



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:48 PM UTC

PDB ID : 8PV5 / pdb\_00008pv5  
EMDB ID : EMD-17954  
Title : Chaetomium thermophilum pre-60S State 8 - pre-5S rotation without Foot - composite structure  
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.  
Deposited on : 2023-07-17  
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

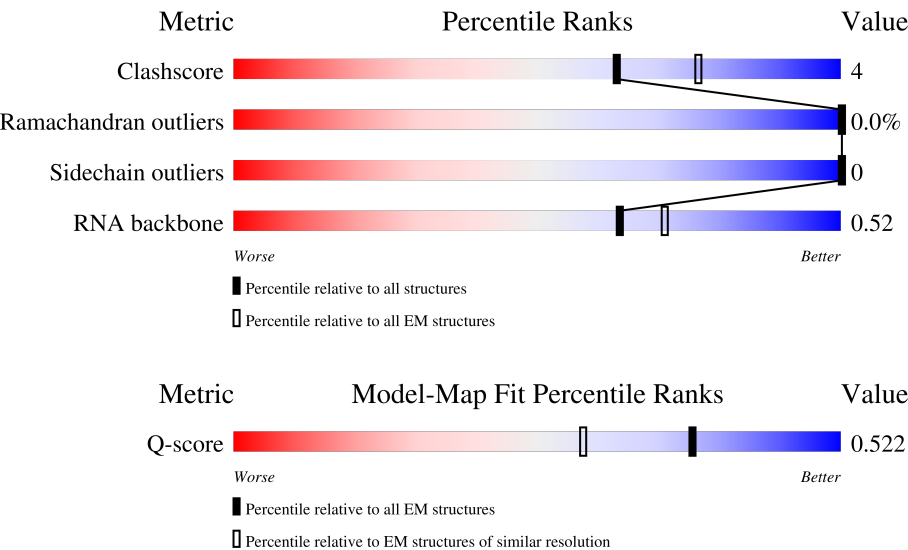
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.86 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                       | 12017 ( 2.36 - 3.36 )                                    |

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   | C1    | 3342   | <div><div>59%28%8%</div></div> |
| 2   | C2    | 156    | <div><div>69%25%</div></div>   |
| 3   | C4    | 119    | <div><div>8%61%36%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | CF    | 270    |                  |
| 5   | CH    | 661    |                  |
| 6   | CK    | 261    |                  |
| 7   | CL    | 558    |                  |
| 8   | CN    | 246    |                  |
| 9   | CO    | 120    |                  |
| 10  | CQ    | 225    |                  |
| 11  | Cb    | 117    |                  |
| 12  | Cd    | 627    |                  |
| 13  | Cf    | 350    |                  |
| 14  | Cg    | 202    |                  |
| 15  | Ch    | 517    |                  |
| 16  | Cz    | 123    |                  |
| 17  | LA    | 254    |                  |
| 18  | LB    | 392    |                  |
| 19  | LC    | 365    |                  |
| 20  | LD    | 304    |                  |
| 21  | LE    | 200    |                  |
| 22  | LF    | 249    |                  |
| 23  | LG    | 262    |                  |
| 24  | LH    | 229    |                  |
| 25  | LJ    | 173    |                  |
| 26  | LK    | 165    |                  |
| 27  | LL    | 213    |                  |
| 28  | LM    | 142    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | LN    | 203    |                  |
| 30  | LO    | 204    |                  |
| 31  | LP    | 187    |                  |
| 32  | LQ    | 213    |                  |
| 33  | LR    | 2898   |                  |
| 34  | LS    | 174    |                  |
| 35  | LT    | 160    |                  |
| 36  | LU    | 127    |                  |
| 37  | LV    | 139    |                  |
| 38  | LX    | 156    |                  |
| 39  | LY    | 138    |                  |
| 40  | LZ    | 135    |                  |
| 41  | La    | 149    |                  |
| 42  | Lc    | 108    |                  |
| 43  | Ld    | 120    |                  |
| 44  | Le    | 131    |                  |
| 45  | Lf    | 109    |                  |
| 46  | Lg    | 119    |                  |
| 47  | Lh    | 935    |                  |
| 48  | Li    | 110    |                  |
| 49  | Lj    | 95     |                  |
| 50  | Lk    | 94     |                  |
| 51  | Ll    | 51     |                  |
| 52  | Lp    | 92     |                  |
| 53  | Lq    | 147    |                  |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 144398 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 RNA chain called 26S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | C1    | 3060     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 65497 | 29256 | 11853 | 21328 | 3060 |         |       |

- Molecule 2 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 2   | C2    | 152      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3239  | 1448 | 579 | 1060 | 152 |         |       |

- Molecule 3 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 3   | C4    | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2536  | 1131 | 453 | 833 | 119 |         |       |

- Molecule 4 is a protein called Large ribosomal subunit protein uL10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | CF    | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1934  | 1215 | 350 | 360 | 9 |         |       |

- Molecule 5 is a protein called Nucleolar GTP-binding protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | CH    | 627      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5053  | 3175 | 920 | 939 | 19 |         |       |

- Molecule 6 is a protein called Ribosome biogenesis protein NSA2 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | CK    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1903  | 1198 | 368 | 333 | 4 |         |       |

- Molecule 7 is a protein called Putative GTP binding protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7   | CL    | 79       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 622   | 389 | 125 | 108 |         |       |

- Molecule 8 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | CN    | 246      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1853  | 1156 | 322 | 368 | 7 |         |       |

- Molecule 9 is a protein called DUF2423 domain-containing protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | CO    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 468   | 290 | 94 | 82 | 2 |         |       |

- Molecule 10 is a protein called Ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 10  | CQ    | 183      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1480  | 925 | 304 | 241 | 10 |         |       |

- Molecule 11 is a protein called Zinc finger domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | Cb    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 517 | 161 | 148 | 4 |         |       |

- Molecule 12 is a protein called Nucleolar GTP-binding protein 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | Cd    | 462      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3691  | 2350 | 671 | 659 | 11 |         |       |

- Molecule 13 is a protein called Ribosome production factor 2 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | Cf    | 285      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2282  | 1443 | 417 | 401 | 21 |         |       |

- Molecule 14 is a protein called Ribosome biogenesis regulatory protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | Cg    | 188      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1478  | 924 | 283 | 270 | 1 |         |       |

- Molecule 15 is a protein called Ribosome assembly protein 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | Ch    | 485      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3812  | 2396 | 696 | 710 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| Ch    | 117     | ASP      | GLU    | engineered mutation | UNP G0SC29 |

- Molecule 16 is a protein called rRNA-processing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | Cz    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 869   | 541 | 180 | 144 | 4 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L2-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | LA    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1454  | 917 | 278 | 256 | 3 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L3-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | LB    | 389      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3104  | 1973 | 579 | 539 | 13 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L4-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | LC    | 363      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2751  | 1737 | 527 | 478 | 9 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein l5-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | LD    | 286      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2266  | 1434 | 407 | 422 | 3 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | LE    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 944 | 267 | 263 | 3 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein l7-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | LF    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2023  | 1297 | 377 | 346 | 3 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | LG    | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1885  | 1207 | 349 | 324 | 5 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein l9-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | LH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 949 | 268 | 272 | 6 |         |       |

- Molecule 25 is a protein called Putative ribosomal protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | LJ    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1357  | 850 | 266 | 235 | 6 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L12-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LK    | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1184  | 743 | 215 | 224 | 2 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LL    | 203      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1587  | 989 | 325 | 271 | 2 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L14-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LM    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1126  | 714 | 216 | 195 | 1 |         |       |

- Molecule 29 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29  | LN    | 202      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1062 | 360 | 278 | 4 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L16-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | LO    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1611  | 1034 | 305 | 267 | 5 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein l17-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | LP    | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1343  | 834 | 274 | 232 | 3 |         |       |

- Molecule 32 is a protein called Ribosomal protein L18-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | LQ    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1200  | 759 | 239 | 200 | 2 |         |       |

- Molecule 33 is a protein called Ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | LR    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1226  | 763 | 259 | 200 | 4 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | LS    | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1426  | 917 | 266 | 238 | 5 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein l21-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | LT    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1027  | 651 | 195 | 179 | 2 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L22-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | LU    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 846   | 548 | 146 | 151 | 1 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein l23-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | LV    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 991   | 630 | 184 | 170 | 7 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L25-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 38  | LX    | 122      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 959   | 614 | 174 | 171 |  |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L26-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | LY    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1056  | 658 | 213 | 183 | 2 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | LZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 713 | 207 | 188 | 4 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L28-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | La    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 872   | 556 | 168 | 147 | 1 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein l30-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | Lc    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 449 | 122 | 129 | 5 |         |       |

- Molecule 43 is a protein called Putative 60S ribosomal protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | Ld    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 875   | 555 | 171 | 148 | 1 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L32-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Le    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1017  | 640 | 208 | 163 | 6 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein l33-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Lf    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 546 | 171 | 144 | 1 |         |       |

- Molecule 46 is a protein called Ribosomal protein l34-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | Lg    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 914   | 567 | 186 | 157 | 4 |         |       |

- Molecule 47 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 47  | Lh    | 118      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 981   | 626 | 194 | 161 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | Li    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 509 | 181 | 136 | 1 |         |       |

- Molecule 49 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | Lj    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 698   | 427 | 154 | 112 | 5 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L38-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | Lk    | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 632   | 400 | 121 | 109 | 2 |         |       |

- Molecule 51 is a protein called Ribosomal protein eL39.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 51  | Ll    | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 436   | 275 | 97 | 64 |         |       |

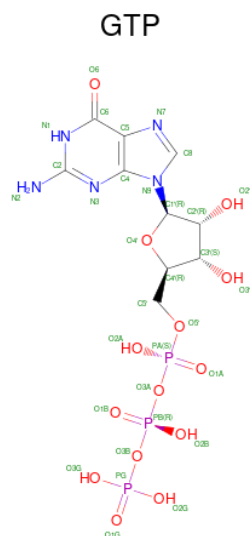
- Molecule 52 is a protein called 60S ribosomal protein L43-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 698   | 430 | 138 | 124 | 6 |         |       |

- Molecule 53 is a protein called Putative 60S ribosomal protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 53  | Lq    | 139      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1049  | 657 | 204 | 188 |         |       |

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 54  | CH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 54  | Cd    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 55  | CH    | 1        | Total Mg<br>1 1 | 0       |
| 55  | Cd    | 2        | Total Mg<br>2 2 | 0       |

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 56  | CQ    | 1        | Total Zn<br>1 1 | 0       |
| 56  | Cb    | 1        | Total Zn<br>1 1 | 0       |
| 56  | Lg    | 1        | Total Zn<br>1 1 | 0       |
| 56  | Lj    | 1        | Total Zn<br>1 1 | 0       |
| 56  | Lp    | 1        | Total Zn<br>1 1 | 0       |

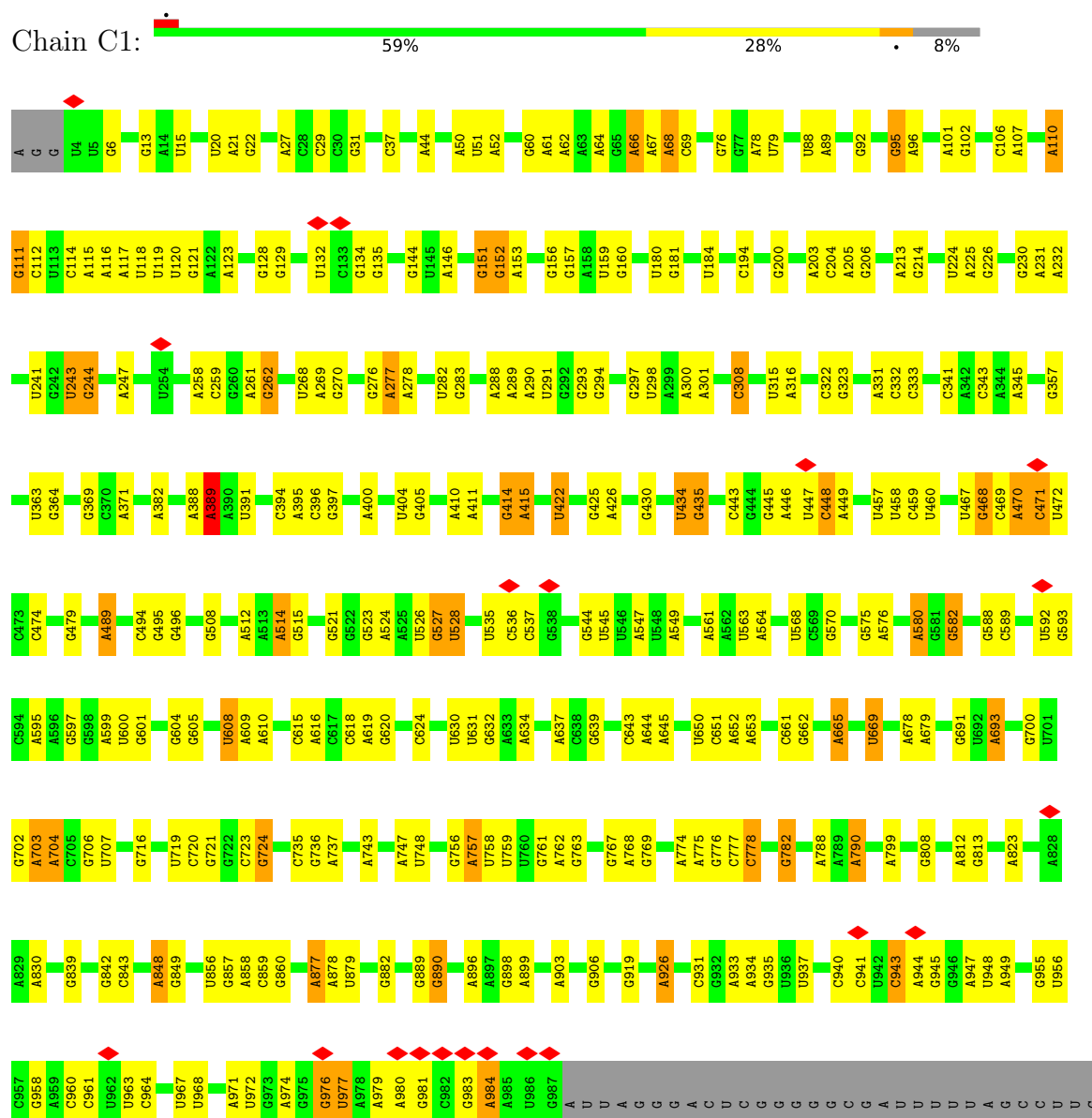
- Molecule 57 is water.

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 57  | CH    | 1        | Total<br>1 | O<br>1 | 0       |
| 57  | Cd    | 2        | Total<br>2 | O<br>2 | 0       |

### 3 Residue-property plots

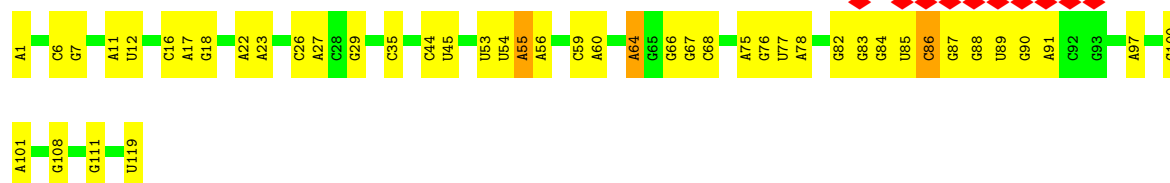
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S rRNA

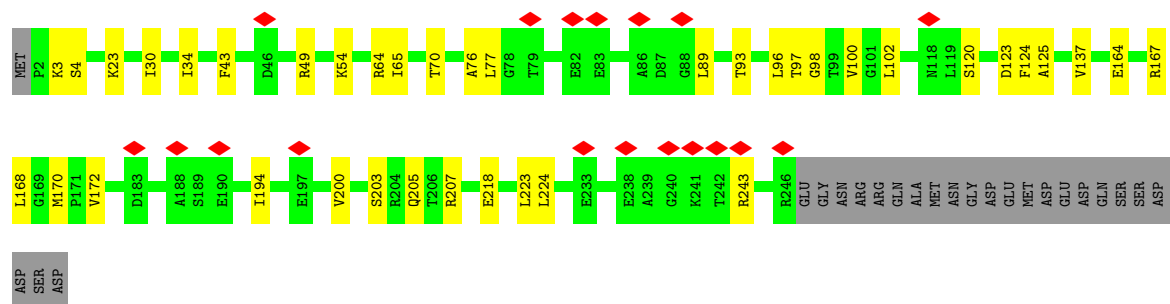
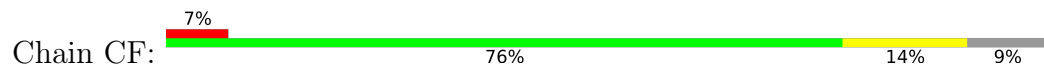




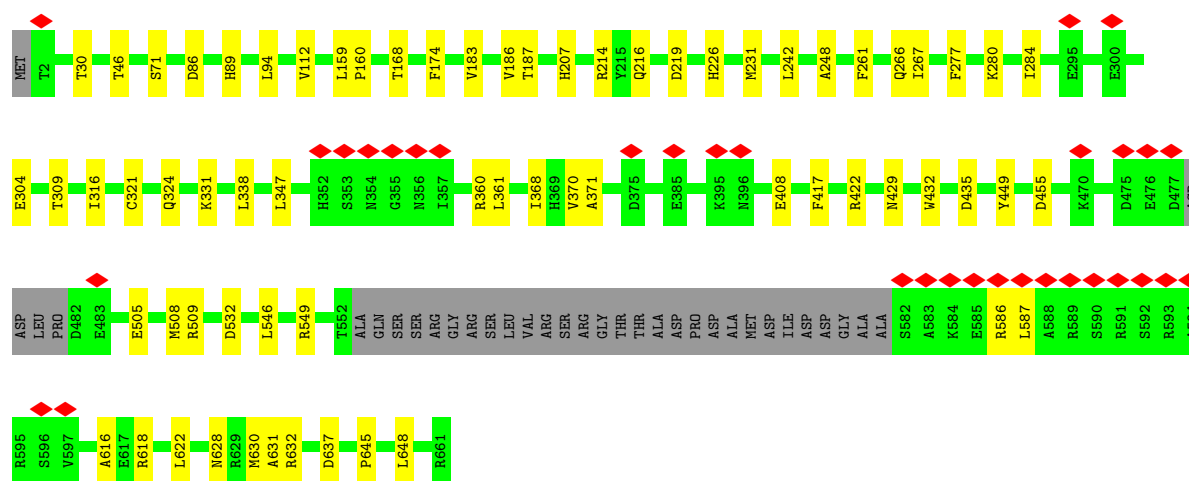
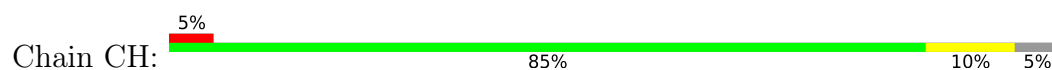
- Molecule 3: 5S rRNA



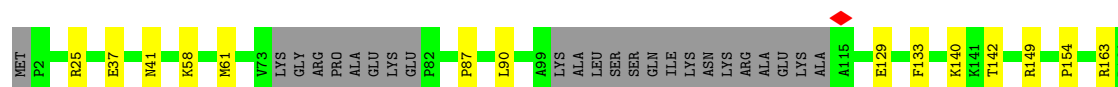
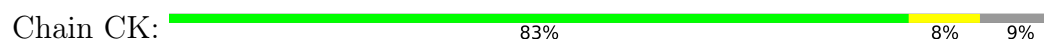
- Molecule 4: Large ribosomal subunit protein uL10



- Molecule 5: Nucleolar GTP-binding protein 1

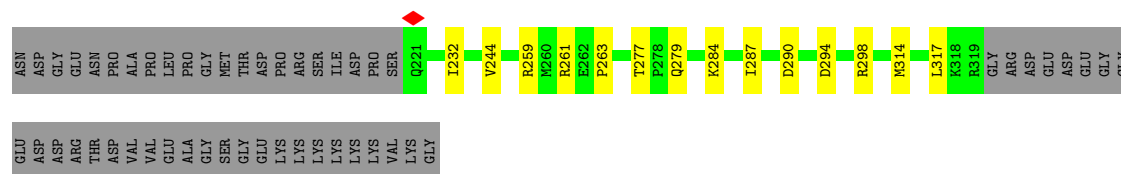


- Molecule 6: Ribosome biogenesis protein NSA2 homolog

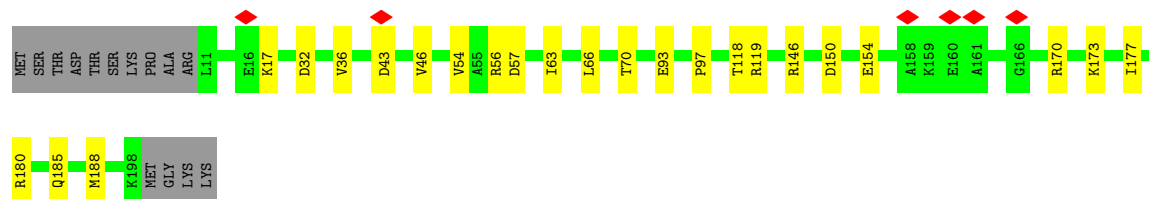
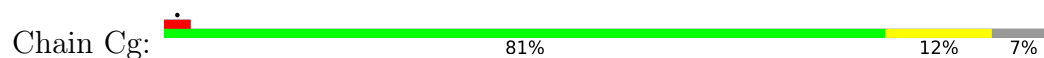




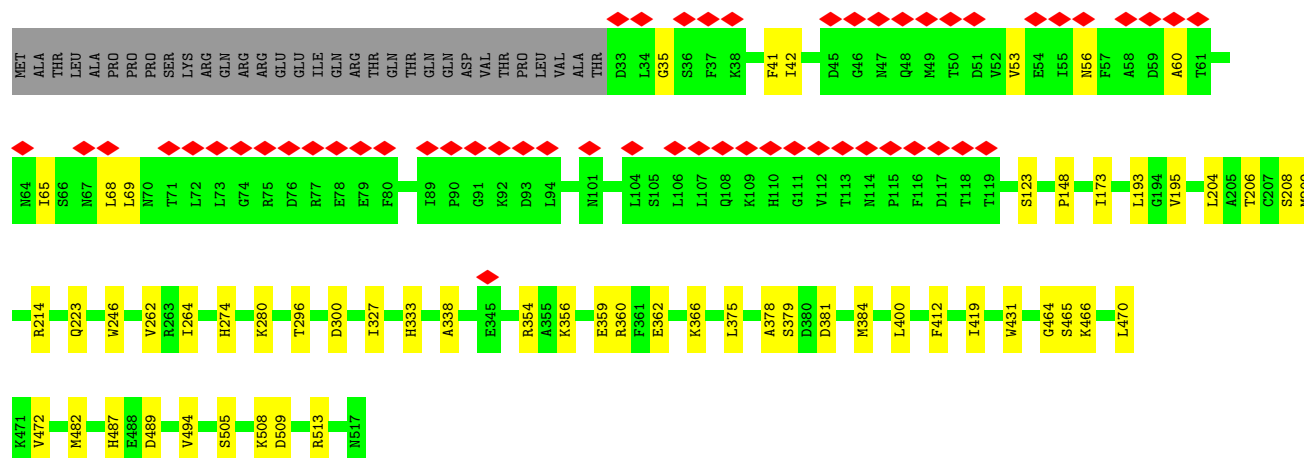
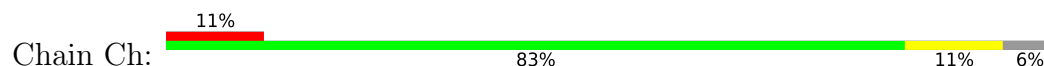




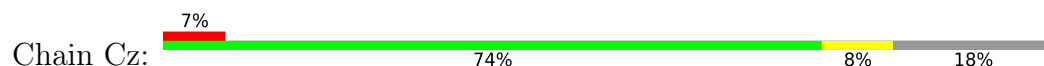
• Molecule 14: Ribosome biogenesis regulatory protein



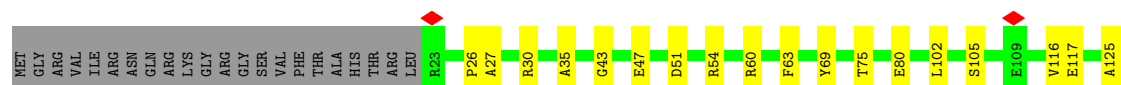
• Molecule 15: Ribosome assembly protein 4

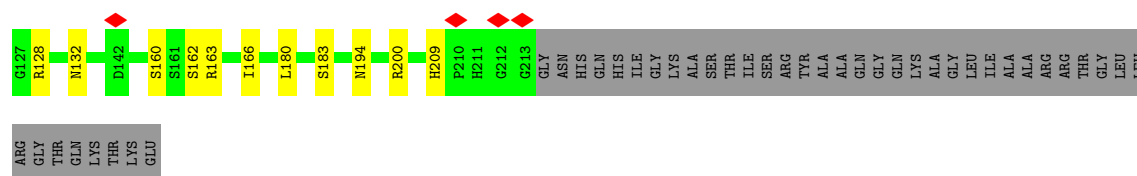


• Molecule 16: rRNA-processing protein

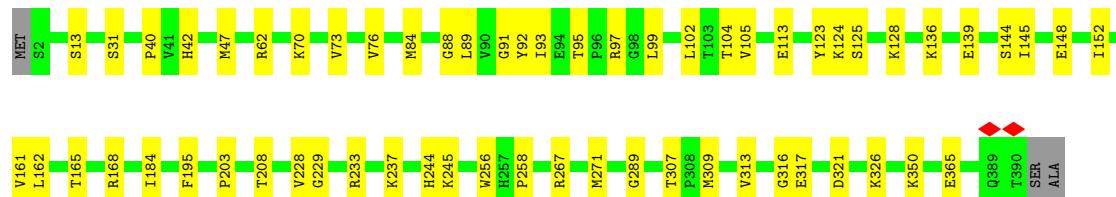
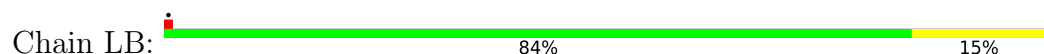


• Molecule 17: 60S ribosomal protein L2-like protein

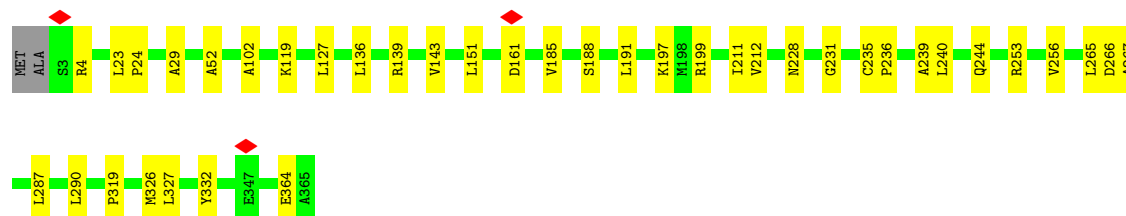




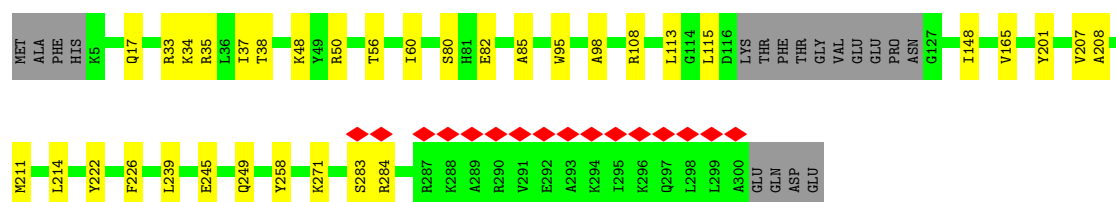
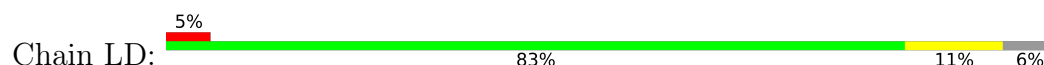
- Molecule 18: 60S ribosomal protein L3-like protein



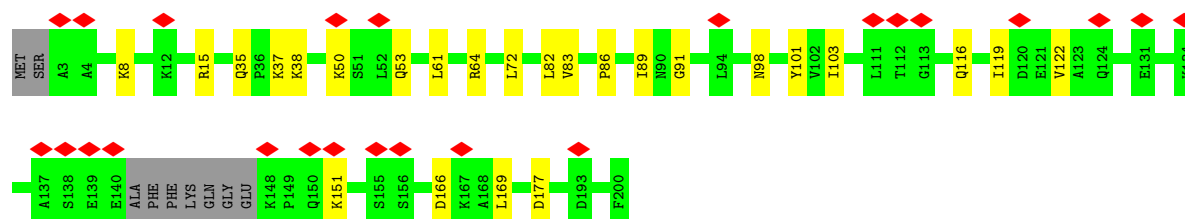
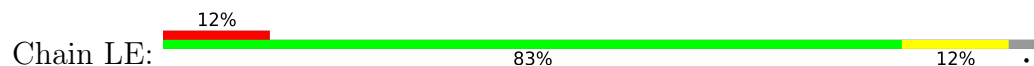
- Molecule 19: 60S ribosomal protein L4-like protein



- Molecule 20: 60S ribosomal protein l5-like protein

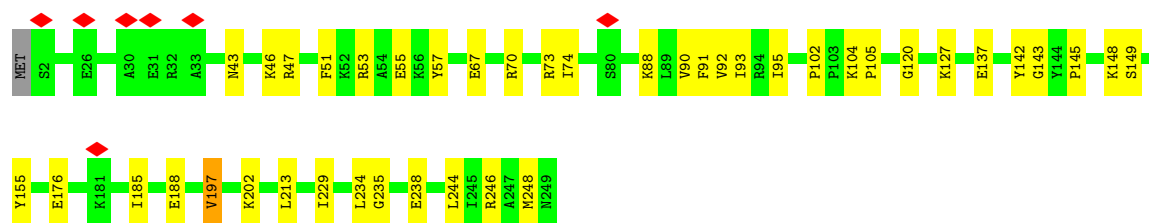


- Molecule 21: 60S ribosomal protein L6



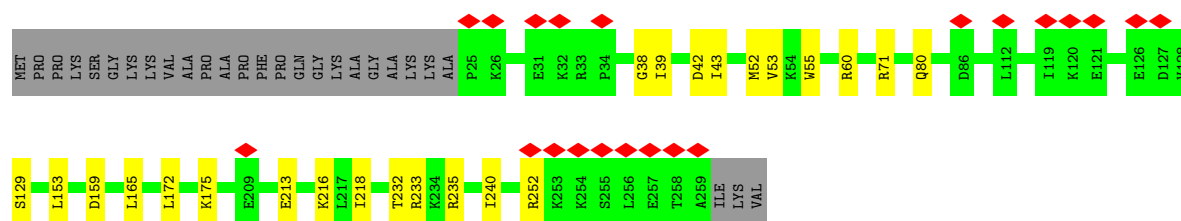
- Molecule 22: 60S ribosomal protein l7-like protein

Chain LF: 



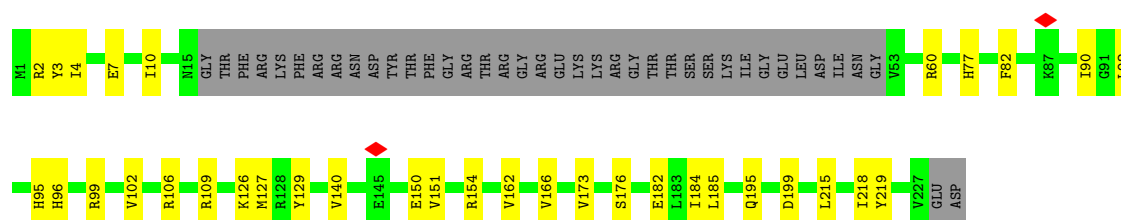
- Molecule 23: 60S ribosomal protein L8

Chain LG: 



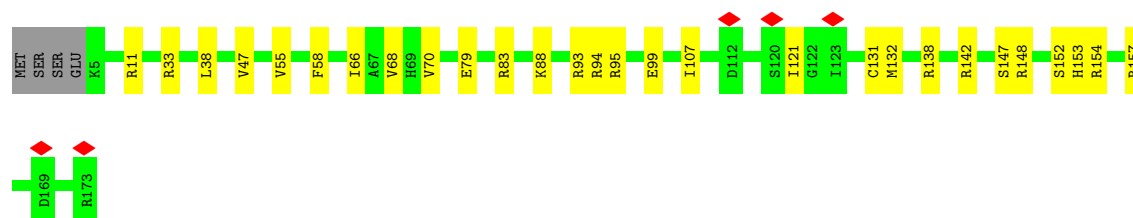
- Molecule 24: 60S ribosomal protein l9-like protein

Chain LH: 

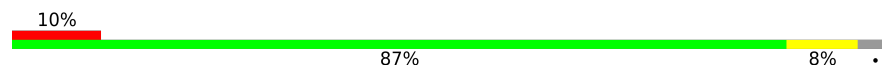


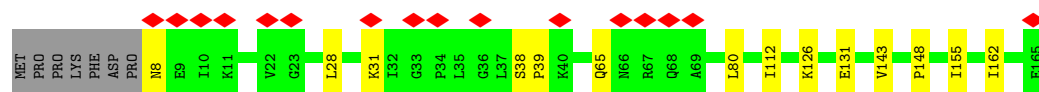
- Molecule 25: Putative ribosomal protein

Chain LJ: 

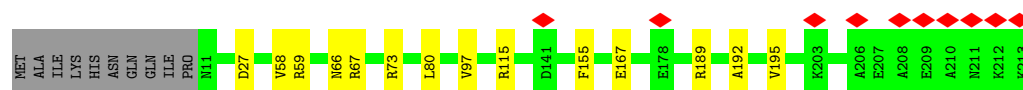
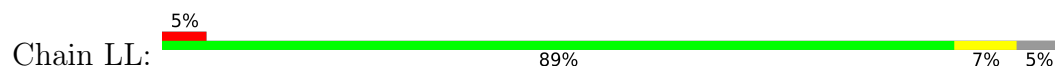


- Molecule 26: 60S ribosomal protein L12-like protein

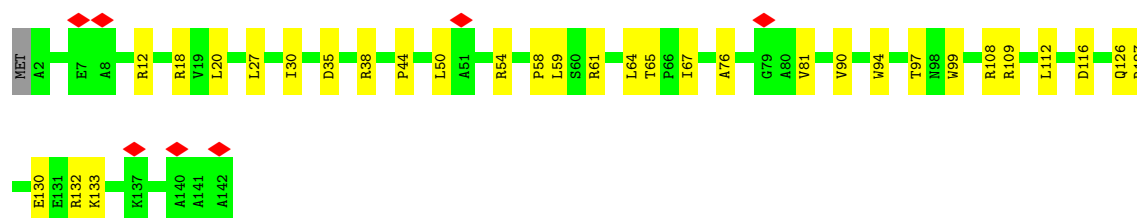
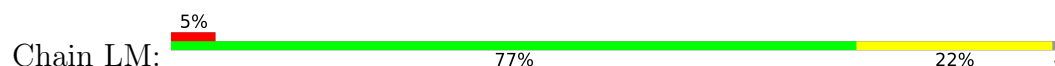
Chain LK: 



- Molecule 27: 60S ribosomal protein L13



- Molecule 28: 60S ribosomal protein L14-like protein



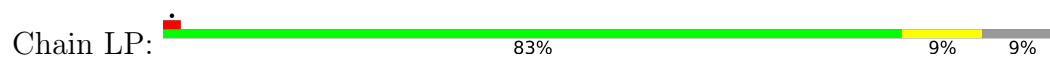
- Molecule 29: Ribosomal protein L15



- Molecule 30: 60S ribosomal protein L16-like protein

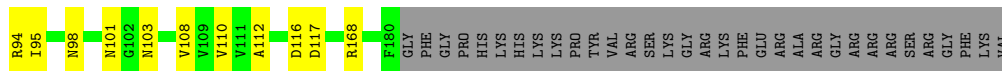


- Molecule 31: 60S ribosomal protein l17-like protein

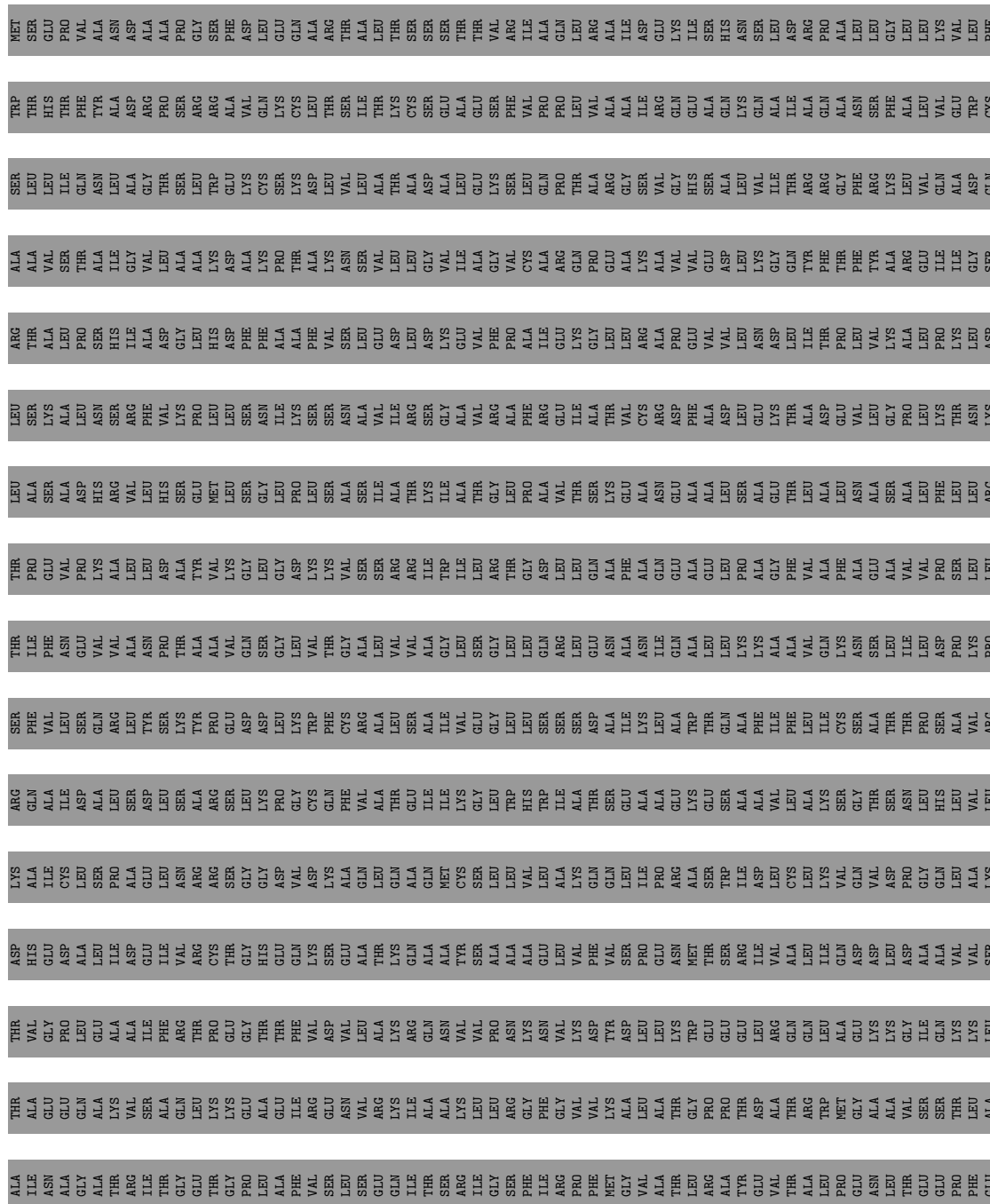


- Molecule 32: Ribosomal protein L18-like protein





Chain LR:  5% • 95%





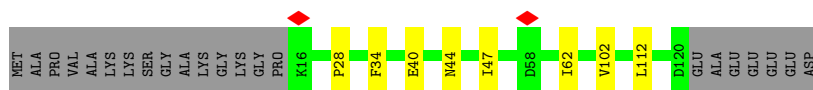
[illegible]

