



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:05 AM UTC

PDB ID : 8PVK / pdb\_00008pvk  
EMDB ID : EMD-17969  
Title : Chaetomium thermophilum pre-60S State 5 - pre-5S rotation - L1 inward - composite structure  
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.  
Deposited on : 2023-07-17  
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

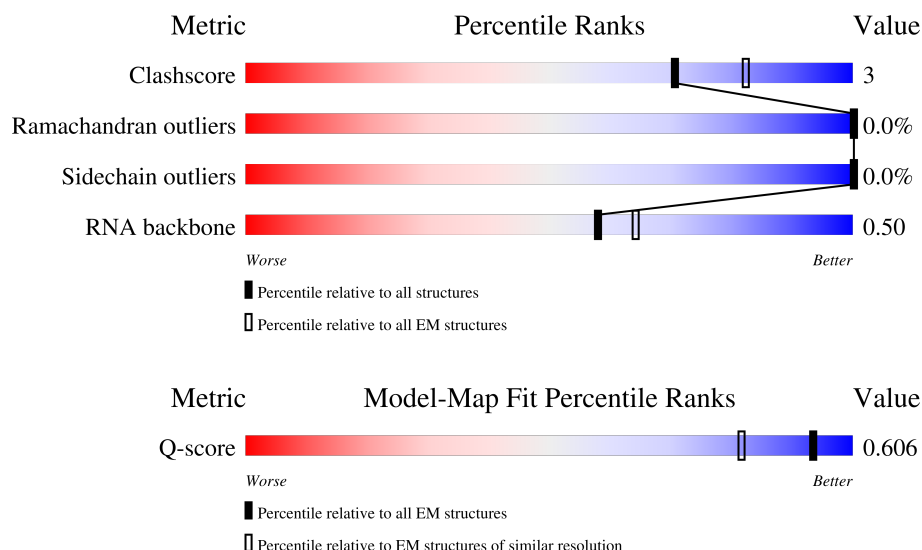
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.55 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.



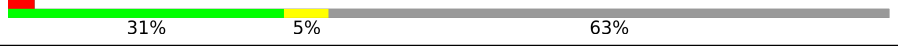
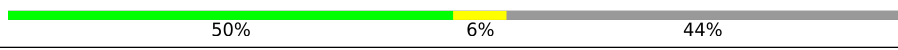
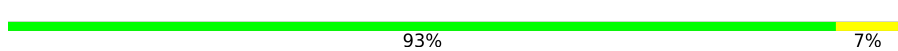
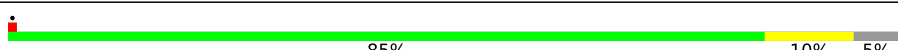
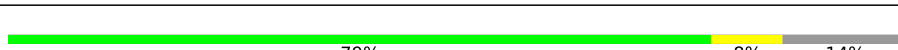
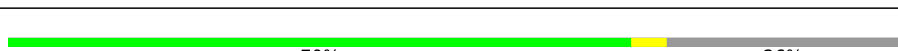
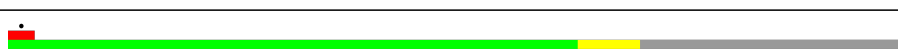
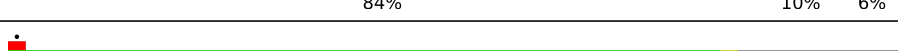
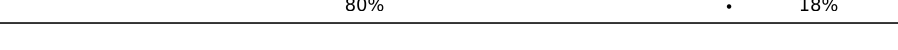
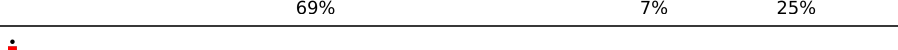
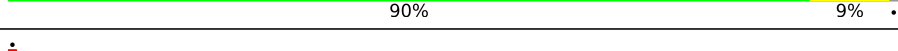
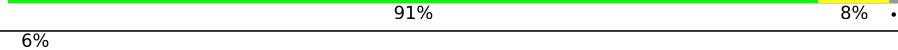
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 7475 ( 2.05 - 3.05 )                                     |

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   |                  |
| 2   | C2    | 156    |                  |
| 3   | C3    | 162    |                  |

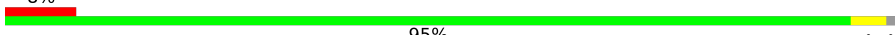
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | C4    | 119    |    |
| 5   | CB    | 391    |    |
| 6   | CF    | 270    |    |
| 7   | CH    | 661    |    |
| 8   | CI    | 414    |    |
| 9   | CJ    | 679    |    |
| 10  | CK    | 261    |    |
| 11  | CL    | 558    |    |
| 12  | CM    | 249    |    |
| 12  | LF    | 249    |    |
| 13  | CN    | 246    |    |
| 14  | CO    | 120    |   |
| 15  | CQ    | 225    |  |
| 16  | Lq    | 147    |  |
| 17  | Cb    | 117    |  |
| 18  | Cd    | 627    |  |
| 19  | Ce    | 443    |  |
| 20  | Cf    | 350    |  |
| 21  | Cg    | 202    |  |
| 22  | Ch    | 517    |  |
| 23  | Cz    | 123    |  |
| 24  | LA    | 254    |  |
| 25  | LB    | 392    |  |
| 26  | LC    | 365    |  |
| 27  | LD    | 304    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 28  | LE    | 200    |    |
| 29  | LG    | 262    |    |
| 30  | LH    | 229    |    |
| 31  | LJ    | 173    |    |
| 32  | LK    | 165    |    |
| 33  | LL    | 213    |    |
| 34  | LM    | 142    |    |
| 35  | LN    | 203    |    |
| 36  | LO    | 204    |    |
| 37  | LP    | 187    |    |
| 38  | LQ    | 213    |    |
| 39  | LR    | 2898   |   |
| 40  | LS    | 174    |  |
| 41  | LT    | 160    |  |
| 42  | LU    | 127    |  |
| 43  | LV    | 139    |  |
| 44  | LX    | 156    |  |
| 45  | LY    | 138    |  |
| 46  | LZ    | 135    |  |
| 47  | La    | 149    |  |
| 48  | Lc    | 108    |  |
| 49  | Ld    | 120    |  |
| 50  | Le    | 131    |  |
| 51  | Lf    | 109    |  |
| 52  | Lg    | 119    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 53  | Lh    | 935    |  |
| 54  | Li    | 110    |  |
| 55  | Lj    | 95     |  |
| 56  | Lk    | 94     |  |
| 57  | Ll    | 51     |  |
| 58  | Lp    | 92     |  |
| 59  | Lr    | 217    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 1   | OMC  | C1    | 1420 | X         | -        | -       | -                |
| 1   | OMG  | C1    | 1433 | X         | -        | -       | -                |
| 1   | OMC  | C1    | 1491 | X         | -        | -       | -                |
| 1   | OMC  | C1    | 1812 | X         | -        | -       | -                |
| 1   | OMC  | C1    | 1836 | X         | -        | -       | -                |
| 1   | OMC  | C1    | 2300 | X         | -        | -       | -                |
| 1   | OMG  | C1    | 2358 | X         | -        | -       | -                |
| 1   | OMG  | C1    | 2578 | X         | -        | -       | -                |
| 1   | OMG  | C1    | 2774 | X         | -        | -       | -                |
| 1   | OMC  | C1    | 2838 | X         | -        | -       | -                |
| 1   | OMG  | C1    | 2876 | X         | -        | -       | -                |
| 1   | OMG  | C1    | 2881 | X         | -        | -       | -                |
| 1   | OMC  | C1    | 2918 | X         | -        | -       | -                |
| 1   | OMG  | C1    | 385  | X         | -        | -       | -                |
| 1   | OMG  | C1    | 627  | X         | -        | -       | -                |
| 1   | OMG  | C1    | 646  | X         | -        | -       | -                |
| 1   | OMC  | C1    | 778  | X         | -        | -       | -                |
| 1   | OMG  | C1    | 787  | X         | -        | -       | -                |

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 160598 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    | 3138     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 67174 | 30003 | 12160 | 21873 | 3138 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 2   | C2    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3319  | 1484 | 589 | 1090 | 156 |         |       |

- Molecule 3 is a RNA chain called ITS2.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C3    | 82       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1754  | 780 | 316 | 576 | 82 |         |       |

- Molecule 4 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4   | C4    | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2536  | 1131 | 453 | 833 | 119 |         |       |

- Molecule 5 is a protein called Utp30.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | CB    | 265      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2107  | 1351 | 371 | 382 | 3 |         |       |

- Molecule 6 is a protein called Large ribosomal subunit protein uL10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | CF    | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1934  | 1215 | 350 | 360 | 9 |         |       |

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | CH    | 627      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5063  | 3181 | 924 | 939 | 19 |         |       |

- Molecule 8 is a protein called Putative RNA-binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | CI    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1234  | 791 | 230 | 208 | 5 |         |       |

- Molecule 9 is a protein called Pescadillo homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | CJ    | 382      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3116  | 2008 | 548 | 550 | 10 |         |       |

- Molecule 10 is a protein called Ribosome biogenesis protein NSA2 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | CK    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1903  | 1198 | 368 | 333 | 4 |         |       |

- Molecule 11 is a protein called Putative GTP binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | CL    | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 622   | 389 | 125 | 108 |   |         |       |

- Molecule 12 is a protein called 60S ribosomal protein l7-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | CM    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1773  | 1144 | 329 | 297 | 3 |         |       |
| 12  | LF    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2023  | 1297 | 377 | 346 | 3 |         |       |

- Molecule 13 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | CN    | 246      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1853  | 1156 | 322 | 368 | 7 |         |       |

- Molecule 14 is a protein called DUF2423 domain-containing protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14  | CO    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 468   | 290 | 94 | 82 | 2 |         |       |

- Molecule 15 is a protein called Ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15  | CQ    | 183      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1480  | 925 | 304 | 241 | 10 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 16  | Lq    | 139      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1073  | 672 | 213 | 188 |         |       |

- Molecule 17 is a protein called Zinc finger domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Cb    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 517 | 161 | 148 | 4 |         |       |

- Molecule 18 is a protein called Nucleolar GTP-binding protein 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | Cd    | 462      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3691  | 2350 | 671 | 659 | 11 |         |       |

- Molecule 19 is a protein called Ribosome biogenesis protein NOP53.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | Ce    | 313      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2549  | 1585 | 487 | 473 | 4 |         |       |

- Molecule 20 is a protein called Ribosome production factor 2 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | Cf    | 285      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2282  | 1443 | 417 | 401 | 21 |         |       |

- Molecule 21 is a protein called Ribosome biogenesis regulatory protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | Cg    | 188      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1478  | 924 | 283 | 270 | 1 |         |       |

- Molecule 22 is a protein called Ribosome assembly protein 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | Ch    | 485      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3813  | 2396 | 697 | 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 23 is a protein called rRNA-processing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Cz    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 869   | 541 | 180 | 144 | 4 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L2-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | LA    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1454  | 917 | 278 | 256 | 3 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L3-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | LB    | 389      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3104  | 1973 | 579 | 539 | 13 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L4-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | LC    | 363      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2751  | 1737 | 527 | 478 | 9 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein l5-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | LD    | 286      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2266  | 1434 | 407 | 422 | 3 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LE    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 944 | 267 | 263 | 3 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29  | LG    | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1889  | 1210 | 350 | 324 | 5 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein l9-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | LH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 949 | 268 | 272 | 6 |         |       |

- Molecule 31 is a protein called Putative ribosomal protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | LJ    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1357  | 850 | 266 | 235 | 6 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L12-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | LK    | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1184  | 743 | 215 | 224 | 2 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | LL    | 203      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1587  | 989 | 325 | 271 | 2 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L14-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | LM    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1126  | 714 | 216 | 195 | 1 |         |       |

- Molecule 35 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | LN    | 202      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1062 | 360 | 278 | 4 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L16-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | LO    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1611  | 1034 | 305 | 267 | 5 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein l17-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | LP    | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1343  | 834 | 274 | 232 | 3 |         |       |

- Molecule 38 is a protein called Ribosomal protein L18-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | LQ    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1200  | 759 | 239 | 200 | 2 |         |       |

- Molecule 39 is a protein called Ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | LR    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1241  | 772 | 262 | 203 | 4 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | LS    | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1426  | 917 | 266 | 238 | 5 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | LT    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1027  | 651 | 195 | 179 | 2 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L22-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | LU    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 846   | 548 | 146 | 151 | 1 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein l23-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | LV    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 991   | 630 | 184 | 170 | 7 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L25-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 44  | LX    | 145      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1133  | 723 | 211 | 199 |  |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L26-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | LY    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1056  | 658 | 213 | 183 | 2 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | LZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 713 | 207 | 188 | 4 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L28-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | La    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 872   | 556 | 168 | 147 | 1 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein l30-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | Lc    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 449 | 122 | 129 | 5 |         |       |

- Molecule 49 is a protein called Putative 60S ribosomal protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | Ld    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 875   | 555 | 171 | 148 | 1 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L32-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | Le    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1017  | 640 | 208 | 163 | 6 |         |       |

- Molecule 51 is a protein called 60S ribosomal protein l33-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | Lf    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 546 | 171 | 144 | 1 |         |       |

- Molecule 52 is a protein called Ribosomal protein l34-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | Lg    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 914   | 567 | 186 | 157 | 4 |         |       |

- Molecule 53 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 53  | Lh    | 122      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1003  | 637 | 198 | 168 |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | Li    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 509 | 181 | 136 | 1 |         |       |

- Molecule 55 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | Lj    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 698   | 427 | 154 | 112 | 5 |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L38-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | Lk    | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 632   | 400 | 121 | 109 | 2 |         |       |

- Molecule 57 is a protein called Ribosomal protein eL39.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 57  | Ll    | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 436   | 275 | 97 | 64 |         |       |

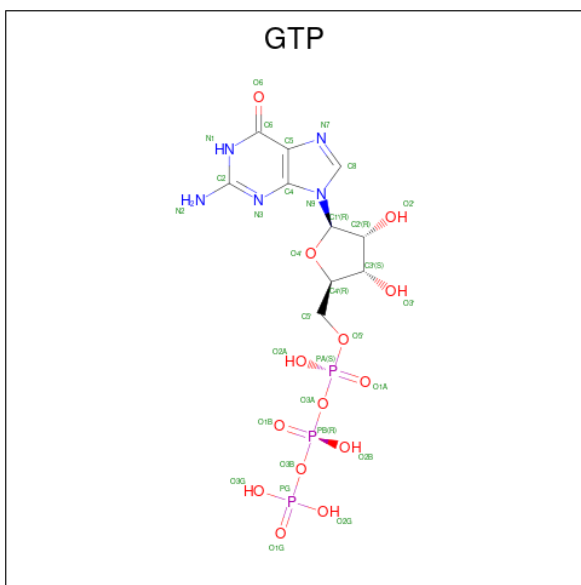
- Molecule 58 is a protein called 60S ribosomal protein L43-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 698   | 430 | 138 | 124 | 6 |         |       |

- Molecule 59 is a protein called Ribosomal protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 59  | Lr    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 1056 | 296 | 300 | 8 |         |       |

- Molecule 60 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 |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 60  | CH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 60  | Cd    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 61  | CH    | 1        | Total Mg<br>1 1 | 0       |
| 61  | Cd    | 2        | Total Mg<br>2 2 | 0       |

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 62  | CQ    | 1        | Total Zn<br>1 1 | 0       |
| 62  | Cb    | 1        | Total Zn<br>1 1 | 0       |
| 62  | Lg    | 1        | Total Zn<br>1 1 | 0       |
| 62  | Lj    | 1        | Total Zn<br>1 1 | 0       |
| 62  | Lp    | 1        | Total Zn<br>1 1 | 0       |

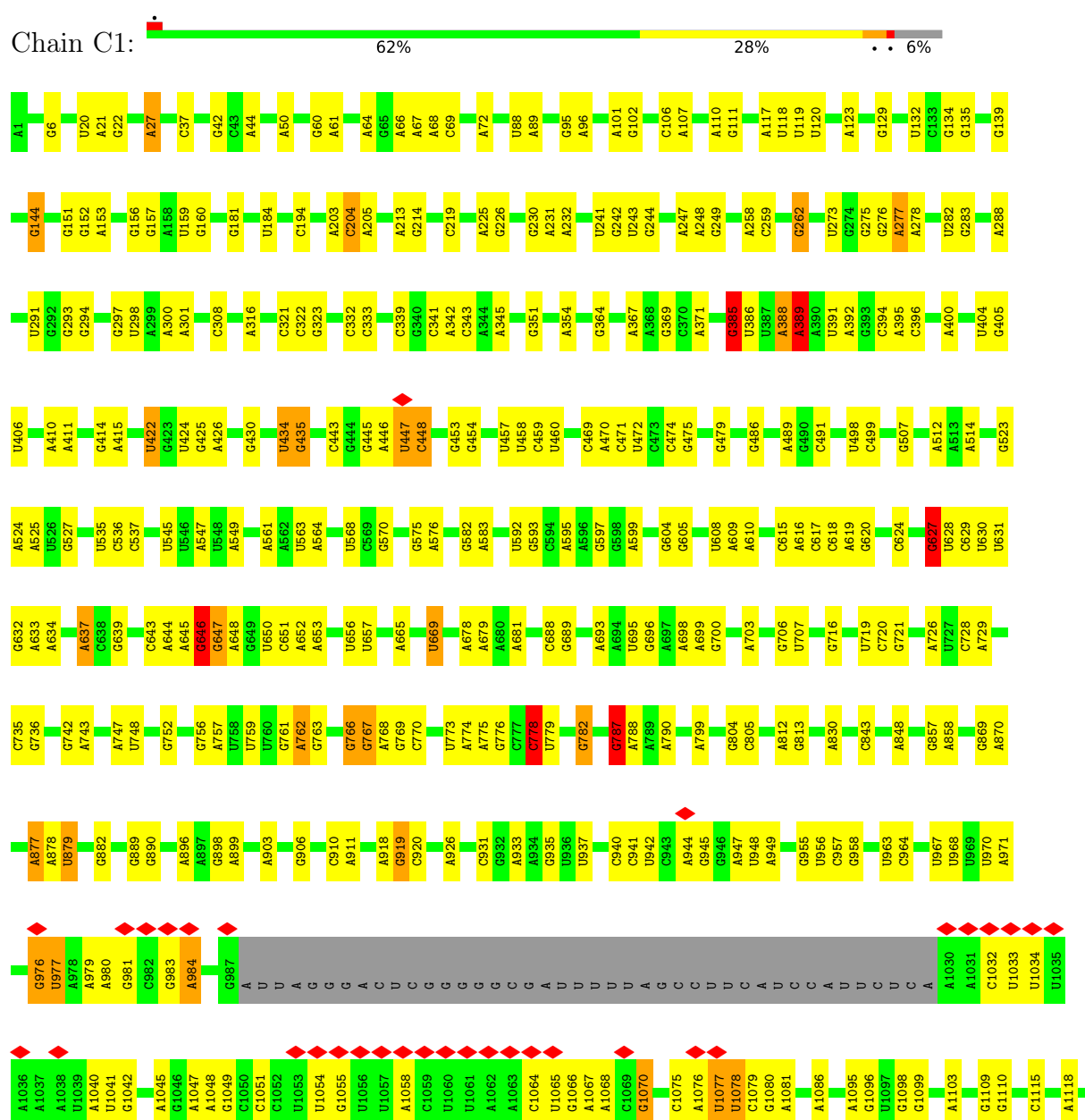
- Molecule 63 is water.

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 63  | CH    | 1        | Total<br>1 | O<br>1 | 0       |
| 63  | 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



|       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2499 | U2409 | U2307 | C2230 | C2125 | G1776 | A1623 | U1506 | G1375 | U1241 | A1126 |
| U2500 | A2410 | A2308 | U2231 | U1241 | A1777 | C1624 | A1517 | A1382 | A1246 | U1127 |
| U2501 | G2411 | U2314 | A     | A1246 | A1778 | U1625 | A1518 | G1383 | G1247 | G1128 |
| G2502 | G2415 | A2315 | A     | G1247 | A1779 | G1638 | G1519 | G1387 | U1248 | G1132 |
| G2503 | U2416 | G2316 | G     | A1248 | A1780 | A1639 | G1526 | A1390 | A1136 | A1137 |
| G2504 | G2417 | G2317 | U2237 | G1783 | G1784 | C1640 | U1536 | A1395 | U1252 |       |
| G2505 | U2418 | A2318 | A2243 | G1792 | G1793 | G1642 | U1537 | G1396 | C1255 | C1143 |
| G2506 | A2419 | A2320 | U     | A1794 | A1795 | G1646 | U1538 | A1401 | U1264 | G1148 |
| G2508 | G2420 | A2321 | G     | U1796 | A1797 | G1647 | U1539 | A1404 | G1265 | G1159 |
|       | A2421 | G2322 | G2045 | U1798 | A1799 | U1661 | A1541 | G1404 | G1266 | G1160 |
| G2515 | A2422 | C2323 | C2046 | U1799 | U1800 | A1677 | G1543 | G1405 | C1267 | G1161 |
| G2516 | U2423 | U2329 | G2047 | U1801 | C1800 | A1677 | G1544 | G1417 | A1269 | A1162 |
| A2517 | U2424 | A2330 | G2049 | U1802 | C1801 | U1681 | G1549 | U1418 | A1270 | U1164 |
| G2518 | G2425 | A2331 | G2050 | C1802 | C1802 | U1682 | G1551 | G1419 | G1278 | G1165 |
| A2521 | G2426 | G2334 | G2051 | A1809 | U1809 | U1685 | G1552 | U1421 | G1283 |       |
| A2522 | U2427 | G2340 | U2052 | G1809 | G1809 | C1697 | G1554 | U1422 | U1173 |       |
| G2523 | G2428 | A2348 | A2053 | G1812 | G1813 | A1698 | G1559 | U1425 | C1175 | A1176 |
| G2524 | G2431 | U2349 | A2054 | G1814 | U1814 | G1699 | U1560 | A1429 | U1288 | G1177 |
|       | G2432 | U2355 | A2055 | G1815 | C1816 | U1704 | G1563 | G1430 | G1290 | A1178 |
| G2533 | U2433 | G2356 | A2056 | G1822 | U1822 | G1707 | A1567 | A1432 | U1292 | C1179 |
| G2544 | G2434 | G2357 | A2069 | G1826 | C1826 | G1710 | A1568 | C1434 | G1296 | A1185 |
| G2545 | U2435 | G2358 | A2070 | G1829 | C1829 | U1722 | A1572 | U1438 | U1305 | A1186 |
| A2552 | G2436 | G2359 | A2076 | A1830 | A1830 | C1726 | A1573 | G1449 | A1313 | A1187 |
| U2556 | G2437 | U2362 | G2079 | G1833 | C1833 | A1730 | G1576 | U1454 | G1316 |       |
| G2557 | U2438 | A2364 | C2080 | G1837 | C1837 | G1731 | C1577 | G1455 |       | G1199 |
| G2562 | G2439 | G2365 | A2089 | U1842 | U1843 | G1737 | G1585 | G1458 | A1331 | C1202 |
| U2566 | G2440 | A2366 | A2089 | G1844 | A1844 | U1743 | U1586 | G1459 | G1332 | G1205 |
| G2567 | U2441 | U2374 | G2084 | G1845 | A1845 | C1744 | C1588 | A1460 | A1333 |       |
| G2568 | G2442 | G2375 | G2085 | G1846 | A1847 | U1745 | U1595 | G1463 | A1335 | G1209 |
| G2569 | U2443 | U2376 | G2086 | U1851 | U1851 | G1746 | U1596 | A1464 | C1336 | G1210 |
| U2570 | A2451 | G2377 | A2089 | U1856 | U1857 | G1751 | G1604 | G1476 | G1337 | A1211 |
| U2571 | G2454 | U2380 | G2092 | G1857 | G1858 | G1758 | U1609 | A1480 | U1339 |       |
| G2575 | G2455 | A2381 | U2092 | U1859 | A1859 | C1759 | G1610 | C1480 | G1345 | G1215 |
| U2576 | U2456 | A2382 | A2101 | U1860 | U1860 | U1761 | C1611 | A1481 | A1346 | G1220 |
| G2577 | G2457 | U2384 | A2102 | A1866 | A1867 | U1762 | G1614 | G1485 | U1361 | A1223 |
| G2578 | U2458 | U2389 | U2103 | A1868 | U1868 | C1763 | G1615 | G1485 | G1362 | A1228 |
| G2579 | G2459 | G2392 | U2104 | A1871 | A1871 | G1766 | A1618 | G1492 | G1370 | A1234 |
| G2582 | U2465 | A2393 | A2105 |       |       | G1767 | C1619 | G1493 | U1371 | C1238 |
| G2583 | G2466 | G2398 | A2112 |       |       |       |       | U1505 |       | G1239 |
| C2584 | U2472 | U2399 | U2117 |       |       |       |       |       |       |       |
| A2585 | U2473 | U2400 | A2118 |       |       |       |       |       |       |       |
| U2592 | A2474 | A2404 | U2119 |       |       |       |       |       |       |       |
| U     | U2477 | A2406 | U2121 |       |       |       |       |       |       |       |
| A     | A     | C2407 | U2122 |       |       |       |       |       |       |       |
| A     | A     | G2226 | G2123 |       |       |       |       |       |       |       |
| A     | A     | A2225 | G2124 |       |       |       |       |       |       |       |
|       |       | U2229 |       |       |       |       |       |       |       |       |

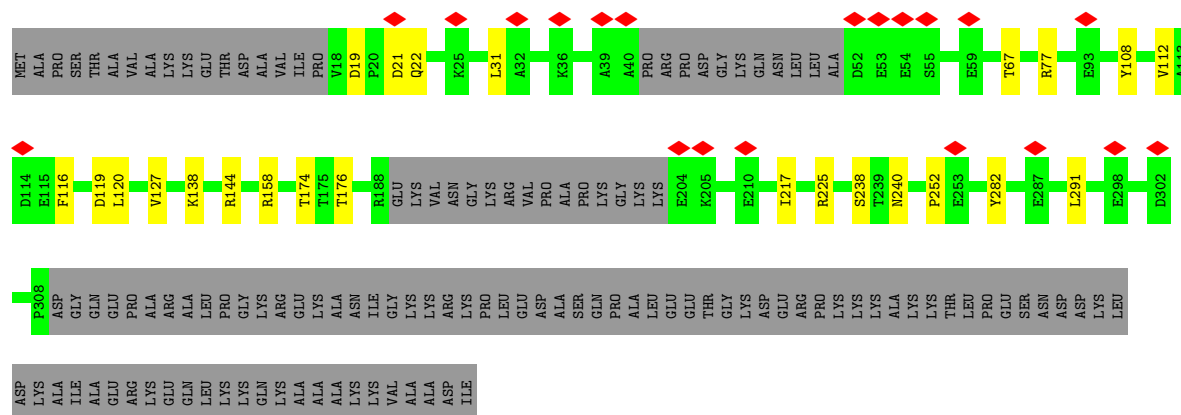


Chain C4: 



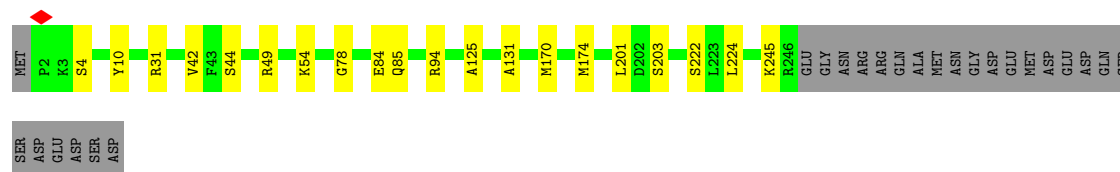
• Molecule 5: Utp30

Chain CB: 



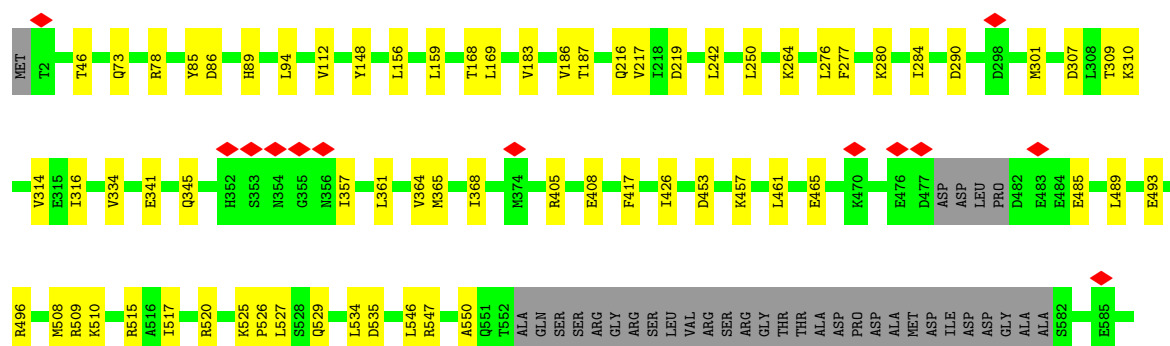
• Molecule 6: Large ribosomal subunit protein uL10

Chain CF: 



• Molecule 7: Nucleolar GTP-binding protein 1

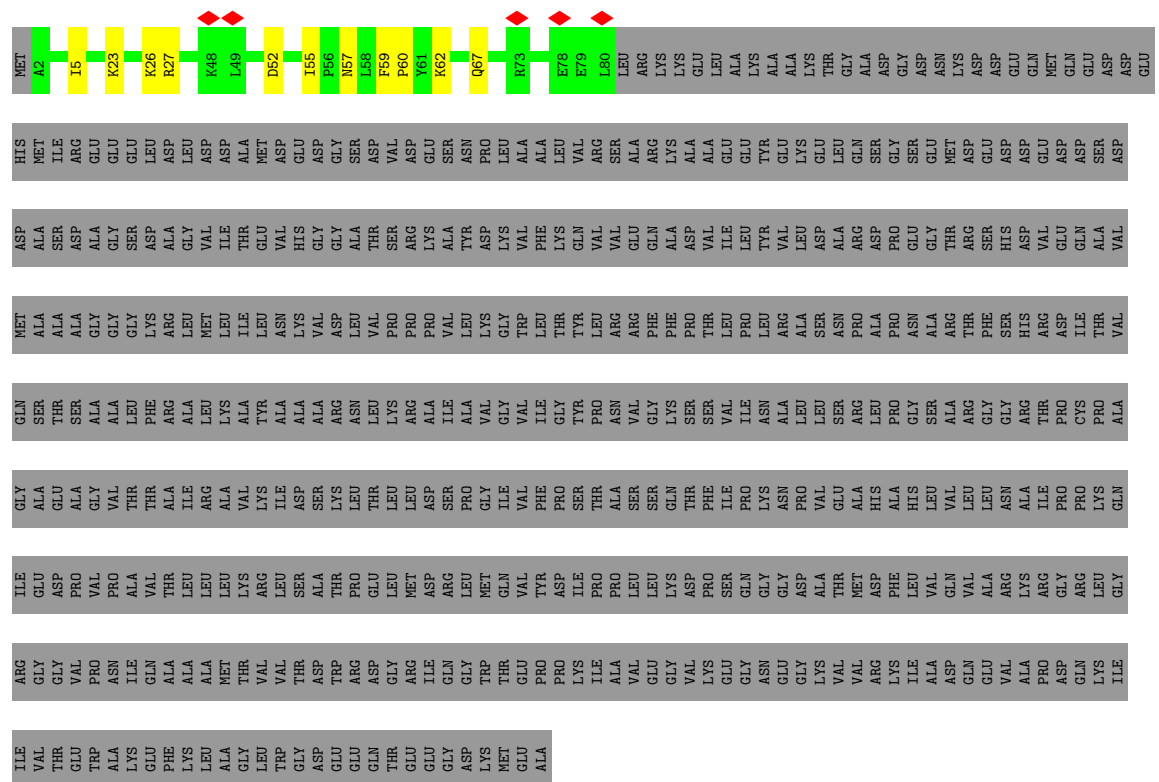
Chain CH: 



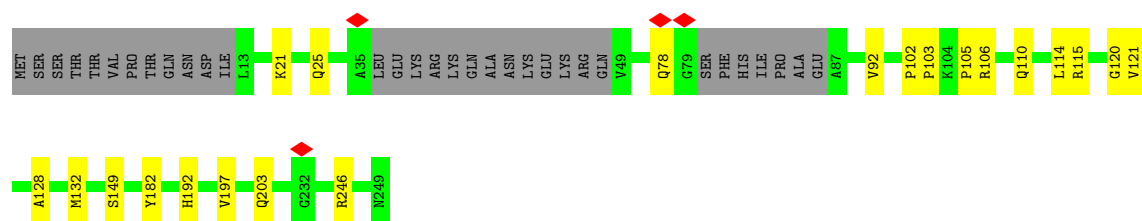


|      |      |      |      |      |            |      |      |                                                                           |                                                                                                                                   |                                                              |
|------|------|------|------|------|------------|------|------|---------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------|
| P154 | P165 | R170 | M190 | P196 | N224       | R241 | T246 | P249                                                                      | V261                                                                                                                              |                                                              |
| Met  | P2   | R16  | E21  | K26  | Q53<br>R54 | Q57  | E69  | V73<br>LYS<br>GLY<br>ARG<br>PRO<br>ALA<br>ALA<br>GLU<br>GLU<br>LYS<br>GLU | P82<br>P87<br>L90<br>A99<br>LYS<br>ALA<br>LEU<br>SER<br>SER<br>GLN<br>ILE<br>LYS<br>ASN<br>LYS<br>ARG<br>ALA<br>GLU<br>LYS<br>ALA | A115<br>I121<br>F133<br>K140<br>T142<br>H143<br>K144<br>R149 |

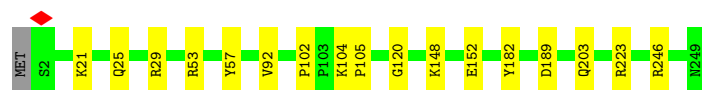
Chain CL:  12% 86%



Chain CM:  79% 8% 13%



Chain LF:  93% 7%



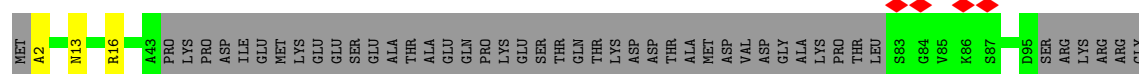
- Molecule 13: Eukaryotic translation initiation factor 6

Chain CN: 88% 12%



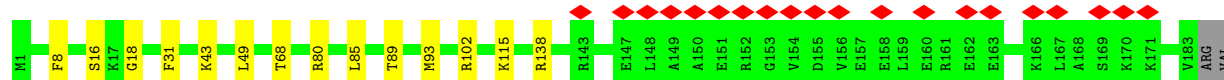
- Molecule 14: DUF2423 domain-containing protein

Chain CO: 48% 48%



- Molecule 15: Ribosome biogenesis protein RLP24

Chain CQ: 9% 75% 6% 19%



- Molecule 16: Putative 60S ribosomal protein

Chain Lq: 85% 10% 5%



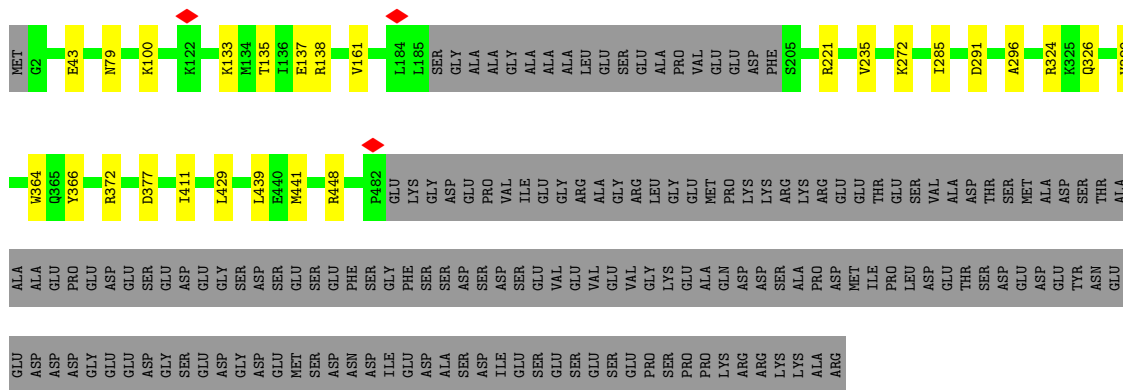
- Molecule 17: Zinc finger domain-containing protein

Chain Cb: 79% 8% 14%

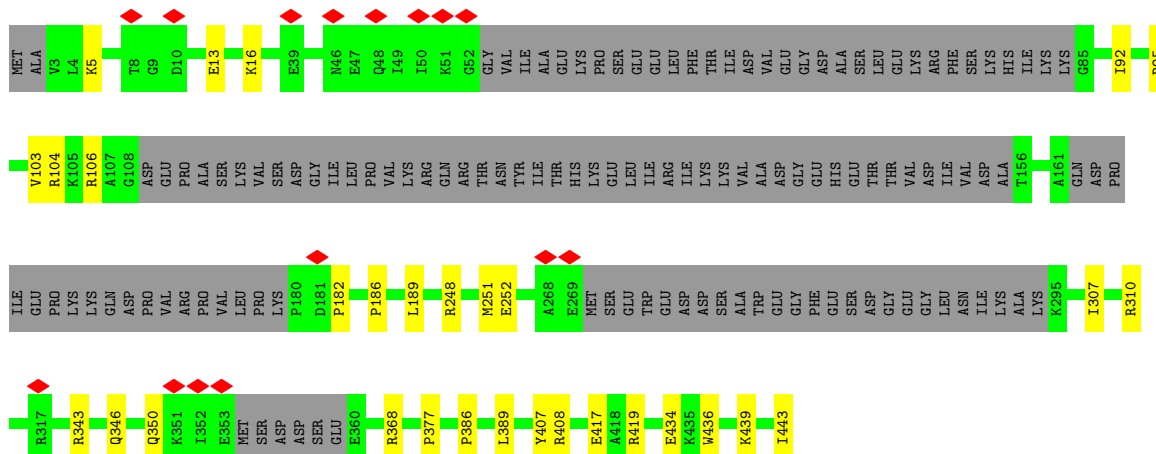


- Molecule 18: Nucleolar GTP-binding protein 2

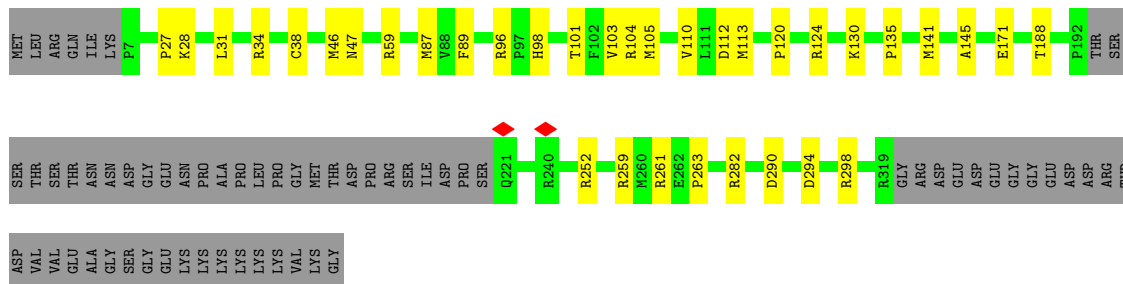
Chain Cd: 70% 26%



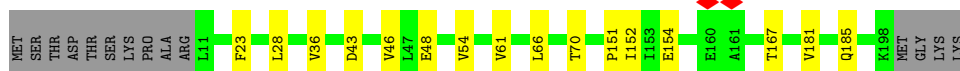
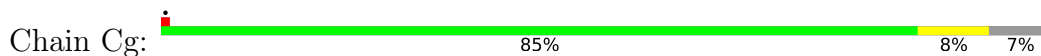
- Molecule 19: Ribosome biogenesis protein NOP53



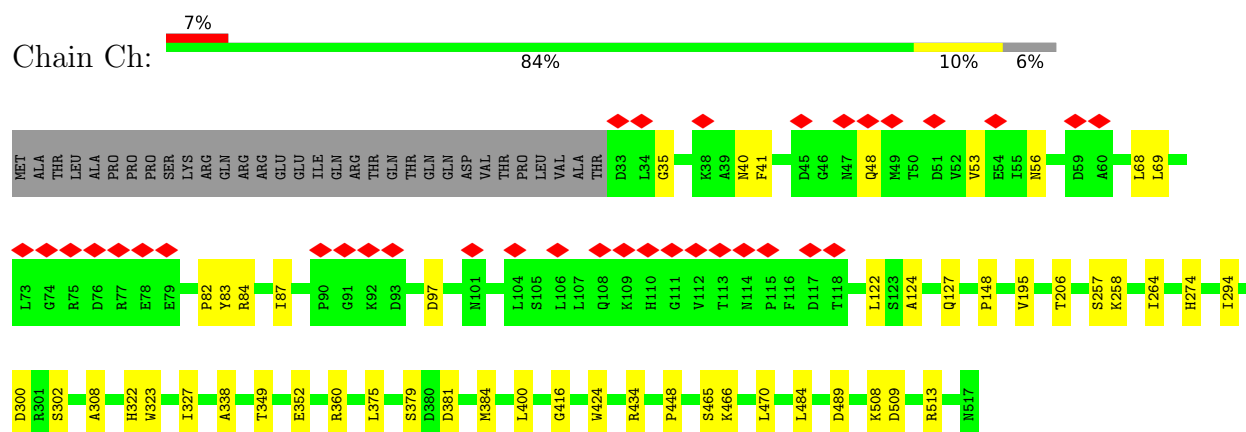
- Molecule 20: Ribosome production factor 2 homolog



