILE:HG12   | 17:Q:93:VAL:HG22   | 1.96                     | 0.47              |
| 30:f:655:C:H2'     | 30:f:656:A:C8      | 2.49                     | 0.47              |
| 30:f:1230:G:H4'    | 52:O:34:SER:HA     | 1.96                     | 0.47              |
| 34:k:219:ALA:HB2   | 34:k:336:VAL:HG23  | 1.96                     | 0.47              |
| 43:t:76:THR:HG22   | 43:t:78:ALA:H      | 1.80                     | 0.47              |
| 46:e:781:ASP:OD2   | 46:e:783:ARG:HB2   | 2.14                     | 0.47              |
| 47:g:88:LEU:HD12   | 47:g:92:VAL:HG21   | 1.96                     | 0.47              |
| 13:M:23:VAL:HG12   | 13:M:45:GLY:HA3    | 1.94                     | 0.47              |
| 26:Z:124:LYS:NZ    | 30:f:2897:A:OP2    | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:f:712:G:OP1     | 43:t:174:ARG:NH1   | 2.47                     | 0.47              |
| 46:e:1045:PHE:HD2  | 46:e:1049:ARG:HG2  | 1.79                     | 0.47              |
| 47:g:14:GLY:HA2    | 47:g:198:VAL:HG13  | 1.96                     | 0.47              |
| 30:f:829:U:H3      | 30:f:895:A:H62     | 1.63                     | 0.47              |
| 41:r:66:GLU:OE1    | 41:r:69:ARG:NH2    | 2.47                     | 0.47              |
| 46:e:910:SER:HB2   | 46:e:955:LEU:HD11  | 1.97                     | 0.47              |
| 46:e:1446:PRO:HD2  | 46:e:1449:TYR:HD1  | 1.78                     | 0.47              |
| 48:v:48:LYS:HA     | 48:v:55:ALA:HA     | 1.96                     | 0.47              |
| 50:x:18:G:O4'      | 50:x:57:G:N2       | 2.47                     | 0.47              |
| 52:0:26:PHE:HZ     | 52:0:93:LEU:HA     | 1.80                     | 0.47              |
| 4:D:19:PRO:HB3     | 4:D:53:PHE:HA      | 1.96                     | 0.47              |
| 5:E:21:LYS:HE3     | 5:E:55:VAL:HA      | 1.97                     | 0.47              |
| 7:G:116:ARG:NH2    | 30:f:1096:U:OP2    | 2.48                     | 0.47              |
| 23:W:81:GLY:O      | 32:i:95:G:O2'      | 2.32                     | 0.47              |
| 30:f:358:G:N2      | 30:f:361:A:OP2     | 2.42                     | 0.47              |
| 34:k:211:GLN:NE2   | 34:k:283:TYR:O     | 2.44                     | 0.47              |
| 45:a:572:TYR:HB2   | 45:a:575:GLU:HG3   | 1.95                     | 0.47              |
| 46:e:115:ILE:O     | 46:e:119:LYS:HG3   | 2.14                     | 0.47              |
| 46:e:137:LEU:HD12  | 46:e:177:LEU:HD21  | 1.97                     | 0.47              |
| 46:e:1279:PHE:HE1  | 46:e:1290:PHE:CB   | 2.28                     | 0.47              |
| 1:A:5:LYS:HE2      | 22:V:40:VAL:HG21   | 1.97                     | 0.47              |
| 4:D:170:ARG:HD2    | 14:N:57:GLY:HA3    | 1.97                     | 0.47              |
| 4:D:180:ARG:NH2    | 30:f:2790:A:OP1    | 2.42                     | 0.47              |
| 9:I:18:PRO:HA      | 9:I:51:ALA:HA      | 1.97                     | 0.47              |
| 32:i:103:G:OP2     | 32:i:105:A:O2'     | 2.33                     | 0.47              |
| 32:i:126:A:O2'     | 32:i:129:C:N4      | 2.48                     | 0.47              |
| 33:j:32:LEU:HD13   | 33:j:163:ARG:HD3   | 1.96                     | 0.47              |
| 41:r:54:SER:HB3    | 41:r:135:ILE:HD11  | 1.97                     | 0.47              |
| 46:e:972:GLU:HA    | 46:e:975:LYS:CG    | 2.44                     | 0.47              |
| 46:e:1167:LEU:HB3  | 46:e:1201:LEU:HD11 | 1.96                     | 0.47              |
| 46:e:1188:ILE:HG22 | 46:e:1192:ARG:NH2  | 2.30                     | 0.47              |
| 46:e:1335:ASN:OD1  | 46:e:1335:ASN:O    | 2.32                     | 0.47              |
| 46:e:1409:ARG:H    | 46:e:1409:ARG:HE   | 1.62                     | 0.47              |
| 46:e:1523:PRO:O    | 46:e:1533:LYS:HB3  | 2.14                     | 0.47              |
| 49:w:89:ASP:O      | 49:w:92:LYS:HB2    | 2.14                     | 0.47              |
| 50:y:47:U:C4       | 50:y:50:C:H5''     | 2.49                     | 0.47              |
| 5:E:151:ARG:NH2    | 5:E:152:GLU:OE2    | 2.44                     | 0.47              |
| 46:e:1213:TYR:O    | 46:e:1217:ILE:HG12 | 2.13                     | 0.47              |
| 50:x:62:C:H2'      | 50:x:63:G:C8       | 2.50                     | 0.47              |
| 30:f:627:U:H2'     | 30:f:628:A:C8      | 2.50                     | 0.47              |
| 36:m:163:LEU:HD11  | 36:m:175:HIS:HB3   | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:m:234:ASP:OD1   | 36:m:234:ASP:N     | 2.47                     | 0.47              |
| 44:u:55:ARG:NH2    | 44:u:76:ALA:O      | 2.48                     | 0.47              |
| 46:e:1178:VAL:HA   | 46:e:1184:ILE:HG21 | 1.97                     | 0.47              |
| 5:E:128:LYS:NZ     | 30:f:1721:U:O4     | 2.38                     | 0.47              |
| 14:N:115:LYS:HA    | 30:f:715:A:H5''    | 1.97                     | 0.47              |
| 30:f:1907:C:O2     | 34:k:240:ARG:NH2   | 2.45                     | 0.47              |
| 30:f:2491:A:H1'    | 49:w:207:LYS:HE2   | 1.97                     | 0.47              |
| 44:u:38:ILE:HA     | 44:u:44:VAL:HG12   | 1.96                     | 0.47              |
| 47:g:219:GLU:HA    | 47:g:224:LEU:HD12  | 1.96                     | 0.47              |
| 30:f:835:G:O2'     | 30:f:857:G:N2      | 2.38                     | 0.46              |
| 30:f:2466:G:H5''   | 49:w:60:ARG:HH12   | 1.80                     | 0.46              |
| 42:s:131:MET:HE3   | 42:s:131:MET:HB3   | 1.81                     | 0.46              |
| 50:y:62:C:H2'      | 50:y:63:G:H8       | 1.80                     | 0.46              |
| 30:f:912:G:OP2     | 33:j:9:ARG:NH2     | 2.45                     | 0.46              |
| 35:l:326:ARG:O     | 38:o:41:ARG:NH2    | 2.48                     | 0.46              |
| 45:a:121:ASN:HD22  | 45:a:136:ARG:NH1   | 2.13                     | 0.46              |
| 45:a:660:CYS:SG    | 45:a:661:PHE:N     | 2.88                     | 0.46              |
| 46:e:1084:LEU:HD22 | 46:e:1130:ASN:HB3  | 1.98                     | 0.46              |
| 46:e:1448:ASN:HB2  | 46:e:1451:LEU:HD12 | 1.97                     | 0.46              |
| 3:C:67:ILE:HD11    | 3:C:80:LYS:HB3     | 1.97                     | 0.46              |
| 5:E:68:GLN:OE1     | 5:E:71:ARG:NH2     | 2.43                     | 0.46              |
| 14:N:96:LYS:HB2    | 14:N:96:LYS:HE2    | 1.70                     | 0.46              |
| 15:O:55:ALA:O      | 15:O:59:LYS:HB3    | 2.16                     | 0.46              |
| 2:B:59[A]:ARG:NH1  | 30:f:1307:G:OP1    | 2.48                     | 0.46              |
| 13:M:133:LYS:NZ    | 30:f:1808:G:OP2    | 2.44                     | 0.46              |
| 30:f:86:G:O2'      | 30:f:98:G:O6       | 2.32                     | 0.46              |
| 39:p:228:GLU:O     | 39:p:232:HIS:ND1   | 2.43                     | 0.46              |
| 41:r:54:SER:OG     | 41:r:130:ASP:O     | 2.33                     | 0.46              |
| 46:e:226:ASN:HB2   | 46:e:229:VAL:HB    | 1.97                     | 0.46              |
| 46:e:940:VAL:HG11  | 46:e:961:LEU:HD21  | 1.97                     | 0.46              |
| 46:e:1431:SER:HA   | 46:e:1439:LEU:O    | 2.14                     | 0.46              |
| 46:e:352:PRO:HG3   | 46:e:397:ASN:OD1   | 2.15                     | 0.46              |
| 46:e:755:ASN:OD1   | 46:e:829:ARG:NH1   | 2.39                     | 0.46              |
| 46:e:1439:LEU:HD13 | 46:e:1464:ILE:HD11 | 1.98                     | 0.46              |
| 50:x:62:C:H2'      | 50:x:63:G:H8       | 1.80                     | 0.46              |
| 4:D:35:PHE:HE1     | 30:f:1348:U:H5'    | 1.80                     | 0.46              |
| 12:L:55:GLU:HB2    | 12:L:108:LYS:HB3   | 1.98                     | 0.46              |
| 20:T:95:ILE:HD11   | 30:f:2555:G:N7     | 2.30                     | 0.46              |
| 30:f:2239:G:O2'    | 45:a:867:GLY:O     | 2.29                     | 0.46              |
| 36:m:207:TYR:HA    | 36:m:210:GLU:HG2   | 1.97                     | 0.46              |
| 44:u:48:GLY:HA3    | 44:u:53:VAL:HB     | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:e:1526:THR:O   | 46:e:1558:ILE:HG21 | 2.11                     | 0.46              |
| 12:L:74:TYR:HB3   | 12:L:77:LYS:HB2    | 1.98                     | 0.46              |
| 18:R:60:ASN:HB3   | 18:R:63:THR:HB     | 1.97                     | 0.46              |
| 30:f:1949:G:H1    | 30:f:2097:U:H3     | 1.63                     | 0.46              |
| 30:f:2815:G:N2    | 30:f:2818:U:O2     | 2.45                     | 0.46              |
| 45:a:4:ARG:NH1    | 45:a:118:SER:HA    | 2.30                     | 0.46              |
| 50:x:17:C:H42     | 50:x:55:U:H1'      | 1.81                     | 0.46              |
| 13:M:28:PRO:O     | 13:M:29:HIS:ND1    | 2.48                     | 0.46              |
| 18:R:9:ILE:HG12   | 18:R:63:THR:HG23   | 1.97                     | 0.46              |
| 30:f:297:G:OP2    | 30:f:297:G:N2      | 2.41                     | 0.46              |
| 36:m:119:TYR:OH   | 36:m:139:PRO:O     | 2.33                     | 0.46              |
| 46:e:750:ALA:C    | 46:e:764:PHE:CE2   | 2.93                     | 0.46              |
| 46:e:995:GLN:O    | 46:e:998:LYS:HG3   | 2.15                     | 0.46              |
| 46:e:1154:LYS:HA  | 46:e:1157:LYS:HD2  | 1.97                     | 0.46              |
| 46:e:1279:PHE:HE1 | 46:e:1290:PHE:HB2  | 1.80                     | 0.46              |
| 47:g:11:ASN:ND2   | 47:g:209:ASP:OD2   | 2.49                     | 0.46              |
| 30:f:696:C:OP2    | 35:l:119:ARG:NH2   | 2.49                     | 0.46              |
| 6:F:22:PRO:O      | 7:G:146:ASN:ND2    | 2.38                     | 0.46              |
| 12:L:16:ARG:NH1   | 30:f:216:G:OP1     | 2.45                     | 0.46              |
| 30:f:40:A:OP1     | 56:f:3401:SPD:N10  | 2.48                     | 0.46              |
| 30:f:1717:U:H2'   | 30:f:1718:G:C8     | 2.50                     | 0.46              |
| 31:h:7:G:OP1      | 36:m:33:ARG:NH1    | 2.48                     | 0.46              |
| 33:j:68:LYS:HE2   | 33:j:70:ARG:HH21   | 1.80                     | 0.46              |
| 38:o:86:VAL:O     | 38:o:114:GLY:HA2   | 2.16                     | 0.46              |
| 46:e:96:ALA:O     | 46:e:99:ILE:HG12   | 2.16                     | 0.46              |
| 48:v:104:ASN:OD1  | 48:v:105:MET:N     | 2.49                     | 0.46              |
| 1:A:62:TYR:OH     | 32:i:141:C:O3'     | 2.34                     | 0.45              |
| 2:B:39[A]:GLU:HG2 | 2:B:40[A]:GLU:HG2  | 1.97                     | 0.45              |
| 15:O:25:LYS:NZ    | 30:f:1106:G:O3'    | 2.44                     | 0.45              |
| 30:f:2218:G:H2'   | 30:f:2219:A:H8     | 1.80                     | 0.45              |
| 34:k:53:MET:HE2   | 34:k:53:MET:HB3    | 1.88                     | 0.45              |
| 17:Q:44:MET:O     | 17:Q:77:ARG:NH1    | 2.49                     | 0.45              |
| 36:m:65:ILE:HG12  | 36:m:74:VAL:HG22   | 1.99                     | 0.45              |
| 39:p:156:ASP:OD1  | 39:p:156:ASP:N     | 2.47                     | 0.45              |
| 45:a:101:LEU:HB2  | 45:a:116:PHE:HE2   | 1.81                     | 0.45              |
| 46:e:457:LYS:O    | 46:e:461:GLU:N     | 2.46                     | 0.45              |
| 49:w:92:LYS:HA    | 49:w:92:LYS:HD3    | 1.71                     | 0.45              |
| 1:A:159:ARG:HB3   | 1:A:164:LEU:HB2    | 1.98                     | 0.45              |
| 8:H:90:ARG:O      | 8:H:91:ASP:HB2     | 2.16                     | 0.45              |
| 8:H:107:PHE:O     | 8:H:108:TYR:C      | 2.58                     | 0.45              |
| 19:S:14:LEU:HD11  | 19:S:31:LYS:HB2    | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:f:494:G:H2'     | 30:f:495:G:H8      | 1.82                     | 0.45              |
| 30:f:1119:C:H2'    | 30:f:1120:A:H8     | 1.81                     | 0.45              |
| 30:f:2392:C:O2'    | 34:k:266:ARG:NH2   | 2.48                     | 0.45              |
| 36:m:83:LEU:HB3    | 36:m:88:ILE:HB     | 1.98                     | 0.45              |
| 46:e:1164:LEU:HD23 | 46:e:1164:LEU:H    | 1.82                     | 0.45              |
| 1:A:202:TYR:HB3    | 35:l:112:LYS:HG3   | 1.97                     | 0.45              |
| 30:f:448:U:O2      | 30:f:488:U:O2'     | 2.33                     | 0.45              |
| 30:f:1497:C:H2'    | 30:f:1498:A:H8     | 1.81                     | 0.45              |
| 46:e:102:ASP:OD1   | 46:e:207:ARG:CZ    | 2.65                     | 0.45              |
| 46:e:713:LEU:HG    | 46:e:717:LYS:HE3   | 1.98                     | 0.45              |
| 46:e:739:SER:HB3   | 46:e:742:ALA:HB3   | 1.98                     | 0.45              |
| 46:e:1192:ARG:CG   | 46:e:1270:TRP:CH2  | 2.80                     | 0.45              |
| 30:f:1008:U:O2'    | 41:r:35:ASP:OD2    | 2.33                     | 0.45              |
| 30:f:2697:A:H2'    | 30:f:2698:G:C8     | 2.52                     | 0.45              |
| 33:j:140:ASN:O     | 33:j:144:ASN:HA    | 2.16                     | 0.45              |
| 35:l:8:VAL:HG23    | 35:l:151:VAL:HG12  | 1.97                     | 0.45              |
| 37:n:175:LYS:O     | 44:u:117:ARG:NH2   | 2.50                     | 0.45              |
| 45:a:346:SER:HB2   | 45:a:564:VAL:HG13  | 1.98                     | 0.45              |
| 46:e:993:VAL:HG23  | 46:e:1048:VAL:HG21 | 1.99                     | 0.45              |
| 46:e:1327:ILE:O    | 46:e:1354:HIS:HA   | 2.17                     | 0.45              |
| 46:e:1507:GLU:HA   | 46:e:1514:ILE:HA   | 1.98                     | 0.45              |
| 13:M:22:LYS:NZ     | 13:M:132:SER:O     | 2.47                     | 0.45              |
| 30:f:3022:G:O2'    | 30:f:3031:G:O6     | 2.32                     | 0.45              |
| 31:h:119:U:OP2     | 36:m:258:LYS:NZ    | 2.45                     | 0.45              |
| 46:e:965:ASN:HB3   | 46:e:1010:PRO:HD2  | 1.99                     | 0.45              |
| 30:f:307:A:H2'     | 30:f:308:A:C8      | 2.52                     | 0.45              |
| 30:f:2094:C:H2'    | 30:f:2095:G:H8     | 1.81                     | 0.45              |
| 31:h:62:U:O2'      | 36:m:285:ARG:NH2   | 2.50                     | 0.45              |
| 33:j:14:SER:OG     | 33:j:15:ILE:N      | 2.50                     | 0.45              |
| 33:j:104:LEU:HD12  | 33:j:158:ILE:HD11  | 1.98                     | 0.45              |
| 23:W:30:GLN:NE2    | 30:f:904:A:OP2     | 2.50                     | 0.45              |
| 29:d:21:ARG:HA     | 29:d:21:ARG:HD2    | 1.80                     | 0.45              |
| 30:f:3116:G:OP1    | 30:f:3116:G:N2     | 2.43                     | 0.45              |
| 46:e:352:PRO:HG3   | 46:e:397:ASN:CG    | 2.41                     | 0.45              |
| 46:e:769:ALA:CB    | 46:e:837:PHE:HB2   | 2.46                     | 0.45              |
| 46:e:783:ARG:HA    | 46:e:786:LEU:HD12  | 1.97                     | 0.45              |
| 46:e:1155:LEU:O    | 46:e:1159:ILE:HG12 | 2.17                     | 0.45              |
| 4:D:180:ARG:HH22   | 30:f:2719:U:H5''   | 1.82                     | 0.45              |
| 30:f:520:U:O4      | 35:l:347:THR:OG1   | 2.34                     | 0.45              |
| 30:f:528:U:H2'     | 30:f:529:A:C8      | 2.51                     | 0.45              |
| 30:f:571:U:H2'     | 30:f:572:A:H8      | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:f:2964:G:N2     | 30:f:2967:A:OP2    | 2.41                     | 0.45              |
| 45:a:199:ILE:HG12  | 45:a:212:LYS:HE3   | 1.99                     | 0.45              |
| 46:e:248:LYS:HA    | 46:e:248:LYS:HD3   | 1.78                     | 0.45              |
| 8:H:42:LYS:NZ      | 30:f:1686:U:OP1    | 2.44                     | 0.45              |
| 22:V:53:TYR:HA     | 22:V:56:ARG:HG2    | 1.99                     | 0.45              |
| 30:f:1693:C:HO2'   | 30:f:1772:U:HO2'   | 1.65                     | 0.45              |
| 38:o:83:LEU:HD11   | 38:o:116:PHE:HB3   | 1.99                     | 0.45              |
| 38:o:232:ARG:O     | 38:o:235:PHE:N     | 2.48                     | 0.45              |
| 46:e:1276:LEU:HD13 | 46:e:1358:GLN:HG2  | 1.99                     | 0.45              |
| 47:g:106:ASN:OD1   | 47:g:150:SER:OG    | 2.34                     | 0.45              |
| 50:x:15:G:H22      | 50:x:48:C:H42      | 1.64                     | 0.45              |
| 40:q:120:ASP:OD1   | 40:q:120:ASP:N     | 2.44                     | 0.44              |
| 46:e:352:PRO:HG3   | 46:e:397:ASN:ND2   | 2.32                     | 0.44              |
| 46:e:972:GLU:HG3   | 46:e:975:LYS:HE2   | 1.99                     | 0.44              |
| 46:e:1024:LEU:HD23 | 46:e:1068:MET:HE1  | 1.99                     | 0.44              |
| 46:e:1059:LEU:HG   | 46:e:1065:VAL:HG21 | 1.99                     | 0.44              |
| 46:e:1184:ILE:HD11 | 46:e:1195:THR:HG23 | 1.99                     | 0.44              |
| 9:I:38:ALA:HB3     | 9:I:59:MET:HB2     | 1.99                     | 0.44              |
| 34:k:215:ILE:HD12  | 34:k:338:LEU:HD12  | 1.98                     | 0.44              |
| 40:q:41:ILE:HD13   | 40:q:71:VAL:HB     | 1.99                     | 0.44              |
| 45:a:704:LEU:HD23  | 45:a:938:ILE:HD11  | 1.99                     | 0.44              |
| 1:A:7:LEU:HD11     | 39:p:162:LEU:HA    | 1.99                     | 0.44              |
| 30:f:1134:G:O2'    | 30:f:2642:A:N3     | 2.44                     | 0.44              |
| 30:f:2660:G:OP1    | 30:f:2750:U:O2'    | 2.35                     | 0.44              |
| 46:e:990:VAL:CB    | 46:e:1039:LEU:HD11 | 2.28                     | 0.44              |
| 46:e:1316:THR:O    | 46:e:1320:LYS:HG3  | 2.17                     | 0.44              |
| 48:v:27:ARG:NH1    | 50:y:5:G:OP1       | 2.50                     | 0.44              |
| 30:f:19:U:H2'      | 30:f:20:A:C8       | 2.52                     | 0.44              |
| 30:f:1786:G:H2'    | 30:f:1787:A:C8     | 2.52                     | 0.44              |
| 39:p:95:ASN:OD1    | 39:p:98:ARG:NH2    | 2.51                     | 0.44              |
| 46:e:321:ASP:OD1   | 46:e:329:TRP:NE1   | 2.46                     | 0.44              |
| 46:e:857:ASP:HA    | 46:e:860:TYR:CD2   | 2.50                     | 0.44              |
| 46:e:933:LEU:HD13  | 46:e:972:GLU:HB2   | 1.98                     | 0.44              |
| 46:e:1192:ARG:HH21 | 46:e:1338:SER:C    | 2.25                     | 0.44              |
| 46:e:1372:LEU:HD13 | 46:e:1372:LEU:HA   | 1.74                     | 0.44              |
| 24:X:10:GLN:HA     | 24:X:13:GLU:HG2    | 1.99                     | 0.44              |
| 30:f:1264:G:N2     | 30:f:1265:U:O4     | 2.40                     | 0.44              |
| 30:f:2284:C:N4     | 30:f:2308:C:OP2    | 2.50                     | 0.44              |
| 48:v:30:GLY:H      | 48:v:41:ILE:HG22   | 1.82                     | 0.44              |
| 51:z:52:GLU:O      | 51:z:53:PHE:C      | 2.60                     | 0.44              |
| 9:I:128:ARG:NE     | 47:g:12:GLU:OE2    | 2.50                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:L:112:ASP:OD2    | 32:i:85:G:N1       | 2.49                     | 0.44              |
| 22:V:9:ILE:HD12     | 43:t:174:ARG:HB2   | 1.99                     | 0.44              |
| 25:Y:37:TYR:O       | 30:f:351:A:N6      | 2.48                     | 0.44              |
| 30:f:1888:U:H5''    | 34:k:247:ARG:HB2   | 2.00                     | 0.44              |
| 30:f:2960:C:H2'     | 30:f:2961:G:C8     | 2.53                     | 0.44              |
| 46:e:141:CYS:SG     | 46:e:221:LYS:CD    | 3.03                     | 0.44              |
| 46:e:1193:LEU:O     | 46:e:1196:THR:HG22 | 2.18                     | 0.44              |
| 46:e:1206:GLN:O     | 46:e:1210:ILE:HG13 | 2.17                     | 0.44              |
| 46:e:1400:PHE:HD1   | 46:e:1400:PHE:HA   | 1.61                     | 0.44              |
| 46:e:1403:ILE:HG23  | 46:e:1488:LEU:HD21 | 2.00                     | 0.44              |
| 50:x:60:U:H5''      | 50:x:61:C:H5       | 1.83                     | 0.44              |
| 2:B:74[A]:ARG:NH1   | 30:f:3008:A:OP2    | 2.51                     | 0.44              |
| 30:f:1899:G:O2'     | 30:f:2334:U:O4     | 2.25                     | 0.44              |
| 33:j:101:VAL:HG22   | 33:j:165:VAL:HG22  | 2.00                     | 0.44              |
| 33:j:135:ILE:HD12   | 33:j:149:ARG:HE    | 1.82                     | 0.44              |
| 36:m:205:SER:HB3    | 36:m:236:LEU:HD21  | 2.00                     | 0.44              |
| 41:r:184:LYS:HE2    | 41:r:184:LYS:HB2   | 1.86                     | 0.44              |
| 46:e:149:LYS:HB3    | 46:e:150:PRO:CD    | 2.47                     | 0.44              |
| 46:e:190:GLU:CB     | 46:e:208:TYR:HB2   | 2.48                     | 0.44              |
| 6:F:80:ARG:HG3      | 6:F:124:LEU:HD21   | 1.99                     | 0.44              |
| 9:I:129:VAL:O       | 9:I:133:SER:HB3    | 2.17                     | 0.44              |
| 14:N:36:GLY:HA3     | 14:N:40:HIS:CE1    | 2.53                     | 0.44              |
| 30:f:2357:A:H2'     | 30:f:2358:A:C8     | 2.53                     | 0.44              |
| 30:f:3379:C:H4'     | 34:k:315:GLY:HA2   | 1.98                     | 0.44              |
| 46:e:129:LEU:HA     | 46:e:129:LEU:HD23  | 1.85                     | 0.44              |
| 46:e:365:THR:HA     | 46:e:368:HIS:CD2   | 2.52                     | 0.44              |
| 46:e:684:SER:CB     | 46:e:715:LEU:HD13  | 2.48                     | 0.44              |
| 47:g:2:ALA:HA       | 47:g:204:ALA:O     | 2.16                     | 0.44              |
| 2:B:127[A]:LEU:HD22 | 6:F:156:VAL:HG13   | 2.00                     | 0.44              |
| 23:W:63:ARG:NH1     | 32:i:58:G:O6       | 2.50                     | 0.44              |
| 30:f:1259:A:N3      | 30:f:1280:C:O2'    | 2.50                     | 0.44              |
| 30:f:3322:A:H2'     | 30:f:3323:A:C8     | 2.53                     | 0.44              |
| 35:l:74:ILE:HD12    | 35:l:75:PRO:HD2    | 2.00                     | 0.44              |
| 39:p:104:GLU:HA     | 39:p:107:GLU:HG3   | 2.00                     | 0.44              |
| 47:g:119:PRO:O      | 47:g:139:ARG:NH1   | 2.50                     | 0.44              |
| 6:F:80:ARG:HD2      | 7:G:155:PRO:HA     | 2.00                     | 0.43              |
| 7:G:68:THR:OG1      | 7:G:69:LYS:N       | 2.51                     | 0.43              |
| 7:G:133:ALA:HB3     | 38:o:121:LYS:HB2   | 2.00                     | 0.43              |
| 30:f:1203:A:N3      | 30:f:2855:U:O2'    | 2.46                     | 0.43              |
| 30:f:2676:A:OP1     | 45:a:652:LYS:NZ    | 2.46                     | 0.43              |
| 46:e:182:LYS:HE2    | 46:e:182:LYS:HB3   | 1.89                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:e:354:PHE:O     | 46:e:358:VAL:HG23  | 2.18                     | 0.43              |
| 46:e:397:ASN:O     | 46:e:400:GLU:N     | 2.52                     | 0.43              |
| 17:Q:46:THR:HG22   | 17:Q:48:ASP:H      | 1.82                     | 0.43              |
| 30:f:595:G:OP2     | 38:o:30:ARG:NH1    | 2.51                     | 0.43              |
| 30:f:799:G:O2'     | 43:t:18:TRP:NE1    | 2.47                     | 0.43              |
| 39:p:82:LEU:HD13   | 39:p:222:PHE:HE2   | 1.84                     | 0.43              |
| 46:e:782:TYR:CE2   | 46:e:786:LEU:HD11  | 2.54                     | 0.43              |
| 49:w:37:GLY:O      | 49:w:202:GLY:N     | 2.52                     | 0.43              |
| 49:w:96:ASN:HD21   | 49:w:99:LEU:HD12   | 1.84                     | 0.43              |
| 8:H:20:SER:HA      | 8:H:23:THR:HG22    | 2.00                     | 0.43              |
| 15:O:14:ARG:NH2    | 30:f:1139:G:OP2    | 2.51                     | 0.43              |
| 30:f:710:A:H2'     | 30:f:711:A:C8      | 2.54                     | 0.43              |
| 30:f:2116:G:OP1    | 30:f:2118:C:N4     | 2.51                     | 0.43              |
| 30:f:3295:A:H2'    | 30:f:3296:A:C8     | 2.53                     | 0.43              |
| 46:e:545:ILE:CB    | 46:e:579:ALA:CA    | 2.90                     | 0.43              |
| 46:e:989:GLU:CA    | 46:e:1034:TRP:CD1  | 3.00                     | 0.43              |
| 46:e:1020:ALA:HB3  | 46:e:1023:ARG:HH11 | 1.83                     | 0.43              |
| 52:0:15:LEU:O      | 52:0:19:LEU:HG     | 2.18                     | 0.43              |
| 52:0:45:LEU:HB3    | 52:0:49:ALA:HB3    | 1.99                     | 0.43              |
| 53:1:42:UNK:O      | 53:1:43:UNK:C      | 2.66                     | 0.43              |
| 23:W:58:THR:OG1    | 23:W:59:THR:N      | 2.51                     | 0.43              |
| 30:f:911:C:OP1     | 33:j:14:SER:OG     | 2.32                     | 0.43              |
| 30:f:1222:G:N2     | 30:f:1285:G:O2'    | 2.51                     | 0.43              |
| 30:f:2514:U:OP2    | 30:f:2586:G:N2     | 2.50                     | 0.43              |
| 30:f:2768:U:H2'    | 30:f:2769:A:H8     | 1.83                     | 0.43              |
| 30:f:3016:A:H2'    | 30:f:3017:A:H8     | 1.83                     | 0.43              |
| 31:h:38:U:N3       | 31:h:41:G:OP2      | 2.41                     | 0.43              |
| 36:m:258:LYS:O     | 36:m:265:TYR:OH    | 2.31                     | 0.43              |
| 39:p:239:GLY:O     | 39:p:243:GLN:HB2   | 2.19                     | 0.43              |
| 46:e:545:ILE:C     | 46:e:582:SER:CB    | 2.90                     | 0.43              |
| 46:e:788:SER:HB2   | 46:e:911:ARG:HD3   | 2.00                     | 0.43              |
| 46:e:944:VAL:HG11  | 46:e:980:LEU:HD23  | 1.19                     | 0.43              |
| 46:e:1079:LEU:HD22 | 46:e:1079:LEU:HA   | 1.73                     | 0.43              |
| 46:e:1080:LEU:O    | 46:e:1084:LEU:HB2  | 2.19                     | 0.43              |
| 30:f:63:A:N3       | 30:f:78:U:O2'      | 2.43                     | 0.43              |
| 30:f:1237:G:H22    | 30:f:1251:A:H2     | 1.66                     | 0.43              |
| 30:f:1657:C:O2'    | 30:f:1797:A:OP2    | 2.30                     | 0.43              |
| 30:f:1666:G:H2'    | 30:f:1667:A:H8     | 1.83                     | 0.43              |
| 45:a:117:PHE:CD1   | 45:a:118:SER:N     | 2.86                     | 0.43              |
| 46:e:332:ASP:HB3   | 46:e:335:SER:HB3   | 2.00                     | 0.43              |
| 46:e:1066:ARG:HH22 | 46:e:1111:GLN:CB   | 1.92                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:e:1094:TYR:O    | 46:e:1098:LEU:HG  | 2.18                     | 0.43              |
| 9:I:117:PRO:HA     | 9:I:135:VAL:HG13  | 2.00                     | 0.43              |
| 20:T:95:ILE:HG21   | 20:T:95:ILE:HD13  | 1.81                     | 0.43              |
| 23:W:27:PHE:HA     | 23:W:34:CYS:HA    | 2.01                     | 0.43              |
| 30:f:1288:U:H2'    | 30:f:1289:G:C8    | 2.54                     | 0.43              |
| 30:f:2514:U:H5'    | 39:p:68:ARG:HG3   | 2.00                     | 0.43              |
| 30:f:2836:C:H5     | 30:f:2852:C:H42   | 1.67                     | 0.43              |
| 39:p:86:THR:HA     | 39:p:89:GLU:HG2   | 2.00                     | 0.43              |
| 45:a:391:LEU:HD23  | 45:a:391:LEU:HA   | 1.87                     | 0.43              |
| 46:e:303:ILE:HD13  | 46:e:345:VAL:HG12 | 2.01                     | 0.43              |
| 46:e:347:ARG:HB3   | 46:e:380:PHE:HE1  | 1.82                     | 0.43              |
| 46:e:728:GLN:O     | 46:e:732:GLN:N    | 2.38                     | 0.43              |
| 47:g:38:PHE:O      | 47:g:42:LEU:HB2   | 2.19                     | 0.43              |
| 1:A:68:ARG:HA      | 1:A:98:LEU:HD21   | 2.00                     | 0.43              |
| 4:D:124:LEU:HD13   | 4:D:127:LEU:HD23  | 2.01                     | 0.43              |
| 4:D:161:LYS:HA     | 4:D:161:LYS:HD3   | 1.82                     | 0.43              |
| 6:F:70:THR:OG1     | 44:u:55:ARG:NH1   | 2.51                     | 0.43              |
| 30:f:2218:G:H2'    | 30:f:2219:A:C8    | 2.54                     | 0.43              |
| 30:f:2875:U:H3     | 53:l:56:UNK:HA    | 1.84                     | 0.43              |
| 30:f:3358:U:H2'    | 30:f:3359:A:H8    | 1.84                     | 0.43              |
| 46:e:740:PRO:HG2   | 46:e:858:LEU:HD23 | 1.99                     | 0.43              |
| 46:e:915:LYS:HA    | 46:e:915:LYS:HD3  | 1.79                     | 0.43              |
| 48:v:80:MET:HE3    | 48:v:80:MET:HB3   | 1.75                     | 0.43              |
| 50:x:41:G:H2'      | 50:x:42:A:C8      | 2.54                     | 0.43              |
| 52:0:75:LYS:O      | 52:0:78:PRO:HD2   | 2.19                     | 0.43              |
| 30:f:716:A:OP1     | 30:f:752:C:O2'    | 2.37                     | 0.43              |
| 46:e:725:LYS:HD2   | 46:e:725:LYS:HA   | 1.76                     | 0.43              |
| 49:w:43:PRO:HD3    | 49:w:163:LEU:HD21 | 2.01                     | 0.43              |
| 52:0:67:LEU:HD22   | 52:0:67:LEU:HA    | 1.85                     | 0.43              |