Chain LS: 

Chain LT: 

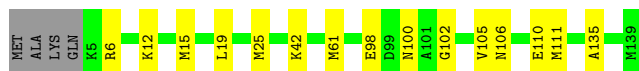
| Residue | Color  | Category      |
|---------|--------|---------------|
| MET     | Grey   | Not in top 20 |
| GLY     | Grey   | Not in top 20 |
| HIS     | Grey   | Not in top 20 |
| ALA     | Grey   | Not in top 20 |
| GLY     | Grey   | Not in top 20 |
| LEU     | Grey   | Not in top 20 |
| ARG     | Grey   | Not in top 20 |
| SER     | Grey   | Not in top 20 |
| GLY     | Grey   | Not in top 20 |
| THR     | Grey   | Not in top 20 |
| ARG     | Grey   | Not in top 20 |
| TYR     | Grey   | Not in top 20 |
| ALA     | Grey   | Not in top 20 |
| PHE     | Grey   | Not in top 20 |
| SER     | Grey   | Not in top 20 |
| ARG     | Grey   | Not in top 20 |
| GLY     | Grey   | Not in top 20 |
| PHE     | Grey   | Not in top 20 |
| ARG     | Grey   | Not in top 20 |
| LYS     | Grey   | Not in top 20 |
| HIS     | Grey   | Not in top 20 |
| GLY     | Grey   | Not in top 20 |
| GLN     | Grey   | Not in top 20 |
| ILE     | Grey   | Not in top 20 |
| PRO     | Grey   | Not in top 20 |
| LEU     | Grey   | Not in top 20 |
| LEU     | Grey   | Not in top 20 |
| THR     | Grey   | Not in top 20 |
| SER     | Grey   | Not in top 20 |
| LEU     | Grey   | Not in top 20 |
| TYR     | Grey   | Not in top 20 |
| R32     | Red    | Top 20        |
| T33     | Green  | Top 20        |
| Y34     | Yellow | Top 20        |
| R35     | Red    | Top 20        |
| V36     | Yellow | Top 20        |
| K43     | Yellow | Top 20        |
| G46     | Green  | Top 20        |
| A47     | Green  | Top 20        |
| V48     | Green  | Top 20        |
| Q49     | Green  | Top 20        |
| K50     | Green  | Top 20        |
| G51     | Green  | Top 20        |
| M52     | Green  | Top 20        |
| P53     | Green  | Top 20        |
| H54     | Green  | Top 20        |
| Y57     | Yellow | Top 20        |
| Y65     | Yellow | Top 20        |
| Y67     | Yellow | Top 20        |

Chain LU:  76% 6% 17%



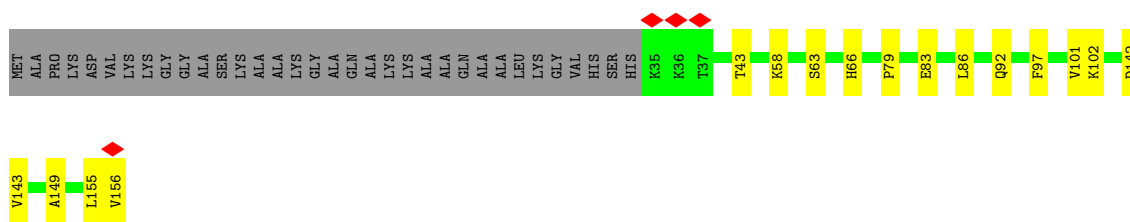
- Molecule 37: 60S ribosomal protein l23-like protein

Chain LV: 86% 11% .



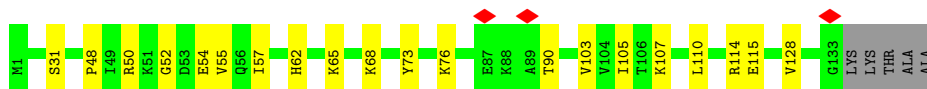
- Molecule 38: 60S ribosomal protein L25-like protein

Chain LX: 68% 10% 22%



- Molecule 39: 60S ribosomal protein L26-like protein

Chain LY: 82% 14% .



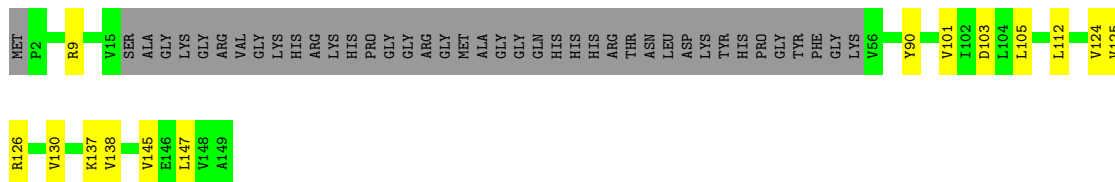
- Molecule 40: 60S ribosomal protein L27

Chain LZ: 7% 82% 18%



- Molecule 41: 60S ribosomal protein L28-like protein

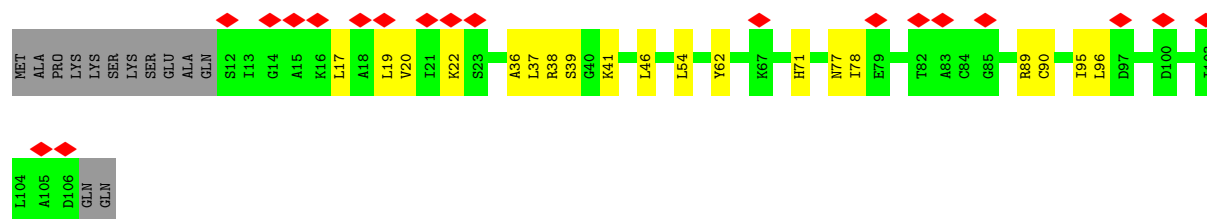
Chain La: 63% 9% 28%



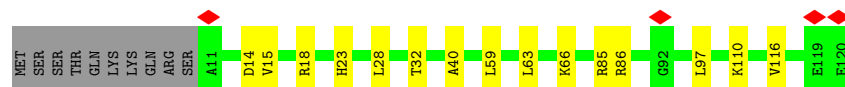
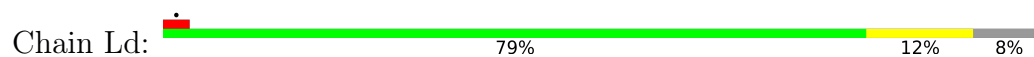
- Molecule 42: 60S ribosomal protein l30-like protein

Chain Lc: 18% 70% 18% 12%

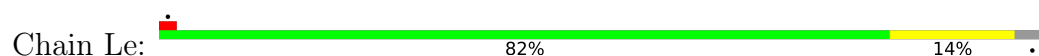




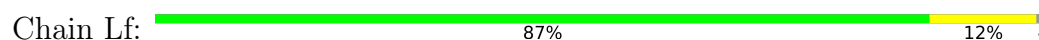
- Molecule 43: Putative 60S ribosomal protein



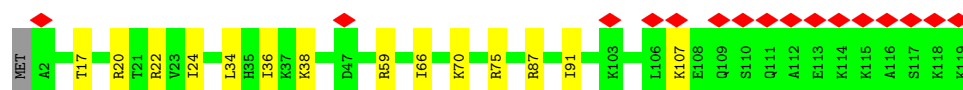
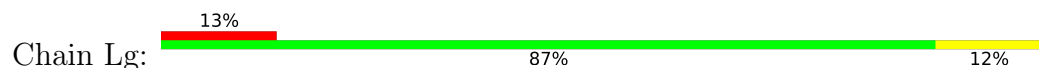
- Molecule 44: 60S ribosomal protein L32-like protein



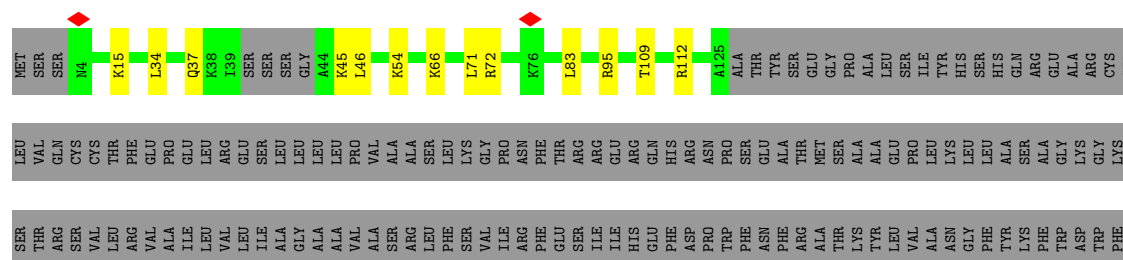
- Molecule 45: 60S ribosomal protein l33-like protein



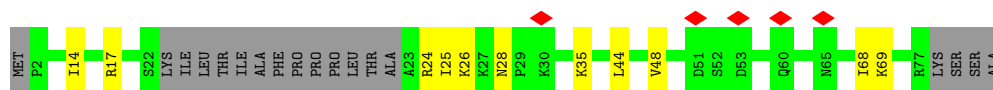
- Molecule 46: Ribosomal protein l34-like protein



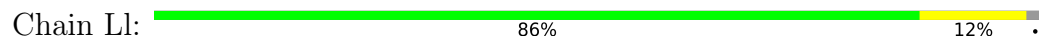
- Molecule 47: dolichyl-diphosphooligosaccharide--protein glycotransferase