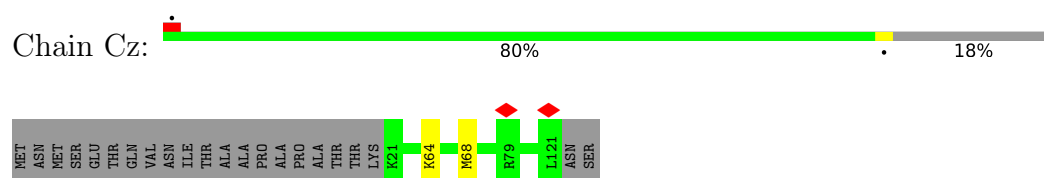
- Molecule 21: Ribosome biogenesis regulatory protein



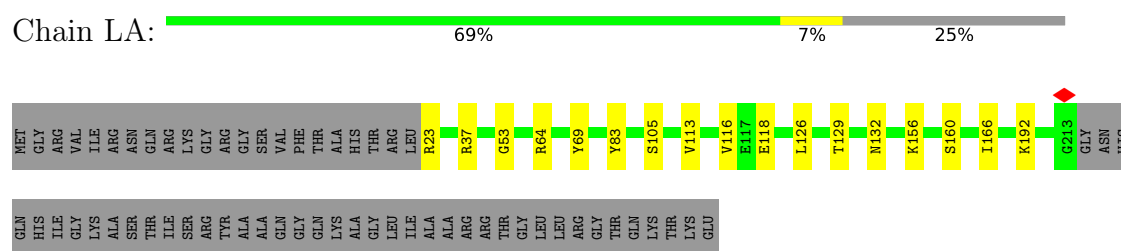
- Molecule 22: Ribosome assembly protein 4



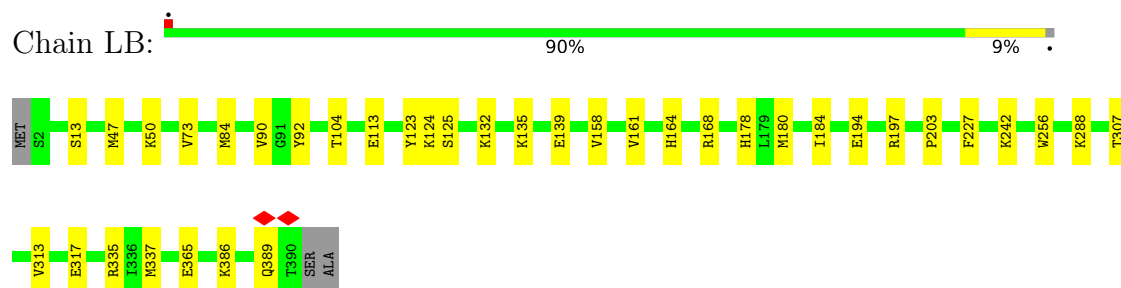
- Molecule 23: rRNA-processing protein



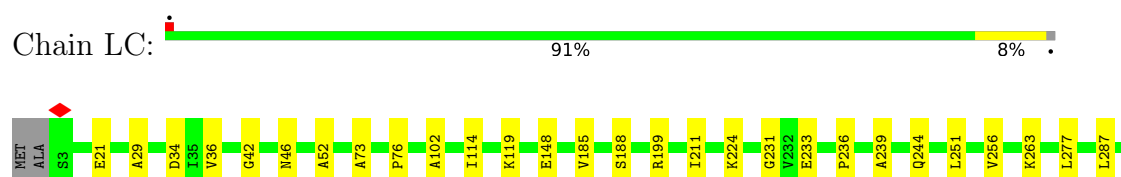
- Molecule 24: 60S ribosomal protein L2-like protein



- Molecule 25: 60S ribosomal protein L3-like protein

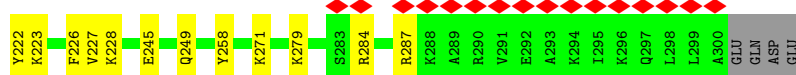
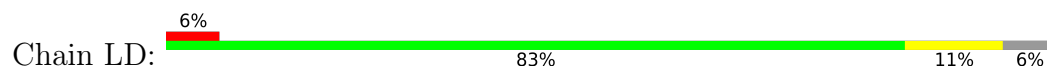


- Molecule 26: 60S ribosomal protein L4-like protein

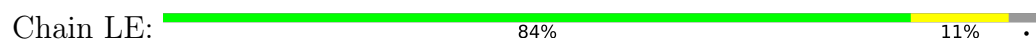




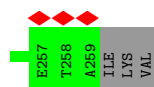
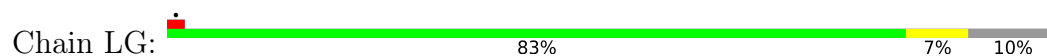
- Molecule 27: 60S ribosomal protein l5-like protein



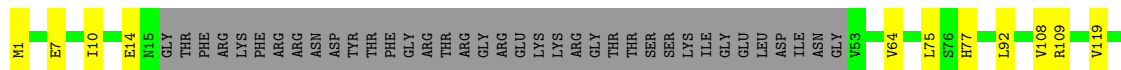
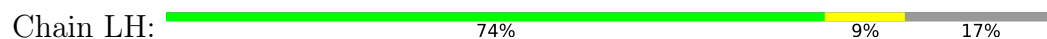
- Molecule 28: 60S ribosomal protein L6



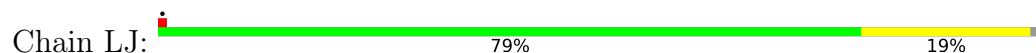
- Molecule 29: 60S ribosomal protein L8

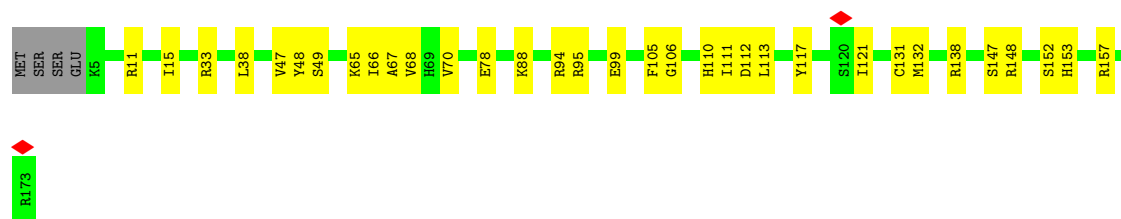


- Molecule 30: 60S ribosomal protein l9-like protein



- Molecule 31: Putative ribosomal protein

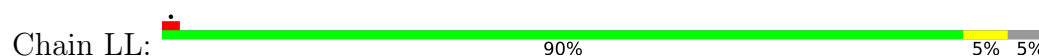




- Molecule 32: 60S ribosomal protein L12-like protein



- Molecule 33: 60S ribosomal protein L13



- Molecule 34: 60S ribosomal protein L14-like protein



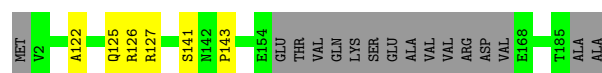
- Molecule 35: Ribosomal protein L15



- Molecule 36: 60S ribosomal protein L16-like protein



- Molecule 37: 60S ribosomal protein l17-like protein











- Molecule 43: 60S ribosomal protein l23-like protein

Chain LV: 84% 13%



- Molecule 44: 60S ribosomal protein L25-like protein

Chain LX: 87% 6% 7%



- Molecule 45: 60S ribosomal protein L26-like protein

Chain LY: 83% 14%



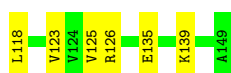
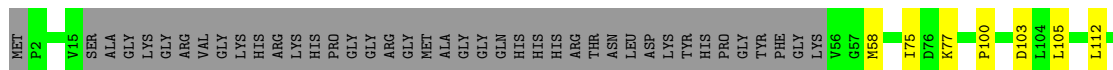
- Molecule 46: 60S ribosomal protein L27

Chain LZ: 87% 13%



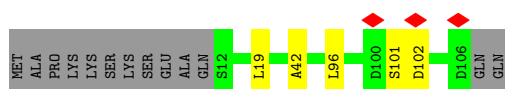
- Molecule 47: 60S ribosomal protein L28-like protein

Chain La: 64% 9% 28%



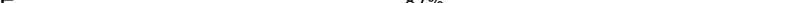
- Molecule 48: 60S ribosomal protein l30-like protein

Chain Lc: 83% 5% 12%

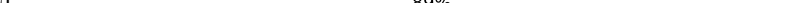


- Molecule 49: Putative 60S ribosomal protein

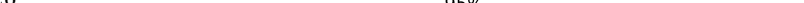
| Amino Acid | Relative Abundance (%) |
|------------|------------------------|
| MET        | ~10                    |
| SER        | ~10                    |
| SER        | ~10                    |
| THR        | ~10                    |
| GLN        | ~10                    |
| LYS        | ~10                    |
| LYS        | ~10                    |
| GLN        | ~10                    |
| ARG        | ~10                    |
| SER        | ~10                    |
| A11        | ~10                    |
| H23        | ~10                    |
| L28        | ~10                    |
| T32        | ~10                    |
| A40        | ~10                    |
| K66        | ~10                    |
| K110       | ~10                    |
| E119       | ~10                    |
| E120       | ~10                    |

- Chain Le:  87% 9% .

| MET | V2 | I39 | D40 | N41 | R42 | R45 | V80 | V83 | I97 | S102 | S103 | R106 | I107 | A125 | K126 | V127 | THR | THR | GLU | VAL |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|

- Chain Lf:  89% 10%

| Position | Information Content (bits) |
|----------|----------------------------|
| MET      | ~1.1                       |
| P2       | ~0.8                       |
| L16      | ~0.3                       |
| K33      | ~0.3                       |
| D38      | ~0.3                       |
| V54      | ~0.3                       |
| Y55      | ~0.3                       |
| K59      | ~0.3                       |
| R67      | ~0.3                       |
| V68      | ~0.3                       |
| K86      | ~0.3                       |
| P90      | ~0.3                       |
| R94      | ~0.3                       |
| I109     | ~0.3                       |

- Chain Lg:  8% 95%

- Chain Lh:  12% 87%

|     |     |     |    |  |     |     |  |     |     |     |     |  |     |     |     |     |     |     |     |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|----|--|-----|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | SER | N4 |  | N16 | K17 |  | S32 | Q33 | Q33 | L34 |  | K38 | S41 | A44 | K45 | K54 | I63 | K79 | D101 | A125 | ALA | THR | TYR | SER | GLU | GLY | PRO | PRO | ALA | LEU | ILE | ILE | TYR | HIS | SER | HIS | GLN | ARG | GLU | ALA | ARG | CYS | CYS | LEU | VAL | GLN | CYS | CYS | THR | PHE | GLU | PRO | TRP |
|-----|-----|-----|----|--|-----|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| LEU | ARG | GLU | SER | LEU | LEU | LEU | PRO | VAL | ALA | ALA | SER | LEU | LYS | GLY | ASN | PHE | THR | ARG | ARG | GLU | ARG | GLN | HIS | ARG | ASN | SER | SER | GLU | ALA | ALA | PRO | LEU | LYS | LEU | LEU | LEU | ALA | ALA | GLY | GLY | LYS | SER | THR | ARG | SER | VAL | LEU | ARG | VAL | ALA | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

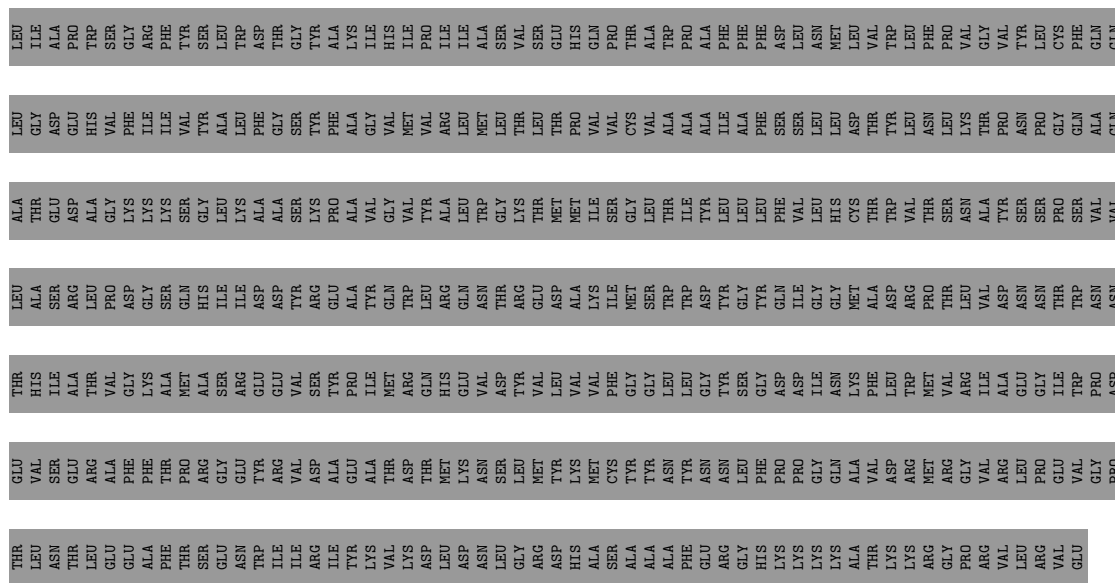
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| LEU | VAL | LEU | LEU | ILE | ALA | GLY | ALA | ALA | VAL | ALA | ALA | SER | ARG | ARG | LEU | PHE | SER | SER | ILE | ILE | ARG | PHE | GLU | GLU | ILE | ILE | HIS | GLU | PHE | PHE | ASP | PRO | TRP | TRP | PHE | ASN | PHE | PHE | ARG | ALA | THR | LYS | TYR | LEU | VAL | VAL | ASN | GLY | GLY | PHE | TYR | LYS | PHE | PHE | TRP | TRP | ASP | ASP | PHE | ASP | ARG | ASP | THR | THR | TRP | HIS | PRO | PRO | LEU | LEU | GLY | ARG |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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

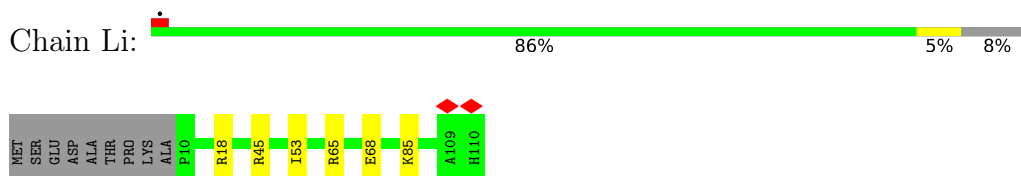
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |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

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| TYR | GLY | TYR | GLY | VAL | ALA | SER | TRP | GLY | GLY | TYR | ALA | PHE | ILE | THR | CYS | LEU | LEU | PRO | LEU | HIS | SER | PHE | VAL | CYS | ILE | CYS | GLY | ARG | TYR | SER | THR | ARG | LEU | TYR | VAL | ALA | TYR | THR | THR | LEU | TRP | TYR | ALA | LEU | GLY | THR | LEU | ALA | SER | GLN | ILE | PRO | PHE | VAL | GLY | PHE | LEU | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

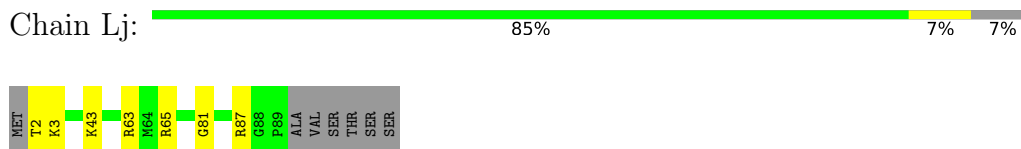
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| VAL | LYS | THR | SER | GLY | HIS | MET | PRO | ALA | LEU | GLY | ILE | PHE | PHE | PHE | LEU | GLN | LEU | LEU | ALA | ALA | PHE | TYR | THR | SER | SER | ARG | ARG | GLN | PHE | PHE | GLN | THR | PHE | LEU | LEU | TRP | LEU | LEU | PHE | ALA | GLY | ILE | PHE | PHE | GLY | LEU | GLY | LEU | GLY | VAL | ILE | ALA | ALA | THR | SER | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



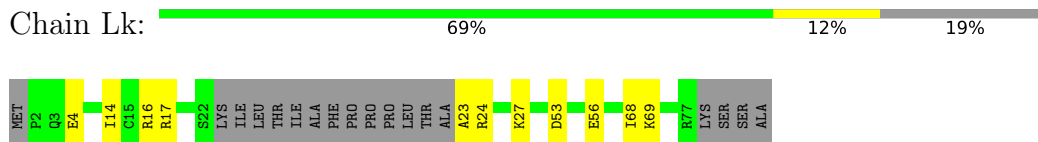
- Molecule 54: 60S ribosomal protein L36



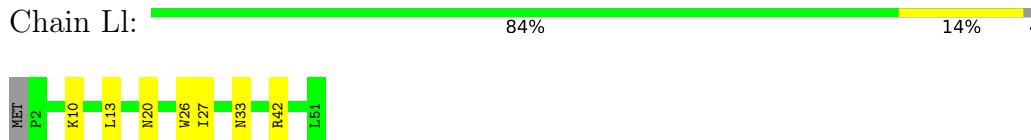
- Molecule 55: Ribosomal protein L37



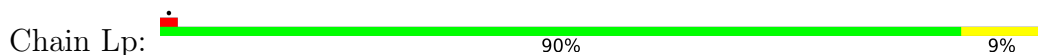
- Molecule 56: 60S ribosomal protein L38-like protein

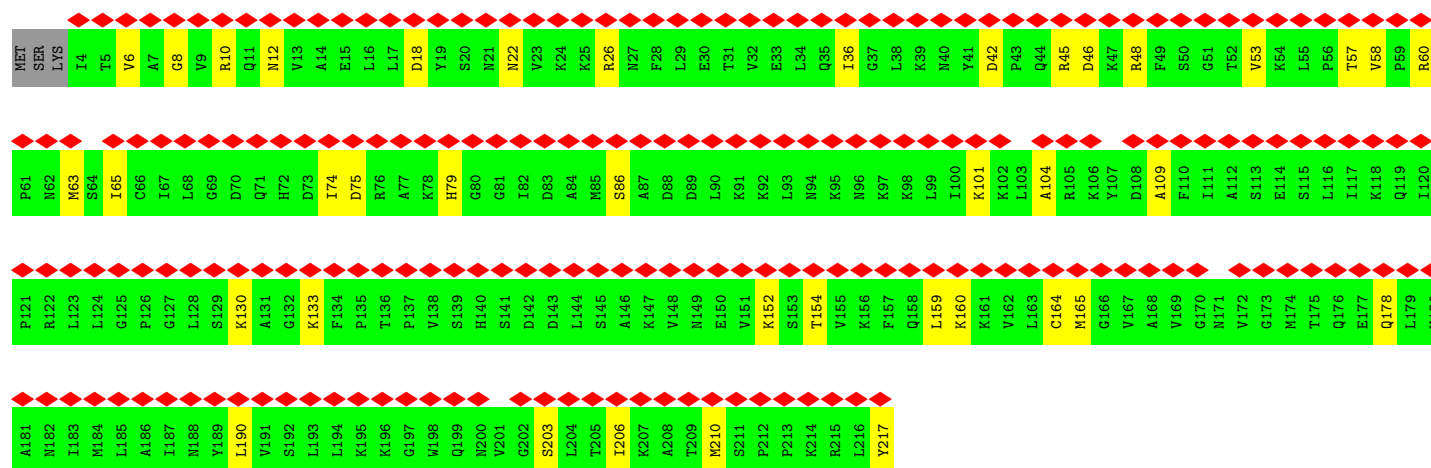


- Molecule 57: Ribosomal protein eL39



- Molecule 58: 60S ribosomal protein L43-like protein





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 74129                                   | 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 ( $e^-/\text{\AA}^2$ ) | 45.6                                    | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 3500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 8.766                                   | Depositor |
| Minimum map value                    | 0.000                                   | Depositor |
| Average map value                    | 0.018                                   | Depositor |
| Map value standard deviation         | 0.167                                   | 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, OMC, ZN, OMG, MG, OMU, A2M

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         | 1/74323 (0.0%) | 0.33        | 0/115881      |
| 2   | C2    | 0.14         | 0/3710         | 0.30        | 0/5778        |
| 3   | C3    | 0.13         | 0/1958         | 0.30        | 0/3050        |
| 4   | C4    | 0.16         | 0/2833         | 0.35        | 0/4414        |
| 5   | CB    | 0.15         | 0/2153         | 0.37        | 0/2926        |
| 6   | CF    | 0.14         | 0/1972         | 0.34        | 0/2660        |
| 7   | CH    | 0.16         | 0/5147         | 0.38        | 0/6926        |
| 8   | CI    | 0.20         | 0/1265         | 0.60        | 4/1702 (0.2%) |
| 9   | CJ    | 0.15         | 0/3196         | 0.33        | 0/4319        |
| 10  | CK    | 0.14         | 0/1939         | 0.34        | 0/2608        |
| 11  | CL    | 0.14         | 0/631          | 0.30        | 0/843         |
| 12  | CM    | 0.15         | 0/1805         | 0.38        | 1/2417 (0.0%) |
| 12  | LF    | 0.17         | 0/2061         | 0.38        | 0/2765        |
| 13  | CN    | 0.14         | 0/1878         | 0.38        | 0/2555        |
| 14  | CO    | 0.14         | 0/470          | 0.32        | 0/619         |
| 15  | CQ    | 0.18         | 0/1504         | 0.38        | 0/2000        |
| 16  | Lq    | 0.15         | 0/1091         | 0.36        | 0/1468        |
| 17  | Cb    | 0.18         | 0/845          | 0.46        | 0/1128        |
| 18  | Cd    | 0.15         | 0/3770         | 0.36        | 0/5082        |
| 19  | Ce    | 0.16         | 0/2579         | 0.37        | 0/3434        |
| 20  | Cf    | 0.14         | 0/2326         | 0.35        | 0/3113        |
| 21  | Cg    | 0.16         | 0/1508         | 0.37        | 0/2051        |
| 22  | Ch    | 0.14         | 0/3914         | 0.40        | 0/5319        |
| 23  | Cz    | 0.17         | 0/877          | 0.33        | 0/1148        |
| 24  | LA    | 0.15         | 0/1488         | 0.39        | 0/2009        |
| 25  | LB    | 0.14         | 0/3172         | 0.37        | 0/4260        |
| 26  | LC    | 0.14         | 0/2808         | 0.34        | 0/3785        |
| 27  | LD    | 0.14         | 0/2308         | 0.33        | 0/3105        |
| 28  | LE    | 0.13         | 0/1504         | 0.30        | 0/2027        |
| 29  | LG    | 0.15         | 0/1918         | 0.35        | 0/2565        |
| 30  | LH    | 0.14         | 0/1515         | 0.38        | 0/2037        |
| 31  | LJ    | 0.15         | 0/1379         | 0.43        | 0/1844        |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 32  | LK    | 0.17         | 0/1198          | 0.41        | 0/1611          |
| 33  | LL    | 0.16         | 0/1614          | 0.37        | 0/2168          |
| 34  | LM    | 0.16         | 0/1145          | 0.34        | 0/1539          |
| 35  | LN    | 0.15         | 0/1741          | 0.37        | 0/2332          |
| 36  | LO    | 0.17         | 0/1645          | 0.41        | 1/2205 (0.0%)   |
| 37  | LP    | 0.15         | 0/1364          | 0.38        | 0/1835          |
| 38  | LQ    | 0.15         | 0/1218          | 0.37        | 0/1639          |
| 39  | LR    | 0.13         | 0/1260          | 0.31        | 0/1683          |
| 40  | LS    | 0.14         | 0/1461          | 0.37        | 0/1966          |
| 41  | LT    | 0.16         | 0/1046          | 0.41        | 0/1409          |
| 42  | LU    | 0.13         | 0/859           | 0.36        | 0/1151          |
| 43  | LV    | 0.13         | 0/1009          | 0.36        | 0/1357          |
| 44  | LX    | 0.16         | 0/1151          | 0.39        | 0/1547          |
| 45  | LY    | 0.17         | 0/1070          | 0.45        | 0/1432          |
| 46  | LZ    | 0.13         | 0/1135          | 0.33        | 0/1519          |
| 47  | La    | 0.14         | 0/892           | 0.33        | 0/1200          |
| 48  | Lc    | 0.14         | 0/714           | 0.34        | 0/960           |
| 49  | Ld    | 0.15         | 0/889           | 0.32        | 0/1192          |
| 50  | Le    | 0.15         | 0/1035          | 0.36        | 0/1379          |
| 51  | Lf    | 0.12         | 0/883           | 0.30        | 0/1187          |
| 52  | Lg    | 0.15         | 0/927           | 0.36        | 0/1244          |
| 53  | Lh    | 0.17         | 0/1014          | 0.39        | 0/1349          |
| 54  | Li    | 0.15         | 0/834           | 0.35        | 0/1099          |
| 55  | Lj    | 0.16         | 0/712           | 0.39        | 0/944           |
| 56  | Lk    | 0.15         | 0/640           | 0.36        | 0/850           |
| 57  | Ll    | 0.13         | 0/446           | 0.27        | 0/593           |
| 58  | Lp    | 0.13         | 0/706           | 0.40        | 0/940           |
| 59  | Lr    | 0.14         | 0/1684          | 0.37        | 0/2266          |
| All | All   | 0.16         | 1/170139 (0.0%) | 0.35        | 6/246434 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | C1    | 36                  | 0                   |
| 53  | Lh    | 0                   | 1                   |
| 56  | Lk    | 0                   | 1                   |
| All | All   | 36                  | 2                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | C1    | 848 | A2M  | O3'-P | 5.15 | 1.61        | 1.56     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8   | CI    | 310 | GLU  | CA-C-N  | -6.13 | 110.40      | 121.14   |
| 8   | CI    | 310 | GLU  | C-N-CA  | -6.13 | 110.40      | 121.14   |
| 8   | CI    | 310 | GLU  | N-CA-CB | 6.05  | 119.65      | 110.28   |
| 8   | CI    | 311 | GLN  | N-CA-CB | 5.32  | 119.08      | 110.40   |
| 12  | CM    | 78  | GLN  | CB-CA-C | -5.15 | 110.22      | 117.23   |
| 36  | LO    | 197 | GLU  | N-CA-CB | 5.12  | 118.74      | 110.40   |

All (36) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom    |
|-----|-------|------|------|---------|
| 1   | C1    | 385  | OMG  | C3',C4' |
| 1   | C1    | 627  | OMG  | C3',C4' |
| 1   | C1    | 646  | OMG  | C3',C4' |
| 1   | C1    | 778  | OMC  | C3',C4' |
| 1   | C1    | 787  | OMG  | C3',C4' |
| 1   | C1    | 1420 | OMC  | C3',C4' |
| 1   | C1    | 1433 | OMG  | C3',C4' |
| 1   | C1    | 1491 | OMC  | C3',C4' |
| 1   | C1    | 1812 | OMC  | C3',C4' |
| 1   | C1    | 1836 | OMC  | C3',C4' |
| 1   | C1    | 2300 | OMC  | C3',C4' |
| 1   | C1    | 2358 | OMG  | C3',C4' |
| 1   | C1    | 2578 | OMG  | C3',C4' |
| 1   | C1    | 2774 | OMG  | C3',C4' |
| 1   | C1    | 2838 | OMC  | C3',C4' |
| 1   | C1    | 2876 | OMG  | C3',C4' |
| 1   | C1    | 2881 | OMG  | C3',C4' |
| 1   | C1    | 2918 | OMC  | C3',C4' |

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 53  | Lh    | 16  | ASN  | Peptide   |
| 56  | Lk    | 16  | ARG  | Sidechain |

## 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    | 67174 | 0        | 33866    | 417     | 0            |
| 2   | C2    | 3319  | 0        | 1678     | 23      | 0            |
| 3   | C3    | 1754  | 0        | 890      | 17      | 0            |
| 4   | C4    | 2536  | 0        | 1286     | 28      | 0            |
| 5   | CB    | 2107  | 0        | 2161     | 17      | 0            |
| 6   | CF    | 1934  | 0        | 1945     | 13      | 0            |
| 7   | CH    | 5063  | 0        | 5157     | 44      | 0            |
| 8   | CI    | 1234  | 0        | 1245     | 13      | 0            |
| 9   | CJ    | 3116  | 0        | 3122     | 27      | 0            |
| 10  | CK    | 1903  | 0        | 1990     | 17      | 0            |
| 11  | CL    | 622   | 0        | 641      | 8       | 0            |
| 12  | CM    | 1773  | 0        | 1879     | 10      | 0            |
| 12  | LF    | 2023  | 0        | 2132     | 11      | 0            |
| 13  | CN    | 1853  | 0        | 1852     | 18      | 0            |
| 14  | CO    | 468   | 0        | 503      | 3       | 0            |
| 15  | CQ    | 1480  | 0        | 1523     | 11      | 0            |
| 16  | Lq    | 1073  | 0        | 1130     | 11      | 0            |
| 17  | Cb    | 830   | 0        | 838      | 6       | 0            |
| 18  | Cd    | 3691  | 0        | 3817     | 19      | 0            |
| 19  | Ce    | 2549  | 0        | 2660     | 22      | 0            |
| 20  | Cf    | 2282  | 0        | 2347     | 26      | 0            |
| 21  | Cg    | 1478  | 0        | 1517     | 12      | 0            |
| 22  | Ch    | 3813  | 0        | 3715     | 27      | 0            |
| 23  | Cz    | 869   | 0        | 956      | 2       | 0            |
| 24  | LA    | 1454  | 0        | 1490     | 11      | 0            |
| 25  | LB    | 3104  | 0        | 3221     | 24      | 0            |
| 26  | LC    | 2751  | 0        | 2875     | 25      | 0            |
| 27  | LD    | 2266  | 0        | 2219     | 22      | 0            |
| 28  | LE    | 1477  | 0        | 1567     | 16      | 0            |
| 29  | LG    | 1889  | 0        | 2043     | 13      | 0            |
| 30  | LH    | 1495  | 0        | 1573     | 13      | 0            |
| 31  | LJ    | 1357  | 0        | 1385     | 23      | 0            |
| 32  | LK    | 1184  | 0        | 1249     | 6       | 0            |
| 33  | LL    | 1587  | 0        | 1655     | 9       | 0            |
| 34  | LM    | 1126  | 0        | 1198     | 12      | 0            |
| 35  | LN    | 1704  | 0        | 1767     | 15      | 0            |
| 36  | LO    | 1611  | 0        | 1702     | 12      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 37  | LP    | 1343   | 0        | 1369     | 5       | 0            |
| 38  | LQ    | 1200   | 0        | 1296     | 11      | 0            |
| 39  | LR    | 1241   | 0        | 1298     | 9       | 0            |
| 40  | LS    | 1426   | 0        | 1481     | 17      | 0            |
| 41  | LT    | 1027   | 0        | 1076     | 7       | 0            |
| 42  | LU    | 846    | 0        | 883      | 3       | 0            |
| 43  | LV    | 991    | 0        | 1044     | 11      | 0            |
| 44  | LX    | 1133   | 0        | 1234     | 8       | 0            |
| 45  | LY    | 1056   | 0        | 1143     | 13      | 0            |
| 46  | LZ    | 1112   | 0        | 1181     | 11      | 0            |
| 47  | La    | 872    | 0        | 903      | 8       | 0            |
| 48  | Lc    | 705    | 0        | 751      | 3       | 0            |
| 49  | Ld    | 875    | 0        | 918      | 5       | 0            |
| 50  | Le    | 1017   | 0        | 1092     | 9       | 0            |
| 51  | Lf    | 862    | 0        | 891      | 9       | 0            |
| 52  | Lg    | 914    | 0        | 960      | 4       | 0            |
| 53  | Lh    | 1003   | 0        | 1116     | 7       | 0            |
| 54  | Li    | 827    | 0        | 906      | 5       | 0            |
| 55  | Lj    | 698    | 0        | 726      | 8       | 0            |
| 56  | Lk    | 632    | 0        | 693      | 6       | 0            |
| 57  | Ll    | 436    | 0        | 473      | 5       | 0            |
| 58  | Lp    | 698    | 0        | 737      | 5       | 0            |
| 59  | Lr    | 1660   | 0        | 1768     | 26      | 0            |
| 60  | CH    | 32     | 0        | 12       | 0       | 0            |
| 60  | Cd    | 32     | 0        | 12       | 1       | 0            |
| 61  | CH    | 1      | 0        | 0        | 0       | 0            |
| 61  | Cd    | 2      | 0        | 0        | 0       | 0            |
| 62  | CQ    | 1      | 0        | 0        | 0       | 0            |
| 62  | Cb    | 1      | 0        | 0        | 0       | 0            |
| 62  | Lg    | 1      | 0        | 0        | 0       | 0            |
| 62  | Lj    | 1      | 0        | 0        | 0       | 0            |
| 62  | Lp    | 1      | 0        | 0        | 0       | 0            |
| 63  | CH    | 1      | 0        | 0        | 0       | 0            |
| 63  | Cd    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 160598 | 0        | 126757   | 973     | 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 3.