| 1:A:158:HIS:HB3    | 1:A:161:ALA:HB3   | 2.00                     | 0.43              |
| 28:c:66:GLY:HA2    | 33:j:80:GLU:HG3   | 2.01                     | 0.43              |
| 30:f:1675:G:H2'    | 30:f:1676:A:H8    | 1.83                     | 0.43              |
| 30:f:1813:A:O2'    | 30:f:1816:A:N3    | 2.46                     | 0.43              |
| 30:f:2129:U:H2'    | 30:f:2130:G:C8    | 2.54                     | 0.43              |
| 30:f:3121:U:H1'    | 30:f:3122:A:H5''  | 2.01                     | 0.43              |
| 45:a:54:VAL:HG22   | 45:a:60:ILE:HG13  | 2.00                     | 0.43              |
| 46:e:351:SER:HG    | 46:e:354:PHE:HB2  | 1.80                     | 0.43              |
| 46:e:835:VAL:HG11  | 46:e:893:MET:HB3  | 2.01                     | 0.43              |
| 46:e:1066:ARG:HH21 | 46:e:1111:GLN:CD  | 2.15                     | 0.43              |
| 46:e:1257:LEU:HA   | 46:e:1260:GLU:HB3 | 2.01                     | 0.43              |
| 46:e:1511:CYS:SG   | 46:e:1535:HIS:CE1 | 3.12                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:y:68:C:H2'      | 50:y:69:G:C8       | 2.53                     | 0.43              |
| 3:C:56:ARG:NH2     | 3:C:75:GLU:OE2     | 2.51                     | 0.43              |
| 5:E:102:LEU:HD22   | 5:E:138:LEU:HD22   | 2.01                     | 0.43              |
| 10:J:34:SER:OG     | 30:f:3085:G:OP1    | 2.32                     | 0.43              |
| 24:X:2:ALA:N       | 24:X:51:LEU:O      | 2.52                     | 0.43              |
| 46:e:146:SER:O     | 46:e:150:PRO:HD2   | 2.18                     | 0.43              |
| 46:e:320:LEU:C     | 46:e:328:ILE:HD13  | 2.44                     | 0.43              |
| 51:z:55:GLY:O      | 51:z:56:ILE:C      | 2.62                     | 0.43              |
| 3:C:179:GLN:HA     | 3:C:182:ILE:HG22   | 2.00                     | 0.42              |
| 6:F:95:ARG:HB2     | 6:F:140:VAL:HG23   | 2.00                     | 0.42              |
| 8:H:81:LYS:HD2     | 8:H:90:ARG:NH1     | 2.33                     | 0.42              |
| 30:f:2747:A:H2'    | 30:f:2748:A:C8     | 2.54                     | 0.42              |
| 30:f:3233:C:H2'    | 30:f:3234:A:C8     | 2.55                     | 0.42              |
| 41:r:72:ALA:HB2    | 41:r:155:ALA:HB2   | 2.01                     | 0.42              |
| 46:e:990:VAL:HG21  | 46:e:1039:LEU:HD13 | 1.20                     | 0.42              |
| 46:e:1040:ALA:O    | 46:e:1041:TYR:HB2  | 2.18                     | 0.42              |
| 46:e:1194:LEU:HD23 | 46:e:1194:LEU:HA   | 1.77                     | 0.42              |
| 1:A:12:ARG:NH1     | 30:f:297:G:O6      | 2.46                     | 0.42              |
| 23:W:45:ARG:NH2    | 30:f:361:A:O3'     | 2.52                     | 0.42              |
| 27:b:28:TYR:HB3    | 27:b:69:VAL:HB     | 2.01                     | 0.42              |
| 30:f:760:G:O2'     | 30:f:770:G:N2      | 2.43                     | 0.42              |
| 46:e:153:ASN:O     | 46:e:157:GLU:HG2   | 2.18                     | 0.42              |
| 46:e:371:LEU:CD1   | 46:e:377:TRP:CZ2   | 2.90                     | 0.42              |
| 46:e:1248:VAL:HG21 | 46:e:1275:ILE:HD11 | 2.00                     | 0.42              |
| 50:x:68:C:H2'      | 50:x:69:G:C8       | 2.54                     | 0.42              |
| 52:0:14:LYS:HE3    | 52:0:52:LEU:HD11   | 2.00                     | 0.42              |
| 2:B:54[A]:TYR:OH   | 2:B:73[A]:PHE:O    | 2.37                     | 0.42              |
| 12:L:86:THR:OG1    | 12:L:94:SER:OG     | 2.36                     | 0.42              |
| 18:R:3:SER:OG      | 18:R:4:LEU:N       | 2.51                     | 0.42              |
| 21:U:78:LYS:HA     | 21:U:81:ARG:HG2    | 2.00                     | 0.42              |
| 22:V:18:THR:HG23   | 43:t:106:GLN:HB3   | 2.01                     | 0.42              |
| 28:c:44:LYS:NZ     | 30:f:1727:G:OP1    | 2.51                     | 0.42              |
| 30:f:2160:G:H2'    | 30:f:2161:G:H8     | 1.84                     | 0.42              |
| 30:f:2213:A:H2'    | 30:f:2214:A:C8     | 2.54                     | 0.42              |
| 30:f:2745:G:N2     | 30:f:2748:A:OP2    | 2.47                     | 0.42              |
| 35:l:276:LEU:HD23  | 35:l:276:LEU:HA    | 1.91                     | 0.42              |
| 44:u:47:ASP:HB2    | 44:u:55:ARG:HG3    | 2.02                     | 0.42              |
| 45:a:117:PHE:HD1   | 45:a:118:SER:O     | 2.02                     | 0.42              |
| 45:a:967:LEU:HD13  | 45:a:1005:LEU:HB2  | 2.01                     | 0.42              |
| 6:F:32:SER:HB2     | 6:F:36:ILE:HD12    | 2.01                     | 0.42              |
| 30:f:417:A:H2'     | 30:f:418:A:C8      | 2.54                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:f:1666:G:H2'   | 30:f:1667:A:C8     | 2.54                     | 0.42              |
| 34:k:106:TRP:O    | 34:k:137:TYR:OH    | 2.24                     | 0.42              |
| 45:a:549:LYS:HA   | 45:a:549:LYS:HD3   | 1.73                     | 0.42              |
| 46:e:282:ASN:HA   | 46:e:285:LYS:HD2   | 2.02                     | 0.42              |
| 9:I:80:ARG:HB2    | 9:I:99:ALA:HB3     | 2.00                     | 0.42              |
| 30:f:2442:G:H2'   | 30:f:2443:A:H8     | 1.83                     | 0.42              |
| 34:k:83:PRO:O     | 34:k:165:GLN:NE2   | 2.47                     | 0.42              |
| 36:m:6:ASP:OD1    | 36:m:6:ASP:N       | 2.48                     | 0.42              |
| 36:m:200:PHE:HB3  | 36:m:237:GLU:HG2   | 2.01                     | 0.42              |
| 46:e:47:LEU:HD11  | 46:e:82:PHE:HB3    | 2.02                     | 0.42              |
| 46:e:328:ILE:HG13 | 46:e:329:TRP:H     | 1.84                     | 0.42              |
| 46:e:354:PHE:CE2  | 46:e:355:PHE:CE1   | 3.07                     | 0.42              |
| 46:e:867:PHE:C    | 46:e:871:LYS:HA    | 2.19                     | 0.42              |
| 46:e:884:ILE:HD12 | 46:e:935:SER:HB3   | 1.79                     | 0.42              |
| 52:0:70:LEU:HB3   | 52:0:73:PHE:CD1    | 2.55                     | 0.42              |
| 6:F:137:ARG:HH21  | 30:f:1213:G:H5'    | 1.85                     | 0.42              |
| 30:f:1203:A:H2'   | 30:f:1204:A:C8     | 2.55                     | 0.42              |
| 30:f:3016:A:H2'   | 30:f:3017:A:C8     | 2.55                     | 0.42              |
| 30:f:3023:U:H2'   | 30:f:3024:A:H8     | 1.84                     | 0.42              |
| 30:f:3337:G:H4'   | 46:e:1377:ARG:HH21 | 1.84                     | 0.42              |
| 33:j:46:LYS:HD2   | 33:j:46:LYS:HA     | 1.81                     | 0.42              |
| 39:p:183:LYS:HB2  | 39:p:194:THR:HG23  | 2.01                     | 0.42              |
| 42:s:96:PHE:HB2   | 42:s:156:LYS:HE3   | 2.01                     | 0.42              |
| 46:e:990:VAL:H    | 46:e:1039:LEU:HD22 | 1.79                     | 0.42              |
| 3:C:182:ILE:HD12  | 3:C:182:ILE:HA     | 1.85                     | 0.42              |
| 4:D:36:LEU:O      | 4:D:40:THR:OG1     | 2.27                     | 0.42              |
| 8:H:41:ILE:HG21   | 8:H:54:VAL:HG21    | 2.02                     | 0.42              |
| 27:b:10:THR:HG21  | 27:b:72:LEU:HD13   | 2.01                     | 0.42              |
| 30:f:158:G:H2'    | 30:f:159:A:H8      | 1.85                     | 0.42              |
| 30:f:673:U:H2'    | 30:f:674:G:C8      | 2.55                     | 0.42              |
| 34:k:214:MET:HE3  | 34:k:214:MET:HB3   | 1.94                     | 0.42              |
| 35:l:261:VAL:HG23 | 35:l:262:TRP:CD1   | 2.55                     | 0.42              |
| 36:m:95:TRP:CE3   | 36:m:198:TYR:HB3   | 2.54                     | 0.42              |
| 36:m:144:VAL:HG11 | 36:m:171:LEU:HD13  | 2.01                     | 0.42              |
| 45:a:45:LYS:HG2   | 45:a:46:PRO:HD2    | 2.00                     | 0.42              |
| 45:a:601:TYR:HA   | 45:a:605:ILE:HB    | 2.02                     | 0.42              |
| 47:g:199:VAL:HG23 | 47:g:204:ALA:HB2   | 2.02                     | 0.42              |
| 52:0:61:ARG:HA    | 52:0:61:ARG:HD2    | 1.92                     | 0.42              |
| 1:A:90:ASN:ND2    | 30:f:2424:A:OP1    | 2.51                     | 0.42              |
| 18:R:45:ARG:O     | 30:f:1145:G:O2'    | 2.36                     | 0.42              |
| 27:b:10:THR:HA    | 27:b:20:HIS:HD2    | 1.84                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:f:129:U:H2'     | 30:f:130:A:C8     | 2.55                     | 0.42              |
| 30:f:1579:C:H2'    | 30:f:1580:A:C8    | 2.55                     | 0.42              |
| 46:e:219:LEU:HD12  | 46:e:219:LEU:HA   | 1.82                     | 0.42              |
| 46:e:1428:VAL:HG23 | 46:e:1443:PHE:HB2 | 2.00                     | 0.42              |
| 7:G:102:ARG:HD2    | 7:G:102:ARG:HA    | 1.77                     | 0.42              |
| 30:f:2413:A:H2'    | 30:f:2414:G:H8    | 1.85                     | 0.42              |
| 30:f:2923:U:O4     | 50:x:74:C:N3      | 2.52                     | 0.42              |
| 36:m:266:ALA:O     | 36:m:270:LYS:HB2  | 2.20                     | 0.42              |
| 46:e:876:PHE:HB3   | 46:e:924:VAL:HG21 | 2.01                     | 0.42              |
| 46:e:883:VAL:HG13  | 46:e:956:LEU:HB3  | 2.01                     | 0.42              |
| 46:e:974:THR:O     | 46:e:978:THR:HG23 | 2.19                     | 0.42              |
| 30:f:531:G:H2'     | 30:f:532:A:C8     | 2.55                     | 0.42              |
| 30:f:2852:C:N3     | 41:r:158:LYS:NZ   | 2.68                     | 0.42              |
| 46:e:957:CYS:O     | 46:e:961:LEU:HG   | 2.20                     | 0.42              |
| 48:v:51:5CT:H5     | 48:v:52:HIS:CE1   | 2.55                     | 0.42              |
| 3:C:116:HIS:HB3    | 3:C:149:VAL:HB    | 2.02                     | 0.41              |
| 6:F:110:MET:HE3    | 6:F:110:MET:HB3   | 1.95                     | 0.41              |
| 12:L:63:LYS:HA     | 12:L:63:LYS:HD3   | 1.92                     | 0.41              |
| 24:X:33:LYS:HA     | 24:X:33:LYS:HD3   | 1.84                     | 0.41              |
| 27:b:61:LYS:NZ     | 27:b:63:LYS:O     | 2.53                     | 0.41              |
| 30:f:296:A:N3      | 30:f:299:G:O2'    | 2.53                     | 0.41              |
| 30:f:1194:G:H2'    | 30:f:1195:A:C8    | 2.55                     | 0.41              |
| 30:f:2772:C:H4'    | 30:f:2773:C:H5'   | 2.02                     | 0.41              |
| 30:f:3218:A:H5''   | 30:f:3219:G:C5    | 2.55                     | 0.41              |
| 37:n:112:THR:HG23  | 37:n:115:GLU:H    | 1.85                     | 0.41              |
| 45:a:113:VAL:HB    | 45:a:123:ILE:HB   | 2.01                     | 0.41              |
| 45:a:840:LYS:HA    | 45:a:840:LYS:HD3  | 1.91                     | 0.41              |
| 46:e:936:VAL:HG22  | 46:e:960:LEU:HD13 | 2.01                     | 0.41              |
| 46:e:1510:ILE:HD12 | 46:e:1538:CYS:HB3 | 2.01                     | 0.41              |
| 46:e:1555:ARG:H    | 46:e:1555:ARG:HD2 | 1.83                     | 0.41              |
| 16:P:29:SER:OG     | 30:f:1730:G:O6    | 2.37                     | 0.41              |
| 16:P:73:GLY:N      | 16:P:76:GLU:OE1   | 2.42                     | 0.41              |
| 30:f:443:G:O6      | 30:f:490:C:N4     | 2.53                     | 0.41              |
| 30:f:689:U:O4      | 35:l:209:TYR:OH   | 2.35                     | 0.41              |
| 30:f:1660:C:H2'    | 30:f:1661:G:H8    | 1.85                     | 0.41              |
| 30:f:2205:U:O4     | 45:a:854:GLN:NE2  | 2.42                     | 0.41              |
| 30:f:2711:C:O2'    | 30:f:2744:U:OP1   | 2.38                     | 0.41              |
| 30:f:3163:A:N6     | 30:f:3288:G:O6    | 2.53                     | 0.41              |
| 42:s:55:ARG:O      | 42:s:58:GLY:N     | 2.53                     | 0.41              |
| 46:e:253:LYS:CB    | 46:e:254:ASN:ND2  | 2.83                     | 0.41              |
| 46:e:819:LEU:C     | 46:e:823:LEU:HD12 | 2.44                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:e:902:ASN:HD22  | 46:e:902:ASN:HA    | 1.62                     | 0.41              |
| 46:e:1319:TRP:CD1  | 46:e:1386:PHE:HE1  | 2.38                     | 0.41              |
| 1:A:98:LEU:HD22    | 1:A:128:LYS:HD2    | 2.02                     | 0.41              |
| 30:f:675:C:O2'     | 30:f:679:U:OP1     | 2.34                     | 0.41              |
| 30:f:1577:G:H2'    | 30:f:1578:C:H6     | 1.85                     | 0.41              |
| 30:f:2451:G:H2'    | 30:f:2452:G:C8     | 2.55                     | 0.41              |
| 30:f:3092:C:O2'    | 30:f:3094:A:OP2    | 2.28                     | 0.41              |
| 46:e:972:GLU:HB3   | 46:e:975:LYS:HE3   | 1.98                     | 0.41              |
| 46:e:1240:LEU:HD23 | 46:e:1241:PRO:HD2  | 2.00                     | 0.41              |
| 20:T:60:ARG:NH1    | 30:f:1593:A:OP1    | 2.53                     | 0.41              |
| 26:Z:100:TYR:OH    | 30:f:2848:G:OP1    | 2.29                     | 0.41              |
| 27:b:100:LYS:HE3   | 27:b:100:LYS:HB3   | 1.90                     | 0.41              |
| 30:f:3198:U:H1'    | 40:q:21:LYS:HB2    | 2.01                     | 0.41              |
| 35:l:6:VAL:N       | 35:l:20:LEU:O      | 2.48                     | 0.41              |
| 35:l:343:LYS:HE2   | 35:l:343:LYS:HB2   | 1.92                     | 0.41              |
| 44:u:93:LYS:HE3    | 44:u:93:LYS:HB2    | 1.87                     | 0.41              |
| 46:e:190:GLU:HG2   | 46:e:191:ASP:N     | 2.35                     | 0.41              |
| 46:e:397:ASN:O     | 46:e:398:SER:C     | 2.62                     | 0.41              |
| 46:e:735:GLN:HG2   | 46:e:815:TYR:CG    | 2.55                     | 0.41              |
| 46:e:1179:LEU:HG   | 46:e:1243:LYS:HB2  | 2.01                     | 0.41              |
| 30:f:20:A:H2'      | 30:f:21:G:C8       | 2.56                     | 0.41              |
| 30:f:1221:A:C4     | 52:0:12:PHE:HZ     | 2.38                     | 0.41              |
| 30:f:1764:U:H3'    | 30:f:1765:U:H4'    | 2.02                     | 0.41              |
| 34:k:284:ARG:HB3   | 34:k:323:MET:HB3   | 2.01                     | 0.41              |
| 41:r:52:LEU:HB3    | 41:r:136:PHE:HB2   | 2.02                     | 0.41              |
| 46:e:1279:PHE:CZ   | 46:e:1290:PHE:HB3  | 2.56                     | 0.41              |
| 49:w:122:ARG:HA    | 49:w:122:ARG:HD2   | 1.64                     | 0.41              |
| 50:x:34:I:H2'      | 50:x:35:G:C8       | 2.56                     | 0.41              |
| 2:B:8[A]:VAL:HG12  | 2:B:117[A]:ARG:HG3 | 2.02                     | 0.41              |
| 7:G:88:ARG:O       | 30:f:2722:U:O2'    | 2.35                     | 0.41              |
| 30:f:599:C:OP1     | 35:l:332:LYS:NZ    | 2.46                     | 0.41              |
| 30:f:745:C:H2'     | 30:f:746:A:H8      | 1.85                     | 0.41              |
| 30:f:1421:G:H2'    | 30:f:1422:G:H8     | 1.85                     | 0.41              |
| 30:f:1497:C:H2'    | 30:f:1498:A:C8     | 2.56                     | 0.41              |
| 46:e:189:ASN:HB2   | 46:e:192:THR:HG23  | 2.02                     | 0.41              |
| 46:e:1307:ILE:O    | 46:e:1311:ILE:HG12 | 2.20                     | 0.41              |
| 3:C:131:ARG:HG3    | 3:C:137:ASN:ND2    | 2.36                     | 0.41              |
| 9:I:135:VAL:HG23   | 47:g:102:SER:HB3   | 2.02                     | 0.41              |
| 14:N:75:LEU:HD23   | 14:N:75:LEU:HA     | 1.92                     | 0.41              |
| 31:h:53:U:O2'      | 31:h:55:A:N7       | 2.53                     | 0.41              |
| 42:s:75:LYS:O      | 42:s:79:ILE:HG13   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 43:t:57:VAL:HG23  | 43:t:147:ILE:HD12   | 2.02                     | 0.41              |
| 44:u:113:THR:OG1  | 44:u:114:ASP:N      | 2.52                     | 0.41              |
| 45:a:246:ASP:HB2  | 45:a:249:GLU:HB2    | 2.02                     | 0.41              |
| 45:a:702:GLY:HA2  | 45:a:952:TYR:O      | 2.21                     | 0.41              |
| 46:e:363:SER:HA   | 46:e:366:LYS:HE2    | 2.03                     | 0.41              |
| 46:e:713:LEU:HA   | 46:e:716:ALA:HB3    | 2.03                     | 0.41              |
| 18:R:99:ASN:O     | 30:f:1388:U:O2'     | 2.36                     | 0.41              |
| 22:V:5:THR:HG23   | 22:V:12:ASN:HB2     | 2.03                     | 0.41              |
| 30:f:352:A:H61    | 30:f:365:A:H5''     | 1.86                     | 0.41              |
| 35:l:34:ILE:HG21  | 35:l:120:TYR:HD2    | 1.85                     | 0.41              |
| 35:l:233:LEU:HD23 | 35:l:233:LEU:HA     | 1.90                     | 0.41              |
| 45:a:893:LYS:HA   | 45:a:893:LYS:HD3    | 1.48                     | 0.41              |
| 46:e:1302:ARG:HA  | 46:e:1302:ARG:HD2   | 1.89                     | 0.41              |
| 48:v:48:LYS:HD2   | 48:v:55:ALA:HB2     | 2.03                     | 0.41              |
| 1:A:18:VAL:HG13   | 1:A:19:LEU:HD12     | 2.01                     | 0.41              |
| 1:A:155:VAL:HG12  | 30:f:58:G:H4'       | 2.03                     | 0.41              |
| 5:E:7:GLN:NE2     | 5:E:35:ALA:O        | 2.53                     | 0.41              |
| 5:E:103:ARG:NH1   | 30:f:1722:U:OP2     | 2.53                     | 0.41              |
| 14:N:114:GLY:O    | 14:N:137:LYS:NZ     | 2.54                     | 0.41              |
| 30:f:946:U:H2'    | 30:f:947:G:H8       | 1.86                     | 0.41              |
| 30:f:1083:G:H2'   | 30:f:1084:A:C8      | 2.56                     | 0.41              |
| 30:f:2357:A:H2'   | 30:f:2358:A:H8      | 1.85                     | 0.41              |
| 31:h:84:A:H2'     | 31:h:85:G:C8        | 2.56                     | 0.41              |
| 40:q:9:GLN:HB3    | 40:q:52:LEU:HD11    | 2.01                     | 0.41              |
| 40:q:90:MET:HE3   | 40:q:179:ILE:HG22   | 2.01                     | 0.41              |
| 41:r:144:ASN:HD22 | 41:r:144:ASN:N      | 2.18                     | 0.41              |
| 45:a:597:THR:HG23 | 45:a:621:TRP:HE1    | 1.86                     | 0.41              |
| 46:e:690:THR:C    | 46:e:692:PHE:N      | 2.79                     | 0.41              |
| 46:e:913:LEU:HD23 | 46:e:913:LEU:HA     | 1.76                     | 0.41              |
| 46:e:1171:TYR:HB2 | 46:e:1201:LEU:HD13  | 2.03                     | 0.41              |
| 49:w:204:LEU:HB2  | 49:w:216:LEU:O      | 2.21                     | 0.41              |
| 50:y:62:C:H2'     | 50:y:63:G:C8        | 2.55                     | 0.41              |
| 2:B:121[A]:PRO:HA | 2:B:124[A]:LEU:HD12 | 2.03                     | 0.41              |
| 3:C:122:ALA:HB3   | 3:C:143:PRO:HB2     | 2.02                     | 0.41              |
| 4:D:155:MET:HE2   | 4:D:163:PRO:HB3     | 2.03                     | 0.41              |
| 6:F:90:MET:HE3    | 30:f:1213:G:H4'     | 2.03                     | 0.41              |
| 17:Q:20:LEU:HD11  | 17:Q:32:ALA:HB2     | 2.03                     | 0.41              |
| 23:W:31:LYS:NZ    | 30:f:815:G:OP2      | 2.52                     | 0.41              |
| 30:f:1238:C:C4'   | 51:z:139:VAL:CB     | 2.98                     | 0.41              |
| 30:f:3217:C:C5    | 30:f:3220:G:H1'     | 2.56                     | 0.41              |
| 36:m:108:ARG:CZ   | 36:m:253:PHE:HB2    | 2.51                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:a:601:TYR:HA    | 45:a:605:ILE:HD12  | 2.03                     | 0.41              |
| 46:e:780:ILE:HD11  | 46:e:904:VAL:HA    | 2.03                     | 0.41              |
| 46:e:838:ILE:HG22  | 46:e:865:THR:N     | 2.36                     | 0.41              |
| 46:e:849:ASN:HB3   | 46:e:855:PRO:HB3   | 2.02                     | 0.41              |
| 46:e:1240:LEU:HG   | 46:e:1290:PHE:CD1  | 2.56                     | 0.41              |
| 1:A:9:GLU:HG3      | 22:V:44:VAL:HG21   | 2.03                     | 0.40              |
| 1:A:174:ILE:HG21   | 30:f:63:A:H5'      | 2.04                     | 0.40              |
| 6:F:43:TYR:OH      | 31:h:96:U:OP1      | 2.35                     | 0.40              |
| 24:X:2:ALA:HB1     | 30:f:1747:G:H21    | 1.86                     | 0.40              |
| 30:f:129:U:H3      | 30:f:139:G:H1      | 1.69                     | 0.40              |
| 30:f:1660:C:H2'    | 30:f:1661:G:C8     | 2.56                     | 0.40              |
| 46:e:121:LEU:O     | 46:e:125:ILE:HG13  | 2.21                     | 0.40              |
| 46:e:388:LEU:O     | 46:e:391:LYS:C     | 2.64                     | 0.40              |
| 46:e:838:ILE:HG23  | 46:e:862:PHE:CD1   | 2.56                     | 0.40              |
| 46:e:1338:SER:HA   | 46:e:1339:PRO:HD3  | 1.87                     | 0.40              |
| 46:e:1527:CYS:N    | 46:e:1558:ILE:HD13 | 2.36                     | 0.40              |
| 48:v:96:ASP:OD1    | 48:v:96:ASP:N      | 2.54                     | 0.40              |
| 7:G:73:GLY:HA2     | 7:G:89:LEU:O       | 2.21                     | 0.40              |
| 18:R:4:LEU:HD12    | 18:R:5:PRO:HD2     | 2.02                     | 0.40              |
| 33:j:52:SER:HB3    | 33:j:191:LEU:HD23  | 2.02                     | 0.40              |
| 34:k:218:ILE:HG12  | 34:k:276:THR:HG23  | 2.03                     | 0.40              |
| 46:e:291:LEU:HD12  | 46:e:291:LEU:HA    | 1.84                     | 0.40              |
| 46:e:381:TRP:CZ3   | 46:e:408:ASN:HB3   | 2.56                     | 0.40              |
| 46:e:722:ILE:HD13  | 46:e:722:ILE:HA    | 1.78                     | 0.40              |
| 46:e:1066:ARG:CZ   | 46:e:1111:GLN:CB   | 2.72                     | 0.40              |
| 46:e:1084:LEU:HA   | 46:e:1087:CYS:HB2  | 2.04                     | 0.40              |
| 49:w:151:VAL:O     | 49:w:154:THR:OG1   | 2.33                     | 0.40              |
| 5:E:31:GLU:HA      | 5:E:34:GLN:HB2     | 2.03                     | 0.40              |
| 20:T:93:PHE:HD2    | 20:T:94:LEU:HD22   | 1.86                     | 0.40              |
| 26:Z:113:ARG:NH2   | 30:f:1190:A:H4'    | 2.36                     | 0.40              |
| 30:f:1249:G:H2'    | 30:f:1250:G:H8     | 1.86                     | 0.40              |
| 30:f:1596:C:H2'    | 30:f:1597:C:C6     | 2.56                     | 0.40              |
| 41:r:181:TYR:CE2   | 41:r:185:ARG:HD2   | 2.56                     | 0.40              |
| 43:t:189:GLU:HA    | 43:t:192:GLU:HG3   | 2.03                     | 0.40              |
| 45:a:25:ARG:HD2    | 50:y:35:G:OP1      | 2.22                     | 0.40              |
| 46:e:770:ILE:HD11  | 46:e:902:ASN:HB2   | 2.03                     | 0.40              |
| 46:e:844:LEU:C     | 46:e:844:LEU:HD23  | 2.46                     | 0.40              |
| 46:e:847:ASP:OD1   | 46:e:911:ARG:NH2   | 2.54                     | 0.40              |
| 50:x:68:C:H2'      | 50:x:69:G:H8       | 1.86                     | 0.40              |
| 2:B:189[A]:ASP:OD1 | 2:B:190[A]:VAL:N   | 2.53                     | 0.40              |
| 12:L:51:ARG:NH2    | 32:i:83:C:O2       | 2.54                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:S:37:THR:HG23   | 19:S:40:ASP:H      | 1.86                     | 0.40              |
| 30:f:94:G:H2'      | 30:f:95:A:C8       | 2.57                     | 0.40              |
| 30:f:182:U:H2'     | 30:f:183:G:H8      | 1.86                     | 0.40              |
| 41:r:44:ASP:OD1    | 41:r:44:ASP:N      | 2.48                     | 0.40              |
| 45:a:574:PHE:HB2   | 45:a:589:MET:HE1   | 2.02                     | 0.40              |
| 46:e:751:VAL:CA    | 46:e:754:ILE:HG22  | 2.27                     | 0.40              |
| 46:e:1167:LEU:CB   | 46:e:1201:LEU:HD21 | 2.51                     | 0.40              |
| 46:e:1192:ARG:HG2  | 46:e:1270:TRP:CZ2  | 2.47                     | 0.40              |
| 5:E:84:THR:HG22    | 30:f:1915:A:H5''   | 2.04                     | 0.40              |
| 30:f:1108:U:H2'    | 30:f:1109:U:C6     | 2.56                     | 0.40              |
| 30:f:2536:A:H2'    | 30:f:2537:U:C4     | 2.56                     | 0.40              |
| 32:i:63:G:H22      | 32:i:97:A:H2       | 1.69                     | 0.40              |
| 39:p:178:ALA:HB2   | 39:p:218:ILE:HG23  | 2.02                     | 0.40              |
| 46:e:347:ARG:HB3   | 46:e:380:PHE:CE1   | 2.56                     | 0.40              |
| 46:e:1441:ILE:O    | 46:e:1441:ILE:HG23 | 2.21                     | 0.40              |
| 46:e:1464:ILE:HD12 | 46:e:1469:TRP:CE3  | 2.54                     | 0.40              |
| 47:g:4:ARG:HD2     | 47:g:208:LEU:HA    | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 201/204 (98%) | 190 (94%) | 11 (6%) | 0        | 100         | 100 |
| 2   | B     | 195/199 (98%) | 192 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 3   | C     | 181/184 (98%) | 172 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 4   | D     | 183/186 (98%) | 176 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 5   | E     | 154/189 (82%) | 151 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 6   | F     | 169/172 (98%) | 163 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 7   | G     | 157/160 (98%) | 149 (95%) | 8 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 8   | H     | 98/121 (81%)  | 93 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 9   | I     | 134/137 (98%) | 132 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 10  | J     | 61/155 (39%)  | 61 (100%) | 0       | 0        | 100         | 100 |
| 11  | K     | 119/142 (84%) | 118 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 12  | L     | 123/127 (97%) | 119 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 13  | M     | 133/136 (98%) | 126 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 14  | N     | 146/149 (98%) | 136 (93%) | 10 (7%) | 0        | 100         | 100 |
| 15  | O     | 56/59 (95%)   | 52 (93%)  | 3 (5%)  | 1 (2%)   | 6           | 14  |
| 16  | P     | 94/105 (90%)  | 93 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 17  | Q     | 107/113 (95%) | 98 (92%)  | 9 (8%)  | 0        | 100         | 100 |
| 18  | R     | 125/130 (96%) | 123 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 19  | S     | 104/107 (97%) | 101 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 20  | T     | 110/121 (91%) | 108 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 21  | U     | 117/120 (98%) | 112 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 22  | V     | 97/100 (97%)  | 93 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 23  | W     | 79/88 (90%)   | 75 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 24  | X     | 75/78 (96%)   | 74 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 25  | Y     | 48/51 (94%)   | 46 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 26  | Z     | 50/128 (39%)  | 47 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 27  | b     | 101/106 (95%) | 95 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 28  | c     | 89/92 (97%)   | 85 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 29  | d     | 20/25 (80%)   | 19 (95%)  | 1 (5%)  | 0        | 100         | 100 |
| 33  | j     | 244/254 (96%) | 226 (93%) | 18 (7%) | 0        | 100         | 100 |
| 34  | k     | 384/387 (99%) | 363 (94%) | 21 (6%) | 0        | 100         | 100 |
| 35  | l     | 359/362 (99%) | 329 (92%) | 29 (8%) | 1 (0%)   | 36          | 58  |
| 36  | m     | 292/297 (98%) | 277 (95%) | 15 (5%) | 0        | 100         | 100 |
| 37  | n     | 163/176 (93%) | 154 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 38  | o     | 220/244 (90%) | 207 (94%) | 13 (6%) | 0        | 100         | 100 |
| 39  | p     | 231/256 (90%) | 220 (95%) | 11 (5%) | 0        | 100         | 100 |
| 40  | q     | 189/191 (99%) | 174 (92%) | 14 (7%) | 1 (0%)   | 24          | 46  |
| 41  | r     | 216/221 (98%) | 206 (95%) | 10 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 42  | s     | 167/174 (96%)    | 161 (96%)  | 5 (3%)   | 1 (1%)   | 21          | 42  |
| 43  | t     | 191/199 (96%)    | 174 (91%)  | 16 (8%)  | 1 (0%)   | 24          | 46  |
| 44  | u     | 134/138 (97%)    | 125 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 45  | a     | 842/1038 (81%)   | 827 (98%)  | 15 (2%)  | 0        | 100         | 100 |
| 46  | e     | 1519/1562 (97%)  | 1501 (99%) | 16 (1%)  | 2 (0%)   | 48          | 70  |
| 47  | g     | 223/245 (91%)    | 215 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 48  | v     | 139/157 (88%)    | 139 (100%) | 0        | 0        | 100         | 100 |
| 49  | w     | 214/217 (99%)    | 211 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 51  | z     | 144/165 (87%)    | 134 (93%)  | 9 (6%)   | 1 (1%)   | 18          | 38  |
| 52  | 0     | 117/312 (38%)    | 116 (99%)  | 0        | 1 (1%)   | 14          | 30  |
| All | All   | 9314/10279 (91%) | 8958 (96%) | 347 (4%) | 9 (0%)   | 49          | 70  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | z     | 88  | PRO  |
| 35  | l     | 4   | PRO  |
| 40  | q     | 107 | ASP  |
| 42  | s     | 108 | GLU  |
| 46  | e     | 437 | LYS  |
| 52  | 0     | 93  | LEU  |
| 46  | e     | 350 | PRO  |
| 15  | O     | 21  | ILE  |
| 43  | t     | 47  | ALA  |