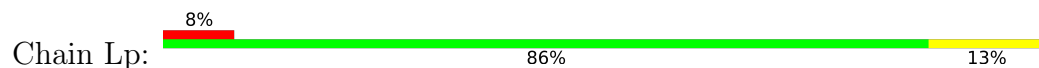




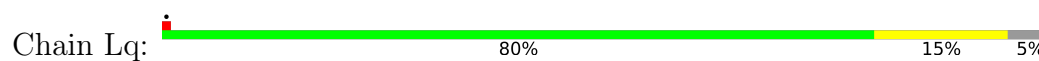
- Molecule 51: Ribosomal protein eL39



- Molecule 52: 60S ribosomal protein L43-like protein



- Molecule 53: Putative 60S ribosomal protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 88358                                   | 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)                 | 3500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 5.628                                   | Depositor |
| Minimum map value                    | -1.791                                  | Depositor |
| Average map value                    | 0.015                                   | Depositor |
| Map value standard deviation         | 0.127                                   | Depositor |
| Recommended contour level            | 0.6                                     | Depositor |
| Map size (Å)                         | 522.5, 522.5, 522.5                     | wwPDB     |
| Map dimensions                       | 500, 500, 500                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.045, 1.045, 1.045                     | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, A2M, OMC, OMG, OMU, ZN, 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   | C1    | 0.16         | 1/72444 (0.0%) | 0.31        | 0/112946      |
| 2   | C2    | 0.13         | 0/3621         | 0.29        | 0/5638        |
| 3   | C4    | 0.14         | 0/2833         | 0.30        | 0/4414        |
| 4   | CF    | 0.18         | 0/1972         | 0.43        | 0/2660        |
| 5   | CH    | 0.17         | 0/5137         | 0.42        | 1/6915 (0.0%) |
| 6   | CK    | 0.15         | 0/1939         | 0.38        | 0/2608        |
| 7   | CL    | 0.18         | 0/631          | 0.41        | 0/843         |
| 8   | CN    | 0.19         | 0/1878         | 0.49        | 0/2555        |
| 9   | CO    | 0.16         | 0/470          | 0.42        | 0/619         |
| 10  | CQ    | 0.22         | 0/1504         | 0.55        | 1/2000 (0.1%) |
| 11  | Cb    | 0.16         | 0/845          | 0.40        | 0/1128        |
| 12  | Cd    | 0.16         | 0/3770         | 0.39        | 0/5082        |
| 13  | Cf    | 0.14         | 0/2326         | 0.39        | 0/3113        |
| 14  | Cg    | 0.15         | 0/1508         | 0.36        | 0/2051        |
| 15  | Ch    | 0.18         | 0/3914         | 0.45        | 0/5319        |
| 16  | Cz    | 0.19         | 0/877          | 0.47        | 0/1148        |
| 17  | LA    | 0.17         | 0/1488         | 0.44        | 0/2009        |
| 18  | LB    | 0.19         | 0/3172         | 0.46        | 0/4260        |
| 19  | LC    | 0.17         | 0/2808         | 0.40        | 0/3785        |
| 20  | LD    | 0.15         | 0/2308         | 0.37        | 0/3105        |
| 21  | LE    | 0.17         | 0/1504         | 0.46        | 2/2027 (0.1%) |
| 22  | LF    | 0.22         | 0/2061         | 0.54        | 0/2765        |
| 23  | LG    | 0.17         | 0/1914         | 0.45        | 0/2561        |
| 24  | LH    | 0.15         | 0/1515         | 0.40        | 0/2037        |
| 25  | LJ    | 0.16         | 0/1379         | 0.43        | 0/1844        |
| 26  | LK    | 0.18         | 0/1198         | 0.48        | 0/1611        |
| 27  | LL    | 0.17         | 0/1614         | 0.39        | 0/2168        |
| 28  | LM    | 0.22         | 0/1145         | 0.53        | 0/1539        |
| 29  | LN    | 0.16         | 0/1741         | 0.38        | 0/2332        |
| 30  | LO    | 0.18         | 0/1645         | 0.44        | 0/2205        |
| 31  | LP    | 0.17         | 0/1364         | 0.42        | 0/1835        |
| 32  | LQ    | 0.18         | 0/1218         | 0.45        | 1/1639 (0.1%) |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 33  | LR    | 0.15         | 0/1245          | 0.39        | 0/1662          |
| 34  | LS    | 0.17         | 0/1461          | 0.46        | 0/1966          |
| 35  | LT    | 0.20         | 0/1046          | 0.53        | 0/1409          |
| 36  | LU    | 0.16         | 0/859           | 0.42        | 0/1151          |
| 37  | LV    | 0.16         | 0/1009          | 0.38        | 0/1357          |
| 38  | LX    | 0.18         | 0/975           | 0.43        | 0/1317          |
| 39  | LY    | 0.18         | 0/1070          | 0.46        | 0/1432          |
| 40  | LZ    | 0.20         | 0/1135          | 0.46        | 0/1519          |
| 41  | La    | 0.16         | 0/892           | 0.40        | 0/1200          |
| 42  | Lc    | 0.17         | 0/714           | 0.48        | 0/960           |
| 43  | Ld    | 0.17         | 0/889           | 0.38        | 0/1192          |
| 44  | Le    | 0.18         | 0/1035          | 0.41        | 0/1379          |
| 45  | Lf    | 0.16         | 0/883           | 0.44        | 0/1187          |
| 46  | Lg    | 0.17         | 0/927           | 0.39        | 0/1244          |
| 47  | Lh    | 0.15         | 0/991           | 0.36        | 0/1317          |
| 48  | Li    | 0.14         | 0/834           | 0.36        | 0/1099          |
| 49  | Lj    | 0.17         | 0/712           | 0.47        | 2/944 (0.2%)    |
| 50  | Lk    | 0.17         | 0/640           | 0.47        | 0/850           |
| 51  | Ll    | 0.13         | 0/446           | 0.30        | 0/593           |
| 52  | Lp    | 0.16         | 0/706           | 0.47        | 0/940           |
| 53  | Lq    | 0.18         | 0/1067          | 0.46        | 0/1442          |
| All | All   | 0.16         | 1/153279 (0.0%) | 0.37        | 7/222921 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | C1    | 1847 | A2M  | O3'-P | 5.11 | 1.61        | 1.56     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 10  | CQ    | 161 | ARG  | CB-CG-CD | 7.69  | 128.99      | 111.30   |
| 49  | Lj    | 69  | THR  | CA-C-N   | 5.56  | 123.74      | 120.24   |
| 49  | Lj    | 69  | THR  | C-N-CA   | 5.56  | 123.74      | 120.24   |
| 5   | CH    | 505 | GLU  | N-CA-CB  | 5.20  | 117.86      | 110.16   |
| 32  | LQ    | 47  | PRO  | CA-N-CD  | -5.07 | 104.91      | 112.00   |
| 21  | LE    | 177 | ASP  | CA-C-N   | 5.03  | 130.46      | 122.61   |
| 21  | LE    | 177 | ASP  | C-N-CA   | 5.03  | 130.46      | 122.61   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C1    | 65497 | 0        | 33046    | 452     | 0            |
| 2   | C2    | 3239  | 0        | 1637     | 24      | 0            |
| 3   | C4    | 2536  | 0        | 1286     | 21      | 0            |
| 4   | CF    | 1934  | 0        | 1945     | 26      | 0            |
| 5   | CH    | 5053  | 0        | 5135     | 46      | 0            |
| 6   | CK    | 1903  | 0        | 1990     | 16      | 0            |
| 7   | CL    | 622   | 0        | 641      | 7       | 0            |
| 8   | CN    | 1853  | 0        | 1852     | 26      | 0            |
| 9   | CO    | 468   | 0        | 503      | 6       | 0            |
| 10  | CQ    | 1480  | 0        | 1523     | 10      | 0            |
| 11  | Cb    | 830   | 0        | 838      | 7       | 0            |
| 12  | Cd    | 3691  | 0        | 3817     | 35      | 0            |
| 13  | Cf    | 2282  | 0        | 2347     | 24      | 0            |
| 14  | Cg    | 1478  | 0        | 1517     | 16      | 0            |
| 15  | Ch    | 3812  | 0        | 3715     | 31      | 0            |
| 16  | Cz    | 869   | 0        | 956      | 10      | 0            |
| 17  | LA    | 1454  | 0        | 1490     | 22      | 0            |
| 18  | LB    | 3104  | 0        | 3221     | 42      | 0            |
| 19  | LC    | 2751  | 0        | 2875     | 30      | 0            |
| 20  | LD    | 2266  | 0        | 2219     | 22      | 0            |
| 21  | LE    | 1477  | 0        | 1567     | 21      | 0            |
| 22  | LF    | 2023  | 0        | 2132     | 33      | 0            |
| 23  | LG    | 1885  | 0        | 2032     | 18      | 0            |
| 24  | LH    | 1495  | 0        | 1573     | 21      | 0            |
| 25  | LJ    | 1357  | 0        | 1385     | 20      | 0            |
| 26  | LK    | 1184  | 0        | 1249     | 8       | 0            |
| 27  | LL    | 1587  | 0        | 1655     | 11      | 0            |
| 28  | LM    | 1126  | 0        | 1198     | 21      | 0            |
| 29  | LN    | 1704  | 0        | 1767     | 22      | 0            |
| 30  | LO    | 1611  | 0        | 1702     | 16      | 0            |
| 31  | LP    | 1343  | 0        | 1369     | 12      | 0            |
| 32  | LQ    | 1200  | 0        | 1296     | 17      | 0            |
| 33  | LR    | 1226  | 0        | 1292     | 16      | 0            |
| 34  | LS    | 1426  | 0        | 1481     | 19      | 0            |
| 35  | LT    | 1027  | 0        | 1076     | 14      | 0            |
| 36  | LU    | 846   | 0        | 883      | 4       | 0            |
| 37  | LV    | 991   | 0        | 1044     | 9       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | LX    | 959    | 0        | 1018     | 12      | 0            |
| 39  | LY    | 1056   | 0        | 1143     | 13      | 0            |
| 40  | LZ    | 1112   | 0        | 1181     | 16      | 0            |
| 41  | La    | 872    | 0        | 903      | 11      | 0            |
| 42  | Lc    | 705    | 0        | 751      | 12      | 0            |
| 43  | Ld    | 875    | 0        | 918      | 11      | 0            |
| 44  | Le    | 1017   | 0        | 1092     | 15      | 0            |
| 45  | Lf    | 862    | 0        | 891      | 9       | 0            |
| 46  | Lg    | 914    | 0        | 960      | 12      | 0            |
| 47  | Lh    | 981    | 0        | 1097     | 10      | 0            |
| 48  | Li    | 827    | 0        | 906      | 11      | 0            |
| 49  | Lj    | 698    | 0        | 726      | 10      | 0            |
| 50  | Lk    | 632    | 0        | 693      | 6       | 0            |
| 51  | Ll    | 436    | 0        | 473      | 6       | 0            |
| 52  | Lp    | 698    | 0        | 737      | 7       | 0            |
| 53  | Lq    | 1049   | 0        | 1075     | 15      | 0            |
| 54  | CH    | 32     | 0        | 12       | 0       | 0            |
| 54  | Cd    | 32     | 0        | 12       | 1       | 0            |
| 55  | CH    | 1      | 0        | 0        | 0       | 0            |
| 55  | Cd    | 2      | 0        | 0        | 0       | 0            |
| 56  | CQ    | 1      | 0        | 0        | 0       | 0            |
| 56  | Cb    | 1      | 0        | 0        | 0       | 0            |
| 56  | Lg    | 1      | 0        | 0        | 0       | 0            |
| 56  | Lj    | 1      | 0        | 0        | 0       | 0            |
| 56  | Lp    | 1      | 0        | 0        | 0       | 0            |
| 57  | CH    | 1      | 0        | 0        | 0       | 0            |
| 57  | Cd    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 144398 | 0        | 111842   | 1052    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1052) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:C1:2400:G:H1   | 1:C1:2473:U:H3     | 1.05                     | 0.93              |
| 1:C1:2389:U:H3   | 1:C1:2562:G:H1     | 1.20                     | 0.90              |
| 1:C1:1054:U:H3   | 1:C1:1070:G:H1     | 0.85                     | 0.85              |
| 18:LB:91:GLY:HA3 | 18:LB:152:ILE:HD11 | 1.60                     | 0.82              |
| 1:C1:2327:G:H22  | 1:C1:2359:G:H1'    | 1.51                     | 0.76              |
| 5:CH:449:TYR:HD2 | 10:CQ:93:MET:HG2   | 1.52                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:CQ:145:LEU:HD22 | 10:CQ:159:LEU:HB3  | 1.70                     | 0.73              |
| 18:LB:95:THR:HG22  | 18:LB:97:ARG:H     | 1.52                     | 0.73              |
| 1:C1:2179:G:H1     | 1:C1:2192:A:H61    | 1.35                     | 0.73              |
| 1:C1:1625:U:H3     | 1:C1:1790:G:H1     | 1.36                     | 0.71              |
| 44:Le:88:MET:HG3   | 53:Lq:36:THR:HA    | 1.71                     | 0.71              |
| 1:C1:1431:U:H2'    | 1:C1:1432:A2M:H8   | 1.74                     | 0.69              |
| 18:LB:105:VAL:HG13 | 18:LB:145:ILE:HD11 | 1.74                     | 0.69              |
| 15:Ch:384:MET:HB2  | 15:Ch:400:LEU:HB2  | 1.75                     | 0.68              |
| 1:C1:2164:G:H21    | 1:C1:2205:A:H62    | 1.42                     | 0.67              |
| 22:LF:92:VAL:O     | 22:LF:120:GLY:HA2  | 1.95                     | 0.67              |
| 1:C1:3204:C:H2'    | 1:C1:3205:G:H8     | 1.60                     | 0.66              |
| 1:C1:3081:A:HO2'   | 24:LH:77:HIS:HD1   | 1.42                     | 0.66              |
| 1:C1:568:U:OP1     | 22:LF:246:ARG:NH2  | 2.28                     | 0.66              |
| 1:C1:1912:A:N1     | 12:Cd:448:ARG:NH2  | 2.44                     | 0.65              |
| 22:LF:149:SER:OG   | 22:LF:246:ARG:NH1  | 2.28                     | 0.65              |
| 1:C1:2101:A:HO2'   | 49:Lj:2:THR:N      | 1.95                     | 0.65              |
| 5:CH:587:LEU:HD11  | 38:LX:86:LEU:HD22  | 1.79                     | 0.65              |
| 13:Cf:314:MET:HB2  | 13:Cf:317:LEU:HD23 | 1.79                     | 0.65              |
| 1:C1:2181:G:OP2    | 48:Li:77:ARG:NH2   | 2.30                     | 0.64              |
| 12:Cd:285:ILE:HD11 | 12:Cd:296:ALA:HB2  | 1.78                     | 0.64              |
| 11:Cb:92:MET:HG3   | 11:Cb:97:TYR:HB3   | 1.79                     | 0.64              |
| 24:LH:10:ILE:HG12  | 24:LH:109:ARG:HG2  | 1.80                     | 0.64              |
| 20:LD:85:ALA:HB2   | 20:LD:258:TYR:HB2  | 1.80                     | 0.64              |
| 1:C1:3209:A:OP1    | 21:LE:64:ARG:NH1   | 2.31                     | 0.63              |
| 5:CH:183:VAL:HG21  | 5:CH:219:ASP:HB2   | 1.80                     | 0.63              |
| 15:Ch:35:GLY:O     | 15:Ch:56:ASN:ND2   | 2.30                     | 0.63              |
| 4:CF:137:VAL:HG21  | 4:CF:170:MET:HE1   | 1.78                     | 0.63              |
| 23:LG:165:LEU:HA   | 29:LN:7:LEU:HD11   | 1.80                     | 0.63              |
| 1:C1:2525:U:H3     | 1:C1:2535:G:H1     | 1.46                     | 0.63              |
| 24:LH:150:GLU:HG2  | 24:LH:166:VAL:HG22 | 1.81                     | 0.63              |
| 17:LA:80:GLU:HG3   | 52:Lp:66:GLY:HA2   | 1.80                     | 0.63              |
| 25:LJ:88:LYS:HE2   | 25:LJ:107:ILE:HG22 | 1.82                     | 0.62              |
| 1:C1:2899:A:H2'    | 18:LB:256:TRP:HB3  | 1.80                     | 0.62              |
| 5:CH:186:VAL:HG23  | 5:CH:187:THR:HG23  | 1.80                     | 0.62              |
| 18:LB:228:VAL:HG21 | 18:LB:271:MET:HE2  | 1.81                     | 0.62              |
| 29:LN:183:THR:HG22 | 29:LN:187:ARG:HB2  | 1.82                     | 0.62              |
| 34:LS:34:GLU:HG2   | 34:LS:61:VAL:HG11  | 1.82                     | 0.61              |
| 1:C1:2087:G:O2'    | 12:Cd:448:ARG:NH1  | 2.33                     | 0.61              |
| 28:LM:44:PRO:HG3   | 28:LM:81:VAL:HG12  | 1.83                     | 0.61              |
| 1:C1:1199:C:OP2    | 7:CL:57:ASN:ND2    | 2.33                     | 0.61              |
| 22:LF:46:LYS:HE3   | 22:LF:185:ILE:HG12 | 1.83                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CN:142:ILE:HG12  | 8:CN:148:VAL:HG12  | 1.82                     | 0.61              |
| 1:C1:3289:G:H1     | 1:C1:3298:U:H3     | 1.47                     | 0.61              |
| 1:C1:1373:A:N6     | 1:C1:1401:A:O2'    | 2.33                     | 0.61              |
| 15:Ch:195:VAL:HG12 | 15:Ch:206:THR:HG22 | 1.82                     | 0.61              |
| 1:C1:2546:U:H4'    | 23:LG:52:MET:HG2   | 1.82                     | 0.61              |
| 8:CN:21:ASN:ND2    | 8:CN:112:ASP:OD2   | 2.34                     | 0.60              |
| 1:C1:1614:G:N7     | 40:LZ:16:ARG:NH1   | 2.49                     | 0.60              |
| 1:C1:3158:C:OP1    | 28:LM:132:ARG:NH2  | 2.33                     | 0.60              |
| 1:C1:2892:A:OP2    | 37:LV:6:ARG:NH1    | 2.34                     | 0.60              |
| 19:LC:29:ALA:O     | 53:Lq:3:ASN:ND2    | 2.34                     | 0.60              |
| 25:LJ:94:ARG:HG2   | 25:LJ:157:ARG:HH21 | 1.65                     | 0.60              |
| 1:C1:2397:U:OP2    | 29:LN:24:ARG:NH1   | 2.34                     | 0.60              |
| 1:C1:2478:A:N1     | 1:C1:2553:C:N4     | 2.50                     | 0.60              |
| 43:Ld:14:ASP:HB3   | 43:Ld:97:LEU:HD21  | 1.82                     | 0.60              |
| 1:C1:508:G:OP1     | 22:LF:73:ARG:NH2   | 2.29                     | 0.60              |
| 6:CK:163:ARG:HH22  | 12:Cd:228:LYS:HG2  | 1.67                     | 0.60              |
| 8:CN:107:VAL:HG23  | 8:CN:108:ILE:HG13  | 1.83                     | 0.60              |
| 17:LA:30:ARG:HD3   | 17:LA:63:PHE:HD2   | 1.67                     | 0.60              |
| 1:C1:1264:U:H2'    | 1:C1:1265:G:H8     | 1.67                     | 0.59              |
| 41:La:103:ASP:HA   | 41:La:126:ARG:HB2  | 1.83                     | 0.59              |
| 1:C1:984:A:N1      | 1:C1:1033:U:O2'    | 2.36                     | 0.59              |
| 24:LH:2:ARG:NH2    | 24:LH:96:HIS:O     | 2.35                     | 0.59              |
| 26:LK:126:LYS:HG3  | 26:LK:162:ILE:HD12 | 1.83                     | 0.59              |
| 1:C1:474:C:OP1     | 53:Lq:88:ARG:NH1   | 2.35                     | 0.59              |
| 19:LC:185:VAL:HG11 | 19:LC:231:GLY:HA3  | 1.83                     | 0.59              |
| 1:C1:203:A:N3      | 19:LC:228:ASN:ND2  | 2.48                     | 0.59              |
| 33:LR:98:ARG:NH1   | 33:LR:130:ASN:OD1  | 2.36                     | 0.59              |
| 1:C1:706:G:N2      | 1:C1:706:G:OP2     | 2.35                     | 0.59              |
| 1:C1:2405:G:H1     | 1:C1:2468:U:H3     | 1.49                     | 0.59              |
| 9:CO:36:LYS:HE2    | 18:LB:208:THR:HG22 | 1.84                     | 0.59              |
| 42:Lc:41:LYS:HG3   | 42:Lc:96:LEU:HD22  | 1.83                     | 0.59              |
| 3:C4:88:G:N2       | 3:C4:91:A:OP2      | 2.36                     | 0.59              |
| 15:Ch:53:VAL:HG21  | 15:Ch:68:LEU:HD21  | 1.85                     | 0.59              |
| 13:Cf:145:ALA:HB3  | 13:Cf:188:THR:HG22 | 1.84                     | 0.59              |
| 24:LH:173:VAL:HG22 | 24:LH:185:LEU:HG   | 1.83                     | 0.59              |
| 1:C1:1260:C:H2'    | 1:C1:1261:A:H8     | 1.68                     | 0.59              |
| 1:C1:1685:U:O2     | 1:C1:1766:G:O2'    | 2.20                     | 0.59              |
| 1:C1:2079:G:OP1    | 1:C1:2081:C:N4     | 2.36                     | 0.59              |
| 1:C1:2833:G:OP2    | 1:C1:2833:G:N2     | 2.35                     | 0.59              |
| 17:LA:117:GLU:HB2  | 17:LA:162:SER:HB2  | 1.85                     | 0.59              |
| 33:LR:105:LEU:HD23 | 33:LR:138:LEU:HD23 | 1.85                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:Lq:31:ASP:HB3   | 53:Lq:34:ASN:HB2   | 1.85                     | 0.59              |
| 21:LE:50:LYS:O     | 21:LE:53:GLN:NE2   | 2.36                     | 0.58              |
| 26:LK:155:ILE:HD13 | 26:LK:162:ILE:HD11 | 1.84                     | 0.58              |
| 1:C1:1661:U:OP1    | 5:CH:509:ARG:NH1   | 2.36                     | 0.58              |
| 1:C1:2477:U:OP2    | 1:C1:2545:G:N2     | 2.30                     | 0.58              |
| 5:CH:628:ASN:O     | 31:LP:125:GLN:NE2  | 2.34                     | 0.58              |
| 1:C1:1305:U:O2'    | 34:LS:1:MET:SD     | 2.62                     | 0.58              |
| 1:C1:2518:G:OP1    | 17:LA:69:TYR:OH    | 2.20                     | 0.58              |
| 29:LN:30:TYR:O     | 29:LN:65:ARG:NH1   | 2.35                     | 0.58              |
| 46:Lg:20:ARG:HG3   | 46:Lg:36:ILE:HG13  | 1.85                     | 0.58              |
| 2:C2:63:G:O2'      | 47:Lh:54:LYS:NZ    | 2.36                     | 0.58              |
| 3:C4:44:C:OP2      | 25:LJ:138:ARG:NH2  | 2.36                     | 0.58              |
| 1:C1:2767:A:N6     | 1:C1:2913:U:O2'    | 2.36                     | 0.58              |
| 2:C2:95:G:OP1      | 49:Lj:76:ASN:ND2   | 2.37                     | 0.57              |
| 4:CF:123:ASP:OD1   | 4:CF:124:PHE:N     | 2.37                     | 0.57              |
| 8:CN:52:THR:HG21   | 18:LB:70:LYS:HE2   | 1.86                     | 0.57              |
| 32:LQ:90:VAL:HG13  | 32:LQ:94:ARG:HD2   | 1.85                     | 0.57              |
| 47:Lh:15:LYS:O     | 47:Lh:66:LYS:NZ    | 2.36                     | 0.57              |
| 1:C1:679:A:N1      | 2:C2:28:C:O2'      | 2.38                     | 0.57              |
| 29:LN:36:ILE:HG12  | 29:LN:64:VAL:HG23  | 1.87                     | 0.57              |
| 1:C1:151:G:H5''    | 1:C1:152:G:H2'     | 1.86                     | 0.57              |
| 1:C1:1240:C:O2     | 4:CF:54:LYS:NZ     | 2.37                     | 0.57              |
| 1:C1:2878:A:H61    | 1:C1:2886:C:H42    | 1.52                     | 0.57              |
| 18:LB:229:GLY:O    | 18:LB:233:ARG:HB2  | 2.03                     | 0.57              |
| 28:LM:59:LEU:O     | 34:LS:155:ARG:NH2  | 2.36                     | 0.57              |
| 42:Lc:39:SER:OG    | 42:Lc:41:LYS:NZ    | 2.36                     | 0.57              |
| 6:CK:202:LYS:NZ    | 12:Cd:71:GLU:OE1   | 2.38                     | 0.57              |
| 5:CH:422:ARG:NH2   | 5:CH:435:ASP:O     | 2.38                     | 0.57              |
| 28:LM:18:ARG:NH1   | 28:LM:65:THR:O     | 2.35                     | 0.57              |
| 50:Lk:35:LYS:HG2   | 50:Lk:48:VAL:HG22  | 1.87                     | 0.57              |
| 21:LE:82:LEU:HD21  | 21:LE:122:VAL:HG13 | 1.87                     | 0.57              |
| 1:C1:926:A:H61     | 1:C1:1358:C:H42    | 1.52                     | 0.56              |
| 1:C1:2524:G:OP2    | 40:LZ:54:ARG:NH1   | 2.38                     | 0.56              |
| 29:LN:159:ARG:HB3  | 29:LN:164:LEU:HB2  | 1.87                     | 0.56              |
| 42:Lc:20:VAL:HG11  | 42:Lc:95:ILE:HD12  | 1.87                     | 0.56              |
| 1:C1:1394:C:H2'    | 1:C1:1395:G:H8     | 1.70                     | 0.56              |
| 11:Cb:15:ARG:NH2   | 11:Cb:18:ASP:OD2   | 2.38                     | 0.56              |
| 15:Ch:338:ALA:O    | 15:Ch:360:ARG:NH1  | 2.37                     | 0.56              |
| 38:LX:149:ALA:HB1  | 38:LX:155:LEU:HB2  | 1.87                     | 0.56              |
| 1:C1:1395:G:H5'    | 44:Le:122:ASN:HD22 | 1.69                     | 0.56              |
| 1:C1:2172:U:O2'    | 1:C1:2175:C:N4     | 2.39                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:1216:G:N2     | 26:LK:131:GLU:OE1  | 2.32                     | 0.56              |
| 5:CH:616:ALA:HB1   | 51:Ll:25:GLN:HB3   | 1.87                     | 0.56              |
| 13:Cf:113:MET:HB2  | 13:Cf:261:ARG:HB3  | 1.86                     | 0.56              |
| 16:Cz:88:LYS:NZ    | 16:Cz:92:GLU:OE2   | 2.39                     | 0.56              |
| 45:Lf:54:VAL:HG22  | 45:Lf:68:VAL:HG22  | 1.86                     | 0.56              |
| 1:C1:282:U:H2'     | 1:C1:283:G:H8      | 1.69                     | 0.56              |
| 1:C1:1785:C:H2'    | 1:C1:1786:G:H8     | 1.71                     | 0.56              |
| 17:LA:27:ALA:O     | 17:LA:128:ARG:NH2  | 2.39                     | 0.56              |
| 27:LL:115:ARG:NH2  | 27:LL:155:PHE:O    | 2.34                     | 0.56              |
| 1:C1:364:G:O2'     | 1:C1:389:A2M:N6    | 2.35                     | 0.56              |
| 1:C1:949:A:H62     | 1:C1:1098:G:H8     | 1.54                     | 0.56              |
| 5:CH:435:ASP:OD2   | 10:CQ:83:ARG:NH1   | 2.34                     | 0.56              |
| 11:Cb:15:ARG:NH1   | 37:LV:98:GLU:OE1   | 2.39                     | 0.56              |
| 1:C1:2368:C:H4'    | 6:CK:142:THR:HG21  | 1.88                     | 0.56              |
| 1:C1:2581:C:H5''   | 14:Cg:177:ILE:HG23 | 1.87                     | 0.56              |
| 40:LZ:22:VAL:HG13  | 40:LZ:44:GLY:HA3   | 1.87                     | 0.56              |
| 1:C1:111:G:OP2     | 27:LL:73:ARG:NH2   | 2.39                     | 0.56              |
| 1:C1:643:C:H2'     | 1:C1:644:A:H8      | 1.70                     | 0.56              |
| 8:CN:219:GLU:HA    | 8:CN:224:LEU:HD12  | 1.88                     | 0.56              |
| 15:Ch:214:ARG:NH1  | 15:Ch:223:GLN:OE1  | 2.35                     | 0.56              |
| 32:LQ:110:VAL:HG12 | 32:LQ:112:ALA:H    | 1.69                     | 0.56              |
| 41:La:112:LEU:HD22 | 41:La:125:VAL:HG11 | 1.88                     | 0.56              |
| 15:Ch:378:ALA:HB2  | 15:Ch:384:MET:HE3  | 1.87                     | 0.56              |
| 28:LM:130:GLU:HA   | 28:LM:133:LYS:HD3  | 1.87                     | 0.56              |
| 8:CN:106:ASN:ND2   | 37:LV:135:ALA:O    | 2.38                     | 0.55              |
| 10:CQ:18:GLY:HA3   | 10:CQ:31:PHE:O     | 2.06                     | 0.55              |
| 22:LF:127:LYS:HE2  | 35:LT:133:ALA:HB3  | 1.87                     | 0.55              |
| 1:C1:1476:G:N2     | 1:C1:1476:G:OP2    | 2.37                     | 0.55              |
| 17:LA:116:VAL:HB   | 17:LA:126:LEU:HB2  | 1.89                     | 0.55              |
| 47:Lh:34:LEU:HA    | 47:Lh:37:GLN:HG3   | 1.88                     | 0.55              |
| 1:C1:977:U:O2      | 1:C1:1037:A:N6     | 2.39                     | 0.55              |
| 24:LH:10:ILE:HB    | 24:LH:90:ILE:HB    | 1.88                     | 0.55              |
| 1:C1:69:C:OP2      | 1:C1:294:G:N2      | 2.39                     | 0.55              |
| 1:C1:405:G:OP1     | 31:LP:62:ARG:NH1   | 2.40                     | 0.55              |
| 1:C1:877:A:O2'     | 1:C1:879:U:OP2     | 2.25                     | 0.55              |
| 1:C1:64:A:H5''     | 29:LN:174:LEU:HD13 | 1.88                     | 0.55              |
| 1:C1:2231:U:O4     | 13:Cf:298:ARG:NH1  | 2.39                     | 0.55              |
| 1:C1:3209:A:OP2    | 21:LE:151:LYS:NZ   | 2.40                     | 0.55              |
| 35:LT:52:MET:HE3   | 35:LT:54:HIS:H     | 1.71                     | 0.55              |
| 12:Cd:47:ILE:HB    | 12:Cd:56:LYS:HB3   | 1.89                     | 0.55              |
| 1:C1:3076:C:H5'    | 16:Cz:27:LYS:HE3   | 1.87                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CF:77:LEU:HD22   | 4:CF:89:LEU:HD11   | 1.88                     | 0.55              |
| 1:C1:1206:A:N1     | 16:Cz:40:ARG:NH2   | 2.54                     | 0.54              |
| 1:C1:2923:G:O2'    | 12:Cd:30:ARG:NH2   | 2.38                     | 0.54              |
| 4:CF:49:ARG:NH2    | 4:CF:125:ALA:O     | 2.40                     | 0.54              |
| 10:CQ:43:LYS:NZ    | 11:Cb:18:ASP:OD1   | 2.35                     | 0.54              |
| 1:C1:1843:G:OP1    | 33:LR:70:ARG:NH2   | 2.40                     | 0.54              |
| 6:CK:241:ARG:NH1   | 12:Cd:79:ASN:OD1   | 2.40                     | 0.54              |
| 18:LB:161:VAL:HG13 | 18:LB:184:ILE:HD11 | 1.89                     | 0.54              |
| 19:LC:319:PRO:HG2  | 22:LF:155:TYR:HB3  | 1.89                     | 0.54              |
| 28:LM:59:LEU:HD13  | 34:LS:152:LEU:HD11 | 1.90                     | 0.54              |
| 32:LQ:95:ILE:HD12  | 32:LQ:108:VAL:HG11 | 1.88                     | 0.54              |
| 1:C1:448:C:H41     | 21:LE:15:ARG:HE    | 1.55                     | 0.54              |
| 12:Cd:442:LEU:HD22 | 12:Cd:460:VAL:HG13 | 1.87                     | 0.54              |
| 1:C1:1211:A:H5''   | 4:CF:203:SER:HB3   | 1.89                     | 0.54              |
| 1:C1:2789:G:H2'    | 1:C1:2790:G:C8     | 2.42                     | 0.54              |
| 4:CF:77:LEU:HD12   | 4:CF:96:LEU:HD11   | 1.90                     | 0.54              |
| 12:Cd:389:THR:HG22 | 12:Cd:391:GLU:H    | 1.72                     | 0.54              |
| 18:LB:233:ARG:HG3  | 18:LB:271:MET:HB2  | 1.89                     | 0.54              |
| 21:LE:98:ASN:HB3   | 21:LE:101:TYR:HD2  | 1.73                     | 0.54              |
| 1:C1:422:U:O2'     | 45:Lf:90:PRO:O     | 2.22                     | 0.54              |
| 1:C1:643:C:H2'     | 1:C1:644:A:C8      | 2.43                     | 0.54              |
| 1:C1:1572:G:OP1    | 46:Lg:59:ARG:NH2   | 2.40                     | 0.54              |
| 12:Cd:397:GLY:HA2  | 12:Cd:469:MET:HE3  | 1.89                     | 0.54              |
| 1:C1:489:A:O2'     | 1:C1:3214:A:N1     | 2.40                     | 0.54              |
| 1:C1:2642:U:HO2'   | 25:LJ:131:CYS:HG   | 1.53                     | 0.54              |
| 7:CL:62:LYS:HB3    | 16:Cz:61:MET:HE3   | 1.90                     | 0.54              |
| 21:LE:61:LEU:HD11  | 21:LE:103:ILE:HG13 | 1.89                     | 0.54              |
| 21:LE:166:ASP:HA   | 21:LE:169:LEU:HB2  | 1.89                     | 0.54              |
| 34:LS:8:GLN:HB2    | 34:LS:64:ILE:HD11  | 1.88                     | 0.54              |
| 1:C1:415:A:N1      | 1:C1:2325:C:O2'    | 2.38                     | 0.54              |
| 1:C1:2591:G:H21    | 1:C1:2605:C:H41    | 1.56                     | 0.54              |
| 1:C1:724:G:OP1     | 32:LQ:101:ASN:ND2  | 2.41                     | 0.54              |
| 12:Cd:336:ASN:ND2  | 12:Cd:356:PRO:O    | 2.40                     | 0.54              |
| 22:LF:148:LYS:HD3  | 22:LF:246:ARG:HH21 | 1.72                     | 0.54              |
| 52:Lp:38:THR:HA    | 52:Lp:45:ASN:HA    | 1.90                     | 0.54              |
| 20:LD:245:GLU:O    | 20:LD:249:GLN:NE2  | 2.40                     | 0.54              |
| 1:C1:2474:A:O2'    | 23:LG:252:ARG:NH1  | 2.41                     | 0.54              |
| 1:C1:2687:G:H22    | 12:Cd:326:GLN:HE22 | 1.56                     | 0.54              |
| 1:C1:471:C:H1'     | 21:LE:8:LYS:HE2    | 1.91                     | 0.53              |
| 1:C1:3151:U:OP1    | 28:LM:99:TRP:NE1   | 2.34                     | 0.53              |
| 10:CQ:179:GLU:OE1  | 43:Ld:86:ARG:NH1   | 2.40                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:Ch:489:ASP:HB3  | 15:Ch:508:LYS:HB3  | 1.89                     | 0.53              |
| 28:LM:108:ARG:NH2  | 30:LO:200:ALA:O    | 2.31                     | 0.53              |
| 28:LM:27:LEU:HD23  | 28:LM:50:LEU:HD22  | 1.89                     | 0.53              |
| 1:C1:960:C:OP1     | 32:LQ:78:ARG:NH1   | 2.37                     | 0.53              |
| 1:C1:979:A:N6      | 1:C1:1033:U:O4     | 2.42                     | 0.53              |
| 1:C1:1316:C:OP1    | 32:LQ:31:GLY:N     | 2.42                     | 0.53              |
| 1:C1:2123:G:H2'    | 1:C1:2124:G:H8     | 1.73                     | 0.53              |
| 18:LB:92:TYR:HB3   | 18:LB:99:LEU:HD22  | 1.90                     | 0.53              |
| 20:LD:37:ILE:HG13  | 20:LD:38:THR:HG23  | 1.89                     | 0.53              |
| 24:LH:3:TYR:OH     | 24:LH:99:ARG:NH1   | 2.41                     | 0.53              |
| 25:LJ:11:ARG:NH2   | 25:LJ:152:SER:O    | 2.41                     | 0.53              |
| 2:C2:103:G:OP2     | 2:C2:105:A:O2'     | 2.24                     | 0.53              |
| 3:C4:86:C:N4       | 3:C4:87:G:O6       | 2.42                     | 0.53              |
| 13:Cf:139:ARG:NH1  | 13:Cf:171:GLU:O    | 2.41                     | 0.53              |
| 19:LC:287:LEU:HD12 | 19:LC:290:LEU:HD11 | 1.91                     | 0.53              |
| 15:Ch:264:ILE:HD12 | 15:Ch:274:HIS:HB2  | 1.91                     | 0.53              |
| 1:C1:1159:C:H4'    | 30:LO:91:PRO:HD3   | 1.90                     | 0.53              |
| 4:CF:64:ARG:NH1    | 4:CF:65:ILE:O      | 2.42                     | 0.53              |
| 4:CF:97:THR:O      | 4:CF:243:ARG:NH2   | 2.42                     | 0.53              |
| 1:C1:582:G:O2'     | 21:LE:35:GLN:O     | 2.26                     | 0.53              |
| 3:C4:100:G:OP1     | 13:Cf:259:ARG:NH2  | 2.41                     | 0.53              |
| 1:C1:2164:G:N2     | 1:C1:2205:A:H62    | 2.06                     | 0.53              |
| 28:LM:12:ARG:NH1   | 28:LM:64:LEU:O     | 2.42                     | 0.53              |
| 31:LP:125:GLN:HB3  | 31:LP:141:SER:HB2  | 1.91                     | 0.53              |
| 41:La:138:VAL:HG11 | 41:La:145:VAL:HG23 | 1.91                     | 0.53              |
| 1:C1:2981:U:H2'    | 1:C1:2982:A:H8     | 1.73                     | 0.53              |
| 4:CF:30:ILE:HG21   | 4:CF:76:ALA:HB1    | 1.90                     | 0.53              |
| 6:CK:87:PRO:HD2    | 6:CK:90:LEU:HD12   | 1.92                     | 0.53              |
| 1:C1:2179:G:H1     | 1:C1:2192:A:N6     | 2.05                     | 0.52              |
| 19:LC:236:PRO:HG2  | 19:LC:239:ALA:HB3  | 1.90                     | 0.52              |
| 28:LM:54:ARG:NH2   | 28:LM:76:ALA:O     | 2.35                     | 0.52              |
| 1:C1:341:C:O2      | 1:C1:345:A:O2'     | 2.26                     | 0.52              |
| 1:C1:2320:A:H2'    | 1:C1:2321:A:H8     | 1.74                     | 0.52              |
| 15:Ch:208:SER:OG   | 15:Ch:209:MET:N    | 2.42                     | 0.52              |
| 15:Ch:379:SER:OG   | 15:Ch:381:ASP:OD1  | 2.28                     | 0.52              |
| 41:La:112:LEU:HB3  | 41:La:130:VAL:HG23 | 1.91                     | 0.52              |
| 1:C1:1438:U:OP1    | 1:C1:1859:A:N6     | 2.42                     | 0.52              |
| 4:CF:224:LEU:HD11  | 4:CF:243:ARG:HH11  | 1.75                     | 0.52              |
| 1:C1:1095:A:H2'    | 1:C1:1096:G:C8     | 2.45                     | 0.52              |
| 6:CK:25:ARG:HH11   | 16:Cz:27:LYS:HZ2   | 1.58                     | 0.52              |
| 6:CK:133:PHE:HB3   | 6:CK:149:ARG:HB3   | 1.90                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:Lq:11:GLU:HA    | 53:Lq:14:ARG:HD2   | 1.91                     | 0.52              |
| 1:C1:1526:G:O2'    | 1:C1:2131:A:O2'    | 2.27                     | 0.52              |
| 50:Lk:26:LYS:NZ    | 50:Lk:28:ASN:OD1   | 2.40                     | 0.52              |
| 7:CL:69:ILE:HG21   | 35:LT:160:ILE:HG21 | 1.91                     | 0.52              |
| 24:LH:4:ILE:HG21   | 34:LS:148:LEU:HD11 | 1.92                     | 0.52              |
| 1:C1:76:G:H5'      | 27:LL:58:VAL:HB    | 1.92                     | 0.52              |
| 1:C1:575:G:H2'     | 1:C1:576:A:H8      | 1.74                     | 0.52              |
| 1:C1:1876:A:H61    | 1:C1:2302:C:H42    | 1.57                     | 0.52              |
| 8:CN:1:MET:HE2     | 8:CN:203:LEU:HD13  | 1.92                     | 0.52              |
| 12:Cd:135:THR:HG22 | 12:Cd:138:ARG:HH12 | 1.75                     | 0.52              |
| 1:C1:2142:C:OP1    | 17:LA:132:ASN:ND2  | 2.42                     | 0.52              |
| 10:CQ:163:GLU:HA   | 10:CQ:166:LYS:HD2  | 1.90                     | 0.52              |
| 22:LF:102:PRO:HB2  | 22:LF:105:PRO:HD2  | 1.92                     | 0.52              |
| 45:Lf:59:LYS:HG3   | 45:Lf:61:VAL:HG23  | 1.92                     | 0.52              |
| 1:C1:608:U:O2      | 45:Lf:62:ARG:NH2   | 2.42                     | 0.52              |
| 1:C1:1879:G:O2'    | 1:C1:2297:U:O4     | 2.27                     | 0.52              |
| 1:C1:2932:G:N7     | 6:CK:140:LYS:NZ    | 2.49                     | 0.52              |
| 34:LS:12:ARG:HB3   | 34:LS:24:LEU:HD13  | 1.92                     | 0.52              |
| 6:CK:129:GLU:HB2   | 12:Cd:62:SER:H     | 1.74                     | 0.52              |
| 18:LB:47:MET:SD    | 18:LB:165:THR:OG1  | 2.67                     | 0.52              |
| 18:LB:76:VAL:HG12  | 18:LB:326:LYS:HA   | 1.92                     | 0.52              |
| 37:LV:106:ASN:OD1  | 37:LV:110:GLU:N    | 2.43                     | 0.52              |
| 41:La:101:VAL:HG22 | 41:La:124:VAL:HB   | 1.92                     | 0.52              |
| 1:C1:278:A:H8      | 1:C1:297:G:H1'     | 1.75                     | 0.51              |
| 1:C1:1252:U:H1'    | 1:C1:1255:C:H5     | 1.75                     | 0.51              |
| 1:C1:2221:U:H2'    | 1:C1:2222:A:H8     | 1.74                     | 0.51              |
| 1:C1:3140:A:N6     | 24:LH:95:HIS:O     | 2.37                     | 0.51              |
| 3:C4:53:U:O2'      | 3:C4:55:A:N7       | 2.42                     | 0.51              |
| 15:Ch:419:ILE:HB   | 15:Ch:431:TRP:HB2  | 1.91                     | 0.51              |
| 17:LA:51:ASP:HB3   | 17:LA:54:ARG:HB3   | 1.91                     | 0.51              |
| 1:C1:106:C:H2'     | 1:C1:107:A:H8      | 1.75                     | 0.51              |
| 1:C1:1083:U:OP2    | 22:LF:202:LYS:NZ   | 2.37                     | 0.51              |
| 1:C1:1460:A:OP1    | 1:C1:3033:G:O2'    | 2.25                     | 0.51              |
| 19:LC:211:ILE:HG13 | 19:LC:256:VAL:HB   | 1.92                     | 0.51              |
| 28:LM:67:ILE:HG21  | 28:LM:90:VAL:HG13  | 1.90                     | 0.51              |
| 47:Lh:45:LYS:HG3   | 47:Lh:46:LEU:HD22  | 1.92                     | 0.51              |
| 1:C1:3202:U:H5''   | 28:LM:126:GLN:HE22 | 1.76                     | 0.51              |
| 1:C1:3209:A:H5''   | 21:LE:64:ARG:HH12  | 1.75                     | 0.51              |
| 5:CH:368:ILE:HD12  | 8:CN:238:LYS:HG3   | 1.91                     | 0.51              |
| 19:LC:24:PRO:HG2   | 19:LC:265:LEU:HD12 | 1.91                     | 0.51              |
| 26:LK:80:LEU:HB3   | 26:LK:112:ILE:HD12 | 1.90                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:LM:35:ASP:OD2   | 28:LM:38:ARG:N     | 2.42                     | 0.51              |
| 1:C1:92:G:N2       | 1:C1:95:G:O2'      | 2.43                     | 0.51              |
| 1:C1:639:G:O2'     | 1:C1:1418:A:OP1    | 2.28                     | 0.51              |
| 40:LZ:22:VAL:HG12  | 40:LZ:42:VAL:HG12  | 1.91                     | 0.51              |
| 1:C1:1290:G:C2     | 30:LO:61:LYS:HE3   | 2.46                     | 0.51              |
| 1:C1:1480:C:H2'    | 1:C1:1481:A:H8     | 1.76                     | 0.51              |
| 15:Ch:509:ASP:OD2  | 15:Ch:513:ARG:NH1  | 2.44                     | 0.51              |
| 17:LA:47:GLU:HG2   | 17:LA:60:ARG:HB3   | 1.92                     | 0.51              |
| 1:C1:277:A:N1      | 1:C1:2744:A:O2'    | 2.39                     | 0.51              |
| 3:C4:11:A:N1       | 3:C4:67:G:O2'      | 2.41                     | 0.51              |
| 24:LH:140:VAL:HG22 | 24:LH:151:VAL:HG22 | 1.91                     | 0.51              |
| 32:LQ:68:THR:HG22  | 32:LQ:70:ALA:H     | 1.75                     | 0.51              |
| 1:C1:582:G:H1'     | 21:LE:37:LYS:HG3   | 1.92                     | 0.51              |
| 1:C1:958:G:H5''    | 32:LQ:168:ARG:HH12 | 1.75                     | 0.51              |
| 1:C1:1929:G:OP2    | 33:LR:135:LYS:NZ   | 2.33                     | 0.51              |
| 1:C1:3126:A:OP1    | 45:Lf:94:ARG:NH1   | 2.44                     | 0.51              |
| 1:C1:3238:U:O4     | 18:LB:124:LYS:NZ   | 2.43                     | 0.51              |
| 2:C2:99:C:OP1      | 38:LX:66:HIS:NE2   | 2.44                     | 0.51              |
| 12:Cd:133:LYS:NZ   | 12:Cd:137:GLU:OE1  | 2.44                     | 0.51              |
| 37:LV:105:VAL:HG12 | 37:LV:111:MET:HA   | 1.93                     | 0.51              |
| 52:Lp:51:ALA:HB3   | 52:Lp:54:ILE:HD12  | 1.92                     | 0.51              |
| 1:C1:37:C:H4'      | 1:C1:790:A:H2      | 1.75                     | 0.51              |
| 1:C1:333:C:OP2     | 19:LC:199:ARG:NH1  | 2.37                     | 0.51              |
| 1:C1:1186:A:H62    | 1:C1:1283:G:H21    | 1.58                     | 0.51              |
| 1:C1:3106:C:OP1    | 9:CO:94:LYS:NZ     | 2.43                     | 0.51              |
| 2:C2:26:U:O2'      | 19:LC:52:ALA:O     | 2.28                     | 0.51              |
| 6:CK:165:PRO:HG2   | 12:Cd:326:GLN:NE2  | 2.26                     | 0.51              |
| 24:LH:176:SER:HB3  | 24:LH:182:GLU:HB3  | 1.93                     | 0.51              |
| 49:Lj:72:ARG:O     | 49:Lj:76:ASN:ND2   | 2.44                     | 0.51              |
| 1:C1:1160:G:O6     | 45:Lf:22:ARG:NH2   | 2.44                     | 0.51              |
| 22:LF:93:ILE:HD13  | 22:LF:213:LEU:HD12 | 1.93                     | 0.51              |
| 29:LN:10:LEU:HB2   | 48:Li:53:ILE:HD12  | 1.91                     | 0.51              |
| 50:Lk:25:ILE:HG13  | 50:Lk:68:ILE:HD11  | 1.93                     | 0.51              |
| 1:C1:1779:A:H2'    | 1:C1:1780:A:H8     | 1.76                     | 0.50              |
| 18:LB:113:GLU:OE2  | 18:LB:168:ARG:NH1  | 2.44                     | 0.50              |
| 43:Ld:28:LEU:HD11  | 43:Ld:40:ALA:HB2   | 1.93                     | 0.50              |
| 1:C1:51:U:H2'      | 1:C1:52:A:H8       | 1.75                     | 0.50              |
| 1:C1:665:A:N1      | 1:C1:691:G:O2'     | 2.38                     | 0.50              |
| 1:C1:2477:U:H5'    | 23:LG:71:ARG:HG3   | 1.92                     | 0.50              |
| 1:C1:3314:G:OP2    | 43:Ld:110:LYS:NZ   | 2.36                     | 0.50              |
| 44:Le:88:MET:HE2   | 53:Lq:114:ARG:HH11 | 1.76                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CH:242:LEU:O     | 5:CH:280:LYS:NZ    | 2.44                     | 0.50              |
| 7:CL:55:ILE:HB     | 7:CL:62:LYS:HE3    | 1.92                     | 0.50              |
| 25:LJ:33:ARG:HD3   | 25:LJ:121:ILE:HA   | 1.94                     | 0.50              |
| 25:LJ:94:ARG:O     | 25:LJ:157:ARG:NH2  | 2.43                     | 0.50              |
| 5:CH:168:THR:HA    | 5:CH:216:GLN:O     | 2.11                     | 0.50              |
| 24:LH:3:TYR:HD2    | 24:LH:102:VAL:HG21 | 1.75                     | 0.50              |
| 1:C1:300:A:H2'     | 1:C1:301:A:H8      | 1.76                     | 0.50              |
| 1:C1:430:G:O6      | 53:Lq:134:ARG:NH1  | 2.45                     | 0.50              |
| 1:C1:1067:A:H2'    | 1:C1:1068:A:C8     | 2.47                     | 0.50              |
| 1:C1:2769:C:OP2    | 1:C1:2914:U:O2'    | 2.29                     | 0.50              |
| 3:C4:108:G:OP1     | 20:LD:284:ARG:NH2  | 2.45                     | 0.50              |
| 14:Cg:66:LEU:O     | 14:Cg:70:THR:OG1   | 2.27                     | 0.50              |
| 1:C1:2308:A:H5''   | 43:Ld:32:THR:HG23  | 1.93                     | 0.50              |
| 40:LZ:49:PRO:HD3   | 40:LZ:67:ILE:HG12  | 1.93                     | 0.50              |
| 44:Le:36:PRO:HD2   | 44:Le:53:MET:HE2   | 1.93                     | 0.50              |
| 44:Le:77:VAL:HG21  | 44:Le:83:VAL:HB    | 1.94                     | 0.50              |
| 44:Le:82:ASP:OD1   | 53:Lq:30:ARG:NH2   | 2.40                     | 0.50              |
| 1:C1:2630:A:O2'    | 25:LJ:99:GLU:OE1   | 2.25                     | 0.50              |
| 13:Cf:277:THR:HG22 | 13:Cf:279:GLN:H    | 1.77                     | 0.50              |
| 24:LH:127:MET:HE3  | 24:LH:185:LEU:HD13 | 1.93                     | 0.50              |
| 28:LM:94:TRP:O     | 28:LM:97:THR:OG1   | 2.29                     | 0.50              |
| 1:C1:1142:A:OP1    | 32:LQ:31:GLY:N     | 2.44                     | 0.50              |
| 1:C1:1193:U:H5     | 4:CF:3:LYS:HB2     | 1.76                     | 0.50              |
| 1:C1:1202:C:O2     | 16:Cz:51:ARG:NH1   | 2.39                     | 0.50              |
| 2:C2:58:G:N7       | 49:Lj:63:ARG:NH2   | 2.47                     | 0.50              |
| 5:CH:637:ASP:HB2   | 51:Ll:46:LYS:HE2   | 1.94                     | 0.50              |
| 17:LA:105:SER:HB3  | 17:LA:160:SER:HB3  | 1.94                     | 0.50              |
| 29:LN:44:ARG:NH1   | 29:LN:120:TRP:O    | 2.44                     | 0.50              |
| 40:LZ:11:LEU:HB2   | 40:LZ:80:MET:HB3   | 1.93                     | 0.50              |
| 1:C1:1643:C:H5''   | 33:LR:96:MET:HE1   | 1.94                     | 0.50              |
| 1:C1:2846:A:N6     | 5:CH:30:THR:OG1    | 2.44                     | 0.50              |
| 1:C1:2920:G:O2'    | 12:Cd:366:TYR:O    | 2.30                     | 0.50              |
| 8:CN:186:VAL:HG12  | 8:CN:218:ILE:HD11  | 1.93                     | 0.50              |
| 26:LK:28:LEU:HD12  | 26:LK:31:LYS:HE3   | 1.94                     | 0.50              |
| 41:La:147:LEU:HD12 | 48:Li:16:LEU:HD22  | 1.92                     | 0.50              |
| 1:C1:1516:U:H2'    | 1:C1:1517:A:H8     | 1.76                     | 0.49              |
| 1:C1:1652:C:OP1    | 33:LR:64:ARG:NH1   | 2.41                     | 0.49              |
| 4:CF:168:LEU:HD21  | 4:CF:207:ARG:HD3   | 1.94                     | 0.49              |
| 13:Cf:103:VAL:HG13 | 13:Cf:113:MET:HG2  | 1.94                     | 0.49              |
| 35:LT:134:MET:HE3  | 35:LT:135:PRO:HD2  | 1.94                     | 0.49              |
| 20:LD:34:LYS:O     | 20:LD:38:THR:OG1   | 2.27                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:LM:112:LEU:HD22 | 28:LM:116:ASP:HB3  | 1.94                     | 0.49              |
| 1:C1:414:G:N7      | 30:LO:69:ARG:NH2   | 2.61                     | 0.49              |
| 1:C1:1598:G:O2'    | 2:C2:126:A:N1      | 2.45                     | 0.49              |
| 8:CN:112:ASP:OD2   | 8:CN:156:ASN:ND2   | 2.39                     | 0.49              |
| 16:Cz:37:LYS:O     | 24:LH:106:ARG:NH1  | 2.42                     | 0.49              |
| 22:LF:88:LYS:HE3   | 22:LF:197:VAL:HB   | 1.92                     | 0.49              |
| 1:C1:66:A:H1'      | 1:C1:78:A:H1'      | 1.93                     | 0.49              |
| 2:C2:63:G:H22      | 2:C2:97:A:H2       | 1.60                     | 0.49              |
| 20:LD:214:LEU:HB3  | 20:LD:222:TYR:HB2  | 1.94                     | 0.49              |
| 43:Ld:18:ARG:HG2   | 43:Ld:116:VAL:HG22 | 1.95                     | 0.49              |
| 1:C1:967:U:H4'     | 22:LF:104:LYS:HG3  | 1.94                     | 0.49              |
| 1:C1:1177:G:H2'    | 1:C1:1178:A:C8     | 2.47                     | 0.49              |
| 1:C1:2120:G:N2     | 1:C1:2140:G:O2'    | 2.45                     | 0.49              |
| 1:C1:101:A:H3'     | 1:C1:102:G:H21     | 1.77                     | 0.49              |
| 1:C1:943:C:O2      | 1:C1:2573:G:N1     | 2.46                     | 0.49              |
| 1:C1:1420:OMC:HM22 | 1:C1:1421:U:H5'    | 1.93                     | 0.49              |
| 1:C1:2145:A:OP2    | 17:LA:194:ASN:ND2  | 2.46                     | 0.49              |
| 5:CH:618:ARG:HH21  | 5:CH:622:LEU:HD11  | 1.76                     | 0.49              |
| 49:Lj:64:MET:SD    | 49:Lj:67:LEU:HB3   | 2.52                     | 0.49              |
| 1:C1:1641:G:H2'    | 1:C1:1642:G:C8     | 2.47                     | 0.49              |
| 1:C1:1766:G:H2'    | 1:C1:1767:A:C8     | 2.48                     | 0.49              |
| 2:C2:52:A:OP1      | 51:Ll:21:ARG:NH1   | 2.38                     | 0.49              |
| 42:Lc:36:ALA:HB1   | 42:Lc:96:LEU:HD21  | 1.95                     | 0.49              |
| 8:CN:106:ASN:OD1   | 8:CN:150:SER:OG    | 2.30                     | 0.49              |
| 12:Cd:60:PHE:O     | 12:Cd:61:GLN:NE2   | 2.46                     | 0.49              |
| 12:Cd:364:TRP:HA   | 12:Cd:377:ASP:O    | 2.13                     | 0.49              |
| 1:C1:300:A:H2'     | 1:C1:301:A:C8      | 2.46                     | 0.49              |
| 1:C1:823:A:H4'     | 33:LR:126:LEU:HD23 | 1.94                     | 0.49              |
| 34:LS:72:VAL:HA    | 34:LS:97:THR:HG22  | 1.95                     | 0.49              |
| 40:LZ:76:TYR:O     | 42:Lc:38:ARG:NH2   | 2.46                     | 0.49              |
| 42:Lc:46:LEU:HD23  | 42:Lc:71:HIS:HB3   | 1.94                     | 0.49              |
| 1:C1:1814:U:OP2    | 51:Ll:10:LYS:NZ    | 2.44                     | 0.49              |
| 1:C1:2066:U:OP2    | 33:LR:76:ARG:NH1   | 2.45                     | 0.49              |
| 5:CH:321:CYS:O     | 5:CH:324:GLN:NE2   | 2.45                     | 0.49              |
| 22:LF:155:TYR:OH   | 22:LF:188:GLU:OE1  | 2.30                     | 0.49              |
| 36:LU:102:VAL:HG22 | 36:LU:112:LEU:HG   | 1.95                     | 0.49              |
| 1:C1:2693:A:H5'    | 14:Cg:118:THR:HA   | 1.95                     | 0.48              |
| 29:LN:5:LYS:HZ1    | 48:Li:46:THR:HG22  | 1.78                     | 0.48              |
| 1:C1:230:G:H2'     | 1:C1:231:A:C8      | 2.48                     | 0.48              |
| 1:C1:661:C:H2'     | 1:C1:662:G:C8      | 2.48                     | 0.48              |
| 1:C1:782:G:H22     | 19:LC:102:ALA:HA   | 1.76                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CH:261:PHE:HB2   | 5:CH:266:GLN:HE22  | 1.79                     | 0.48              |
| 17:LA:43:GLY:HA3   | 17:LA:63:PHE:CD1   | 2.48                     | 0.48              |
| 19:LC:244:GLN:O    | 19:LC:253:ARG:NH1  | 2.44                     | 0.48              |
| 1:C1:2511:U:OP1    | 46:Lg:107:LYS:NZ   | 2.46                     | 0.48              |
| 1:C1:2860:G:O2'    | 1:C1:2982:A:N1     | 2.38                     | 0.48              |
| 4:CF:77:LEU:HD11   | 4:CF:102:LEU:HD21  | 1.94                     | 0.48              |
| 29:LN:178:HIS:O    | 29:LN:181:ASN:ND2  | 2.46                     | 0.48              |
| 1:C1:1045:A:N3     | 35:LT:130:ARG:NH2  | 2.61                     | 0.48              |
| 5:CH:174:PHE:HE2   | 5:CH:266:GLN:HA    | 1.77                     | 0.48              |
| 13:Cf:232:ILE:HG23 | 13:Cf:244:VAL:HG13 | 1.95                     | 0.48              |
| 32:LQ:87:ARG:HB3   | 32:LQ:112:ALA:HB2  | 1.95                     | 0.48              |
| 37:LV:19:LEU:HD11  | 37:LV:100:ASN:HB3  | 1.95                     | 0.48              |
| 47:Lh:37:GLN:HE22  | 47:Lh:45:LYS:HB2   | 1.78                     | 0.48              |
| 1:C1:702:G:HO2'    | 1:C1:735:C:HO2'    | 1.62                     | 0.48              |
| 1:C1:2801:U:O2'    | 1:C1:2805:U:N3     | 2.45                     | 0.48              |
| 8:CN:97:ILE:HD11   | 8:CN:104:LEU:HD11  | 1.96                     | 0.48              |
| 10:CQ:16:SER:HB3   | 18:LB:73:VAL:HG11  | 1.95                     | 0.48              |
| 15:Ch:148:PRO:HB3  | 15:Ch:508:LYS:HA   | 1.94                     | 0.48              |
| 1:C1:526:U:H5      | 34:LS:132:THR:HG21 | 1.78                     | 0.48              |
| 1:C1:693:A:N6      | 1:C1:703:A:OP2     | 2.44                     | 0.48              |
| 5:CH:508:MET:HE1   | 43:Ld:66:LYS:HB2   | 1.94                     | 0.48              |
| 23:LG:42:ASP:OD1   | 23:LG:43:ILE:N     | 2.43                     | 0.48              |
| 27:LL:167:GLU:OE1  | 41:La:90:TYR:OH    | 2.31                     | 0.48              |
| 1:C1:230:G:H2'     | 1:C1:231:A:H8      | 1.79                     | 0.48              |
| 1:C1:2640:U:H5'    | 25:LJ:66:ILE:HD11  | 1.96                     | 0.48              |
| 7:CL:4:THR:HG22    | 30:LO:53:LEU:HD11  | 1.96                     | 0.48              |
| 18:LB:136:LYS:HA   | 18:LB:139:GLU:HG2  | 1.95                     | 0.48              |
| 19:LC:364:GLU:O    | 34:LS:28:ARG:NH1   | 2.47                     | 0.48              |
| 22:LF:229:ILE:HG23 | 34:LS:36:VAL:HG13  | 1.94                     | 0.48              |
| 1:C1:2919:C:H2'    | 1:C1:2920:G:H8     | 1.79                     | 0.48              |
| 1:C1:2355:C:O2'    | 18:LB:267:ARG:NH1  | 2.39                     | 0.48              |
| 1:C1:2647:U:N3     | 20:LD:17:GLN:O     | 2.40                     | 0.48              |
| 1:C1:2100:U:OP2    | 1:C1:2105:A:N6     | 2.38                     | 0.48              |
| 1:C1:2210:G:P      | 12:Cd:371:LYS:HD2  | 2.53                     | 0.48              |
| 13:Cf:98:HIS:HB2   | 13:Cf:118:LEU:HB2  | 1.96                     | 0.48              |
| 29:LN:23:LEU:O     | 29:LN:122:ASN:ND2  | 2.36                     | 0.48              |
| 34:LS:93:GLU:HG3   | 34:LS:137:ARG:HG2  | 1.95                     | 0.48              |
| 1:C1:1796:A:H2'    | 1:C1:1797:A:C8     | 2.49                     | 0.47              |
| 1:C1:2147:U:OP1    | 17:LA:209:HIS:NE2  | 2.38                     | 0.47              |
| 5:CH:71:SER:O      | 12:Cd:178:ARG:NH1  | 2.47                     | 0.47              |
| 19:LC:151:LEU:HD23 | 19:LC:256:VAL:HG22 | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LZ:14:ARG:HH11  | 46:Lg:87:ARG:HH21  | 1.60                     | 0.47              |
| 1:C1:580:A:H1'     | 1:C1:1320:G:H5''   | 1.96                     | 0.47              |
| 1:C1:1291:A:N1     | 1:C1:2344:G:O2'    | 2.47                     | 0.47              |
| 20:LD:208:ALA:HB2  | 20:LD:239:LEU:HD12 | 1.97                     | 0.47              |
| 35:LT:115:LEU:HA   | 35:LT:118:LYS:HG2  | 1.96                     | 0.47              |
| 1:C1:842:G:H8      | 17:LA:183:SER:HB2  | 1.79                     | 0.47              |
| 25:LJ:38:LEU:HD13  | 25:LJ:70:VAL:HG23  | 1.96                     | 0.47              |
| 1:C1:88:U:H2'      | 1:C1:89:A:H8       | 1.80                     | 0.47              |
| 1:C1:2796:A:O2'    | 1:C1:2810:A:N6     | 2.47                     | 0.47              |
| 8:CN:217:VAL:HA    | 8:CN:233:ILE:HD11  | 1.97                     | 0.47              |
| 39:LY:110:LEU:HD11 | 39:LY:115:GLU:HG3  | 1.97                     | 0.47              |
| 1:C1:468:G:O2'     | 1:C1:470:A:N1      | 2.48                     | 0.47              |
| 14:Cg:17:LYS:NZ    | 14:Cg:32:ASP:OD2   | 2.47                     | 0.47              |
| 24:LH:154:ARG:HG2  | 24:LH:162:VAL:HG22 | 1.96                     | 0.47              |
| 39:LY:62:HIS:HB3   | 39:LY:65:LYS:HD2   | 1.96                     | 0.47              |
| 1:C1:563:U:H2'     | 1:C1:564:A:H8      | 1.79                     | 0.47              |
| 1:C1:976:G:H4'     | 1:C1:977:U:H5'     | 1.95                     | 0.47              |
| 1:C1:1372:G:H5''   | 44:Le:102:SER:HB3  | 1.97                     | 0.47              |
| 1:C1:1476:G:H2'    | 51:Ll:13:LEU:HD22  | 1.96                     | 0.47              |
| 1:C1:1677:A:OP1    | 46:Lg:22:ARG:NH2   | 2.48                     | 0.47              |
| 1:C1:2577:G:H21    | 1:C1:2578:OMG:HM23 | 1.78                     | 0.47              |
| 5:CH:159:LEU:HD12  | 5:CH:160:PRO:HD2   | 1.95                     | 0.47              |
| 6:CK:165:PRO:HG2   | 12:Cd:326:GLN:HE21 | 1.79                     | 0.47              |
| 13:Cf:28:LYS:HE2   | 14:Cg:93:GLU:HB3   | 1.97                     | 0.47              |
| 13:Cf:182:ARG:HG3  | 13:Cf:183:PHE:CD2  | 2.50                     | 0.47              |
| 24:LH:129:TYR:HB3  | 24:LH:218:ILE:HG23 | 1.97                     | 0.47              |
| 1:C1:1816:C:O2'    | 1:C1:1822:A:N1     | 2.44                     | 0.47              |
| 12:Cd:238:HIS:HD1  | 12:Cd:332:ILE:HG13 | 1.79                     | 0.47              |
| 15:Ch:41:PHE:HD2   | 15:Ch:69:LEU:HD13  | 1.79                     | 0.47              |
| 38:LX:79:PRO:HA    | 38:LX:97:PHE:HA    | 1.97                     | 0.47              |
| 1:C1:1054:U:O4     | 1:C1:1070:G:O6     | 2.33                     | 0.47              |
| 1:C1:3120:C:H2'    | 1:C1:3121:G:H8     | 1.80                     | 0.47              |
| 1:C1:3209:A:H5''   | 21:LE:64:ARG:HH22  | 1.80                     | 0.47              |