All (973) 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:C1:3289:G:H1     | 1:C1:3298:U:H3     | 1.05                     | 1.00              |
| 1:C1:1054:U:H3     | 1:C1:1070:G:H1     | 0.90                     | 0.84              |
| 1:C1:1809:G:HO2'   | 9:CJ:2:GLY:N       | 1.76                     | 0.82              |
| 33:LL:199:GLU:HG2  | 33:LL:203:LYS:HZ3  | 1.43                     | 0.81              |
| 20:Cf:87:MET:HB2   | 20:Cf:103:VAL:HB   | 1.72                     | 0.71              |
| 1:C1:1420:OMC:H5'  | 26:LC:73:ALA:HB2   | 1.71                     | 0.71              |
| 17:Cb:52:CYS:SG    | 17:Cb:74:HIS:HE1   | 2.14                     | 0.70              |
| 53:Lh:34:LEU:O     | 53:Lh:45:LYS:NZ    | 2.22                     | 0.69              |
| 8:CI:242:ASP:OD2   | 8:CI:246:ARG:NH1   | 2.26                     | 0.69              |
| 1:C1:2101:A:HO2'   | 55:Lj:2:THR:N      | 1.92                     | 0.68              |
| 1:C1:1588:C:O2'    | 44:LX:92:GLN:NE2   | 2.23                     | 0.68              |
| 59:Lr:160:LYS:H    | 59:Lr:165:MET:HE1  | 1.59                     | 0.68              |
| 1:C1:2087:G:O2'    | 18:Cd:448:ARG:NH1  | 2.29                     | 0.66              |
| 3:C3:40:G:H1       | 3:C3:45:U:H3       | 1.45                     | 0.65              |
| 21:Cg:151:PRO:HB2  | 21:Cg:152:ILE:HD12 | 1.79                     | 0.65              |
| 1:C1:643:C:H2'     | 1:C1:644:A:H8      | 1.62                     | 0.65              |
| 8:CI:246:ARG:NH2   | 19:Ce:443:ILE:OXT  | 2.30                     | 0.64              |
| 18:Cd:411:ILE:HG13 | 18:Cd:439:LEU:HD11 | 1.79                     | 0.64              |
| 1:C1:2577:G:H4'    | 1:C1:2578:OMG:H5'  | 1.79                     | 0.64              |
| 43:LV:106:ASN:HD21 | 43:LV:110:GLU:HB2  | 1.63                     | 0.64              |
| 1:C1:1661:U:OP1    | 7:CH:509:ARG:NH1   | 2.30                     | 0.63              |
| 16:Lq:31:ASP:HB3   | 16:Lq:34:ASN:HB2   | 1.80                     | 0.63              |
| 7:CH:242:LEU:O     | 7:CH:280:LYS:NZ    | 2.29                     | 0.63              |
| 6:CF:94:ARG:HD2    | 6:CF:245:LYS:HD3   | 1.80                     | 0.63              |
| 30:LH:129:TYR:HB3  | 30:LH:218:ILE:HG12 | 1.81                     | 0.63              |
| 31:LJ:94:ARG:HG3   | 31:LJ:157:ARG:HH21 | 1.64                     | 0.62              |
| 59:Lr:75:ASP:O     | 59:Lr:79:HIS:ND1   | 2.29                     | 0.62              |
| 1:C1:1067:A:O2'    | 41:LT:35:ARG:NH2   | 2.32                     | 0.62              |
| 4:C4:80:U:H3       | 4:C4:98:G:H1       | 1.46                     | 0.62              |
| 10:CK:54:ARG:NH1   | 10:CK:57:GLN:OE1   | 2.32                     | 0.62              |
| 26:LC:185:VAL:HG11 | 26:LC:231:GLY:HA3  | 1.81                     | 0.62              |
| 18:Cd:285:ILE:HD11 | 18:Cd:296:ALA:HB2  | 1.81                     | 0.62              |
| 54:Li:65:ARG:NH1   | 54:Li:68:GLU:OE1   | 2.33                     | 0.62              |
| 22:Ch:84:ARG:NH1   | 22:Ch:97:ASP:OD1   | 2.33                     | 0.62              |
| 4:C4:61:C:O2'      | 27:LD:279:LYS:NZ   | 2.33                     | 0.61              |
| 1:C1:2734:U:H1'    | 47:La:58:MET:HE1   | 1.82                     | 0.61              |
| 6:CF:10:TYR:OH     | 10:CK:69:GLU:OE2   | 2.18                     | 0.61              |
| 27:LD:83:LEU:HB3   | 27:LD:88:ILE:HB    | 1.81                     | 0.61              |
| 37:LP:125:GLN:HB3  | 37:LP:141:SER:HB2  | 1.83                     | 0.61              |
| 45:LY:71:SER:HB3   | 45:LY:80:HIS:HB2   | 1.82                     | 0.61              |
| 49:Ld:28:LEU:HD11  | 49:Ld:40:ALA:HB2   | 1.83                     | 0.61              |
| 1:C1:2221:U:H2'    | 1:C1:2222:A:H8     | 1.65                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:LC:301:ARG:NH2  | 38:LQ:66:ARG:O     | 2.33                     | 0.61              |
| 13:CN:109:VAL:HB   | 13:CN:149:GLY:HA2  | 1.82                     | 0.61              |
| 23:Cz:68:MET:HE2   | 41:LT:160:ILE:HG12 | 1.82                     | 0.61              |
| 30:LH:10:ILE:HG12  | 30:LH:109:ARG:HG2  | 1.82                     | 0.61              |
| 59:Lr:60:ARG:HD3   | 59:Lr:63:MET:HG3   | 1.82                     | 0.61              |
| 27:LD:214:LEU:HB3  | 27:LD:222:TYR:HB2  | 1.81                     | 0.61              |
| 30:LH:127:MET:HG2  | 30:LH:220:VAL:HA   | 1.82                     | 0.61              |
| 1:C1:1812:OMC:OP1  | 44:LX:133:LYS:NZ   | 2.32                     | 0.60              |
| 1:C1:1842:U:OP1    | 39:LR:70:ARG:NH2   | 2.34                     | 0.60              |
| 1:C1:1148:G:OP1    | 51:Lf:86:LYS:NZ    | 2.32                     | 0.60              |
| 45:LY:86:ARG:HB3   | 45:LY:96:ILE:HD11  | 1.82                     | 0.60              |
| 27:LD:37:ILE:HG13  | 27:LD:38:THR:HG23  | 1.84                     | 0.60              |
| 13:CN:142:ILE:HG12 | 13:CN:148:VAL:HG12 | 1.82                     | 0.60              |
| 1:C1:2789:G:H2'    | 1:C1:2790:G:C8     | 2.36                     | 0.60              |
| 21:Cg:181:VAL:O    | 21:Cg:185:GLN:NE2  | 2.33                     | 0.60              |
| 1:C1:2899:A:H2'    | 25:LB:256:TRP:HB3  | 1.84                     | 0.60              |
| 18:Cd:364:TRP:HA   | 18:Cd:377:ASP:O    | 2.01                     | 0.60              |
| 4:C4:53:U:O2'      | 4:C4:55:A:N7       | 2.34                     | 0.59              |
| 19:Ce:346:GLN:O    | 19:Ce:350:GLN:NE2  | 2.35                     | 0.59              |
| 8:CI:214:THR:OG1   | 8:CI:234:GLU:OE1   | 2.19                     | 0.59              |
| 1:C1:2477:U:OP2    | 1:C1:2545:G:N2     | 2.31                     | 0.59              |
| 1:C1:262:G:O6      | 35:LN:15:GLN:NE2   | 2.33                     | 0.59              |
| 1:C1:949:A:H62     | 1:C1:1098:G:H8     | 1.49                     | 0.59              |
| 1:C1:2308:A:H5''   | 49:Ld:32:THR:HG23  | 1.84                     | 0.59              |
| 7:CH:186:VAL:HG23  | 7:CH:187:THR:HG23  | 1.83                     | 0.59              |
| 10:CK:170:ARG:NH1  | 18:Cd:43:GLU:OE2   | 2.36                     | 0.59              |
| 22:Ch:489:ASP:HB3  | 22:Ch:508:LYS:HB3  | 1.83                     | 0.59              |
| 1:C1:1264:U:H2'    | 1:C1:1265:G:H8     | 1.68                     | 0.59              |
| 19:Ce:103:VAL:HG23 | 19:Ce:104:ARG:HG2  | 1.84                     | 0.58              |
| 31:LJ:110:HIS:HA   | 31:LJ:113:LEU:HD23 | 1.84                     | 0.58              |
| 35:LN:36:ILE:HG12  | 35:LN:64:VAL:HG23  | 1.85                     | 0.58              |
| 1:C1:2932:G:N7     | 10:CK:140:LYS:NZ   | 2.45                     | 0.58              |
| 4:C4:99:C:H5'      | 20:Cf:96:ARG:HH22  | 1.69                     | 0.58              |
| 2:C2:154:C:H5'     | 29:LG:184:LYS:HD3  | 1.85                     | 0.58              |
| 1:C1:2682:U:H5''   | 20:Cf:282:ARG:HD3  | 1.84                     | 0.58              |
| 13:CN:107:VAL:HG23 | 13:CN:108:ILE:HG13 | 1.86                     | 0.58              |
| 19:Ce:307:ILE:HG12 | 19:Ce:310:ARG:HH21 | 1.68                     | 0.58              |
| 24:LA:105:SER:HB3  | 24:LA:160:SER:HB3  | 1.85                     | 0.58              |
| 30:LH:127:MET:HE1  | 30:LH:200:ILE:HB   | 1.86                     | 0.58              |
| 46:LZ:49:PRO:HD3   | 46:LZ:67:ILE:HG12  | 1.85                     | 0.58              |
| 7:CH:264:LYS:HD3   | 7:CH:301:MET:HE1   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:Ch:384:MET:HB2  | 22:Ch:400:LEU:HB2  | 1.86                     | 0.58              |
| 1:C1:2079:G:OP1    | 1:C1:2081:C:N4     | 2.37                     | 0.58              |
| 22:Ch:195:VAL:HG12 | 22:Ch:206:THR:HG22 | 1.85                     | 0.58              |
| 1:C1:984:A:N1      | 1:C1:1033:U:O2'    | 2.37                     | 0.58              |
| 25:LB:84:MET:O     | 25:LB:203:PRO:HA   | 2.03                     | 0.58              |
| 1:C1:563:U:H2'     | 1:C1:564:A:H8      | 1.69                     | 0.57              |
| 1:C1:948:U:H2'     | 1:C1:949:A:H8      | 1.68                     | 0.57              |
| 7:CH:465:GLU:OE2   | 15:CQ:102:ARG:NH1  | 2.37                     | 0.57              |
| 34:LM:54:ARG:HG2   | 40:LS:70:LEU:HD22  | 1.86                     | 0.57              |
| 1:C1:766:G:N3      | 38:LQ:93:SER:OG    | 2.36                     | 0.57              |
| 15:CQ:16:SER:HB3   | 25:LB:73:VAL:HG11  | 1.86                     | 0.57              |
| 43:LV:64:VAL:O     | 43:LV:72:ARG:NH1   | 2.38                     | 0.57              |
| 5:CB:282:TYR:OH    | 8:CI:316:ARG:NH1   | 2.38                     | 0.57              |
| 39:LR:98:ARG:NH1   | 39:LR:130:ASN:OD1  | 2.36                     | 0.57              |
| 43:LV:34:ARG:HB2   | 43:LV:66:LYS:HG3   | 1.87                     | 0.57              |
| 5:CB:291:LEU:HD21  | 8:CI:323:MET:HE2   | 1.87                     | 0.57              |
| 20:Cf:89:PHE:HB3   | 20:Cf:101:THR:HB   | 1.85                     | 0.57              |
| 22:Ch:41:PHE:HE1   | 22:Ch:122:LEU:HD12 | 1.70                     | 0.57              |
| 31:LJ:94:ARG:O     | 31:LJ:157:ARG:NH2  | 2.38                     | 0.57              |
| 1:C1:259:C:OP1     | 35:LN:5:LYS:NZ     | 2.36                     | 0.57              |
| 1:C1:1619:C:OP2    | 52:Lg:75:ARG:NH1   | 2.37                     | 0.57              |
| 1:C1:1814:U:OP2    | 57:Ll:10:LYS:NZ    | 2.35                     | 0.57              |
| 1:C1:1614:G:N7     | 46:LZ:16:ARG:NH1   | 2.52                     | 0.57              |
| 7:CH:632:ARG:HB3   | 7:CH:637:ASP:HB3   | 1.86                     | 0.57              |
| 14:CO:13:ASN:OD1   | 14:CO:16:ARG:NH2   | 2.37                     | 0.57              |
| 1:C1:957:C:OP2     | 38:LQ:78:ARG:NH2   | 2.37                     | 0.56              |
| 2:C2:63:G:O2'      | 53:Lh:54:LYS:NZ    | 2.37                     | 0.56              |
| 9:CJ:397:TRP:HB2   | 9:CJ:401:LEU:HD12  | 1.86                     | 0.56              |
| 7:CH:85:TYR:O      | 7:CH:148:TYR:OH    | 2.23                     | 0.56              |
| 18:Cd:100:LYS:NZ   | 18:Cd:291:ASP:O    | 2.39                     | 0.56              |
| 20:Cf:124:ARG:HG3  | 20:Cf:252:ARG:HH21 | 1.71                     | 0.56              |
| 20:Cf:252:ARG:NH1  | 21:Cg:48:GLU:OE2   | 2.33                     | 0.56              |
| 21:Cg:23:PHE:HZ    | 21:Cg:61:VAL:HG12  | 1.69                     | 0.56              |
| 31:LJ:33:ARG:HD3   | 31:LJ:121:ILE:HA   | 1.88                     | 0.56              |
| 1:C1:1278:G:OP2    | 40:LS:84:ARG:NH1   | 2.39                     | 0.56              |
| 20:Cf:112:ASP:HB3  | 20:Cf:263:PRO:HG3  | 1.88                     | 0.56              |
| 36:LO:13:LYS:O     | 40:LS:169:ARG:NH2  | 2.39                     | 0.56              |
| 36:LO:129:LEU:HD11 | 40:LS:170:PRO:HG2  | 1.86                     | 0.56              |
| 29:LG:165:LEU:HA   | 35:LN:7:LEU:HD11   | 1.88                     | 0.56              |
| 1:C1:2544:G:H5'    | 19:Ce:436:TRP:HE1  | 1.70                     | 0.56              |
| 29:LG:249:GLU:HG3  | 29:LG:253:LYS:HE2  | 1.87                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:LV:25:MET:HE1   | 43:LV:80:ILE:HG12  | 1.87                     | 0.56              |
| 10:CK:53:GLN:HE22  | 10:CK:57:GLN:HE21  | 1.51                     | 0.56              |
| 34:LM:59:LEU:O     | 40:LS:155:ARG:NH2  | 2.37                     | 0.56              |
| 7:CH:453:ASP:OD2   | 7:CH:457:LYS:NZ    | 2.39                     | 0.55              |
| 26:LC:36:VAL:HG21  | 26:LC:251:LEU:HD21 | 1.87                     | 0.55              |
| 1:C1:813:G:O2'     | 1:C1:1844:A:N3     | 2.39                     | 0.55              |
| 1:C1:2473:U:H2'    | 1:C1:2474:A:H8     | 1.70                     | 0.55              |
| 34:LM:54:ARG:NH2   | 34:LM:76:ALA:O     | 2.38                     | 0.55              |
| 51:Lf:59:LYS:O     | 51:Lf:67:ARG:NH2   | 2.39                     | 0.55              |
| 1:C1:69:C:OP2      | 1:C1:294:G:N2      | 2.40                     | 0.55              |
| 22:Ch:264:ILE:HD12 | 22:Ch:274:HIS:HB2  | 1.88                     | 0.55              |
| 39:LR:44:LEU:HD22  | 39:LR:49:LEU:HD12  | 1.88                     | 0.55              |
| 41:LT:45:ASN:ND2   | 41:LT:94:GLU:O     | 2.40                     | 0.55              |
| 1:C1:976:G:H4'     | 1:C1:977:U:H5'     | 1.89                     | 0.55              |
| 1:C1:1305:U:O2'    | 40:LS:1:MET:SD     | 2.64                     | 0.55              |
| 1:C1:1611:C:OP2    | 46:LZ:47:ARG:NH2   | 2.39                     | 0.55              |
| 15:CQ:43:LYS:NZ    | 17:Cb:18:ASP:OD1   | 2.35                     | 0.55              |
| 1:C1:1459:G:OP2    | 7:CH:515:ARG:NH1   | 2.36                     | 0.55              |
| 1:C1:2434:U:OP2    | 59:Lr:26:ARG:NH1   | 2.39                     | 0.55              |
| 1:C1:775:A:H2'     | 1:C1:776:G:H8      | 1.72                     | 0.55              |
| 7:CH:156:LEU:HD23  | 7:CH:159:LEU:HD12  | 1.88                     | 0.55              |
| 27:LD:95:TRP:CE3   | 27:LD:201:TYR:HB3  | 2.42                     | 0.55              |
| 1:C1:2411:G:H2'    | 1:C1:2412:G:H8     | 1.72                     | 0.55              |
| 2:C2:126:A:O2'     | 2:C2:128:U:OP2     | 2.25                     | 0.55              |
| 35:LN:56:LYS:NZ    | 35:LN:145:ASP:OD1  | 2.40                     | 0.55              |
| 45:LY:47:ILE:HD13  | 45:LY:114:ARG:HH21 | 1.72                     | 0.55              |
| 27:LD:85:ALA:HB2   | 27:LD:258:TYR:HB2  | 1.88                     | 0.55              |
| 1:C1:643:C:H2'     | 1:C1:644:A:C8      | 2.41                     | 0.54              |
| 1:C1:1041:U:OP2    | 12:LF:104:LYS:NZ   | 2.40                     | 0.54              |
| 3:C3:57:A:OP2      | 5:CB:144:ARG:NH2   | 2.40                     | 0.54              |
| 13:CN:32:GLU:OE1   | 13:CN:50:ARG:NH1   | 2.39                     | 0.54              |
| 45:LY:52:GLY:HA2   | 45:LY:68:LYS:HE3   | 1.88                     | 0.54              |
| 1:C1:2368:C:H4'    | 10:CK:142:THR:HG21 | 1.89                     | 0.54              |
| 1:C1:3025:C:H3'    | 39:LR:62:ARG:HH22  | 1.70                     | 0.54              |
| 30:LH:126:LYS:HB2  | 30:LH:222:GLU:HB3  | 1.90                     | 0.54              |
| 31:LJ:11:ARG:NH2   | 31:LJ:152:SER:O    | 2.40                     | 0.54              |
| 1:C1:1095:A:H2'    | 1:C1:1096:G:C8     | 2.41                     | 0.54              |
| 1:C1:1431:U:H2'    | 1:C1:1432:A2M:H8   | 1.88                     | 0.54              |
| 2:C2:71:A:O2'      | 2:C2:83:C:N4       | 2.39                     | 0.54              |
| 26:LC:236:PRO:HG2  | 26:LC:239:ALA:HB3  | 1.89                     | 0.54              |
| 1:C1:3153:G:N7     | 40:LS:168:LYS:NZ   | 2.49                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CJ:25:LYS:HE3    | 9:CJ:73:LEU:HD11   | 1.88                     | 0.54              |
| 12:CM:103:PRO:HA   | 12:CM:106:ARG:HG2  | 1.89                     | 0.54              |
| 34:LM:123:LEU:HD22 | 36:LO:195:VAL:HG22 | 1.89                     | 0.54              |
| 4:C4:23:A:N3       | 4:C4:119:U:O2'     | 2.39                     | 0.54              |
| 9:CJ:136:ASP:OD1   | 9:CJ:139:ARG:NH2   | 2.41                     | 0.54              |
| 1:C1:3109:U:H3     | 1:C1:3338:C:H42    | 1.56                     | 0.54              |
| 22:Ch:379:SER:OG   | 22:Ch:381:ASP:OD1  | 2.26                     | 0.54              |
| 26:LC:211:ILE:HG13 | 26:LC:256:VAL:HB   | 1.89                     | 0.54              |
| 27:LD:245:GLU:HG3  | 27:LD:249:GLN:HE21 | 1.73                     | 0.54              |
| 28:LE:74:LYS:NZ    | 28:LE:120:ASP:OD1  | 2.38                     | 0.54              |
| 29:LG:27:ASN:HB3   | 29:LG:30:LEU:HG    | 1.90                     | 0.54              |
| 35:LN:23:LEU:O     | 35:LN:122:ASN:ND2  | 2.39                     | 0.54              |
| 1:C1:507:G:H5''    | 26:LC:346:ALA:HB2  | 1.89                     | 0.54              |
| 1:C1:877:A:O2'     | 1:C1:879:U:OP2     | 2.26                     | 0.54              |
| 9:CJ:36:LEU:HD11   | 9:CJ:75:GLU:HG2    | 1.90                     | 0.54              |
| 1:C1:248:A:H2'     | 1:C1:249:G:H8      | 1.73                     | 0.53              |
| 1:C1:277:A:N1      | 1:C1:2744:A:O2'    | 2.41                     | 0.53              |
| 10:CK:133:PHE:HB3  | 10:CK:149:ARG:HB3  | 1.90                     | 0.53              |
| 1:C1:2420:G:O2'    | 1:C1:2444:G:N2     | 2.36                     | 0.53              |
| 1:C1:2796:A:O2'    | 1:C1:2810:A:N6     | 2.41                     | 0.53              |
| 58:Lp:51:ALA:HB3   | 58:Lp:54:ILE:HD12  | 1.88                     | 0.53              |
| 1:C1:2981:U:H2'    | 1:C1:2982:A:H8     | 1.73                     | 0.53              |
| 1:C1:2882:U:OP2    | 18:Cd:221:ARG:NE   | 2.35                     | 0.53              |
| 1:C1:371:A:H4'     | 45:LY:90:THR:HG22  | 1.91                     | 0.53              |
| 41:LT:42:ILE:HD11  | 41:LT:74:VAL:HG11  | 1.90                     | 0.53              |
| 1:C1:2953:A:O2'    | 2:C2:1:A:N1        | 2.41                     | 0.53              |
| 22:Ch:35:GLY:O     | 22:Ch:56:ASN:ND2   | 2.42                     | 0.53              |
| 1:C1:3289:G:O6     | 1:C1:3298:U:O4     | 2.27                     | 0.53              |
| 2:C2:86:U:O2       | 55:Lj:87:ARG:NH1   | 2.41                     | 0.53              |
| 2:C2:120:G:H5'     | 19:Ce:182:PRO:HB3  | 1.90                     | 0.53              |
| 9:CJ:380:ARG:HD2   | 9:CJ:401:LEU:HB3   | 1.91                     | 0.53              |
| 30:LH:14:GLU:HA    | 34:LM:2:ALA:HB2    | 1.91                     | 0.53              |
| 1:C1:688:C:H2'     | 1:C1:689:G:H8      | 1.73                     | 0.53              |
| 1:C1:726:A:OP1     | 38:LQ:94:ARG:NH1   | 2.42                     | 0.53              |
| 2:C2:119:C:OP1     | 9:CJ:70:GLN:NE2    | 2.41                     | 0.53              |
| 7:CH:183:VAL:HG21  | 7:CH:219:ASP:HB2   | 1.90                     | 0.53              |
| 13:CN:11:ASN:ND2   | 13:CN:209:ASP:OD2  | 2.42                     | 0.53              |
| 13:CN:21:ASN:ND2   | 13:CN:112:ASP:OD2  | 2.39                     | 0.53              |
| 22:Ch:53:VAL:HG21  | 22:Ch:68:LEU:HD21  | 1.89                     | 0.53              |
| 3:C3:55:U:O2'      | 3:C3:58:A:N7       | 2.39                     | 0.53              |
| 42:LU:45:GLU:HG3   | 42:LU:46:ARG:HG2   | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:716:G:H5''    | 38:LQ:71:PRO:HB2   | 1.91                     | 0.53              |
| 25:LB:307:THR:HG21 | 25:LB:317:GLU:HG2  | 1.90                     | 0.53              |
| 1:C1:457:U:H5'     | 16:Lq:67:LYS:HD3   | 1.91                     | 0.52              |
| 9:CJ:75:GLU:HG3    | 9:CJ:77:LEU:H      | 1.74                     | 0.52              |
| 44:LX:79:PRO:HA    | 44:LX:97:PHE:HA    | 1.91                     | 0.52              |
| 45:LY:1:MET:HE3    | 45:LY:2:LYS:HG3    | 1.91                     | 0.52              |
| 1:C1:422:U:O2'     | 51:Lf:90:PRO:O     | 2.23                     | 0.52              |
| 1:C1:1766:G:H2'    | 1:C1:1767:A:C8     | 2.44                     | 0.52              |
| 33:LL:115:ARG:NH2  | 33:LL:155:PHE:O    | 2.34                     | 0.52              |
| 51:Lf:16:LEU:HD11  | 51:Lf:33:LYS:HB2   | 1.91                     | 0.52              |
| 1:C1:2112:A:N6     | 1:C1:2150:G:O2'    | 2.38                     | 0.52              |
| 3:C3:36:C:H2'      | 3:C3:37:G:H8       | 1.74                     | 0.52              |
| 3:C3:64:G:N2       | 8:CI:281:LYS:O     | 2.41                     | 0.52              |
| 35:LN:9:GLU:HB2    | 54:Li:53:ILE:HG13  | 1.91                     | 0.52              |
| 46:LZ:13:THR:HB    | 52:Lg:87:ARG:HG3   | 1.91                     | 0.52              |
| 1:C1:1866:A:O2'    | 25:LB:227:PHE:O    | 2.25                     | 0.52              |
| 1:C1:2327:G:H22    | 1:C1:2359:G:H1'    | 1.74                     | 0.52              |
| 1:C1:2489:C:OP1    | 24:LA:37:ARG:NH1   | 2.37                     | 0.52              |
| 18:Cd:324:ARG:O    | 18:Cd:372:ARG:NH2  | 2.39                     | 0.52              |
| 12:LF:53:ARG:NH1   | 12:LF:189:ASP:OD2  | 2.40                     | 0.52              |
| 1:C1:242:G:O6      | 33:LL:132:LYS:NZ   | 2.42                     | 0.52              |
| 1:C1:1779:A:H2'    | 1:C1:1780:A:H8     | 1.75                     | 0.52              |
| 1:C1:2920:G:O2'    | 18:Cd:366:TYR:O    | 2.26                     | 0.52              |
| 27:LD:223:LYS:O    | 27:LD:227:VAL:HB   | 2.09                     | 0.52              |
| 35:LN:140:LYS:NZ   | 53:Lh:101:ASP:OD2  | 2.41                     | 0.52              |
| 1:C1:282:U:H2'     | 1:C1:283:G:H8      | 1.75                     | 0.52              |
| 1:C1:1045:A:O2'    | 41:LT:108:ARG:NH2  | 2.43                     | 0.52              |
| 1:C1:2231:U:O4     | 20:Cf:298:ARG:NH1  | 2.43                     | 0.52              |
| 7:CH:307:ASP:HA    | 7:CH:310:LYS:HG2   | 1.90                     | 0.52              |
| 7:CH:520:ARG:O     | 7:CH:525:LYS:NZ    | 2.43                     | 0.52              |
| 28:LE:199:LYS:O    | 34:LM:117:ARG:NH2  | 2.42                     | 0.52              |
| 31:LJ:48:TYR:HD1   | 31:LJ:65:LYS:HD3   | 1.75                     | 0.52              |
| 57:Ll:27:ILE:O     | 57:Ll:33:ASN:ND2   | 2.42                     | 0.52              |
| 59:Lr:42:ASP:O     | 59:Lr:45:ARG:NH1   | 2.43                     | 0.52              |
| 1:C1:1685:U:O2     | 1:C1:1766:G:O2'    | 2.28                     | 0.52              |
| 44:LX:105:LYS:NZ   | 44:LX:125:THR:OG1  | 2.43                     | 0.52              |
| 12:CM:102:PRO:HB2  | 12:CM:105:PRO:HD2  | 1.92                     | 0.52              |
| 13:CN:1:MET:HE2    | 13:CN:203:LEU:HD13 | 1.92                     | 0.52              |
| 19:Ce:417:GLU:OE2  | 19:Ce:419:ARG:NH1  | 2.42                     | 0.52              |
| 22:Ch:470:LEU:HB2  | 22:Ch:484:LEU:HB2  | 1.92                     | 0.52              |
| 1:C1:388:A:H2'     | 1:C1:389:A2M:H8    | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:967:U:H2'     | 1:C1:968:U:H6      | 1.75                     | 0.51              |
| 2:C2:58:G:O6       | 55:Lj:63:ARG:NH1   | 2.37                     | 0.51              |
| 3:C3:49:G:H4'      | 5:CB:238:SER:HB2   | 1.92                     | 0.51              |
| 6:CF:78:GLY:HA3    | 6:CF:84:GLU:HA     | 1.91                     | 0.51              |
| 35:LN:177:GLY:O    | 35:LN:184:ARG:NH1  | 2.44                     | 0.51              |
| 1:C1:404:U:H2'     | 1:C1:405:G:H8      | 1.76                     | 0.51              |
| 1:C1:787:OMG:HM23  | 1:C1:918:A:H61     | 1.75                     | 0.51              |
| 1:C1:1054:U:O4     | 1:C1:1070:G:O6     | 2.28                     | 0.51              |
| 1:C1:2404:A:H2'    | 1:C1:2405:G:H8     | 1.75                     | 0.51              |
| 19:Ce:386:PRO:HA   | 19:Ce:389:LEU:HD13 | 1.91                     | 0.51              |
| 59:Lr:57:THR:OG1   | 59:Lr:178:GLN:OE1  | 2.29                     | 0.51              |
| 1:C1:2518:G:OP1    | 24:LA:69:TYR:OH    | 2.26                     | 0.51              |
| 1:C1:3000:U:OP2    | 1:C1:3050:C:N4     | 2.44                     | 0.51              |
| 15:CQ:18:GLY:HA3   | 15:CQ:31:PHE:O     | 2.10                     | 0.51              |
| 46:LZ:69:PRO:HG3   | 46:LZ:114:LYS:HB2  | 1.93                     | 0.51              |
| 46:LZ:120:ARG:NH1  | 46:LZ:126:ASN:OD1  | 2.43                     | 0.51              |
| 1:C1:742:G:O2'     | 1:C1:752:G:N2      | 2.40                     | 0.51              |
| 13:CN:219:GLU:HA   | 13:CN:224:LEU:HD12 | 1.93                     | 0.51              |
| 1:C1:2389:U:H3     | 1:C1:2562:G:H1     | 1.57                     | 0.51              |
| 13:CN:61:ARG:NH2   | 13:CN:105:GLY:O    | 2.43                     | 0.51              |
| 1:C1:1372:G:H5''   | 50:Le:102:SER:HB3  | 1.91                     | 0.51              |
| 1:C1:2425:G:O6     | 1:C1:2456:U:O2     | 2.28                     | 0.51              |
| 3:C3:70:G:H2'      | 3:C3:71:G:H8       | 1.76                     | 0.51              |
| 1:C1:2092:U:H2'    | 1:C1:2093:G:C8     | 2.46                     | 0.51              |
| 3:C3:64:G:O6       | 8:CI:278:ARG:NH1   | 2.44                     | 0.51              |
| 12:CM:149:SER:OG   | 12:CM:246:ARG:NH1  | 2.43                     | 0.51              |
| 1:C1:3202:U:OP1    | 34:LM:122:ARG:NH2  | 2.41                     | 0.51              |
| 27:LD:50:ARG:NH2   | 27:LD:72:ASP:OD2   | 2.44                     | 0.51              |
| 57:Ll:20:ASN:ND2   | 57:Ll:42:ARG:O     | 2.43                     | 0.51              |
| 1:C1:300:A:H2'     | 1:C1:301:A:C8      | 2.45                     | 0.50              |
| 58:Lp:82:THR:HA    | 58:Lp:85:ARG:HG2   | 1.93                     | 0.50              |
| 1:C1:1758:G:O2'    | 1:C1:1760:G:OP2    | 2.27                     | 0.50              |
| 22:Ch:148:PRO:HB3  | 22:Ch:508:LYS:HA   | 1.91                     | 0.50              |
| 1:C1:1826:C:OP1    | 1:C1:1829:C:N4     | 2.42                     | 0.50              |
| 1:C1:3137:A:OP1    | 36:LO:38:ARG:NH2   | 2.43                     | 0.50              |
| 25:LB:90:VAL:HG13  | 25:LB:104:THR:HG22 | 1.93                     | 0.50              |
| 1:C1:448:C:H41     | 28:LE:15:ARG:HH21  | 1.59                     | 0.50              |
| 2:C2:83:C:OP1      | 2:C2:85:G:N2       | 2.44                     | 0.50              |
| 47:La:112:LEU:HD22 | 47:La:125:VAL:HG11 | 1.92                     | 0.50              |
| 59:Lr:65:ILE:HG12  | 59:Lr:109:ALA:HB3  | 1.94                     | 0.50              |
| 1:C1:219:C:OP1     | 45:LY:46:SER:OG    | 2.29                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:410:A:H2'     | 1:C1:411:A:C8      | 2.47                     | 0.50              |
| 1:C1:1912:A:N1     | 18:Cd:448:ARG:NH2  | 2.60                     | 0.50              |
| 1:C1:3145:C:OP1    | 36:LO:178:ARG:NH1  | 2.45                     | 0.50              |
| 21:Cg:43:ASP:HB3   | 21:Cg:46:VAL:HG22  | 1.94                     | 0.50              |
| 26:LC:21:GLU:OE2   | 26:LC:263:LYS:NZ   | 2.44                     | 0.50              |
| 40:LS:66:GLU:HB3   | 40:LS:69:PRO:HG3   | 1.92                     | 0.50              |
| 1:C1:1211:A:H5''   | 6:CF:203:SER:HB3   | 1.94                     | 0.50              |
| 1:C1:2771:C:H2'    | 1:C1:2772:A:H8     | 1.76                     | 0.50              |
| 2:C2:26:U:O2'      | 26:LC:52:ALA:O     | 2.30                     | 0.50              |
| 38:LQ:78:ARG:HG3   | 38:LQ:82:MET:HE3   | 1.93                     | 0.50              |
| 47:La:75:ILE:HD12  | 47:La:118:LEU:HG   | 1.94                     | 0.50              |
| 1:C1:639:G:O2'     | 1:C1:1418:A:OP1    | 2.30                     | 0.50              |
| 2:C2:63:G:H22      | 2:C2:97:A:H2       | 1.59                     | 0.50              |
| 22:Ch:327:ILE:HB   | 22:Ch:375:LEU:HD11 | 1.94                     | 0.50              |
| 30:LH:7:GLU:HA     | 30:LH:92:LEU:O     | 2.12                     | 0.50              |
| 56:Lk:14:ILE:HA    | 56:Lk:17:ARG:HD3   | 1.93                     | 0.50              |
| 1:C1:1783:C:H2'    | 1:C1:1784:G:H8     | 1.76                     | 0.50              |
| 1:C1:1794:A:OP1    | 19:Ce:368:ARG:NH1  | 2.44                     | 0.50              |
| 1:C1:3002:A:H4'    | 25:LB:13:SER:HB2   | 1.92                     | 0.50              |
| 1:C1:3079:U:H1'    | 1:C1:3080:A:H5''   | 1.93                     | 0.50              |
| 4:C4:77:U:H2'      | 4:C4:78:A:H8       | 1.77                     | 0.50              |
| 6:CF:44:SER:OG     | 6:CF:222:SER:OG    | 2.29                     | 0.50              |
| 19:Ce:13:GLU:OE1   | 19:Ce:16:LYS:NZ    | 2.45                     | 0.50              |
| 24:LA:129:THR:OG1  | 24:LA:132:ASN:ND2  | 2.42                     | 0.50              |
| 32:LK:143:VAL:HG23 | 32:LK:148:PRO:HG3  | 1.94                     | 0.50              |
| 1:C1:604:G:H2'     | 1:C1:605:G:C8      | 2.47                     | 0.50              |
| 1:C1:1779:A:H2'    | 1:C1:1780:A:C8     | 2.46                     | 0.50              |
| 4:C4:115:U:OP1     | 20:Cf:130:LYS:NZ   | 2.33                     | 0.50              |
| 10:CK:16:ARG:NH2   | 10:CK:21:GLU:OE2   | 2.45                     | 0.50              |
| 17:Cb:24:ARG:HG2   | 17:Cb:27:ARG:HH12  | 1.76                     | 0.50              |
| 20:Cf:47:ASN:OD1   | 20:Cf:59:ARG:NH2   | 2.44                     | 0.50              |
| 59:Lr:58:VAL:HG13  | 59:Lr:152:LYS:HB3  | 1.94                     | 0.50              |
| 11:CL:52:ASP:OD2   | 40:LS:80:ARG:NH1   | 2.45                     | 0.49              |
| 27:LD:34:LYS:O     | 27:LD:38:THR:OG1   | 2.28                     | 0.49              |
| 1:C1:489:A:O2'     | 1:C1:3214:A:N1     | 2.38                     | 0.49              |
| 1:C1:1491:OMC:H5'  | 1:C1:2317:C:H1'    | 1.95                     | 0.49              |
| 4:C4:45:U:H2'      | 4:C4:46:G:H8       | 1.77                     | 0.49              |
| 1:C1:1577:C:H5'    | 1:C1:1676:A:H1'    | 1.94                     | 0.49              |
| 1:C1:1799:U:O4     | 9:CJ:50:ARG:NH1    | 2.42                     | 0.49              |
| 34:LM:94:TRP:O     | 34:LM:97:THR:OG1   | 2.29                     | 0.49              |
| 43:LV:7:GLY:H      | 43:LV:42:LYS:HE3   | 1.77                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:C1:101:A:H3'    | 1:C1:102:G:H21     | 1.78                     | 0.49              |
| 1:C1:333:C:OP2    | 26:LC:199:ARG:NH1  | 2.35                     | 0.49              |
| 3:C3:23:U:OP1     | 5:CB:77:ARG:NH2    | 2.46                     | 0.49              |
| 5:CB:19:ASP:N     | 5:CB:19:ASP:OD1    | 2.45                     | 0.49              |
| 10:CK:141:LYS:O   | 10:CK:144:LYS:NZ   | 2.39                     | 0.49              |
| 20:Cf:145:ALA:HB3 | 20:Cf:188:THR:HG22 | 1.95                     | 0.49              |
| 1:C1:979:A:N6     | 1:C1:1033:U:O4     | 2.45                     | 0.49              |
| 1:C1:2767:A:N6    | 1:C1:2913:U:O2'    | 2.43                     | 0.49              |
| 3:C3:71:G:H1      | 3:C3:134:U:H3      | 1.60                     | 0.49              |
| 11:CL:67:GLN:OE1  | 23:Cz:64:LYS:NZ    | 2.31                     | 0.49              |
| 16:Lq:11:GLU:HA   | 16:Lq:14:ARG:HD2   | 1.95                     | 0.49              |
| 22:Ch:40:ASN:OD1  | 22:Ch:48:GLN:NE2   | 2.40                     | 0.49              |
| 1:C1:21:A:H2'     | 1:C1:22:G:C8       | 2.48                     | 0.49              |
| 1:C1:681:A:OP1    | 26:LC:46:ASN:ND2   | 2.39                     | 0.49              |
| 1:C1:1604:G:OP1   | 19:Ce:343:ARG:NH2  | 2.45                     | 0.49              |
| 26:LC:114:ILE:HB  | 26:LC:119:LYS:HE3  | 1.95                     | 0.49              |
| 45:LY:54:GLU:HB2  | 45:LY:107:LYS:HB3  | 1.95                     | 0.49              |
| 1:C1:630:U:H2'    | 1:C1:631:U:C2      | 2.48                     | 0.49              |
| 1:C1:1641:G:H2'   | 1:C1:1642:G:C8     | 2.48                     | 0.49              |
| 7:CH:426:ILE:O    | 15:CQ:80:ARG:NH1   | 2.45                     | 0.49              |
| 10:CK:165:PRO:HG2 | 18:Cd:326:GLN:HE21 | 1.78                     | 0.49              |
| 47:La:135:GLU:HG2 | 47:La:139:LYS:HE2  | 1.95                     | 0.49              |
| 1:C1:669:U:O4     | 26:LC:119:LYS:NZ   | 2.42                     | 0.49              |
| 13:CN:61:ARG:HD3  | 43:LV:133:SER:HA   | 1.95                     | 0.49              |
| 51:Lf:54:VAL:HG22 | 51:Lf:68:VAL:HG22  | 1.95                     | 0.49              |
| 59:Lr:18:ASP:OD1  | 59:Lr:22:ASN:ND2   | 2.41                     | 0.49              |
| 1:C1:2219:A:N6    | 1:C1:2221:U:OP1    | 2.47                     | 0.48              |
| 1:C1:2621:G:H2'   | 1:C1:2622:G:H8     | 1.78                     | 0.48              |
| 9:CJ:171:LEU:HB3  | 9:CJ:238:LEU:HD23  | 1.95                     | 0.48              |
| 1:C1:619:A:H2'    | 1:C1:620:G:C8      | 2.47                     | 0.48              |
| 1:C1:2100:U:OP2   | 1:C1:2105:A:N6     | 2.38                     | 0.48              |
| 1:C1:2556:U:H2'   | 1:C1:2557:G:H8     | 1.77                     | 0.48              |
| 25:LB:92:TYR:HB2  | 25:LB:158:VAL:HB   | 1.95                     | 0.48              |
| 1:C1:575:G:H2'    | 1:C1:576:A:H8      | 1.78                     | 0.48              |
| 1:C1:2801:U:O2'   | 1:C1:2805:U:N3     | 2.45                     | 0.48              |
| 1:C1:2833:G:OP2   | 1:C1:2833:G:N2     | 2.35                     | 0.48              |
| 1:C1:64:A:H5''    | 35:LN:174:LEU:HD13 | 1.95                     | 0.48              |
| 1:C1:706:G:OP2    | 1:C1:706:G:N2      | 2.33                     | 0.48              |
| 1:C1:1067:A:H2'   | 1:C1:1068:A:H8     | 1.77                     | 0.48              |
| 1:C1:2318:G:OP1   | 37:LP:141:SER:OG   | 2.23                     | 0.48              |
| 1:C1:2631:G:H5'   | 31:LJ:95:ARG:NH1   | 2.29                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LS:162:LYS:HG3  | 51:Lf:38:ASP:HB3   | 1.95                     | 0.48              |
| 42:LU:21:PHE:HB2   | 42:LU:72:ILE:HB    | 1.95                     | 0.48              |
| 1:C1:1202:C:O2'    | 1:C1:1269:A:N1     | 2.42                     | 0.48              |
| 1:C1:2771:C:H2'    | 1:C1:2772:A:C8     | 2.48                     | 0.48              |
| 4:C4:100:G:OP1     | 20:Cf:259:ARG:NH2  | 2.44                     | 0.48              |
| 7:CH:365:MET:HA    | 7:CH:368:ILE:HG12  | 1.94                     | 0.48              |
| 16:Lq:73:LYS:HG2   | 26:LC:148:GLU:HG3  | 1.94                     | 0.48              |
| 43:LV:47:ARG:HD2   | 43:LV:48:LEU:H     | 1.77                     | 0.48              |
| 1:C1:1128:G:OP1    | 50:Le:45:ARG:NH2   | 2.47                     | 0.48              |
| 1:C1:1491:OMC:OP1  | 37:LP:127:ARG:NH1  | 2.35                     | 0.48              |
| 1:C1:1698:A:H4'    | 39:LR:117:LYS:HD2  | 1.94                     | 0.48              |
| 8:CI:225:GLY:HA3   | 8:CI:282:VAL:HG22  | 1.94                     | 0.48              |
| 9:CJ:200:ASN:ND2   | 9:CJ:205:ASP:OD1   | 2.45                     | 0.48              |
| 1:C1:782:G:H22     | 26:LC:102:ALA:HA   | 1.79                     | 0.48              |
| 9:CJ:400:VAL:HG21  | 12:CM:192:HIS:HA   | 1.95                     | 0.48              |
| 18:Cd:235:VAL:O    | 18:Cd:329:VAL:HA   | 2.14                     | 0.48              |
| 59:Lr:53:VAL:O     | 59:Lr:154:THR:HA   | 2.13                     | 0.48              |
| 1:C1:2789:G:H2'    | 1:C1:2790:G:H8     | 1.77                     | 0.48              |
| 34:LM:113:THR:H    | 34:LM:116:ASP:HB2  | 1.79                     | 0.48              |
| 1:C1:42:G:H21      | 1:C1:2571:U:H4'    | 1.79                     | 0.48              |
| 1:C1:1186:A:H62    | 1:C1:1283:G:H21    | 1.62                     | 0.48              |
| 4:C4:89:U:H3'      | 4:C4:90:G:C8       | 2.49                     | 0.48              |
| 21:Cg:181:VAL:HG12 | 21:Cg:185:GLN:HE22 | 1.79                     | 0.48              |
| 36:LO:62:MET:HA    | 36:LO:72:PRO:HD2   | 1.95                     | 0.48              |
| 53:Lh:34:LEU:HD23  | 53:Lh:45:LYS:HE2   | 1.96                     | 0.48              |
| 22:Ch:416:GLY:O    | 22:Ch:434:ARG:NH1  | 2.47                     | 0.48              |
| 29:LG:136:LYS:HD2  | 29:LG:141:HIS:HE1  | 1.78                     | 0.48              |
| 31:LJ:49:SER:HB2   | 31:LJ:67:ALA:HB3   | 1.96                     | 0.48              |
| 32:LK:130:LYS:NZ   | 32:LK:156:GLU:OE2  | 2.43                     | 0.48              |
| 1:C1:967:U:H2'     | 1:C1:968:U:C6      | 2.49                     | 0.47              |
| 1:C1:2123:G:H2'    | 1:C1:2124:G:H8     | 1.79                     | 0.47              |
| 8:CI:297:LEU:HD12  | 8:CI:301:GLN:HG3   | 1.95                     | 0.47              |
| 19:Ce:186:PRO:HD2  | 19:Ce:189:LEU:HD12 | 1.95                     | 0.47              |
| 24:LA:83:TYR:HB3   | 58:Lp:64:MET:HG3   | 1.96                     | 0.47              |
| 59:Lr:8:GLY:O      | 59:Lr:12:ASN:ND2   | 2.45                     | 0.47              |
| 1:C1:1316:C:OP1    | 38:LQ:31:GLY:N     | 2.47                     | 0.47              |
| 1:C1:1778:A:H2'    | 1:C1:1779:A:C8     | 2.49                     | 0.47              |
| 21:Cg:66:LEU:O     | 21:Cg:70:THR:OG1   | 2.29                     | 0.47              |
| 28:LE:58:LEU:HD11  | 28:LE:72:LEU:HB2   | 1.95                     | 0.47              |
| 47:La:103:ASP:OD2  | 47:La:126:ARG:NH1  | 2.47                     | 0.47              |
| 1:C1:2181:G:H2'    | 1:C1:2182:A:H8     | 1.80                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CN:186:VAL:HG12 | 13:CN:218:ILE:HD11 | 1.95                     | 0.47              |
| 56:Lk:27:LYS:NZ    | 56:Lk:56:GLU:OE2   | 2.41                     | 0.47              |
| 1:C1:1077:U:O2'    | 1:C1:1078:U:O2     | 2.29                     | 0.47              |
| 1:C1:1159:C:H4'    | 36:LO:91:PRO:HD3   | 1.96                     | 0.47              |
| 1:C1:1624:C:H5'    | 1:C1:1625:U:H5''   | 1.95                     | 0.47              |
| 7:CH:527:LEU:HD13  | 7:CH:550:ALA:HB2   | 1.95                     | 0.47              |
| 9:CJ:42:ILE:HG13   | 9:CJ:72:LEU:HD11   | 1.95                     | 0.47              |
| 10:CK:165:PRO:HG2  | 18:Cd:326:GLN:NE2  | 2.29                     | 0.47              |
| 27:LD:95:TRP:CD1   | 27:LD:161:ARG:HA   | 2.50                     | 0.47              |
| 44:LX:73:HIS:HD1   | 53:Lh:32:SER:HG    | 1.58                     | 0.47              |
| 1:C1:37:C:H4'      | 1:C1:790:A:H2      | 1.78                     | 0.47              |
| 1:C1:424:U:H2'     | 1:C1:425:G:C8      | 2.49                     | 0.47              |
| 1:C1:627:OMG:OP1   | 50:Le:41:ASN:ND2   | 2.37                     | 0.47              |
| 1:C1:1278:G:O2'    | 40:LS:115:ARG:NH1  | 2.47                     | 0.47              |
| 1:C1:1783:C:H2'    | 1:C1:1784:G:C8     | 2.50                     | 0.47              |
| 1:C1:2627:U:H2'    | 1:C1:2628:G:H8     | 1.79                     | 0.47              |
| 7:CH:73:GLN:O      | 7:CH:78:ARG:NH2    | 2.47                     | 0.47              |
| 28:LE:86:PRO:HD2   | 28:LE:89:ILE:HD12  | 1.95                     | 0.47              |
| 1:C1:300:A:H2'     | 1:C1:301:A:H8      | 1.80                     | 0.47              |
| 1:C1:787:OMG:H5''  | 26:LC:76:PRO:HD3   | 1.96                     | 0.47              |
| 1:C1:1404:G:H2'    | 1:C1:1405:G:H8     | 1.79                     | 0.47              |
| 31:LJ:147:SER:OG   | 31:LJ:148:ARG:N    | 2.47                     | 0.47              |
| 1:C1:351:G:N2      | 1:C1:354:A:OP2     | 2.39                     | 0.47              |
| 1:C1:767:G:O6      | 47:La:77:LYS:NZ    | 2.47                     | 0.47              |
| 1:C1:1067:A:H2'    | 1:C1:1068:A:C8     | 2.50                     | 0.47              |
| 1:C1:1802:C:H2'    | 1:C1:1803:A:H8     | 1.78                     | 0.47              |
| 5:CB:108:TYR:OH    | 5:CB:158:ARG:NH2   | 2.47                     | 0.47              |
| 11:CL:55:ILE:HB    | 11:CL:62:LYS:HE3   | 1.97                     | 0.47              |
| 24:LA:23:ARG:HH21  | 24:LA:53:GLY:HA3   | 1.80                     | 0.47              |
| 30:LH:173:VAL:HG22 | 30:LH:185:LEU:HG   | 1.97                     | 0.47              |
| 59:Lr:159:LEU:HD12 | 59:Lr:165:MET:HE3  | 1.96                     | 0.47              |
| 25:LB:194:GLU:OE2  | 25:LB:197:ARG:NH2  | 2.41                     | 0.47              |
| 40:LS:12:ARG:HB3   | 40:LS:24:LEU:HD23  | 1.95                     | 0.47              |
| 1:C1:646:OMG:H2'   | 1:C1:647:G:H8      | 1.80                     | 0.47              |
| 1:C1:2314:U:H2'    | 1:C1:2315:A:H8     | 1.80                     | 0.47              |
| 3:C3:40:G:O6       | 3:C3:45:U:O4       | 2.33                     | 0.47              |
| 4:C4:6:C:O2'       | 27:LD:50:ARG:NH2   | 2.48                     | 0.47              |
| 7:CH:508:MET:HE1   | 49:Ld:66:LYS:HB2   | 1.96                     | 0.47              |
| 14:CO:106:ILE:HG23 | 14:CO:107:VAL:HG13 | 1.97                     | 0.47              |
| 26:LC:233:GLU:OE1  | 26:LC:244:GLN:NE2  | 2.48                     | 0.47              |
| 1:C1:1395:G:H5''   | 50:Le:125:ALA:HB2  | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:Lr:104:ALA:O    | 59:Lr:133:LYS:NZ   | 2.43                     | 0.47              |
| 1:C1:652:A:H2'     | 1:C1:653:A:H8      | 1.79                     | 0.46              |
| 4:C4:78:A:H62      | 4:C4:100:G:H21     | 1.63                     | 0.46              |
| 7:CH:290:ASP:OD1   | 7:CH:290:ASP:N     | 2.48                     | 0.46              |
| 1:C1:582:G:O2'     | 28:LE:35:GLN:O     | 2.33                     | 0.46              |
| 1:C1:1460:A:OP1    | 1:C1:3033:G:O2'    | 2.30                     | 0.46              |
| 1:C1:1491:OMC:H2'  | 1:C1:1492:G:H8     | 1.81                     | 0.46              |
| 1:C1:1638:G:H2'    | 1:C1:1639:A:C8     | 2.51                     | 0.46              |
| 1:C1:1879:G:O2'    | 1:C1:2297:U:O4     | 2.26                     | 0.46              |
| 1:C1:2642:U:HO2'   | 31:LJ:131:CYS:HG   | 1.62                     | 0.46              |
| 24:LA:53:GLY:O     | 24:LA:192:LYS:NZ   | 2.48                     | 0.46              |
| 32:LK:28:LEU:HD12  | 32:LK:31:LYS:HE3   | 1.97                     | 0.46              |
| 59:Lr:6:VAL:O      | 59:Lr:10:ARG:HG2   | 2.16                     | 0.46              |
| 1:C1:20:U:H2'      | 1:C1:21:A:C8       | 2.51                     | 0.46              |
| 1:C1:491:C:H5''    | 28:LE:100:ARG:HG3  | 1.97                     | 0.46              |
| 1:C1:1707:G:OP1    | 58:Lp:44:LYS:NZ    | 2.44                     | 0.46              |
| 1:C1:3133:U:O4     | 28:LE:191:LYS:NZ   | 2.40                     | 0.46              |
| 33:LL:199:GLU:HG2  | 33:LL:203:LYS:NZ   | 2.24                     | 0.46              |
| 1:C1:2280:A:H5''   | 1:C1:2282:U:H5'    | 1.97                     | 0.46              |
| 1:C1:2728:A:H2'    | 1:C1:2729:G:C8     | 2.50                     | 0.46              |
| 28:LE:86:PRO:HG3   | 28:LE:169:LEU:HD23 | 1.98                     | 0.46              |
| 56:Lk:24:ARG:HA    | 56:Lk:69:LYS:O     | 2.15                     | 0.46              |
| 1:C1:523:G:H2'     | 1:C1:524:A:C8      | 2.51                     | 0.46              |
| 1:C1:1240:C:O2     | 6:CF:54:LYS:NZ     | 2.49                     | 0.46              |
| 1:C1:1491:OMC:O3'  | 1:C1:2316:G:O2'    | 2.30                     | 0.46              |
| 9:CJ:258:ASP:HB3   | 9:CJ:261:LYS:HB2   | 1.98                     | 0.46              |
| 1:C1:231:A:H2'     | 1:C1:232:A:C8      | 2.50                     | 0.46              |
| 1:C1:568:U:OP1     | 12:LF:246:ARG:NH2  | 2.46                     | 0.46              |
| 1:C1:1576:C:H2'    | 1:C1:1577:C:C6     | 2.51                     | 0.46              |
| 1:C1:1877:G:OP2    | 17:Cb:11:LYS:NZ    | 2.35                     | 0.46              |
| 1:C1:2878:A:H61    | 1:C1:2886:C:H42    | 1.63                     | 0.46              |
| 5:CB:120:LEU:HD11  | 5:CB:225:ARG:HG3   | 1.96                     | 0.46              |
| 22:Ch:322:HIS:HD1  | 22:Ch:323:TRP:H    | 1.64                     | 0.46              |
| 25:LB:47:MET:HE2   | 25:LB:180:MET:HG2  | 1.98                     | 0.46              |
| 26:LC:188:SER:O    | 26:LC:188:SER:OG   | 2.33                     | 0.46              |
| 12:LF:182:TYR:CZ   | 12:LF:203:GLN:HG2  | 2.51                     | 0.46              |
| 1:C1:1697:C:H2'    | 1:C1:1698:A:C8     | 2.50                     | 0.46              |
| 1:C1:2711:U:H2'    | 1:C1:2712:G:C8     | 2.51                     | 0.46              |
| 1:C1:2881:OMG:H5'' | 1:C1:2882:U:C6     | 2.51                     | 0.46              |
| 7:CH:341:GLU:O     | 7:CH:345:GLN:HG3   | 2.16                     | 0.46              |
| 26:LC:287:LEU:HD11 | 38:LQ:60:LEU:HB2   | 1.96                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:652:A:H2'     | 1:C1:653:A:C8      | 2.50                     | 0.46              |
| 6:CF:42:VAL:HG12   | 6:CF:224:LEU:HD12  | 1.98                     | 0.46              |
| 22:Ch:87:ILE:HG22  | 22:Ch:122:LEU:HD22 | 1.98                     | 0.46              |
| 25:LB:132:LYS:HA   | 25:LB:135:LYS:HE2  | 1.96                     | 0.46              |
| 1:C1:430:G:O6      | 16:Lq:134:ARG:NH1  | 2.39                     | 0.46              |
| 1:C1:1480:C:H2'    | 1:C1:1481:A:H8     | 1.81                     | 0.46              |
| 1:C1:2974:A:H2'    | 1:C1:2975:G:H8     | 1.80                     | 0.46              |
| 7:CH:493:GLU:OE2   | 7:CH:496:ARG:NH1   | 2.48                     | 0.46              |
| 11:CL:23:LYS:HE2   | 11:CL:27:ARG:HH21  | 1.81                     | 0.46              |
| 13:CN:99:GLU:HG3   | 13:CN:101:LEU:H    | 1.80                     | 0.46              |
| 16:Lq:113:ALA:HB1  | 28:LE:30:ALA:HA    | 1.98                     | 0.46              |
| 18:Cd:135:THR:HG22 | 18:Cd:138:ARG:HH12 | 1.80                     | 0.46              |
| 22:Ch:82:PRO:HB2   | 22:Ch:127:GLN:HB3  | 1.98                     | 0.46              |
| 44:LX:109:LYS:HE3  | 44:LX:109:LYS:HB2  | 1.81                     | 0.46              |
| 1:C1:1577:C:H2'    | 1:C1:1578:G:C8     | 2.51                     | 0.46              |
| 1:C1:3236:A:OP1    | 25:LB:125:SER:OG   | 2.32                     | 0.46              |
| 29:LG:85:LEU:HD22  | 29:LG:89:LEU:HD23  | 1.97                     | 0.46              |
| 44:LX:103:ALA:O    | 44:LX:133:LYS:NZ   | 2.44                     | 0.46              |
| 48:Lc:19:LEU:HD22  | 48:Lc:101:SER:HB2  | 1.98                     | 0.46              |
| 1:C1:88:U:H2'      | 1:C1:89:A:H8       | 1.81                     | 0.45              |
| 1:C1:735:C:H2'     | 1:C1:736:G:H8      | 1.81                     | 0.45              |
| 1:C1:1177:G:H2'    | 1:C1:1178:A:C8     | 2.51                     | 0.45              |
| 1:C1:3120:C:H2'    | 1:C1:3121:G:H8     | 1.81                     | 0.45              |
| 1:C1:3314:G:OP2    | 49:Ld:110:LYS:NZ   | 2.38                     | 0.45              |
| 4:C4:108:G:OP1     | 27:LD:284:ARG:NH2  | 2.49                     | 0.45              |
| 9:CJ:17:MET:HE3    | 9:CJ:66:THR:HA     | 1.97                     | 0.45              |
| 1:C1:410:A:H2'     | 1:C1:411:A:H8      | 1.81                     | 0.45              |
| 1:C1:575:G:H2'     | 1:C1:576:A:C8      | 2.51                     | 0.45              |
| 1:C1:1454:U:H2'    | 1:C1:1455:G:C8     | 2.51                     | 0.45              |
| 4:C4:89:U:OP1      | 4:C4:91:A:N6       | 2.50                     | 0.45              |
| 7:CH:510:LYS:HG2   | 7:CH:517:ILE:HD11  | 1.98                     | 0.45              |
| 1:C1:119:U:O4      | 1:C1:144:G:N2      | 2.48                     | 0.45              |
| 1:C1:341:C:O2      | 1:C1:345:A:O2'     | 2.33                     | 0.45              |
| 1:C1:651:C:H2'     | 1:C1:652:A:H8      | 1.79                     | 0.45              |
| 10:CK:154:PRO:HG2  | 10:CK:249:PRO:HB2  | 1.98                     | 0.45              |
| 16:Lq:3:ASN:ND2    | 26:LC:29:ALA:O     | 2.49                     | 0.45              |
| 46:LZ:52:ILE:HD12  | 46:LZ:61:ILE:HG12  | 1.99                     | 0.45              |
| 59:Lr:6:VAL:HG13   | 59:Lr:10:ARG:HH11  | 1.81                     | 0.45              |
| 1:C1:159:U:H2'     | 1:C1:160:G:C8      | 2.51                     | 0.45              |
| 1:C1:1917:OMU:H1'  | 1:C1:1917:OMU:HM23 | 1.62                     | 0.45              |
| 1:C1:2182:A:H2'    | 1:C1:2183:A:H8     | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:2769:C:OP2    | 1:C1:2914:U:O2'    | 2.33                     | 0.45              |
| 18:Cd:429:LEU:HD11 | 18:Cd:441:MET:HB3  | 1.99                     | 0.45              |
| 25:LB:313:VAL:HG23 | 25:LB:365:GLU:HG3  | 1.99                     | 0.45              |
| 28:LE:61:LEU:HD11  | 28:LE:103:ILE:HG13 | 1.99                     | 0.45              |
| 12:LF:57:TYR:OH    | 12:LF:189:ASP:OD1  | 2.31                     | 0.45              |
| 1:C1:106:C:H2'     | 1:C1:107:A:H8      | 1.81                     | 0.45              |
| 1:C1:615:C:H2'     | 1:C1:616:A:C8      | 2.52                     | 0.45              |
| 1:C1:651:C:H2'     | 1:C1:652:A:C8      | 2.52                     | 0.45              |
| 1:C1:679:A:N1      | 2:C2:28:C:O2'      | 2.47                     | 0.45              |
| 16:Lq:10:TRP:HB2   | 16:Lq:47:VAL:HG11  | 1.98                     | 0.45              |
| 22:Ch:509:ASP:OD2  | 22:Ch:513:ARG:NH1  | 2.49                     | 0.45              |
| 31:LJ:15:ILE:HD12  | 31:LJ:78:GLU:HG2   | 1.99                     | 0.45              |
| 43:LV:19:LEU:HD12  | 43:LV:80:ILE:HD13  | 1.99                     | 0.45              |
| 1:C1:425:G:H5''    | 51:Lf:59:LYS:HG2   | 1.99                     | 0.45              |
| 1:C1:1137:A:OP2    | 1:C1:2334:G:N1     | 2.42                     | 0.45              |
| 1:C1:1337:G:N2     | 1:C1:1339:U:O2'    | 2.37                     | 0.45              |
| 1:C1:1698:A:H2'    | 1:C1:1699:G:C8     | 2.51                     | 0.45              |
| 1:C1:2069:A:H2'    | 1:C1:2070:A:C8     | 2.51                     | 0.45              |
| 1:C1:3179:G:H2'    | 1:C1:3180:G:H8     | 1.82                     | 0.45              |
| 2:C2:59:A:O2'      | 44:LX:69:ARG:NH1   | 2.50                     | 0.45              |
| 12:CM:110:GLN:HG2  | 12:CM:115:ARG:HH21 | 1.81                     | 0.45              |
| 15:CQ:89:THR:O     | 15:CQ:93:MET:HG3   | 2.16                     | 0.45              |
| 33:LL:124:ILE:HG23 | 33:LL:138:THR:HG21 | 1.99                     | 0.45              |
| 1:C1:404:U:H2'     | 1:C1:405:G:C8      | 2.52                     | 0.45              |
| 1:C1:1920:G:H21    | 1:C1:3303:A:H8     | 1.63                     | 0.45              |
| 1:C1:3238:U:O4     | 25:LB:124:LYS:NZ   | 2.50                     | 0.45              |
| 2:C2:58:G:N7       | 55:Lj:63:ARG:NH2   | 2.42                     | 0.45              |
| 3:C3:57:A:N6       | 5:CB:138:LYS:O     | 2.46                     | 0.45              |
| 59:Lr:26:ARG:HG3   | 59:Lr:210:MET:HG3  | 1.97                     | 0.45              |
| 1:C1:1126:A:H5''   | 50:Le:39:ILE:HD11  | 1.98                     | 0.45              |
| 1:C1:1526:G:HO2'   | 1:C1:2131:A:HO2'   | 1.64                     | 0.45              |
| 6:CF:174:MET:HE3   | 6:CF:174:MET:HB3   | 1.83                     | 0.45              |
| 22:Ch:465:SER:OG   | 22:Ch:466:LYS:N    | 2.50                     | 0.45              |
| 31:LJ:38:LEU:HD13  | 31:LJ:70:VAL:HG23  | 1.98                     | 0.45              |
| 1:C1:644:A:H2'     | 1:C1:645:A:C8      | 2.52                     | 0.45              |
| 1:C1:2568:A:H2'    | 1:C1:2569:G:C8     | 2.52                     | 0.45              |
| 6:CF:31:ARG:NH1    | 6:CF:85:GLN:OE1    | 2.49                     | 0.45              |
| 1:C1:728:C:H2'     | 1:C1:729:A:H8      | 1.82                     | 0.45              |
| 1:C1:1361:U:H2'    | 1:C1:1362:G:H8     | 1.81                     | 0.45              |
| 1:C1:1476:G:OP2    | 1:C1:1476:G:N2     | 2.46                     | 0.45              |
| 1:C1:2405:G:H2'    | 1:C1:2406:A:H8     | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:2446:G:H22    | 1:C1:2449:A:H5'    | 1.81                     | 0.45              |
| 19:Ce:377:PRO:O    | 19:Ce:408:ARG:NH1  | 2.46                     | 0.45              |
| 52:Lg:77:TYR:HB3   | 52:Lg:81:ARG:HB2   | 1.98                     | 0.45              |
| 7:CH:250:LEU:HD11  | 7:CH:334:VAL:HG11  | 1.99                     | 0.44              |
| 24:LA:118:GLU:OE2  | 24:LA:156:LYS:NZ   | 2.48                     | 0.44              |
| 12:LF:102:PRO:HB2  | 12:LF:105:PRO:HD2  | 1.99                     | 0.44              |
| 1:C1:230:G:H2'     | 1:C1:231:A:C8      | 2.52                     | 0.44              |
| 1:C1:617:C:H2'     | 1:C1:618:C:H6      | 1.82                     | 0.44              |
| 1:C1:1476:G:H2'    | 57:Ll:13:LEU:HD22  | 1.99                     | 0.44              |
| 1:C1:1697:C:H2'    | 1:C1:1698:A:H8     | 1.82                     | 0.44              |
| 1:C1:2427:U:H2'    | 1:C1:2428:G:C8     | 2.52                     | 0.44              |
| 1:C1:3144:U:OP1    | 36:LO:170:TYR:OH   | 2.30                     | 0.44              |
| 8:CI:211:GLY:HA3   | 8:CI:240:VAL:HG11  | 1.99                     | 0.44              |
| 1:C1:453:G:H2'     | 1:C1:454:G:H8      | 1.82                     | 0.44              |
| 1:C1:615:C:H2'     | 1:C1:616:A:H8      | 1.83                     | 0.44              |
| 1:C1:629:C:H2'     | 1:C1:630:U:C6      | 2.53                     | 0.44              |
| 1:C1:698:A:H2'     | 1:C1:699:A:C8      | 2.53                     | 0.44              |
| 1:C1:2176:A:H2'    | 1:C1:2177:A:C8     | 2.53                     | 0.44              |
| 1:C1:2860:G:O2'    | 1:C1:2982:A:N1     | 2.46                     | 0.44              |
| 1:C1:2971:U:H2'    | 1:C1:2972:U:C6     | 2.53                     | 0.44              |
| 2:C2:99:C:O2'      | 55:Lj:65:ARG:NH2   | 2.51                     | 0.44              |
| 4:C4:12:U:OP2      | 4:C4:68:C:O2'      | 2.35                     | 0.44              |
| 8:CI:203:LEU:HD22  | 8:CI:233:ILE:HD11  | 1.99                     | 0.44              |
| 50:Le:103:SER:O    | 50:Le:107:ILE:HG13 | 2.17                     | 0.44              |
| 1:C1:2169:G:H2'    | 1:C1:2170:A:C8     | 2.53                     | 0.44              |
| 7:CH:527:LEU:HD21  | 7:CH:547:ARG:HD2   | 1.98                     | 0.44              |
| 10:CK:241:ARG:NH1  | 18:Cd:79:ASN:OD1   | 2.49                     | 0.44              |
| 12:CM:21:LYS:O     | 12:CM:25:GLN:HG3   | 2.18                     | 0.44              |
| 35:LN:159:ARG:HB3  | 35:LN:164:LEU:HB2  | 2.00                     | 0.44              |
| 1:C1:1894:G:O2'    | 39:LR:82:LYS:O     | 2.31                     | 0.44              |
| 1:C1:2633:A:H5''   | 31:LJ:106:GLY:HA3  | 1.98                     | 0.44              |
| 3:C3:10:C:H2'      | 3:C3:11:A:H8       | 1.82                     | 0.44              |
| 17:Cb:8:THR:HB     | 17:Cb:11:LYS:HD2   | 1.99                     | 0.44              |
| 22:Ch:424:TRP:HA   | 22:Ch:448:PRO:HB3  | 2.00                     | 0.44              |
| 59:Lr:36:ILE:HG21  | 59:Lr:190:LEU:HD21 | 2.00                     | 0.44              |
| 1:C1:2320:A:H2'    | 1:C1:2321:A:H8     | 1.82                     | 0.44              |
| 39:LR:105:LEU:HD23 | 39:LR:138:LEU:HD23 | 2.00                     | 0.44              |
| 40:LS:77:ILE:HG12  | 40:LS:126:VAL:HG22 | 2.00                     | 0.44              |
| 1:C1:980:A:H2'     | 1:C1:981:G:C8      | 2.53                     | 0.44              |
| 1:C1:1449:G:N2     | 1:C1:1493:G:H5''   | 2.32                     | 0.44              |
| 1:C1:2392:G:H2'    | 1:C1:2393:A:H8     | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:2516:G:O2'    | 46:LZ:135:PHE:OXT  | 2.33                     | 0.44              |
| 18:Cd:133:LYS:NZ   | 18:Cd:137:GLU:OE2  | 2.50                     | 0.44              |
| 22:Ch:338:ALA:O    | 22:Ch:360:ARG:NH1  | 2.43                     | 0.44              |
| 24:LA:116:VAL:HB   | 24:LA:126:LEU:HB2  | 1.99                     | 0.44              |
| 26:LC:42:GLY:HA3   | 26:LC:114:ILE:HD11 | 2.00                     | 0.44              |
| 12:LF:223:ARG:HD2  | 12:LF:223:ARG:HA   | 1.63                     | 0.44              |
| 34:LM:44:PRO:HG3   | 34:LM:81:VAL:HG12  | 1.98                     | 0.44              |
| 1:C1:219:C:H5'     | 45:LY:33:PRO:HD3   | 1.99                     | 0.44              |
| 1:C1:1345:G:H2'    | 1:C1:1346:A:C8     | 2.53                     | 0.44              |
| 1:C1:2576:U:H1'    | 1:C1:2577:G:H5'    | 1.99                     | 0.44              |
| 1:C1:2790:G:H2'    | 1:C1:2791:C:C6     | 2.53                     | 0.44              |
| 1:C1:3284:G:H21    | 1:C1:3303:A:H2     | 1.66                     | 0.44              |
| 3:C3:37:G:O2'      | 5:CB:67:THR:OG1    | 2.32                     | 0.44              |
| 7:CH:242:LEU:HD22  | 7:CH:277:PHE:HE1   | 1.81                     | 0.44              |
| 7:CH:535:ASP:OD2   | 15:CQ:138:ARG:NH1  | 2.47                     | 0.44              |
| 10:CK:121:ILE:HD11 | 10:CK:246:THR:HG22 | 2.00                     | 0.44              |
| 48:Lc:42:ALA:HA    | 48:Lc:96:LEU:HD23  | 1.99                     | 0.44              |
| 1:C1:1252:U:H1'    | 1:C1:1255:C:H5     | 1.83                     | 0.44              |
| 1:C1:1463:G:O2'    | 1:C1:1851:U:O4     | 2.25                     | 0.44              |
| 1:C1:2330:A:H2'    | 1:C1:2331:A:C8     | 2.52                     | 0.44              |
| 1:C1:2404:A:H2'    | 1:C1:2405:G:C8     | 2.53                     | 0.44              |
| 1:C1:2925:G:H2'    | 1:C1:2926:A:C8     | 2.52                     | 0.44              |
| 5:CB:31:LEU:HD12   | 5:CB:252:PRO:HG3   | 2.00                     | 0.44              |
| 9:CJ:187:LYS:HD2   | 9:CJ:488:PRO:HB2   | 2.00                     | 0.44              |
| 12:CM:128:ALA:O    | 12:CM:132:MET:HG3  | 2.18                     | 0.44              |
| 20:Cf:34:ARG:HE    | 20:Cf:38:CYS:HB3   | 1.83                     | 0.44              |
| 25:LB:50:LYS:HB2   | 25:LB:337:MET:HE2  | 1.99                     | 0.44              |
| 25:LB:288:LYS:HA   | 25:LB:288:LYS:HD2  | 1.80                     | 0.44              |
| 1:C1:453:G:H2'     | 1:C1:454:G:C8      | 2.53                     | 0.43              |
| 1:C1:1041:U:H2'    | 1:C1:1042:G:H8     | 1.82                     | 0.43              |
| 1:C1:1615:G:N2     | 1:C1:1618:A:OP2    | 2.38                     | 0.43              |
| 4:C4:4:U:H2'       | 4:C4:5:A:C8        | 2.53                     | 0.43              |
| 5:CB:119:ASP:N     | 5:CB:119:ASP:OD1   | 2.50                     | 0.43              |
| 28:LE:139:GLU:HG3  | 28:LE:152:LYS:HE2  | 1.99                     | 0.43              |
| 1:C1:1871:A:OP2    | 25:LB:242:LYS:NZ   | 2.52                     | 0.43              |
| 1:C1:1901:A:H2'    | 1:C1:1902:A:C8     | 2.54                     | 0.43              |
| 1:C1:2376:A:H2'    | 1:C1:2377:G:H8     | 1.83                     | 0.43              |
| 36:LO:127:ARG:HG2  | 36:LO:131:LEU:HD13 | 2.00                     | 0.43              |
| 1:C1:120:U:OP2     | 19:Ce:106:ARG:NH2  | 2.51                     | 0.43              |
| 7:CH:461:LEU:HD11  | 15:CQ:68:THR:HG22  | 1.99                     | 0.43              |
| 15:CQ:115:LYS:HE2  | 15:CQ:115:LYS:HB3  | 1.84                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:Cb:33:GLN:O    | 17:Cb:37:GLU:HG3   | 2.19                     | 0.43              |
| 28:LE:127:TYR:OH  | 28:LE:161:ASP:OD2  | 2.35                     | 0.43              |
| 1:C1:2621:G:H2'   | 1:C1:2622:G:C8     | 2.53                     | 0.43              |
| 1:C1:2822:G:C2    | 7:CH:94:LEU:HD13   | 2.53                     | 0.43              |
| 1:C1:2838:OMC:H2' | 1:C1:2839:U:C6     | 2.52                     | 0.43              |
| 1:C1:3126:A:OP1   | 51:Lf:94:ARG:NH2   | 2.39                     | 0.43              |
| 4:C4:56:A:H4'     | 31:LJ:153:HIS:HB2  | 2.01                     | 0.43              |
| 4:C4:59:C:H2'     | 4:C4:60:A:C8       | 2.53                     | 0.43              |
| 15:CQ:8:PHE:HE1   | 15:CQ:49:LEU:HD12  | 1.83                     | 0.43              |
| 20:Cf:27:PRO:HB3  | 20:Cf:171:GLU:HG2  | 2.00                     | 0.43              |
| 30:LH:1:MET:HE1   | 40:LS:138:PRO:HB2  | 2.01                     | 0.43              |
| 31:LJ:88:LYS:HE3  | 31:LJ:105:PHE:HB2  | 2.00                     | 0.43              |
| 33:LL:141:ASP:OD1 | 33:LL:141:ASP:N    | 2.51                     | 0.43              |
| 45:LY:85:THR:HG22 | 45:LY:95:PRO:HA    | 2.00                     | 0.43              |
| 1:C1:656:U:H2'    | 1:C1:657:U:C6      | 2.53                     | 0.43              |
| 1:C1:2570:U:H2'   | 1:C1:2571:U:C6     | 2.53                     | 0.43              |
| 7:CH:357:ILE:HG23 | 7:CH:361:LEU:HD23  | 2.01                     | 0.43              |
| 27:LD:186:TYR:HA  | 27:LD:193:LEU:HA   | 1.99                     | 0.43              |
| 30:LH:75:LEU:HD13 | 30:LH:108:VAL:HG13 | 2.01                     | 0.43              |
| 31:LJ:132:MET:HB3 | 31:LJ:132:MET:HE3  | 1.81                     | 0.43              |
| 1:C1:2080:A:C8    | 1:C1:3022:U:H1'    | 2.53                     | 0.43              |
| 1:C1:2411:G:H2'   | 1:C1:2412:G:C8     | 2.50                     | 0.43              |
| 6:CF:131:ALA:HB2  | 6:CF:201:LEU:HD21  | 2.00                     | 0.43              |
| 7:CH:276:LEU:HG   | 18:Cd:161:VAL:HG13 | 2.00                     | 0.43              |
| 9:CJ:179:LEU:HD22 | 9:CJ:184:SER:HB2   | 2.00                     | 0.43              |
| 40:LS:1:MET:HG3   | 40:LS:118:PHE:HB2  | 2.00                     | 0.43              |
| 1:C1:27:A:N3      | 1:C1:321:C:O2'     | 2.46                     | 0.43              |
| 1:C1:2307:U:H2'   | 1:C1:2308:A:C8     | 2.53                     | 0.43              |
| 9:CJ:411:SER:HA   | 9:CJ:450:TYR:HE2   | 1.83                     | 0.43              |
| 20:Cf:34:ARG:HG2  | 20:Cf:46:MET:HE1   | 2.00                     | 0.43              |
| 20:Cf:98:HIS:CD2  | 20:Cf:120:PRO:HG3  | 2.53                     | 0.43              |
| 1:C1:1264:U:H2'   | 1:C1:1265:G:C8     | 2.51                     | 0.43              |
| 8:CI:207:PHE:HB2  | 8:CI:213:ILE:HD11  | 1.99                     | 0.43              |
| 29:LG:33:ARG:HH21 | 46:LZ:51:LYS:HD2   | 1.83                     | 0.43              |
| 34:LM:20:LEU:HD21 | 34:LM:30:ILE:HD11  | 1.99                     | 0.43              |
| 35:LN:28:TRP:O    | 35:LN:32:GLN:HG2   | 2.19                     | 0.43              |
| 1:C1:88:U:H2'     | 1:C1:89:A:C8       | 2.54                     | 0.43              |
| 1:C1:768:A:H4'    | 1:C1:769:G:H5'     | 2.01                     | 0.43              |
| 1:C1:1559:G:OP2   | 1:C1:1559:G:N2     | 2.42                     | 0.43              |
| 1:C1:2544:G:O6    | 29:LG:66:LYS:NZ    | 2.48                     | 0.43              |
| 1:C1:2620:G:H2'   | 1:C1:2621:G:H8     | 1.84                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:CJ:380:ARG:HB2   | 9:CJ:401:LEU:HD13 | 2.01                     | 0.43              |
| 25:LB:123:TYR:CZ   | 25:LB:124:LYS:HG3 | 2.54                     | 0.43              |
| 58:Lp:73:THR:HG22  | 58:Lp:75:ALA:H    | 1.82                     | 0.43              |
| 59:Lr:203:SER:HA   | 59:Lr:217:TYR:HB3 | 2.00                     | 0.43              |
| 1:C1:203:A:H4'     | 1:C1:205:A:N7     | 2.34                     | 0.43              |
| 1:C1:2706:A:H2'    | 1:C1:2707:A:C8    | 2.54                     | 0.43              |
| 7:CH:86:ASP:OD2    | 7:CH:89:HIS:ND1   | 2.51                     | 0.43              |
| 19:Ce:103:VAL:HG12 | 54:Li:45:ARG:HD2  | 2.01                     | 0.43              |
| 38:LQ:126:MET:O    | 38:LQ:146:GLY:HA3 | 2.18                     | 0.43              |
| 39:LR:112:SER:OG   | 39:LR:114:LYS:NZ  | 2.51                     | 0.43              |
| 46:LZ:22:VAL:HG12  | 46:LZ:44:GLY:HA3  | 2.01                     | 0.43              |
| 1:C1:1726:C:O2'    | 56:Lk:4:GLU:OE1   | 2.34                     | 0.42              |
| 1:C1:2495:U:H2'    | 1:C1:2496:G:C8    | 2.54                     | 0.42              |
| 2:C2:57:C:H4'      | 2:C2:63:G:N7      | 2.34                     | 0.42              |
| 4:C4:44:C:OP2      | 31:LJ:138:ARG:NH2 | 2.52                     | 0.42              |
| 1:C1:695:U:H2'     | 1:C1:696:G:C8     | 2.54                     | 0.42              |
| 1:C1:1572:G:OP1    | 52:Lg:59:ARG:NH2  | 2.42                     | 0.42              |
| 1:C1:2130:A:H2'    | 1:C1:2131:A:C8    | 2.54                     | 0.42              |
| 4:C4:1:A:C8        | 27:LD:271:LYS:HG2 | 2.54                     | 0.42              |
| 29:LG:188:ARG:O    | 29:LG:191:THR:OG1 | 2.37                     | 0.42              |
| 56:Lk:23:ALA:O     | 56:Lk:68:ILE:HA   | 2.18                     | 0.42              |
| 1:C1:1737:G:OP1    | 42:LU:101:ARG:NH2 | 2.34                     | 0.42              |
| 4:C4:97:A:H2'      | 4:C4:98:G:H8      | 1.84                     | 0.42              |
| 9:CJ:223:ASP:HB3   | 9:CJ:226:ILE:HG22 | 2.01                     | 0.42              |
| 1:C1:405:G:H2'     | 1:C1:406:U:C6     | 2.54                     | 0.42              |
| 1:C1:804:G:H2'     | 1:C1:805:C:H6     | 1.85                     | 0.42              |
| 1:C1:1421:U:H2'    | 1:C1:1422:U:C6    | 2.55                     | 0.42              |
| 1:C1:1425:U:OP1    | 37:LP:126:ARG:NH2 | 2.52                     | 0.42              |
| 1:C1:2101:A:C4     | 55:Lj:3:LYS:HB3   | 2.54                     | 0.42              |
| 1:C1:2956:U:H2'    | 1:C1:2957:C:C6    | 2.55                     | 0.42              |
| 7:CH:526:PRO:HB2   | 7:CH:529:GLN:HG3  | 2.02                     | 0.42              |
| 10:CK:196:PRO:HD2  | 10:CK:224:ASN:HB3 | 2.00                     | 0.42              |
| 1:C1:637:A2M:HM'3  | 1:C1:637:A2M:H1'  | 1.89                     | 0.42              |
| 1:C1:1816:C:O2'    | 1:C1:1822:A:N1    | 2.44                     | 0.42              |
| 1:C1:2405:G:H2'    | 1:C1:2406:A:C8    | 2.54                     | 0.42              |
| 3:C3:49:G:H21      | 5:CB:240:ASN:HD22 | 1.68                     | 0.42              |
| 11:CL:5:ILE:HD13   | 36:LO:49:PHE:HB2  | 2.00                     | 0.42              |
| 15:CQ:85:LEU:O     | 15:CQ:89:THR:OG1  | 2.33                     | 0.42              |
| 20:Cf:28:LYS:HB2   | 20:Cf:28:LYS:HE3  | 1.81                     | 0.42              |
| 31:LJ:99:GLU:OE2   | 31:LJ:157:ARG:NH1 | 2.49                     | 0.42              |
| 33:LL:67:ARG:NE    | 47:La:105:LEU:O   | 2.53                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:LV:59:MET:HA    | 43:LV:78:ALA:O     | 2.19                     | 0.42              |
| 47:La:100:PRO:HG2  | 47:La:123:VAL:HG12 | 2.01                     | 0.42              |
| 50:Le:80:VAL:HA    | 50:Le:83:VAL:HG12  | 2.01                     | 0.42              |
| 1:C1:278:A:H8      | 1:C1:297:G:H1'     | 1.84                     | 0.42              |
| 1:C1:604:G:H2'     | 1:C1:605:G:H8      | 1.84                     | 0.42              |
| 1:C1:882:G:H1'     | 1:C1:1569:A:N6     | 2.34                     | 0.42              |
| 1:C1:957:C:H2'     | 1:C1:958:G:C8      | 2.54                     | 0.42              |
| 1:C1:1766:G:H2'    | 1:C1:1767:A:H8     | 1.84                     | 0.42              |
| 1:C1:2182:A:H2'    | 1:C1:2183:A:C8     | 2.54                     | 0.42              |
| 13:CN:241:ILE:HG23 | 13:CN:245:PHE:HD2  | 1.84                     | 0.42              |
| 25:LB:386:LYS:HA   | 25:LB:389:GLN:HB2  | 2.01                     | 0.42              |
| 26:LC:34:ASP:OD1   | 26:LC:34:ASP:N     | 2.52                     | 0.42              |
| 32:LK:38:SER:HB3   | 32:LK:41:LYS:HG2   | 2.02                     | 0.42              |
| 32:LK:146:LYS:HB2  | 32:LK:146:LYS:HE2  | 1.75                     | 0.42              |
| 1:C1:118:U:O2'     | 1:C1:120:U:OP2     | 2.33                     | 0.42              |
| 1:C1:1199:C:OP2    | 11:CL:57:ASN:ND2   | 2.52                     | 0.42              |
| 1:C1:1577:C:H2'    | 1:C1:1578:G:H8     | 1.85                     | 0.42              |
| 1:C1:2426:G:N2     | 59:Lr:164:CYS:SG   | 2.72                     | 0.42              |
| 1:C1:2973:C:OP2    | 14:CO:2:ALA:N      | 2.53                     | 0.42              |
| 1:C1:3179:G:H2'    | 1:C1:3180:G:C8     | 2.55                     | 0.42              |
| 2:C2:95:G:O2'      | 55:Lj:81:GLY:O     | 2.30                     | 0.42              |
| 20:Cf:290:ASP:OD1  | 20:Cf:294:ASP:N    | 2.52                     | 0.42              |
| 22:Ch:294:ILE:HG13 | 22:Ch:308:ALA:HB2  | 2.02                     | 0.42              |
| 22:Ch:300:ASP:OD1  | 22:Ch:302:SER:OG   | 2.33                     | 0.42              |
| 24:LA:113:VAL:HG12 | 24:LA:166:ILE:HD13 | 2.01                     | 0.42              |
| 1:C1:293:G:H2'     | 1:C1:294:G:H8      | 1.85                     | 0.42              |
| 1:C1:582:G:H1'     | 28:LE:37:LYS:HG3   | 2.02                     | 0.42              |
| 1:C1:787:OMG:CM2   | 1:C1:918:A:H61     | 2.32                     | 0.42              |
| 1:C1:1623:A:H5''   | 1:C1:1624:C:C5     | 2.55                     | 0.42              |
| 1:C1:2518:G:C6     | 24:LA:64:ARG:HD2   | 2.54                     | 0.42              |
| 1:C1:3078:C:OP2    | 10:CK:26:LYS:NZ    | 2.52                     | 0.42              |
| 3:C3:36:C:H2'      | 3:C3:37:G:C8       | 2.53                     | 0.42              |
| 5:CB:112:VAL:HG21  | 5:CB:127:VAL:HG21  | 2.02                     | 0.42              |
| 9:CJ:79:GLN:OE1    | 9:CJ:82:ARG:NH1    | 2.52                     | 0.42              |
| 13:CN:104:LEU:HA   | 13:CN:107:VAL:HG22 | 2.01                     | 0.42              |
| 20:Cf:103:VAL:HG13 | 20:Cf:113:MET:HG2  | 2.01                     | 0.42              |
| 25:LB:113:GLU:OE2  | 25:LB:168:ARG:NH1  | 2.52                     | 0.42              |
| 33:LL:189:ARG:HB2  | 54:Li:18:ARG:HD3   | 2.02                     | 0.42              |
| 59:Lr:74:ILE:HD11  | 59:Lr:86:SER:HB3   | 2.01                     | 0.42              |
| 1:C1:1214:A:H5''   | 1:C1:1215:C:H5'    | 2.01                     | 0.42              |
| 1:C1:1877:G:H2'    | 1:C1:1878:G:C8     | 2.55                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:2123:G:H2'    | 1:C1:2124:G:C8     | 2.55                     | 0.42              |
| 9:CJ:472:PRO:HA    | 9:CJ:473:PRO:HD3   | 1.85                     | 0.42              |
| 13:CN:101:LEU:HA   | 43:LV:137:VAL:HG22 | 2.01                     | 0.42              |
| 29:LG:159:ASP:N    | 29:LG:159:ASP:OD1  | 2.53                     | 0.42              |
| 45:LY:73:TYR:CD2   | 45:LY:76:LYS:HG2   | 2.55                     | 0.42              |
| 1:C1:474:C:H2'     | 1:C1:475:G:H8      | 1.85                     | 0.42              |
| 1:C1:1762:U:H2'    | 1:C1:1763:C:C6     | 2.54                     | 0.42              |
| 1:C1:2518:G:N2     | 29:LG:41:GLN:O     | 2.53                     | 0.42              |
| 4:C4:63:G:H2'      | 4:C4:64:A:C8       | 2.55                     | 0.42              |
| 5:CB:21:ASP:OD1    | 5:CB:22:GLN:N      | 2.53                     | 0.42              |
| 19:Ce:248:ARG:HA   | 19:Ce:251:MET:HE2  | 2.01                     | 0.42              |
| 25:LB:161:VAL:HG13 | 25:LB:184:ILE:HD11 | 2.00                     | 0.42              |
| 40:LS:78:TRP:HE1   | 40:LS:89:ASN:ND2   | 2.17                     | 0.42              |
| 1:C1:129:G:OP2     | 53:Lh:79:LYS:NZ    | 2.46                     | 0.41              |
| 1:C1:2117:U:H2'    | 1:C1:2118:G:H8     | 1.85                     | 0.41              |
| 1:C1:3204:C:H2'    | 1:C1:3205:G:C8     | 2.55                     | 0.41              |
| 4:C4:59:C:H2'      | 4:C4:60:A:H8       | 1.84                     | 0.41              |
| 13:CN:14:GLY:O     | 13:CN:61:ARG:NH1   | 2.53                     | 0.41              |
| 18:Cd:272:LYS:HG2  | 60:Cd:1000:GTP:C5  | 2.55                     | 0.41              |
| 20:Cf:104:ARG:HB3  | 20:Cf:112:ASP:OD1  | 2.20                     | 0.41              |
| 20:Cf:105:MET:HE1  | 20:Cf:110:VAL:HG22 | 2.01                     | 0.41              |
| 21:Cg:36:VAL:HG13  | 21:Cg:54:VAL:HG21  | 2.01                     | 0.41              |
| 22:Ch:83:TYR:HD1   | 22:Ch:124:ALA:HB1  | 1.86                     | 0.41              |
| 26:LC:277:LEU:HD23 | 26:LC:277:LEU:HA   | 1.90                     | 0.41              |
| 27:LD:60:ILE:HB    | 27:LD:80:SER:HB3   | 2.01                     | 0.41              |
| 1:C1:434:U:H2'     | 1:C1:435:G:H8      | 1.84                     | 0.41              |
| 1:C1:762:A:N7      | 38:LQ:179:HIS:ND1  | 2.69                     | 0.41              |
| 1:C1:1387:G:N2     | 1:C1:1390:A:OP2    | 2.40                     | 0.41              |
| 1:C1:2683:OMU:H1'  | 1:C1:2683:OMU:HM23 | 1.60                     | 0.41              |
| 1:C1:2876:OMG:OP1  | 43:LV:49:ASN:N     | 2.47                     | 0.41              |
| 9:CJ:227:MET:HE3   | 19:Ce:407:TYR:HD1  | 1.85                     | 0.41              |
| 19:Ce:248:ARG:NH1  | 19:Ce:252:GLU:OE2  | 2.53                     | 0.41              |
| 31:LJ:47:VAL:O     | 31:LJ:68:VAL:HA    | 2.19                     | 0.41              |
| 34:LM:13:ARG:NH2   | 40:LS:149:SER:O    | 2.53                     | 0.41              |
| 46:LZ:24:ILE:HA    | 46:LZ:42:VAL:HG12  | 2.01                     | 0.41              |
| 1:C1:364:G:N1      | 1:C1:367:A:OP2     | 2.48                     | 0.41              |
| 1:C1:1595:C:H2'    | 1:C1:1596:U:C6     | 2.55                     | 0.41              |
| 1:C1:2329:C:H2'    | 1:C1:2330:A:H8     | 1.85                     | 0.41              |
| 1:C1:2447:A:H4'    | 59:Lr:130:LYS:HE3  | 2.02                     | 0.41              |
| 1:C1:2697:A:H2'    | 1:C1:2698:A:C8     | 2.56                     | 0.41              |
| 1:C1:3245:C:O3'    | 25:LB:335:ARG:NH2  | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:Cf:135:PRO:HA   | 27:LD:68:GLU:HA    | 2.02                     | 0.41              |
| 22:Ch:349:THR:HG23 | 22:Ch:352:GLU:H    | 1.84                     | 0.41              |
| 12:LF:148:LYS:O    | 12:LF:152:GLU:HG2  | 2.20                     | 0.41              |
| 1:C1:646:OMG:H2'   | 1:C1:647:G:C8      | 2.56                     | 0.41              |
| 1:C1:773:U:H2'     | 1:C1:774:A:C8      | 2.55                     | 0.41              |
| 1:C1:910:C:H2'     | 1:C1:911:A:C8      | 2.56                     | 0.41              |
| 1:C1:1676:A:H2'    | 1:C1:1677:A:C8     | 2.56                     | 0.41              |
| 1:C1:1900:U:O2'    | 1:C1:1912:A:N7     | 2.44                     | 0.41              |
| 1:C1:2209:G:H2'    | 1:C1:2210:G:C8     | 2.55                     | 0.41              |
| 1:C1:2307:U:H2'    | 1:C1:2308:A:H8     | 1.85                     | 0.41              |
| 1:C1:3145:C:H3'    | 1:C1:3146:C:H6     | 1.86                     | 0.41              |
| 2:C2:75:G:OP2      | 45:LY:73:TYR:OH    | 2.30                     | 0.41              |
| 4:C4:11:A:N1       | 4:C4:67:G:O2'      | 2.48                     | 0.41              |
| 7:CH:169:LEU:HB2   | 7:CH:217:VAL:HG22  | 2.03                     | 0.41              |
| 19:Ce:434:GLU:HB3  | 19:Ce:439:LYS:HE3  | 2.02                     | 0.41              |
| 20:Cf:141:MET:HG2  | 21:Cg:28:LEU:HD13  | 2.02                     | 0.41              |
| 21:Cg:154:GLU:HG3  | 41:LT:89:ILE:HG22  | 2.02                     | 0.41              |
| 27:LD:193:LEU:HD21 | 27:LD:198:LEU:HD22 | 2.02                     | 0.41              |
| 38:LQ:108:VAL:HB   | 38:LQ:128:VAL:HG22 | 2.01                     | 0.41              |
| 1:C1:447:U:H3      | 16:Lq:84:LYS:HG3   | 1.86                     | 0.41              |
| 1:C1:2974:A:H2'    | 1:C1:2975:G:C8     | 2.54                     | 0.41              |
| 7:CH:284:ILE:HB    | 7:CH:316:ILE:HD13  | 2.01                     | 0.41              |
| 35:LN:73:ARG:HA    | 35:LN:74:PRO:HD3   | 1.93                     | 0.41              |
| 36:LO:98:ALA:O     | 36:LO:102:GLU:HG2  | 2.20                     | 0.41              |
| 1:C1:869:G:H2'     | 1:C1:870:A:C8      | 2.55                     | 0.41              |
| 1:C1:1238:C:H4'    | 32:LK:130:LYS:HE2  | 2.02                     | 0.41              |
| 1:C1:1698:A:H2'    | 1:C1:1699:G:H8     | 1.85                     | 0.41              |
| 1:C1:1796:A:H2'    | 1:C1:1797:A:C8     | 2.55                     | 0.41              |
| 1:C1:2504:G:H2'    | 1:C1:2505:U:H6     | 1.85                     | 0.41              |
| 1:C1:2605:C:H2'    | 1:C1:2606:A:C8     | 2.56                     | 0.41              |
| 1:C1:2958:G:H2'    | 1:C1:2959:U:C6     | 2.56                     | 0.41              |
| 2:C2:26:U:H2'      | 2:C2:27:U:C6       | 2.55                     | 0.41              |
| 2:C2:29:U:H5''     | 33:LL:27:ASP:HB3   | 2.03                     | 0.41              |
| 5:CB:116:PHE:HE1   | 5:CB:217:ILE:HG23  | 1.85                     | 0.41              |
| 10:CK:87:PRO:HD2   | 10:CK:90:LEU:HD12  | 2.02                     | 0.41              |
| 11:CL:59:PHE:HA    | 11:CL:60:PRO:HD3   | 1.95                     | 0.41              |
| 22:Ch:257:SER:OG   | 22:Ch:258:LYS:N    | 2.53                     | 0.41              |
| 25:LB:135:LYS:O    | 25:LB:139:GLU:HG3  | 2.20                     | 0.41              |
| 26:LC:303:PRO:HB2  | 12:LF:29:ARG:HE    | 1.85                     | 0.41              |
| 12:LF:92:VAL:O     | 12:LF:120:GLY:HA2  | 2.20                     | 0.41              |
| 36:LO:77:ALA:HB1   | 36:LO:108:GLU:OE2  | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Lf:55:TYR:CZ    | 51:Lf:67:ARG:HB2   | 2.54                     | 0.41              |
| 1:C1:118:U:O2'     | 19:Ce:106:ARG:NH2  | 2.53                     | 0.41              |
| 1:C1:617:C:H2'     | 1:C1:618:C:C6      | 2.55                     | 0.41              |
| 1:C1:1517:A:H2'    | 1:C1:1518:A:C8     | 2.56                     | 0.41              |
| 1:C1:1646:G:H2'    | 1:C1:1647:G:H8     | 1.85                     | 0.41              |
| 1:C1:3037:U:O2'    | 1:C1:3039:C:OP2    | 2.37                     | 0.41              |
| 12:CM:114:LEU:HD21 | 12:CM:121:VAL:HG22 | 2.02                     | 0.41              |
| 20:Cf:113:MET:HB2  | 20:Cf:261:ARG:HB3  | 2.02                     | 0.41              |
| 59:Lr:12:ASN:HB3   | 59:Lr:206:ILE:HD11 | 2.03                     | 0.41              |
| 1:C1:769:G:H2'     | 1:C1:770:C:C6      | 2.56                     | 0.41              |
| 1:C1:970:U:H2'     | 1:C1:971:A:H8      | 1.86                     | 0.41              |
| 1:C1:1191:C:H4'    | 6:CF:4:SER:HA      | 2.01                     | 0.41              |
| 1:C1:2298:G:O4'    | 1:C1:2300:OMC:H5   | 2.03                     | 0.41              |
| 1:C1:2627:U:H2'    | 1:C1:2628:G:C8     | 2.55                     | 0.41              |
| 1:C1:2842:U:H2'    | 1:C1:2843:C:H6     | 1.85                     | 0.41              |
| 4:C4:10:C:OP2      | 20:Cf:59:ARG:NH1   | 2.54                     | 0.41              |
| 4:C4:17:A:H2'      | 4:C4:18:G:H8       | 1.86                     | 0.41              |
| 35:LN:145:ASP:HB3  | 35:LN:148:ILE:HG22 | 2.03                     | 0.41              |
| 1:C1:282:U:H2'     | 1:C1:283:G:C8      | 2.53                     | 0.41              |
| 1:C1:425:G:H2'     | 1:C1:426:A:C8      | 2.56                     | 0.41              |
| 1:C1:524:A:H2'     | 1:C1:525:A:C8      | 2.56                     | 0.41              |
| 1:C1:1103:A:OP1    | 11:CL:26:LYS:NZ    | 2.46                     | 0.41              |
| 1:C1:1220:G:H22    | 1:C1:1234:A:H2     | 1.69                     | 0.41              |
| 1:C1:2069:A:H2'    | 1:C1:2070:A:H8     | 1.86                     | 0.41              |
| 1:C1:2181:G:H2'    | 1:C1:2182:A:C8     | 2.56                     | 0.41              |
| 1:C1:2456:U:H1'    | 59:Lr:164:CYS:HB3  | 2.02                     | 0.41              |
| 1:C1:2704:G:N2     | 1:C1:2707:A:OP2    | 2.39                     | 0.41              |
| 1:C1:2838:OMC:H2'  | 1:C1:2839:U:H6     | 1.85                     | 0.41              |
| 1:C1:3081:A:O2'    | 30:LH:77:HIS:ND1   | 2.49                     | 0.41              |
| 4:C4:38:U:N3       | 4:C4:41:G:OP2      | 2.45                     | 0.41              |
| 4:C4:109:G:OP1     | 27:LD:287:ARG:NH2  | 2.54                     | 0.41              |
| 5:CB:174:THR:HG22  | 5:CB:176:THR:H     | 1.86                     | 0.41              |
| 7:CH:168:THR:HG23  | 7:CH:216:GLN:HG3   | 2.03                     | 0.41              |
| 7:CH:361:LEU:HA    | 7:CH:364:VAL:HG12  | 2.03                     | 0.41              |
| 7:CH:485:GLU:O     | 7:CH:489:LEU:HG    | 2.21                     | 0.41              |
| 16:Lq:88:ARG:HH12  | 28:LE:23:LYS:HD3   | 1.86                     | 0.41              |
| 16:Lq:106:ASP:OD1  | 16:Lq:106:ASP:N    | 2.51                     | 0.41              |
| 30:LH:207:ARG:HE   | 30:LH:207:ARG:HB3  | 1.71                     | 0.41              |
| 31:LJ:111:ILE:HG12 | 31:LJ:117:TYR:HB2  | 2.02                     | 0.41              |
| 35:LN:35:VAL:O     | 35:LN:64:VAL:HA    | 2.21                     | 0.41              |
| 39:LR:108:LYS:HE2  | 39:LR:108:LYS:HB3  | 1.74                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:LY:73:TYR:CE2  | 45:LY:76:LYS:HG2   | 2.56                     | 0.41              |
| 55:Lj:43:LYS:HB2  | 55:Lj:43:LYS:HE3   | 1.81                     | 0.41              |
| 59:Lr:45:ARG:NH1  | 59:Lr:46:ASP:OD2   | 2.53                     | 0.41              |
| 1:C1:619:A:H2'    | 1:C1:620:G:H8      | 1.84                     | 0.41              |
| 1:C1:1480:C:H2'   | 1:C1:1481:A:C8     | 2.56                     | 0.41              |
| 1:C1:3315:U:OP1   | 49:Ld:23:HIS:NE2   | 2.41                     | 0.41              |
| 7:CH:534:LEU:HD12 | 7:CH:546:LEU:HD11  | 2.02                     | 0.41              |
| 12:CM:92:VAL:O    | 12:CM:120:GLY:HA2  | 2.20                     | 0.41              |
| 13:CN:126:GLU:HG3 | 13:CN:137:VAL:HG11 | 2.02                     | 0.41              |
| 27:LD:48:LYS:HE2  | 27:LD:148:ILE:HD13 | 2.03                     | 0.41              |
| 30:LH:64:VAL:HG12 | 30:LH:119:VAL:HG21 | 2.02                     | 0.41              |
| 50:Le:97:ILE:HG21 | 50:Le:106:ARG:HG2  | 2.02                     | 0.41              |
| 54:Li:85:LYS:HA   | 54:Li:85:LYS:HD3   | 1.83                     | 0.41              |
| 1:C1:204:C:C2     | 26:LC:224:LYS:HE3  | 2.56                     | 0.40              |
| 1:C1:957:C:H2'    | 1:C1:958:G:H8      | 1.86                     | 0.40              |
| 1:C1:970:U:H2'    | 1:C1:971:A:C8      | 2.56                     | 0.40              |
| 1:C1:2523:G:H2'   | 1:C1:2524:G:H8     | 1.85                     | 0.40              |
| 1:C1:2640:U:H5'   | 31:LJ:66:ILE:HD11  | 2.03                     | 0.40              |
| 7:CH:309:THR:HG22 | 7:CH:314:VAL:HB    | 2.03                     | 0.40              |
| 7:CH:606:GLY:HA3  | 57:Ll:26:TRP:CD1   | 2.56                     | 0.40              |
| 9:CJ:197:TYR:O    | 9:CJ:207:LEU:HA    | 2.20                     | 0.40              |
| 21:Cg:154:GLU:OE1 | 41:LT:54:HIS:ND1   | 2.54                     | 0.40              |
| 22:Ch:41:PHE:CD2  | 22:Ch:69:LEU:HD13  | 2.56                     | 0.40              |
| 25:LB:164:HIS:HA  | 25:LB:178:HIS:O    | 2.21                     | 0.40              |
| 50:Le:42:ARG:HA   | 50:Le:42:ARG:HD2   | 1.97                     | 0.40              |
| 1:C1:400:A:C2     | 2:C2:17:A:H1'      | 2.56                     | 0.40              |
| 1:C1:1661:U:H5''  | 7:CH:510:LYS:HD3   | 2.03                     | 0.40              |
| 1:C1:2631:G:H5'   | 31:LJ:95:ARG:HH12  | 1.86                     | 0.40              |
| 1:C1:3236:A:H2'   | 1:C1:3237:A:C8     | 2.56                     | 0.40              |
| 6:CF:49:ARG:NH2   | 6:CF:125:ALA:O     | 2.46                     | 0.40              |
| 7:CH:46:THR:HG23  | 7:CH:112:VAL:HG22  | 2.03                     | 0.40              |
| 9:CJ:84:GLN:OE1   | 9:CJ:120:ARG:NH2   | 2.51                     | 0.40              |
| 9:CJ:179:LEU:HD21 | 9:CJ:201:ILE:HD11  | 2.03                     | 0.40              |
| 12:CM:182:TYR:CZ  | 12:CM:203:GLN:HG2  | 2.57                     | 0.40              |
| 19:Ce:5:LYS:HE2   | 19:Ce:5:LYS:HB3    | 1.91                     | 0.40              |
| 20:Cf:31:LEU:HB3  | 20:Cf:87:MET:SD    | 2.61                     | 0.40              |
| 31:LJ:112:ASP:OD1 | 31:LJ:112:ASP:N    | 2.51                     | 0.40              |
| 48:Lc:102:ASP:OD1 | 48:Lc:102:ASP:N    | 2.48                     | 0.40              |
| 53:Lh:17:LYS:NZ   | 53:Lh:63:ILE:O     | 2.54                     | 0.40              |
| 59:Lr:48:ARG:HA   | 59:Lr:159:LEU:HD23 | 2.02                     | 0.40              |
| 1:C1:498:U:H2'    | 1:C1:499:C:C6      | 2.56                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:2446:G:N7     | 59:Lr:101:LYS:NZ   | 2.64                     | 0.40              |
| 1:C1:2609:U:H4'    | 21:Cg:167:THR:HG22 | 2.04                     | 0.40              |
| 1:C1:2694:U:H2'    | 1:C1:2695:A:C8     | 2.56                     | 0.40              |
| 1:C1:2814:C:H2'    | 1:C1:2815:G:H8     | 1.86                     | 0.40              |
| 2:C2:9:A:H2'       | 2:C2:10:A:C8       | 2.57                     | 0.40              |
| 3:C3:3:C:N4        | 29:LG:88:ASN:OD1   | 2.50                     | 0.40              |
| 6:CF:170:MET:HE2   | 6:CF:170:MET:HB3   | 1.98                     | 0.40              |
| 8:CI:237:ASP:OD2   | 8:CI:239:GLU:HG3   | 2.20                     | 0.40              |
| 27:LD:90:HIS:CE1   | 27:LD:228:LYS:HB3  | 2.56                     | 0.40              |
| 27:LD:214:LEU:HD12 | 27:LD:226:PHE:HE2  | 1.86                     | 0.40              |
| 29:LG:169:LEU:HD23 | 29:LG:169:LEU:HA   | 1.91                     | 0.40              |
| 37:LP:122:ALA:HB3  | 37:LP:143:PRO:HG2  | 2.02                     | 0.40              |
| 56:Lk:53:ASP:OD1   | 56:Lk:53:ASP:N     | 2.53                     | 0.40              |
| 1:C1:1681:U:H2'    | 1:C1:1682:C:C6     | 2.57                     | 0.40              |
| 1:C1:1793:A:O2'    | 1:C1:1796:A:N3     | 2.49                     | 0.40              |
| 1:C1:2727:U:H2'    | 1:C1:2728:A:H8     | 1.86                     | 0.40              |
| 1:C1:2790:G:H2'    | 1:C1:2791:C:H6     | 1.87                     | 0.40              |
| 7:CH:408:GLU:HG3   | 7:CH:417:PHE:HB3   | 2.03                     | 0.40              |
| 9:CJ:396:GLY:HA2   | 9:CJ:405:ALA:HB1   | 2.03                     | 0.40              |
| 28:LE:86:PRO:HB3   | 28:LE:166:ASP:HB2  | 2.03                     | 0.40              |
| 1:C1:273:U:O2'     | 1:C1:275:G:N7      | 2.46                     | 0.40              |
| 1:C1:919:G:OP2     | 1:C1:920:C:N4      | 2.49                     | 0.40              |
| 1:C1:1095:A:O2'    | 1:C1:1353:G:H4'    | 2.21                     | 0.40              |
| 1:C1:2419:A:N3     | 1:C1:2445:U:O2'    | 2.40                     | 0.40              |
| 1:C1:2612:C:H2'    | 1:C1:2613:C:C6     | 2.56                     | 0.40              |
| 1:C1:2738:A:H2'    | 1:C1:2739:A:H8     | 1.87                     | 0.40              |
| 7:CH:405:ARG:HD2   | 13:CN:33:ASN:HA    | 2.02                     | 0.40              |
| 19:Ce:92:ILE:O     | 19:Ce:95:ARG:NH1   | 2.41                     | 0.40              |
| 12:LF:21:LYS:O     | 12:LF:25:GLN:HG3   | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 5   | CB    | 259/391 (66%) | 255 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 6   | CF    | 243/270 (90%) | 241 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 7   | CH    | 621/661 (94%) | 617 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 8   | CI    | 150/414 (36%) | 147 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 9   | CJ    | 376/679 (55%) | 373 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 10  | CK    | 231/261 (88%) | 225 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 11  | CL    | 77/558 (14%)  | 76 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 12  | CM    | 211/249 (85%) | 207 (98%)  | 3 (1%)  | 1 (0%)   | 24          | 34  |
| 12  | LF    | 246/249 (99%) | 240 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 13  | CN    | 244/246 (99%) | 238 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 14  | CO    | 56/120 (47%)  | 56 (100%)  | 0       | 0        | 100         | 100 |
| 15  | CQ    | 181/225 (80%) | 180 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 16  | Lq    | 137/147 (93%) | 134 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 17  | Cb    | 99/117 (85%)  | 98 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 18  | Cd    | 458/627 (73%) | 450 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 19  | Ce    | 301/443 (68%) | 299 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 20  | Cf    | 281/350 (80%) | 276 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 21  | Cg    | 186/202 (92%) | 185 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 22  | Ch    | 484/517 (94%) | 468 (97%)  | 16 (3%) | 0        | 100         | 100 |
| 23  | Cz    | 99/123 (80%)  | 98 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 24  | LA    | 189/254 (74%) | 185 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 25  | LB    | 387/392 (99%) | 380 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 26  | LC    | 361/365 (99%) | 355 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 27  | LD    | 282/304 (93%) | 280 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 28  | LE    | 187/200 (94%) | 182 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 29  | LG    | 233/262 (89%) | 230 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 30  | LH    | 188/229 (82%) | 184 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 31  | LJ    | 167/173 (96%) | 166 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 32  | LK    | 156/165 (94%) | 155 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 33  | LL    | 201/213 (94%) | 199 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 34  | LM    | 139/142 (98%) | 136 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 35  | LN    | 200/203 (98%) | 193 (96%)  | 7 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 36  | LO    | 201/204 (98%)     | 199 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 37  | LP    | 167/187 (89%)     | 166 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 38  | LQ    | 148/213 (70%)     | 145 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 39  | LR    | 153/2898 (5%)     | 152 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 40  | LS    | 172/174 (99%)     | 169 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 41  | LT    | 127/160 (79%)     | 125 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 42  | LU    | 103/127 (81%)     | 100 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 43  | LV    | 133/139 (96%)     | 132 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 44  | LX    | 143/156 (92%)     | 140 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 45  | LY    | 131/138 (95%)     | 125 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 46  | LZ    | 133/135 (98%)     | 132 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 47  | La    | 104/149 (70%)     | 102 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 48  | Lc    | 93/108 (86%)      | 92 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 49  | Ld    | 108/120 (90%)     | 107 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 50  | Le    | 124/131 (95%)     | 123 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 51  | Lf    | 106/109 (97%)     | 105 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 52  | Lg    | 116/119 (98%)     | 114 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 53  | Lh    | 120/935 (13%)     | 116 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 54  | Li    | 99/110 (90%)      | 99 (100%)   | 0        | 0        | 100         | 100 |
| 55  | Lj    | 86/95 (90%)       | 84 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 56  | Lk    | 74/94 (79%)       | 73 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 57  | Ll    | 48/51 (94%)       | 46 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 58  | Lp    | 89/92 (97%)       | 85 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 59  | Lr    | 212/217 (98%)     | 201 (95%)   | 11 (5%)  | 0        | 100         | 100 |
| All | All   | 10620/16612 (64%) | 10440 (98%) | 179 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | CM    | 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 5   | CB    | 227/329 (69%)  | 227 (100%) | 0        | 100         | 100 |
| 6   | CF    | 212/236 (90%)  | 212 (100%) | 0        | 100         | 100 |
| 7   | CH    | 549/575 (96%)  | 549 (100%) | 0        | 100         | 100 |
| 8   | CI    | 124/336 (37%)  | 124 (100%) | 0        | 100         | 100 |
| 9   | CJ    | 331/579 (57%)  | 331 (100%) | 0        | 100         | 100 |
| 10  | CK    | 206/225 (92%)  | 205 (100%) | 1 (0%)   | 81          | 88  |
| 11  | CL    | 61/458 (13%)   | 61 (100%)  | 0        | 100         | 100 |
| 12  | CM    | 185/215 (86%)  | 185 (100%) | 0        | 100         | 100 |
| 12  | LF    | 213/215 (99%)  | 213 (100%) | 0        | 100         | 100 |
| 13  | CN    | 205/206 (100%) | 205 (100%) | 0        | 100         | 100 |
| 14  | CO    | 48/99 (48%)    | 48 (100%)  | 0        | 100         | 100 |
| 15  | CQ    | 144/192 (75%)  | 144 (100%) | 0        | 100         | 100 |
| 16  | Lq    | 109/112 (97%)  | 109 (100%) | 0        | 100         | 100 |
| 17  | Cb    | 85/101 (84%)   | 85 (100%)  | 0        | 100         | 100 |
| 18  | Cd    | 403/541 (74%)  | 403 (100%) | 0        | 100         | 100 |
| 19  | Ce    | 267/383 (70%)  | 267 (100%) | 0        | 100         | 100 |
| 20  | Cf    | 250/310 (81%)  | 250 (100%) | 0        | 100         | 100 |
| 21  | Cg    | 158/176 (90%)  | 158 (100%) | 0        | 100         | 100 |
| 22  | Ch    | 408/436 (94%)  | 408 (100%) | 0        | 100         | 100 |
| 23  | Cz    | 89/107 (83%)   | 89 (100%)  | 0        | 100         | 100 |
| 24  | LA    | 150/198 (76%)  | 150 (100%) | 0        | 100         | 100 |
| 25  | LB    | 329/331 (99%)  | 329 (100%) | 0        | 100         | 100 |
| 26  | LC    | 282/285 (99%)  | 282 (100%) | 0        | 100         | 100 |
| 27  | LD    | 221/253 (87%)  | 221 (100%) | 0        | 100         | 100 |
| 28  | LE    | 157/166 (95%)  | 157 (100%) | 0        | 100         | 100 |
| 29  | LG    | 200/222 (90%)  | 200 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 30  | LH    | 167/200 (84%)    | 167 (100%)  | 0        | 100         | 100 |
| 31  | LJ    | 140/150 (93%)    | 140 (100%)  | 0        | 100         | 100 |
| 32  | LK    | 127/136 (93%)    | 127 (100%)  | 0        | 100         | 100 |
| 33  | LL    | 158/176 (90%)    | 158 (100%)  | 0        | 100         | 100 |
| 34  | LM    | 116/117 (99%)    | 116 (100%)  | 0        | 100         | 100 |
| 35  | LN    | 179/180 (99%)    | 179 (100%)  | 0        | 100         | 100 |
| 36  | LO    | 162/163 (99%)    | 162 (100%)  | 0        | 100         | 100 |
| 37  | LP    | 133/152 (88%)    | 133 (100%)  | 0        | 100         | 100 |
| 38  | LQ    | 128/178 (72%)    | 128 (100%)  | 0        | 100         | 100 |
| 39  | LR    | 125/2396 (5%)    | 125 (100%)  | 0        | 100         | 100 |
| 40  | LS    | 152/154 (99%)    | 152 (100%)  | 0        | 100         | 100 |
| 41  | LT    | 110/135 (82%)    | 110 (100%)  | 0        | 100         | 100 |
| 42  | LU    | 92/108 (85%)     | 92 (100%)   | 0        | 100         | 100 |
| 43  | LV    | 98/102 (96%)     | 98 (100%)   | 0        | 100         | 100 |
| 44  | LX    | 122/129 (95%)    | 122 (100%)  | 0        | 100         | 100 |
| 45  | LY    | 116/119 (98%)    | 116 (100%)  | 0        | 100         | 100 |
| 46  | LZ    | 121/121 (100%)   | 121 (100%)  | 0        | 100         | 100 |
| 47  | La    | 93/122 (76%)     | 93 (100%)   | 0        | 100         | 100 |
| 48  | Lc    | 76/88 (86%)      | 76 (100%)   | 0        | 100         | 100 |
| 49  | Ld    | 90/105 (86%)     | 90 (100%)   | 0        | 100         | 100 |
| 50  | Le    | 109/114 (96%)    | 109 (100%)  | 0        | 100         | 100 |
| 51  | Lf    | 89/90 (99%)      | 89 (100%)   | 0        | 100         | 100 |
| 52  | Lg    | 95/102 (93%)     | 95 (100%)   | 0        | 100         | 100 |
| 53  | Lh    | 109/781 (14%)    | 109 (100%)  | 0        | 100         | 100 |
| 54  | Li    | 85/93 (91%)      | 85 (100%)   | 0        | 100         | 100 |
| 55  | Lj    | 72/78 (92%)      | 72 (100%)   | 0        | 100         | 100 |
| 56  | Lk    | 73/88 (83%)      | 73 (100%)   | 0        | 100         | 100 |
| 57  | Ll    | 45/46 (98%)      | 45 (100%)   | 0        | 100         | 100 |
| 58  | Lp    | 73/74 (99%)      | 73 (100%)   | 0        | 100         | 100 |
| 59  | Lr    | 186/189 (98%)    | 186 (100%)  | 0        | 100         | 100 |
| All | All   | 9054/13972 (65%) | 9053 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | CK    | 190 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | CF    | 205 | GLN  |
| 7   | CH    | 73  | GLN  |
| 7   | CH    | 77  | HIS  |
| 7   | CH    | 82  | ASN  |
| 7   | CH    | 266 | GLN  |
| 7   | CH    | 411 | ASN  |
| 7   | CH    | 608 | GLN  |
| 7   | CH    | 619 | GLN  |
| 9   | CJ    | 173 | HIS  |
| 10  | CK    | 14  | HIS  |
| 10  | CK    | 53  | GLN  |
| 10  | CK    | 95  | ASN  |
| 10  | CK    | 248 | ASN  |
| 12  | CM    | 178 | ASN  |
| 15  | CQ    | 39  | ASN  |
| 15  | CQ    | 82  | ASN  |
| 16  | Lq    | 15  | ASN  |
| 16  | Lq    | 43  | HIS  |
| 17  | Cb    | 68  | HIS  |
| 18  | Cd    | 9   | ASN  |
| 18  | Cd    | 22  | HIS  |
| 19  | Ce    | 329 | GLN  |
| 20  | Cf    | 40  | GLN  |
| 21  | Cg    | 106 | GLN  |
| 21  | Cg    | 185 | GLN  |
| 22  | Ch    | 56  | ASN  |
| 22  | Ch    | 127 | GLN  |
| 22  | Ch    | 274 | HIS  |
| 22  | Ch    | 326 | HIS  |
| 22  | Ch    | 432 | ASN  |
| 23  | Cz    | 58  | GLN  |
| 23  | Cz    | 81  | GLN  |
| 24  | LA    | 205 | ASN  |
| 25  | LB    | 166 | GLN  |
| 25  | LB    | 183 | GLN  |
| 26  | LC    | 38  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | LC    | 217 | HIS  |
| 26  | LC    | 330 | ASN  |
| 27  | LD    | 57  | ASN  |
| 27  | LD    | 89  | ASN  |
| 27  | LD    | 90  | HIS  |
| 28  | LE    | 35  | GLN  |
| 28  | LE    | 124 | GLN  |
| 12  | LF    | 200 | ASN  |
| 12  | LF    | 249 | ASN  |
| 29  | LG    | 36  | ASN  |
| 29  | LG    | 194 | HIS  |
| 30  | LH    | 133 | HIS  |
| 30  | LH    | 179 | GLN  |
| 32  | LK    | 8   | ASN  |
| 32  | LK    | 14  | HIS  |
| 32  | LK    | 66  | ASN  |
| 32  | LK    | 142 | GLN  |
| 33  | LL    | 114 | GLN  |
| 34  | LM    | 5   | ASN  |
| 35  | LN    | 32  | GLN  |
| 35  | LN    | 91  | GLN  |
| 35  | LN    | 95  | GLN  |
| 35  | LN    | 138 | ASN  |
| 37  | LP    | 75  | GLN  |
| 38  | LQ    | 98  | ASN  |
| 38  | LQ    | 122 | GLN  |
| 39  | LR    | 125 | HIS  |
| 40  | LS    | 88  | HIS  |
| 40  | LS    | 89  | ASN  |
| 41  | LT    | 131 | GLN  |
| 45  | LY    | 18  | HIS  |
| 47  | La    | 11  | HIS  |
| 47  | La    | 62  | HIS  |
| 49  | Ld    | 64  | ASN  |
| 51  | Lf    | 7   | HIS  |
| 58  | Lp    | 45  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | C1    | 3130/3342 (93%) | 590 (18%)         | 41 (1%)         |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2   | C2    | 155/156 (99%)   | 21 (13%)          | 0               |
| 3   | C3    | 80/162 (49%)    | 19 (23%)          | 0               |
| 4   | C4    | 118/119 (99%)   | 25 (21%)          | 2 (1%)          |
| All | All   | 3483/3779 (92%) | 655 (18%)         | 43 (1%)         |