### 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     | 175/176 (99%) | 175 (100%) | 0        | 100         | 100 |
| 2   | B     | 160/162 (99%) | 160 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | C     | 138/146 (94%)  | 138 (100%) | 0        | 100         | 100 |
| 4   | D     | 150/151 (99%)  | 150 (100%) | 0        | 100         | 100 |
| 5   | E     | 129/154 (84%)  | 129 (100%) | 0        | 100         | 100 |
| 6   | F     | 155/156 (99%)  | 155 (100%) | 0        | 100         | 100 |
| 7   | G     | 135/137 (98%)  | 135 (100%) | 0        | 100         | 100 |
| 8   | H     | 87/107 (81%)   | 87 (100%)  | 0        | 100         | 100 |
| 9   | I     | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 10  | J     | 54/129 (42%)   | 54 (100%)  | 0        | 100         | 100 |
| 11  | K     | 104/118 (88%)  | 104 (100%) | 0        | 100         | 100 |
| 12  | L     | 108/110 (98%)  | 108 (100%) | 0        | 100         | 100 |
| 13  | M     | 112/116 (97%)  | 112 (100%) | 0        | 100         | 100 |
| 14  | N     | 117/119 (98%)  | 117 (100%) | 0        | 100         | 100 |
| 15  | O     | 46/47 (98%)    | 46 (100%)  | 0        | 100         | 100 |
| 16  | P     | 81/88 (92%)    | 81 (100%)  | 0        | 100         | 100 |
| 17  | Q     | 92/97 (95%)    | 92 (100%)  | 0        | 100         | 100 |
| 18  | R     | 107/111 (96%)  | 107 (100%) | 0        | 100         | 100 |
| 19  | S     | 90/91 (99%)    | 90 (100%)  | 0        | 100         | 100 |
| 20  | T     | 95/103 (92%)   | 95 (100%)  | 0        | 100         | 100 |
| 21  | U     | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 22  | V     | 80/82 (98%)    | 80 (100%)  | 0        | 100         | 100 |
| 23  | W     | 67/71 (94%)    | 67 (100%)  | 0        | 100         | 100 |
| 24  | X     | 68/69 (99%)    | 68 (100%)  | 0        | 100         | 100 |
| 25  | Y     | 45/46 (98%)    | 45 (100%)  | 0        | 100         | 100 |
| 26  | Z     | 45/116 (39%)   | 45 (100%)  | 0        | 100         | 100 |
| 27  | b     | 87/91 (96%)    | 87 (100%)  | 0        | 100         | 100 |
| 28  | c     | 71/72 (99%)    | 71 (100%)  | 0        | 100         | 100 |
| 29  | d     | 20/23 (87%)    | 20 (100%)  | 0        | 100         | 100 |
| 33  | j     | 189/196 (96%)  | 189 (100%) | 0        | 100         | 100 |
| 34  | k     | 321/323 (99%)  | 321 (100%) | 0        | 100         | 100 |
| 35  | l     | 288/289 (100%) | 288 (100%) | 0        | 100         | 100 |
| 36  | m     | 241/245 (98%)  | 241 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 37  | n     | 139/155 (90%)   | 139 (100%) | 0        | 100         | 100 |
| 38  | o     | 186/205 (91%)   | 186 (100%) | 0        | 100         | 100 |
| 39  | p     | 187/208 (90%)   | 187 (100%) | 0        | 100         | 100 |
| 40  | q     | 168/171 (98%)   | 168 (100%) | 0        | 100         | 100 |
| 41  | r     | 185/187 (99%)   | 184 (100%) | 1 (0%)   | 81          | 92  |
| 42  | s     | 145/150 (97%)   | 142 (98%)  | 3 (2%)   | 47          | 73  |
| 43  | t     | 154/159 (97%)   | 154 (100%) | 0        | 100         | 100 |
| 44  | u     | 107/109 (98%)   | 107 (100%) | 0        | 100         | 100 |
| 45  | a     | 678/949 (71%)   | 675 (100%) | 3 (0%)   | 84          | 93  |
| 46  | e     | 1149/1451 (79%) | 1055 (92%) | 94 (8%)  | 10          | 24  |
| 47  | g     | 180/211 (85%)   | 180 (100%) | 0        | 100         | 100 |
| 48  | v     | 119/132 (90%)   | 118 (99%)  | 1 (1%)   | 73          | 88  |
| 49  | w     | 197/198 (100%)  | 196 (100%) | 1 (0%)   | 81          | 92  |
| 52  | 0     | 104/254 (41%)   | 94 (90%)   | 10 (10%) | 8           | 17  |
| All | All   | 7563/8690 (87%) | 7450 (98%) | 113 (2%) | 55          | 80  |