| 1:C1:3315:U:OP1    | 43:Ld:23:HIS:NE2   | 2.28                     | 0.47              |
| 2:C2:38:U:H5'      | 47:Lh:83:LEU:HD13  | 1.97                     | 0.47              |
| 5:CH:267:ILE:HD13  | 5:CH:304:GLU:HG2   | 1.96                     | 0.47              |
| 5:CH:645:PRO:HG2   | 5:CH:648:LEU:HD12  | 1.97                     | 0.47              |
| 28:LM:20:LEU:HD11  | 28:LM:30:ILE:HD11  | 1.96                     | 0.47              |
| 28:LM:54:ARG:HG2   | 34:LS:70:LEU:HD22  | 1.97                     | 0.47              |
| 52:Lp:6:LYS:HE3    | 52:Lp:7:LYS:HE3    | 1.97                     | 0.47              |
| 1:C1:1779:A:H2'    | 1:C1:1780:A:C8     | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:2516:G:O2'    | 40:LZ:135:PHE:OXT  | 2.31                     | 0.47              |
| 37:LV:42:LYS:HE2   | 37:LV:61:MET:HE3   | 1.97                     | 0.47              |
| 42:Lc:37:LEU:HD11  | 42:Lc:62:TYR:HD1   | 1.80                     | 0.47              |
| 43:Ld:85:ARG:HG2   | 43:Ld:97:LEU:HD22  | 1.97                     | 0.47              |
| 44:Le:80:VAL:HA    | 44:Le:83:VAL:HG12  | 1.97                     | 0.47              |
| 1:C1:404:U:H2'     | 1:C1:405:G:H8      | 1.80                     | 0.46              |
| 1:C1:523:G:H2'     | 1:C1:524:A:C8      | 2.50                     | 0.46              |
| 1:C1:618:C:H2'     | 1:C1:619:A:H8      | 1.78                     | 0.46              |
| 1:C1:1576:C:O2'    | 1:C1:1676:A:N3     | 2.48                     | 0.46              |
| 15:Ch:465:SER:OG   | 15:Ch:466:LYS:N    | 2.46                     | 0.46              |
| 32:LQ:116:ASP:OD1  | 32:LQ:117:ASP:N    | 2.48                     | 0.46              |
| 44:Le:20:ARG:HB3   | 44:Le:23:SER:HB2   | 1.98                     | 0.46              |
| 1:C1:357:G:OP2     | 49:Lj:52:LYS:NZ    | 2.34                     | 0.46              |
| 1:C1:2495:U:H2'    | 1:C1:2496:G:C8     | 2.50                     | 0.46              |
| 1:C1:3179:G:H2'    | 1:C1:3180:G:H8     | 1.80                     | 0.46              |
| 2:C2:13:A:O2'      | 31:LP:121:GLN:O    | 2.32                     | 0.46              |
| 7:CL:5:ILE:HA      | 30:LO:53:LEU:HD22  | 1.97                     | 0.46              |
| 20:LD:214:LEU:HD12 | 20:LD:226:PHE:HE2  | 1.80                     | 0.46              |
| 27:LL:59:ARG:NH1   | 27:LL:66:ASN:O     | 2.39                     | 0.46              |
| 27:LL:80:LEU:HD11  | 27:LL:97:VAL:HG22  | 1.97                     | 0.46              |
| 36:LU:47:ILE:HD12  | 36:LU:62:ILE:HD11  | 1.97                     | 0.46              |
| 40:LZ:23:VAL:HG11  | 40:LZ:86:LEU:HD23  | 1.98                     | 0.46              |
| 46:Lg:66:ILE:HB    | 46:Lg:70:LYS:HD2   | 1.96                     | 0.46              |
| 1:C1:644:A:H2'     | 1:C1:645:A:C8      | 2.50                     | 0.46              |
| 1:C1:1345:G:H2'    | 1:C1:1346:A:C8     | 2.50                     | 0.46              |
| 1:C1:3275:U:H4'    | 1:C1:3276:A:H5'    | 1.96                     | 0.46              |
| 15:Ch:246:TRP:O    | 15:Ch:354:ARG:NH1  | 2.46                     | 0.46              |
| 28:LM:127:ARG:HH22 | 30:LO:204:TYR:HB3  | 1.80                     | 0.46              |
| 38:LX:142:ASP:OD1  | 38:LX:143:VAL:N    | 2.48                     | 0.46              |
| 44:Le:10:ILE:HA    | 44:Le:64:THR:HG21  | 1.98                     | 0.46              |
| 1:C1:119:U:O4      | 1:C1:144:G:N2      | 2.48                     | 0.46              |
| 1:C1:262:G:H5''    | 29:LN:14:LYS:HE2   | 1.97                     | 0.46              |
| 1:C1:775:A:H2'     | 1:C1:776:G:H8      | 1.80                     | 0.46              |
| 1:C1:948:U:H2'     | 1:C1:949:A:H8      | 1.80                     | 0.46              |
| 1:C1:1550:U:H5'    | 1:C1:1551:C:H5     | 1.80                     | 0.46              |
| 8:CN:88:LEU:HD12   | 8:CN:94:ILE:HD11   | 1.97                     | 0.46              |
| 15:Ch:327:ILE:HB   | 15:Ch:375:LEU:HD11 | 1.97                     | 0.46              |
| 15:Ch:487:HIS:ND1  | 15:Ch:509:ASP:OD2  | 2.44                     | 0.46              |
| 24:LH:195:GLN:NE2  | 24:LH:199:ASP:OD1  | 2.46                     | 0.46              |
| 25:LJ:38:LEU:HD12  | 25:LJ:68:VAL:HG22  | 1.98                     | 0.46              |
| 35:LT:111:GLU:HA   | 35:LT:114:GLU:HG3  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:Lj:64:MET:HG3   | 49:Lj:68:SER:HB3   | 1.98                     | 0.46              |
| 1:C1:604:G:H2'     | 1:C1:605:G:C8      | 2.51                     | 0.46              |
| 1:C1:774:A:H2'     | 1:C1:775:A:H8      | 1.78                     | 0.46              |
| 1:C1:1894:G:N2     | 33:LR:81:ARG:O     | 2.37                     | 0.46              |
| 1:C1:2858:C:O2'    | 1:C1:2860:G:OP2    | 2.29                     | 0.46              |
| 3:C4:1:A:C8        | 20:LD:271:LYS:HG2  | 2.50                     | 0.46              |
| 15:Ch:472:VAL:HB   | 15:Ch:482:MET:HB2  | 1.98                     | 0.46              |
| 23:LG:80:GLN:HG2   | 23:LG:233:ARG:HB2  | 1.97                     | 0.46              |
| 35:LT:143:ILE:HG23 | 35:LT:148:PRO:HD3  | 1.96                     | 0.46              |
| 4:CF:200:VAL:HG13  | 16:Cz:21:LYS:HE2   | 1.97                     | 0.46              |
| 5:CH:631:ALA:HB2   | 31:LP:125:GLN:HE21 | 1.80                     | 0.46              |
| 18:LB:62:ARG:HH12  | 18:LB:350:LYS:HG2  | 1.81                     | 0.46              |
| 23:LG:172:LEU:HA   | 48:Li:52:LEU:HD11  | 1.97                     | 0.46              |
| 46:Lg:24:ILE:HD13  | 46:Lg:34:LEU:HD22  | 1.97                     | 0.46              |
| 27:LL:67:ARG:NE    | 41:La:105:LEU:O    | 2.45                     | 0.46              |
| 27:LL:189:ARG:HB2  | 48:Li:18:ARG:HD3   | 1.97                     | 0.46              |
| 42:Lc:78:ILE:HG13  | 42:Lc:89:ARG:HG2   | 1.98                     | 0.46              |
| 48:Li:67:ILE:HD11  | 48:Li:99:LEU:HD22  | 1.98                     | 0.46              |
| 23:LG:213:GLU:HG3  | 23:LG:216:LYS:HE3  | 1.97                     | 0.46              |
| 53:Lq:64:ILE:HA    | 53:Lq:79:TYR:O     | 2.16                     | 0.46              |
| 1:C1:669:U:O4      | 19:LC:119:LYS:NZ   | 2.43                     | 0.46              |
| 1:C1:2092:U:H2'    | 1:C1:2093:G:C8     | 2.51                     | 0.46              |
| 13:Cf:112:ASP:HB3  | 13:Cf:263:PRO:HG3  | 1.98                     | 0.46              |
| 18:LB:244:HIS:CD2  | 18:LB:245:LYS:HG2  | 2.50                     | 0.46              |
| 52:Lp:73:THR:HG22  | 52:Lp:75:ALA:H     | 1.79                     | 0.46              |
| 1:C1:110:A:N1      | 1:C1:315:U:O2'     | 2.42                     | 0.46              |
| 1:C1:652:A:H2'     | 1:C1:653:A:C8      | 2.51                     | 0.46              |
| 1:C1:967:U:H2'     | 1:C1:968:U:H6      | 1.81                     | 0.46              |
| 4:CF:164:GLU:OE2   | 4:CF:167:ARG:NH2   | 2.48                     | 0.46              |
| 39:LY:73:TYR:CD2   | 39:LY:76:LYS:HG2   | 2.51                     | 0.46              |
| 1:C1:1480:C:H2'    | 1:C1:1481:A:C8     | 2.51                     | 0.45              |
| 1:C1:2976:C:OP1    | 8:CN:9:ASN:ND2     | 2.43                     | 0.45              |
| 1:C1:3289:G:O6     | 1:C1:3298:U:O4     | 2.34                     | 0.45              |
| 4:CF:30:ILE:O      | 4:CF:34:ILE:HG12   | 2.16                     | 0.45              |
| 23:LG:71:ARG:NH1   | 23:LG:240:ILE:O    | 2.49                     | 0.45              |
| 39:LY:52:GLY:HA2   | 39:LY:68:LYS:HE2   | 1.98                     | 0.45              |
| 53:Lq:9:ILE:HG22   | 53:Lq:47:VAL:HG22  | 1.98                     | 0.45              |
| 1:C1:29:C:O2'      | 1:C1:62:A:N3       | 2.45                     | 0.45              |
| 1:C1:64:A:N3       | 1:C1:79:U:O2'      | 2.41                     | 0.45              |
| 1:C1:735:C:H2'     | 1:C1:736:G:H8      | 1.82                     | 0.45              |
| 1:C1:980:A:H2'     | 1:C1:981:G:C8      | 2.51                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:1778:A:H2'    | 1:C1:1779:A:C8     | 2.52                     | 0.45              |
| 1:C1:1824:C:O2'    | 49:Lj:11:ARG:NH1   | 2.47                     | 0.45              |
| 1:C1:2123:G:H2'    | 1:C1:2124:G:C8     | 2.51                     | 0.45              |
| 8:CN:85:ARG:NH2    | 8:CN:89:PRO:O      | 2.49                     | 0.45              |
| 17:LA:30:ARG:O     | 17:LA:163:ARG:NH1  | 2.39                     | 0.45              |
| 19:LC:4:ARG:NH2    | 19:LC:23:LEU:O     | 2.48                     | 0.45              |
| 1:C1:21:A:H2'      | 1:C1:22:G:C8       | 2.51                     | 0.45              |
| 1:C1:180:U:H1'     | 39:LY:128:VAL:HG11 | 1.99                     | 0.45              |
| 1:C1:2159:C:H2'    | 1:C1:2160:C:C6     | 2.51                     | 0.45              |
| 1:C1:2164:G:H21    | 1:C1:2205:A:N6     | 2.11                     | 0.45              |
| 1:C1:2510:C:H1'    | 23:LG:38:GLY:HA3   | 1.98                     | 0.45              |
| 4:CF:194:ILE:O     | 4:CF:205:GLN:NE2   | 2.37                     | 0.45              |
| 19:LC:266:ASP:OD1  | 19:LC:267:ALA:N    | 2.49                     | 0.45              |
| 20:LD:98:ALA:HB1   | 20:LD:165:VAL:HG23 | 1.98                     | 0.45              |
| 1:C1:121:G:N2      | 23:LG:129:SER:OG   | 2.49                     | 0.45              |
| 1:C1:495:G:H2'     | 1:C1:496:G:H8      | 1.81                     | 0.45              |
| 1:C1:644:A:H2'     | 1:C1:645:A:H8      | 1.82                     | 0.45              |
| 5:CH:408:GLU:HG3   | 5:CH:417:PHE:HB3   | 1.99                     | 0.45              |
| 8:CN:4:ARG:NH1     | 8:CN:210:THR:O     | 2.46                     | 0.45              |
| 19:LC:127:LEU:HD11 | 19:LC:240:LEU:HD13 | 1.98                     | 0.45              |
| 5:CH:532:ASP:OD1   | 10:CQ:138:ARG:NH2  | 2.50                     | 0.45              |
| 7:CL:38:LEU:O      | 7:CL:42:ASN:HB2    | 2.17                     | 0.45              |
| 12:Cd:358:PRO:HD2  | 12:Cd:400:ARG:HG2  | 1.99                     | 0.45              |
| 40:LZ:8:ARG:NH2    | 40:LZ:85:THR:OG1   | 2.50                     | 0.45              |
| 41:La:125:VAL:HB   | 41:La:145:VAL:HG22 | 1.98                     | 0.45              |
| 42:Lc:77:ASN:HB2   | 42:Lc:90:CYS:H     | 1.81                     | 0.45              |
| 1:C1:382:A:H5''    | 31:LP:16:ARG:HG3   | 1.98                     | 0.45              |
| 1:C1:1054:U:O2     | 1:C1:1070:G:N2     | 2.40                     | 0.45              |
| 1:C1:1326:A:H2'    | 1:C1:1327:G:C8     | 2.52                     | 0.45              |
| 18:LB:40:PRO:O     | 18:LB:42:HIS:ND1   | 2.50                     | 0.45              |
| 18:LB:307:THR:HG21 | 18:LB:317:GLU:HG2  | 1.99                     | 0.45              |
| 25:LJ:79:GLU:OE2   | 25:LJ:83:ARG:NE    | 2.48                     | 0.45              |
| 1:C1:128:G:H2'     | 1:C1:129:G:H8      | 1.82                     | 0.45              |
| 1:C1:774:A:H2'     | 1:C1:775:A:C8      | 2.52                     | 0.45              |
| 1:C1:1187:A:N6     | 1:C1:2810:A:O4'    | 2.50                     | 0.45              |
| 1:C1:1191:C:H4'    | 4:CF:4:SER:HA      | 1.98                     | 0.45              |
| 1:C1:3299:U:H2'    | 1:C1:3300:A:H8     | 1.81                     | 0.45              |
| 4:CF:43:PHE:HB3    | 4:CF:223:LEU:HD23  | 1.98                     | 0.45              |
| 5:CH:248:ALA:HB2   | 5:CH:338:LEU:HD21  | 1.99                     | 0.45              |
| 13:Cf:141:MET:HE1  | 14:Cg:63:ILE:HD11  | 1.99                     | 0.45              |
| 17:LA:26:PRO:O     | 17:LA:75:THR:OG1   | 2.34                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:LB:313:VAL:HG23 | 18:LB:365:GLU:HG3  | 1.99                     | 0.45              |
| 31:LP:116:HIS:HB3  | 31:LP:149:ILE:HB   | 1.98                     | 0.45              |
| 36:LU:40:GLU:O     | 36:LU:44:ASN:ND2   | 2.37                     | 0.45              |
| 43:Ld:15:VAL:HA    | 43:Ld:85:ARG:O     | 2.17                     | 0.45              |
| 1:C1:1582:A:N6     | 38:LX:83:GLU:OE2   | 2.30                     | 0.45              |
| 1:C1:2580:G:H4'    | 14:Cg:180:ARG:HD2  | 1.97                     | 0.45              |
| 1:C1:2961:G:O2'    | 18:LB:92:TYR:OH    | 2.24                     | 0.45              |
| 1:C1:2973:C:OP2    | 9:CO:2:ALA:N       | 2.50                     | 0.45              |
| 20:LD:207:VAL:O    | 20:LD:211:MET:HG3  | 2.16                     | 0.45              |
| 24:LH:60:ARG:HG2   | 24:LH:82:PHE:HE2   | 1.82                     | 0.45              |
| 30:LO:62:MET:HA    | 30:LO:72:PRO:HD2   | 1.98                     | 0.45              |
| 1:C1:2728:A:H2'    | 1:C1:2729:G:C8     | 2.52                     | 0.45              |
| 5:CH:347:LEU:HD13  | 5:CH:361:LEU:HD11  | 1.99                     | 0.45              |
| 20:LD:60:ILE:HB    | 20:LD:80:SER:HB3   | 1.98                     | 0.45              |
| 23:LG:53:VAL:HG22  | 38:LX:43:THR:HA    | 1.98                     | 0.45              |
| 1:C1:20:U:H2'      | 1:C1:21:A:C8       | 2.52                     | 0.45              |
| 1:C1:723:C:O2'     | 32:LQ:103:ASN:ND2  | 2.40                     | 0.45              |
| 1:C1:2211:C:H2'    | 12:Cd:315:ARG:NH2  | 2.31                     | 0.45              |
| 1:C1:2396:U:OP2    | 1:C1:2397:U:O2'    | 2.29                     | 0.45              |
| 3:C4:16:C:N3       | 3:C4:64:A:N6       | 2.63                     | 0.45              |
| 3:C4:27:A:O3'      | 25:LJ:142:ARG:NH1  | 2.50                     | 0.45              |
| 14:Cg:36:VAL:HG13  | 14:Cg:54:VAL:HG21  | 1.99                     | 0.45              |
| 20:LD:48:LYS:HE2   | 20:LD:148:ILE:HD13 | 1.99                     | 0.45              |
| 20:LD:82:GLU:OE1   | 20:LD:108:ARG:NH1  | 2.50                     | 0.45              |
| 22:LF:43:ASN:O     | 22:LF:47:ARG:HG2   | 2.17                     | 0.45              |
| 22:LF:238:GLU:HG3  | 34:LS:35:VAL:HG22  | 1.98                     | 0.45              |
| 30:LO:58:TYR:O     | 30:LO:74:HIS:NE2   | 2.40                     | 0.45              |
| 34:LS:60:SER:OG    | 34:LS:62:ASN:OD1   | 2.34                     | 0.45              |
| 37:LV:25:MET:HE3   | 37:LV:102:GLY:HA3  | 1.98                     | 0.45              |
| 1:C1:282:U:H2'     | 1:C1:283:G:C8      | 2.51                     | 0.44              |
| 1:C1:410:A:H2'     | 1:C1:411:A:C8      | 2.52                     | 0.44              |
| 1:C1:788:A:N3      | 1:C1:2771:C:O2'    | 2.47                     | 0.44              |
| 5:CH:370:VAL:HG11  | 8:CN:230:PRO:HB2   | 1.99                     | 0.44              |
| 15:Ch:42:ILE:O     | 15:Ch:123:SER:HA   | 2.16                     | 0.44              |
| 18:LB:93:ILE:HG23  | 18:LB:102:LEU:HB2  | 1.99                     | 0.44              |
| 40:LZ:21:LYS:HE3   | 40:LZ:133:LEU:HB2  | 1.99                     | 0.44              |
| 1:C1:115:A:H4'     | 29:LN:49:ARG:HG2   | 1.99                     | 0.44              |
| 1:C1:859:C:N4      | 1:C1:860:G:O6      | 2.50                     | 0.44              |
| 1:C1:2314:U:H2'    | 1:C1:2315:A:H8     | 1.83                     | 0.44              |
| 1:C1:3002:A:H4'    | 18:LB:13:SER:HB2   | 1.99                     | 0.44              |
| 5:CH:360:ARG:NE    | 8:CN:246:TYR:O     | 2.43                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:Cg:185:GLN:HA   | 14:Cg:188:MET:HG2  | 1.99                     | 0.44              |
| 29:LN:177:GLY:O    | 29:LN:184:ARG:NH1  | 2.50                     | 0.44              |
| 1:C1:400:A:C2      | 2:C2:17:A:H1'      | 2.52                     | 0.44              |
| 1:C1:3211:U:N3     | 21:LE:64:ARG:HD3   | 2.32                     | 0.44              |
| 3:C4:77:U:H2'      | 3:C4:78:A:H8       | 1.82                     | 0.44              |
| 8:CN:11:ASN:ND2    | 8:CN:209:ASP:OD2   | 2.50                     | 0.44              |
| 18:LB:144:SER:O    | 18:LB:148:GLU:HG2  | 2.18                     | 0.44              |
| 22:LF:229:ILE:HA   | 34:LS:36:VAL:HG22  | 1.99                     | 0.44              |
| 40:LZ:50:SER:HB2   | 40:LZ:64:ARG:HB3   | 1.99                     | 0.44              |
| 1:C1:2751:A:H2'    | 1:C1:2752:G:H8     | 1.82                     | 0.44              |
| 18:LB:84:MET:O     | 18:LB:203:PRO:HA   | 2.18                     | 0.44              |
| 18:LB:289:GLY:N    | 18:LB:321:ASP:OD1  | 2.38                     | 0.44              |
| 22:LF:43:ASN:HA    | 22:LF:46:LYS:HB3   | 2.00                     | 0.44              |
| 49:Lj:29:ASN:O     | 49:Lj:32:LYS:NZ    | 2.41                     | 0.44              |
| 1:C1:589:C:H4'     | 19:LC:327:LEU:HD13 | 1.99                     | 0.44              |
| 1:C1:1316:C:O2'    | 22:LF:213:LEU:O    | 2.35                     | 0.44              |
| 1:C1:1758:G:O2'    | 1:C1:1760:G:OP2    | 2.30                     | 0.44              |
| 1:C1:1920:G:H21    | 1:C1:3303:A:H8     | 1.65                     | 0.44              |
| 1:C1:2169:G:H2'    | 1:C1:2170:A:C8     | 2.53                     | 0.44              |
| 1:C1:2181:G:H2'    | 1:C1:2182:A:H8     | 1.82                     | 0.44              |
| 1:C1:2729:G:H2'    | 1:C1:2732:C:H5     | 1.83                     | 0.44              |
| 1:C1:3123:U:H2'    | 1:C1:3124:G:C8     | 2.52                     | 0.44              |
| 4:CF:93:THR:HA     | 4:CF:96:LEU:HG     | 1.98                     | 0.44              |
| 5:CH:429:ASN:HB3   | 5:CH:432:TRP:CD2   | 2.53                     | 0.44              |
| 1:C1:974:A:H5''    | 35:LT:43:LYS:HD2   | 2.00                     | 0.44              |
| 1:C1:1596:U:H2'    | 1:C1:1597:G:C8     | 2.53                     | 0.44              |
| 4:CF:70:THR:OG1    | 4:CF:98:GLY:O      | 2.26                     | 0.44              |
| 28:LM:109:ARG:HH21 | 30:LO:202:TYR:C    | 2.25                     | 0.44              |
| 1:C1:1619:C:OP2    | 46:Lg:75:ARG:NH1   | 2.38                     | 0.44              |
| 1:C1:1874:U:OP1    | 11:Cb:7:ARG:NH1    | 2.50                     | 0.44              |
| 3:C4:26:C:H5'      | 20:LD:56:THR:HB    | 1.99                     | 0.44              |
| 15:Ch:470:LEU:HD21 | 15:Ch:505:SER:HB3  | 2.00                     | 0.44              |
| 21:LE:86:PRO:HD2   | 21:LE:89:ILE:HD12  | 2.00                     | 0.44              |
| 31:LP:52:ILE:HA    | 31:LP:85:VAL:HG12  | 2.00                     | 0.44              |
| 32:LQ:64:LEU:O     | 32:LQ:68:THR:HB    | 2.18                     | 0.44              |
| 1:C1:434:U:H2'     | 1:C1:435:G:C8      | 2.53                     | 0.44              |
| 1:C1:1345:G:H2'    | 1:C1:1346:A:H8     | 1.83                     | 0.44              |
| 1:C1:1588:C:O3'    | 38:LX:92:GLN:NE2   | 2.51                     | 0.44              |
| 1:C1:3288:A:H2'    | 1:C1:3289:G:H8     | 1.83                     | 0.44              |
| 5:CH:309:THR:HG21  | 5:CH:316:ILE:HG12  | 2.00                     | 0.44              |
| 12:Cd:298:ARG:NH1  | 12:Cd:299:ALA:O    | 2.51                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:Lk:14:ILE:HA    | 50:Lk:17:ARG:HD3   | 2.00                     | 0.44              |
| 1:C1:231:A:H2'     | 1:C1:232:A:C8      | 2.52                     | 0.44              |
| 1:C1:661:C:H2'     | 1:C1:662:G:H8      | 1.82                     | 0.44              |
| 1:C1:1447:G:N2     | 1:C1:1450:A:OP2    | 2.50                     | 0.44              |
| 1:C1:1571:G:OP1    | 46:Lg:17:THR:OG1   | 2.35                     | 0.44              |
| 1:C1:1636:A:OP2    | 46:Lg:38:LYS:NZ    | 2.49                     | 0.44              |
| 1:C1:2182:A:H2'    | 1:C1:2183:A:H8     | 1.83                     | 0.44              |
| 1:C1:2713:G:OP2    | 14:Cg:119:ARG:NH2  | 2.39                     | 0.44              |
| 3:C4:12:U:OP2      | 3:C4:68:C:O2'      | 2.35                     | 0.44              |
| 9:CO:6:ARG:HA      | 9:CO:11:LYS:HE3    | 2.00                     | 0.44              |
| 12:Cd:273:ILE:HD13 | 12:Cd:296:ALA:HB1  | 2.00                     | 0.44              |
| 19:LC:332:TYR:CE1  | 22:LF:55:GLU:HG2   | 2.52                     | 0.44              |
| 25:LJ:55:VAL:HG12  | 25:LJ:58:PHE:H     | 1.83                     | 0.44              |
| 47:Lh:109:THR:HG22 | 47:Lh:112:ARG:HH21 | 1.83                     | 0.44              |
| 1:C1:514:A:H3'     | 1:C1:515:G:H8      | 1.83                     | 0.43              |
| 1:C1:882:G:H1'     | 1:C1:1569:A:N6     | 2.32                     | 0.43              |
| 1:C1:1367:U:H5'    | 19:LC:139:ARG:HH12 | 1.83                     | 0.43              |
| 2:C2:9:A:H2'       | 2:C2:10:A:C8       | 2.53                     | 0.43              |
| 13:Cf:34:ARG:HE    | 13:Cf:38:CYS:HB3   | 1.83                     | 0.43              |
| 19:LC:136:LEU:HD23 | 19:LC:143:VAL:HG11 | 2.00                     | 0.43              |
| 20:LD:95:TRP:CE3   | 20:LD:201:TYR:HB3  | 2.53                     | 0.43              |
| 50:Lk:24:ARG:HA    | 50:Lk:69:LYS:O     | 2.18                     | 0.43              |
| 1:C1:2386:U:H2'    | 1:C1:2387:A:H8     | 1.82                     | 0.43              |
| 1:C1:2822:G:C2     | 5:CH:94:LEU:HD13   | 2.53                     | 0.43              |
| 5:CH:371:ALA:HB3   | 8:CN:181:LEU:HB2   | 2.00                     | 0.43              |
| 17:LA:180:LEU:HD22 | 52:Lp:26:VAL:HG21  | 2.00                     | 0.43              |
| 21:LE:72:LEU:HA    | 21:LE:83:VAL:HG12  | 1.99                     | 0.43              |
| 39:LY:55:VAL:HG12  | 39:LY:105:ILE:HG12 | 2.00                     | 0.43              |
| 1:C1:575:G:H2'     | 1:C1:576:A:C8      | 2.53                     | 0.43              |
| 1:C1:1197:U:H2'    | 1:C1:1198:A:C8     | 2.53                     | 0.43              |
| 1:C1:2889:A:H2'    | 1:C1:2890:C:C6     | 2.54                     | 0.43              |
| 2:C2:97:A:OP1      | 47:Lh:72:ARG:NH2   | 2.44                     | 0.43              |
| 8:CN:26:VAL:HG21   | 8:CN:35:TYR:HD2    | 1.83                     | 0.43              |
| 15:Ch:173:ILE:HD11 | 15:Ch:204:LEU:HD22 | 2.01                     | 0.43              |
| 22:LF:53:ARG:HG2   | 22:LF:57:TYR:CZ    | 2.54                     | 0.43              |
| 24:LH:126:LYS:HG2  | 24:LH:184:ILE:HG12 | 2.00                     | 0.43              |
| 31:LP:18:ARG:NH1   | 31:LP:147:GLU:OE1  | 2.51                     | 0.43              |
| 44:Le:24:ASP:OD1   | 44:Le:24:ASP:N     | 2.50                     | 0.43              |
| 53:Lq:54:ILE:HD12  | 53:Lq:114:ARG:HB3  | 2.00                     | 0.43              |
| 1:C1:88:U:H2'      | 1:C1:89:A:C8       | 2.53                     | 0.43              |
| 1:C1:371:A:H4'     | 39:LY:90:THR:HG22  | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:1288:U:C2     | 18:LB:258:PRO:HG3  | 2.54                     | 0.43              |
| 1:C1:2176:A:N3     | 1:C1:2560:A:O2'    | 2.45                     | 0.43              |
| 14:Cg:154:GLU:OE1  | 35:LT:57:TYR:OH    | 2.25                     | 0.43              |
| 21:LE:38:LYS:HA    | 21:LE:38:LYS:HD3   | 1.91                     | 0.43              |
| 25:LJ:147:SER:OG   | 25:LJ:148:ARG:N    | 2.50                     | 0.43              |
| 29:LN:36:ILE:HD11  | 29:LN:105:ARG:HB3  | 1.99                     | 0.43              |
| 40:LZ:41:LEU:HG    | 40:LZ:73:VAL:HG22  | 1.99                     | 0.43              |
| 1:C1:1205:G:OP1    | 4:CF:23:LYS:NZ     | 2.51                     | 0.43              |
| 1:C1:3187:A:OP1    | 18:LB:97:ARG:NH2   | 2.48                     | 0.43              |
| 5:CH:242:LEU:HD22  | 5:CH:277:PHE:HE1   | 1.84                     | 0.43              |
| 5:CH:546:LEU:HA    | 5:CH:549:ARG:HD2   | 1.99                     | 0.43              |
| 42:Lc:17:LEU:HD21  | 42:Lc:46:LEU:HD11  | 2.01                     | 0.43              |
| 1:C1:404:U:H2'     | 1:C1:405:G:C8      | 2.54                     | 0.43              |
| 1:C1:1202:C:O2'    | 1:C1:1269:A:N1     | 2.50                     | 0.43              |
| 1:C1:2376:A:H2'    | 1:C1:2377:G:H8     | 1.83                     | 0.43              |
| 4:CF:170:MET:HB3   | 4:CF:172:VAL:HG13  | 2.00                     | 0.43              |
| 8:CN:14:GLY:HA2    | 8:CN:198:VAL:HG13  | 2.01                     | 0.43              |
| 17:LA:43:GLY:HA3   | 17:LA:63:PHE:HD1   | 1.83                     | 0.43              |
| 52:Lp:79:MET:O     | 52:Lp:83:LEU:HB2   | 2.19                     | 0.43              |
| 1:C1:757:A:H2'     | 1:C1:758:U:C6      | 2.54                     | 0.43              |
| 1:C1:777:C:H2'     | 1:C1:778:OMC:H6    | 1.83                     | 0.43              |
| 1:C1:1577:C:H5'    | 1:C1:1676:A:H1'    | 2.00                     | 0.43              |
| 1:C1:1595:C:H2'    | 1:C1:1596:U:C6     | 2.54                     | 0.43              |
| 1:C1:1804:C:H2'    | 1:C1:1805:G:H8     | 1.83                     | 0.43              |
| 1:C1:2400:G:N2     | 1:C1:2473:U:O2     | 2.35                     | 0.43              |
| 1:C1:3079:U:H1'    | 1:C1:3080:A:H5''   | 2.00                     | 0.43              |
| 1:C1:3145:C:H5'    | 30:LO:178:ARG:HE   | 1.82                     | 0.43              |
| 2:C2:58:G:O6       | 49:Lj:63:ARG:NH1   | 2.51                     | 0.43              |
| 4:CF:96:LEU:HD22   | 4:CF:100:VAL:HG11  | 2.01                     | 0.43              |
| 13:Cf:284:LYS:HB2  | 13:Cf:287:ILE:HB   | 2.01                     | 0.43              |
| 33:LR:44:LEU:HD22  | 33:LR:49:LEU:HD22  | 2.01                     | 0.43              |
| 1:C1:425:G:H2'     | 1:C1:426:A:C8      | 2.54                     | 0.43              |
| 1:C1:457:U:H5'     | 53:Lq:67:LYS:HD3   | 2.01                     | 0.43              |
| 1:C1:527:G:N1      | 1:C1:544:G:O2'     | 2.48                     | 0.43              |
| 1:C1:704:A:OP1     | 41:La:137:LYS:NZ   | 2.52                     | 0.43              |
| 1:C1:1366:G:O2'    | 19:LC:139:ARG:NH1  | 2.51                     | 0.43              |
| 1:C1:2683:OMU:HM23 | 1:C1:2683:OMU:H1'  | 1.64                     | 0.43              |
| 1:C1:3026:C:OP1    | 33:LR:59:SER:N     | 2.44                     | 0.43              |
| 3:C4:35:C:O2       | 3:C4:45:U:O2'      | 2.35                     | 0.43              |
| 23:LG:153:LEU:HB2  | 23:LG:218:ILE:HD11 | 1.99                     | 0.43              |
| 35:LT:34:TYR:HE2   | 35:LT:93:ILE:HG23  | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:1376:A:H5''   | 44:Le:100:ASN:HB2  | 2.01                     | 0.43              |
| 1:C1:2771:C:H2'    | 1:C1:2772:A:C8     | 2.54                     | 0.43              |
| 6:CK:154:PRO:HG2   | 6:CK:249:PRO:HB2   | 2.00                     | 0.43              |
| 10:CQ:89:THR:O     | 10:CQ:93:MET:HG3   | 2.19                     | 0.43              |
| 14:Cg:150:ASP:O    | 14:Cg:170:ARG:NH1  | 2.41                     | 0.43              |
| 39:LY:57:ILE:HG12  | 39:LY:103:VAL:HG12 | 2.01                     | 0.43              |
| 53:Lq:96:SER:HA    | 53:Lq:100:LYS:HG2  | 2.00                     | 0.43              |
| 1:C1:159:U:H2'     | 1:C1:160:G:C8      | 2.53                     | 0.43              |
| 1:C1:293:G:H2'     | 1:C1:294:G:H8      | 1.83                     | 0.43              |
| 1:C1:1077:U:O2'    | 1:C1:1078:U:O2     | 2.27                     | 0.43              |
| 1:C1:1545:G:H2'    | 1:C1:1546:G:H8     | 1.84                     | 0.43              |
| 1:C1:1576:C:H2'    | 1:C1:1577:C:C6     | 2.53                     | 0.43              |
| 19:LC:188:SER:O    | 19:LC:188:SER:OG   | 2.33                     | 0.43              |
| 33:LR:108:LYS:HE2  | 33:LR:108:LYS:HB3  | 1.73                     | 0.43              |
| 35:LT:155:ALA:O    | 35:LT:158:THR:OG1  | 2.34                     | 0.43              |
| 1:C1:269:A:H2'     | 1:C1:270:G:C8      | 2.54                     | 0.42              |
| 1:C1:1319:C:H2'    | 1:C1:1320:G:H8     | 1.84                     | 0.42              |
| 1:C1:1454:U:H2'    | 1:C1:1455:G:C8     | 2.54                     | 0.42              |
| 1:C1:1592:C:H5''   | 50:Lk:44:LEU:HD22  | 2.00                     | 0.42              |
| 3:C4:23:A:N3       | 3:C4:119:U:O2'     | 2.42                     | 0.42              |
| 3:C4:59:C:H2'      | 3:C4:60:A:C8       | 2.54                     | 0.42              |
| 8:CN:109:VAL:HB    | 8:CN:149:GLY:HA2   | 2.00                     | 0.42              |
| 29:LN:35:VAL:HA    | 29:LN:65:ARG:HG2   | 2.01                     | 0.42              |
| 45:Lf:104:LEU:O    | 45:Lf:107:SER:OG   | 2.30                     | 0.42              |
| 1:C1:128:G:H2'     | 1:C1:129:G:C8      | 2.54                     | 0.42              |
| 1:C1:203:A:H4'     | 1:C1:205:A:N7      | 2.34                     | 0.42              |
| 1:C1:1173:A:C8     | 1:C1:1176:A:HI1'   | 2.53                     | 0.42              |
| 1:C1:1323:C:H2'    | 1:C1:1324:U:C6     | 2.54                     | 0.42              |
| 1:C1:1697:C:H2'    | 1:C1:1698:A:C8     | 2.54                     | 0.42              |
| 1:C1:2696:C:O2'    | 13:Cf:279:GLN:OE1  | 2.29                     | 0.42              |
| 1:C1:2727:U:H2'    | 1:C1:2728:A:H8     | 1.84                     | 0.42              |
| 1:C1:3026:C:OP2    | 33:LR:62:ARG:NH2   | 2.52                     | 0.42              |
| 1:C1:3236:A:OP1    | 18:LB:125:SER:OG   | 2.29                     | 0.42              |
| 5:CH:587:LEU:HD12  | 5:CH:587:LEU:HA    | 1.84                     | 0.42              |
| 13:Cf:47:ASN:OD1   | 13:Cf:59:ARG:NH1   | 2.51                     | 0.42              |
| 15:Ch:193:LEU:HD11 | 15:Ch:209:MET:HG2  | 2.00                     | 0.42              |
| 15:Ch:356:LYS:HA   | 15:Ch:359:GLU:HG2  | 2.01                     | 0.42              |
| 18:LB:152:ILE:HA   | 18:LB:152:ILE:HD12 | 1.85                     | 0.42              |
| 29:LN:9:GLU:HB2    | 48:Li:53:ILE:HG13  | 2.02                     | 0.42              |
| 31:LP:122:ALA:HB3  | 31:LP:143:PRO:HB2  | 2.00                     | 0.42              |
| 31:LP:178:VAL:HG23 | 31:LP:182:ARG:HH12 | 1.82                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:261:A:O2'     | 29:LN:14:LYS:NZ    | 2.52                     | 0.42              |
| 1:C1:527:G:N2      | 1:C1:528:U:O4      | 2.41                     | 0.42              |
| 1:C1:1148:G:OP1    | 45:Lf:86:LYS:NZ    | 2.42                     | 0.42              |
| 1:C1:1361:U:H2'    | 1:C1:1362:G:H8     | 1.84                     | 0.42              |
| 1:C1:1395:G:H5''   | 44:Le:125:ALA:HB2  | 2.01                     | 0.42              |
| 1:C1:3126:A:H1'    | 30:LO:103:ARG:HH21 | 1.84                     | 0.42              |
| 3:C4:56:A:H4'      | 25:LJ:153:HIS:HB2  | 2.00                     | 0.42              |
| 12:Cd:418:VAL:HG22 | 12:Cd:475:TRP:HB3  | 2.00                     | 0.42              |
| 13:Cf:143:VAL:HB   | 13:Cf:186:VAL:HG22 | 2.01                     | 0.42              |
| 27:LL:192:ALA:HB2  | 48:Li:19:GLY:HA2   | 2.01                     | 0.42              |
| 1:C1:630:U:H2'     | 1:C1:631:U:C2      | 2.55                     | 0.42              |
| 1:C1:890:G:N2      | 29:LN:76:PRO:O     | 2.52                     | 0.42              |
| 1:C1:1698:A:H2'    | 1:C1:1699:G:C8     | 2.54                     | 0.42              |
| 1:C1:2277:OMU:O5'  | 1:C1:2277:OMU:H6   | 2.19                     | 0.42              |
| 1:C1:3179:G:H2'    | 1:C1:3180:G:C8     | 2.55                     | 0.42              |
| 5:CH:284:ILE:HB    | 5:CH:316:ILE:HD13  | 2.02                     | 0.42              |
| 26:LK:38:SER:HA    | 26:LK:39:PRO:HD3   | 1.88                     | 0.42              |
| 33:LR:133:LYS:HG3  | 33:LR:134:HIS:CD2  | 2.54                     | 0.42              |
| 1:C1:1135:G:O2'    | 1:C1:2334:G:N2     | 2.53                     | 0.42              |
| 1:C1:2112:A:N6     | 1:C1:2150:G:O2'    | 2.40                     | 0.42              |
| 1:C1:2489:C:H2'    | 1:C1:2490:G:H8     | 1.84                     | 0.42              |
| 1:C1:2523:G:H2'    | 1:C1:2524:G:C8     | 2.54                     | 0.42              |
| 1:C1:2875:U:H2'    | 1:C1:2876:OMG:H8   | 1.84                     | 0.42              |
| 5:CH:226:HIS:CE1   | 5:CH:231:MET:HG2   | 2.54                     | 0.42              |
| 19:LC:161:ASP:OD2  | 19:LC:161:ASP:N    | 2.45                     | 0.42              |
| 23:LG:232:THR:HG22 | 23:LG:235:ARG:HH12 | 1.83                     | 0.42              |
| 1:C1:1100:G:H2'    | 1:C1:1101:C:C6     | 2.55                     | 0.42              |
| 1:C1:1642:G:H1     | 1:C1:1767:A:H61    | 1.68                     | 0.42              |
| 13:Cf:23:ILE:HD13  | 14:Cg:97:PRO:HD2   | 2.00                     | 0.42              |
| 20:LD:283:SER:OG   | 20:LD:284:ARG:N    | 2.53                     | 0.42              |
| 1:C1:1225:G:N7     | 12:Cd:152:LYS:NZ   | 2.67                     | 0.42              |
| 1:C1:1242:A:H2'    | 1:C1:1243:A:C8     | 2.54                     | 0.42              |
| 1:C1:2971:U:H2'    | 1:C1:2972:U:C6     | 2.55                     | 0.42              |
| 5:CH:455:ASP:N     | 5:CH:455:ASP:OD1   | 2.53                     | 0.42              |
| 18:LB:123:TYR:CZ   | 18:LB:124:LYS:HG3  | 2.54                     | 0.42              |
| 19:LC:287:LEU:HD11 | 32:LQ:60:LEU:HB2   | 2.02                     | 0.42              |
| 1:C1:243:U:O2'     | 1:C1:244:G:O5'     | 2.30                     | 0.42              |
| 1:C1:289:A:H2'     | 1:C1:290:A:C8      | 2.54                     | 0.42              |
| 1:C1:1626:G:O2'    | 1:C1:1788:G:N2     | 2.50                     | 0.42              |
| 21:LE:116:GLN:HA   | 21:LE:119:ILE:HB   | 2.02                     | 0.42              |
| 1:C1:13:G:H1       | 2:C2:146:U:H3      | 1.68                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:1243:A:H2'    | 1:C1:1244:G:C4     | 2.55                     | 0.42              |
| 1:C1:1619:C:H2'    | 1:C1:1620:G:H8     | 1.85                     | 0.42              |
| 1:C1:2225:A:H2'    | 1:C1:2226:C:C6     | 2.53                     | 0.42              |
| 1:C1:2280:A:H5''   | 1:C1:2282:U:H5'    | 2.02                     | 0.42              |
| 2:C2:91:C:H2'      | 2:C2:92:A:C8       | 2.55                     | 0.42              |
| 3:C4:17:A:OP1      | 25:LJ:154:ARG:NH2  | 2.51                     | 0.42              |
| 3:C4:17:A:H2'      | 3:C4:18:G:H8       | 1.84                     | 0.42              |
| 6:CK:174:PRO:HG2   | 6:CK:177:LEU:HD12  | 2.02                     | 0.42              |
| 14:Cg:56:ARG:NH2   | 14:Cg:57:ASP:OD1   | 2.41                     | 0.42              |
| 26:LK:143:VAL:HG23 | 26:LK:148:PRO:HG3  | 2.02                     | 0.42              |
| 27:LL:195:VAL:HG21 | 48:Li:20:LEU:HD11  | 2.02                     | 0.42              |
| 38:LX:63:SER:HB2   | 47:Lh:71:LEU:HD13  | 2.02                     | 0.42              |
| 45:Lf:51:VAL:HG23  | 45:Lf:102:ILE:HG13 | 2.02                     | 0.42              |
| 1:C1:716:G:H5''    | 32:LQ:71:PRO:HB2   | 2.02                     | 0.42              |
| 1:C1:1137:A:OP2    | 1:C1:2334:G:N1     | 2.43                     | 0.42              |
| 1:C1:2110:A:OP2    | 17:LA:200:ARG:NH2  | 2.51                     | 0.42              |
| 1:C1:2224:G:H3'    | 1:C1:2225:A:H8     | 1.85                     | 0.42              |
| 1:C1:2489:C:H2'    | 1:C1:2490:G:C8     | 2.55                     | 0.42              |
| 1:C1:3144:U:OP1    | 30:LO:170:TYR:OH   | 2.26                     | 0.42              |
| 1:C1:3235:A:H5''   | 18:LB:128:LYS:HG3  | 2.01                     | 0.42              |
| 5:CH:86:ASP:HB3    | 5:CH:89:HIS:HB2    | 2.02                     | 0.42              |
| 31:LP:91:LEU:HD23  | 31:LP:91:LEU:HA    | 1.94                     | 0.42              |
| 43:Ld:59:LEU:HG    | 43:Ld:63:LEU:HD23  | 2.02                     | 0.42              |
| 1:C1:21:A:P        | 47:Lh:95:ARG:HE    | 2.42                     | 0.41              |
| 1:C1:736:G:H2'     | 1:C1:737:A:H8      | 1.84                     | 0.41              |
| 1:C1:813:G:O2'     | 1:C1:1844:A:N3     | 2.42                     | 0.41              |
| 1:C1:1610:G:N1     | 1:C1:1792:G:H2'    | 2.35                     | 0.41              |
| 1:C1:1877:G:OP2    | 11:Cb:11:LYS:NZ    | 2.40                     | 0.41              |
| 1:C1:2701:C:H2'    | 1:C1:2702:A:H8     | 1.85                     | 0.41              |
| 1:C1:3220:G:H2'    | 1:C1:3221:A:C8     | 2.55                     | 0.41              |
| 25:LJ:132:MET:HB3  | 25:LJ:132:MET:HE3  | 1.79                     | 0.41              |
| 40:LZ:70:PHE:HA    | 40:LZ:110:LYS:HE2  | 2.01                     | 0.41              |
| 1:C1:615:C:H2'     | 1:C1:616:A:C8      | 2.55                     | 0.41              |
| 1:C1:650:U:H2'     | 1:C1:651:C:C6      | 2.55                     | 0.41              |
| 1:C1:2677:U:O2'    | 12:Cd:80:THR:O     | 2.38                     | 0.41              |
| 2:C2:75:G:OP2      | 39:LY:73:TYR:OH    | 2.25                     | 0.41              |
| 5:CH:331:LYS:HE2   | 5:CH:331:LYS:HB3   | 1.92                     | 0.41              |
| 20:LD:113:LEU:HB3  | 20:LD:115:LEU:HD13 | 2.03                     | 0.41              |
| 35:LT:65:TYR:HB3   | 35:LT:75:ILE:HD11  | 2.02                     | 0.41              |
| 1:C1:68:A:O2'      | 1:C1:308:C:O2      | 2.36                     | 0.41              |
| 1:C1:116:A:H2'     | 1:C1:258:A:H2'     | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:3250:G:H3'    | 1:C1:3251:A:H8     | 1.86                     | 0.41              |
| 6:CK:58:LYS:HA     | 6:CK:61:MET:HE2    | 2.02                     | 0.41              |
| 22:LF:70:ARG:O     | 22:LF:74:ILE:HG12  | 2.20                     | 0.41              |
| 22:LF:95:ILE:HD11  | 22:LF:234:LEU:HD23 | 2.01                     | 0.41              |
| 22:LF:176:GLU:HG3  | 22:LF:185:ILE:HG13 | 2.02                     | 0.41              |
| 24:LH:7:GLU:HA     | 24:LH:92:LEU:O     | 2.20                     | 0.41              |
| 30:LO:77:ALA:HB3   | 30:LO:80:ARG:HD3   | 2.02                     | 0.41              |
| 44:Le:98:ALA:HB3   | 44:Le:101:VAL:HG23 | 2.03                     | 0.41              |
| 1:C1:1157:G:N2     | 30:LO:89:MET:HE2   | 2.35                     | 0.41              |
| 1:C1:2383:C:H2'    | 1:C1:2384:OMU:H6   | 2.03                     | 0.41              |
| 1:C1:2392:G:H2'    | 1:C1:2393:A:C8     | 2.56                     | 0.41              |
| 1:C1:3327:C:H2'    | 1:C1:3328:G:H8     | 1.85                     | 0.41              |
| 2:C2:29:U:H5''     | 27:LL:27:ASP:HB3   | 2.02                     | 0.41              |
| 5:CH:46:THR:HG23   | 5:CH:112:VAL:HG22  | 2.02                     | 0.41              |
| 14:Cg:43:ASP:HB3   | 14:Cg:46:VAL:HG12  | 2.02                     | 0.41              |
| 15:Ch:60:ALA:HA    | 15:Ch:65:ILE:HD11  | 2.02                     | 0.41              |
| 15:Ch:262:VAL:HG21 | 15:Ch:296:THR:HG21 | 2.01                     | 0.41              |
| 18:LB:89:LEU:O     | 18:LB:104:THR:HA   | 2.20                     | 0.41              |
| 23:LG:159:ASP:OD2  | 23:LG:159:ASP:N    | 2.53                     | 0.41              |
| 28:LM:58:PRO:HD2   | 28:LM:61:ARG:HB2   | 2.03                     | 0.41              |
| 29:LN:73:ARG:HA    | 29:LN:74:PRO:HD3   | 1.89                     | 0.41              |
| 39:LY:73:TYR:CE2   | 39:LY:76:LYS:HG2   | 2.55                     | 0.41              |
| 1:C1:848:A2M:HM'2  | 1:C1:849:G:H5'     | 2.01                     | 0.41              |
| 1:C1:1306:C:H2'    | 1:C1:1307:C:C6     | 2.54                     | 0.41              |
| 1:C1:1413:U:H2'    | 41:La:9:ARG:HH22   | 1.86                     | 0.41              |
| 1:C1:1783:C:H2'    | 1:C1:1784:G:C8     | 2.55                     | 0.41              |
| 1:C1:2642:U:H2'    | 1:C1:2643:C:C6     | 2.56                     | 0.41              |
| 1:C1:3118:C:O2'    | 1:C1:3119:A:H8     | 2.03                     | 0.41              |
| 2:C2:85:G:H2'      | 2:C2:87:G:C4       | 2.55                     | 0.41              |
| 14:Cg:146:ARG:O    | 14:Cg:173:LYS:NZ   | 2.49                     | 0.41              |
| 15:Ch:280:LYS:HE2  | 15:Ch:300:ASP:HB2  | 2.03                     | 0.41              |
| 21:LE:86:PRO:HB3   | 21:LE:166:ASP:HB2  | 2.01                     | 0.41              |
| 21:LE:86:PRO:HG3   | 21:LE:169:LEU:HD13 | 2.03                     | 0.41              |
| 22:LF:67:GLU:HA    | 22:LF:70:ARG:HG2   | 2.01                     | 0.41              |
| 36:LU:28:PRO:HB2   | 36:LU:34:PHE:HB2   | 2.03                     | 0.41              |
| 38:LX:101:VAL:HG13 | 38:LX:102:LYS:HD3  | 2.02                     | 0.41              |
| 39:LY:31:SER:HA    | 39:LY:48:PRO:HA    | 2.01                     | 0.41              |
| 40:LZ:14:ARG:HH11  | 46:Lg:87:ARG:NH2   | 2.18                     | 0.41              |
| 1:C1:3042:C:H2'    | 1:C1:3043:G:O4'    | 2.21                     | 0.41              |
| 1:C1:3044:A:H3'    | 1:C1:3045:A:H8     | 1.85                     | 0.41              |
| 2:C2:53:A:OP1      | 51:Ll:19:GLN:NE2   | 2.49                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C4:6:C:O2'      | 20:LD:50:ARG:NH2   | 2.53                     | 0.41              |
| 5:CH:630:MET:HE2  | 5:CH:632:ARG:HH21  | 1.86                     | 0.41              |
| 12:Cd:328:SER:HB3 | 12:Cd:376:ILE:HD11 | 2.02                     | 0.41              |
| 15:Ch:464:GLY:HA3 | 15:Ch:494:VAL:HG21 | 2.03                     | 0.41              |
| 17:LA:35:ALA:HA   | 23:LG:39:ILE:HD12  | 2.01                     | 0.41              |
| 24:LH:215:LEU:O   | 24:LH:219:TYR:OH   | 2.39                     | 0.41              |
| 25:LJ:93:ARG:HH12 | 25:LJ:95:ARG:HD3   | 1.84                     | 0.41              |
| 42:Lc:54:LEU:HD11 | 46:Lg:91:ILE:HG22  | 2.02                     | 0.41              |
| 1:C1:1305:U:OP1   | 34:LS:117:ARG:NH1  | 2.39                     | 0.41              |
| 1:C1:1577:C:H2'   | 1:C1:1578:G:C8     | 2.56                     | 0.41              |
| 4:CF:120:SER:OG   | 4:CF:218:GLU:OE1   | 2.30                     | 0.41              |
| 5:CH:586:ARG:HE   | 38:LX:156:VAL:HB   | 1.84                     | 0.41              |
| 12:Cd:443:ALA:HB2 | 12:Cd:460:VAL:HG21 | 2.02                     | 0.41              |
| 13:Cf:34:ARG:HH12 | 13:Cf:63:LYS:HG2   | 1.86                     | 0.41              |
| 15:Ch:362:GLU:O   | 15:Ch:366:LYS:HG3  | 2.19                     | 0.41              |
| 19:LC:191:LEU:HG  | 19:LC:197:LYS:HD3  | 2.01                     | 0.41              |
| 32:LQ:94:ARG:O    | 32:LQ:98:ASN:ND2   | 2.50                     | 0.41              |
| 35:LT:36:VAL:HG13 | 35:LT:65:TYR:HA    | 2.02                     | 0.41              |
| 1:C1:3145:C:H3'   | 1:C1:3146:C:H6     | 1.86                     | 0.41              |
| 1:C1:3315:U:H2'   | 1:C1:3319:C:H41    | 1.84                     | 0.41              |
| 8:CN:76:THR:O     | 8:CN:96:ARG:NH1    | 2.46                     | 0.41              |
| 18:LB:88:GLY:HA3  | 18:LB:162:LEU:HB2  | 2.03                     | 0.41              |
| 19:LC:319:PRO:HB2 | 19:LC:326:MET:HE2  | 2.03                     | 0.41              |
| 22:LF:51:PHE:O    | 22:LF:55:GLU:HG3   | 2.20                     | 0.41              |
| 23:LG:175:LYS:HD2 | 48:Li:52:LEU:HD12  | 2.02                     | 0.41              |
| 42:Lc:19:LEU:HA   | 42:Lc:22:LYS:HG2   | 2.03                     | 0.41              |
| 53:Lq:35:LEU:HD12 | 53:Lq:107:LEU:HB3  | 2.02                     | 0.41              |
| 1:C1:118:U:O2'    | 1:C1:120:U:OP2     | 2.37                     | 0.41              |
| 1:C1:971:A:H2'    | 1:C1:972:U:C6      | 2.56                     | 0.41              |
| 1:C1:1367:U:H5'   | 19:LC:139:ARG:NH1  | 2.35                     | 0.41              |
| 1:C1:1430:G:O2'   | 1:C1:2318:G:O6     | 2.35                     | 0.41              |
| 1:C1:2570:U:H2'   | 1:C1:2571:U:C6     | 2.56                     | 0.41              |
| 1:C1:2697:A:H2'   | 1:C1:2698:A:C8     | 2.56                     | 0.41              |
| 1:C1:2738:A:H2'   | 1:C1:2739:A:H8     | 1.86                     | 0.41              |
| 1:C1:2751:A:H2'   | 1:C1:2752:G:C8     | 2.56                     | 0.41              |
| 1:C1:3270:U:H4'   | 18:LB:309:MET:HB3  | 2.02                     | 0.41              |
| 2:C2:57:C:H4'     | 2:C2:63:G:N7       | 2.36                     | 0.41              |
| 8:CN:177:LEU:HD12 | 8:CN:181:LEU:HD11  | 2.03                     | 0.41              |
| 12:Cd:272:LYS:HG2 | 54:Cd:1000:GTP:C5  | 2.56                     | 0.41              |
| 13:Cf:290:ASP:OD1 | 13:Cf:294:ASP:N    | 2.53                     | 0.41              |
| 22:LF:90:VAL:HA   | 22:LF:143:GLY:O    | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LG:55:TRP:O     | 23:LG:60:ARG:NH1   | 2.52                     | 0.41              |
| 1:C1:2727:U:H2'    | 1:C1:2728:A:C8     | 2.55                     | 0.41              |
| 1:C1:2839:U:H5''   | 18:LB:237:LYS:HG2  | 2.03                     | 0.41              |
| 1:C1:3236:A:H2'    | 1:C1:3237:A:C8     | 2.56                     | 0.41              |
| 12:Cd:45:LYS:HD2   | 12:Cd:46:PRO:HD2   | 2.02                     | 0.41              |
| 19:LC:212:VAL:HA   | 19:LC:235:CYS:O    | 2.21                     | 0.41              |
| 20:LD:33:ARG:O     | 20:LD:37:ILE:HG12  | 2.21                     | 0.41              |
| 26:LK:8:ASN:C      | 26:LK:65:GLN:HE22  | 2.29                     | 0.41              |
| 32:LQ:79:ARG:HG2   | 32:LQ:82:MET:HE2   | 2.03                     | 0.41              |
| 1:C1:3320:C:H4'    | 18:LB:316:GLY:HA2  | 2.03                     | 0.40              |
| 2:C2:141:C:H4'     | 29:LN:110:CYS:HB3  | 2.02                     | 0.40              |
| 6:CK:25:ARG:NH1    | 16:Cz:27:LYS:HZ2   | 2.19                     | 0.40              |
| 13:Cf:39:SER:OG    | 13:Cf:98:HIS:ND1   | 2.46                     | 0.40              |
| 22:LF:137:GLU:OE1  | 22:LF:235:GLY:HA2  | 2.21                     | 0.40              |
| 22:LF:244:LEU:HD11 | 22:LF:248:MET:HE2  | 2.03                     | 0.40              |
| 39:LY:50:ARG:HG2   | 39:LY:114:ARG:HH22 | 1.86                     | 0.40              |
| 53:Lq:119:LEU:HD22 | 53:Lq:123:ARG:HH12 | 1.87                     | 0.40              |
| 1:C1:363:U:H4'     | 1:C1:397:G:H5'     | 2.02                     | 0.40              |
| 1:C1:768:A:H4'     | 1:C1:769:G:H5'     | 2.03                     | 0.40              |
| 1:C1:1182:C:H2'    | 1:C1:1183:A:C8     | 2.57                     | 0.40              |
| 1:C1:1584:U:H2'    | 1:C1:1585:A:O4'    | 2.21                     | 0.40              |
| 1:C1:1802:C:H2'    | 1:C1:1803:A:C8     | 2.56                     | 0.40              |
| 1:C1:2682:U:H2'    | 1:C1:2683:OMU:H6   | 2.03                     | 0.40              |
| 1:C1:2694:U:H2'    | 1:C1:2695:A:C8     | 2.56                     | 0.40              |
| 1:C1:3247:G:O2'    | 1:C1:3250:G:N1     | 2.47                     | 0.40              |
| 5:CH:207:HIS:HB3   | 5:CH:214:ARG:HD2   | 2.03                     | 0.40              |
| 9:CO:37:LEU:HD12   | 9:CO:37:LEU:HA     | 1.95                     | 0.40              |
| 11:Cb:81:LEU:HD23  | 11:Cb:81:LEU:HA    | 1.92                     | 0.40              |
| 15:Ch:333:HIS:NE2  | 15:Ch:412:PHE:O    | 2.49                     | 0.40              |
| 22:LF:213:LEU:HB3  | 22:LF:248:MET:HB3  | 2.03                     | 0.40              |
| 39:LY:54:GLU:HB2   | 39:LY:107:LYS:HB3  | 2.03                     | 0.40              |
| 1:C1:268:U:H2'     | 1:C1:269:A:C8      | 2.55                     | 0.40              |
| 1:C1:600:U:H2'     | 1:C1:601:G:H8      | 1.86                     | 0.40              |
| 1:C1:619:A:H2'     | 1:C1:620:G:C8      | 2.56                     | 0.40              |
| 1:C1:1214:A:H5''   | 1:C1:1215:C:H5'    | 2.03                     | 0.40              |
| 1:C1:2140:G:C6     | 17:LA:125:ALA:HB1  | 2.57                     | 0.40              |
| 1:C1:3087:A:C6     | 1:C1:3089:U:H1'    | 2.56                     | 0.40              |
| 1:C1:3094:G:OP1    | 18:LB:31:SER:OG    | 2.29                     | 0.40              |
| 9:CO:37:LEU:HG     | 18:LB:195:PHE:HZ   | 1.86                     | 0.40              |
| 16:Cz:77:GLN:HA    | 16:Cz:80:ILE:HG12  | 2.02                     | 0.40              |
| 22:LF:91:PHE:H     | 22:LF:145:PRO:HD3  | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:LJ:47:VAL:O     | 25:LJ:68:VAL:HA    | 2.20                     | 0.40              |
| 1:C1:106:C:H2'     | 1:C1:107:A:C8      | 2.56                     | 0.40              |
| 1:C1:224:U:H2'     | 1:C1:225:A:C8      | 2.56                     | 0.40              |
| 1:C1:410:A:H2'     | 1:C1:411:A:H8      | 1.86                     | 0.40              |
| 1:C1:2219:A:N6     | 1:C1:2221:U:OP1    | 2.54                     | 0.40              |
| 1:C1:2620:G:OP1    | 20:LD:35:ARG:NH1   | 2.53                     | 0.40              |
| 1:C1:2945:U:H2'    | 1:C1:2946:A:H8     | 1.86                     | 0.40              |
| 13:Cf:104:ARG:HB3  | 13:Cf:112:ASP:OD1  | 2.22                     | 0.40              |
| 22:LF:137:GLU:OE2  | 22:LF:142:TYR:OH   | 2.29                     | 0.40              |
| 33:LR:4:LEU:HD11   | 33:LR:29:VAL:HG13  | 2.03                     | 0.40              |
| 34:LS:1:MET:HG3    | 34:LS:118:PHE:HB2  | 2.02                     | 0.40              |
| 37:LV:12:LYS:NZ    | 37:LV:15:MET:SD    | 2.94                     | 0.40              |
| 1:C1:129:G:H5''    | 38:LX:58:LYS:HE3   | 2.03                     | 0.40              |
| 1:C1:3208:U:O2'    | 21:LE:91:GLY:O     | 2.31                     | 0.40              |
| 3:C4:59:C:H2'      | 3:C4:60:A:H8       | 1.85                     | 0.40              |
| 6:CK:37:GLU:O      | 6:CK:41:ASN:HB2    | 2.22                     | 0.40              |
| 17:LA:102:LEU:HD12 | 17:LA:166:ILE:HD11 | 2.03                     | 0.40              |
| 30:LO:61:LYS:HB3   | 30:LO:72:PRO:HG2   | 2.02                     | 0.40              |
| 33:LR:105:LEU:HD22 | 33:LR:135:LYS:HG3  | 2.02                     | 0.40              |
| 34:LS:90:MET:HE1   | 34:LS:114:HIS:CD2  | 2.56                     | 0.40              |
| 44:Le:122:ASN:OD1  | 44:Le:122:ASN:N    | 2.54                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 4   | CF    | 243/270 (90%) | 242 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 5   | CH    | 621/661 (94%) | 616 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 6   | CK    | 231/261 (88%) | 224 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 7   | CL    | 77/558 (14%)  | 76 (99%)   | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 8   | CN    | 244/246 (99%) | 239 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 9   | CO    | 56/120 (47%)  | 55 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 10  | CQ    | 181/225 (80%) | 181 (100%) | 0       | 0        | 100         | 100 |
| 11  | Cb    | 99/117 (85%)  | 98 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 12  | Cd    | 458/627 (73%) | 446 (97%)  | 12 (3%) | 0        | 100         | 100 |
| 13  | Cf    | 281/350 (80%) | 277 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 14  | Cg    | 186/202 (92%) | 185 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 15  | Ch    | 484/517 (94%) | 469 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 16  | Cz    | 99/123 (80%)  | 99 (100%)  | 0       | 0        | 100         | 100 |
| 17  | LA    | 189/254 (74%) | 185 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 18  | LB    | 387/392 (99%) | 381 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 19  | LC    | 361/365 (99%) | 354 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 20  | LD    | 282/304 (93%) | 280 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 21  | LE    | 187/200 (94%) | 182 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 22  | LF    | 246/249 (99%) | 240 (98%)  | 5 (2%)  | 1 (0%)   | 30          | 48  |
| 23  | LG    | 233/262 (89%) | 230 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 24  | LH    | 188/229 (82%) | 185 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 25  | LJ    | 167/173 (96%) | 165 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 26  | LK    | 156/165 (94%) | 154 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 27  | LL    | 201/213 (94%) | 199 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 28  | LM    | 139/142 (98%) | 137 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 29  | LN    | 200/203 (98%) | 195 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 30  | LO    | 201/204 (98%) | 197 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 31  | LP    | 167/187 (89%) | 164 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 32  | LQ    | 148/213 (70%) | 147 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 33  | LR    | 150/2898 (5%) | 148 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 34  | LS    | 172/174 (99%) | 167 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 35  | LT    | 127/160 (79%) | 124 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 36  | LU    | 103/127 (81%) | 99 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 37  | LV    | 133/139 (96%) | 132 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 38  | LX    | 120/156 (77%) | 117 (98%)  | 3 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 39  | LY    | 131/138 (95%)    | 125 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 40  | LZ    | 133/135 (98%)    | 130 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 41  | La    | 104/149 (70%)    | 104 (100%) | 0        | 0        | 100         | 100 |
| 42  | Lc    | 93/108 (86%)     | 93 (100%)  | 0        | 0        | 100         | 100 |
| 43  | Ld    | 108/120 (90%)    | 108 (100%) | 0        | 0        | 100         | 100 |
| 44  | Le    | 124/131 (95%)    | 121 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 45  | Lf    | 106/109 (97%)    | 105 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 46  | Lg    | 116/119 (98%)    | 113 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 47  | Lh    | 114/935 (12%)    | 112 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 48  | Li    | 99/110 (90%)     | 99 (100%)  | 0        | 0        | 100         | 100 |
| 49  | Lj    | 86/95 (90%)      | 85 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 50  | Lk    | 74/94 (79%)      | 73 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 51  | Ll    | 48/51 (94%)      | 46 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 52  | Lp    | 89/92 (97%)      | 86 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 53  | Lq    | 137/147 (93%)    | 132 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| All | All   | 9079/14219 (64%) | 8921 (98%) | 157 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | LF    | 197 | VAL  |