All (655) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 6   | G    |
| 1   | C1    | 27  | A    |
| 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    | 72  | A    |
| 1   | C1    | 95  | G    |
| 1   | C1    | 96  | A    |
| 1   | C1    | 110 | A    |
| 1   | C1    | 111 | G    |
| 1   | C1    | 117 | A    |
| 1   | C1    | 123 | A    |
| 1   | C1    | 132 | U    |
| 1   | C1    | 134 | G    |
| 1   | C1    | 135 | G    |
| 1   | C1    | 139 | G    |
| 1   | C1    | 144 | G    |
| 1   | C1    | 152 | G    |
| 1   | C1    | 153 | A    |
| 1   | C1    | 156 | G    |
| 1   | C1    | 157 | G    |
| 1   | C1    | 181 | G    |
| 1   | C1    | 184 | U    |
| 1   | C1    | 194 | C    |
| 1   | C1    | 204 | C    |
| 1   | C1    | 213 | A    |
| 1   | C1    | 214 | G    |
| 1   | C1    | 225 | A    |
| 1   | C1    | 226 | G    |
| 1   | C1    | 241 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 244 | G    |
| 1   | C1    | 247 | A    |
| 1   | C1    | 258 | A    |
| 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    | 332 | C    |
| 1   | C1    | 339 | C    |
| 1   | C1    | 342 | A    |
| 1   | C1    | 343 | C    |
| 1   | C1    | 369 | G    |
| 1   | C1    | 385 | OMG  |
| 1   | C1    | 386 | U    |
| 1   | C1    | 388 | A    |
| 1   | C1    | 389 | A2M  |
| 1   | C1    | 391 | U    |
| 1   | C1    | 392 | A    |
| 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    |
| 1   | C1    | 448 | C    |
| 1   | C1    | 458 | U    |
| 1   | C1    | 459 | C    |
| 1   | C1    | 460 | U    |
| 1   | C1    | 469 | C    |
| 1   | C1    | 470 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 471 | C    |
| 1   | C1    | 472 | U    |
| 1   | C1    | 479 | G    |
| 1   | C1    | 486 | G    |
| 1   | C1    | 512 | A    |
| 1   | C1    | 514 | A    |
| 1   | C1    | 527 | G    |
| 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    | 583 | A    |
| 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    | 627 | OMG  |
| 1   | C1    | 628 | U    |
| 1   | C1    | 632 | G    |
| 1   | C1    | 633 | A    |
| 1   | C1    | 634 | A    |
| 1   | C1    | 646 | OMG  |
| 1   | C1    | 647 | G    |
| 1   | C1    | 648 | A    |
| 1   | C1    | 650 | U    |
| 1   | C1    | 665 | A    |
| 1   | C1    | 669 | U    |
| 1   | C1    | 678 | A    |
| 1   | C1    | 693 | A    |
| 1   | C1    | 700 | G    |
| 1   | C1    | 703 | A    |
| 1   | C1    | 707 | U    |
| 1   | C1    | 719 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 720 | C    |
| 1   | C1    | 721 | 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    | 766 | G    |
| 1   | C1    | 767 | G    |
| 1   | C1    | 778 | OMC  |
| 1   | C1    | 779 | U    |
| 1   | C1    | 782 | G    |
| 1   | C1    | 787 | OMG  |
| 1   | C1    | 788 | A    |
| 1   | C1    | 799 | A    |
| 1   | C1    | 812 | A    |
| 1   | C1    | 830 | A    |
| 1   | C1    | 843 | C    |
| 1   | C1    | 857 | G    |
| 1   | C1    | 877 | A    |
| 1   | C1    | 878 | A    |
| 1   | C1    | 879 | U    |
| 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    |
| 1   | C1    | 931 | C    |
| 1   | C1    | 933 | A    |
| 1   | C1    | 935 | G    |
| 1   | C1    | 937 | U    |
| 1   | C1    | 940 | C    |
| 1   | C1    | 941 | C    |
| 1   | C1    | 942 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 944  | A    |
| 1   | C1    | 945  | G    |
| 1   | C1    | 947  | A    |
| 1   | C1    | 955  | G    |
| 1   | C1    | 956  | U    |
| 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    | 1086 | A    |
| 1   | C1    | 1099 | G    |
| 1   | C1    | 1109 | G    |
| 1   | C1    | 1110 | G    |
| 1   | C1    | 1115 | C    |
| 1   | C1    | 1118 | A    |
| 1   | C1    | 1127 | U    |
| 1   | C1    | 1132 | G    |
| 1   | C1    | 1136 | A    |
| 1   | C1    | 1143 | C    |
| 1   | C1    | 1161 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 1163 | G    |
| 1   | C1    | 1164 | U    |
| 1   | C1    | 1165 | G    |
| 1   | C1    | 1173 | A    |
| 1   | C1    | 1175 | C    |
| 1   | C1    | 1176 | A    |
| 1   | C1    | 1179 | C    |
| 1   | C1    | 1185 | A    |
| 1   | C1    | 1187 | A    |
| 1   | C1    | 1194 | U    |
| 1   | C1    | 1205 | G    |
| 1   | C1    | 1209 | G    |
| 1   | C1    | 1228 | A    |
| 1   | C1    | 1241 | U    |
| 1   | C1    | 1246 | A    |
| 1   | C1    | 1248 | U    |
| 1   | C1    | 1255 | C    |
| 1   | C1    | 1268 | G    |
| 1   | C1    | 1269 | A    |
| 1   | C1    | 1270 | A    |
| 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    | 1331 | A    |
| 1   | C1    | 1332 | G    |
| 1   | C1    | 1333 | A    |
| 1   | C1    | 1334 | A    |
| 1   | C1    | 1335 | A    |
| 1   | C1    | 1336 | C    |
| 1   | C1    | 1337 | G    |
| 1   | C1    | 1370 | G    |
| 1   | C1    | 1375 | G    |
| 1   | C1    | 1382 | A    |
| 1   | C1    | 1383 | G    |
| 1   | C1    | 1401 | A    |
| 1   | C1    | 1417 | G    |
| 1   | C1    | 1420 | OMC  |
| 1   | C1    | 1421 | U    |
| 1   | C1    | 1429 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 1433 | OMG  |
| 1   | C1    | 1434 | C    |
| 1   | C1    | 1438 | U    |
| 1   | C1    | 1458 | G    |
| 1   | C1    | 1464 | A    |
| 1   | C1    | 1466 | G    |
| 1   | C1    | 1485 | G    |
| 1   | C1    | 1491 | OMC  |
| 1   | C1    | 1492 | G    |
| 1   | C1    | 1505 | U    |
| 1   | C1    | 1506 | U    |
| 1   | C1    | 1519 | G    |
| 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    | 1552 | G    |
| 1   | C1    | 1554 | G    |
| 1   | C1    | 1560 | U    |
| 1   | C1    | 1563 | 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    |
| 1   | C1    | 1609 | U    |
| 1   | C1    | 1619 | C    |
| 1   | C1    | 1623 | A    |
| 1   | C1    | 1624 | C    |
| 1   | C1    | 1685 | U    |
| 1   | C1    | 1697 | C    |
| 1   | C1    | 1704 | U    |
| 1   | C1    | 1710 | G    |
| 1   | C1    | 1722 | U    |
| 1   | C1    | 1730 | A    |
| 1   | C1    | 1731 | G    |
| 1   | C1    | 1745 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 1746 | G    |
| 1   | C1    | 1751 | G    |
| 1   | C1    | 1760 | G    |
| 1   | C1    | 1776 | G    |
| 1   | C1    | 1777 | A    |
| 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    | 1812 | OMC  |
| 1   | C1    | 1813 | G    |
| 1   | C1    | 1822 | A    |
| 1   | C1    | 1826 | C    |
| 1   | C1    | 1829 | C    |
| 1   | C1    | 1830 | A    |
| 1   | C1    | 1836 | OMC  |
| 1   | C1    | 1837 | C    |
| 1   | C1    | 1846 | C    |
| 1   | C1    | 1847 | A2M  |
| 1   | C1    | 1856 | U    |
| 1   | C1    | 1858 | G    |
| 1   | C1    | 1859 | A    |
| 1   | C1    | 1860 | U    |
| 1   | C1    | 1886 | G    |
| 1   | C1    | 1887 | C    |
| 1   | C1    | 1917 | OMU  |
| 1   | C1    | 1934 | G    |
| 1   | C1    | 1935 | C    |
| 1   | C1    | 1937 | C    |
| 1   | C1    | 2046 | C    |
| 1   | C1    | 2047 | G    |
| 1   | C1    | 2048 | U    |
| 1   | C1    | 2050 | C    |
| 1   | C1    | 2052 | G    |
| 1   | C1    | 2054 | U    |
| 1   | C1    | 2056 | A    |
| 1   | C1    | 2076 | A    |
| 1   | C1    | 2084 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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    | 2147 | U    |
| 1   | C1    | 2151 | A    |
| 1   | C1    | 2156 | U    |
| 1   | C1    | 2157 | G    |
| 1   | C1    | 2158 | C    |
| 1   | C1    | 2161 | A    |
| 1   | C1    | 2167 | C    |
| 1   | C1    | 2169 | G    |
| 1   | C1    | 2171 | A    |
| 1   | C1    | 2172 | U    |
| 1   | C1    | 2186 | A    |
| 1   | C1    | 2188 | U    |
| 1   | C1    | 2192 | A    |
| 1   | C1    | 2203 | G    |
| 1   | C1    | 2205 | A    |
| 1   | C1    | 2206 | A    |
| 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    |
| 1   | C1    | 2225 | A    |
| 1   | C1    | 2226 | C    |
| 1   | C1    | 2229 | U    |
| 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 2297 | U    |
| 1   | C1    | 2298 | G    |
| 1   | C1    | 2299 | U    |
| 1   | C1    | 2300 | OMC  |
| 1   | C1    | 2301 | C    |
| 1   | C1    | 2327 | G    |
| 1   | C1    | 2340 | G    |
| 1   | C1    | 2348 | A    |
| 1   | C1    | 2355 | C    |
| 1   | C1    | 2356 | G    |
| 1   | C1    | 2358 | OMG  |
| 1   | C1    | 2359 | 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    | 2398 | G    |
| 1   | C1    | 2407 | C    |
| 1   | C1    | 2409 | U    |
| 1   | C1    | 2410 | A    |
| 1   | C1    | 2411 | G    |
| 1   | C1    | 2415 | G    |
| 1   | C1    | 2416 | U    |
| 1   | C1    | 2421 | A    |
| 1   | C1    | 2422 | A    |
| 1   | C1    | 2425 | G    |
| 1   | C1    | 2426 | G    |
| 1   | C1    | 2431 | A    |
| 1   | C1    | 2432 | G    |
| 1   | C1    | 2435 | U    |
| 1   | C1    | 2437 | G    |
| 1   | C1    | 2438 | G    |
| 1   | C1    | 2440 | G    |
| 1   | C1    | 2446 | G    |
| 1   | C1    | 2450 | U    |
| 1   | C1    | 2454 | A    |
| 1   | C1    | 2457 | A    |
| 1   | C1    | 2458 | C    |
| 1   | C1    | 2459 | U    |
| 1   | C1    | 2465 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 2466 | G    |
| 1   | C1    | 2472 | U    |
| 1   | C1    | 2477 | U    |
| 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    | 2515 | G    |
| 1   | C1    | 2521 | A    |
| 1   | C1    | 2527 | C    |
| 1   | C1    | 2533 | G    |
| 1   | C1    | 2544 | G    |
| 1   | C1    | 2545 | G    |
| 1   | C1    | 2552 | A    |
| 1   | C1    | 2565 | G    |
| 1   | C1    | 2566 | G    |
| 1   | C1    | 2576 | U    |
| 1   | C1    | 2577 | G    |
| 1   | C1    | 2578 | OMG  |
| 1   | C1    | 2579 | G    |
| 1   | C1    | 2582 | G    |
| 1   | C1    | 2584 | C    |
| 1   | C1    | 2585 | A    |
| 1   | C1    | 2605 | C    |
| 1   | C1    | 2613 | C    |
| 1   | C1    | 2615 | A    |
| 1   | C1    | 2631 | G    |
| 1   | C1    | 2633 | A    |
| 1   | C1    | 2635 | A    |
| 1   | C1    | 2636 | G    |
| 1   | C1    | 2647 | U    |
| 1   | C1    | 2651 | A    |
| 1   | C1    | 2656 | A    |
| 1   | C1    | 2663 | A    |
| 1   | C1    | 2664 | A    |
| 1   | C1    | 2667 | C    |
| 1   | C1    | 2672 | U    |
| 1   | C1    | 2673 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 2674 | A    |
| 1   | C1    | 2675 | U    |
| 1   | C1    | 2680 | A    |
| 1   | C1    | 2689 | G    |
| 1   | C1    | 2691 | G    |
| 1   | C1    | 2713 | G    |
| 1   | C1    | 2717 | A    |
| 1   | C1    | 2731 | C    |
| 1   | C1    | 2732 | C    |
| 1   | C1    | 2736 | G    |
| 1   | C1    | 2737 | A    |
| 1   | C1    | 2754 | U    |
| 1   | C1    | 2755 | G    |
| 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    | 2773 | G    |
| 1   | C1    | 2774 | OMG  |
| 1   | C1    | 2775 | G    |
| 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    | 2817 | U    |
| 1   | C1    | 2821 | U    |
| 1   | C1    | 2826 | C    |
| 1   | C1    | 2828 | U    |
| 1   | C1    | 2836 | G    |
| 1   | C1    | 2838 | OMC  |
| 1   | C1    | 2839 | U    |
| 1   | C1    | 2846 | A    |
| 1   | C1    | 2857 | G    |
| 1   | C1    | 2858 | C    |
| 1   | C1    | 2863 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 2876 | OMG  |
| 1   | C1    | 2877 | G    |
| 1   | C1    | 2881 | OMG  |
| 1   | C1    | 2882 | U    |
| 1   | C1    | 2883 | U    |
| 1   | C1    | 2884 | C    |
| 1   | C1    | 2885 | A    |
| 1   | C1    | 2894 | U    |
| 1   | C1    | 2895 | A    |
| 1   | C1    | 2903 | U    |
| 1   | C1    | 2905 | A    |
| 1   | C1    | 2909 | G    |
| 1   | C1    | 2918 | OMC  |
| 1   | C1    | 2919 | C    |
| 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    | 2949 | G    |
| 1   | C1    | 2951 | U    |
| 1   | C1    | 2955 | C    |
| 1   | C1    | 2956 | U    |
| 1   | C1    | 2970 | A    |
| 1   | C1    | 2980 | G    |
| 1   | C1    | 3014 | U    |
| 1   | C1    | 3017 | G    |
| 1   | C1    | 3032 | 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    | 3080 | A    |
| 1   | C1    | 3087 | A    |
| 1   | C1    | 3088 | A    |
| 1   | C1    | 3089 | U    |
| 1   | C1    | 3100 | A    |
| 1   | C1    | 3101 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 3102 | G    |
| 1   | C1    | 3112 | U    |
| 1   | C1    | 3113 | A    |
| 1   | C1    | 3119 | A    |
| 1   | C1    | 3124 | G    |
| 1   | C1    | 3125 | U    |
| 1   | C1    | 3126 | A    |
| 1   | C1    | 3127 | G    |
| 1   | C1    | 3131 | U    |
| 1   | C1    | 3133 | U    |
| 1   | C1    | 3135 | A    |
| 1   | C1    | 3141 | G    |
| 1   | C1    | 3146 | C    |
| 1   | C1    | 3155 | A    |
| 1   | C1    | 3162 | C    |
| 1   | C1    | 3163 | A    |
| 1   | C1    | 3164 | G    |
| 1   | C1    | 3186 | A    |
| 1   | C1    | 3190 | G    |
| 1   | C1    | 3200 | A    |
| 1   | C1    | 3206 | C    |
| 1   | C1    | 3210 | U    |
| 1   | C1    | 3211 | U    |
| 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    | 3244 | G    |
| 1   | C1    | 3245 | C    |
| 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    | 3295 | U    |
| 1   | C1    | 3297 | G    |
| 1   | C1    | 3299 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 3302 | G    |
| 1   | C1    | 3310 | G    |
| 1   | C1    | 3312 | G    |
| 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    | 52   | A    |
| 2   | C2    | 59   | A    |
| 2   | C2    | 62   | A    |
| 2   | C2    | 63   | G    |
| 2   | C2    | 81   | U    |
| 2   | C2    | 82   | U    |
| 2   | C2    | 83   | C    |
| 2   | C2    | 84   | C    |
| 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    | 125  | U    |
| 2   | C2    | 151  | C    |
| 2   | C2    | 154  | C    |
| 3   | C3    | 2    | U    |
| 3   | C3    | 3    | C    |
| 3   | C3    | 7    | C    |
| 3   | C3    | 10   | C    |
| 3   | C3    | 14   | C    |
| 3   | C3    | 19   | G    |
| 3   | C3    | 20   | G    |
| 3   | C3    | 25   | U    |
| 3   | C3    | 33   | A    |
| 3   | C3    | 36   | C    |
| 3   | C3    | 40   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C3    | 57  | A    |
| 3   | C3    | 58  | A    |
| 3   | C3    | 59  | A    |
| 3   | C3    | 63  | A    |
| 3   | C3    | 68  | C    |
| 3   | C3    | 69  | G    |
| 3   | C3    | 135 | G    |
| 3   | C3    | 138 | A    |
| 4   | C4    | 7   | G    |
| 4   | C4    | 9   | C    |
| 4   | C4    | 29  | G    |
| 4   | C4    | 52  | G    |
| 4   | C4    | 54  | U    |
| 4   | C4    | 55  | A    |
| 4   | C4    | 64  | A    |
| 4   | C4    | 66  | G    |
| 4   | C4    | 75  | A    |
| 4   | C4    | 76  | G    |
| 4   | C4    | 78  | A    |
| 4   | C4    | 83  | G    |
| 4   | C4    | 84  | G    |
| 4   | C4    | 85  | U    |
| 4   | C4    | 86  | C    |
| 4   | C4    | 87  | G    |
| 4   | C4    | 89  | U    |
| 4   | C4    | 90  | G    |
| 4   | C4    | 91  | A    |
| 4   | C4    | 95  | C    |
| 4   | C4    | 96  | C    |
| 4   | C4    | 98  | G    |
| 4   | C4    | 100 | G    |
| 4   | C4    | 101 | A    |
| 4   | C4    | 111 | G    |