All (113) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | r     | 112 | GLN  |
| 42  | s     | 29  | ARG  |
| 42  | s     | 55  | ARG  |
| 42  | s     | 60  | ARG  |
| 45  | a     | 98  | ASP  |
| 45  | a     | 136 | ARG  |
| 45  | a     | 893 | LYS  |
| 46  | e     | 77  | ASN  |
| 46  | e     | 105 | VAL  |
| 46  | e     | 125 | ILE  |
| 46  | e     | 156 | THR  |
| 46  | e     | 178 | LEU  |
| 46  | e     | 227 | LYS  |
| 46  | e     | 229 | VAL  |
| 46  | e     | 254 | ASN  |
| 46  | e     | 264 | VAL  |
| 46  | e     | 277 | MET  |
| 46  | e     | 281 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | e     | 299 | THR  |
| 46  | e     | 309 | VAL  |
| 46  | e     | 327 | THR  |
| 46  | e     | 372 | ASP  |
| 46  | e     | 387 | ARG  |
| 46  | e     | 397 | ASN  |
| 46  | e     | 412 | PHE  |
| 46  | e     | 707 | LYS  |
| 46  | e     | 730 | ILE  |
| 46  | e     | 731 | LEU  |
| 46  | e     | 736 | VAL  |
| 46  | e     | 737 | TYR  |
| 46  | e     | 738 | PHE  |
| 46  | e     | 743 | LYS  |
| 46  | e     | 754 | ILE  |
| 46  | e     | 757 | CYS  |
| 46  | e     | 760 | THR  |
| 46  | e     | 764 | PHE  |
| 46  | e     | 770 | ILE  |
| 46  | e     | 771 | GLU  |
| 46  | e     | 782 | TYR  |
| 46  | e     | 785 | SER  |
| 46  | e     | 799 | THR  |
| 46  | e     | 801 | ASP  |
| 46  | e     | 826 | LEU  |
| 46  | e     | 844 | LEU  |
| 46  | e     | 858 | LEU  |
| 46  | e     | 861 | ASP  |
| 46  | e     | 862 | PHE  |
| 46  | e     | 867 | PHE  |
| 46  | e     | 869 | HIS  |
| 46  | e     | 895 | THR  |
| 46  | e     | 902 | ASN  |
| 46  | e     | 924 | VAL  |
| 46  | e     | 933 | LEU  |
| 46  | e     | 950 | THR  |
| 46  | e     | 955 | LEU  |
| 46  | e     | 973 | ILE  |
| 46  | e     | 979 | LEU  |
| 46  | e     | 987 | ILE  |
| 46  | e     | 989 | GLU  |
| 46  | e     | 993 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | e     | 998  | LYS  |
| 46  | e     | 1000 | LEU  |
| 46  | e     | 1006 | LEU  |
| 46  | e     | 1028 | PHE  |
| 46  | e     | 1033 | LYS  |
| 46  | e     | 1059 | LEU  |
| 46  | e     | 1075 | LEU  |
| 46  | e     | 1077 | GLU  |
| 46  | e     | 1079 | LEU  |
| 46  | e     | 1094 | TYR  |
| 46  | e     | 1102 | CYS  |
| 46  | e     | 1123 | TYR  |
| 46  | e     | 1132 | ILE  |
| 46  | e     | 1179 | LEU  |
| 46  | e     | 1189 | ASN  |
| 46  | e     | 1195 | THR  |
| 46  | e     | 1242 | GLN  |
| 46  | e     | 1252 | VAL  |
| 46  | e     | 1258 | GLU  |
| 46  | e     | 1274 | LEU  |
| 46  | e     | 1294 | LEU  |
| 46  | e     | 1300 | ILE  |
| 46  | e     | 1303 | MET  |
| 46  | e     | 1367 | THR  |
| 46  | e     | 1372 | LEU  |
| 46  | e     | 1379 | LEU  |
| 46  | e     | 1391 | ILE  |
| 46  | e     | 1400 | PHE  |
| 46  | e     | 1408 | ASP  |
| 46  | e     | 1409 | ARG  |
| 46  | e     | 1419 | ILE  |
| 46  | e     | 1421 | LEU  |
| 46  | e     | 1428 | VAL  |
| 46  | e     | 1439 | LEU  |
| 46  | e     | 1454 | ILE  |
| 46  | e     | 1464 | ILE  |
| 46  | e     | 1470 | LYS  |
| 46  | e     | 1477 | GLN  |
| 46  | e     | 1480 | ILE  |
| 46  | e     | 1527 | CYS  |
| 46  | e     | 1539 | LEU  |
| 48  | v     | 54   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | w     | 92  | LYS  |
| 52  | 0     | 30  | VAL  |
| 52  | 0     | 51  | VAL  |
| 52  | 0     | 52  | LEU  |
| 52  | 0     | 67  | LEU  |
| 52  | 0     | 76  | LEU  |
| 52  | 0     | 80  | VAL  |
| 52  | 0     | 93  | LEU  |
| 52  | 0     | 95  | GLU  |
| 52  | 0     | 105 | VAL  |
| 52  | 0     | 189 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 95     | GLN  |
| 2   | B     | 26[A]  | GLN  |
| 2   | B     | 193[A] | GLN  |
| 3   | C     | 55     | GLN  |
| 3   | C     | 97     | ASN  |
| 4   | D     | 5      | HIS  |
| 5   | E     | 150    | GLN  |
| 7   | G     | 66     | ASN  |
| 7   | G     | 149    | GLN  |
| 8   | H     | 87     | ASN  |
| 8   | H     | 101    | ASN  |
| 11  | K     | 65     | GLN  |
| 11  | K     | 85     | GLN  |
| 13  | M     | 122    | HIS  |
| 13  | M     | 127    | ASN  |
| 14  | N     | 38     | GLN  |
| 15  | O     | 12     | GLN  |
| 15  | O     | 17     | HIS  |
| 17  | Q     | 15     | ASN  |
| 17  | Q     | 21     | HIS  |
| 18  | R     | 35     | GLN  |
| 18  | R     | 49     | ASN  |
| 20  | T     | 61     | GLN  |
| 21  | U     | 16     | GLN  |
| 21  | U     | 59     | ASN  |
| 21  | U     | 99     | GLN  |
| 23  | W     | 12     | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | W     | 13  | ASN  |
| 25  | Y     | 4   | GLN  |
| 25  | Y     | 20  | ASN  |
| 27  | b     | 3   | ASN  |
| 27  | b     | 22  | GLN  |
| 27  | b     | 102 | GLN  |
| 34  | k     | 139 | GLN  |
| 34  | k     | 198 | HIS  |
| 34  | k     | 224 | HIS  |
| 35  | l     | 5   | GLN  |
| 35  | l     | 196 | ASN  |
| 35  | l     | 316 | ASN  |
| 38  | o     | 64  | GLN  |
| 38  | o     | 225 | GLN  |
| 38  | o     | 244 | ASN  |
| 39  | p     | 77  | GLN  |
| 40  | q     | 49  | ASN  |
| 40  | q     | 169 | ASN  |
| 40  | q     | 183 | HIS  |
| 42  | s     | 43  | GLN  |
| 42  | s     | 62  | ASN  |
| 42  | s     | 90  | GLN  |
| 44  | u     | 62  | GLN  |
| 45  | a     | 94  | GLN  |
| 45  | a     | 121 | ASN  |
| 45  | a     | 147 | GLN  |
| 45  | a     | 382 | GLN  |
| 45  | a     | 395 | ASN  |
| 45  | a     | 438 | ASN  |
| 45  | a     | 562 | HIS  |
| 46  | e     | 13  | ASN  |
| 46  | e     | 79  | ASN  |
| 46  | e     | 174 | GLN  |
| 46  | e     | 189 | ASN  |
| 46  | e     | 254 | ASN  |
| 46  | e     | 368 | HIS  |
| 46  | e     | 403 | ASN  |
| 46  | e     | 795 | HIS  |
| 46  | e     | 805 | ASN  |
| 46  | e     | 810 | GLN  |
| 46  | e     | 832 | ASN  |
| 46  | e     | 888 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | e     | 902  | ASN  |
| 46  | e     | 1141 | GLN  |
| 46  | e     | 1145 | ASN  |
| 46  | e     | 1189 | ASN  |
| 46  | e     | 1235 | ASN  |
| 46  | e     | 1288 | GLN  |
| 47  | g     | 9    | ASN  |
| 47  | g     | 75   | GLN  |
| 48  | v     | 52   | HIS  |
| 48  | v     | 78   | HIS  |
| 48  | v     | 125  | GLN  |
| 52  | 0     | 36   | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 30  | f     | 3212/3395 (94%) | 591 (18%)         | 0               |
| 31  | h     | 120/121 (99%)   | 12 (10%)          | 0               |
| 32  | i     | 157/158 (99%)   | 32 (20%)          | 0               |
| 50  | x     | 70/76 (92%)     | 19 (27%)          | 0               |
| 50  | y     | 69/76 (90%)     | 18 (26%)          | 0               |
| All | All   | 3628/3826 (94%) | 672 (18%)         | 0               |