### 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 |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 4   | CF    | 212/236 (90%) | 212 (100%) | 0        | 100         | 100 |
| 5   | CH    | 547/575 (95%) | 547 (100%) | 0        | 100         | 100 |
| 6   | CK    | 206/225 (92%) | 206 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 7   | CL    | 61/458 (13%)   | 61 (100%)  | 0        | 100         | 100 |
| 8   | CN    | 205/206 (100%) | 205 (100%) | 0        | 100         | 100 |
| 9   | CO    | 48/99 (48%)    | 48 (100%)  | 0        | 100         | 100 |
| 10  | CQ    | 144/192 (75%)  | 144 (100%) | 0        | 100         | 100 |
| 11  | Cb    | 85/101 (84%)   | 85 (100%)  | 0        | 100         | 100 |
| 12  | Cd    | 403/541 (74%)  | 403 (100%) | 0        | 100         | 100 |
| 13  | Cf    | 250/310 (81%)  | 250 (100%) | 0        | 100         | 100 |
| 14  | Cg    | 158/176 (90%)  | 158 (100%) | 0        | 100         | 100 |
| 15  | Ch    | 408/436 (94%)  | 408 (100%) | 0        | 100         | 100 |
| 16  | Cz    | 89/107 (83%)   | 89 (100%)  | 0        | 100         | 100 |
| 17  | LA    | 150/198 (76%)  | 150 (100%) | 0        | 100         | 100 |
| 18  | LB    | 329/331 (99%)  | 329 (100%) | 0        | 100         | 100 |
| 19  | LC    | 282/285 (99%)  | 282 (100%) | 0        | 100         | 100 |
| 20  | LD    | 221/253 (87%)  | 221 (100%) | 0        | 100         | 100 |
| 21  | LE    | 157/166 (95%)  | 157 (100%) | 0        | 100         | 100 |
| 22  | LF    | 213/215 (99%)  | 213 (100%) | 0        | 100         | 100 |
| 23  | LG    | 199/222 (90%)  | 199 (100%) | 0        | 100         | 100 |
| 24  | LH    | 167/200 (84%)  | 167 (100%) | 0        | 100         | 100 |
| 25  | LJ    | 140/150 (93%)  | 140 (100%) | 0        | 100         | 100 |
| 26  | LK    | 127/136 (93%)  | 127 (100%) | 0        | 100         | 100 |
| 27  | LL    | 158/176 (90%)  | 158 (100%) | 0        | 100         | 100 |
| 28  | LM    | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 29  | LN    | 179/180 (99%)  | 179 (100%) | 0        | 100         | 100 |
| 30  | LO    | 162/163 (99%)  | 162 (100%) | 0        | 100         | 100 |
| 31  | LP    | 133/152 (88%)  | 133 (100%) | 0        | 100         | 100 |
| 32  | LQ    | 128/178 (72%)  | 128 (100%) | 0        | 100         | 100 |
| 33  | LR    | 125/2396 (5%)  | 125 (100%) | 0        | 100         | 100 |
| 34  | LS    | 152/154 (99%)  | 152 (100%) | 0        | 100         | 100 |
| 35  | LT    | 110/135 (82%)  | 110 (100%) | 0        | 100         | 100 |
| 36  | LU    | 92/108 (85%)   | 92 (100%)  | 0        | 100         | 100 |
| 37  | LV    | 98/102 (96%)   | 98 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 38  | LX    | 104/129 (81%)    | 104 (100%)  | 0        | 100         | 100 |
| 39  | LY    | 116/119 (98%)    | 116 (100%)  | 0        | 100         | 100 |
| 40  | LZ    | 121/121 (100%)   | 121 (100%)  | 0        | 100         | 100 |
| 41  | La    | 93/122 (76%)     | 93 (100%)   | 0        | 100         | 100 |
| 42  | Lc    | 76/88 (86%)      | 76 (100%)   | 0        | 100         | 100 |
| 43  | Ld    | 90/105 (86%)     | 90 (100%)   | 0        | 100         | 100 |
| 44  | Le    | 109/114 (96%)    | 109 (100%)  | 0        | 100         | 100 |
| 45  | Lf    | 89/90 (99%)      | 89 (100%)   | 0        | 100         | 100 |
| 46  | Lg    | 95/102 (93%)     | 95 (100%)   | 0        | 100         | 100 |
| 47  | Lh    | 106/781 (14%)    | 106 (100%)  | 0        | 100         | 100 |
| 48  | Li    | 85/93 (91%)      | 85 (100%)   | 0        | 100         | 100 |
| 49  | Lj    | 72/78 (92%)      | 72 (100%)   | 0        | 100         | 100 |
| 50  | Lk    | 73/88 (83%)      | 73 (100%)   | 0        | 100         | 100 |
| 51  | Ll    | 45/46 (98%)      | 45 (100%)   | 0        | 100         | 100 |
| 52  | Lp    | 73/74 (99%)      | 73 (100%)   | 0        | 100         | 100 |
| 53  | Lq    | 104/112 (93%)    | 104 (100%)  | 0        | 100         | 100 |
| All | All   | 7705/11941 (64%) | 7705 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CF    | 121 | GLN  |
| 5   | CH    | 14  | GLN  |
| 5   | CH    | 82  | ASN  |
| 5   | CH    | 389 | ASN  |
| 5   | CH    | 499 | HIS  |
| 5   | CH    | 551 | GLN  |
| 5   | CH    | 619 | GLN  |
| 6   | CK    | 95  | ASN  |
| 10  | CQ    | 5   | ASN  |
| 10  | CQ    | 39  | ASN  |
| 11  | Cb    | 33  | GLN  |
| 12  | Cd    | 22  | HIS  |
| 12  | Cd    | 176 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | Cd    | 387 | HIS  |
| 13  | Cf    | 54  | GLN  |
| 14  | Cg    | 192 | GLN  |
| 15  | Ch    | 114 | ASN  |
| 15  | Ch    | 133 | HIS  |
| 15  | Ch    | 408 | ASN  |
| 15  | Ch    | 517 | ASN  |
| 17  | LA    | 205 | ASN  |
| 19  | LC    | 60  | GLN  |
| 19  | LC    | 111 | HIS  |
| 19  | LC    | 315 | GLN  |
| 20  | LD    | 89  | ASN  |
| 22  | LF    | 242 | ASN  |
| 23  | LG    | 44  | GLN  |
| 23  | LG    | 64  | GLN  |
| 24  | LH    | 95  | HIS  |
| 26  | LK    | 14  | HIS  |
| 27  | LL    | 114 | GLN  |
| 29  | LN    | 95  | GLN  |
| 31  | LP    | 72  | GLN  |
| 31  | LP    | 75  | GLN  |
| 31  | LP    | 97  | ASN  |
| 32  | LQ    | 73  | ASN  |
| 35  | LT    | 112 | ASN  |
| 35  | LT    | 127 | GLN  |
| 39  | LY    | 43  | ASN  |
| 39  | LY    | 92  | GLN  |
| 41  | La    | 62  | HIS  |
| 43  | Ld    | 62  | GLN  |
| 43  | Ld    | 88  | ASN  |
| 44  | Le    | 50  | ASN  |
| 44  | Le    | 122 | ASN  |
| 45  | Lf    | 26  | HIS  |
| 46  | Lg    | 84  | ASN  |
| 47  | Lh    | 33  | GLN  |
| 47  | Lh    | 47  | ASN  |
| 49  | Lj    | 13  | ASN  |
| 49  | Lj    | 30  | GLN  |
| 49  | Lj    | 76  | ASN  |
| 50  | Lk    | 32  | GLN  |
| 51  | Ll    | 11  | GLN  |
| 51  | Ll    | 33  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | Lq    | 43  | HIS  |
| 53  | Lq    | 97  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | C1    | 3051/3342 (91%) | 580 (19%)         | 24 (0%)         |
| 2   | C2    | 150/156 (96%)   | 22 (14%)          | 1 (0%)          |
| 3   | C4    | 118/119 (99%)   | 19 (16%)          | 0               |
| All | All   | 3319/3617 (91%) | 621 (18%)         | 25 (0%)         |