All (43) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C1    | 151 | G    |
| 1   | C1    | 243 | U    |
| 1   | C1    | 385 | OMG  |
| 1   | C1    | 627 | OMG  |
| 1   | C1    | 646 | OMG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C1    | 778  | OMC  |
| 1   | C1    | 787  | OMG  |
| 1   | C1    | 898  | G    |
| 1   | C1    | 1047 | A    |
| 1   | C1    | 1064 | C    |
| 1   | C1    | 1077 | U    |
| 1   | C1    | 1267 | C    |
| 1   | C1    | 1420 | OMC  |
| 1   | C1    | 1433 | OMG  |
| 1   | C1    | 1491 | OMC  |
| 1   | C1    | 1537 | U    |
| 1   | C1    | 1812 | OMC  |
| 1   | C1    | 1836 | OMC  |
| 1   | C1    | 2157 | G    |
| 1   | C1    | 2160 | C    |
| 1   | C1    | 2225 | A    |
| 1   | C1    | 2280 | A    |
| 1   | C1    | 2300 | OMC  |
| 1   | C1    | 2358 | OMG  |
| 1   | C1    | 2409 | U    |
| 1   | C1    | 2575 | C    |
| 1   | C1    | 2578 | OMG  |
| 1   | C1    | 2774 | OMG  |
| 1   | C1    | 2838 | OMC  |
| 1   | C1    | 2876 | OMG  |
| 1   | C1    | 2881 | OMG  |
| 1   | C1    | 2883 | U    |
| 1   | C1    | 2918 | OMC  |
| 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    |
| 4   | C4    | 85   | U    |
| 4   | C4    | 90   | G    |