All (672) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | f     | 6   | A    |
| 30  | f     | 13  | A    |
| 30  | f     | 14  | U    |
| 30  | f     | 26  | A    |
| 30  | f     | 40  | A    |
| 30  | f     | 43  | A    |
| 30  | f     | 49  | A    |
| 30  | f     | 59  | G    |
| 30  | f     | 60  | A    |
| 30  | f     | 65  | A    |
| 30  | f     | 66  | A    |
| 30  | f     | 92  | G    |
| 30  | f     | 99  | A    |
| 30  | f     | 109 | A    |
| 30  | f     | 110 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | f     | 111 | C    |
| 30  | f     | 116 | A    |
| 30  | f     | 120 | G    |
| 30  | f     | 121 | A    |
| 30  | f     | 122 | A    |
| 30  | f     | 133 | U    |
| 30  | f     | 134 | U    |
| 30  | f     | 135 | C    |
| 30  | f     | 136 | G    |
| 30  | f     | 156 | G    |
| 30  | f     | 157 | A    |
| 30  | f     | 165 | A    |
| 30  | f     | 166 | C    |
| 30  | f     | 172 | G    |
| 30  | f     | 173 | G    |
| 30  | f     | 187 | A    |
| 30  | f     | 190 | U    |
| 30  | f     | 191 | U    |
| 30  | f     | 200 | C    |
| 30  | f     | 206 | G    |
| 30  | f     | 210 | U    |
| 30  | f     | 211 | A    |
| 30  | f     | 213 | A    |
| 30  | f     | 218 | G    |
| 30  | f     | 219 | A    |
| 30  | f     | 234 | G    |
| 30  | f     | 240 | U    |
| 30  | f     | 241 | G    |
| 30  | f     | 242 | C    |
| 30  | f     | 243 | G    |
| 30  | f     | 245 | U    |
| 30  | f     | 249 | U    |
| 30  | f     | 252 | U    |
| 30  | f     | 269 | G    |
| 30  | f     | 283 | G    |
| 30  | f     | 286 | U    |
| 30  | f     | 295 | A    |
| 30  | f     | 305 | U    |
| 30  | f     | 323 | A    |
| 30  | f     | 329 | U    |
| 30  | f     | 339 | C    |
| 30  | f     | 350 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | f     | 374 | A    |
| 30  | f     | 376 | G    |
| 30  | f     | 398 | A    |
| 30  | f     | 399 | A    |
| 30  | f     | 401 | U    |
| 30  | f     | 402 | A    |
| 30  | f     | 403 | C    |
| 30  | f     | 421 | G    |
| 30  | f     | 422 | A    |
| 30  | f     | 439 | C    |
| 30  | f     | 440 | A    |
| 30  | f     | 441 | U    |
| 30  | f     | 442 | G    |
| 30  | f     | 443 | G    |
| 30  | f     | 445 | G    |
| 30  | f     | 446 | U    |
| 30  | f     | 447 | U    |
| 30  | f     | 448 | U    |
| 30  | f     | 450 | G    |
| 30  | f     | 487 | U    |
| 30  | f     | 488 | U    |
| 30  | f     | 489 | U    |
| 30  | f     | 490 | C    |
| 30  | f     | 494 | G    |
| 30  | f     | 518 | G    |
| 30  | f     | 520 | U    |
| 30  | f     | 521 | A    |
| 30  | f     | 523 | A    |
| 30  | f     | 535 | G    |
| 30  | f     | 536 | U    |
| 30  | f     | 543 | C    |
| 30  | f     | 544 | C    |
| 30  | f     | 546 | C    |
| 30  | f     | 547 | G    |
| 30  | f     | 548 | G    |
| 30  | f     | 551 | A    |
| 30  | f     | 552 | G    |
| 30  | f     | 555 | U    |
| 30  | f     | 557 | A    |
| 30  | f     | 559 | A    |
| 30  | f     | 578 | A    |
| 30  | f     | 579 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | f     | 589 | A    |
| 30  | f     | 597 | G    |
| 30  | f     | 604 | G    |
| 30  | f     | 608 | A    |
| 30  | f     | 609 | G    |
| 30  | f     | 611 | A    |
| 30  | f     | 620 | U    |
| 30  | f     | 621 | A    |
| 30  | f     | 622 | A    |
| 30  | f     | 637 | C    |
| 30  | f     | 638 | C    |
| 30  | f     | 649 | A    |
| 30  | f     | 660 | A    |
| 30  | f     | 677 | A    |
| 30  | f     | 681 | U    |
| 30  | f     | 684 | G    |
| 30  | f     | 690 | A    |
| 30  | f     | 691 | A    |
| 30  | f     | 705 | A    |
| 30  | f     | 712 | G    |
| 30  | f     | 715 | A    |
| 30  | f     | 716 | A    |
| 30  | f     | 719 | U    |
| 30  | f     | 720 | A    |
| 30  | f     | 758 | C    |
| 30  | f     | 763 | G    |
| 30  | f     | 764 | U    |
| 30  | f     | 765 | C    |
| 30  | f     | 766 | U    |
| 30  | f     | 767 | U    |
| 30  | f     | 776 | U    |
| 30  | f     | 777 | U    |
| 30  | f     | 780 | A    |
| 30  | f     | 781 | G    |
| 30  | f     | 785 | G    |
| 30  | f     | 786 | A    |
| 30  | f     | 806 | A    |
| 30  | f     | 817 | A    |
| 30  | f     | 830 | A    |
| 30  | f     | 846 | A    |
| 30  | f     | 849 | C    |
| 30  | f     | 850 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 861  | C    |
| 30  | f     | 874  | U    |
| 30  | f     | 879  | U    |
| 30  | f     | 896  | A    |
| 30  | f     | 907  | G    |
| 30  | f     | 908  | G    |
| 30  | f     | 914  | A    |
| 30  | f     | 916  | G    |
| 30  | f     | 917  | A    |
| 30  | f     | 920  | A    |
| 30  | f     | 921  | A    |
| 30  | f     | 924  | G    |
| 30  | f     | 925  | A    |
| 30  | f     | 937  | G    |
| 30  | f     | 944  | C    |
| 30  | f     | 959  | C    |
| 30  | f     | 960  | U    |
| 30  | f     | 981  | U    |
| 30  | f     | 982  | C    |
| 30  | f     | 991  | G    |
| 30  | f     | 994  | G    |
| 30  | f     | 1001 | G    |
| 30  | f     | 1002 | A    |
| 30  | f     | 1010 | G    |
| 30  | f     | 1015 | U    |
| 30  | f     | 1016 | C    |
| 30  | f     | 1017 | C    |
| 30  | f     | 1018 | G    |
| 30  | f     | 1021 | G    |
| 30  | f     | 1024 | G    |
| 30  | f     | 1025 | A    |
| 30  | f     | 1028 | U    |
| 30  | f     | 1036 | A    |
| 30  | f     | 1041 | U    |
| 30  | f     | 1047 | A    |
| 30  | f     | 1049 | C    |
| 30  | f     | 1063 | G    |
| 30  | f     | 1064 | A    |
| 30  | f     | 1065 | A    |
| 30  | f     | 1072 | G    |
| 30  | f     | 1081 | U    |
| 30  | f     | 1087 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 1093 | A    |
| 30  | f     | 1094 | U    |
| 30  | f     | 1095 | U    |
| 30  | f     | 1097 | G    |
| 30  | f     | 1098 | A    |
| 30  | f     | 1103 | A    |
| 30  | f     | 1104 | G    |
| 30  | f     | 1117 | G    |
| 30  | f     | 1131 | G    |
| 30  | f     | 1144 | U    |
| 30  | f     | 1153 | A    |
| 30  | f     | 1159 | A    |
| 30  | f     | 1160 | C    |
| 30  | f     | 1177 | G    |
| 30  | f     | 1180 | A    |
| 30  | f     | 1181 | U    |
| 30  | f     | 1192 | C    |
| 30  | f     | 1193 | A    |
| 30  | f     | 1196 | C    |
| 30  | f     | 1197 | A    |
| 30  | f     | 1201 | C    |
| 30  | f     | 1202 | A    |
| 30  | f     | 1208 | U    |
| 30  | f     | 1217 | A    |
| 30  | f     | 1218 | U    |
| 30  | f     | 1219 | C    |
| 30  | f     | 1222 | G    |
| 30  | f     | 1225 | A    |
| 30  | f     | 1227 | C    |
| 30  | f     | 1235 | U    |
| 30  | f     | 1236 | G    |
| 30  | f     | 1238 | C    |
| 30  | f     | 1241 | U    |
| 30  | f     | 1242 | G    |
| 30  | f     | 1244 | A    |
| 30  | f     | 1245 | A    |
| 30  | f     | 1251 | A    |
| 30  | f     | 1252 | A    |
| 30  | f     | 1254 | C    |
| 30  | f     | 1258 | U    |
| 30  | f     | 1259 | A    |
| 30  | f     | 1263 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 1264 | G    |
| 30  | f     | 1265 | U    |
| 30  | f     | 1269 | U    |
| 30  | f     | 1272 | C    |
| 30  | f     | 1277 | C    |
| 30  | f     | 1278 | A    |
| 30  | f     | 1279 | C    |
| 30  | f     | 1282 | G    |
| 30  | f     | 1285 | G    |
| 30  | f     | 1286 | A    |
| 30  | f     | 1287 | A    |
| 30  | f     | 1295 | G    |
| 30  | f     | 1307 | G    |
| 30  | f     | 1308 | A    |
| 30  | f     | 1309 | U    |
| 30  | f     | 1313 | G    |
| 30  | f     | 1330 | A    |
| 30  | f     | 1348 | U    |
| 30  | f     | 1349 | G    |
| 30  | f     | 1351 | U    |
| 30  | f     | 1352 | A    |
| 30  | f     | 1354 | G    |
| 30  | f     | 1355 | A    |
| 30  | f     | 1356 | U    |
| 30  | f     | 1357 | G    |
| 30  | f     | 1386 | A    |
| 30  | f     | 1392 | G    |
| 30  | f     | 1399 | A    |
| 30  | f     | 1400 | G    |
| 30  | f     | 1419 | A    |
| 30  | f     | 1434 | G    |
| 30  | f     | 1437 | C    |
| 30  | f     | 1446 | A    |
| 30  | f     | 1450 | G    |
| 30  | f     | 1481 | A    |
| 30  | f     | 1482 | A    |
| 30  | f     | 1483 | G    |
| 30  | f     | 1487 | G    |
| 30  | f     | 1488 | G    |
| 30  | f     | 1502 | C    |
| 30  | f     | 1508 | C    |
| 30  | f     | 1536 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 1539 | A    |
| 30  | f     | 1555 | U    |
| 30  | f     | 1556 | C    |
| 30  | f     | 1557 | A    |
| 30  | f     | 1560 | G    |
| 30  | f     | 1562 | C    |
| 30  | f     | 1563 | C    |
| 30  | f     | 1566 | A    |
| 30  | f     | 1568 | U    |
| 30  | f     | 1569 | U    |
| 30  | f     | 1572 | U    |
| 30  | f     | 1573 | G    |
| 30  | f     | 1575 | A    |
| 30  | f     | 1576 | G    |
| 30  | f     | 1580 | A    |
| 30  | f     | 1581 | C    |
| 30  | f     | 1582 | C    |
| 30  | f     | 1583 | A    |
| 30  | f     | 1589 | A    |
| 30  | f     | 1590 | G    |
| 30  | f     | 1605 | A    |
| 30  | f     | 1607 | U    |
| 30  | f     | 1620 | U    |
| 30  | f     | 1629 | U    |
| 30  | f     | 1639 | C    |
| 30  | f     | 1642 | A    |
| 30  | f     | 1643 | A    |
| 30  | f     | 1645 | U    |
| 30  | f     | 1657 | C    |
| 30  | f     | 1683 | A    |
| 30  | f     | 1716 | U    |
| 30  | f     | 1717 | U    |
| 30  | f     | 1724 | U    |
| 30  | f     | 1725 | C    |
| 30  | f     | 1736 | G    |
| 30  | f     | 1741 | A    |
| 30  | f     | 1750 | A    |
| 30  | f     | 1751 | G    |
| 30  | f     | 1760 | A    |
| 30  | f     | 1761 | C    |
| 30  | f     | 1764 | U    |
| 30  | f     | 1765 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 1766 | G    |
| 30  | f     | 1770 | G    |
| 30  | f     | 1775 | G    |
| 30  | f     | 1780 | G    |
| 30  | f     | 1797 | A    |
| 30  | f     | 1814 | A    |
| 30  | f     | 1816 | A    |
| 30  | f     | 1819 | U    |
| 30  | f     | 1820 | U    |
| 30  | f     | 1821 | U    |
| 30  | f     | 1835 | A    |
| 30  | f     | 1839 | A    |
| 30  | f     | 1840 | U    |
| 30  | f     | 1841 | A    |
| 30  | f     | 1842 | A    |
| 30  | f     | 1846 | C    |
| 30  | f     | 1849 | C    |
| 30  | f     | 1850 | A    |
| 30  | f     | 1866 | C    |
| 30  | f     | 1867 | A    |
| 30  | f     | 1880 | U    |
| 30  | f     | 1881 | A    |
| 30  | f     | 1893 | A    |
| 30  | f     | 1906 | G    |
| 30  | f     | 1943 | C    |
| 30  | f     | 1952 | G    |
| 30  | f     | 1953 | G    |
| 30  | f     | 1954 | G    |
| 30  | f     | 2094 | C    |
| 30  | f     | 2101 | C    |
| 30  | f     | 2102 | U    |
| 30  | f     | 2111 | G    |
| 30  | f     | 2112 | U    |
| 30  | f     | 2113 | A    |
| 30  | f     | 2114 | C    |
| 30  | f     | 2121 | G    |
| 30  | f     | 2122 | G    |
| 30  | f     | 2131 | A    |
| 30  | f     | 2134 | G    |
| 30  | f     | 2140 | U    |
| 30  | f     | 2144 | A    |
| 30  | f     | 2158 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 2160 | G    |
| 30  | f     | 2169 | G    |
| 30  | f     | 2176 | U    |
| 30  | f     | 2201 | G    |
| 30  | f     | 2206 | G    |
| 30  | f     | 2207 | A    |
| 30  | f     | 2208 | A    |
| 30  | f     | 2209 | U    |
| 30  | f     | 2222 | A    |
| 30  | f     | 2223 | A    |
| 30  | f     | 2225 | U    |
| 30  | f     | 2228 | A    |
| 30  | f     | 2249 | G    |
| 30  | f     | 2272 | G    |
| 30  | f     | 2273 | G    |
| 30  | f     | 2274 | U    |
| 30  | f     | 2281 | A    |
| 30  | f     | 2282 | U    |
| 30  | f     | 2288 | G    |
| 30  | f     | 2307 | G    |
| 30  | f     | 2308 | C    |
| 30  | f     | 2310 | U    |
| 30  | f     | 2313 | A    |
| 30  | f     | 2314 | U    |
| 30  | f     | 2315 | G    |
| 30  | f     | 2334 | U    |
| 30  | f     | 2335 | G    |
| 30  | f     | 2336 | U    |
| 30  | f     | 2373 | A    |
| 30  | f     | 2374 | C    |
| 30  | f     | 2375 | G    |
| 30  | f     | 2385 | G    |
| 30  | f     | 2388 | U    |
| 30  | f     | 2393 | G    |
| 30  | f     | 2397 | A    |
| 30  | f     | 2402 | A    |
| 30  | f     | 2403 | G    |
| 30  | f     | 2404 | A    |
| 30  | f     | 2411 | U    |
| 30  | f     | 2419 | A    |
| 30  | f     | 2437 | G    |
| 30  | f     | 2446 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 2447 | A    |
| 30  | f     | 2450 | G    |
| 30  | f     | 2461 | A    |
| 30  | f     | 2463 | G    |
| 30  | f     | 2464 | U    |
| 30  | f     | 2468 | A    |
| 30  | f     | 2469 | G    |
| 30  | f     | 2470 | C    |
| 30  | f     | 2471 | U    |
| 30  | f     | 2472 | U    |
| 30  | f     | 2474 | G    |
| 30  | f     | 2479 | C    |
| 30  | f     | 2480 | A    |
| 30  | f     | 2484 | A    |
| 30  | f     | 2486 | A    |
| 30  | f     | 2487 | U    |
| 30  | f     | 2488 | A    |
| 30  | f     | 2494 | A    |
| 30  | f     | 2495 | C    |
| 30  | f     | 2496 | C    |
| 30  | f     | 2499 | U    |
| 30  | f     | 2501 | U    |
| 30  | f     | 2502 | A    |
| 30  | f     | 2503 | G    |
| 30  | f     | 2505 | U    |
| 30  | f     | 2514 | U    |
| 30  | f     | 2515 | A    |
| 30  | f     | 2522 | G    |
| 30  | f     | 2526 | C    |
| 30  | f     | 2531 | C    |
| 30  | f     | 2537 | U    |
| 30  | f     | 2538 | U    |
| 30  | f     | 2539 | C    |
| 30  | f     | 2540 | A    |
| 30  | f     | 2541 | U    |
| 30  | f     | 2542 | U    |
| 30  | f     | 2544 | U    |
| 30  | f     | 2547 | A    |
| 30  | f     | 2548 | C    |
| 30  | f     | 2549 | G    |
| 30  | f     | 2552 | C    |
| 30  | f     | 2554 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 2555 | G    |
| 30  | f     | 2561 | A    |
| 30  | f     | 2569 | A    |
| 30  | f     | 2570 | U    |
| 30  | f     | 2571 | U    |
| 30  | f     | 2572 | C    |
| 30  | f     | 2573 | G    |
| 30  | f     | 2581 | U    |
| 30  | f     | 2585 | G    |
| 30  | f     | 2593 | A    |
| 30  | f     | 2594 | C    |
| 30  | f     | 2606 | G    |
| 30  | f     | 2607 | G    |
| 30  | f     | 2614 | G    |
| 30  | f     | 2648 | G    |
| 30  | f     | 2651 | G    |
| 30  | f     | 2652 | U    |
| 30  | f     | 2656 | A    |
| 30  | f     | 2674 | A    |
| 30  | f     | 2677 | G    |
| 30  | f     | 2678 | A    |
| 30  | f     | 2689 | A    |
| 30  | f     | 2691 | A    |
| 30  | f     | 2694 | A    |
| 30  | f     | 2696 | A    |
| 30  | f     | 2704 | A    |
| 30  | f     | 2714 | G    |
| 30  | f     | 2719 | U    |
| 30  | f     | 2728 | G    |
| 30  | f     | 2729 | U    |
| 30  | f     | 2740 | A    |
| 30  | f     | 2752 | U    |
| 30  | f     | 2753 | G    |
| 30  | f     | 2755 | C    |
| 30  | f     | 2772 | C    |
| 30  | f     | 2773 | C    |
| 30  | f     | 2777 | G    |
| 30  | f     | 2778 | G    |
| 30  | f     | 2788 | C    |
| 30  | f     | 2796 | G    |
| 30  | f     | 2800 | G    |
| 30  | f     | 2801 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 2803 | A    |
| 30  | f     | 2810 | C    |
| 30  | f     | 2814 | G    |
| 30  | f     | 2816 | G    |
| 30  | f     | 2817 | A    |
| 30  | f     | 2818 | U    |
| 30  | f     | 2821 | C    |
| 30  | f     | 2834 | G    |
| 30  | f     | 2842 | U    |
| 30  | f     | 2844 | C    |
| 30  | f     | 2845 | A    |
| 30  | f     | 2849 | C    |
| 30  | f     | 2860 | U    |
| 30  | f     | 2867 | C    |
| 30  | f     | 2871 | G    |
| 30  | f     | 2872 | A    |
| 30  | f     | 2875 | U    |
| 30  | f     | 2887 | A    |
| 30  | f     | 2898 | G    |
| 30  | f     | 2899 | C    |
| 30  | f     | 2911 | A    |
| 30  | f     | 2914 | G    |
| 30  | f     | 2923 | U    |
| 30  | f     | 2935 | U    |
| 30  | f     | 2936 | A    |
| 30  | f     | 2941 | A    |
| 30  | f     | 2942 | C    |
| 30  | f     | 2947 | G    |
| 30  | f     | 2971 | A    |
| 30  | f     | 2983 | C    |
| 30  | f     | 2990 | G    |
| 30  | f     | 2992 | U    |
| 30  | f     | 2996 | U    |
| 30  | f     | 2997 | G    |
| 30  | f     | 3006 | A    |
| 30  | f     | 3012 | A    |
| 30  | f     | 3056 | U    |
| 30  | f     | 3059 | G    |
| 30  | f     | 3078 | U    |
| 30  | f     | 3079 | U    |
| 30  | f     | 3080 | G    |
| 30  | f     | 3086 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 3092 | C    |
| 30  | f     | 3104 | U    |
| 30  | f     | 3113 | A    |
| 30  | f     | 3122 | A    |
| 30  | f     | 3130 | A    |
| 30  | f     | 3131 | U    |
| 30  | f     | 3142 | A    |
| 30  | f     | 3143 | C    |
| 30  | f     | 3151 | U    |
| 30  | f     | 3154 | C    |
| 30  | f     | 3155 | U    |
| 30  | f     | 3156 | U    |
| 30  | f     | 3157 | U    |
| 30  | f     | 3165 | A    |
| 30  | f     | 3170 | A    |
| 30  | f     | 3173 | G    |
| 30  | f     | 3174 | A    |
| 30  | f     | 3175 | U    |
| 30  | f     | 3176 | G    |
| 30  | f     | 3179 | U    |
| 30  | f     | 3181 | C    |
| 30  | f     | 3186 | A    |
| 30  | f     | 3187 | A    |
| 30  | f     | 3196 | U    |
| 30  | f     | 3207 | U    |
| 30  | f     | 3209 | A    |
| 30  | f     | 3217 | C    |
| 30  | f     | 3218 | A    |
| 30  | f     | 3219 | G    |
| 30  | f     | 3228 | C    |
| 30  | f     | 3229 | G    |
| 30  | f     | 3243 | A    |
| 30  | f     | 3245 | A    |
| 30  | f     | 3247 | G    |
| 30  | f     | 3259 | U    |
| 30  | f     | 3263 | G    |
| 30  | f     | 3269 | U    |
| 30  | f     | 3270 | U    |
| 30  | f     | 3273 | A    |
| 30  | f     | 3276 | G    |
| 30  | f     | 3281 | U    |
| 30  | f     | 3287 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | f     | 3288 | G    |
| 30  | f     | 3289 | G    |
| 30  | f     | 3294 | A    |
| 30  | f     | 3295 | A    |
| 30  | f     | 3303 | G    |
| 30  | f     | 3304 | U    |
| 30  | f     | 3307 | A    |
| 30  | f     | 3313 | U    |
| 30  | f     | 3316 | A    |
| 30  | f     | 3317 | U    |
| 30  | f     | 3318 | G    |
| 30  | f     | 3319 | U    |
| 30  | f     | 3320 | A    |
| 30  | f     | 3341 | U    |
| 30  | f     | 3342 | A    |
| 30  | f     | 3345 | G    |
| 30  | f     | 3351 | U    |
| 30  | f     | 3352 | U    |
| 30  | f     | 3353 | G    |
| 30  | f     | 3354 | U    |
| 30  | f     | 3355 | U    |
| 30  | f     | 3369 | G    |
| 30  | f     | 3375 | A    |
| 30  | f     | 3378 | C    |
| 30  | f     | 3382 | U    |
| 30  | f     | 3383 | G    |
| 30  | f     | 3386 | G    |
| 30  | f     | 3389 | U    |
| 30  | f     | 3390 | G    |
| 30  | f     | 3396 | U    |
| 31  | h     | 7    | G    |
| 31  | h     | 29   | C    |
| 31  | h     | 53   | U    |
| 31  | h     | 54   | U    |
| 31  | h     | 55   | A    |
| 31  | h     | 65   | G    |
| 31  | h     | 73   | C    |
| 31  | h     | 74   | C    |
| 31  | h     | 95   | A    |
| 31  | h     | 102  | A    |
| 31  | h     | 112  | G    |
| 31  | h     | 121  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | i     | 23  | U    |
| 32  | i     | 34  | U    |
| 32  | i     | 35  | C    |
| 32  | i     | 39  | G    |
| 32  | i     | 48  | A    |
| 32  | i     | 52  | A    |
| 32  | i     | 53  | A    |
| 32  | i     | 59  | A    |
| 32  | i     | 62  | C    |
| 32  | i     | 63  | G    |
| 32  | i     | 80  | A    |
| 32  | i     | 81  | U    |
| 32  | i     | 82  | U    |
| 32  | i     | 83  | C    |
| 32  | i     | 84  | C    |
| 32  | i     | 85  | G    |
| 32  | i     | 86  | U    |
| 32  | i     | 87  | G    |
| 32  | i     | 90  | U    |
| 32  | i     | 95  | G    |
| 32  | i     | 104 | A    |
| 32  | i     | 105 | A    |
| 32  | i     | 106 | C    |
| 32  | i     | 111 | A    |
| 32  | i     | 113 | U    |
| 32  | i     | 125 | U    |
| 32  | i     | 126 | A    |
| 32  | i     | 138 | A    |
| 32  | i     | 151 | C    |
| 32  | i     | 152 | G    |
| 32  | i     | 157 | U    |
| 32  | i     | 158 | U    |
| 50  | x     | 5   | G    |
| 50  | x     | 9   | G    |
| 50  | x     | 15  | G    |
| 50  | x     | 16  | U    |
| 50  | x     | 17  | C    |
| 50  | x     | 18  | G    |
| 50  | x     | 22  | G    |
| 50  | x     | 28  | U    |
| 50  | x     | 33  | U    |
| 50  | x     | 37  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | x     | 38  | U    |
| 50  | x     | 39  | G    |
| 50  | x     | 46  | G    |
| 50  | x     | 48  | C    |
| 50  | x     | 56  | C    |
| 50  | x     | 57  | G    |
| 50  | x     | 58  | A    |
| 50  | x     | 60  | U    |
| 50  | x     | 74  | C    |
| 50  | y     | 7   | G    |
| 50  | y     | 9   | G    |
| 50  | y     | 13  | U    |
| 50  | y     | 17  | C    |
| 50  | y     | 23  | C    |
| 50  | y     | 26  | G    |
| 50  | y     | 36  | C    |
| 50  | y     | 38  | U    |
| 50  | y     | 43  | G    |
| 50  | y     | 45  | G    |
| 50  | y     | 46  | G    |
| 50  | y     | 47  | U    |
| 50  | y     | 48  | C    |
| 50  | y     | 56  | C    |
| 50  | y     | 58  | A    |
| 50  | y     | 61  | C    |
| 50  | y     | 75  | C    |
| 50  | y     | 76  | A    |