All (621) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 6   | G    |
| 1   | C1    | 15  | U    |
| 1   | C1    | 27  | A    |
| 1   | C1    | 31  | G    |
| 1   | C1    | 44  | A    |
| 1   | C1    | 50  | A    |
| 1   | C1    | 60  | G    |
| 1   | C1    | 61  | A    |
| 1   | C1    | 66  | A    |
| 1   | C1    | 67  | A    |
| 1   | C1    | 68  | A    |
| 1   | C1    | 95  | G    |
| 1   | C1    | 96  | A    |
| 1   | C1    | 110 | A    |
| 1   | C1    | 111 | G    |
| 1   | C1    | 112 | C    |
| 1   | C1    | 114 | C    |
| 1   | C1    | 117 | A    |
| 1   | C1    | 123 | A    |
| 1   | C1    | 132 | U    |
| 1   | C1    | 134 | G    |
| 1   | C1    | 135 | G    |
| 1   | C1    | 146 | A    |
| 1   | C1    | 152 | G    |
| 1   | C1    | 153 | A    |
| 1   | C1    | 156 | G    |
| 1   | C1    | 157 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 181 | G    |
| 1   | C1    | 184 | U    |
| 1   | C1    | 194 | C    |
| 1   | C1    | 200 | G    |
| 1   | C1    | 204 | C    |
| 1   | C1    | 206 | G    |
| 1   | C1    | 213 | A    |
| 1   | C1    | 214 | G    |
| 1   | C1    | 226 | G    |
| 1   | C1    | 241 | U    |
| 1   | C1    | 244 | G    |
| 1   | C1    | 247 | A    |
| 1   | C1    | 259 | C    |
| 1   | C1    | 262 | G    |
| 1   | C1    | 276 | G    |
| 1   | C1    | 277 | A    |
| 1   | C1    | 288 | A    |
| 1   | C1    | 291 | U    |
| 1   | C1    | 298 | U    |
| 1   | C1    | 308 | C    |
| 1   | C1    | 316 | A    |
| 1   | C1    | 322 | C    |
| 1   | C1    | 323 | G    |
| 1   | C1    | 331 | A    |
| 1   | C1    | 332 | C    |
| 1   | C1    | 343 | C    |
| 1   | C1    | 369 | G    |
| 1   | C1    | 388 | A    |
| 1   | C1    | 389 | A2M  |
| 1   | C1    | 391 | U    |
| 1   | C1    | 394 | C    |
| 1   | C1    | 395 | A    |
| 1   | C1    | 396 | C    |
| 1   | C1    | 414 | G    |
| 1   | C1    | 415 | A    |
| 1   | C1    | 422 | U    |
| 1   | C1    | 434 | U    |
| 1   | C1    | 435 | G    |
| 1   | C1    | 443 | C    |
| 1   | C1    | 445 | G    |
| 1   | C1    | 446 | A    |
| 1   | C1    | 447 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 448 | C    |
| 1   | C1    | 449 | A    |
| 1   | C1    | 458 | U    |
| 1   | C1    | 459 | C    |
| 1   | C1    | 460 | U    |
| 1   | C1    | 467 | U    |
| 1   | C1    | 468 | G    |
| 1   | C1    | 469 | C    |
| 1   | C1    | 470 | A    |
| 1   | C1    | 471 | C    |
| 1   | C1    | 472 | U    |
| 1   | C1    | 479 | G    |
| 1   | C1    | 489 | A    |
| 1   | C1    | 494 | C    |
| 1   | C1    | 512 | A    |
| 1   | C1    | 514 | A    |
| 1   | C1    | 521 | G    |
| 1   | C1    | 527 | G    |
| 1   | C1    | 528 | U    |
| 1   | C1    | 535 | U    |
| 1   | C1    | 536 | C    |
| 1   | C1    | 537 | C    |
| 1   | C1    | 545 | U    |
| 1   | C1    | 547 | A    |
| 1   | C1    | 549 | A    |
| 1   | C1    | 561 | A    |
| 1   | C1    | 570 | G    |
| 1   | C1    | 580 | A    |
| 1   | C1    | 582 | G    |
| 1   | C1    | 588 | G    |
| 1   | C1    | 592 | U    |
| 1   | C1    | 593 | G    |
| 1   | C1    | 595 | A    |
| 1   | C1    | 597 | G    |
| 1   | C1    | 599 | A    |
| 1   | C1    | 608 | U    |
| 1   | C1    | 609 | A    |
| 1   | C1    | 610 | A    |
| 1   | C1    | 624 | C    |
| 1   | C1    | 632 | G    |
| 1   | C1    | 634 | A    |
| 1   | C1    | 665 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 669 | U    |
| 1   | C1    | 678 | A    |
| 1   | C1    | 693 | A    |
| 1   | C1    | 700 | G    |
| 1   | C1    | 703 | A    |
| 1   | C1    | 704 | A    |
| 1   | C1    | 707 | U    |
| 1   | C1    | 719 | U    |
| 1   | C1    | 720 | C    |
| 1   | C1    | 721 | G    |
| 1   | C1    | 724 | G    |
| 1   | C1    | 743 | A    |
| 1   | C1    | 747 | A    |
| 1   | C1    | 748 | U    |
| 1   | C1    | 756 | G    |
| 1   | C1    | 757 | A    |
| 1   | C1    | 759 | U    |
| 1   | C1    | 761 | G    |
| 1   | C1    | 762 | A    |
| 1   | C1    | 763 | G    |
| 1   | C1    | 767 | G    |
| 1   | C1    | 782 | G    |
| 1   | C1    | 790 | A    |
| 1   | C1    | 799 | A    |
| 1   | C1    | 808 | G    |
| 1   | C1    | 812 | A    |
| 1   | C1    | 830 | A    |
| 1   | C1    | 839 | G    |
| 1   | C1    | 843 | C    |
| 1   | C1    | 856 | U    |
| 1   | C1    | 857 | G    |
| 1   | C1    | 877 | A    |
| 1   | C1    | 878 | A    |
| 1   | C1    | 889 | G    |
| 1   | C1    | 890 | G    |
| 1   | C1    | 896 | A    |
| 1   | C1    | 898 | G    |
| 1   | C1    | 899 | A    |
| 1   | C1    | 903 | A    |
| 1   | C1    | 906 | G    |
| 1   | C1    | 919 | G    |
| 1   | C1    | 926 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 931  | C    |
| 1   | C1    | 933  | A    |
| 1   | C1    | 934  | A    |
| 1   | C1    | 935  | G    |
| 1   | C1    | 937  | U    |
| 1   | C1    | 940  | C    |
| 1   | C1    | 941  | C    |
| 1   | C1    | 943  | C    |
| 1   | C1    | 944  | A    |
| 1   | C1    | 945  | G    |
| 1   | C1    | 947  | A    |
| 1   | C1    | 955  | G    |
| 1   | C1    | 956  | U    |
| 1   | C1    | 961  | C    |
| 1   | C1    | 963  | U    |
| 1   | C1    | 964  | C    |
| 1   | C1    | 976  | G    |
| 1   | C1    | 977  | U    |
| 1   | C1    | 983  | G    |
| 1   | C1    | 984  | A    |
| 1   | C1    | 1032 | C    |
| 1   | C1    | 1034 | U    |
| 1   | C1    | 1040 | A    |
| 1   | C1    | 1047 | A    |
| 1   | C1    | 1048 | A    |
| 1   | C1    | 1049 | G    |
| 1   | C1    | 1051 | C    |
| 1   | C1    | 1055 | G    |
| 1   | C1    | 1058 | A    |
| 1   | C1    | 1064 | C    |
| 1   | C1    | 1065 | U    |
| 1   | C1    | 1066 | G    |
| 1   | C1    | 1070 | G    |
| 1   | C1    | 1075 | C    |
| 1   | C1    | 1076 | A    |
| 1   | C1    | 1077 | U    |
| 1   | C1    | 1078 | U    |
| 1   | C1    | 1079 | C    |
| 1   | C1    | 1080 | G    |
| 1   | C1    | 1081 | A    |
| 1   | C1    | 1084 | G    |
| 1   | C1    | 1086 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 1099 | G    |
| 1   | C1    | 1109 | G    |
| 1   | C1    | 1110 | G    |
| 1   | C1    | 1115 | C    |
| 1   | C1    | 1118 | A    |
| 1   | C1    | 1119 | A    |
| 1   | C1    | 1127 | U    |
| 1   | C1    | 1132 | G    |
| 1   | C1    | 1133 | A    |
| 1   | C1    | 1136 | A    |
| 1   | C1    | 1151 | U    |
| 1   | C1    | 1163 | G    |
| 1   | C1    | 1164 | U    |
| 1   | C1    | 1165 | G    |
| 1   | C1    | 1175 | C    |
| 1   | C1    | 1176 | A    |
| 1   | C1    | 1179 | C    |
| 1   | C1    | 1182 | C    |
| 1   | C1    | 1185 | A    |
| 1   | C1    | 1188 | A    |
| 1   | C1    | 1194 | U    |
| 1   | C1    | 1205 | G    |
| 1   | C1    | 1228 | A    |
| 1   | C1    | 1229 | G    |
| 1   | C1    | 1241 | U    |
| 1   | C1    | 1242 | A    |
| 1   | C1    | 1246 | A    |
| 1   | C1    | 1248 | U    |
| 1   | C1    | 1268 | G    |
| 1   | C1    | 1278 | G    |
| 1   | C1    | 1287 | A    |
| 1   | C1    | 1288 | U    |
| 1   | C1    | 1290 | G    |
| 1   | C1    | 1292 | U    |
| 1   | C1    | 1296 | G    |
| 1   | C1    | 1313 | A    |
| 1   | C1    | 1315 | A    |
| 1   | C1    | 1331 | A    |
| 1   | C1    | 1332 | G    |
| 1   | C1    | 1333 | A    |
| 1   | C1    | 1334 | A    |
| 1   | C1    | 1335 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 1336 | C    |
| 1   | C1    | 1337 | G    |
| 1   | C1    | 1369 | A    |
| 1   | C1    | 1370 | G    |
| 1   | C1    | 1375 | G    |
| 1   | C1    | 1382 | A    |
| 1   | C1    | 1383 | G    |
| 1   | C1    | 1400 | G    |
| 1   | C1    | 1401 | A    |
| 1   | C1    | 1417 | G    |
| 1   | C1    | 1420 | OMC  |
| 1   | C1    | 1429 | A    |
| 1   | C1    | 1433 | OMG  |
| 1   | C1    | 1438 | U    |
| 1   | C1    | 1458 | G    |
| 1   | C1    | 1464 | A    |
| 1   | C1    | 1477 | U    |
| 1   | C1    | 1479 | C    |
| 1   | C1    | 1485 | G    |
| 1   | C1    | 1491 | OMC  |
| 1   | C1    | 1505 | U    |
| 1   | C1    | 1506 | U    |
| 1   | C1    | 1507 | A    |
| 1   | C1    | 1536 | U    |
| 1   | C1    | 1538 | U    |
| 1   | C1    | 1539 | C    |
| 1   | C1    | 1540 | A    |
| 1   | C1    | 1542 | A    |
| 1   | C1    | 1543 | G    |
| 1   | C1    | 1549 | C    |
| 1   | C1    | 1550 | U    |
| 1   | C1    | 1551 | C    |
| 1   | C1    | 1553 | U    |
| 1   | C1    | 1556 | C    |
| 1   | C1    | 1559 | G    |
| 1   | C1    | 1561 | G    |
| 1   | C1    | 1567 | A    |
| 1   | C1    | 1568 | A    |
| 1   | C1    | 1569 | A    |
| 1   | C1    | 1573 | A    |
| 1   | C1    | 1585 | A    |
| 1   | C1    | 1586 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 1601 | G    |
| 1   | C1    | 1609 | U    |
| 1   | C1    | 1618 | A    |
| 1   | C1    | 1619 | C    |
| 1   | C1    | 1622 | A    |
| 1   | C1    | 1623 | A    |
| 1   | C1    | 1624 | C    |
| 1   | C1    | 1625 | U    |
| 1   | C1    | 1637 | C    |
| 1   | C1    | 1684 | A    |
| 1   | C1    | 1685 | U    |
| 1   | C1    | 1693 | G    |
| 1   | C1    | 1696 | A    |
| 1   | C1    | 1697 | C    |
| 1   | C1    | 1704 | U    |
| 1   | C1    | 1722 | U    |
| 1   | C1    | 1730 | A    |
| 1   | C1    | 1731 | G    |
| 1   | C1    | 1745 | U    |
| 1   | C1    | 1746 | G    |
| 1   | C1    | 1751 | G    |
| 1   | C1    | 1760 | G    |
| 1   | C1    | 1776 | G    |
| 1   | C1    | 1777 | A    |
| 1   | C1    | 1788 | G    |
| 1   | C1    | 1792 | G    |
| 1   | C1    | 1793 | A    |
| 1   | C1    | 1794 | A    |
| 1   | C1    | 1795 | U    |
| 1   | C1    | 1796 | A    |
| 1   | C1    | 1799 | U    |
| 1   | C1    | 1800 | C    |
| 1   | C1    | 1801 | U    |
| 1   | C1    | 1803 | A    |
| 1   | C1    | 1822 | A    |
| 1   | C1    | 1826 | C    |
| 1   | C1    | 1829 | C    |
| 1   | C1    | 1830 | A    |
| 1   | C1    | 1846 | C    |
| 1   | C1    | 1847 | A2M  |
| 1   | C1    | 1856 | U    |
| 1   | C1    | 1858 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 1860 | U    |
| 1   | C1    | 1873 | A    |
| 1   | C1    | 1886 | G    |
| 1   | C1    | 1887 | C    |
| 1   | C1    | 2056 | A    |
| 1   | C1    | 2076 | A    |
| 1   | C1    | 2084 | G    |
| 1   | C1    | 2085 | G    |
| 1   | C1    | 2089 | A    |
| 1   | C1    | 2094 | A    |
| 1   | C1    | 2103 | U    |
| 1   | C1    | 2121 | A    |
| 1   | C1    | 2126 | C    |
| 1   | C1    | 2132 | G    |
| 1   | C1    | 2139 | U    |
| 1   | C1    | 2156 | U    |
| 1   | C1    | 2157 | G    |
| 1   | C1    | 2158 | C    |
| 1   | C1    | 2161 | A    |
| 1   | C1    | 2167 | C    |
| 1   | C1    | 2168 | U    |
| 1   | C1    | 2169 | G    |
| 1   | C1    | 2170 | A    |
| 1   | C1    | 2171 | A    |
| 1   | C1    | 2172 | U    |
| 1   | C1    | 2173 | G    |
| 1   | C1    | 2186 | A    |
| 1   | C1    | 2192 | A    |
| 1   | C1    | 2203 | G    |
| 1   | C1    | 2205 | A    |
| 1   | C1    | 2206 | A    |
| 1   | C1    | 2210 | G    |
| 1   | C1    | 2212 | G    |
| 1   | C1    | 2216 | G    |
| 1   | C1    | 2217 | U    |
| 1   | C1    | 2218 | A    |
| 1   | C1    | 2219 | A    |
| 1   | C1    | 2220 | C    |
| 1   | C1    | 2221 | U    |
| 1   | C1    | 2222 | A    |
| 1   | C1    | 2223 | U    |
| 1   | C1    | 2224 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 2225 | A    |
| 1   | C1    | 2226 | C    |
| 1   | C1    | 2230 | C    |
| 1   | C1    | 2231 | U    |
| 1   | C1    | 2237 | U    |
| 1   | C1    | 2279 | G    |
| 1   | C1    | 2281 | U    |
| 1   | C1    | 2282 | U    |
| 1   | C1    | 2284 | A    |
| 1   | C1    | 2297 | U    |
| 1   | C1    | 2298 | G    |
| 1   | C1    | 2299 | U    |
| 1   | C1    | 2340 | G    |
| 1   | C1    | 2348 | A    |
| 1   | C1    | 2351 | U    |
| 1   | C1    | 2355 | C    |
| 1   | C1    | 2356 | G    |
| 1   | C1    | 2357 | G    |
| 1   | C1    | 2362 | A    |
| 1   | C1    | 2364 | A    |
| 1   | C1    | 2373 | U    |
| 1   | C1    | 2374 | U    |
| 1   | C1    | 2381 | G    |
| 1   | C1    | 2382 | A    |
| 1   | C1    | 2400 | G    |
| 1   | C1    | 2401 | A    |
| 1   | C1    | 2403 | A    |
| 1   | C1    | 2405 | G    |
| 1   | C1    | 2472 | U    |
| 1   | C1    | 2473 | U    |
| 1   | C1    | 2474 | A    |
| 1   | C1    | 2477 | U    |
| 1   | C1    | 2478 | A    |
| 1   | C1    | 2489 | C    |
| 1   | C1    | 2499 | C    |
| 1   | C1    | 2501 | U    |
| 1   | C1    | 2502 | G    |
| 1   | C1    | 2503 | C    |
| 1   | C1    | 2506 | C    |
| 1   | C1    | 2507 | C    |
| 1   | C1    | 2508 | A    |
| 1   | C1    | 2513 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 2516 | G    |
| 1   | C1    | 2521 | A    |
| 1   | C1    | 2524 | G    |
| 1   | C1    | 2530 | C    |
| 1   | C1    | 2531 | G    |
| 1   | C1    | 2533 | G    |
| 1   | C1    | 2539 | A    |
| 1   | C1    | 2544 | G    |
| 1   | C1    | 2545 | G    |
| 1   | C1    | 2552 | A    |
| 1   | C1    | 2565 | G    |
| 1   | C1    | 2566 | G    |
| 1   | C1    | 2569 | G    |
| 1   | C1    | 2573 | G    |
| 1   | C1    | 2575 | C    |
| 1   | C1    | 2576 | U    |
| 1   | C1    | 2577 | G    |
| 1   | C1    | 2578 | OMG  |
| 1   | C1    | 2582 | G    |
| 1   | C1    | 2584 | C    |
| 1   | C1    | 2585 | A    |
| 1   | C1    | 2589 | C    |
| 1   | C1    | 2613 | C    |
| 1   | C1    | 2615 | A    |
| 1   | C1    | 2633 | A    |
| 1   | C1    | 2635 | A    |
| 1   | C1    | 2636 | G    |
| 1   | C1    | 2647 | U    |
| 1   | C1    | 2650 | A    |
| 1   | C1    | 2651 | A    |
| 1   | C1    | 2656 | A    |
| 1   | C1    | 2657 | G    |
| 1   | C1    | 2663 | A    |
| 1   | C1    | 2664 | A    |
| 1   | C1    | 2668 | C    |
| 1   | C1    | 2671 | U    |
| 1   | C1    | 2672 | U    |
| 1   | C1    | 2673 | G    |
| 1   | C1    | 2674 | A    |
| 1   | C1    | 2675 | U    |
| 1   | C1    | 2680 | A    |
| 1   | C1    | 2682 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 2690 | OMU  |
| 1   | C1    | 2691 | G    |
| 1   | C1    | 2708 | G    |
| 1   | C1    | 2713 | G    |
| 1   | C1    | 2717 | A    |
| 1   | C1    | 2730 | U    |
| 1   | C1    | 2731 | C    |
| 1   | C1    | 2732 | C    |
| 1   | C1    | 2736 | G    |
| 1   | C1    | 2737 | A    |
| 1   | C1    | 2750 | G    |
| 1   | C1    | 2754 | U    |
| 1   | C1    | 2755 | G    |
| 1   | C1    | 2756 | C    |
| 1   | C1    | 2757 | C    |
| 1   | C1    | 2758 | A    |
| 1   | C1    | 2761 | A    |
| 1   | C1    | 2762 | A    |
| 1   | C1    | 2763 | A    |
| 1   | C1    | 2769 | C    |
| 1   | C1    | 2783 | G    |
| 1   | C1    | 2784 | C    |
| 1   | C1    | 2785 | U    |
| 1   | C1    | 2802 | U    |
| 1   | C1    | 2803 | C    |
| 1   | C1    | 2804 | A    |
| 1   | C1    | 2805 | U    |
| 1   | C1    | 2806 | A    |
| 1   | C1    | 2812 | G    |
| 1   | C1    | 2815 | G    |
| 1   | C1    | 2816 | C    |
| 1   | C1    | 2817 | U    |
| 1   | C1    | 2826 | C    |
| 1   | C1    | 2834 | U    |
| 1   | C1    | 2836 | G    |
| 1   | C1    | 2846 | A    |
| 1   | C1    | 2857 | G    |
| 1   | C1    | 2858 | C    |
| 1   | C1    | 2863 | U    |
| 1   | C1    | 2882 | U    |
| 1   | C1    | 2883 | U    |
| 1   | C1    | 2884 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 2885 | A    |
| 1   | C1    | 2894 | U    |
| 1   | C1    | 2895 | A    |
| 1   | C1    | 2903 | U    |
| 1   | C1    | 2905 | A    |
| 1   | C1    | 2929 | C    |
| 1   | C1    | 2930 | A    |
| 1   | C1    | 2931 | G    |
| 1   | C1    | 2938 | U    |
| 1   | C1    | 2939 | U    |
| 1   | C1    | 2940 | U    |
| 1   | C1    | 2942 | C    |
| 1   | C1    | 2955 | C    |
| 1   | C1    | 2956 | U    |
| 1   | C1    | 2970 | A    |
| 1   | C1    | 2980 | G    |
| 1   | C1    | 3007 | A    |
| 1   | C1    | 3014 | U    |
| 1   | C1    | 3017 | G    |
| 1   | C1    | 3036 | G    |
| 1   | C1    | 3044 | A    |
| 1   | C1    | 3049 | A    |
| 1   | C1    | 3050 | C    |
| 1   | C1    | 3051 | C    |
| 1   | C1    | 3067 | G    |
| 1   | C1    | 3076 | C    |
| 1   | C1    | 3080 | A    |
| 1   | C1    | 3087 | A    |
| 1   | C1    | 3088 | A    |
| 1   | C1    | 3089 | U    |
| 1   | C1    | 3100 | A    |
| 1   | C1    | 3101 | C    |
| 1   | C1    | 3102 | G    |
| 1   | C1    | 3112 | U    |
| 1   | C1    | 3113 | A    |
| 1   | C1    | 3119 | A    |
| 1   | C1    | 3126 | A    |
| 1   | C1    | 3127 | G    |
| 1   | C1    | 3131 | U    |
| 1   | C1    | 3133 | U    |
| 1   | C1    | 3135 | A    |
| 1   | C1    | 3141 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 3146 | C    |
| 1   | C1    | 3155 | A    |
| 1   | C1    | 3162 | C    |
| 1   | C1    | 3163 | A    |
| 1   | C1    | 3164 | G    |
| 1   | C1    | 3168 | A    |
| 1   | C1    | 3185 | G    |
| 1   | C1    | 3186 | A    |
| 1   | C1    | 3187 | A    |
| 1   | C1    | 3188 | G    |
| 1   | C1    | 3190 | G    |
| 1   | C1    | 3200 | A    |
| 1   | C1    | 3201 | A    |
| 1   | C1    | 3206 | C    |
| 1   | C1    | 3210 | U    |
| 1   | C1    | 3211 | U    |
| 1   | C1    | 3213 | C    |
| 1   | C1    | 3214 | A    |
| 1   | C1    | 3217 | U    |
| 1   | C1    | 3218 | U    |
| 1   | C1    | 3228 | C    |
| 1   | C1    | 3229 | G    |
| 1   | C1    | 3231 | G    |
| 1   | C1    | 3245 | C    |
| 1   | C1    | 3248 | A    |
| 1   | C1    | 3254 | U    |
| 1   | C1    | 3257 | A    |
| 1   | C1    | 3258 | U    |
| 1   | C1    | 3259 | G    |
| 1   | C1    | 3260 | U    |
| 1   | C1    | 3276 | A    |
| 1   | C1    | 3282 | U    |
| 1   | C1    | 3292 | U    |
| 1   | C1    | 3293 | U    |
| 1   | C1    | 3295 | U    |
| 1   | C1    | 3297 | G    |
| 1   | C1    | 3299 | U    |
| 1   | C1    | 3302 | G    |
| 1   | C1    | 3304 | U    |
| 1   | C1    | 3310 | G    |
| 1   | C1    | 3312 | G    |
| 1   | C1    | 3316 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 3319 | C    |
| 1   | C1    | 3323 | C    |
| 1   | C1    | 3324 | C    |
| 1   | C1    | 3325 | U    |
| 1   | C1    | 3331 | U    |
| 1   | C1    | 3332 | A    |
| 1   | C1    | 3338 | C    |
| 2   | C2    | 34   | U    |
| 2   | C2    | 35   | C    |
| 2   | C2    | 38   | U    |
| 2   | C2    | 49   | G    |
| 2   | C2    | 59   | A    |
| 2   | C2    | 62   | A    |
| 2   | C2    | 63   | G    |
| 2   | C2    | 86   | U    |
| 2   | C2    | 87   | G    |
| 2   | C2    | 90   | U    |
| 2   | C2    | 95   | G    |
| 2   | C2    | 104  | A    |
| 2   | C2    | 106  | C    |
| 2   | C2    | 113  | U    |
| 2   | C2    | 116  | G    |
| 2   | C2    | 123  | G    |
| 2   | C2    | 125  | U    |
| 2   | C2    | 126  | A    |
| 2   | C2    | 128  | U    |
| 2   | C2    | 129  | C    |
| 2   | C2    | 148  | G    |
| 2   | C2    | 151  | C    |
| 3   | C4    | 7    | G    |
| 3   | C4    | 22   | A    |
| 3   | C4    | 29   | G    |
| 3   | C4    | 54   | U    |
| 3   | C4    | 55   | A    |
| 3   | C4    | 64   | A    |
| 3   | C4    | 66   | G    |
| 3   | C4    | 75   | A    |
| 3   | C4    | 76   | G    |
| 3   | C4    | 82   | G    |
| 3   | C4    | 83   | G    |
| 3   | C4    | 84   | G    |
| 3   | C4    | 85   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C4    | 86  | C    |
| 3   | C4    | 89  | U    |
| 3   | C4    | 90  | G    |
| 3   | C4    | 97  | A    |
| 3   | C4    | 101 | A    |
| 3   | C4    | 111 | G    |

All (25) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 151  | G    |
| 1   | C1    | 243  | U    |
| 1   | C1    | 898  | G    |
| 1   | C1    | 1047 | A    |
| 1   | C1    | 1064 | C    |
| 1   | C1    | 1077 | U    |
| 1   | C1    | 1267 | C    |
| 1   | C1    | 1537 | U    |
| 1   | C1    | 1622 | A    |
| 1   | C1    | 2157 | G    |
| 1   | C1    | 2160 | C    |
| 1   | C1    | 2225 | A    |
| 1   | C1    | 2280 | A    |
| 1   | C1    | 2575 | C    |
| 1   | C1    | 2883 | U    |
| 1   | C1    | 3079 | U    |
| 1   | C1    | 3132 | A    |
| 1   | C1    | 3205 | G    |
| 1   | C1    | 3210 | U    |
| 1   | C1    | 3230 | G    |
| 1   | C1    | 3258 | U    |
| 1   | C1    | 3298 | U    |
| 1   | C1    | 3301 | C    |
| 1   | C1    | 3324 | C    |
| 2   | C2    | 127  | U    |

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

34 non-standard protein/DNA/RNA residues are 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 |
| 1   | OMU  | C1    | 1868 | 1    | 19,22,23     | 3.12 | 6 (31%)  | 25,31,34    | 1.84 | 5 (20%)  |
| 1   | OMC  | C1    | 2300 | 1    | 19,22,23     | 0.52 | 0        | 25,31,34    | 0.70 | 0        |
| 1   | OMU  | C1    | 2277 | 1    | 19,22,23     | 3.11 | 6 (31%)  | 25,31,34    | 1.71 | 5 (20%)  |
| 1   | OMG  | C1    | 2774 | 1    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.49 | 0        |
| 1   | OMG  | C1    | 2881 | 1    | 23,26,27     | 0.45 | 0        | 32,38,41    | 0.48 | 0        |
| 1   | OMU  | C1    | 2688 | 1    | 19,22,23     | 3.12 | 6 (31%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 1   | OMG  | C1    | 2876 | 1    | 23,26,27     | 0.47 | 0        | 32,38,41    | 0.48 | 0        |
| 1   | A2M  | C1    | 1432 | 1    | 22,25,26     | 4.01 | 12 (54%) | 30,36,39    | 3.38 | 12 (40%) |
| 1   | OMG  | C1    | 646  | 1    | 23,26,27     | 0.47 | 0        | 32,38,41    | 0.48 | 0        |
| 1   | A2M  | C1    | 1223 | 1    | 22,25,26     | 3.97 | 11 (50%) | 30,36,39    | 3.37 | 13 (43%) |
| 1   | A2M  | C1    | 1847 | 1    | 22,25,26     | 3.99 | 12 (54%) | 30,36,39    | 3.49 | 14 (46%) |
| 1   | OMC  | C1    | 2918 | 1    | 19,22,23     | 0.53 | 0        | 25,31,34    | 0.79 | 1 (4%)   |
| 1   | OMG  | C1    | 787  | 1    | 23,26,27     | 0.47 | 0        | 32,38,41    | 0.53 | 0        |
| 1   | OMG  | C1    | 2578 | 1    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.54 | 0        |
| 1   | OMC  | C1    | 1812 | 1    | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.62 | 0        |
| 1   | OMG  | C1    | 1433 | 1    | 23,26,27     | 0.48 | 0        | 32,38,41    | 0.48 | 0        |
| 1   | A2M  | C1    | 389  | 1    | 22,25,26     | 4.00 | 12 (54%) | 30,36,39    | 3.41 | 13 (43%) |
| 1   | OMU  | C1    | 2380 | 1    | 19,22,23     | 3.11 | 6 (31%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 1   | OMU  | C1    | 1917 | 1    | 19,22,23     | 3.14 | 6 (31%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 1   | OMG  | C1    | 2358 | 1    | 23,26,27     | 0.48 | 0        | 32,38,41    | 0.50 | 0        |
| 1   | A2M  | C1    | 858  | 1    | 22,25,26     | 4.01 | 11 (50%) | 30,36,39    | 3.41 | 13 (43%) |
| 1   | OMU  | C1    | 2384 | 1    | 19,22,23     | 3.13 | 6 (31%)  | 25,31,34    | 1.77 | 4 (16%)  |
| 1   | OMG  | C1    | 385  | 1    | 23,26,27     | 0.47 | 0        | 32,38,41    | 0.57 | 0        |
| 1   | OMU  | C1    | 2683 | 1    | 19,22,23     | 3.10 | 6 (31%)  | 25,31,34    | 1.74 | 4 (16%)  |
| 1   | A2M  | C1    | 2289 | 1    | 22,25,26     | 4.01 | 11 (50%) | 30,36,39    | 3.33 | 13 (43%) |
| 1   | OMC  | C1    | 1491 | 1    | 19,22,23     | 0.52 | 0        | 25,31,34    | 0.72 | 0        |
| 1   | OMC  | C1    | 778  | 1    | 19,22,23     | 0.53 | 0        | 25,31,34    | 0.95 | 1 (4%)   |
| 1   | OMU  | C1    | 2690 | 1    | 19,22,23     | 3.11 | 6 (31%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 1   | OMG  | C1    | 627  | 1    | 23,26,27     | 0.47 | 0        | 32,38,41    | 0.52 | 0        |
| 1   | A2M  | C1    | 848  | 1    | 22,25,26     | 4.00 | 12 (54%) | 30,36,39    | 3.44 | 14 (46%) |
| 1   | A2M  | C1    | 637  | 1    | 22,25,26     | 4.00 | 11 (50%) | 30,36,39    | 3.46 | 13 (43%) |
| 1   | OMC  | C1    | 1420 | 1    | 19,22,23     | 0.61 | 0        | 25,31,34    | 1.56 | 4 (16%)  |
| 1   | OMC  | C1    | 1836 | 1    | 19,22,23     | 0.54 | 0        | 25,31,34    | 0.89 | 1 (4%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMC  | C1    | 2838 | 1    | 19,22,23     | 0.64 | 0        | 25,31,34    | 1.55 | 4 (16%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | OMU  | C1    | 1868 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMC  | C1    | 2300 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMU  | C1    | 2277 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 2774 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMG  | C1    | 2881 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMU  | C1    | 2688 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 2876 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 1432 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMG  | C1    | 646  | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 1223 | 1    | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 1847 | 1    | -       | 3/9/27/28 | 0/3/3/3 |
| 1   | OMC  | C1    | 2918 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 787  | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMG  | C1    | 2578 | 1    | -       | 3/9/27/28 | 0/3/3/3 |
| 1   | OMC  | C1    | 1812 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 1433 | 1    | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 389  | 1    | -       | 4/9/27/28 | 0/3/3/3 |
| 1   | OMU  | C1    | 2380 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMU  | C1    | 1917 | 1    | -       | 2/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 2358 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 858  | 1    | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | OMU  | C1    | 2384 | 1    | -       | 1/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 385  | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMU  | C1    | 2683 | 1    | -       | 1/9/27/28 | 0/2/2/2 |
| 1   | A2M  | C1    | 2289 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMC  | C1    | 1491 | 1    | -       | 1/9/27/28 | 0/2/2/2 |
| 1   | OMC  | C1    | 778  | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMU  | C1    | 2690 | 1    | -       | 2/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 627  | 1    | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 848  | 1    | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 637  | 1    | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | OMC  | C1    | 1420 | 1    | -       | 2/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | OMC  | C1    | 1836 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMC  | C1    | 2838 | 1    | -       | 2/9/27/28 | 0/2/2/2 |