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

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   | OMC  | C1    | 2918 | 1    | 19,22,23     | 3.13 | 8 (42%)     | 25,31,34    | 2.67 | 9 (36%)     |
| 1   | A2M  | C1    | 1223 | 1    | 22,25,26     | 3.96 | 10 (45%)    | 30,36,39    | 3.33 | 13 (43%)    |
| 1   | OMC  | C1    | 2300 | 1    | 19,22,23     | 3.04 | 8 (42%)     | 25,31,34    | 2.79 | 11 (44%)    |
| 1   | OMC  | C1    | 1812 | 1    | 19,22,23     | 3.14 | 8 (42%)     | 25,31,34    | 2.60 | 10 (40%)    |
| 1   | OMG  | C1    | 787  | 1    | 23,26,27     | 2.48 | 9 (39%)     | 32,38,41    | 2.98 | 16 (50%)    |
| 1   | OMC  | C1    | 778  | 1    | 19,22,23     | 3.12 | 8 (42%)     | 25,31,34    | 2.63 | 9 (36%)     |
| 1   | OMU  | C1    | 2683 | 1    | 19,22,23     | 3.10 | 6 (31%)     | 25,31,34    | 1.76 | 5 (20%)     |
| 1   | OMC  | C1    | 1420 | 1    | 19,22,23     | 3.03 | 8 (42%)     | 25,31,34    | 2.61 | 9 (36%)     |
| 1   | A2M  | C1    | 389  | 1    | 22,25,26     | 4.00 | 12 (54%)    | 30,36,39    | 3.41 | 12 (40%)    |
| 1   | OMC  | C1    | 1491 | 1    | 19,22,23     | 3.08 | 8 (42%)     | 25,31,34    | 2.71 | 10 (40%)    |
| 1   | A2M  | C1    | 848  | 1    | 22,25,26     | 3.99 | 12 (54%)    | 30,36,39    | 3.44 | 14 (46%)    |
| 1   | A2M  | C1    | 1432 | 1    | 22,25,26     | 3.98 | 12 (54%)    | 30,36,39    | 3.43 | 13 (43%)    |
| 1   | A2M  | C1    | 2289 | 1    | 22,25,26     | 4.00 | 11 (50%)    | 30,36,39    | 3.32 | 13 (43%)    |
| 1   | OMC  | C1    | 2838 | 1    | 19,22,23     | 3.16 | 8 (42%)     | 25,31,34    | 2.63 | 8 (32%)     |
| 1   | OMC  | C1    | 1836 | 1    | 19,22,23     | 3.11 | 8 (42%)     | 25,31,34    | 2.75 | 10 (40%)    |
| 1   | OMU  | C1    | 1868 | 1    | 19,22,23     | 3.14 | 6 (31%)     | 25,31,34    | 1.86 | 5 (20%)     |
| 1   | A2M  | C1    | 1847 | 1    | 22,25,26     | 3.97 | 12 (54%)    | 30,36,39    | 3.47 | 14 (46%)    |
| 1   | OMG  | C1    | 2358 | 1    | 23,26,27     | 2.50 | 9 (39%)     | 32,38,41    | 2.82 | 18 (56%)    |
| 1   | OMG  | C1    | 385  | 1    | 23,26,27     | 2.49 | 9 (39%)     | 32,38,41    | 2.92 | 19 (59%)    |
| 1   | OMG  | C1    | 2881 | 1    | 23,26,27     | 2.48 | 9 (39%)     | 32,38,41    | 2.86 | 17 (53%)    |
| 1   | OMG  | C1    | 2774 | 1    | 23,26,27     | 2.51 | 9 (39%)     | 32,38,41    | 2.87 | 18 (56%)    |
| 1   | A2M  | C1    | 858  | 1    | 22,25,26     | 4.00 | 12 (54%)    | 30,36,39    | 3.37 | 12 (40%)    |
| 1   | OMG  | C1    | 1433 | 1    | 23,26,27     | 2.51 | 9 (39%)     | 32,38,41    | 2.86 | 18 (56%)    |
| 1   | OMU  | C1    | 2277 | 1    | 19,22,23     | 3.13 | 6 (31%)     | 25,31,34    | 1.76 | 5 (20%)     |
| 1   | OMG  | C1    | 2578 | 1    | 23,26,27     | 2.53 | 9 (39%)     | 32,38,41    | 2.90 | 18 (56%)    |
| 1   | OMG  | C1    | 2876 | 1    | 23,26,27     | 2.55 | 8 (34%)     | 32,38,41    | 3.15 | 16 (50%)    |
| 1   | OMG  | C1    | 627  | 1    | 23,26,27     | 2.52 | 9 (39%)     | 32,38,41    | 2.85 | 17 (53%)    |
| 1   | OMU  | C1    | 1917 | 1    | 19,22,23     | 3.17 | 6 (31%)     | 25,31,34    | 1.80 | 5 (20%)     |
| 1   | OMU  | C1    | 2380 | 1    | 19,22,23     | 3.10 | 6 (31%)     | 25,31,34    | 1.78 | 5 (20%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMU  | C1    | 2690 | 1    | 19,22,23     | 3.11 | 6 (31%)  | 25,31,34    | 1.78 | 4 (16%)  |
| 1   | OMU  | C1    | 2688 | 1    | 19,22,23     | 3.13 | 6 (31%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 1   | OMG  | C1    | 646  | 1    | 23,26,27     | 2.54 | 9 (39%)  | 32,38,41    | 2.85 | 17 (53%) |
| 1   | A2M  | C1    | 637  | 1    | 22,25,26     | 3.98 | 11 (50%) | 30,36,39    | 3.36 | 13 (43%) |
| 1   | OMU  | C1    | 2384 | 1    | 19,22,23     | 3.16 | 6 (31%)  | 25,31,34    | 1.75 | 5 (20%)  |

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   | OMC  | C1    | 2918 | 1    | 2/2/5/5 | 5/9/27/28 | 0/2/2/2 |
| 1   | OMC  | C1    | 2300 | 1    | 2/2/5/5 | 5/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 646  | 1    | 2/2/5/5 | 4/9/27/28 | 0/3/3/3 |
| 1   | OMC  | C1    | 1812 | 1    | 2/2/5/5 | 3/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 787  | 1    | 2/2/5/5 | 1/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 1223 | 1    | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | OMC  | C1    | 778  | 1    | 2/2/5/5 | 4/9/27/28 | 0/2/2/2 |
| 1   | OMU  | C1    | 2683 | 1    | -       | 1/9/27/28 | 0/2/2/2 |
| 1   | OMC  | C1    | 1420 | 1    | 2/2/5/5 | 5/9/27/28 | 0/2/2/2 |
| 1   | A2M  | C1    | 389  | 1    | -       | 3/9/27/28 | 0/3/3/3 |
| 1   | OMC  | C1    | 1491 | 1    | 2/2/5/5 | 6/9/27/28 | 0/2/2/2 |
| 1   | A2M  | C1    | 848  | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 1432 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 2289 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMC  | C1    | 2838 | 1    | 2/2/5/5 | 5/9/27/28 | 0/2/2/2 |
| 1   | OMC  | C1    | 1836 | 1    | 2/2/5/5 | 5/9/27/28 | 0/2/2/2 |
| 1   | OMU  | C1    | 1868 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | A2M  | C1    | 1847 | 1    | -       | 3/9/27/28 | 0/3/3/3 |
| 1   | OMG  | C1    | 385  | 1    | 2/2/5/5 | 4/9/27/28 | 0/3/3/3 |
| 1   | OMG  | C1    | 2881 | 1    | 2/2/5/5 | 3/9/27/28 | 0/3/3/3 |
| 1   | OMG  | C1    | 2774 | 1    | 2/2/5/5 | 4/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 858  | 1    | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | OMG  | C1    | 1433 | 1    | 2/2/5/5 | 3/9/27/28 | 0/3/3/3 |
| 1   | OMU  | C1    | 2277 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 2578 | 1    | 2/2/5/5 | 4/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | OMG  | C1    | 2876 | 1    | 2/2/5/5 | 3/9/27/28 | 0/3/3/3 |
| 1   | OMG  | C1    | 627  | 1    | 2/2/5/5 | 2/9/27/28 | 0/3/3/3 |
| 1   | OMU  | C1    | 1917 | 1    | -       | 3/9/27/28 | 0/2/2/2 |
| 1   | OMU  | C1    | 2380 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMU  | C1    | 2690 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMU  | C1    | 2688 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMG  | C1    | 2358 | 1    | 2/2/5/5 | 4/9/27/28 | 0/3/3/3 |
| 1   | A2M  | C1    | 637  | 1    | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | OMU  | C1    | 2384 | 1    | -       | 1/9/27/28 | 0/2/2/2 |

All (293) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | C1    | 2289 | A2M  | C3'-C2' | -13.08 | 1.24        | 1.53     |
| 1   | C1    | 858  | A2M  | C3'-C2' | -13.04 | 1.24        | 1.53     |
| 1   | C1    | 637  | A2M  | C3'-C2' | -12.99 | 1.24        | 1.53     |
| 1   | C1    | 848  | A2M  | C3'-C2' | -12.98 | 1.24        | 1.53     |
| 1   | C1    | 389  | A2M  | C3'-C2' | -12.89 | 1.24        | 1.53     |
| 1   | C1    | 1223 | A2M  | C3'-C2' | -12.83 | 1.24        | 1.53     |
| 1   | C1    | 1432 | A2M  | C3'-C2' | -12.81 | 1.25        | 1.53     |
| 1   | C1    | 1847 | A2M  | C3'-C2' | -12.81 | 1.25        | 1.53     |
| 1   | C1    | 1917 | OMU  | C2-N1   | 7.81   | 1.50        | 1.38     |
| 1   | C1    | 2384 | OMU  | C2-N1   | 7.66   | 1.50        | 1.38     |
| 1   | C1    | 1868 | OMU  | C2-N1   | 7.60   | 1.50        | 1.38     |
| 1   | C1    | 2277 | OMU  | C2-N1   | 7.50   | 1.50        | 1.38     |
| 1   | C1    | 2688 | OMU  | C2-N1   | 7.44   | 1.50        | 1.38     |
| 1   | C1    | 2690 | OMU  | C2-N1   | 7.44   | 1.50        | 1.38     |
| 1   | C1    | 2384 | OMU  | C2-N3   | 7.41   | 1.50        | 1.38     |
| 1   | C1    | 2683 | OMU  | C2-N1   | 7.40   | 1.50        | 1.38     |
| 1   | C1    | 2688 | OMU  | C2-N3   | 7.36   | 1.50        | 1.38     |
| 1   | C1    | 2380 | OMU  | C2-N3   | 7.34   | 1.50        | 1.38     |
| 1   | C1    | 2277 | OMU  | C2-N3   | 7.31   | 1.50        | 1.38     |
| 1   | C1    | 2380 | OMU  | C2-N1   | 7.30   | 1.49        | 1.38     |
| 1   | C1    | 2683 | OMU  | C2-N3   | 7.29   | 1.50        | 1.38     |
| 1   | C1    | 1868 | OMU  | C2-N3   | 7.28   | 1.50        | 1.38     |
| 1   | C1    | 2690 | OMU  | C2-N3   | 7.27   | 1.50        | 1.38     |
| 1   | C1    | 1917 | OMU  | C2-N3   | 7.24   | 1.50        | 1.38     |
| 1   | C1    | 646  | OMG  | C4-N3   | 6.82   | 1.49        | 1.34     |
| 1   | C1    | 2578 | OMG  | C4-N3   | 6.74   | 1.49        | 1.34     |
| 1   | C1    | 2876 | OMG  | C4-N3   | 6.70   | 1.49        | 1.34     |
| 1   | C1    | 2774 | OMG  | C4-N3   | 6.68   | 1.49        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C1    | 787  | OMG  | C4-N3   | 6.68  | 1.49        | 1.34     |
| 1   | C1    | 1433 | OMG  | C4-N3   | 6.65  | 1.49        | 1.34     |
| 1   | C1    | 2881 | OMG  | C4-N3   | 6.63  | 1.49        | 1.34     |
| 1   | C1    | 2358 | OMG  | C4-N3   | 6.63  | 1.49        | 1.34     |
| 1   | C1    | 627  | OMG  | C4-N3   | 6.63  | 1.49        | 1.34     |
| 1   | C1    | 637  | A2M  | O4'-C4' | -6.61 | 1.30        | 1.45     |
| 1   | C1    | 389  | A2M  | O4'-C4' | -6.57 | 1.30        | 1.45     |
| 1   | C1    | 385  | OMG  | C4-N3   | 6.55  | 1.49        | 1.34     |
| 1   | C1    | 1223 | A2M  | O4'-C4' | -6.54 | 1.30        | 1.45     |
| 1   | C1    | 858  | A2M  | O4'-C4' | -6.47 | 1.30        | 1.45     |
| 1   | C1    | 1847 | A2M  | O4'-C4' | -6.46 | 1.30        | 1.45     |
| 1   | C1    | 1432 | A2M  | O4'-C4' | -6.45 | 1.30        | 1.45     |
| 1   | C1    | 2289 | A2M  | O4'-C4' | -6.34 | 1.30        | 1.45     |
| 1   | C1    | 848  | A2M  | O4'-C4' | -6.30 | 1.31        | 1.45     |
| 1   | C1    | 1917 | OMU  | C6-C5   | 6.25  | 1.49        | 1.35     |
| 1   | C1    | 1868 | OMU  | C6-C5   | 6.21  | 1.49        | 1.35     |
| 1   | C1    | 2380 | OMU  | C6-C5   | 6.21  | 1.49        | 1.35     |
| 1   | C1    | 2277 | OMU  | C6-C5   | 6.19  | 1.49        | 1.35     |
| 1   | C1    | 2688 | OMU  | C6-C5   | 6.18  | 1.49        | 1.35     |
| 1   | C1    | 2690 | OMU  | C6-C5   | 6.17  | 1.49        | 1.35     |
| 1   | C1    | 2384 | OMU  | C6-C5   | 6.16  | 1.49        | 1.35     |
| 1   | C1    | 2683 | OMU  | C6-C5   | 6.12  | 1.49        | 1.35     |
| 1   | C1    | 2838 | OMC  | C4-N4   | 6.11  | 1.48        | 1.33     |
| 1   | C1    | 1812 | OMC  | C2-N3   | 6.10  | 1.48        | 1.36     |
| 1   | C1    | 1836 | OMC  | C4-N4   | 6.02  | 1.48        | 1.33     |
| 1   | C1    | 1812 | OMC  | C4-N4   | 6.01  | 1.48        | 1.33     |
| 1   | C1    | 1836 | OMC  | C2-N3   | 6.01  | 1.48        | 1.36     |
| 1   | C1    | 2918 | OMC  | C4-N4   | 6.00  | 1.48        | 1.33     |
| 1   | C1    | 778  | OMC  | C2-N3   | 5.96  | 1.48        | 1.36     |
| 1   | C1    | 778  | OMC  | C4-N4   | 5.95  | 1.48        | 1.33     |
| 1   | C1    | 2918 | OMC  | C2-N3   | 5.92  | 1.48        | 1.36     |
| 1   | C1    | 2300 | OMC  | C4-N4   | 5.88  | 1.48        | 1.33     |
| 1   | C1    | 1491 | OMC  | C2-N3   | 5.83  | 1.47        | 1.36     |
| 1   | C1    | 1491 | OMC  | C4-N4   | 5.81  | 1.48        | 1.33     |
| 1   | C1    | 2300 | OMC  | C2-N3   | 5.74  | 1.47        | 1.36     |
| 1   | C1    | 1420 | OMC  | C2-N3   | 5.72  | 1.47        | 1.36     |
| 1   | C1    | 2838 | OMC  | C2-N3   | 5.70  | 1.47        | 1.36     |
| 1   | C1    | 1420 | OMC  | C4-N4   | 5.69  | 1.47        | 1.33     |
| 1   | C1    | 1432 | A2M  | C3'-C4' | 5.63  | 1.67        | 1.53     |
| 1   | C1    | 2838 | OMC  | C2-N1   | 5.57  | 1.51        | 1.40     |
| 1   | C1    | 2876 | OMG  | C2-N3   | 5.55  | 1.46        | 1.33     |
| 1   | C1    | 2838 | OMC  | C6-C5   | 5.44  | 1.47        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 1   | C1    | 646  | OMG  | C2-N3   | 5.40 | 1.46        | 1.33     |
| 1   | C1    | 787  | OMG  | C2-N3   | 5.39 | 1.46        | 1.33     |
| 1   | C1    | 848  | A2M  | C3'-C4' | 5.37 | 1.66        | 1.53     |
| 1   | C1    | 2289 | A2M  | C3'-C4' | 5.36 | 1.66        | 1.53     |
| 1   | C1    | 858  | A2M  | C3'-C4' | 5.35 | 1.66        | 1.53     |
| 1   | C1    | 1223 | A2M  | C3'-C4' | 5.31 | 1.66        | 1.53     |
| 1   | C1    | 2918 | OMC  | C2-N1   | 5.30 | 1.51        | 1.40     |
| 1   | C1    | 627  | OMG  | C2-N3   | 5.30 | 1.46        | 1.33     |
| 1   | C1    | 2578 | OMG  | C2-N3   | 5.26 | 1.45        | 1.33     |
| 1   | C1    | 2300 | OMC  | C2-N1   | 5.25 | 1.51        | 1.40     |
| 1   | C1    | 2876 | OMG  | C2-N2   | 5.23 | 1.46        | 1.34     |
| 1   | C1    | 2578 | OMG  | C2-N2   | 5.23 | 1.46        | 1.34     |
| 1   | C1    | 2881 | OMG  | C2-N3   | 5.22 | 1.45        | 1.33     |
| 1   | C1    | 627  | OMG  | C2-N2   | 5.22 | 1.46        | 1.34     |
| 1   | C1    | 1847 | A2M  | C3'-C4' | 5.21 | 1.66        | 1.53     |
| 1   | C1    | 2774 | OMG  | C2-N3   | 5.20 | 1.45        | 1.33     |
| 1   | C1    | 2774 | OMG  | C2-N2   | 5.20 | 1.46        | 1.34     |
| 1   | C1    | 385  | OMG  | C2-N2   | 5.20 | 1.46        | 1.34     |
| 1   | C1    | 1433 | OMG  | C2-N3   | 5.20 | 1.45        | 1.33     |
| 1   | C1    | 637  | A2M  | C3'-C4' | 5.20 | 1.66        | 1.53     |
| 1   | C1    | 1491 | OMC  | C2-N1   | 5.19 | 1.51        | 1.40     |
| 1   | C1    | 1433 | OMG  | C2-N2   | 5.19 | 1.46        | 1.34     |
| 1   | C1    | 2918 | OMC  | C6-C5   | 5.19 | 1.47        | 1.35     |
| 1   | C1    | 2358 | OMG  | C2-N2   | 5.19 | 1.46        | 1.34     |
| 1   | C1    | 389  | A2M  | C3'-C4' | 5.18 | 1.66        | 1.53     |
| 1   | C1    | 778  | OMC  | C2-N1   | 5.18 | 1.50        | 1.40     |
| 1   | C1    | 1812 | OMC  | C6-C5   | 5.13 | 1.47        | 1.35     |
| 1   | C1    | 385  | OMG  | C2-N3   | 5.12 | 1.45        | 1.33     |
| 1   | C1    | 2358 | OMG  | C2-N3   | 5.09 | 1.45        | 1.33     |
| 1   | C1    | 1836 | OMC  | C2-N1   | 5.09 | 1.50        | 1.40     |
| 1   | C1    | 1812 | OMC  | C2-N1   | 5.08 | 1.50        | 1.40     |
| 1   | C1    | 646  | OMG  | C2-N2   | 5.07 | 1.46        | 1.34     |
| 1   | C1    | 2881 | OMG  | C2-N2   | 5.06 | 1.46        | 1.34     |
| 1   | C1    | 778  | OMC  | C6-C5   | 5.06 | 1.46        | 1.35     |
| 1   | C1    | 1491 | OMC  | C6-C5   | 5.03 | 1.46        | 1.35     |
| 1   | C1    | 1836 | OMC  | C6-C5   | 5.01 | 1.46        | 1.35     |
| 1   | C1    | 1420 | OMC  | C6-C5   | 4.95 | 1.46        | 1.35     |
| 1   | C1    | 787  | OMG  | C2-N2   | 4.95 | 1.45        | 1.34     |
| 1   | C1    | 1420 | OMC  | C2-N1   | 4.92 | 1.50        | 1.40     |
| 1   | C1    | 1812 | OMC  | C4-N3   | 4.87 | 1.44        | 1.34     |
| 1   | C1    | 1836 | OMC  | C4-N3   | 4.87 | 1.44        | 1.34     |
| 1   | C1    | 2300 | OMC  | C6-C5   | 4.83 | 1.46        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C1    | 778  | OMC  | C4-N3   | 4.81  | 1.44        | 1.34     |
| 1   | C1    | 2918 | OMC  | C4-N3   | 4.74  | 1.43        | 1.34     |
| 1   | C1    | 1420 | OMC  | C4-N3   | 4.74  | 1.43        | 1.34     |
| 1   | C1    | 2300 | OMC  | C4-N3   | 4.65  | 1.43        | 1.34     |
| 1   | C1    | 1491 | OMC  | C4-N3   | 4.63  | 1.43        | 1.34     |
| 1   | C1    | 2289 | A2M  | O4'-C1' | 4.55  | 1.52        | 1.42     |
| 1   | C1    | 848  | A2M  | O4'-C1' | 4.54  | 1.52        | 1.42     |
| 1   | C1    | 1847 | A2M  | O4'-C1' | 4.53  | 1.52        | 1.42     |
| 1   | C1    | 389  | A2M  | O4'-C1' | 4.52  | 1.52        | 1.42     |
| 1   | C1    | 858  | A2M  | O4'-C1' | 4.49  | 1.52        | 1.42     |
| 1   | C1    | 2384 | OMU  | C4-N3   | 4.45  | 1.46        | 1.38     |
| 1   | C1    | 2277 | OMU  | C4-N3   | 4.45  | 1.46        | 1.38     |
| 1   | C1    | 2683 | OMU  | C4-N3   | 4.45  | 1.46        | 1.38     |
| 1   | C1    | 2688 | OMU  | C4-N3   | 4.45  | 1.46        | 1.38     |
| 1   | C1    | 637  | A2M  | C6-N6   | 4.44  | 1.45        | 1.34     |
| 1   | C1    | 389  | A2M  | C6-N6   | 4.42  | 1.45        | 1.34     |
| 1   | C1    | 2289 | A2M  | C6-N6   | 4.40  | 1.45        | 1.34     |
| 1   | C1    | 637  | A2M  | O4'-C1' | 4.40  | 1.52        | 1.42     |
| 1   | C1    | 848  | A2M  | C6-N6   | 4.39  | 1.45        | 1.34     |
| 1   | C1    | 1223 | A2M  | C6-N6   | 4.39  | 1.45        | 1.34     |
| 1   | C1    | 858  | A2M  | C6-N6   | 4.39  | 1.45        | 1.34     |
| 1   | C1    | 1847 | A2M  | C6-N6   | 4.39  | 1.45        | 1.34     |
| 1   | C1    | 1868 | OMU  | C4-N3   | 4.38  | 1.46        | 1.38     |
| 1   | C1    | 1432 | A2M  | C6-N6   | 4.37  | 1.45        | 1.34     |
| 1   | C1    | 2380 | OMU  | C4-N3   | 4.35  | 1.46        | 1.38     |
| 1   | C1    | 1847 | A2M  | C1'-N9  | -4.35 | 1.34        | 1.46     |
| 1   | C1    | 1917 | OMU  | C4-N3   | 4.34  | 1.46        | 1.38     |
| 1   | C1    | 2690 | OMU  | C4-N3   | 4.34  | 1.46        | 1.38     |
| 1   | C1    | 2838 | OMC  | C4-N3   | 4.32  | 1.43        | 1.34     |
| 1   | C1    | 848  | A2M  | C1'-N9  | -4.30 | 1.34        | 1.46     |
| 1   | C1    | 1432 | A2M  | O4'-C1' | 4.30  | 1.51        | 1.42     |
| 1   | C1    | 1223 | A2M  | C1'-N9  | -4.29 | 1.34        | 1.46     |
| 1   | C1    | 1223 | A2M  | O4'-C1' | 4.27  | 1.51        | 1.42     |
| 1   | C1    | 858  | A2M  | C1'-N9  | -4.27 | 1.34        | 1.46     |
| 1   | C1    | 2289 | A2M  | C1'-N9  | -4.26 | 1.34        | 1.46     |
| 1   | C1    | 1432 | A2M  | C1'-N9  | -4.23 | 1.34        | 1.46     |
| 1   | C1    | 1491 | OMC  | O2-C2   | -4.21 | 1.15        | 1.23     |
| 1   | C1    | 389  | A2M  | C1'-N9  | -4.20 | 1.34        | 1.46     |
| 1   | C1    | 2300 | OMC  | O2-C2   | -4.19 | 1.15        | 1.23     |
| 1   | C1    | 1836 | OMC  | O2-C2   | -4.17 | 1.16        | 1.23     |
| 1   | C1    | 1420 | OMC  | O2-C2   | -4.13 | 1.16        | 1.23     |
| 1   | C1    | 2838 | OMC  | O2-C2   | -4.12 | 1.16        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C1    | 637  | A2M  | C1'-N9  | -4.11 | 1.35        | 1.46     |
| 1   | C1    | 778  | OMC  | O2-C2   | -4.09 | 1.16        | 1.23     |
| 1   | C1    | 2918 | OMC  | O2-C2   | -4.07 | 1.16        | 1.23     |
| 1   | C1    | 1812 | OMC  | O2-C2   | -4.04 | 1.16        | 1.23     |
| 1   | C1    | 389  | A2M  | O2'-C2' | 3.93  | 1.52        | 1.42     |
| 1   | C1    | 1432 | A2M  | O2'-C2' | 3.71  | 1.51        | 1.42     |
| 1   | C1    | 858  | A2M  | O2'-C2' | 3.68  | 1.51        | 1.42     |
| 1   | C1    | 637  | A2M  | O2'-C2' | 3.67  | 1.51        | 1.42     |
| 1   | C1    | 1223 | A2M  | O2'-C2' | 3.64  | 1.51        | 1.42     |
| 1   | C1    | 2289 | A2M  | O2'-C2' | 3.63  | 1.51        | 1.42     |
| 1   | C1    | 848  | A2M  | O2'-C2' | 3.60  | 1.51        | 1.42     |
| 1   | C1    | 1847 | A2M  | O2'-C2' | 3.58  | 1.51        | 1.42     |
| 1   | C1    | 389  | A2M  | C2'-C1' | 3.29  | 1.61        | 1.53     |
| 1   | C1    | 2838 | OMC  | C5-C4   | 3.16  | 1.50        | 1.42     |
| 1   | C1    | 2876 | OMG  | C5-N7   | -3.16 | 1.32        | 1.39     |
| 1   | C1    | 1847 | A2M  | C2'-C1' | 3.16  | 1.60        | 1.53     |
| 1   | C1    | 848  | A2M  | C2'-C1' | 3.15  | 1.60        | 1.53     |
| 1   | C1    | 646  | OMG  | C5-N7   | -3.09 | 1.32        | 1.39     |
| 1   | C1    | 627  | OMG  | C5-N7   | -3.05 | 1.33        | 1.39     |
| 1   | C1    | 1432 | A2M  | C2'-C1' | 3.00  | 1.60        | 1.53     |
| 1   | C1    | 2289 | A2M  | C2'-C1' | 3.00  | 1.60        | 1.53     |
| 1   | C1    | 2289 | A2M  | C5-C4   | -2.97 | 1.33        | 1.39     |
| 1   | C1    | 2881 | OMG  | O6-C6   | -2.96 | 1.18        | 1.23     |
| 1   | C1    | 787  | OMG  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 1   | C1    | 858  | A2M  | C5-C4   | -2.94 | 1.33        | 1.39     |
| 1   | C1    | 2876 | OMG  | O6-C6   | -2.93 | 1.18        | 1.23     |
| 1   | C1    | 637  | A2M  | C2'-C1' | 2.93  | 1.60        | 1.53     |
| 1   | C1    | 848  | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 1   | C1    | 1223 | A2M  | C5-C4   | -2.91 | 1.33        | 1.39     |
| 1   | C1    | 1223 | A2M  | C2'-C1' | 2.91  | 1.60        | 1.53     |
| 1   | C1    | 2838 | OMC  | C6-N1   | 2.91  | 1.45        | 1.38     |
| 1   | C1    | 1432 | A2M  | C5-C4   | -2.90 | 1.33        | 1.39     |
| 1   | C1    | 2918 | OMC  | C5-C4   | 2.90  | 1.49        | 1.42     |
| 1   | C1    | 389  | A2M  | C5-C4   | -2.89 | 1.33        | 1.39     |
| 1   | C1    | 858  | A2M  | C2'-C1' | 2.89  | 1.60        | 1.53     |
| 1   | C1    | 1847 | A2M  | C5-C4   | -2.88 | 1.33        | 1.39     |
| 1   | C1    | 2881 | OMG  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 1   | C1    | 637  | A2M  | C5-C4   | -2.86 | 1.34        | 1.39     |
| 1   | C1    | 646  | OMG  | O6-C6   | -2.86 | 1.18        | 1.23     |
| 1   | C1    | 1433 | OMG  | C5-N7   | -2.83 | 1.33        | 1.39     |
| 1   | C1    | 778  | OMC  | C5-C4   | 2.83  | 1.49        | 1.42     |
| 1   | C1    | 2358 | OMG  | C5-N7   | -2.83 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | C1    | 2358 | OMG  | O6-C6 | -2.82 | 1.18        | 1.23     |
| 1   | C1    | 2876 | OMG  | C2-N1 | 2.81  | 1.44        | 1.37     |
| 1   | C1    | 1812 | OMC  | C5-C4 | 2.81  | 1.49        | 1.42     |
| 1   | C1    | 2774 | OMG  | C5-N7 | -2.80 | 1.33        | 1.39     |
| 1   | C1    | 627  | OMG  | O6-C6 | -2.79 | 1.18        | 1.23     |
| 1   | C1    | 385  | OMG  | C2-N1 | 2.79  | 1.44        | 1.37     |
| 1   | C1    | 1491 | OMC  | C5-C4 | 2.79  | 1.49        | 1.42     |
| 1   | C1    | 1917 | OMU  | C6-N1 | 2.78  | 1.44        | 1.38     |
| 1   | C1    | 2578 | OMG  | C5-N7 | -2.78 | 1.33        | 1.39     |
| 1   | C1    | 2918 | OMC  | C6-N1 | 2.77  | 1.44        | 1.38     |
| 1   | C1    | 2578 | OMG  | O6-C6 | -2.76 | 1.18        | 1.23     |
| 1   | C1    | 2688 | OMU  | C6-N1 | 2.75  | 1.44        | 1.38     |
| 1   | C1    | 778  | OMC  | C6-N1 | 2.75  | 1.44        | 1.38     |
| 1   | C1    | 1420 | OMC  | C6-N1 | 2.74  | 1.44        | 1.38     |
| 1   | C1    | 1491 | OMC  | C6-N1 | 2.74  | 1.44        | 1.38     |
| 1   | C1    | 1433 | OMG  | O6-C6 | -2.74 | 1.18        | 1.23     |
| 1   | C1    | 2774 | OMG  | O6-C6 | -2.74 | 1.18        | 1.23     |
| 1   | C1    | 2690 | OMU  | C6-N1 | 2.74  | 1.44        | 1.38     |
| 1   | C1    | 1868 | OMU  | C6-N1 | 2.73  | 1.44        | 1.38     |
| 1   | C1    | 1812 | OMC  | C6-N1 | 2.73  | 1.44        | 1.38     |
| 1   | C1    | 1836 | OMC  | C5-C4 | 2.73  | 1.49        | 1.42     |
| 1   | C1    | 787  | OMG  | O6-C6 | -2.73 | 1.18        | 1.23     |
| 1   | C1    | 1433 | OMG  | C2-N1 | 2.72  | 1.44        | 1.37     |
| 1   | C1    | 2384 | OMU  | C6-N1 | 2.72  | 1.44        | 1.38     |
| 1   | C1    | 385  | OMG  | C5-N7 | -2.72 | 1.33        | 1.39     |
| 1   | C1    | 385  | OMG  | O6-C6 | -2.70 | 1.18        | 1.23     |
| 1   | C1    | 2380 | OMU  | C6-N1 | 2.70  | 1.44        | 1.38     |
| 1   | C1    | 2277 | OMU  | C6-N1 | 2.70  | 1.44        | 1.38     |
| 1   | C1    | 1836 | OMC  | C6-N1 | 2.70  | 1.44        | 1.38     |
| 1   | C1    | 2578 | OMG  | C2-N1 | 2.68  | 1.44        | 1.37     |
| 1   | C1    | 389  | A2M  | C5-N7 | -2.66 | 1.34        | 1.39     |
| 1   | C1    | 2683 | OMU  | C6-N1 | 2.66  | 1.44        | 1.38     |
| 1   | C1    | 385  | OMG  | C6-N1 | 2.64  | 1.43        | 1.38     |
| 1   | C1    | 637  | A2M  | C5-N7 | -2.64 | 1.34        | 1.39     |
| 1   | C1    | 1223 | A2M  | C5-N7 | -2.62 | 1.34        | 1.39     |
| 1   | C1    | 1420 | OMC  | C5-C4 | 2.62  | 1.49        | 1.42     |
| 1   | C1    | 2774 | OMG  | C6-N1 | 2.61  | 1.43        | 1.38     |
| 1   | C1    | 1432 | A2M  | C5-N7 | -2.61 | 1.34        | 1.39     |
| 1   | C1    | 646  | OMG  | C2-N1 | 2.61  | 1.44        | 1.37     |
| 1   | C1    | 627  | OMG  | C2-N1 | 2.59  | 1.43        | 1.37     |
| 1   | C1    | 1847 | A2M  | C5-N7 | -2.58 | 1.34        | 1.39     |
| 1   | C1    | 858  | A2M  | C5-N7 | -2.58 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C1    | 787  | OMG  | C2-N1   | 2.57  | 1.43        | 1.37     |
| 1   | C1    | 2300 | OMC  | C5-C4   | 2.57  | 1.48        | 1.42     |
| 1   | C1    | 2578 | OMG  | C6-N1   | 2.56  | 1.43        | 1.38     |
| 1   | C1    | 2881 | OMG  | C2-N1   | 2.56  | 1.43        | 1.37     |
| 1   | C1    | 385  | OMG  | C5-C6   | 2.54  | 1.53        | 1.44     |
| 1   | C1    | 2774 | OMG  | C2-N1   | 2.54  | 1.43        | 1.37     |
| 1   | C1    | 2289 | A2M  | C5-N7   | -2.53 | 1.34        | 1.39     |
| 1   | C1    | 1433 | OMG  | C6-N1   | 2.53  | 1.43        | 1.38     |
| 1   | C1    | 2300 | OMC  | C6-N1   | 2.51  | 1.44        | 1.38     |
| 1   | C1    | 2358 | OMG  | C2-N1   | 2.49  | 1.43        | 1.37     |
| 1   | C1    | 848  | A2M  | C5-N7   | -2.47 | 1.34        | 1.39     |
| 1   | C1    | 2881 | OMG  | C4-N9   | -2.42 | 1.31        | 1.38     |
| 1   | C1    | 2876 | OMG  | C6-N1   | 2.41  | 1.43        | 1.38     |
| 1   | C1    | 627  | OMG  | C6-N1   | 2.40  | 1.43        | 1.38     |
| 1   | C1    | 2358 | OMG  | C6-N1   | 2.37  | 1.43        | 1.38     |
| 1   | C1    | 2358 | OMG  | C5-C6   | 2.37  | 1.53        | 1.44     |
| 1   | C1    | 787  | OMG  | C6-N1   | 2.37  | 1.43        | 1.38     |
| 1   | C1    | 2578 | OMG  | C5-C6   | 2.36  | 1.53        | 1.44     |
| 1   | C1    | 2774 | OMG  | C5-C6   | 2.35  | 1.53        | 1.44     |
| 1   | C1    | 646  | OMG  | C4-N9   | -2.34 | 1.32        | 1.38     |
| 1   | C1    | 627  | OMG  | C4-N9   | -2.34 | 1.32        | 1.38     |
| 1   | C1    | 1433 | OMG  | C4-N9   | -2.33 | 1.32        | 1.38     |
| 1   | C1    | 2690 | OMU  | C5-C4   | 2.32  | 1.48        | 1.43     |
| 1   | C1    | 1433 | OMG  | C5-C6   | 2.32  | 1.53        | 1.44     |
| 1   | C1    | 1868 | OMU  | C5-C4   | 2.32  | 1.48        | 1.43     |
| 1   | C1    | 2688 | OMU  | C5-C4   | 2.31  | 1.48        | 1.43     |
| 1   | C1    | 1917 | OMU  | C5-C4   | 2.29  | 1.48        | 1.43     |
| 1   | C1    | 1432 | A2M  | O3'-C3' | 2.28  | 1.48        | 1.43     |
| 1   | C1    | 2774 | OMG  | C4-N9   | -2.27 | 1.32        | 1.38     |
| 1   | C1    | 2277 | OMU  | C5-C4   | 2.26  | 1.48        | 1.43     |
| 1   | C1    | 2380 | OMU  | C5-C4   | 2.25  | 1.48        | 1.43     |
| 1   | C1    | 2683 | OMU  | C5-C4   | 2.24  | 1.48        | 1.43     |
| 1   | C1    | 2881 | OMG  | C5-C6   | 2.24  | 1.52        | 1.44     |
| 1   | C1    | 787  | OMG  | C5-C6   | 2.24  | 1.52        | 1.44     |
| 1   | C1    | 2384 | OMU  | C5-C4   | 2.21  | 1.48        | 1.43     |
| 1   | C1    | 2358 | OMG  | C4-N9   | -2.20 | 1.32        | 1.38     |
| 1   | C1    | 1847 | A2M  | O3'-C3' | 2.20  | 1.48        | 1.43     |
| 1   | C1    | 2876 | OMG  | C4-N9   | -2.18 | 1.32        | 1.38     |
| 1   | C1    | 1432 | A2M  | C8-N9   | -2.16 | 1.33        | 1.37     |
| 1   | C1    | 385  | OMG  | C4-N9   | -2.13 | 1.32        | 1.38     |
| 1   | C1    | 787  | OMG  | C4-N9   | -2.13 | 1.32        | 1.38     |
| 1   | C1    | 1847 | A2M  | C8-N9   | -2.12 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C1    | 627  | OMG  | C5-C6   | 2.11  | 1.52        | 1.44     |
| 1   | C1    | 646  | OMG  | C6-N1   | 2.10  | 1.42        | 1.38     |
| 1   | C1    | 848  | A2M  | O3'-C3' | 2.10  | 1.48        | 1.43     |
| 1   | C1    | 646  | OMG  | C5-C6   | 2.06  | 1.52        | 1.44     |
| 1   | C1    | 389  | A2M  | O3'-C3' | 2.06  | 1.48        | 1.43     |
| 1   | C1    | 2881 | OMG  | C6-N1   | 2.06  | 1.42        | 1.38     |
| 1   | C1    | 637  | A2M  | C8-N9   | -2.06 | 1.34        | 1.37     |
| 1   | C1    | 2578 | OMG  | C4-N9   | -2.06 | 1.32        | 1.38     |
| 1   | C1    | 848  | A2M  | C8-N9   | -2.05 | 1.34        | 1.37     |
| 1   | C1    | 389  | A2M  | C8-N9   | -2.04 | 1.34        | 1.37     |
| 1   | C1    | 858  | A2M  | O3'-C3' | 2.03  | 1.48        | 1.43     |
| 1   | C1    | 2289 | A2M  | O3'-C3' | 2.03  | 1.48        | 1.43     |
| 1   | C1    | 858  | A2M  | C8-N9   | -2.01 | 1.34        | 1.37     |