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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 |
| 48  | 5CT  | v     | 51  | 48   | 13,14,15     | 0.78 | 0        | 8,15,17     | 1.28 | 1 (12%)  |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 48  | 5CT  | v     | 51  | 48   | -       | 9/13/14/16 | -     |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|----------|-------|------------------------|---------------------|
| 48  | v     | 51  | 5CT  | C4-C3-C2 | -2.20 | 108.84                 | 113.47              |

There are no chirality outliers.

All (9) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 48  | v     | 51  | 5CT  | NZ-C1-C2-C3 |
| 48  | v     | 51  | 5CT  | O1-C2-C3-C4 |
| 48  | v     | 51  | 5CT  | C2-C3-C4-N1 |
| 48  | v     | 51  | 5CT  | C-CA-CB-CG  |
| 48  | v     | 51  | 5CT  | N-CA-CB-CG  |
| 48  | v     | 51  | 5CT  | NZ-C1-C2-O1 |
| 48  | v     | 51  | 5CT  | C1-C2-C3-C4 |
| 48  | v     | 51  | 5CT  | C2-C1-NZ-CE |
| 48  | v     | 51  | 5CT  | CE-CD-CG-CB |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 48  | v     | 51  | 5CT  | 1       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 21 ligands modelled in this entry, 20 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  | SPD  | f     | 3401 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.85 | 0           |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 56  | SPD  | f     | 3401 | -    | -       | 5/7/7/7  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 56  | f     | 3401 | SPD  | C3-C4-C5-N6 |
| 56  | f     | 3401 | SPD  | N6-C7-C8-C9 |
| 56  | f     | 3401 | SPD  | C2-C3-C4-C5 |
| 56  | f     | 3401 | SPD  | C4-C5-N6-C7 |
| 56  | f     | 3401 | SPD  | C8-C7-N6-C5 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | f     | 3401 | SPD  | 1       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

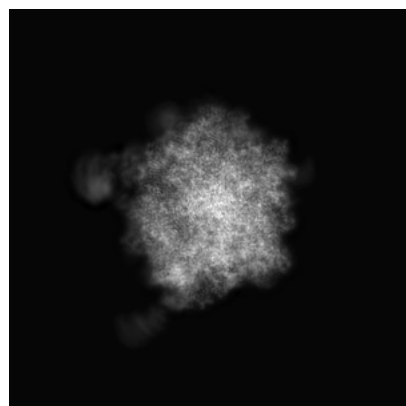
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15428. These allow visual inspection of the internal detail of the map and identification of artifacts.

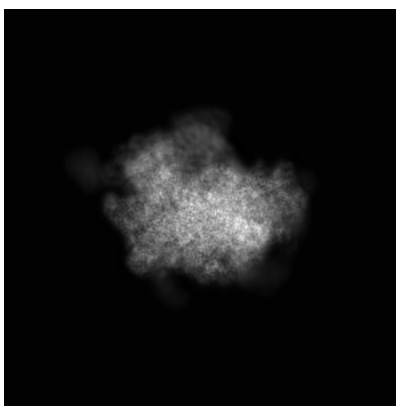
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

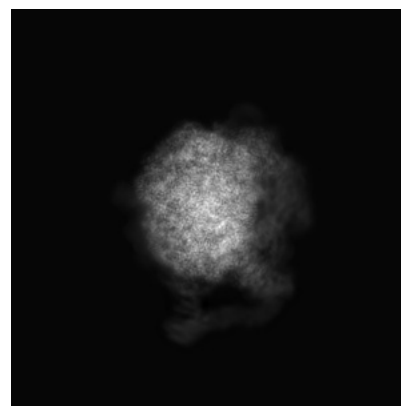
#### 6.1.1 Primary map



X

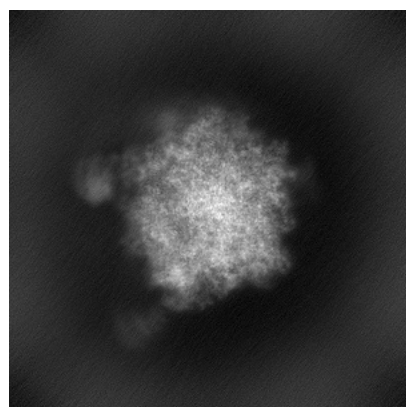


Y

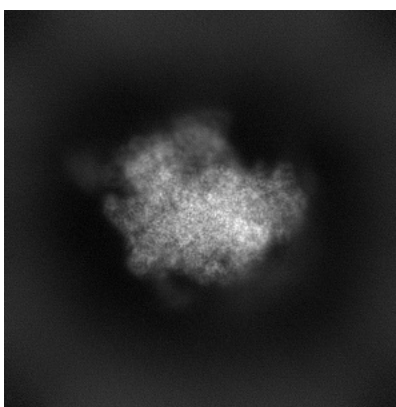


Z

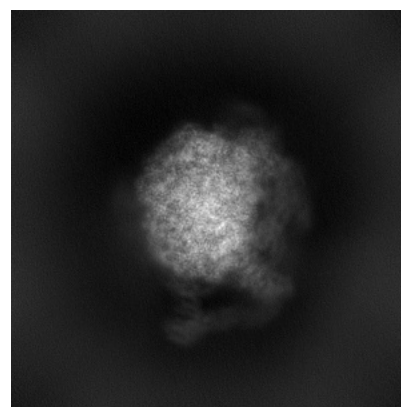
#### 6.1.2 Raw map



X



Y

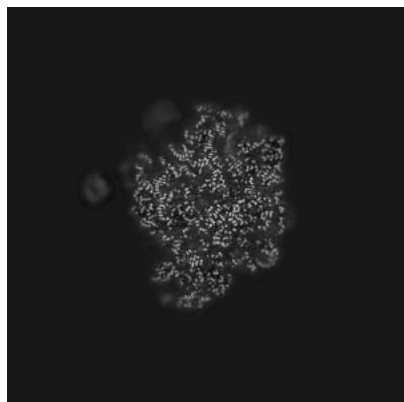


Z

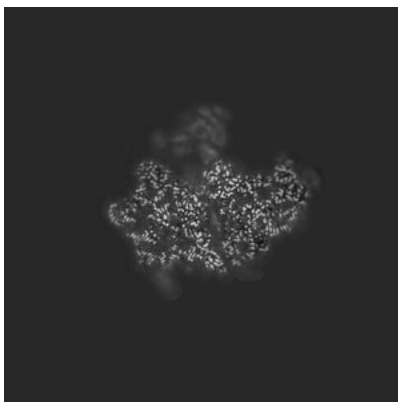
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

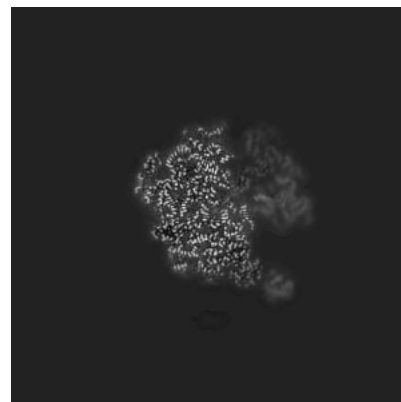
### 6.2.1 Primary map



X Index: 225

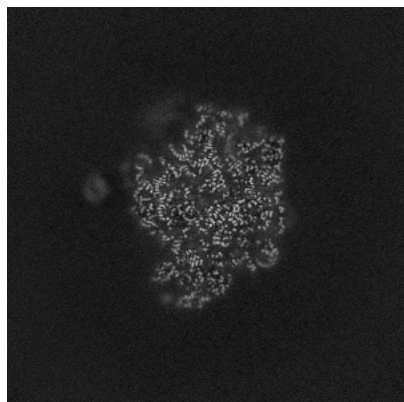


Y Index: 225

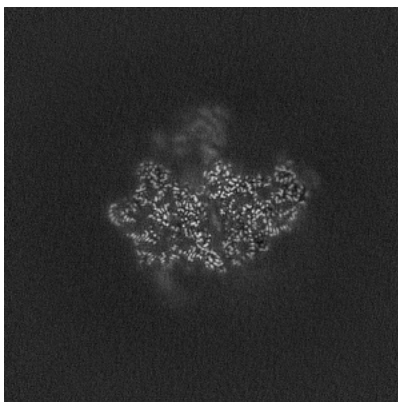


Z Index: 225

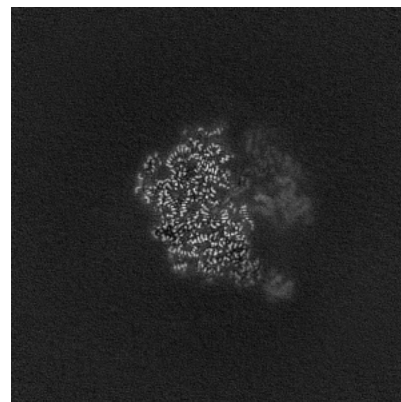
### 6.2.2 Raw map



X Index: 225



Y Index: 225

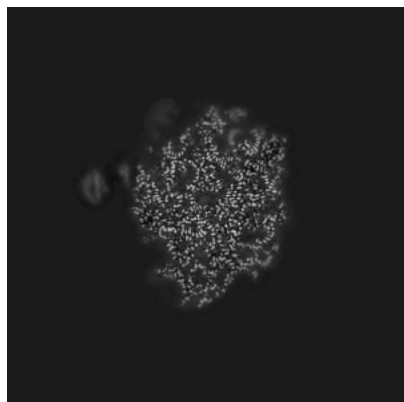


Z Index: 225

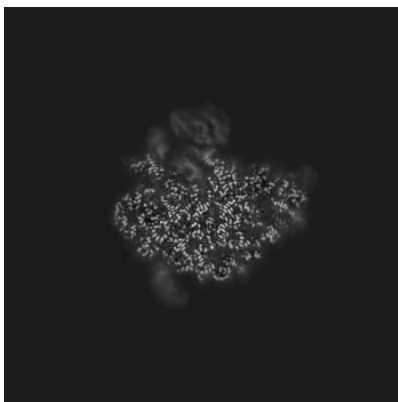
The images above show central slices of the map in three orthogonal directions.