All (140) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | C1    | 858  | A2M  | C3'-C2' | -13.07 | 1.24        | 1.53     |
| 1   | C1    | 2289 | A2M  | C3'-C2' | -13.04 | 1.24        | 1.53     |
| 1   | C1    | 848  | A2M  | C3'-C2' | -13.00 | 1.24        | 1.53     |
| 1   | C1    | 1432 | A2M  | C3'-C2' | -12.99 | 1.24        | 1.53     |
| 1   | C1    | 637  | A2M  | C3'-C2' | -12.96 | 1.24        | 1.53     |
| 1   | C1    | 389  | A2M  | C3'-C2' | -12.93 | 1.24        | 1.53     |
| 1   | C1    | 1847 | A2M  | C3'-C2' | -12.91 | 1.24        | 1.53     |
| 1   | C1    | 1223 | A2M  | C3'-C2' | -12.87 | 1.24        | 1.53     |
| 1   | C1    | 1917 | OMU  | C2-N1   | 7.69   | 1.50        | 1.38     |
| 1   | C1    | 2384 | OMU  | C2-N1   | 7.54   | 1.50        | 1.38     |
| 1   | C1    | 1868 | OMU  | C2-N1   | 7.45   | 1.50        | 1.38     |
| 1   | C1    | 2690 | OMU  | C2-N1   | 7.42   | 1.50        | 1.38     |
| 1   | C1    | 2277 | OMU  | C2-N1   | 7.41   | 1.50        | 1.38     |
| 1   | C1    | 2380 | OMU  | C2-N1   | 7.39   | 1.50        | 1.38     |
| 1   | C1    | 2688 | OMU  | C2-N1   | 7.39   | 1.50        | 1.38     |
| 1   | C1    | 2683 | OMU  | C2-N1   | 7.38   | 1.50        | 1.38     |
| 1   | C1    | 2384 | OMU  | C2-N3   | 7.35   | 1.50        | 1.38     |
| 1   | C1    | 2683 | OMU  | C2-N3   | 7.32   | 1.50        | 1.38     |
| 1   | C1    | 2688 | OMU  | C2-N3   | 7.31   | 1.50        | 1.38     |
| 1   | C1    | 1868 | OMU  | C2-N3   | 7.31   | 1.50        | 1.38     |
| 1   | C1    | 2380 | OMU  | C2-N3   | 7.30   | 1.50        | 1.38     |
| 1   | C1    | 2277 | OMU  | C2-N3   | 7.29   | 1.50        | 1.38     |
| 1   | C1    | 1917 | OMU  | C2-N3   | 7.28   | 1.50        | 1.38     |
| 1   | C1    | 2690 | OMU  | C2-N3   | 7.27   | 1.50        | 1.38     |
| 1   | C1    | 637  | A2M  | O4'-C4' | -6.67  | 1.30        | 1.45     |
| 1   | C1    | 1223 | A2M  | O4'-C4' | -6.60  | 1.30        | 1.45     |
| 1   | C1    | 389  | A2M  | O4'-C4' | -6.57  | 1.30        | 1.45     |
| 1   | C1    | 1432 | A2M  | O4'-C4' | -6.57  | 1.30        | 1.45     |
| 1   | C1    | 858  | A2M  | O4'-C4' | -6.52  | 1.30        | 1.45     |
| 1   | C1    | 1847 | A2M  | O4'-C4' | -6.45  | 1.30        | 1.45     |
| 1   | C1    | 2289 | A2M  | O4'-C4' | -6.44  | 1.30        | 1.45     |
| 1   | C1    | 848  | A2M  | O4'-C4' | -6.40  | 1.30        | 1.45     |
| 1   | C1    | 2688 | OMU  | C6-C5   | 6.23   | 1.49        | 1.35     |
| 1   | C1    | 2277 | OMU  | C6-C5   | 6.22   | 1.49        | 1.35     |
| 1   | C1    | 1917 | OMU  | C6-C5   | 6.21   | 1.49        | 1.35     |
| 1   | C1    | 2384 | OMU  | C6-C5   | 6.21   | 1.49        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C1    | 2690 | OMU  | C6-C5   | 6.20  | 1.49        | 1.35     |
| 1   | C1    | 2380 | OMU  | C6-C5   | 6.20  | 1.49        | 1.35     |
| 1   | C1    | 1868 | OMU  | C6-C5   | 6.18  | 1.49        | 1.35     |
| 1   | C1    | 2683 | OMU  | C6-C5   | 6.15  | 1.49        | 1.35     |
| 1   | C1    | 2289 | A2M  | C3'-C4' | 5.38  | 1.66        | 1.53     |
| 1   | C1    | 848  | A2M  | C3'-C4' | 5.31  | 1.66        | 1.53     |
| 1   | C1    | 1223 | A2M  | C3'-C4' | 5.30  | 1.66        | 1.53     |
| 1   | C1    | 858  | A2M  | C3'-C4' | 5.29  | 1.66        | 1.53     |
| 1   | C1    | 1432 | A2M  | C3'-C4' | 5.28  | 1.66        | 1.53     |
| 1   | C1    | 1847 | A2M  | C3'-C4' | 5.18  | 1.66        | 1.53     |
| 1   | C1    | 389  | A2M  | C3'-C4' | 5.16  | 1.66        | 1.53     |
| 1   | C1    | 637  | A2M  | C3'-C4' | 5.07  | 1.65        | 1.53     |
| 1   | C1    | 848  | A2M  | O4'-C1' | 4.52  | 1.52        | 1.42     |
| 1   | C1    | 1847 | A2M  | O4'-C1' | 4.48  | 1.52        | 1.42     |
| 1   | C1    | 1847 | A2M  | C1'-N9  | -4.47 | 1.34        | 1.46     |
| 1   | C1    | 1432 | A2M  | O4'-C1' | 4.47  | 1.52        | 1.42     |
| 1   | C1    | 2380 | OMU  | C4-N3   | 4.47  | 1.46        | 1.38     |
| 1   | C1    | 2289 | A2M  | O4'-C1' | 4.46  | 1.52        | 1.42     |
| 1   | C1    | 389  | A2M  | O4'-C1' | 4.45  | 1.52        | 1.42     |
| 1   | C1    | 1223 | A2M  | C6-N6   | 4.45  | 1.45        | 1.34     |
| 1   | C1    | 848  | A2M  | C1'-N9  | -4.44 | 1.34        | 1.46     |
| 1   | C1    | 2289 | A2M  | C6-N6   | 4.43  | 1.45        | 1.34     |
| 1   | C1    | 2683 | OMU  | C4-N3   | 4.43  | 1.46        | 1.38     |
| 1   | C1    | 637  | A2M  | C1'-N9  | -4.43 | 1.34        | 1.46     |
| 1   | C1    | 858  | A2M  | O4'-C1' | 4.42  | 1.52        | 1.42     |
| 1   | C1    | 637  | A2M  | O4'-C1' | 4.42  | 1.52        | 1.42     |
| 1   | C1    | 2384 | OMU  | C4-N3   | 4.41  | 1.46        | 1.38     |
| 1   | C1    | 2277 | OMU  | C4-N3   | 4.41  | 1.46        | 1.38     |
| 1   | C1    | 2289 | A2M  | C1'-N9  | -4.40 | 1.34        | 1.46     |
| 1   | C1    | 637  | A2M  | C6-N6   | 4.40  | 1.45        | 1.34     |
| 1   | C1    | 848  | A2M  | C6-N6   | 4.40  | 1.45        | 1.34     |
| 1   | C1    | 1847 | A2M  | C6-N6   | 4.40  | 1.45        | 1.34     |
| 1   | C1    | 389  | A2M  | C6-N6   | 4.39  | 1.45        | 1.34     |
| 1   | C1    | 858  | A2M  | C6-N6   | 4.39  | 1.45        | 1.34     |
| 1   | C1    | 1432 | A2M  | C1'-N9  | -4.38 | 1.34        | 1.46     |
| 1   | C1    | 2690 | OMU  | C4-N3   | 4.36  | 1.46        | 1.38     |
| 1   | C1    | 1432 | A2M  | C6-N6   | 4.36  | 1.45        | 1.34     |
| 1   | C1    | 1868 | OMU  | C4-N3   | 4.36  | 1.46        | 1.38     |
| 1   | C1    | 1917 | OMU  | C4-N3   | 4.35  | 1.46        | 1.38     |
| 1   | C1    | 858  | A2M  | C1'-N9  | -4.35 | 1.34        | 1.46     |
| 1   | C1    | 2688 | OMU  | C4-N3   | 4.34  | 1.46        | 1.38     |
| 1   | C1    | 389  | A2M  | C1'-N9  | -4.30 | 1.34        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C1    | 1223 | A2M  | C1'-N9  | -4.29 | 1.34        | 1.46     |
| 1   | C1    | 1223 | A2M  | O4'-C1' | 4.23  | 1.51        | 1.42     |
| 1   | C1    | 389  | A2M  | O2'-C2' | 3.73  | 1.51        | 1.42     |
| 1   | C1    | 858  | A2M  | O2'-C2' | 3.65  | 1.51        | 1.42     |
| 1   | C1    | 637  | A2M  | O2'-C2' | 3.61  | 1.51        | 1.42     |
| 1   | C1    | 1847 | A2M  | O2'-C2' | 3.60  | 1.51        | 1.42     |
| 1   | C1    | 1223 | A2M  | O2'-C2' | 3.59  | 1.51        | 1.42     |
| 1   | C1    | 2289 | A2M  | O2'-C2' | 3.58  | 1.51        | 1.42     |
| 1   | C1    | 848  | A2M  | O2'-C2' | 3.56  | 1.51        | 1.42     |
| 1   | C1    | 1432 | A2M  | O2'-C2' | 3.55  | 1.51        | 1.42     |
| 1   | C1    | 1847 | A2M  | C2'-C1' | 3.11  | 1.60        | 1.53     |
| 1   | C1    | 848  | A2M  | C2'-C1' | 3.10  | 1.60        | 1.53     |
| 1   | C1    | 389  | A2M  | C2'-C1' | 3.06  | 1.60        | 1.53     |
| 1   | C1    | 389  | A2M  | C5-C4   | -3.02 | 1.33        | 1.39     |
| 1   | C1    | 2289 | A2M  | C5-C4   | -3.02 | 1.33        | 1.39     |
| 1   | C1    | 637  | A2M  | C2'-C1' | 3.01  | 1.60        | 1.53     |
| 1   | C1    | 1432 | A2M  | C5-C4   | -3.00 | 1.33        | 1.39     |
| 1   | C1    | 848  | A2M  | C5-C4   | -2.98 | 1.33        | 1.39     |
| 1   | C1    | 1223 | A2M  | C2'-C1' | 2.97  | 1.60        | 1.53     |
| 1   | C1    | 1223 | A2M  | C5-C4   | -2.97 | 1.33        | 1.39     |
| 1   | C1    | 858  | A2M  | C5-C4   | -2.95 | 1.33        | 1.39     |
| 1   | C1    | 1432 | A2M  | C2'-C1' | 2.94  | 1.60        | 1.53     |
| 1   | C1    | 1847 | A2M  | C5-C4   | -2.93 | 1.33        | 1.39     |
| 1   | C1    | 637  | A2M  | C5-C4   | -2.93 | 1.33        | 1.39     |
| 1   | C1    | 2289 | A2M  | C2'-C1' | 2.84  | 1.60        | 1.53     |
| 1   | C1    | 858  | A2M  | C2'-C1' | 2.82  | 1.60        | 1.53     |
| 1   | C1    | 389  | A2M  | C5-N7   | -2.81 | 1.33        | 1.39     |
| 1   | C1    | 2688 | OMU  | C6-N1   | 2.74  | 1.44        | 1.38     |
| 1   | C1    | 2277 | OMU  | C6-N1   | 2.72  | 1.44        | 1.38     |
| 1   | C1    | 1917 | OMU  | C6-N1   | 2.72  | 1.44        | 1.38     |
| 1   | C1    | 2683 | OMU  | C6-N1   | 2.70  | 1.44        | 1.38     |
| 1   | C1    | 1868 | OMU  | C6-N1   | 2.70  | 1.44        | 1.38     |
| 1   | C1    | 637  | A2M  | C5-N7   | -2.69 | 1.34        | 1.39     |
| 1   | C1    | 1432 | A2M  | C5-N7   | -2.68 | 1.34        | 1.39     |
| 1   | C1    | 2380 | OMU  | C6-N1   | 2.68  | 1.44        | 1.38     |
| 1   | C1    | 2690 | OMU  | C6-N1   | 2.67  | 1.44        | 1.38     |
| 1   | C1    | 2384 | OMU  | C6-N1   | 2.67  | 1.44        | 1.38     |
| 1   | C1    | 1223 | A2M  | C5-N7   | -2.63 | 1.34        | 1.39     |
| 1   | C1    | 858  | A2M  | C5-N7   | -2.61 | 1.34        | 1.39     |
| 1   | C1    | 2289 | A2M  | C5-N7   | -2.58 | 1.34        | 1.39     |
| 1   | C1    | 848  | A2M  | C5-N7   | -2.49 | 1.34        | 1.39     |
| 1   | C1    | 1847 | A2M  | C5-N7   | -2.48 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C1    | 2688 | OMU  | C5-C4   | 2.34  | 1.48        | 1.43     |
| 1   | C1    | 1868 | OMU  | C5-C4   | 2.33  | 1.48        | 1.43     |
| 1   | C1    | 1432 | A2M  | C8-N9   | -2.32 | 1.33        | 1.37     |
| 1   | C1    | 2277 | OMU  | C5-C4   | 2.26  | 1.48        | 1.43     |
| 1   | C1    | 2690 | OMU  | C5-C4   | 2.26  | 1.48        | 1.43     |
| 1   | C1    | 1917 | OMU  | C5-C4   | 2.23  | 1.48        | 1.43     |
| 1   | C1    | 2380 | OMU  | C5-C4   | 2.22  | 1.48        | 1.43     |
| 1   | C1    | 2384 | OMU  | C5-C4   | 2.22  | 1.48        | 1.43     |
| 1   | C1    | 1847 | A2M  | C8-N9   | -2.21 | 1.33        | 1.37     |
| 1   | C1    | 637  | A2M  | C8-N9   | -2.19 | 1.33        | 1.37     |
| 1   | C1    | 858  | A2M  | C8-N9   | -2.16 | 1.33        | 1.37     |
| 1   | C1    | 2683 | OMU  | C5-C4   | 2.16  | 1.48        | 1.43     |
| 1   | C1    | 389  | A2M  | C8-N9   | -2.14 | 1.33        | 1.37     |
| 1   | C1    | 848  | A2M  | C8-N9   | -2.14 | 1.33        | 1.37     |
| 1   | C1    | 1847 | A2M  | O3'-C3' | 2.13  | 1.48        | 1.43     |
| 1   | C1    | 848  | A2M  | O3'-C3' | 2.10  | 1.48        | 1.43     |
| 1   | C1    | 389  | A2M  | O3'-C3' | 2.07  | 1.48        | 1.43     |
| 1   | C1    | 1223 | A2M  | C8-N9   | -2.05 | 1.34        | 1.37     |
| 1   | C1    | 1432 | A2M  | O3'-C3' | 2.03  | 1.48        | 1.43     |
| 1   | C1    | 2289 | A2M  | O3'-C3' | 2.03  | 1.48        | 1.43     |

All (154) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | C1    | 1847 | A2M  | C1'-N9-C8 | -9.60 | 105.80      | 127.09   |
| 1   | C1    | 637  | A2M  | C1'-N9-C8 | -9.57 | 105.86      | 127.09   |
| 1   | C1    | 389  | A2M  | C1'-N9-C8 | -9.49 | 106.02      | 127.09   |
| 1   | C1    | 1432 | A2M  | C1'-N9-C8 | -9.38 | 106.28      | 127.09   |
| 1   | C1    | 858  | A2M  | C1'-N9-C8 | -9.31 | 106.43      | 127.09   |
| 1   | C1    | 848  | A2M  | C1'-N9-C8 | -9.23 | 106.60      | 127.09   |
| 1   | C1    | 1223 | A2M  | C1'-N9-C8 | -9.05 | 107.01      | 127.09   |
| 1   | C1    | 2289 | A2M  | C1'-N9-C8 | -8.82 | 107.51      | 127.09   |
| 1   | C1    | 389  | A2M  | C4-N9-C1' | 8.20  | 145.81      | 126.63   |
| 1   | C1    | 637  | A2M  | C4-N9-C1' | 8.20  | 145.81      | 126.63   |
| 1   | C1    | 1847 | A2M  | C4-N9-C1' | 8.18  | 145.75      | 126.63   |
| 1   | C1    | 1432 | A2M  | C4-N9-C1' | 8.11  | 145.60      | 126.63   |
| 1   | C1    | 858  | A2M  | C4-N9-C1' | 7.99  | 145.32      | 126.63   |
| 1   | C1    | 848  | A2M  | C4-N9-C1' | 7.83  | 144.94      | 126.63   |
| 1   | C1    | 1223 | A2M  | C4-N9-C1' | 7.77  | 144.81      | 126.63   |
| 1   | C1    | 2289 | A2M  | C4-N9-C1' | 7.46  | 144.09      | 126.63   |
| 1   | C1    | 2289 | A2M  | N3-C2-N1  | -5.93 | 119.61      | 128.58   |
| 1   | C1    | 637  | A2M  | N3-C2-N1  | -5.86 | 119.70      | 128.58   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | C1    | 1847 | A2M  | N3-C2-N1  | -5.79 | 119.82      | 128.58   |
| 1   | C1    | 858  | A2M  | N3-C2-N1  | -5.78 | 119.84      | 128.58   |
| 1   | C1    | 848  | A2M  | N3-C2-N1  | -5.77 | 119.84      | 128.58   |
| 1   | C1    | 1223 | A2M  | N3-C2-N1  | -5.74 | 119.89      | 128.58   |
| 1   | C1    | 1432 | A2M  | N3-C2-N1  | -5.73 | 119.90      | 128.58   |
| 1   | C1    | 389  | A2M  | N3-C2-N1  | -5.73 | 119.91      | 128.58   |
| 1   | C1    | 1847 | A2M  | N6-C6-N1  | -5.66 | 105.77      | 118.38   |
| 1   | C1    | 1868 | OMU  | C4-N3-C2  | -5.64 | 119.62      | 126.61   |
| 1   | C1    | 2688 | OMU  | C4-N3-C2  | -5.57 | 119.70      | 126.61   |
| 1   | C1    | 848  | A2M  | N6-C6-N1  | -5.55 | 106.02      | 118.38   |
| 1   | C1    | 2690 | OMU  | C4-N3-C2  | -5.53 | 119.74      | 126.61   |
| 1   | C1    | 1223 | A2M  | N6-C6-N1  | -5.52 | 106.09      | 118.38   |
| 1   | C1    | 2380 | OMU  | C4-N3-C2  | -5.51 | 119.77      | 126.61   |
| 1   | C1    | 2289 | A2M  | N6-C6-N1  | -5.45 | 106.23      | 118.38   |
| 1   | C1    | 858  | A2M  | N6-C6-N1  | -5.43 | 106.28      | 118.38   |
| 1   | C1    | 637  | A2M  | N6-C6-N1  | -5.38 | 106.39      | 118.38   |
| 1   | C1    | 1432 | A2M  | N6-C6-N1  | -5.36 | 106.43      | 118.38   |
| 1   | C1    | 1917 | OMU  | C4-N3-C2  | -5.36 | 119.95      | 126.61   |
| 1   | C1    | 2384 | OMU  | C4-N3-C2  | -5.31 | 120.02      | 126.61   |
| 1   | C1    | 2683 | OMU  | C4-N3-C2  | -5.26 | 120.09      | 126.61   |
| 1   | C1    | 2277 | OMU  | C4-N3-C2  | -5.15 | 120.22      | 126.61   |
| 1   | C1    | 389  | A2M  | N6-C6-N1  | -5.14 | 106.92      | 118.38   |
| 1   | C1    | 389  | A2M  | C5-C4-N3  | -4.98 | 119.86      | 126.72   |
| 1   | C1    | 637  | A2M  | C5-C4-N3  | -4.97 | 119.87      | 126.72   |
| 1   | C1    | 1847 | A2M  | C5-C4-N3  | -4.87 | 120.00      | 126.72   |
| 1   | C1    | 848  | A2M  | C5-C4-N3  | -4.81 | 120.09      | 126.72   |
| 1   | C1    | 858  | A2M  | C5-C4-N3  | -4.79 | 120.12      | 126.72   |
| 1   | C1    | 1432 | A2M  | C5-C4-N3  | -4.78 | 120.14      | 126.72   |
| 1   | C1    | 2838 | OMC  | C1'-N1-C2 | 4.73  | 128.89      | 118.44   |
| 1   | C1    | 1223 | A2M  | C5-C4-N3  | -4.70 | 120.24      | 126.72   |
| 1   | C1    | 1420 | OMC  | C1'-N1-C2 | 4.64  | 128.70      | 118.44   |
| 1   | C1    | 2289 | A2M  | C5-C4-N3  | -4.50 | 120.52      | 126.72   |
| 1   | C1    | 1847 | A2M  | N9-C8-N7  | -4.42 | 107.67      | 113.94   |
| 1   | C1    | 1847 | A2M  | C5-C6-N6  | 4.42  | 134.22      | 123.29   |
| 1   | C1    | 848  | A2M  | N9-C8-N7  | -4.41 | 107.68      | 113.94   |
| 1   | C1    | 2289 | A2M  | N9-C8-N7  | -4.39 | 107.71      | 113.94   |
| 1   | C1    | 1223 | A2M  | C5-C6-N6  | 4.34  | 134.03      | 123.29   |
| 1   | C1    | 2289 | A2M  | C5-C6-N6  | 4.32  | 133.98      | 123.29   |
| 1   | C1    | 1223 | A2M  | N9-C8-N7  | -4.29 | 107.85      | 113.94   |
| 1   | C1    | 858  | A2M  | C5-C6-N6  | 4.29  | 133.90      | 123.29   |
| 1   | C1    | 858  | A2M  | N9-C8-N7  | -4.28 | 107.87      | 113.94   |
| 1   | C1    | 637  | A2M  | N9-C8-N7  | -4.26 | 107.89      | 113.94   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | C1    | 848  | A2M  | C5-C6-N6   | 4.24  | 133.80      | 123.29   |
| 1   | C1    | 637  | A2M  | C5-C6-N6   | 4.21  | 133.70      | 123.29   |
| 1   | C1    | 389  | A2M  | N9-C8-N7   | -4.17 | 108.02      | 113.94   |
| 1   | C1    | 1432 | A2M  | C5-C6-N6   | 4.15  | 133.56      | 123.29   |
| 1   | C1    | 2289 | A2M  | O4'-C1'-N9 | 4.07  | 115.92      | 108.09   |
| 1   | C1    | 1432 | A2M  | N9-C8-N7   | -4.01 | 108.24      | 113.94   |
| 1   | C1    | 848  | A2M  | O4'-C1'-N9 | 3.97  | 115.72      | 108.09   |
| 1   | C1    | 2688 | OMU  | N3-C2-N1   | 3.96  | 120.04      | 114.89   |
| 1   | C1    | 389  | A2M  | C5-C6-N6   | 3.94  | 133.03      | 123.29   |
| 1   | C1    | 1223 | A2M  | O4'-C1'-N9 | 3.92  | 115.61      | 108.09   |
| 1   | C1    | 858  | A2M  | O4'-C1'-N9 | 3.88  | 115.55      | 108.09   |
| 1   | C1    | 1917 | OMU  | N3-C2-N1   | 3.87  | 119.93      | 114.89   |
| 1   | C1    | 1868 | OMU  | N3-C2-N1   | 3.86  | 119.92      | 114.89   |
| 1   | C1    | 2384 | OMU  | N3-C2-N1   | 3.85  | 119.90      | 114.89   |
| 1   | C1    | 2690 | OMU  | N3-C2-N1   | 3.83  | 119.87      | 114.89   |
| 1   | C1    | 1432 | A2M  | O4'-C1'-N9 | 3.78  | 115.35      | 108.09   |
| 1   | C1    | 2380 | OMU  | N3-C2-N1   | 3.77  | 119.80      | 114.89   |
| 1   | C1    | 389  | A2M  | O4'-C1'-N9 | 3.71  | 115.21      | 108.09   |
| 1   | C1    | 2277 | OMU  | N3-C2-N1   | 3.70  | 119.71      | 114.89   |
| 1   | C1    | 2683 | OMU  | N3-C2-N1   | 3.68  | 119.68      | 114.89   |
| 1   | C1    | 1868 | OMU  | C5-C4-N3   | 3.67  | 119.94      | 114.80   |
| 1   | C1    | 2380 | OMU  | C5-C4-N3   | 3.60  | 119.85      | 114.80   |
| 1   | C1    | 2690 | OMU  | C5-C4-N3   | 3.55  | 119.78      | 114.80   |
| 1   | C1    | 2688 | OMU  | C5-C4-N3   | 3.55  | 119.77      | 114.80   |
| 1   | C1    | 637  | A2M  | O4'-C1'-N9 | 3.53  | 114.86      | 108.09   |
| 1   | C1    | 2838 | OMC  | C1'-N1-C6  | -3.51 | 113.28      | 120.78   |
| 1   | C1    | 2683 | OMU  | C5-C4-N3   | 3.51  | 119.71      | 114.80   |
| 1   | C1    | 1847 | A2M  | C2-N3-C4   | 3.45  | 120.25      | 111.83   |
| 1   | C1    | 637  | A2M  | C2-N3-C4   | 3.44  | 120.23      | 111.83   |
| 1   | C1    | 2384 | OMU  | C5-C4-N3   | 3.44  | 119.62      | 114.80   |
| 1   | C1    | 1917 | OMU  | C5-C4-N3   | 3.42  | 119.59      | 114.80   |
| 1   | C1    | 848  | A2M  | C2-N3-C4   | 3.40  | 120.13      | 111.83   |
| 1   | C1    | 389  | A2M  | C2-N3-C4   | 3.40  | 120.12      | 111.83   |
| 1   | C1    | 1420 | OMC  | C1'-N1-C6  | -3.37 | 113.58      | 120.78   |
| 1   | C1    | 858  | A2M  | C2-N3-C4   | 3.35  | 120.01      | 111.83   |
| 1   | C1    | 2277 | OMU  | C5-C4-N3   | 3.35  | 119.49      | 114.80   |
| 1   | C1    | 1432 | A2M  | C2-N3-C4   | 3.34  | 119.99      | 111.83   |
| 1   | C1    | 1223 | A2M  | C2-N3-C4   | 3.30  | 119.90      | 111.83   |
| 1   | C1    | 2289 | A2M  | C2-N3-C4   | 3.28  | 119.83      | 111.83   |
| 1   | C1    | 389  | A2M  | N3-C4-N9   | 3.25  | 132.69      | 127.17   |
| 1   | C1    | 637  | A2M  | N3-C4-N9   | 3.18  | 132.58      | 127.17   |
| 1   | C1    | 1847 | A2M  | O4'-C1'-N9 | 3.06  | 113.97      | 108.09   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | C1    | 1847 | A2M  | C5-N7-C8   | 3.04  | 108.23      | 103.45   |
| 1   | C1    | 1847 | A2M  | N3-C4-N9   | 3.01  | 132.29      | 127.17   |
| 1   | C1    | 848  | A2M  | N3-C4-N9   | 3.01  | 132.29      | 127.17   |
| 1   | C1    | 1432 | A2M  | N3-C4-N9   | 2.98  | 132.24      | 127.17   |
| 1   | C1    | 848  | A2M  | C5-N7-C8   | 2.97  | 108.12      | 103.45   |
| 1   | C1    | 1868 | OMU  | O4-C4-C5   | -2.97 | 120.05      | 125.16   |
| 1   | C1    | 2380 | OMU  | O4-C4-C5   | -2.95 | 120.08      | 125.16   |
| 1   | C1    | 2690 | OMU  | O4-C4-C5   | -2.94 | 120.09      | 125.16   |
| 1   | C1    | 858  | A2M  | N3-C4-N9   | 2.93  | 132.15      | 127.17   |
| 1   | C1    | 1223 | A2M  | C5-N7-C8   | 2.92  | 108.04      | 103.45   |
| 1   | C1    | 2384 | OMU  | O4-C4-C5   | -2.91 | 120.14      | 125.16   |
| 1   | C1    | 2683 | OMU  | O4-C4-C5   | -2.91 | 120.15      | 125.16   |
| 1   | C1    | 858  | A2M  | C5-N7-C8   | 2.90  | 108.02      | 103.45   |
| 1   | C1    | 637  | A2M  | C5-N7-C8   | 2.90  | 108.00      | 103.45   |
| 1   | C1    | 848  | A2M  | C2'-C1'-N9 | -2.87 | 109.03      | 113.75   |
| 1   | C1    | 2688 | OMU  | O4-C4-C5   | -2.85 | 120.25      | 125.16   |
| 1   | C1    | 2289 | A2M  | C5-N7-C8   | 2.85  | 107.92      | 103.45   |
| 1   | C1    | 389  | A2M  | C5-N7-C8   | 2.83  | 107.91      | 103.45   |
| 1   | C1    | 1847 | A2M  | C2'-C1'-N9 | -2.82 | 109.11      | 113.75   |
| 1   | C1    | 1223 | A2M  | N3-C4-N9   | 2.82  | 131.96      | 127.17   |
| 1   | C1    | 1917 | OMU  | O4-C4-C5   | -2.78 | 120.37      | 125.16   |
| 1   | C1    | 2289 | A2M  | N3-C4-N9   | 2.76  | 131.86      | 127.17   |
| 1   | C1    | 2277 | OMU  | O4-C4-C5   | -2.75 | 120.41      | 125.16   |
| 1   | C1    | 778  | OMC  | C1'-N1-C2  | 2.69  | 124.39      | 118.44   |
| 1   | C1    | 1420 | OMC  | O2-C2-N1   | 2.67  | 124.14      | 118.90   |
| 1   | C1    | 1836 | OMC  | C1'-N1-C2  | 2.67  | 124.34      | 118.44   |
| 1   | C1    | 2838 | OMC  | O2-C2-N3   | -2.67 | 118.13      | 122.33   |
| 1   | C1    | 1432 | A2M  | C5-N7-C8   | 2.66  | 107.63      | 103.45   |
| 1   | C1    | 848  | A2M  | C4-N9-C8   | 2.59  | 108.46      | 105.74   |
| 1   | C1    | 1847 | A2M  | C4-N9-C8   | 2.58  | 108.45      | 105.74   |
| 1   | C1    | 2289 | A2M  | C4-N9-C8   | 2.54  | 108.40      | 105.74   |
| 1   | C1    | 1420 | OMC  | O2-C2-N3   | -2.49 | 118.40      | 122.33   |
| 1   | C1    | 637  | A2M  | C4-N9-C8   | 2.45  | 108.31      | 105.74   |
| 1   | C1    | 2838 | OMC  | O2-C2-N1   | 2.39  | 123.58      | 118.90   |
| 1   | C1    | 858  | A2M  | C4-N9-C8   | 2.39  | 108.25      | 105.74   |
| 1   | C1    | 1223 | A2M  | C4-N9-C8   | 2.33  | 108.18      | 105.74   |
| 1   | C1    | 2289 | A2M  | C2'-C1'-N9 | -2.30 | 109.97      | 113.75   |
| 1   | C1    | 1847 | A2M  | C4-C5-N7   | -2.30 | 107.95      | 110.58   |
| 1   | C1    | 389  | A2M  | C4-N9-C8   | 2.30  | 108.15      | 105.74   |
| 1   | C1    | 1432 | A2M  | C4-N9-C8   | 2.27  | 108.12      | 105.74   |
| 1   | C1    | 1917 | OMU  | C1'-N1-C2  | 2.26  | 121.66      | 117.59   |
| 1   | C1    | 2688 | OMU  | O2-C2-N1   | -2.26 | 119.85      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | C1    | 1868 | OMU  | O2-C2-N1  | -2.20 | 119.93      | 122.80   |
| 1   | C1    | 2690 | OMU  | O2-C2-N1  | -2.20 | 119.94      | 122.80   |
| 1   | C1    | 848  | A2M  | C4-C5-N7  | -2.15 | 108.12      | 110.58   |
| 1   | C1    | 2380 | OMU  | O2-C2-N1  | -2.14 | 120.01      | 122.80   |
| 1   | C1    | 1223 | A2M  | C4-C5-N7  | -2.14 | 108.14      | 110.58   |
| 1   | C1    | 858  | A2M  | C4-C5-N7  | -2.13 | 108.15      | 110.58   |
| 1   | C1    | 389  | A2M  | C6-C5-C4  | 2.12  | 120.08      | 117.18   |
| 1   | C1    | 2918 | OMC  | C1'-N1-C2 | 2.12  | 123.12      | 118.44   |
| 1   | C1    | 2277 | OMU  | O2-C2-N1  | -2.04 | 120.14      | 122.80   |
| 1   | C1    | 637  | A2M  | C4-C5-N7  | -2.04 | 108.25      | 110.58   |

There are no chirality outliers.

All (30) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | C1    | 389  | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 389  | A2M  | C1'-C2'-O2'-CM' |
| 1   | C1    | 858  | A2M  | C1'-C2'-O2'-CM' |
| 1   | C1    | 1223 | A2M  | C1'-C2'-O2'-CM' |
| 1   | C1    | 1433 | OMG  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1917 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | C1    | 2578 | OMG  | O4'-C4'-C5'-O5' |
| 1   | C1    | 2683 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | C1    | 2690 | OMU  | O4'-C4'-C5'-O5' |
| 1   | C1    | 2838 | OMC  | O4'-C1'-N1-C2   |
| 1   | C1    | 2838 | OMC  | O4'-C1'-N1-C6   |
| 1   | C1    | 389  | A2M  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2690 | OMU  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1433 | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2578 | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1847 | A2M  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1491 | OMC  | O4'-C4'-C5'-O5' |
| 1   | C1    | 637  | A2M  | C1'-C2'-O2'-CM' |
| 1   | C1    | 848  | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 637  | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1223 | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1917 | OMU  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1847 | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1420 | OMC  | C2'-C1'-N1-C6   |
| 1   | C1    | 389  | A2M  | C4'-C5'-O5'-P   |
| 1   | C1    | 2578 | OMG  | C4'-C5'-O5'-P   |
| 1   | C1    | 1847 | A2M  | C4'-C5'-O5'-P   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | C1    | 1420 | OMC  | C2'-C1'-N1-C2   |
| 1   | C1    | 2384 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | C1    | 627  | OMG  | O4'-C4'-C5'-O5' |

There are no ring outliers.

10 monomers are involved in 11 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | C1    | 2277 | OMU  | 1       | 0            |
| 1   | C1    | 2876 | OMG  | 1       | 0            |
| 1   | C1    | 1432 | A2M  | 1       | 0            |
| 1   | C1    | 2578 | OMG  | 1       | 0            |
| 1   | C1    | 389  | A2M  | 1       | 0            |
| 1   | C1    | 2384 | OMU  | 1       | 0            |
| 1   | C1    | 2683 | OMU  | 2       | 0            |
| 1   | C1    | 778  | OMC  | 1       | 0            |
| 1   | C1    | 848  | A2M  | 1       | 0            |
| 1   | C1    | 1420 | OMC  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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 | $\# Z  > 2$ |
| 54  | GTP  | Cd    | 1000 | 55   | 33,34,34     | 0.97 | 2 (6%)      | 50,54,54    | 1.59 | 8 (16%)     |
| 54  | GTP  | CH    | 701  | 55   | 33,34,34     | 0.91 | 1 (3%)      | 50,54,54    | 1.58 | 9 (18%)     |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 54  | GTP  | Cd    | 1000 | 55   | -       | 5/22/38/38 | 0/3/3/3 |
| 54  | GTP  | CH    | 701  | 55   | -       | 5/22/38/38 | 0/3/3/3 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 54  | CH    | 701  | GTP  | C2-N3  | 2.10 | 1.38        | 1.33     |
| 54  | Cd    | 1000 | GTP  | PA-O3A | 2.03 | 1.61        | 1.59     |
| 54  | Cd    | 1000 | GTP  | C2-N3  | 2.02 | 1.38        | 1.33     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | Cd    | 1000 | GTP  | C5-C4-N3    | -4.96 | 120.49      | 128.39   |
| 54  | CH    | 701  | GTP  | C5-C4-N3    | -4.90 | 120.58      | 128.39   |
| 54  | Cd    | 1000 | GTP  | C2-N3-C4    | 4.60  | 120.23      | 112.30   |
| 54  | CH    | 701  | GTP  | C2-N3-C4    | 4.53  | 120.10      | 112.30   |
| 54  | Cd    | 1000 | GTP  | N9-C4-N3    | 3.12  | 132.20      | 125.95   |
| 54  | CH    | 701  | GTP  | N9-C4-N3    | 3.09  | 132.14      | 125.95   |
| 54  | Cd    | 1000 | GTP  | C2-N1-C6    | -2.93 | 119.80      | 125.11   |
| 54  | CH    | 701  | GTP  | C2-N1-C6    | -2.86 | 119.93      | 125.11   |
| 54  | CH    | 701  | GTP  | N9-C8-N7    | -2.66 | 108.47      | 113.40   |
| 54  | Cd    | 1000 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 54  | Cd    | 1000 | GTP  | C8-N7-C5    | 2.50  | 108.71      | 104.26   |
| 54  | Cd    | 1000 | GTP  | C5-C6-N1    | 2.49  | 119.60      | 113.25   |
| 54  | CH    | 701  | GTP  | C8-N7-C5    | 2.49  | 108.70      | 104.26   |
| 54  | CH    | 701  | GTP  | C5-C6-N1    | 2.45  | 119.49      | 113.25   |
| 54  | Cd    | 1000 | GTP  | O6-C6-C5    | -2.42 | 120.14      | 126.53   |
| 54  | CH    | 701  | GTP  | O6-C6-C5    | -2.36 | 120.31      | 126.53   |
| 54  | CH    | 701  | GTP  | C3'-C2'-C1' | 2.18  | 105.58      | 101.46   |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 54  | CH    | 701  | GTP  | C5'-O5'-PA-O3A |
| 54  | CH    | 701  | GTP  | C5'-O5'-PA-O1A |
| 54  | Cd    | 1000 | GTP  | C5'-O5'-PA-O3A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 54  | Cd    | 1000 | GTP  | C5'-O5'-PA-O1A  |
| 54  | Cd    | 1000 | GTP  | C5'-O5'-PA-O2A  |
| 54  | CH    | 701  | GTP  | O4'-C4'-C5'-O5' |
| 54  | CH    | 701  | GTP  | PB-O3A-PA-O2A   |
| 54  | Cd    | 1000 | GTP  | C4'-C5'-O5'-PA  |
| 54  | Cd    | 1000 | GTP  | PG-O3B-PB-O1B   |
| 54  | CH    | 701  | GTP  | PB-O3A-PA-O1A   |

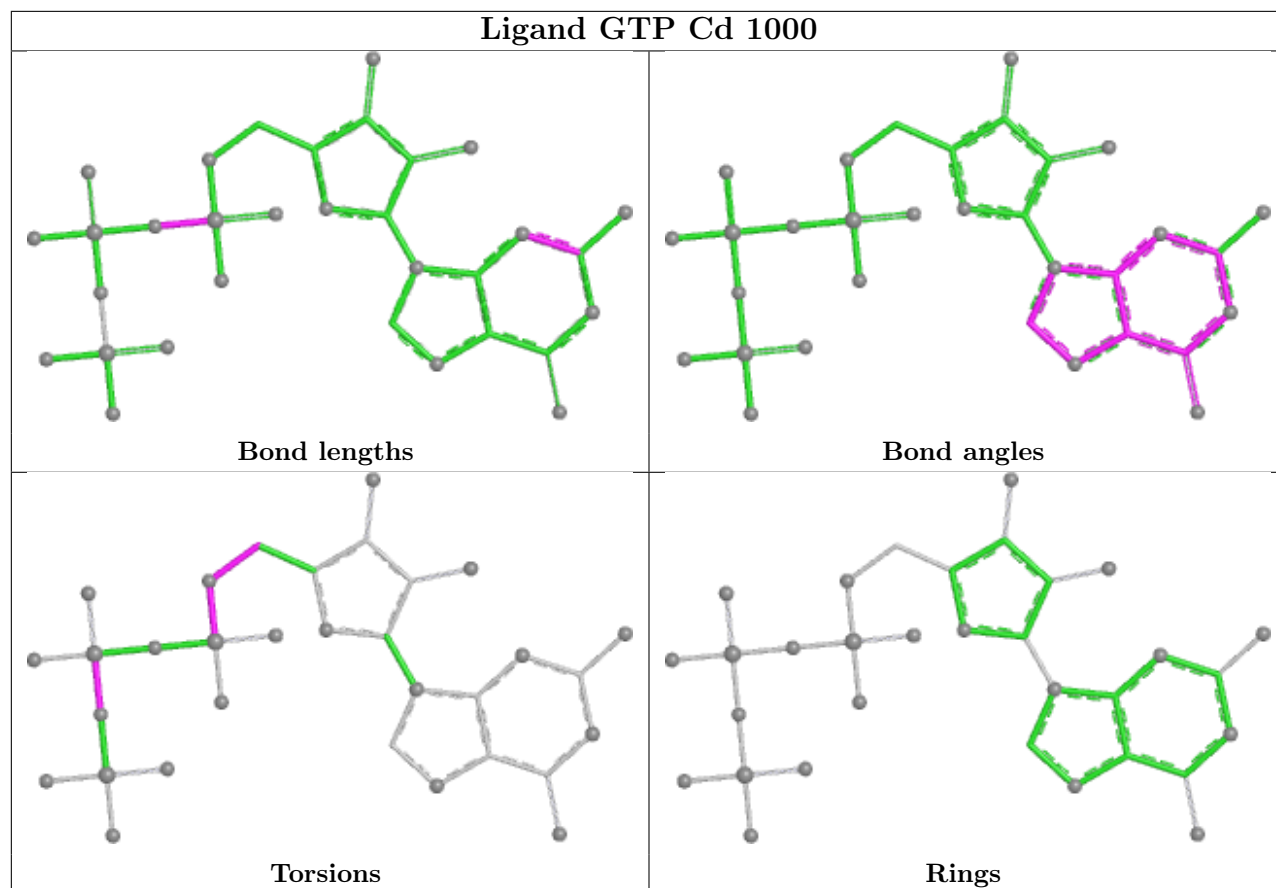
There are no ring outliers.