All (393) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | C1    | 1847 | A2M  | C1'-N9-C8   | -9.56 | 105.88      | 127.09   |
| 1   | C1    | 389  | A2M  | C1'-N9-C8   | -9.33 | 106.40      | 127.09   |
| 1   | C1    | 1432 | A2M  | C1'-N9-C8   | -9.29 | 106.47      | 127.09   |
| 1   | C1    | 637  | A2M  | C1'-N9-C8   | -9.20 | 106.67      | 127.09   |
| 1   | C1    | 858  | A2M  | C1'-N9-C8   | -9.16 | 106.76      | 127.09   |
| 1   | C1    | 848  | A2M  | C1'-N9-C8   | -9.12 | 106.85      | 127.09   |
| 1   | C1    | 1223 | A2M  | C1'-N9-C8   | -8.88 | 107.38      | 127.09   |
| 1   | C1    | 2289 | A2M  | C1'-N9-C8   | -8.77 | 107.63      | 127.09   |
| 1   | C1    | 1847 | A2M  | C4-N9-C1'   | 8.23  | 145.89      | 126.63   |
| 1   | C1    | 389  | A2M  | C4-N9-C1'   | 8.06  | 145.47      | 126.63   |
| 1   | C1    | 1432 | A2M  | C4-N9-C1'   | 8.04  | 145.44      | 126.63   |
| 1   | C1    | 637  | A2M  | C4-N9-C1'   | 7.98  | 145.29      | 126.63   |
| 1   | C1    | 858  | A2M  | C4-N9-C1'   | 7.85  | 144.99      | 126.63   |
| 1   | C1    | 848  | A2M  | C4-N9-C1'   | 7.79  | 144.86      | 126.63   |
| 1   | C1    | 1223 | A2M  | C4-N9-C1'   | 7.62  | 144.44      | 126.63   |
| 1   | C1    | 2289 | A2M  | C4-N9-C1'   | 7.55  | 144.28      | 126.63   |
| 1   | C1    | 2876 | OMG  | C1'-N9-C8   | -7.07 | 106.64      | 126.73   |
| 1   | C1    | 2300 | OMC  | O2'-C2'-C1' | 6.26  | 120.88      | 108.99   |
| 1   | C1    | 2918 | OMC  | O2'-C2'-C1' | 6.24  | 120.85      | 108.99   |
| 1   | C1    | 2918 | OMC  | C2'-C1'-N1  | 6.18  | 125.97      | 114.24   |
| 1   | C1    | 1836 | OMC  | O2'-C2'-C1' | 6.13  | 120.63      | 108.99   |
| 1   | C1    | 2838 | OMC  | O2'-C2'-C1' | 6.12  | 120.60      | 108.99   |
| 1   | C1    | 778  | OMC  | O2'-C2'-C1' | 6.08  | 120.54      | 108.99   |
| 1   | C1    | 1812 | OMC  | O2'-C2'-C1' | 6.07  | 120.52      | 108.99   |
| 1   | C1    | 1420 | OMC  | O2'-C2'-C1' | 6.06  | 120.51      | 108.99   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | C1    | 1491 | OMC  | O2'-C2'-C1' | 6.06  | 120.50      | 108.99   |
| 1   | C1    | 1836 | OMC  | C2'-C1'-N1  | 6.02  | 125.67      | 114.24   |
| 1   | C1    | 787  | OMG  | C1'-N9-C8   | -5.93 | 109.89      | 126.73   |
| 1   | C1    | 385  | OMG  | O2'-C2'-C1' | 5.88  | 120.15      | 108.99   |
| 1   | C1    | 2881 | OMG  | O2'-C2'-C1' | 5.83  | 120.07      | 108.99   |
| 1   | C1    | 2289 | A2M  | N3-C2-N1    | -5.83 | 119.76      | 128.58   |
| 1   | C1    | 858  | A2M  | N3-C2-N1    | -5.82 | 119.77      | 128.58   |
| 1   | C1    | 627  | OMG  | O2'-C2'-C1' | 5.80  | 120.00      | 108.99   |
| 1   | C1    | 2876 | OMG  | O2'-C2'-C1' | 5.79  | 119.99      | 108.99   |
| 1   | C1    | 1223 | A2M  | N3-C2-N1    | -5.79 | 119.81      | 128.58   |
| 1   | C1    | 2300 | OMC  | C2'-C1'-N1  | 5.78  | 125.20      | 114.24   |
| 1   | C1    | 1432 | A2M  | N3-C2-N1    | -5.77 | 119.85      | 128.58   |
| 1   | C1    | 848  | A2M  | N3-C2-N1    | -5.76 | 119.86      | 128.58   |
| 1   | C1    | 389  | A2M  | N3-C2-N1    | -5.76 | 119.86      | 128.58   |
| 1   | C1    | 2774 | OMG  | O2'-C2'-C1' | 5.74  | 119.89      | 108.99   |
| 1   | C1    | 1847 | A2M  | N3-C2-N1    | -5.73 | 119.91      | 128.58   |
| 1   | C1    | 1433 | OMG  | O2'-C2'-C1' | 5.70  | 119.81      | 108.99   |
| 1   | C1    | 2358 | OMG  | O2'-C2'-C1' | 5.70  | 119.81      | 108.99   |
| 1   | C1    | 1868 | OMU  | C4-N3-C2    | -5.69 | 119.54      | 126.61   |
| 1   | C1    | 2876 | OMG  | C1'-N9-C4   | 5.68  | 143.26      | 126.49   |
| 1   | C1    | 2578 | OMG  | O2'-C2'-C1' | 5.67  | 119.76      | 108.99   |
| 1   | C1    | 787  | OMG  | O2'-C2'-C1' | 5.67  | 119.75      | 108.99   |
| 1   | C1    | 1847 | A2M  | N6-C6-N1    | -5.63 | 105.85      | 118.38   |
| 1   | C1    | 637  | A2M  | N3-C2-N1    | -5.61 | 120.09      | 128.58   |
| 1   | C1    | 848  | A2M  | N6-C6-N1    | -5.58 | 105.95      | 118.38   |
| 1   | C1    | 1432 | A2M  | N6-C6-N1    | -5.57 | 105.98      | 118.38   |
| 1   | C1    | 646  | OMG  | C1'-N9-C8   | -5.56 | 110.93      | 126.73   |
| 1   | C1    | 646  | OMG  | O2'-C2'-C1' | 5.56  | 119.55      | 108.99   |
| 1   | C1    | 2690 | OMU  | C4-N3-C2    | -5.53 | 119.75      | 126.61   |
| 1   | C1    | 637  | A2M  | N6-C6-N1    | -5.50 | 106.13      | 118.38   |
| 1   | C1    | 858  | A2M  | N6-C6-N1    | -5.49 | 106.14      | 118.38   |
| 1   | C1    | 1223 | A2M  | N6-C6-N1    | -5.49 | 106.15      | 118.38   |
| 1   | C1    | 2688 | OMU  | C4-N3-C2    | -5.48 | 119.81      | 126.61   |
| 1   | C1    | 2380 | OMU  | C4-N3-C2    | -5.47 | 119.82      | 126.61   |
| 1   | C1    | 389  | A2M  | N6-C6-N1    | -5.46 | 106.21      | 118.38   |
| 1   | C1    | 2289 | A2M  | N6-C6-N1    | -5.42 | 106.30      | 118.38   |
| 1   | C1    | 2277 | OMU  | C4-N3-C2    | -5.37 | 119.95      | 126.61   |
| 1   | C1    | 778  | OMC  | C2'-C1'-N1  | 5.34  | 124.38      | 114.24   |
| 1   | C1    | 2683 | OMU  | C4-N3-C2    | -5.33 | 119.99      | 126.61   |
| 1   | C1    | 1917 | OMU  | C4-N3-C2    | -5.32 | 120.01      | 126.61   |
| 1   | C1    | 2838 | OMC  | C2'-C1'-N1  | 5.32  | 124.34      | 114.24   |
| 1   | C1    | 627  | OMG  | C1'-N9-C8   | -5.30 | 111.67      | 126.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | C1    | 1491 | OMC  | C2'-C1'-N1  | 5.22  | 124.15      | 114.24   |
| 1   | C1    | 1420 | OMC  | C2'-C1'-N1  | 5.18  | 124.07      | 114.24   |
| 1   | C1    | 2384 | OMU  | C4-N3-C2    | -5.17 | 120.20      | 126.61   |
| 1   | C1    | 1812 | OMC  | C2'-C1'-N1  | 5.15  | 124.01      | 114.24   |
| 1   | C1    | 2838 | OMC  | O4'-C1'-N1  | 5.04  | 119.79      | 108.36   |
| 1   | C1    | 2881 | OMG  | C1'-N9-C8   | -4.99 | 112.56      | 126.73   |
| 1   | C1    | 389  | A2M  | C5-C4-N3    | -4.98 | 119.86      | 126.72   |
| 1   | C1    | 1432 | A2M  | C5-C4-N3    | -4.98 | 119.86      | 126.72   |
| 1   | C1    | 385  | OMG  | C5-C4-N3    | -4.98 | 120.47      | 128.39   |
| 1   | C1    | 848  | A2M  | C5-C4-N3    | -4.96 | 119.89      | 126.72   |
| 1   | C1    | 637  | A2M  | C5-C4-N3    | -4.94 | 119.91      | 126.72   |
| 1   | C1    | 2876 | OMG  | C5-C4-N3    | -4.93 | 120.54      | 128.39   |
| 1   | C1    | 2578 | OMG  | C5-C4-N3    | -4.92 | 120.56      | 128.39   |
| 1   | C1    | 1847 | A2M  | C5-C4-N3    | -4.92 | 119.94      | 126.72   |
| 1   | C1    | 2876 | OMG  | C2'-C1'-N9  | 4.92  | 123.57      | 114.24   |
| 1   | C1    | 787  | OMG  | C5-C4-N3    | -4.82 | 120.71      | 128.39   |
| 1   | C1    | 385  | OMG  | C2-N3-C4    | 4.82  | 120.61      | 112.30   |
| 1   | C1    | 2578 | OMG  | O4'-C1'-N9  | 4.81  | 119.27      | 108.36   |
| 1   | C1    | 2881 | OMG  | C2'-C1'-N9  | 4.79  | 123.33      | 114.24   |
| 1   | C1    | 787  | OMG  | C1'-N9-C4   | 4.78  | 140.61      | 126.49   |
| 1   | C1    | 858  | A2M  | C5-C4-N3    | -4.76 | 120.16      | 126.72   |
| 1   | C1    | 2774 | OMG  | O4'-C1'-N9  | 4.76  | 119.14      | 108.36   |
| 1   | C1    | 385  | OMG  | O4'-C1'-N9  | 4.74  | 119.09      | 108.36   |
| 1   | C1    | 2289 | A2M  | C5-C4-N3    | -4.72 | 120.21      | 126.72   |
| 1   | C1    | 1223 | A2M  | C5-C4-N3    | -4.72 | 120.22      | 126.72   |
| 1   | C1    | 2358 | OMG  | C2-N3-C4    | 4.71  | 120.42      | 112.30   |
| 1   | C1    | 2358 | OMG  | C5-C4-N3    | -4.70 | 120.90      | 128.39   |
| 1   | C1    | 1433 | OMG  | C1'-N9-C8   | -4.69 | 113.41      | 126.73   |
| 1   | C1    | 2578 | OMG  | C2-N3-C4    | 4.69  | 120.37      | 112.30   |
| 1   | C1    | 2358 | OMG  | O4'-C1'-N9  | 4.58  | 118.74      | 108.36   |
| 1   | C1    | 646  | OMG  | C5-C4-N3    | -4.52 | 121.19      | 128.39   |
| 1   | C1    | 787  | OMG  | C2'-C1'-N9  | 4.52  | 122.81      | 114.24   |
| 1   | C1    | 627  | OMG  | C5-C4-N3    | -4.48 | 121.25      | 128.39   |
| 1   | C1    | 2774 | OMG  | C5-C4-N3    | -4.47 | 121.28      | 128.39   |
| 1   | C1    | 2774 | OMG  | C2'-C1'-N9  | 4.46  | 122.70      | 114.24   |
| 1   | C1    | 1433 | OMG  | C5-C4-N3    | -4.44 | 121.33      | 128.39   |
| 1   | C1    | 646  | OMG  | O3'-C3'-C4' | 4.42  | 123.78      | 111.08   |
| 1   | C1    | 2774 | OMG  | C1'-N9-C8   | -4.41 | 114.21      | 126.73   |
| 1   | C1    | 2774 | OMG  | C2-N3-C4    | 4.38  | 119.85      | 112.30   |
| 1   | C1    | 2578 | OMG  | C1'-N9-C8   | -4.37 | 114.30      | 126.73   |
| 1   | C1    | 1847 | A2M  | C5-C6-N6    | 4.37  | 134.10      | 123.29   |
| 1   | C1    | 1433 | OMG  | O4'-C1'-N9  | 4.36  | 118.23      | 108.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | C1    | 2358 | OMG  | C1'-N9-C8   | -4.34 | 114.39      | 126.73   |
| 1   | C1    | 1432 | A2M  | C5-C6-N6    | 4.34  | 134.03      | 123.29   |
| 1   | C1    | 2358 | OMG  | O3'-C3'-C4' | 4.32  | 123.50      | 111.08   |
| 1   | C1    | 858  | A2M  | C5-C6-N6    | 4.32  | 133.98      | 123.29   |
| 1   | C1    | 2881 | OMG  | C5-C4-N3    | -4.31 | 121.53      | 128.39   |
| 1   | C1    | 1847 | A2M  | N9-C8-N7    | -4.31 | 107.82      | 113.94   |
| 1   | C1    | 1223 | A2M  | C5-C6-N6    | 4.30  | 133.94      | 123.29   |
| 1   | C1    | 2881 | OMG  | O3'-C3'-C2' | 4.29  | 123.21      | 111.19   |
| 1   | C1    | 637  | A2M  | C5-C6-N6    | 4.29  | 133.91      | 123.29   |
| 1   | C1    | 2578 | OMG  | O3'-C3'-C4' | 4.29  | 123.40      | 111.08   |
| 1   | C1    | 848  | A2M  | N9-C8-N7    | -4.29 | 107.85      | 113.94   |
| 1   | C1    | 2289 | A2M  | C5-C6-N6    | 4.28  | 133.89      | 123.29   |
| 1   | C1    | 848  | A2M  | C5-C6-N6    | 4.27  | 133.87      | 123.29   |
| 1   | C1    | 787  | OMG  | O3'-C3'-C2' | 4.26  | 123.12      | 111.19   |
| 1   | C1    | 1433 | OMG  | O3'-C3'-C4' | 4.25  | 123.30      | 111.08   |
| 1   | C1    | 2918 | OMC  | O4'-C1'-N1  | 4.24  | 117.97      | 108.36   |
| 1   | C1    | 858  | A2M  | N9-C8-N7    | -4.24 | 107.92      | 113.94   |
| 1   | C1    | 1223 | A2M  | N9-C8-N7    | -4.23 | 107.94      | 113.94   |
| 1   | C1    | 1433 | OMG  | C2-N3-C4    | 4.23  | 119.58      | 112.30   |
| 1   | C1    | 389  | A2M  | C5-C6-N6    | 4.22  | 133.73      | 123.29   |
| 1   | C1    | 646  | OMG  | O4'-C1'-N9  | 4.21  | 117.90      | 108.36   |
| 1   | C1    | 2876 | OMG  | O3'-C3'-C2' | 4.21  | 122.97      | 111.19   |
| 1   | C1    | 627  | OMG  | O3'-C3'-C4' | 4.20  | 123.14      | 111.08   |
| 1   | C1    | 2289 | A2M  | N9-C8-N7    | -4.20 | 107.98      | 113.94   |
| 1   | C1    | 389  | A2M  | N9-C8-N7    | -4.18 | 108.00      | 113.94   |
| 1   | C1    | 1491 | OMC  | O3'-C3'-C4' | 4.17  | 123.06      | 111.08   |
| 1   | C1    | 1433 | OMG  | C2'-C1'-N9  | 4.17  | 122.15      | 114.24   |
| 1   | C1    | 2918 | OMC  | O3'-C3'-C2' | 4.17  | 122.85      | 111.19   |
| 1   | C1    | 1491 | OMC  | O3'-C3'-C2' | 4.17  | 122.85      | 111.19   |
| 1   | C1    | 385  | OMG  | C2'-C1'-N9  | 4.16  | 122.14      | 114.24   |
| 1   | C1    | 2881 | OMG  | O4'-C1'-N9  | 4.16  | 117.79      | 108.36   |
| 1   | C1    | 1432 | A2M  | N9-C8-N7    | -4.15 | 108.04      | 113.94   |
| 1   | C1    | 787  | OMG  | O4'-C1'-N9  | 4.15  | 117.76      | 108.36   |
| 1   | C1    | 2876 | OMG  | C5'-C4'-C3' | 4.13  | 130.09      | 115.21   |
| 1   | C1    | 1836 | OMC  | O3'-C3'-C2' | 4.10  | 122.67      | 111.19   |
| 1   | C1    | 2774 | OMG  | O3'-C3'-C4' | 4.10  | 122.87      | 111.08   |
| 1   | C1    | 2289 | A2M  | O4'-C1'-N9  | 4.10  | 115.97      | 108.09   |
| 1   | C1    | 848  | A2M  | O4'-C1'-N9  | 4.10  | 115.96      | 108.09   |
| 1   | C1    | 1420 | OMC  | O3'-C3'-C2' | 4.09  | 122.64      | 111.19   |
| 1   | C1    | 2300 | OMC  | C1'-N1-C2   | 4.09  | 127.48      | 118.44   |
| 1   | C1    | 637  | A2M  | N9-C8-N7    | -4.08 | 108.15      | 113.94   |
| 1   | C1    | 627  | OMG  | C2-N3-C4    | 4.07  | 119.30      | 112.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | C1    | 2881 | OMG  | O3'-C3'-C4' | 4.06  | 122.75      | 111.08   |
| 1   | C1    | 385  | OMG  | O3'-C3'-C2' | 4.06  | 122.55      | 111.19   |
| 1   | C1    | 1223 | A2M  | O4'-C1'-N9  | 4.06  | 115.88      | 108.09   |
| 1   | C1    | 2838 | OMC  | O3'-C3'-C2' | 4.05  | 122.53      | 111.19   |
| 1   | C1    | 385  | OMG  | C1'-N9-C8   | -4.03 | 115.27      | 126.73   |
| 1   | C1    | 2300 | OMC  | C1'-N1-C6   | -4.02 | 112.18      | 120.78   |
| 1   | C1    | 1433 | OMG  | O3'-C3'-C2' | 4.02  | 122.45      | 111.19   |
| 1   | C1    | 787  | OMG  | C2-N3-C4    | 4.01  | 119.20      | 112.30   |
| 1   | C1    | 385  | OMG  | O3'-C3'-C4' | 3.99  | 122.55      | 111.08   |
| 1   | C1    | 2876 | OMG  | C2-N3-C4    | 3.99  | 119.17      | 112.30   |
| 1   | C1    | 778  | OMC  | O3'-C3'-C2' | 3.98  | 122.34      | 111.19   |
| 1   | C1    | 1917 | OMU  | N3-C2-N1    | 3.98  | 120.07      | 114.89   |
| 1   | C1    | 1812 | OMC  | O3'-C3'-C4' | 3.96  | 122.46      | 111.08   |
| 1   | C1    | 778  | OMC  | O3'-C3'-C4' | 3.96  | 122.45      | 111.08   |
| 1   | C1    | 627  | OMG  | O3'-C3'-C2' | 3.95  | 122.24      | 111.19   |
| 1   | C1    | 1868 | OMU  | N3-C2-N1    | 3.95  | 120.03      | 114.89   |
| 1   | C1    | 2881 | OMG  | C2-N3-C4    | 3.94  | 119.09      | 112.30   |
| 1   | C1    | 1433 | OMG  | C5'-C4'-C3' | 3.94  | 129.40      | 115.21   |
| 1   | C1    | 2876 | OMG  | N9-C4-N3    | 3.94  | 133.83      | 125.95   |
| 1   | C1    | 2774 | OMG  | O3'-C3'-C2' | 3.93  | 122.17      | 111.19   |
| 1   | C1    | 1812 | OMC  | O4'-C1'-N1  | 3.92  | 117.25      | 108.36   |
| 1   | C1    | 627  | OMG  | O4'-C1'-N9  | 3.92  | 117.23      | 108.36   |
| 1   | C1    | 778  | OMC  | O4'-C1'-N1  | 3.91  | 117.23      | 108.36   |
| 1   | C1    | 1420 | OMC  | O3'-C3'-C4' | 3.91  | 122.32      | 111.08   |
| 1   | C1    | 627  | OMG  | C5'-C4'-C3' | 3.89  | 129.22      | 115.21   |
| 1   | C1    | 2300 | OMC  | O3'-C3'-C4' | 3.89  | 122.25      | 111.08   |
| 1   | C1    | 1836 | OMC  | C1'-N1-C2   | 3.88  | 127.02      | 118.44   |
| 1   | C1    | 1491 | OMC  | C1'-N1-C2   | 3.88  | 127.00      | 118.44   |
| 1   | C1    | 2300 | OMC  | O3'-C3'-C2' | 3.87  | 122.03      | 111.19   |
| 1   | C1    | 2838 | OMC  | O3'-C3'-C4' | 3.86  | 122.18      | 111.08   |
| 1   | C1    | 1420 | OMC  | O4'-C1'-N1  | 3.86  | 117.11      | 108.36   |
| 1   | C1    | 2876 | OMG  | O3'-C3'-C4' | 3.85  | 122.14      | 111.08   |
| 1   | C1    | 787  | OMG  | O3'-C3'-C4' | 3.85  | 122.13      | 111.08   |
| 1   | C1    | 2578 | OMG  | O3'-C3'-C2' | 3.85  | 121.95      | 111.19   |
| 1   | C1    | 646  | OMG  | C2-N3-C4    | 3.84  | 118.91      | 112.30   |
| 1   | C1    | 1432 | A2M  | O4'-C1'-N9  | 3.83  | 115.45      | 108.09   |
| 1   | C1    | 858  | A2M  | O4'-C1'-N9  | 3.83  | 115.45      | 108.09   |
| 1   | C1    | 1836 | OMC  | O3'-C3'-C4' | 3.83  | 122.09      | 111.08   |
| 1   | C1    | 2881 | OMG  | C1'-N9-C4   | 3.83  | 137.79      | 126.49   |
| 1   | C1    | 646  | OMG  | C1'-N9-C4   | 3.82  | 137.76      | 126.49   |
| 1   | C1    | 646  | OMG  | C5'-C4'-C3' | 3.81  | 128.93      | 115.21   |
| 1   | C1    | 2300 | OMC  | O4'-C1'-N1  | 3.80  | 116.98      | 108.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | C1    | 627  | OMG  | C1'-N9-C4   | 3.80  | 137.72      | 126.49   |
| 1   | C1    | 1491 | OMC  | C5'-C4'-C3' | 3.79  | 128.87      | 115.21   |
| 1   | C1    | 2918 | OMC  | O3'-C3'-C4' | 3.79  | 121.97      | 111.08   |
| 1   | C1    | 1491 | OMC  | O4'-C1'-N1  | 3.78  | 116.94      | 108.36   |
| 1   | C1    | 1836 | OMC  | C5'-C4'-C3' | 3.78  | 128.82      | 115.21   |
| 1   | C1    | 2688 | OMU  | N3-C2-N1    | 3.78  | 119.81      | 114.89   |
| 1   | C1    | 1812 | OMC  | O3'-C3'-C2' | 3.77  | 121.75      | 111.19   |
| 1   | C1    | 2380 | OMU  | N3-C2-N1    | 3.76  | 119.79      | 114.89   |
| 1   | C1    | 627  | OMG  | C2'-C1'-N9  | 3.76  | 121.37      | 114.24   |
| 1   | C1    | 2384 | OMU  | N3-C2-N1    | 3.76  | 119.78      | 114.89   |
| 1   | C1    | 2690 | OMU  | N3-C2-N1    | 3.75  | 119.78      | 114.89   |
| 1   | C1    | 2578 | OMG  | C2'-C1'-N9  | 3.75  | 121.35      | 114.24   |
| 1   | C1    | 1836 | OMC  | O4'-C1'-N1  | 3.74  | 116.83      | 108.36   |
| 1   | C1    | 646  | OMG  | O3'-C3'-C2' | 3.74  | 121.65      | 111.19   |
| 1   | C1    | 2881 | OMG  | C5'-C4'-C3' | 3.73  | 128.65      | 115.21   |
| 1   | C1    | 389  | A2M  | O4'-C1'-N9  | 3.71  | 115.22      | 108.09   |
| 1   | C1    | 2358 | OMG  | O3'-C3'-C2' | 3.71  | 121.57      | 111.19   |
| 1   | C1    | 385  | OMG  | O4'-C4'-C5' | 3.70  | 121.19      | 109.33   |
| 1   | C1    | 2277 | OMU  | N3-C2-N1    | 3.70  | 119.71      | 114.89   |
| 1   | C1    | 2683 | OMU  | N3-C2-N1    | 3.69  | 119.69      | 114.89   |
| 1   | C1    | 637  | A2M  | O4'-C1'-N9  | 3.67  | 115.14      | 108.09   |
| 1   | C1    | 2300 | OMC  | C5'-C4'-C3' | 3.67  | 128.41      | 115.21   |
| 1   | C1    | 2918 | OMC  | C5'-C4'-C3' | 3.67  | 128.41      | 115.21   |
| 1   | C1    | 2578 | OMG  | C5'-C4'-C3' | 3.66  | 128.38      | 115.21   |
| 1   | C1    | 1836 | OMC  | C1'-N1-C6   | -3.65 | 112.97      | 120.78   |
| 1   | C1    | 778  | OMC  | C5'-C4'-C3' | 3.64  | 128.33      | 115.21   |
| 1   | C1    | 2380 | OMU  | C5-C4-N3    | 3.64  | 119.90      | 114.80   |
| 1   | C1    | 787  | OMG  | C5'-C4'-C3' | 3.63  | 128.29      | 115.21   |
| 1   | C1    | 1812 | OMC  | C5'-C4'-C3' | 3.62  | 128.25      | 115.21   |
| 1   | C1    | 2358 | OMG  | C5'-C4'-C3' | 3.61  | 128.22      | 115.21   |
| 1   | C1    | 2690 | OMU  | C5-C4-N3    | 3.60  | 119.84      | 114.80   |
| 1   | C1    | 787  | OMG  | O4'-C4'-C5' | 3.60  | 120.86      | 109.33   |
| 1   | C1    | 2578 | OMG  | O4'-C4'-C5' | 3.60  | 120.85      | 109.33   |
| 1   | C1    | 1868 | OMU  | C5-C4-N3    | 3.59  | 119.83      | 114.80   |
| 1   | C1    | 2774 | OMG  | C5'-C4'-C3' | 3.59  | 128.15      | 115.21   |
| 1   | C1    | 2838 | OMC  | C5'-C4'-C3' | 3.59  | 128.14      | 115.21   |
| 1   | C1    | 1491 | OMC  | C1'-N1-C6   | -3.57 | 113.14      | 120.78   |
| 1   | C1    | 1420 | OMC  | C5'-C4'-C3' | 3.57  | 128.07      | 115.21   |
| 1   | C1    | 2688 | OMU  | C5-C4-N3    | 3.56  | 119.79      | 114.80   |
| 1   | C1    | 1491 | OMC  | O4'-C4'-C5' | 3.55  | 120.72      | 109.33   |
| 1   | C1    | 2774 | OMG  | O4'-C4'-C5' | 3.54  | 120.67      | 109.33   |
| 1   | C1    | 2358 | OMG  | O4'-C4'-C5' | 3.52  | 120.61      | 109.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | C1    | 2683 | OMU  | C5-C4-N3    | 3.52  | 119.73      | 114.80   |
| 1   | C1    | 646  | OMG  | N9-C8-N7    | -3.51 | 106.90      | 113.40   |
| 1   | C1    | 2277 | OMU  | C5-C4-N3    | 3.51  | 119.71      | 114.80   |
| 1   | C1    | 1433 | OMG  | C1'-N9-C4   | 3.50  | 136.83      | 126.49   |
| 1   | C1    | 778  | OMC  | C1'-N1-C2   | 3.50  | 126.16      | 118.44   |
| 1   | C1    | 1432 | A2M  | C2-N3-C4    | 3.48  | 120.33      | 111.83   |
| 1   | C1    | 646  | OMG  | N9-C4-N3    | 3.48  | 132.91      | 125.95   |
| 1   | C1    | 2876 | OMG  | O6-C6-C5    | -3.47 | 117.36      | 126.53   |
| 1   | C1    | 2838 | OMC  | O4'-C4'-C5' | 3.46  | 120.43      | 109.33   |
| 1   | C1    | 2774 | OMG  | N9-C8-N7    | -3.46 | 106.98      | 113.40   |
| 1   | C1    | 2881 | OMG  | O4'-C4'-C5' | 3.45  | 120.39      | 109.33   |
| 1   | C1    | 385  | OMG  | C5'-C4'-C3' | 3.45  | 127.63      | 115.21   |
| 1   | C1    | 389  | A2M  | C2-N3-C4    | 3.44  | 120.22      | 111.83   |
| 1   | C1    | 848  | A2M  | C2-N3-C4    | 3.43  | 120.22      | 111.83   |
| 1   | C1    | 1812 | OMC  | C1'-N1-C2   | 3.43  | 126.02      | 118.44   |
| 1   | C1    | 1847 | A2M  | C2-N3-C4    | 3.42  | 120.19      | 111.83   |
| 1   | C1    | 1433 | OMG  | N9-C8-N7    | -3.42 | 107.06      | 113.40   |
| 1   | C1    | 787  | OMG  | N9-C4-N3    | 3.41  | 132.78      | 125.95   |
| 1   | C1    | 2918 | OMC  | O4'-C4'-C5' | 3.41  | 120.26      | 109.33   |
| 1   | C1    | 1917 | OMU  | C5-C4-N3    | 3.39  | 119.55      | 114.80   |
| 1   | C1    | 1812 | OMC  | O4'-C4'-C5' | 3.39  | 120.19      | 109.33   |
| 1   | C1    | 627  | OMG  | N9-C8-N7    | -3.38 | 107.12      | 113.40   |
| 1   | C1    | 2384 | OMU  | C5-C4-N3    | 3.38  | 119.54      | 114.80   |
| 1   | C1    | 637  | A2M  | C2-N3-C4    | 3.38  | 120.09      | 111.83   |
| 1   | C1    | 778  | OMC  | O4'-C4'-C5' | 3.36  | 120.09      | 109.33   |
| 1   | C1    | 1836 | OMC  | O4'-C4'-C5' | 3.35  | 120.06      | 109.33   |
| 1   | C1    | 858  | A2M  | C2-N3-C4    | 3.35  | 120.00      | 111.83   |
| 1   | C1    | 1420 | OMC  | O4'-C4'-C5' | 3.34  | 120.05      | 109.33   |
| 1   | C1    | 2358 | OMG  | N9-C8-N7    | -3.34 | 107.20      | 113.40   |
| 1   | C1    | 627  | OMG  | O4'-C4'-C5' | 3.33  | 120.02      | 109.33   |
| 1   | C1    | 1223 | A2M  | C2-N3-C4    | 3.33  | 119.97      | 111.83   |
| 1   | C1    | 2289 | A2M  | C2-N3-C4    | 3.32  | 119.95      | 111.83   |
| 1   | C1    | 2300 | OMC  | O4'-C4'-C5' | 3.32  | 119.97      | 109.33   |
| 1   | C1    | 1433 | OMG  | O4'-C4'-C5' | 3.31  | 119.93      | 109.33   |
| 1   | C1    | 1420 | OMC  | C1'-N1-C6   | -3.30 | 113.74      | 120.78   |
| 1   | C1    | 646  | OMG  | O4'-C4'-C5' | 3.29  | 119.87      | 109.33   |
| 1   | C1    | 2578 | OMG  | N9-C8-N7    | -3.28 | 107.31      | 113.40   |
| 1   | C1    | 385  | OMG  | N9-C8-N7    | -3.28 | 107.31      | 113.40   |
| 1   | C1    | 2358 | OMG  | C2'-C1'-N9  | 3.28  | 120.46      | 114.24   |
| 1   | C1    | 646  | OMG  | C2'-C1'-N9  | 3.28  | 120.46      | 114.24   |
| 1   | C1    | 2774 | OMG  | C1'-N9-C4   | 3.27  | 136.14      | 126.49   |
| 1   | C1    | 2578 | OMG  | C1'-N9-C4   | 3.26  | 136.10      | 126.49   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | C1    | 1847 | A2M  | O4'-C1'-N9  | 3.25  | 114.33      | 108.09   |
| 1   | C1    | 2881 | OMG  | N9-C8-N7    | -3.24 | 107.39      | 113.40   |
| 1   | C1    | 778  | OMC  | C1'-N1-C6   | -3.22 | 113.90      | 120.78   |
| 1   | C1    | 1420 | OMC  | C1'-N1-C2   | 3.21  | 125.52      | 118.44   |
| 1   | C1    | 2876 | OMG  | O4'-C4'-C5' | 3.20  | 119.59      | 109.33   |
| 1   | C1    | 389  | A2M  | N3-C4-N9    | 3.16  | 132.54      | 127.17   |
| 1   | C1    | 385  | OMG  | C1'-N9-C4   | 3.15  | 135.78      | 126.49   |
| 1   | C1    | 2876 | OMG  | O4'-C1'-N9  | 3.13  | 115.46      | 108.36   |
| 1   | C1    | 787  | OMG  | N9-C8-N7    | -3.12 | 107.61      | 113.40   |
| 1   | C1    | 1812 | OMC  | C1'-N1-C6   | -3.11 | 114.14      | 120.78   |
| 1   | C1    | 848  | A2M  | N3-C4-N9    | 3.11  | 132.45      | 127.17   |
| 1   | C1    | 2838 | OMC  | O2-C2-N3    | -3.10 | 117.45      | 122.33   |
| 1   | C1    | 2358 | OMG  | C1'-N9-C4   | 3.08  | 135.58      | 126.49   |
| 1   | C1    | 637  | A2M  | N3-C4-N9    | 3.08  | 132.40      | 127.17   |
| 1   | C1    | 1432 | A2M  | N3-C4-N9    | 3.07  | 132.38      | 127.17   |
| 1   | C1    | 627  | OMG  | N9-C4-N3    | 3.05  | 132.05      | 125.95   |
| 1   | C1    | 2578 | OMG  | N9-C4-N3    | 3.05  | 132.05      | 125.95   |
| 1   | C1    | 1847 | A2M  | N3-C4-N9    | 3.04  | 132.33      | 127.17   |
| 1   | C1    | 2683 | OMU  | O4-C4-C5    | -2.98 | 120.02      | 125.16   |
| 1   | C1    | 1847 | A2M  | C5-N7-C8    | 2.97  | 108.12      | 103.45   |
| 1   | C1    | 858  | A2M  | N3-C4-N9    | 2.96  | 132.21      | 127.17   |
| 1   | C1    | 2688 | OMU  | O4-C4-C5    | -2.94 | 120.10      | 125.16   |
| 1   | C1    | 848  | A2M  | C2'-C1'-N9  | -2.92 | 108.94      | 113.75   |
| 1   | C1    | 848  | A2M  | C5-N7-C8    | 2.92  | 108.04      | 103.45   |
| 1   | C1    | 2876 | OMG  | C2-N1-C6    | -2.92 | 119.81      | 125.11   |
| 1   | C1    | 1868 | OMU  | O4-C4-C5    | -2.91 | 120.14      | 125.16   |
| 1   | C1    | 2277 | OMU  | O4-C4-C5    | -2.91 | 120.15      | 125.16   |
| 1   | C1    | 385  | OMG  | C2-N1-C6    | -2.91 | 119.84      | 125.11   |
| 1   | C1    | 1432 | A2M  | C5-N7-C8    | 2.90  | 108.01      | 103.45   |
| 1   | C1    | 2380 | OMU  | O4-C4-C5    | -2.89 | 120.18      | 125.16   |
| 1   | C1    | 2384 | OMU  | O4-C4-C5    | -2.88 | 120.20      | 125.16   |
| 1   | C1    | 1223 | A2M  | N3-C4-N9    | 2.88  | 132.06      | 127.17   |
| 1   | C1    | 389  | A2M  | C5-N7-C8    | 2.87  | 107.96      | 103.45   |
| 1   | C1    | 2289 | A2M  | N3-C4-N9    | 2.85  | 132.02      | 127.17   |
| 1   | C1    | 2876 | OMG  | N9-C8-N7    | -2.85 | 108.12      | 113.40   |
| 1   | C1    | 637  | A2M  | C5-N7-C8    | 2.84  | 107.91      | 103.45   |
| 1   | C1    | 1223 | A2M  | C5-N7-C8    | 2.83  | 107.89      | 103.45   |
| 1   | C1    | 2690 | OMU  | O4-C4-C5    | -2.82 | 120.29      | 125.16   |
| 1   | C1    | 2358 | OMG  | N9-C4-N3    | 2.81  | 131.58      | 125.95   |
| 1   | C1    | 2881 | OMG  | N9-C4-N3    | 2.81  | 131.57      | 125.95   |
| 1   | C1    | 858  | A2M  | C5-N7-C8    | 2.81  | 107.86      | 103.45   |
| 1   | C1    | 646  | OMG  | O6-C6-C5    | -2.81 | 119.12      | 126.53   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | C1    | 2774 | OMG  | N9-C4-N3   | 2.78  | 131.52      | 125.95   |
| 1   | C1    | 2289 | A2M  | C5-N7-C8   | 2.78  | 107.81      | 103.45   |
| 1   | C1    | 1433 | OMG  | N9-C4-N3   | 2.75  | 131.46      | 125.95   |
| 1   | C1    | 385  | OMG  | N9-C4-N3   | 2.71  | 131.38      | 125.95   |
| 1   | C1    | 2578 | OMG  | C2-N1-C6   | -2.67 | 120.27      | 125.11   |
| 1   | C1    | 1917 | OMU  | O4-C4-C5   | -2.67 | 120.55      | 125.16   |
| 1   | C1    | 627  | OMG  | O6-C6-C5   | -2.64 | 119.57      | 126.53   |
| 1   | C1    | 385  | OMG  | C5-C6-N1   | 2.63  | 119.95      | 113.25   |
| 1   | C1    | 2578 | OMG  | C5-C6-N1   | 2.62  | 119.93      | 113.25   |
| 1   | C1    | 2918 | OMC  | C1'-N1-C2  | 2.59  | 124.16      | 118.44   |
| 1   | C1    | 787  | OMG  | C2-N1-C6   | -2.59 | 120.42      | 125.11   |
| 1   | C1    | 2876 | OMG  | C5-C6-N1   | 2.58  | 119.83      | 113.25   |
| 1   | C1    | 1433 | OMG  | C2-N1-C6   | -2.58 | 120.44      | 125.11   |
| 1   | C1    | 787  | OMG  | O6-C6-C5   | -2.54 | 119.81      | 126.53   |
| 1   | C1    | 1433 | OMG  | O6-C6-C5   | -2.51 | 119.89      | 126.53   |
| 1   | C1    | 1433 | OMG  | C5-C6-N1   | 2.50  | 119.62      | 113.25   |
| 1   | C1    | 2578 | OMG  | O6-C6-C5   | -2.50 | 119.93      | 126.53   |
| 1   | C1    | 1917 | OMU  | C1'-N1-C2  | 2.50  | 122.08      | 117.59   |
| 1   | C1    | 2774 | OMG  | O6-C6-C5   | -2.48 | 119.98      | 126.53   |
| 1   | C1    | 2358 | OMG  | N1-C2-N3   | -2.48 | 118.78      | 123.32   |
| 1   | C1    | 848  | A2M  | C4-N9-C8   | 2.43  | 108.29      | 105.74   |
| 1   | C1    | 2358 | OMG  | C5-C6-N1   | 2.43  | 119.44      | 113.25   |
| 1   | C1    | 2774 | OMG  | C5-C6-N1   | 2.43  | 119.44      | 113.25   |
| 1   | C1    | 385  | OMG  | O6-C6-C5   | -2.42 | 120.14      | 126.53   |
| 1   | C1    | 627  | OMG  | C2-N1-C6   | -2.39 | 120.78      | 125.11   |
| 1   | C1    | 858  | A2M  | C4-N9-C8   | 2.39  | 108.25      | 105.74   |
| 1   | C1    | 627  | OMG  | C5-C6-N1   | 2.39  | 119.33      | 113.25   |
| 1   | C1    | 646  | OMG  | C5-C6-N1   | 2.39  | 119.33      | 113.25   |
| 1   | C1    | 1847 | A2M  | C4-N9-C8   | 2.38  | 108.24      | 105.74   |
| 1   | C1    | 2881 | OMG  | C5-C6-N1   | 2.37  | 119.28      | 113.25   |
| 1   | C1    | 787  | OMG  | C5-C6-N1   | 2.36  | 119.27      | 113.25   |
| 1   | C1    | 646  | OMG  | C2-N1-C6   | -2.36 | 120.83      | 125.11   |
| 1   | C1    | 2384 | OMU  | C1'-N1-C2  | 2.34  | 121.80      | 117.59   |
| 1   | C1    | 1223 | A2M  | C4-N9-C8   | 2.32  | 108.18      | 105.74   |
| 1   | C1    | 2774 | OMG  | C2-N1-C6   | -2.32 | 120.90      | 125.11   |
| 1   | C1    | 385  | OMG  | N2-C2-N1   | 2.32  | 121.65      | 116.76   |
| 1   | C1    | 2380 | OMU  | O2-C2-N1   | -2.31 | 119.80      | 122.80   |
| 1   | C1    | 2918 | OMC  | C1'-N1-C6  | -2.30 | 115.87      | 120.78   |
| 1   | C1    | 389  | A2M  | C4-N9-C8   | 2.27  | 108.12      | 105.74   |
| 1   | C1    | 2358 | OMG  | O6-C6-C5   | -2.26 | 120.56      | 126.53   |
| 1   | C1    | 1847 | A2M  | C2'-C1'-N9 | -2.26 | 110.04      | 113.75   |
| 1   | C1    | 2881 | OMG  | O6-C6-C5   | -2.24 | 120.62      | 126.53   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | C1    | 2289 | A2M  | C4-N9-C8   | 2.24  | 108.09      | 105.74   |
| 1   | C1    | 1432 | A2M  | C4-N9-C8   | 2.24  | 108.08      | 105.74   |
| 1   | C1    | 385  | OMG  | C8-N7-C5   | 2.23  | 108.22      | 104.26   |
| 1   | C1    | 2774 | OMG  | N1-C2-N3   | -2.22 | 119.27      | 123.32   |
| 1   | C1    | 2881 | OMG  | C2-N1-C6   | -2.21 | 121.10      | 125.11   |
| 1   | C1    | 2683 | OMU  | O2-C2-N1   | -2.20 | 119.93      | 122.80   |
| 1   | C1    | 2358 | OMG  | C2-N1-C6   | -2.19 | 121.14      | 125.11   |
| 1   | C1    | 2578 | OMG  | N1-C2-N3   | -2.19 | 119.31      | 123.32   |
| 1   | C1    | 1847 | A2M  | C4-C5-N7   | -2.18 | 108.09      | 110.58   |
| 1   | C1    | 2289 | A2M  | C2'-C1'-N9 | -2.17 | 110.18      | 113.75   |
| 1   | C1    | 1432 | A2M  | C4-C5-N7   | -2.16 | 108.11      | 110.58   |
| 1   | C1    | 637  | A2M  | C4-N9-C8   | 2.15  | 108.00      | 105.74   |
| 1   | C1    | 1836 | OMC  | N4-C4-N3   | 2.14  | 121.74      | 117.91   |
| 1   | C1    | 646  | OMG  | C8-N9-C4   | 2.14  | 110.04      | 106.03   |
| 1   | C1    | 848  | A2M  | C4-C5-N7   | -2.13 | 108.15      | 110.58   |
| 1   | C1    | 2688 | OMU  | O2-C2-N1   | -2.11 | 120.05      | 122.80   |
| 1   | C1    | 2774 | OMG  | C8-N7-C5   | 2.10  | 107.99      | 104.26   |
| 1   | C1    | 2277 | OMU  | O2-C2-N1   | -2.09 | 120.08      | 122.80   |
| 1   | C1    | 1491 | OMC  | O2-C2-N3   | -2.09 | 119.04      | 122.33   |
| 1   | C1    | 2300 | OMC  | O2-C2-N3   | -2.08 | 119.04      | 122.33   |
| 1   | C1    | 2578 | OMG  | C8-N7-C5   | 2.08  | 107.97      | 104.26   |
| 1   | C1    | 2358 | OMG  | C8-N7-C5   | 2.07  | 107.94      | 104.26   |
| 1   | C1    | 1433 | OMG  | C8-N7-C5   | 2.07  | 107.94      | 104.26   |
| 1   | C1    | 627  | OMG  | N1-C2-N3   | -2.05 | 119.57      | 123.32   |
| 1   | C1    | 637  | A2M  | C4-C5-N7   | -2.04 | 108.24      | 110.58   |
| 1   | C1    | 385  | OMG  | N1-C2-N3   | -2.03 | 119.60      | 123.32   |
| 1   | C1    | 2881 | OMG  | N1-C2-N3   | -2.03 | 119.61      | 123.32   |
| 1   | C1    | 1223 | A2M  | C4-C5-N7   | -2.03 | 108.27      | 110.58   |
| 1   | C1    | 1812 | OMC  | N4-C4-N3   | 2.02  | 121.52      | 117.91   |
| 1   | C1    | 2300 | OMC  | O2-C2-N1   | 2.02  | 122.86      | 118.90   |
| 1   | C1    | 1868 | OMU  | O2-C2-N1   | -2.01 | 120.19      | 122.80   |
| 1   | C1    | 1433 | OMG  | N1-C2-N3   | -2.00 | 119.65      | 123.32   |