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

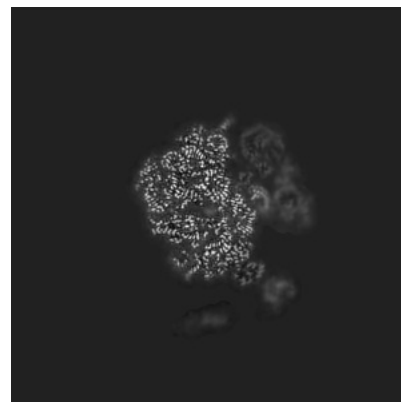
### 6.3.1 Primary map



X Index: 219

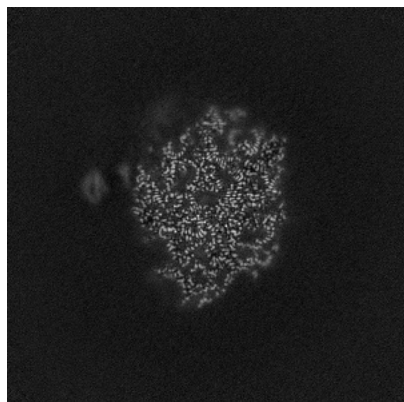


Y Index: 237

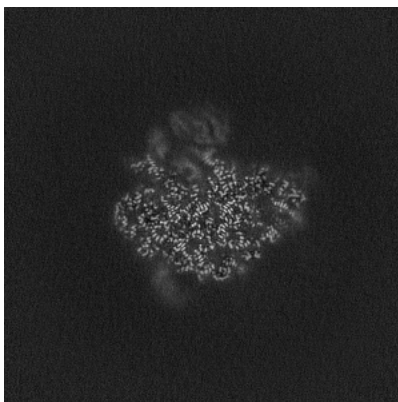


Z Index: 231

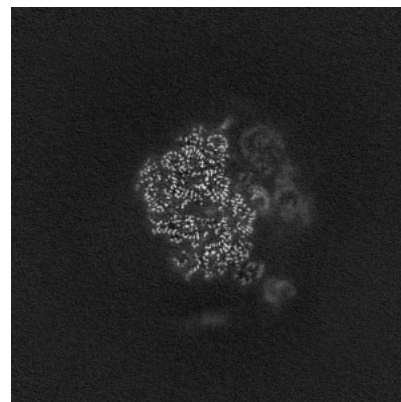
### 6.3.2 Raw map



X Index: 219



Y Index: 237



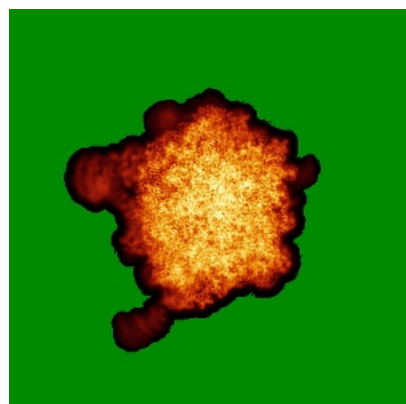
Z Index: 231

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

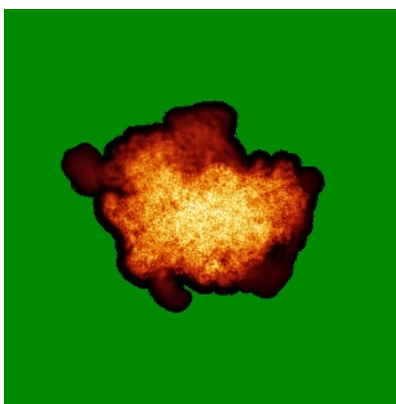


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

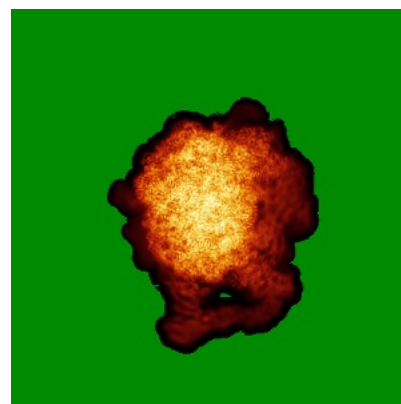
### 6.4.1 Primary map



X

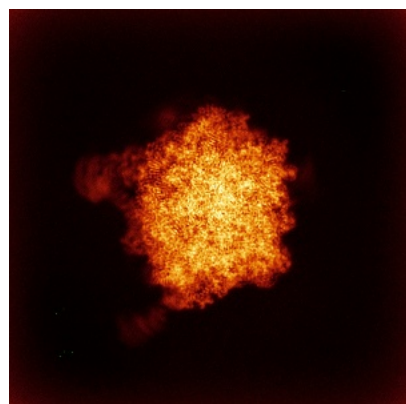


Y

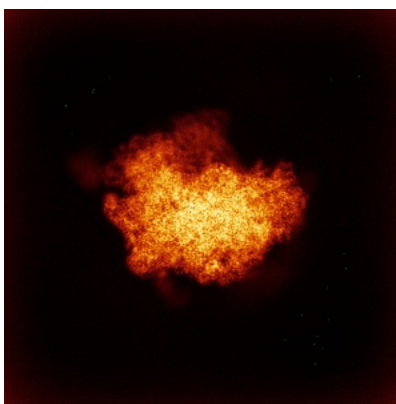


Z

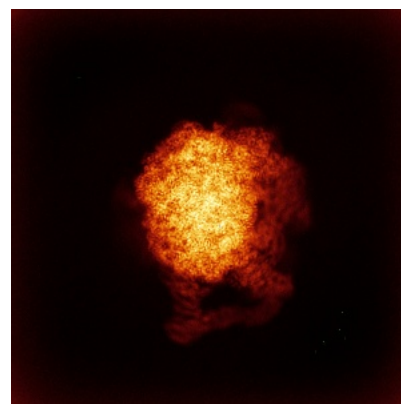
### 6.4.2 Raw map



X



Y

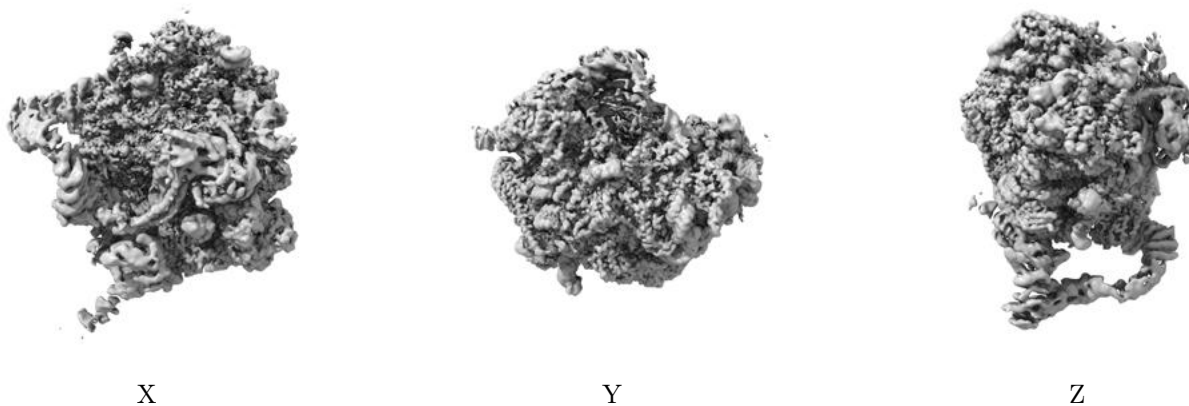


Z

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

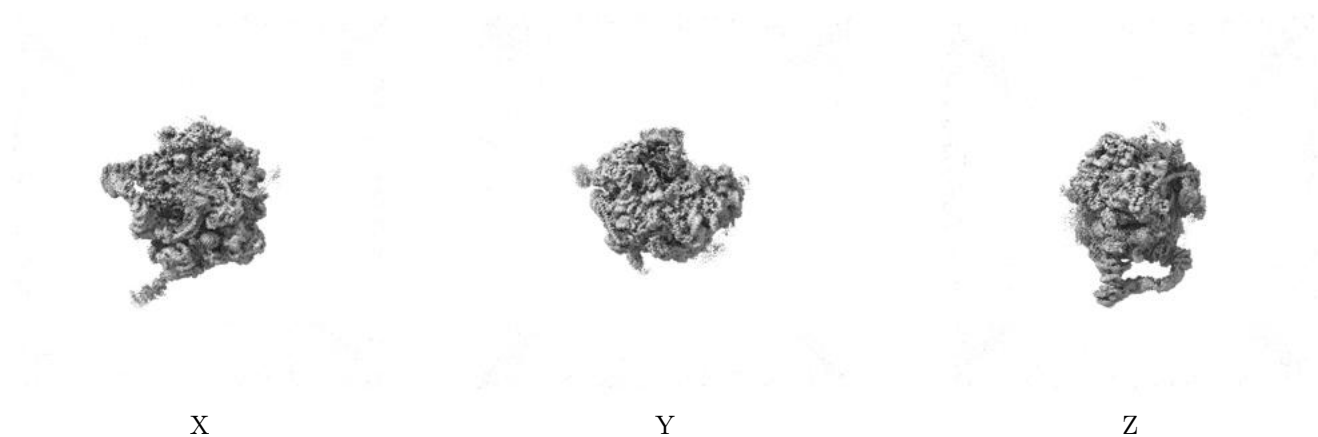
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

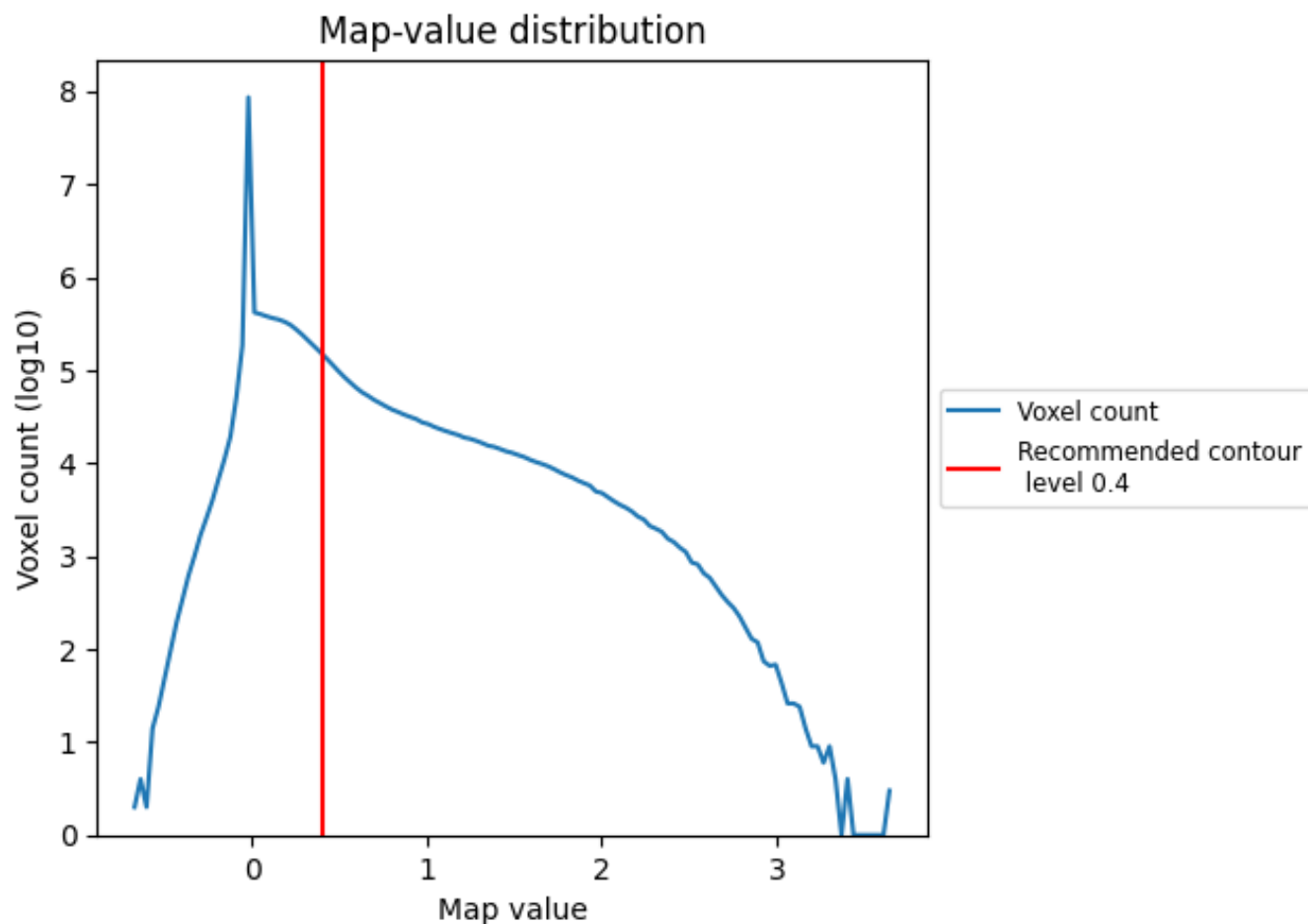
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

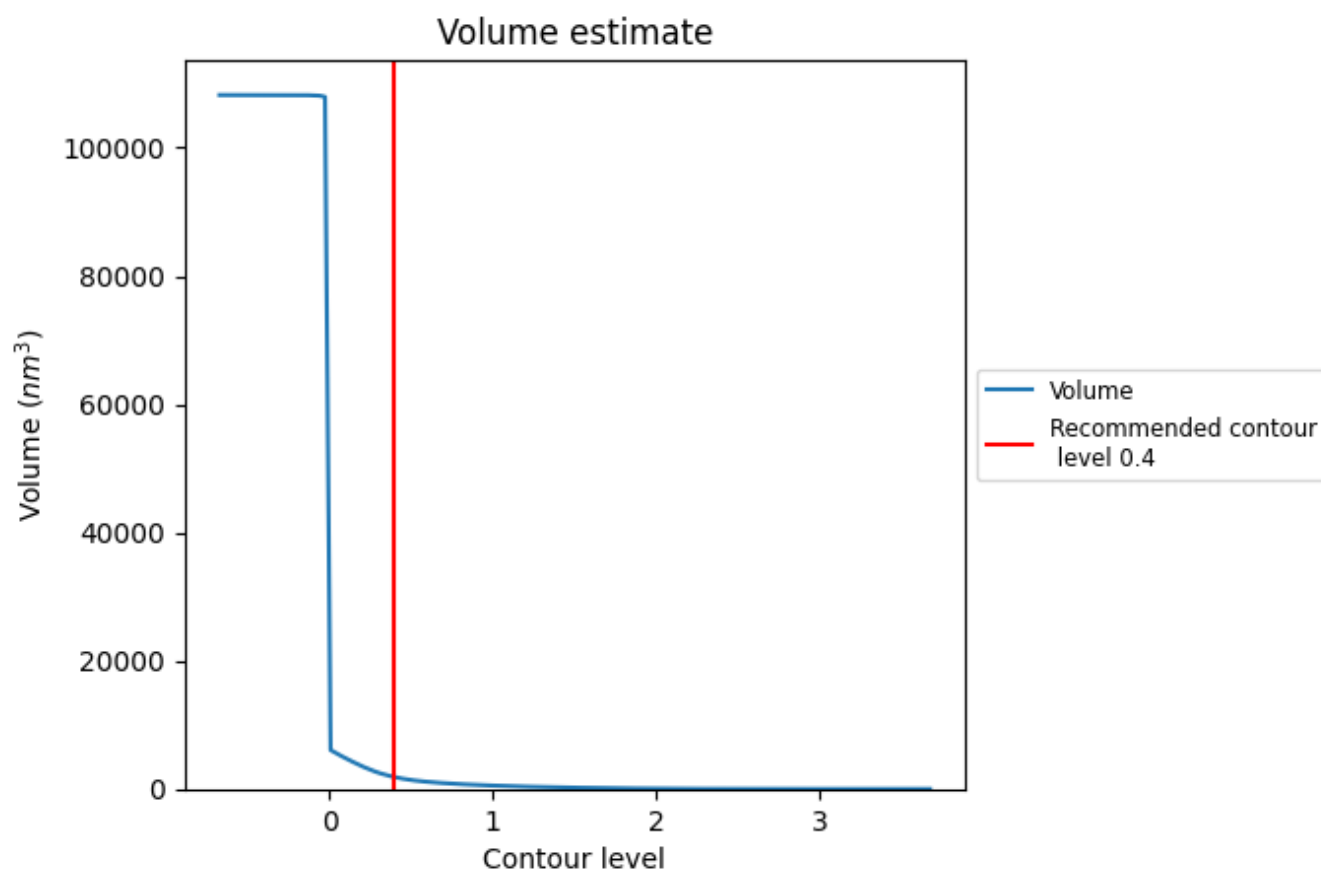
This section contains the results of statistical analysis of the map.