1 monomer is involved in 1 short contact:

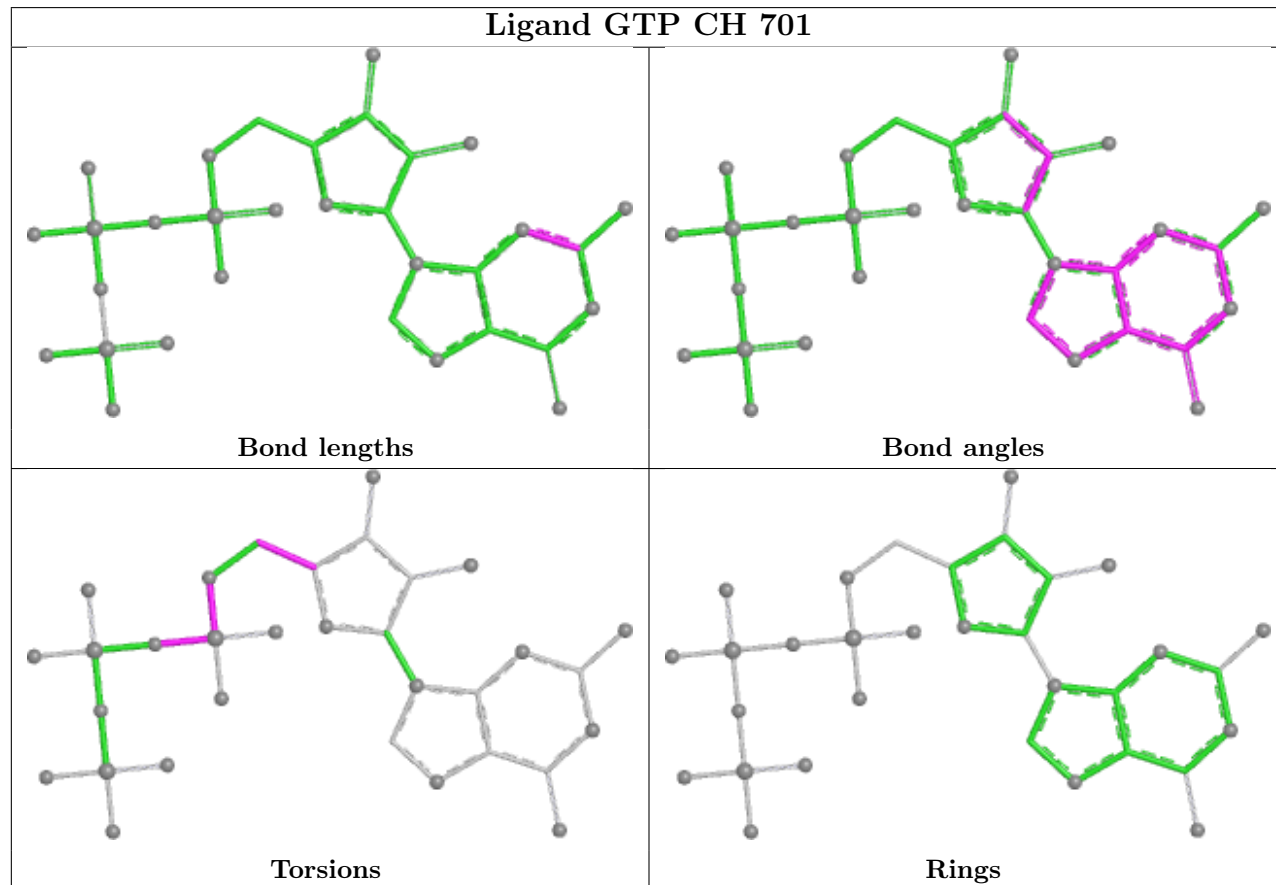
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 54  | Cd    | 1000 | GTP  | 1       | 0            |

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

## Ligand GTP Cd 1000



## Ligand GTP CH 701



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

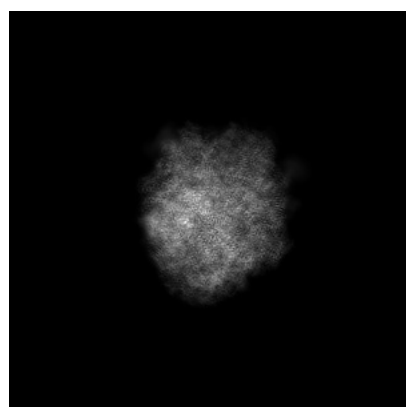
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17954. These allow visual inspection of the internal detail of the map and identification of artifacts.

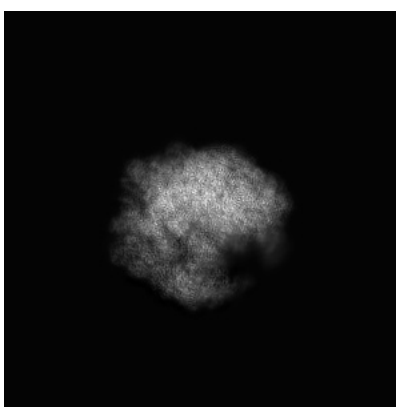
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

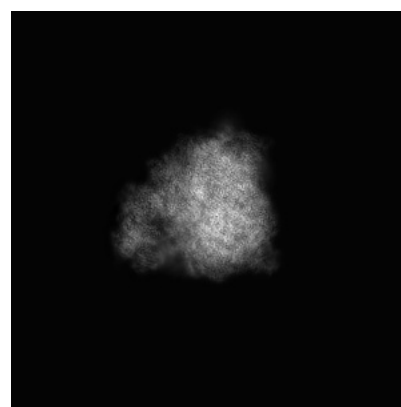
#### 6.1.1 Primary map



X



Y

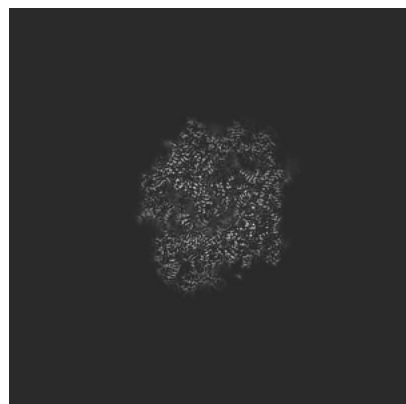


Z

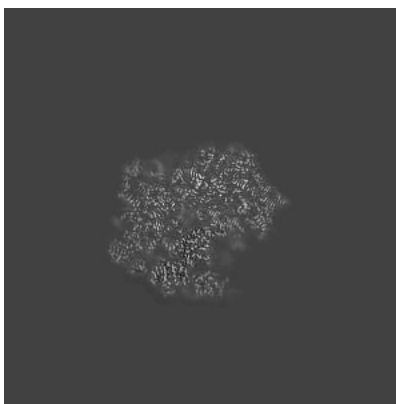
The images above show the map projected in three orthogonal directions.

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

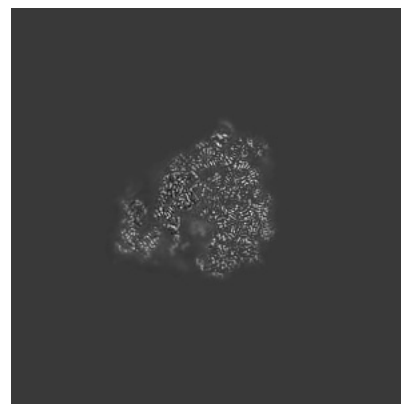
#### 6.2.1 Primary map



X Index: 250



Y Index: 250

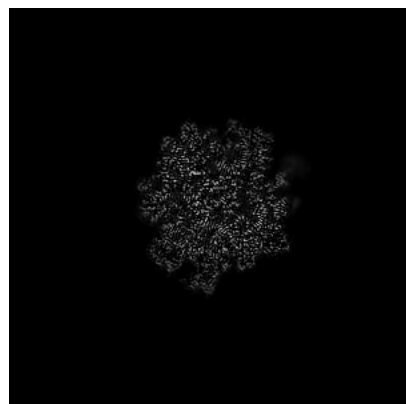


Z Index: 250

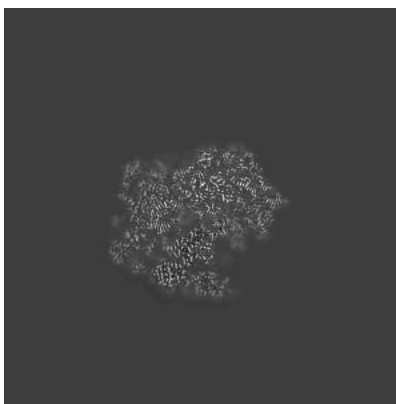
The images above show central slices of the map in three orthogonal directions.

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

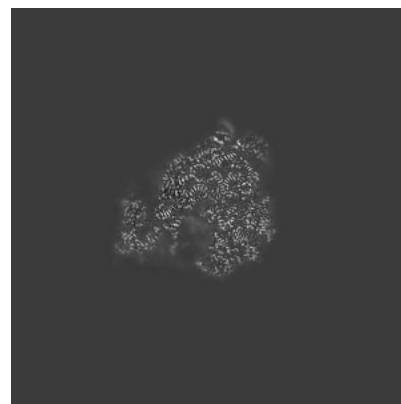
### 6.3.1 Primary map



X Index: 264



Y Index: 248

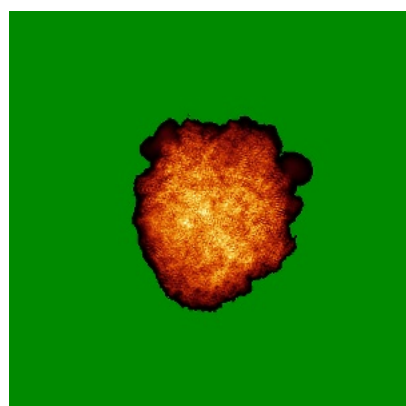


Z Index: 252

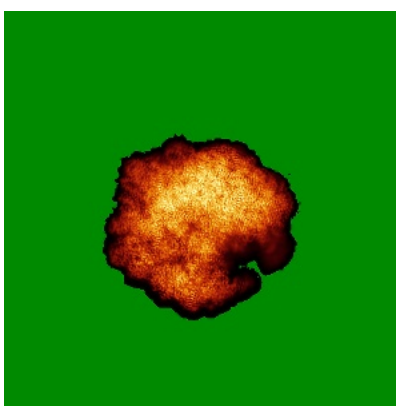
The images above show the largest variance slices of the map in three orthogonal directions.

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

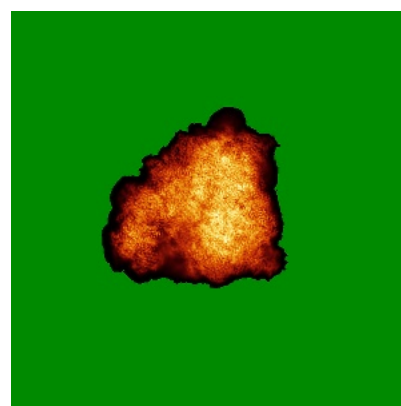
### 6.4.1 Primary map



X



Y

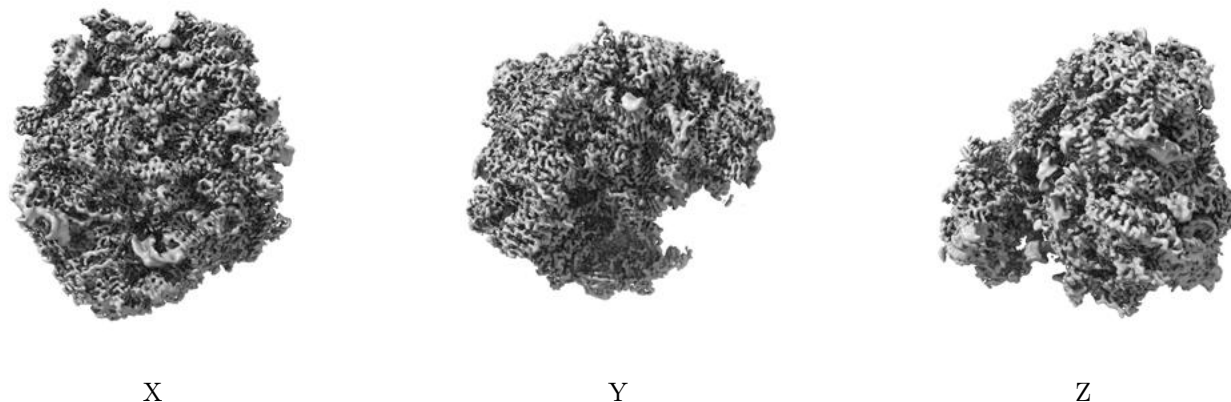


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

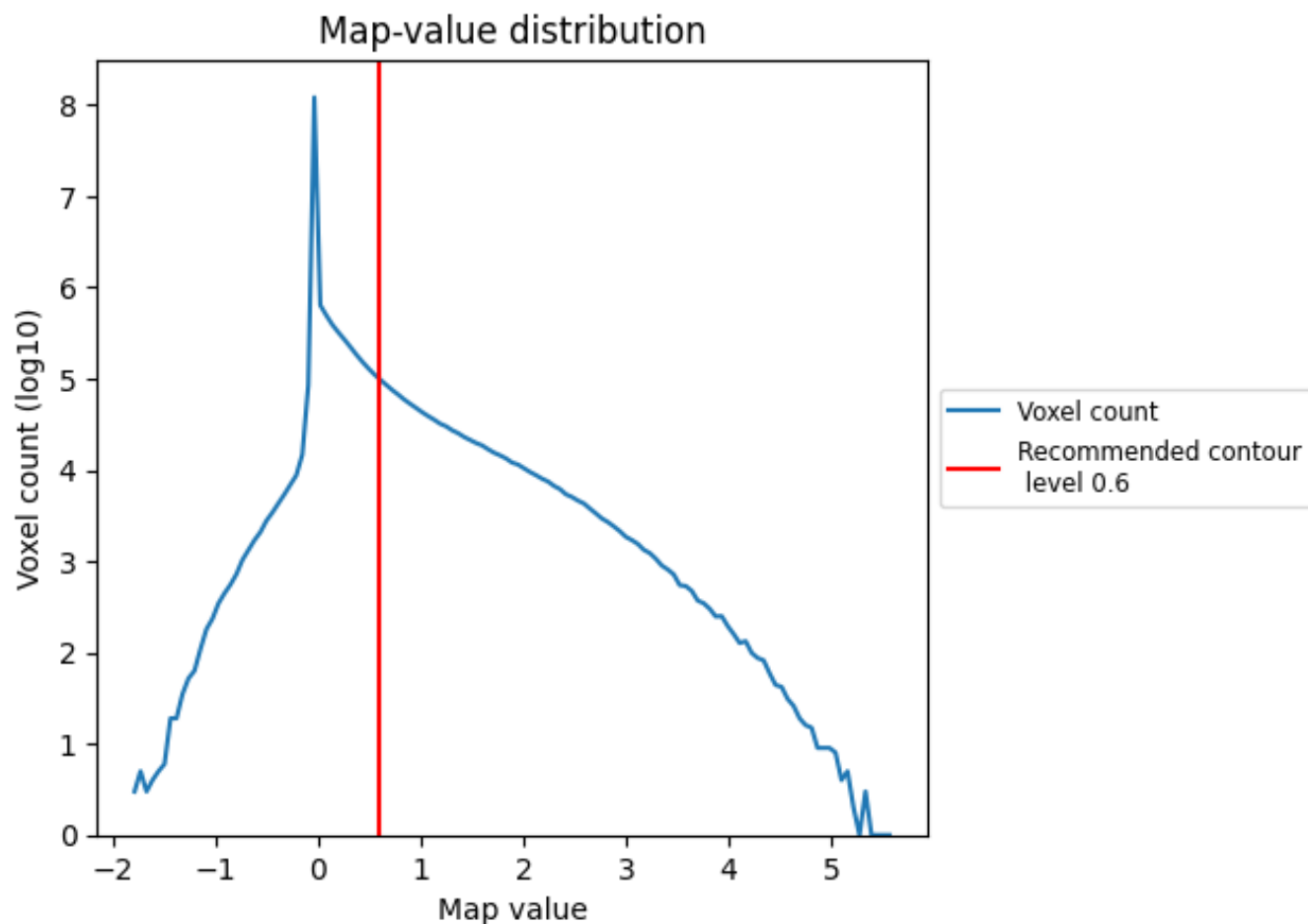
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

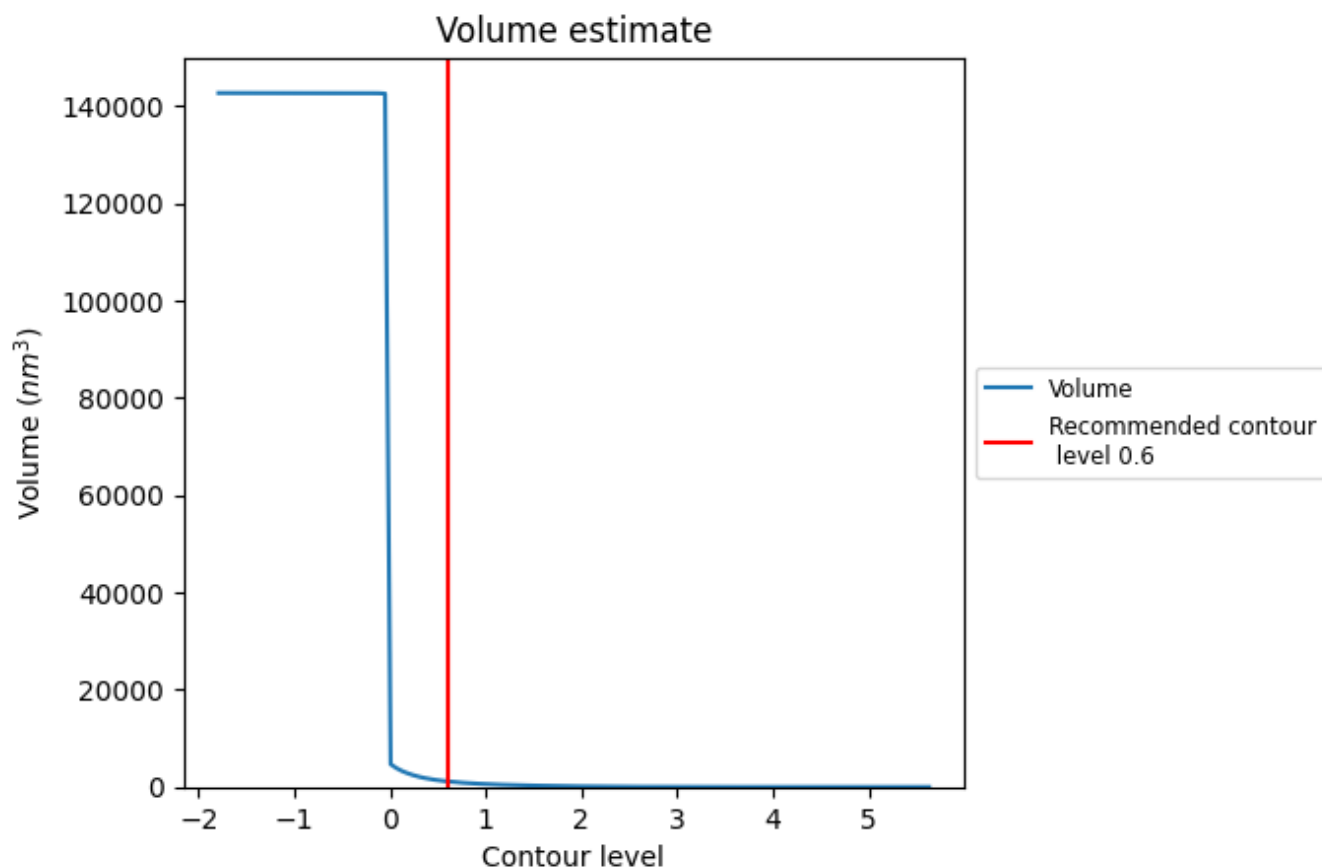
This section contains the results of statistical analysis of the map.

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



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

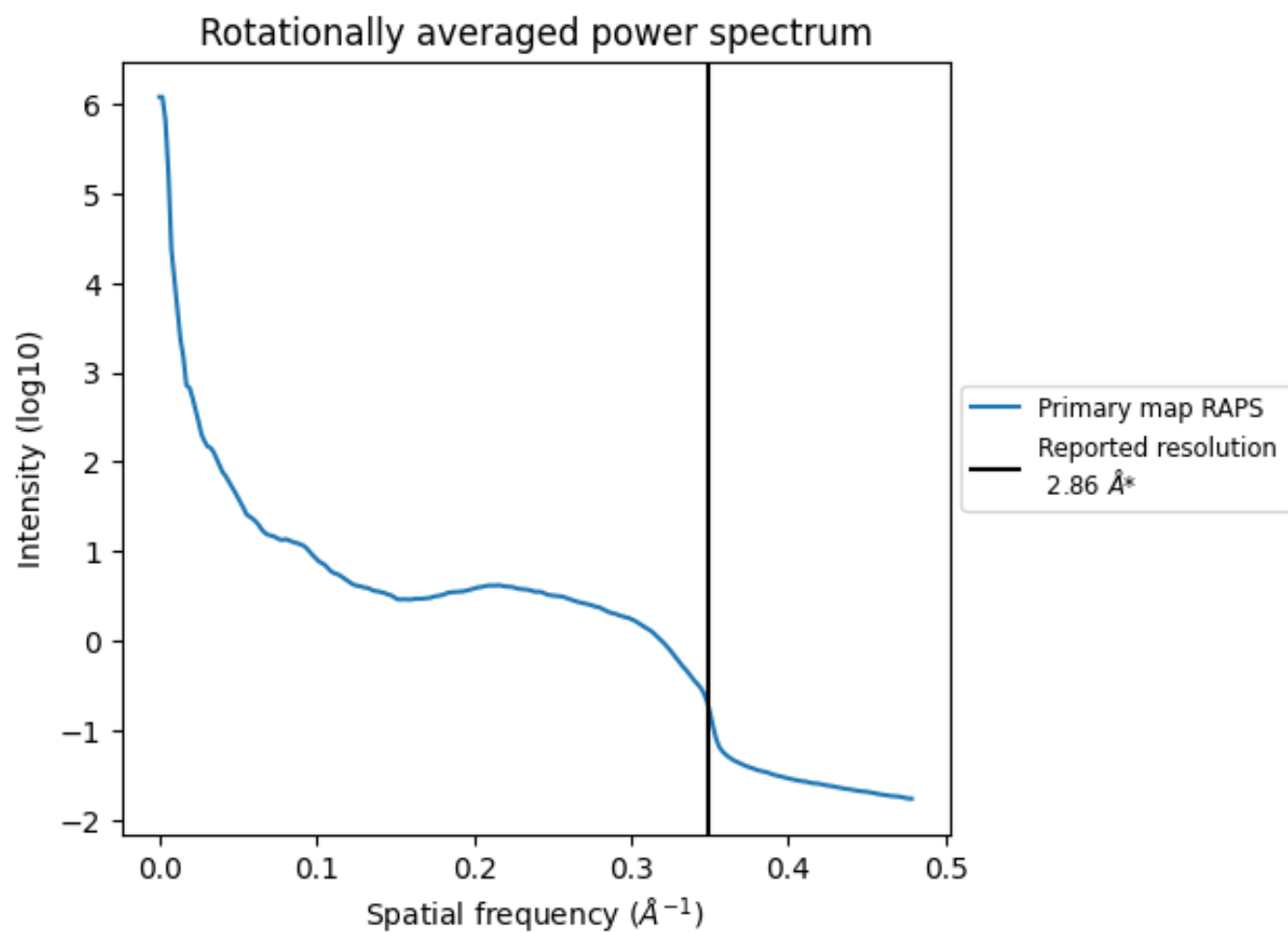
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1142  $\text{nm}^3$ ; this corresponds to an approximate mass of 1032 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 0.350 Å<sup>-1</sup>

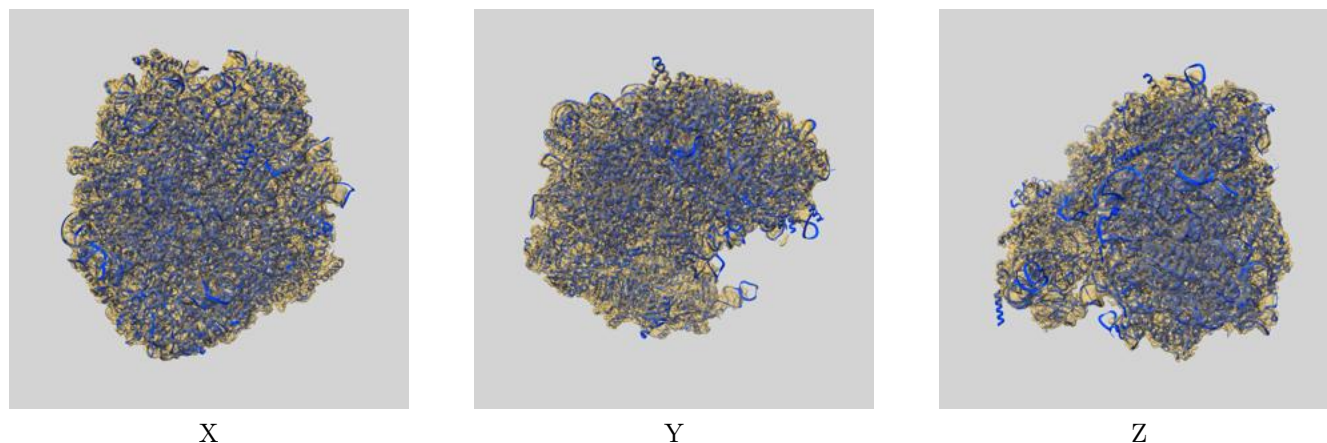
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

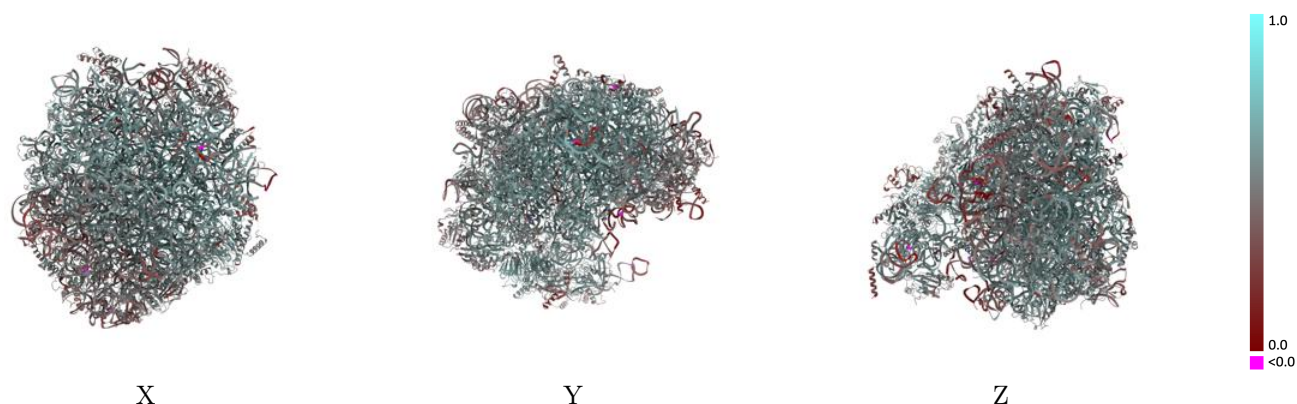
This section contains information regarding the fit between EMDB map EMD-17954 and PDB model 8PV5. Per-residue inclusion information can be found in section 3 on page 15.

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



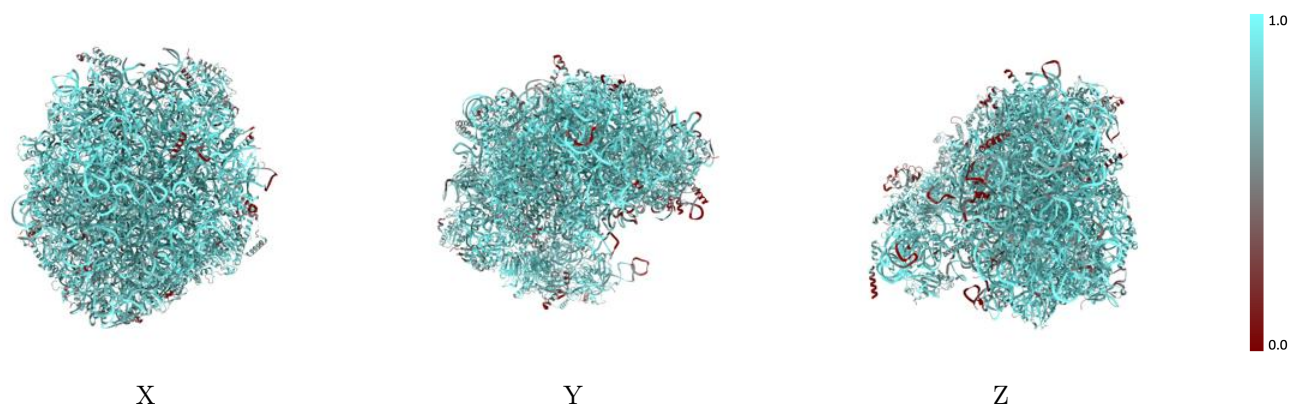
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



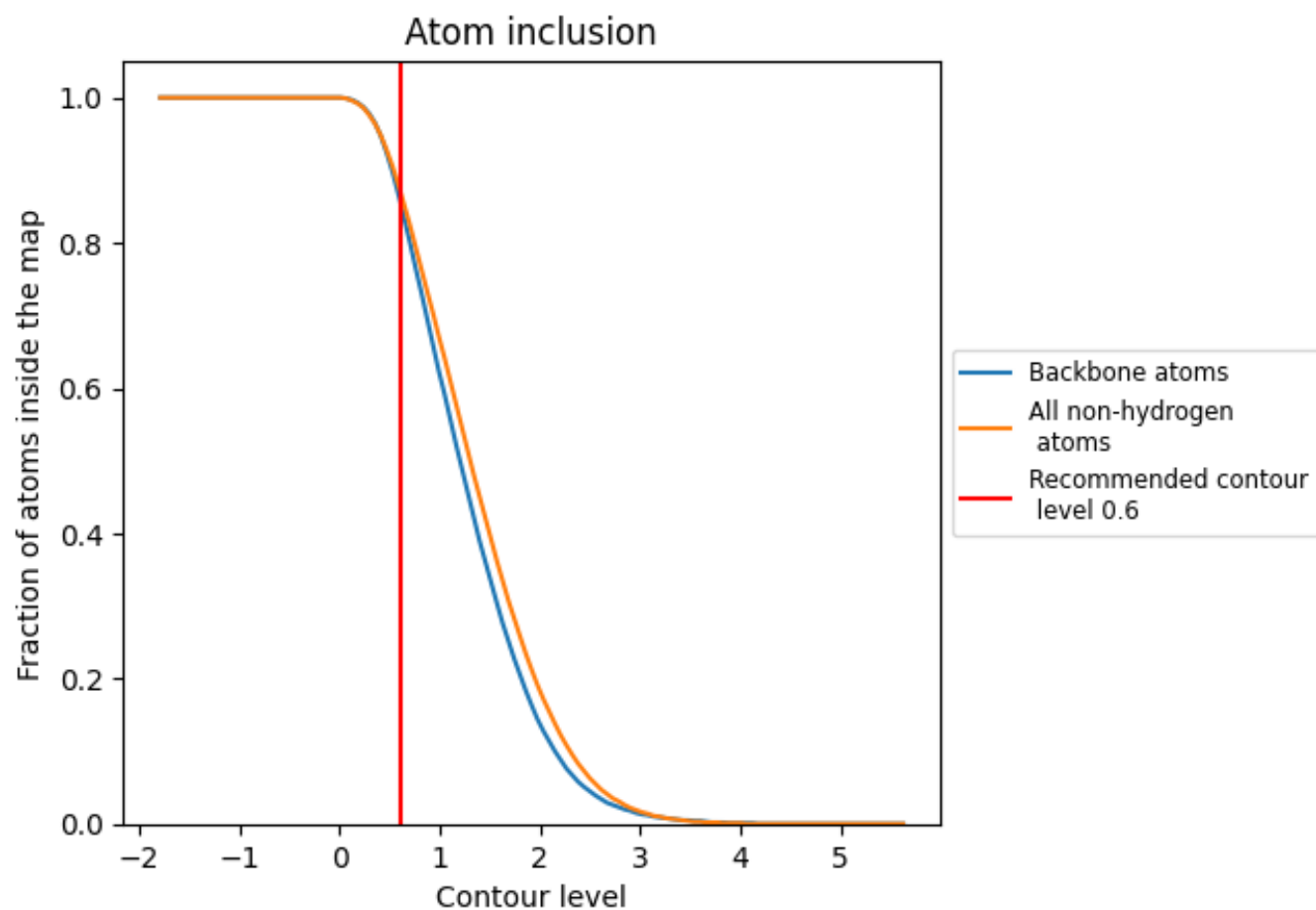
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 87% 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 (0.6) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8740   |  0.5220   |
| C1    |  0.9120   |  0.5220   |
| C2    |  0.9640   |  0.5810   |
| C4    |  0.8710   |  0.4960   |
| CF    |  0.7370   |  0.4460   |
| CH    |  0.8320   |  0.5440   |
| CK    |  0.9350   |  0.5860   |
| CL    |  0.6160   |  0.4490   |
| CN    |  0.8680   |  0.5710   |
| CO    |  0.7460   |  0.4820   |
| CQ    |  0.8180   |  0.5360   |
| Cb    |  0.8680   |  0.5740   |
| Cd    |  0.8970   |  0.5640   |
| Cf    |  0.8730   |  0.5440   |
| Cg    |  0.8490   |  0.5300   |
| Ch    |  0.8250   |  0.5380   |
| Cz    |  0.6850 |  0.4190 |
| LA    |  0.8330 |  0.4940 |
| LB    |  0.9190 |  0.5540 |
| LC    |  0.9000 |  0.5350 |
| LD    |  0.8680 |  0.5390 |
| LE    |  0.7190 |  0.4190 |
| LF    |  0.8260 |  0.4470 |
| LG    |  0.7330 |  0.4460 |
| LH    |  0.8280 |  0.5050 |
| LJ    |  0.7900 |  0.4790 |
| LK    |  0.7430 |  0.4920 |
| LL    |  0.8750 |  0.5660 |
| LM    |  0.7550 |  0.4440 |
| LN    |  0.9310 |  0.5840 |
| LO    |  0.8650 |  0.4880 |
| LP    |  0.9090 |  0.5440 |
| LQ    |  0.8350 |  0.5030 |
| LR    |  0.8970 |  0.5590 |
| LS    |  0.8430 |  0.4710 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| LT    |  0.6820   |  0.4350   |
| LU    |  0.8580   |  0.5430   |
| LV    |  0.9230   |  0.6050   |
| LX    |  0.8800   |  0.5570   |
| LY    |  0.8830   |  0.5470   |
| LZ    |  0.7370   |  0.4290   |
| La    |  0.8900   |  0.5630   |
| Lc    |  0.6570   |  0.4070   |
| Ld    |  0.9070   |  0.5920   |
| Le    |  0.8810   |  0.5020   |
| Lf    |  0.8950   |  0.4740   |
| Lg    |  0.7950   |  0.5030   |
| Lh    |  0.8570   |  0.5330   |
| Li    |  0.8330   |  0.5080   |
| Lj    |  0.9720   |  0.6150   |
| Lk    |  0.7340   |  0.5000   |
| Ll    |  0.9810   |  0.6260   |
| Lp    |  0.8100  |  0.4970  |
| Lq    |  0.8730 |  0.4660 |