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



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

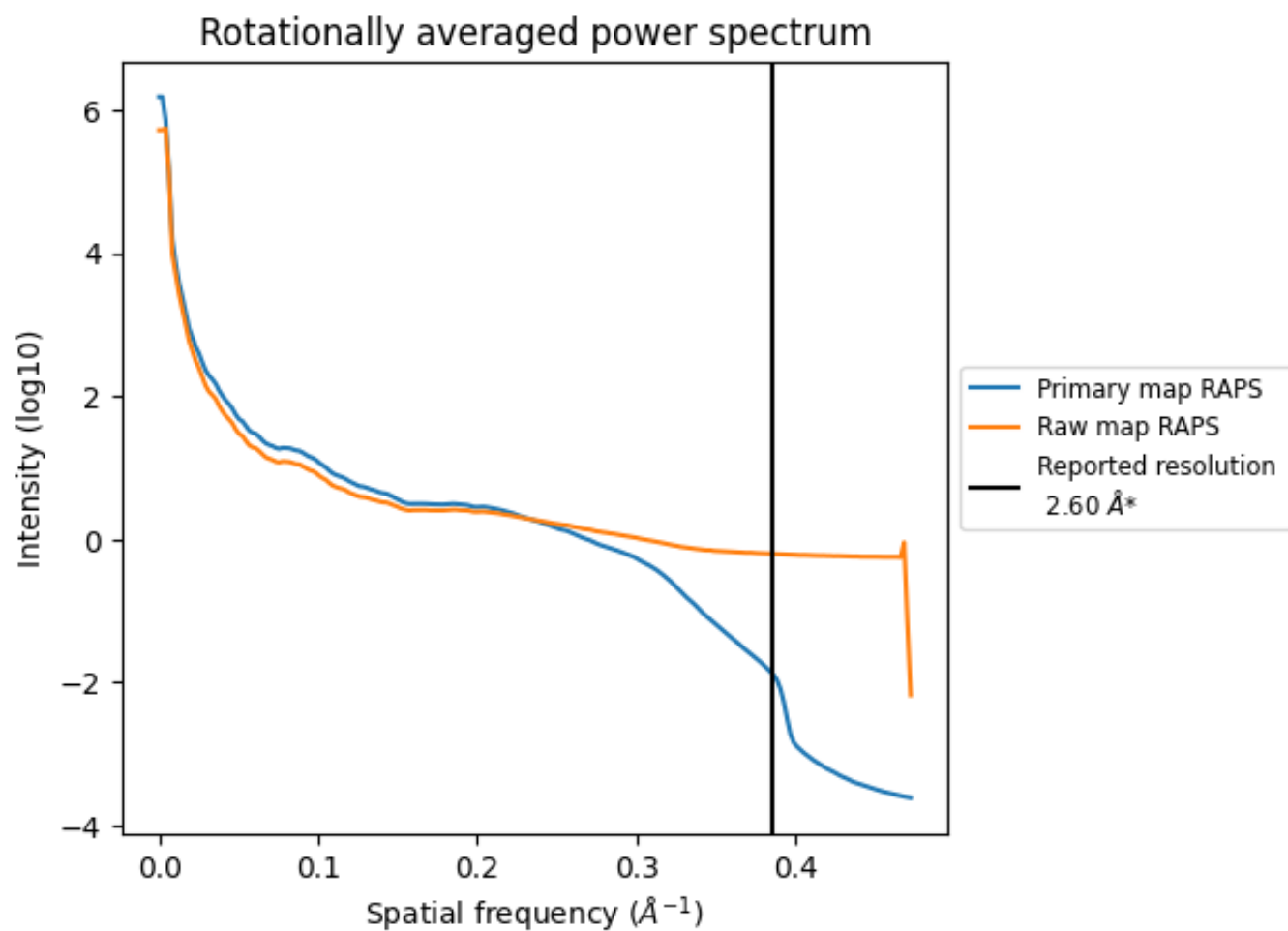
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1851 nm<sup>3</sup>; this corresponds to an approximate mass of 1672 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 ⓘ

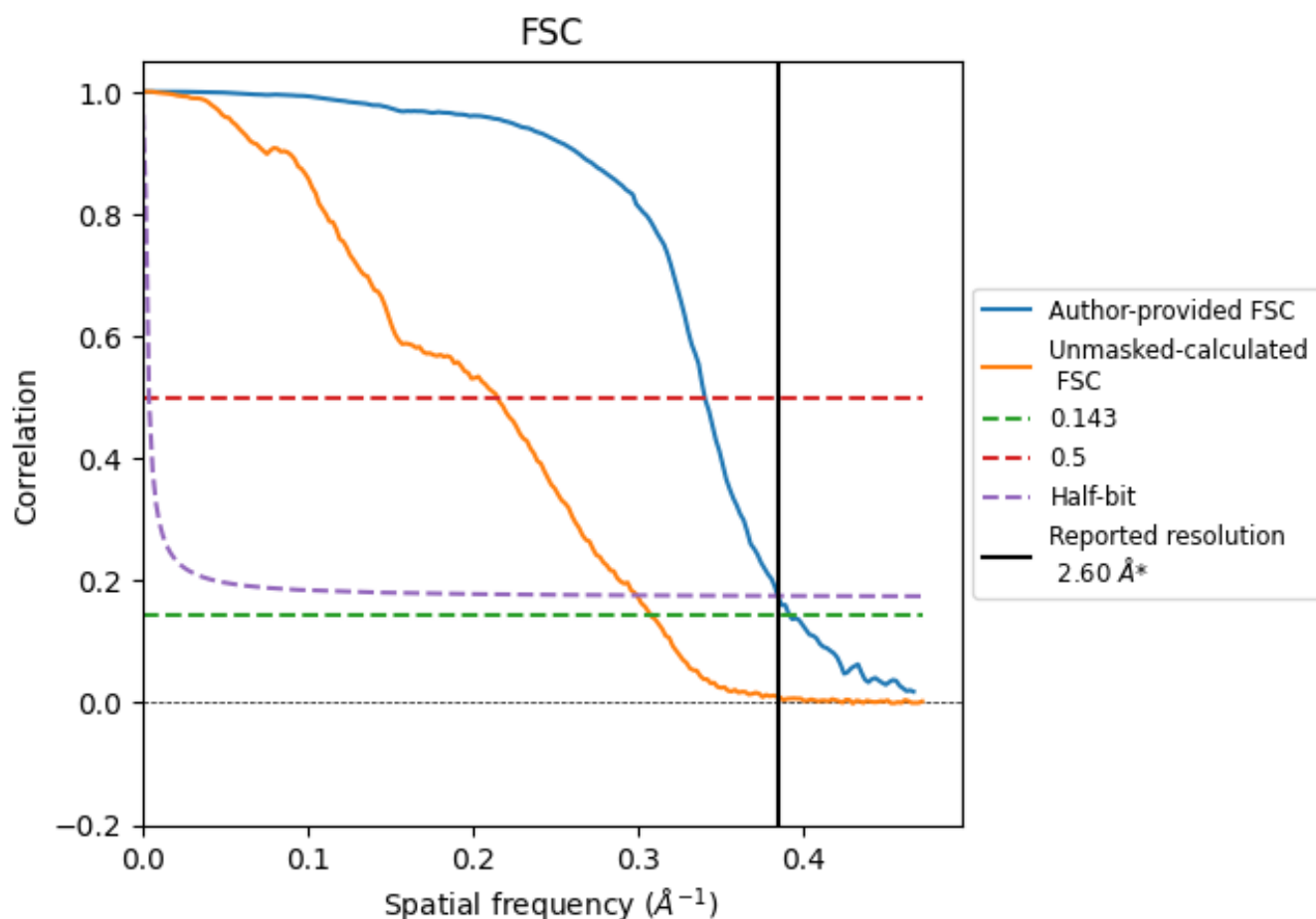


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

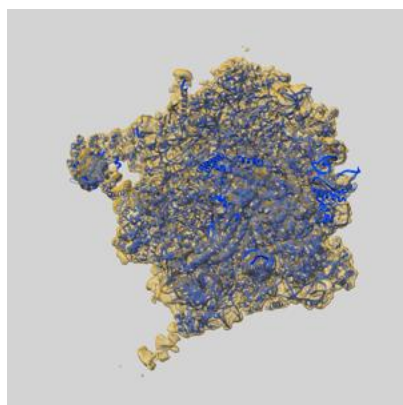
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.60                               | -    | -        |
| Author-provided FSC curve | 2.55                               | 2.94 | 2.60     |
| Unmasked-calculated*      | 3.25                               | 4.65 | 3.34     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.6 by more than 10 %

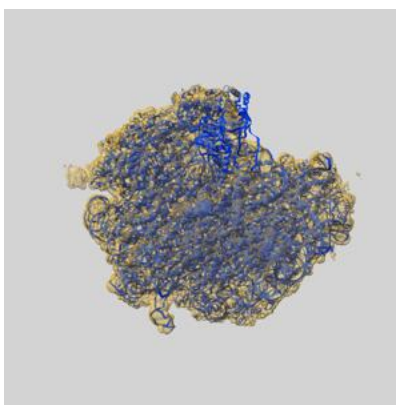
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15428 and PDB model 8AGZ. Per-residue inclusion information can be found in section 3 on page 16.

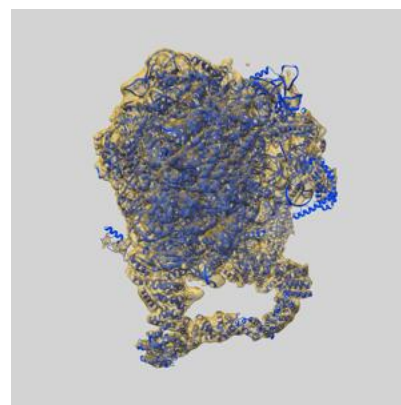
### 9.1 Map-model overlay [i](#)



X



Y

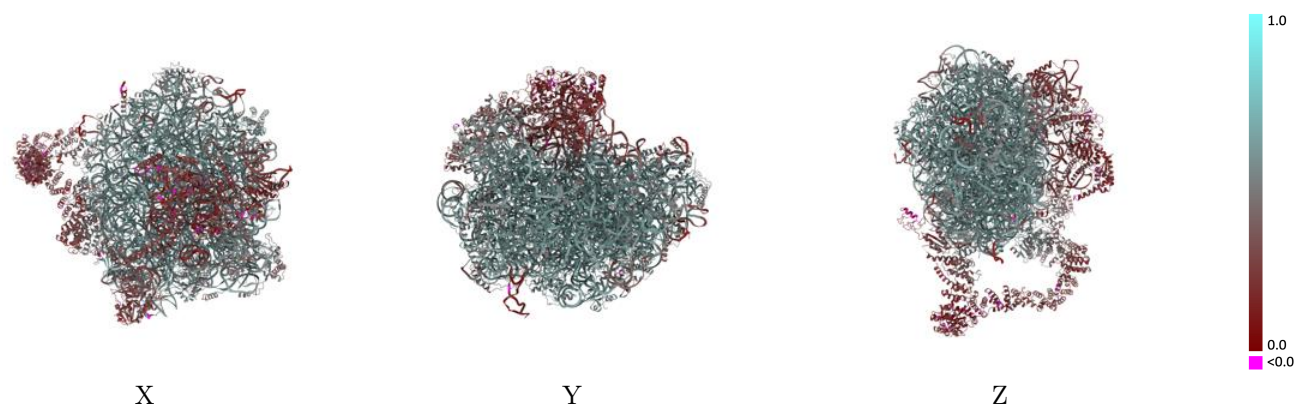


Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

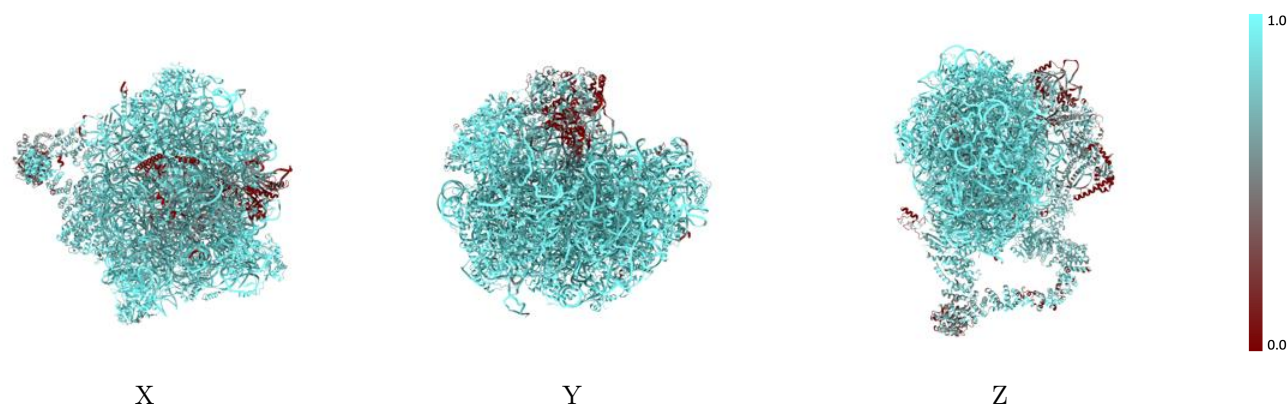


## 9.2 Q-score mapped to coordinate model [i](#)



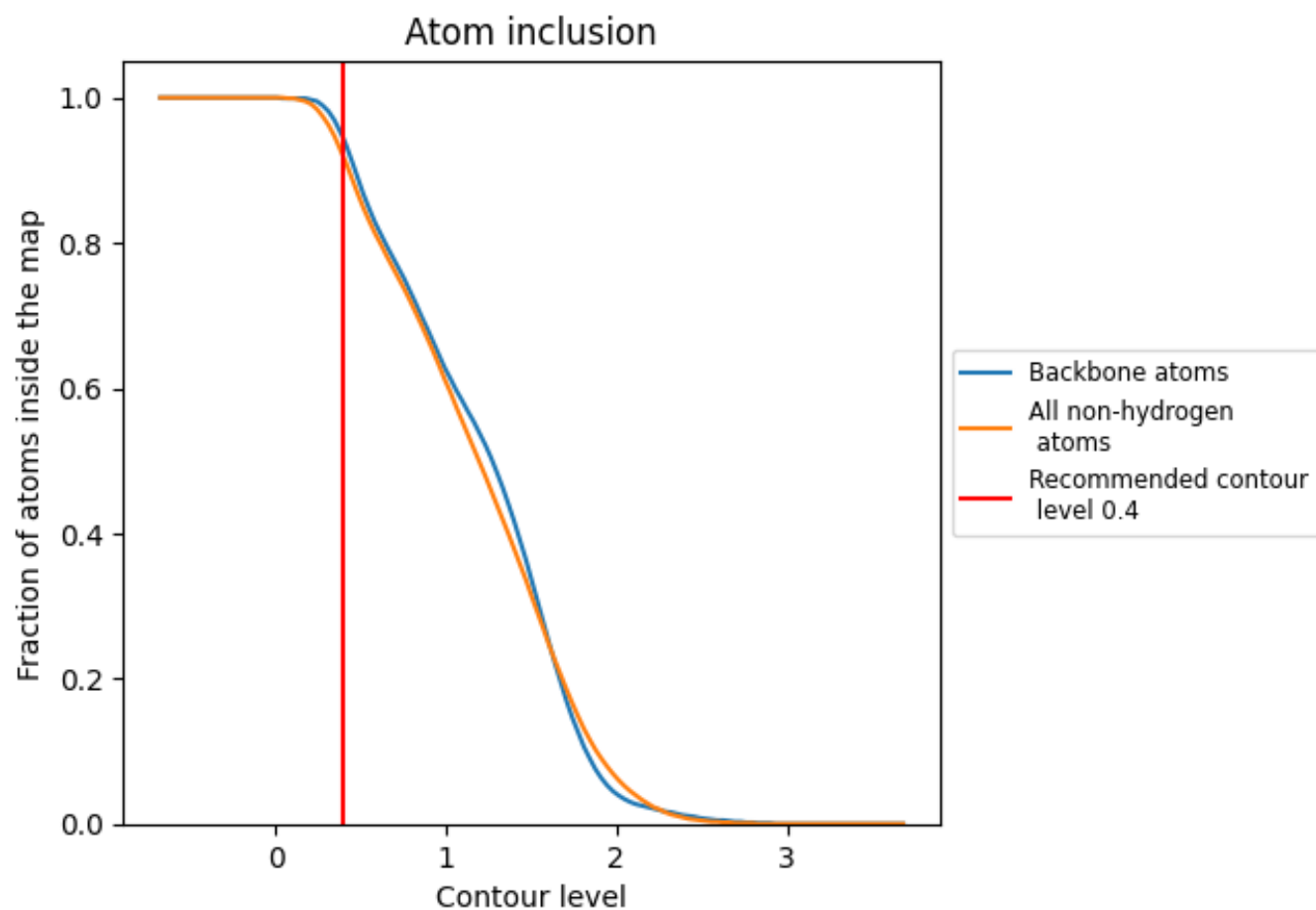
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9190   |  0.5120   |
| 0     |  0.8470   |  0.2900   |
| 1     |  1.0000   |  0.4020   |
| A     |  0.9930   |  0.6120   |
| B     |  0.9790   |  0.5890   |
| C     |  0.9640   |  0.5890   |
| D     |  0.9820   |  0.5850   |
| E     |  0.9390   |  0.5500   |
| F     |  0.9810   |  0.5800   |
| G     |  0.9680   |  0.5650   |
| H     |  0.9220   |  0.4640   |
| I     |  0.9680   |  0.5780   |
| J     |  0.9660   |  0.5780   |
| K     |  0.9660   |  0.5740   |
| L     |  0.9770  |  0.5700  |
| M     |  0.9560 |  0.5210 |
| N     |  0.9810 |  0.5940 |
| O     |  0.9580 |  0.5420 |
| P     |  0.9390 |  0.5230 |
| Q     |  0.9260 |  0.5490 |
| R     |  0.9820 |  0.5990 |
| S     |  0.9920 |  0.6150 |
| T     |  0.9770 |  0.5760 |
| U     |  0.9670 |  0.5580 |
| V     |  0.9600 |  0.5300 |
| W     |  1.0000 |  0.6280 |
| X     |  0.9210 |  0.4970 |
| Y     |  1.0000 |  0.6020 |
| Z     |  0.9700 |  0.5760 |
| a     |  0.5850 |  0.2180 |
| b     |  0.9640 |  0.5730 |
| c     |  0.9720 |  0.5700 |
| d     |  0.7610 |  0.4030 |
| e     |  0.6980 |  0.2570 |
| f     |  0.9820 |  0.5700 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                            | Q-score                                                                                   |
|-------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| g     |  0.8440  |  0.4880  |
| h     |  0.9990  |  0.5720  |
| i     |  0.9970  |  0.5980  |
| j     |  0.9910  |  0.6050  |
| k     |  0.9790  |  0.5880  |
| l     |  0.9780  |  0.5770  |
| m     |  0.9400  |  0.4870  |
| n     |  0.9500  |  0.5290  |
| o     |  0.9690  |  0.5710  |
| p     |  0.9460  |  0.5210  |
| q     |  0.9610  |  0.5500  |
| r     |  0.9610  |  0.5470  |
| s     |  0.9300  |  0.4480  |
| t     |  0.9710  |  0.5610  |
| u     |  0.9700  |  0.5500  |
| v     |  0.4610  |  0.3610  |
| w     |  0.1230  |  0.2290  |
| x     |  0.7470  |  0.2550  |
| y     |  0.8690  |  0.2310  |
| z     |  0.9090 |  0.2990 |