All (36) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | C1    | 385 | OMG  | C3'  |
| 1   | C1    | 385 | OMG  | C4'  |
| 1   | C1    | 627 | OMG  | C3'  |
| 1   | C1    | 627 | OMG  | C4'  |
| 1   | C1    | 646 | OMG  | C3'  |
| 1   | C1    | 646 | OMG  | C4'  |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | C1    | 778  | OMC  | C3'  |
| 1   | C1    | 778  | OMC  | C4'  |
| 1   | C1    | 787  | OMG  | C3'  |
| 1   | C1    | 787  | OMG  | C4'  |
| 1   | C1    | 1420 | OMC  | C3'  |
| 1   | C1    | 1420 | OMC  | C4'  |
| 1   | C1    | 1433 | OMG  | C3'  |
| 1   | C1    | 1433 | OMG  | C4'  |
| 1   | C1    | 1491 | OMC  | C3'  |
| 1   | C1    | 1491 | OMC  | C4'  |
| 1   | C1    | 1812 | OMC  | C3'  |
| 1   | C1    | 1812 | OMC  | C4'  |
| 1   | C1    | 1836 | OMC  | C3'  |
| 1   | C1    | 1836 | OMC  | C4'  |
| 1   | C1    | 2300 | OMC  | C3'  |
| 1   | C1    | 2300 | OMC  | C4'  |
| 1   | C1    | 2358 | OMG  | C3'  |
| 1   | C1    | 2358 | OMG  | C4'  |
| 1   | C1    | 2578 | OMG  | C3'  |
| 1   | C1    | 2578 | OMG  | C4'  |
| 1   | C1    | 2774 | OMG  | C3'  |
| 1   | C1    | 2774 | OMG  | C4'  |
| 1   | C1    | 2838 | OMC  | C3'  |
| 1   | C1    | 2838 | OMC  | C4'  |
| 1   | C1    | 2876 | OMG  | C3'  |
| 1   | C1    | 2876 | OMG  | C4'  |
| 1   | C1    | 2881 | OMG  | C3'  |
| 1   | C1    | 2881 | OMG  | C4'  |
| 1   | C1    | 2918 | OMC  | C3'  |
| 1   | C1    | 2918 | OMC  | C4'  |

All (85) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | C1    | 385 | OMG  | O4'-C4'-C5'-O5' |
| 1   | C1    | 389 | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 389 | A2M  | C1'-C2'-O2'-CM' |
| 1   | C1    | 627 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 637 | A2M  | C1'-C2'-O2'-CM' |
| 1   | C1    | 646 | OMG  | C4'-C5'-O5'-P   |
| 1   | C1    | 646 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 778 | OMC  | C3'-C2'-O2'-CM2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | C1    | 1223 | A2M  | C1'-C2'-O2'-CM' |
| 1   | C1    | 1420 | OMC  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 1420 | OMC  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1433 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 1491 | OMC  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 1491 | OMC  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1812 | OMC  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 1812 | OMC  | C4'-C5'-O5'-P   |
| 1   | C1    | 1836 | OMC  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 1836 | OMC  | C4'-C5'-O5'-P   |
| 1   | C1    | 1917 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | C1    | 2300 | OMC  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 2358 | OMG  | C4'-C5'-O5'-P   |
| 1   | C1    | 2358 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 2578 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 2683 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | C1    | 2774 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 2838 | OMC  | O4'-C1'-N1-C2   |
| 1   | C1    | 2838 | OMC  | O4'-C1'-N1-C6   |
| 1   | C1    | 2838 | OMC  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 2876 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 2881 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 2918 | OMC  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 385  | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 646  | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 778  | OMC  | C3'-C4'-C5'-O5' |
| 1   | C1    | 787  | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1812 | OMC  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1836 | OMC  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1917 | OMU  | O4'-C4'-C5'-O5' |
| 1   | C1    | 2300 | OMC  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2358 | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2578 | OMG  | O4'-C4'-C5'-O5' |
| 1   | C1    | 2774 | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2838 | OMC  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2881 | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2918 | OMC  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2881 | OMG  | C4'-C5'-O5'-P   |
| 1   | C1    | 2774 | OMG  | C4'-C5'-O5'-P   |
| 1   | C1    | 385  | OMG  | C3'-C2'-O2'-CM2 |
| 1   | C1    | 1491 | OMC  | C4'-C5'-O5'-P   |
| 1   | C1    | 2838 | OMC  | C4'-C5'-O5'-P   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | C1    | 389  | A2M  | C3'-C4'-C5'-O5' |
| 1   | C1    | 627  | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1847 | A2M  | C3'-C4'-C5'-O5' |
| 1   | C1    | 778  | OMC  | C4'-C5'-O5'-P   |
| 1   | C1    | 2918 | OMC  | C4'-C5'-O5'-P   |
| 1   | C1    | 1917 | OMU  | C3'-C4'-C5'-O5' |
| 1   | C1    | 2300 | OMC  | C4'-C5'-O5'-P   |
| 1   | C1    | 1420 | OMC  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1433 | OMG  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1491 | OMC  | C3'-C4'-C5'-O5' |
| 1   | C1    | 1847 | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 2876 | OMG  | C3'-C4'-C5'-O5' |
| 1   | C1    | 385  | OMG  | C4'-C5'-O5'-P   |
| 1   | C1    | 2578 | OMG  | C4'-C5'-O5'-P   |
| 1   | C1    | 2300 | OMC  | C2'-C1'-N1-C2   |
| 1   | C1    | 2300 | OMC  | C2'-C1'-N1-C6   |
| 1   | C1    | 1420 | OMC  | C4'-C5'-O5'-P   |
| 1   | C1    | 1847 | A2M  | C4'-C5'-O5'-P   |
| 1   | C1    | 1491 | OMC  | C2'-C1'-N1-C2   |
| 1   | C1    | 1433 | OMG  | C2'-C1'-N9-C4   |
| 1   | C1    | 858  | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1223 | A2M  | O4'-C4'-C5'-O5' |
| 1   | C1    | 2918 | OMC  | C2'-C1'-N1-C6   |
| 1   | C1    | 2384 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | C1    | 646  | OMG  | C2'-C1'-N9-C4   |
| 1   | C1    | 2774 | OMG  | C2'-C1'-N9-C4   |
| 1   | C1    | 1491 | OMC  | C2'-C1'-N1-C6   |
| 1   | C1    | 2876 | OMG  | O4'-C4'-C5'-O5' |
| 1   | C1    | 1836 | OMC  | C2'-C1'-N1-C6   |
| 1   | C1    | 2358 | OMG  | C2'-C1'-N9-C4   |
| 1   | C1    | 1836 | OMC  | C2'-C1'-N1-C2   |
| 1   | C1    | 778  | OMC  | C2'-C1'-N1-C6   |
| 1   | C1    | 1420 | OMC  | C2'-C1'-N1-C2   |
| 1   | C1    | 2918 | OMC  | C2'-C1'-N1-C2   |
| 1   | C1    | 2578 | OMG  | C2'-C1'-N9-C4   |

There are no ring outliers.

16 monomers are involved in 23 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | C1    | 2300 | OMC  | 1       | 0            |
| 1   | C1    | 1812 | OMC  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | C1    | 787  | OMG  | 3       | 0            |
| 1   | C1    | 2683 | OMU  | 1       | 0            |
| 1   | C1    | 1420 | OMC  | 1       | 0            |
| 1   | C1    | 389  | A2M  | 1       | 0            |
| 1   | C1    | 1491 | OMC  | 4       | 0            |
| 1   | C1    | 1432 | A2M  | 1       | 0            |
| 1   | C1    | 2838 | OMC  | 2       | 0            |
| 1   | C1    | 2881 | OMG  | 1       | 0            |
| 1   | C1    | 2578 | OMG  | 1       | 0            |
| 1   | C1    | 2876 | OMG  | 1       | 0            |
| 1   | C1    | 627  | OMG  | 1       | 0            |
| 1   | C1    | 1917 | OMU  | 1       | 0            |
| 1   | C1    | 646  | OMG  | 2       | 0            |
| 1   | C1    | 637  | A2M  | 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 |
| 60  | GTP  | CH    | 701  | 61   | 33,34,34     | 0.92 | 1 (3%)   | 50,54,54    | 1.57 | 9 (18%)  |
| 60  | GTP  | Cd    | 1000 | 61   | 33,34,34     | 0.92 | 1 (3%)   | 50,54,54    | 1.65 | 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   |
|-----|------|-------|------|------|---------|------------|---------|
| 60  | GTP  | CH    | 701  | 61   | -       | 7/22/38/38 | 0/3/3/3 |
| 60  | GTP  | Cd    | 1000 | 61   | -       | 1/22/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 60  | CH    | 701  | GTP  | C2-N3 | 2.18 | 1.38        | 1.33     |
| 60  | Cd    | 1000 | GTP  | C2-N3 | 2.04 | 1.38        | 1.33     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 60  | CH    | 701  | GTP  | C5-C4-N3    | -4.99 | 120.44      | 128.39   |
| 60  | Cd    | 1000 | GTP  | C5-C4-N3    | -4.97 | 120.48      | 128.39   |
| 60  | Cd    | 1000 | GTP  | C2-N3-C4    | 4.65  | 120.31      | 112.30   |
| 60  | CH    | 701  | GTP  | C2-N3-C4    | 4.57  | 120.17      | 112.30   |
| 60  | CH    | 701  | GTP  | N9-C4-N3    | 3.21  | 132.37      | 125.95   |
| 60  | Cd    | 1000 | GTP  | N9-C4-N3    | 3.14  | 132.24      | 125.95   |
| 60  | Cd    | 1000 | GTP  | C2-N1-C6    | -2.90 | 119.85      | 125.11   |
| 60  | CH    | 701  | GTP  | C2-N1-C6    | -2.88 | 119.89      | 125.11   |
| 60  | Cd    | 1000 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 60  | CH    | 701  | GTP  | N9-C8-N7    | -2.57 | 108.64      | 113.40   |
| 60  | Cd    | 1000 | GTP  | C8-N7-C5    | 2.49  | 108.70      | 104.26   |
| 60  | CH    | 701  | GTP  | C5-C6-N1    | 2.49  | 119.59      | 113.25   |
| 60  | Cd    | 1000 | GTP  | C5-C6-N1    | 2.47  | 119.55      | 113.25   |
| 60  | Cd    | 1000 | GTP  | O6-C6-C5    | -2.46 | 120.04      | 126.53   |
| 60  | CH    | 701  | GTP  | C8-N7-C5    | 2.44  | 108.61      | 104.26   |
| 60  | CH    | 701  | GTP  | O6-C6-C5    | -2.40 | 120.21      | 126.53   |
| 60  | Cd    | 1000 | GTP  | C3'-C2'-C1' | 2.33  | 105.86      | 101.46   |
| 60  | CH    | 701  | GTP  | C3'-C2'-C1' | 2.24  | 105.70      | 101.46   |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 60  | CH    | 701 | GTP  | C5'-O5'-PA-O3A  |
| 60  | CH    | 701 | GTP  | C5'-O5'-PA-O1A  |
| 60  | CH    | 701 | GTP  | C5'-O5'-PA-O2A  |
| 60  | CH    | 701 | GTP  | C3'-C4'-C5'-O5' |
| 60  | CH    | 701 | GTP  | O4'-C4'-C5'-O5' |
| 60  | CH    | 701 | GTP  | PB-O3A-PA-O2A   |
| 60  | CH    | 701 | GTP  | PB-O3A-PA-O1A   |

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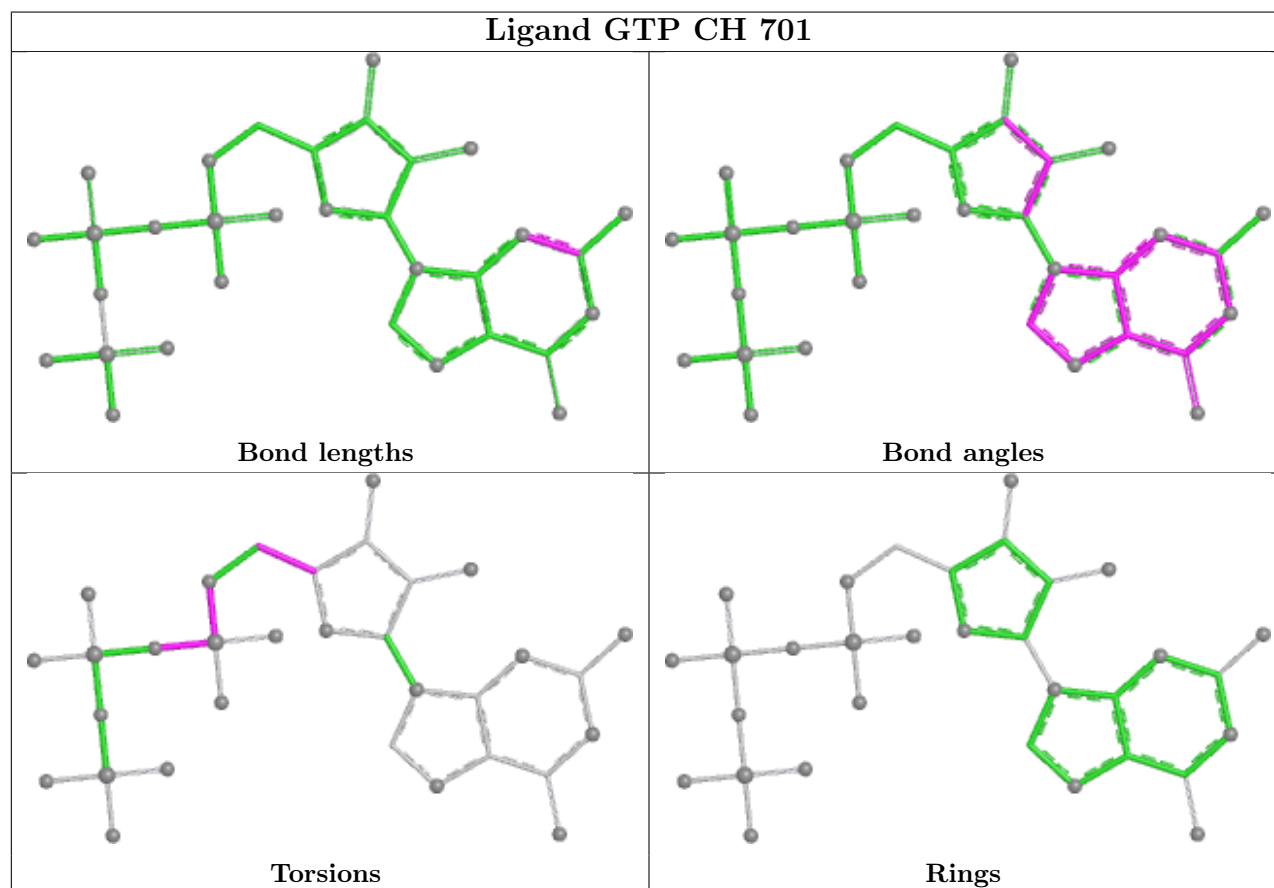
| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 60  | Cd    | 1000 | GTP  | PB-O3A-PA-O2A |

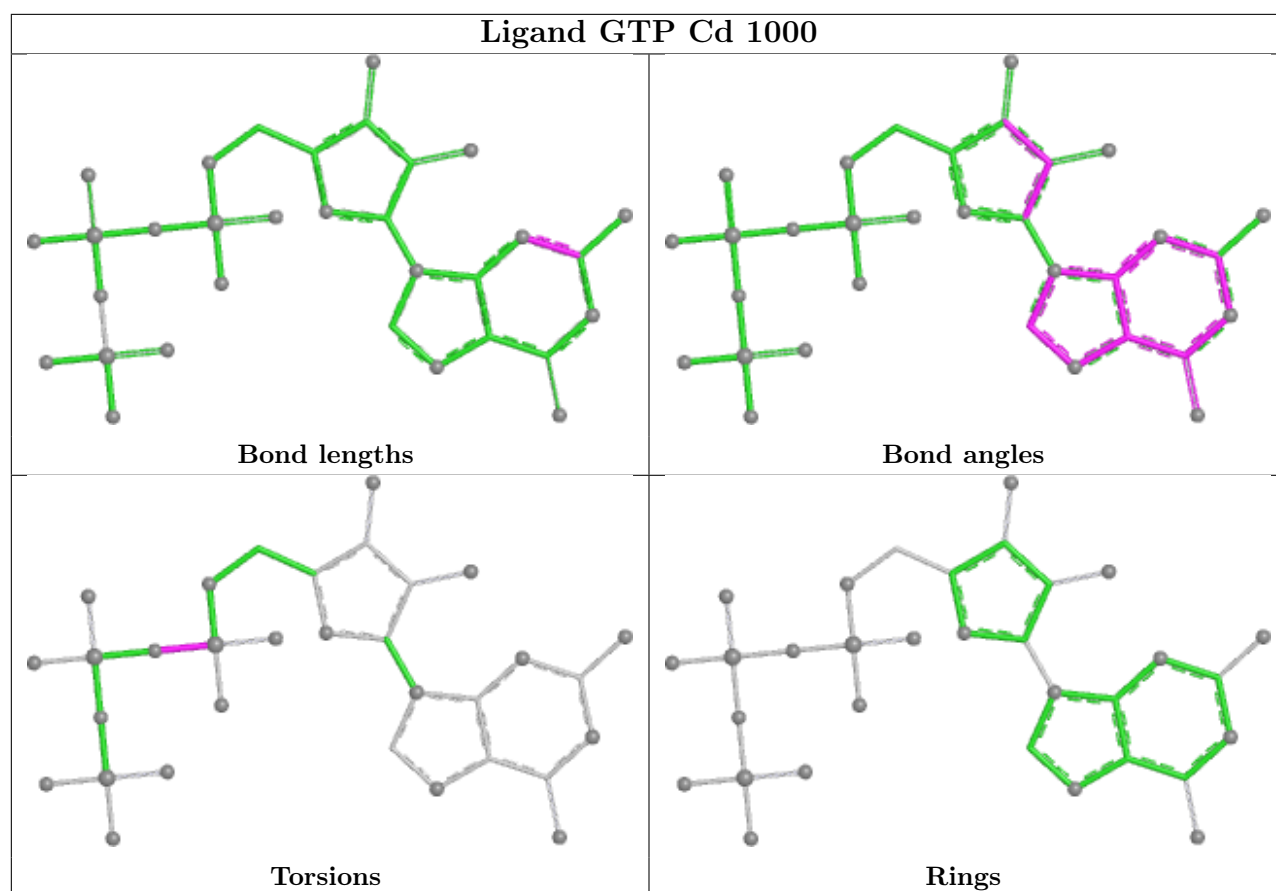
There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 60  | 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.





## 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.

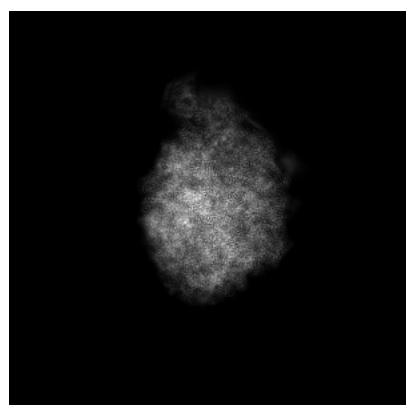
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17969. These allow visual inspection of the internal detail of the map and identification of artifacts.

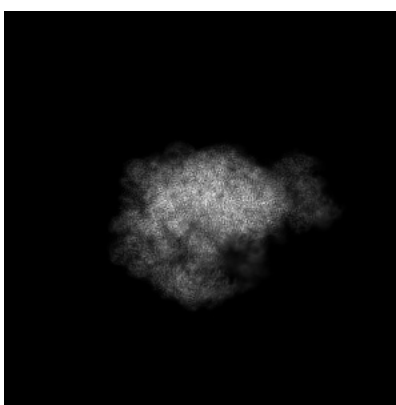
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

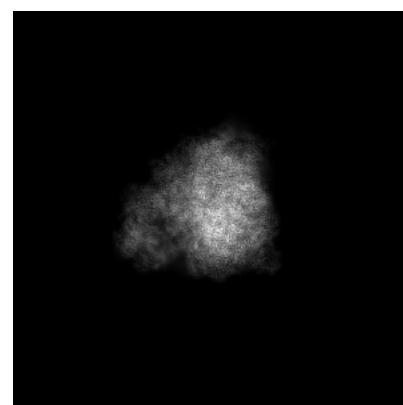
#### 6.1.1 Primary map



X



Y

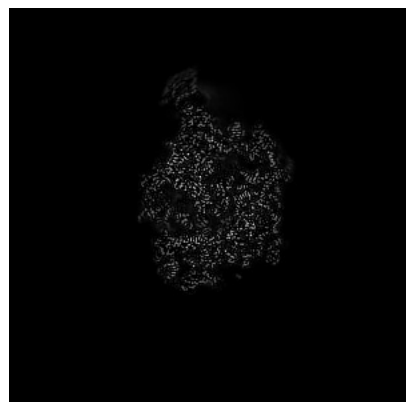


Z

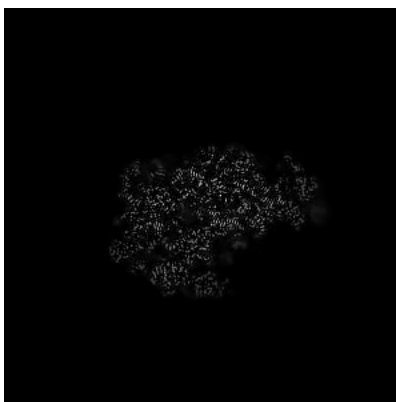
The images above show the map projected in three orthogonal directions.

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

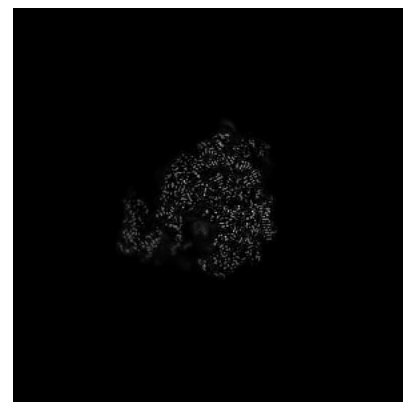
#### 6.2.1 Primary map



X Index: 250



Y Index: 250

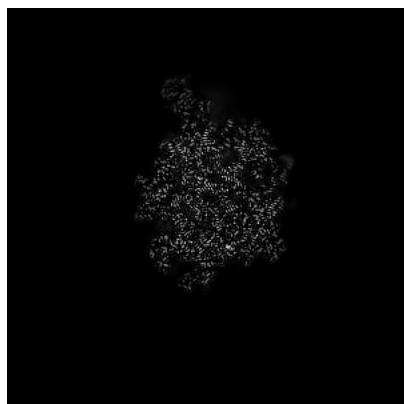


Z Index: 250

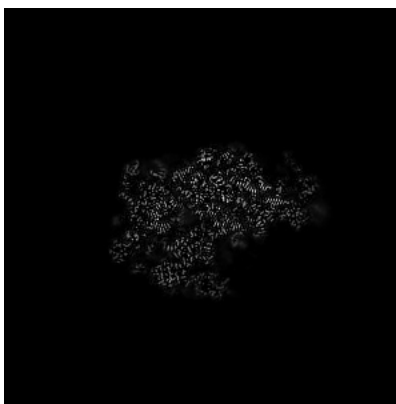
The images above show central slices of the map in three orthogonal directions.

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

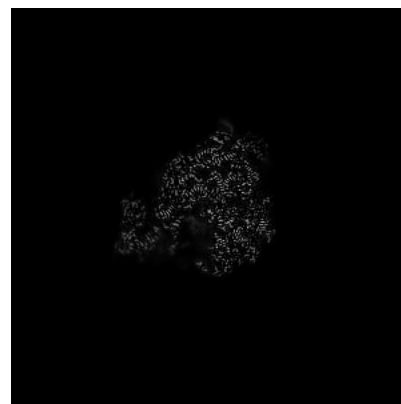
### 6.3.1 Primary map



X Index: 259



Y Index: 248

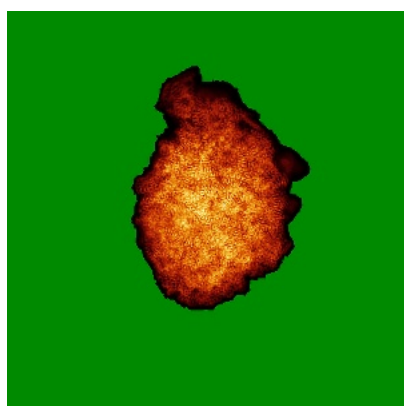


Z Index: 252

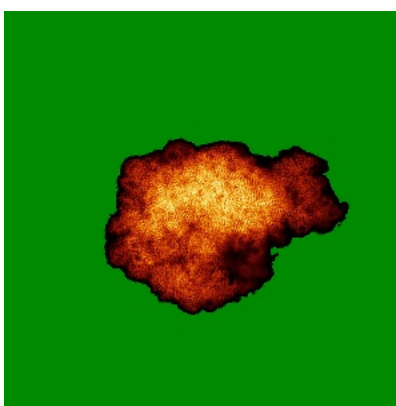
The images above show the largest variance slices of the map in three orthogonal directions.

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

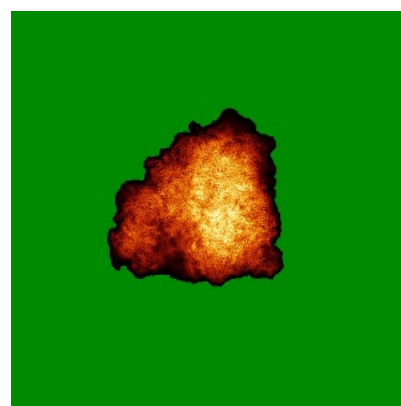
### 6.4.1 Primary map



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

This section was not generated.

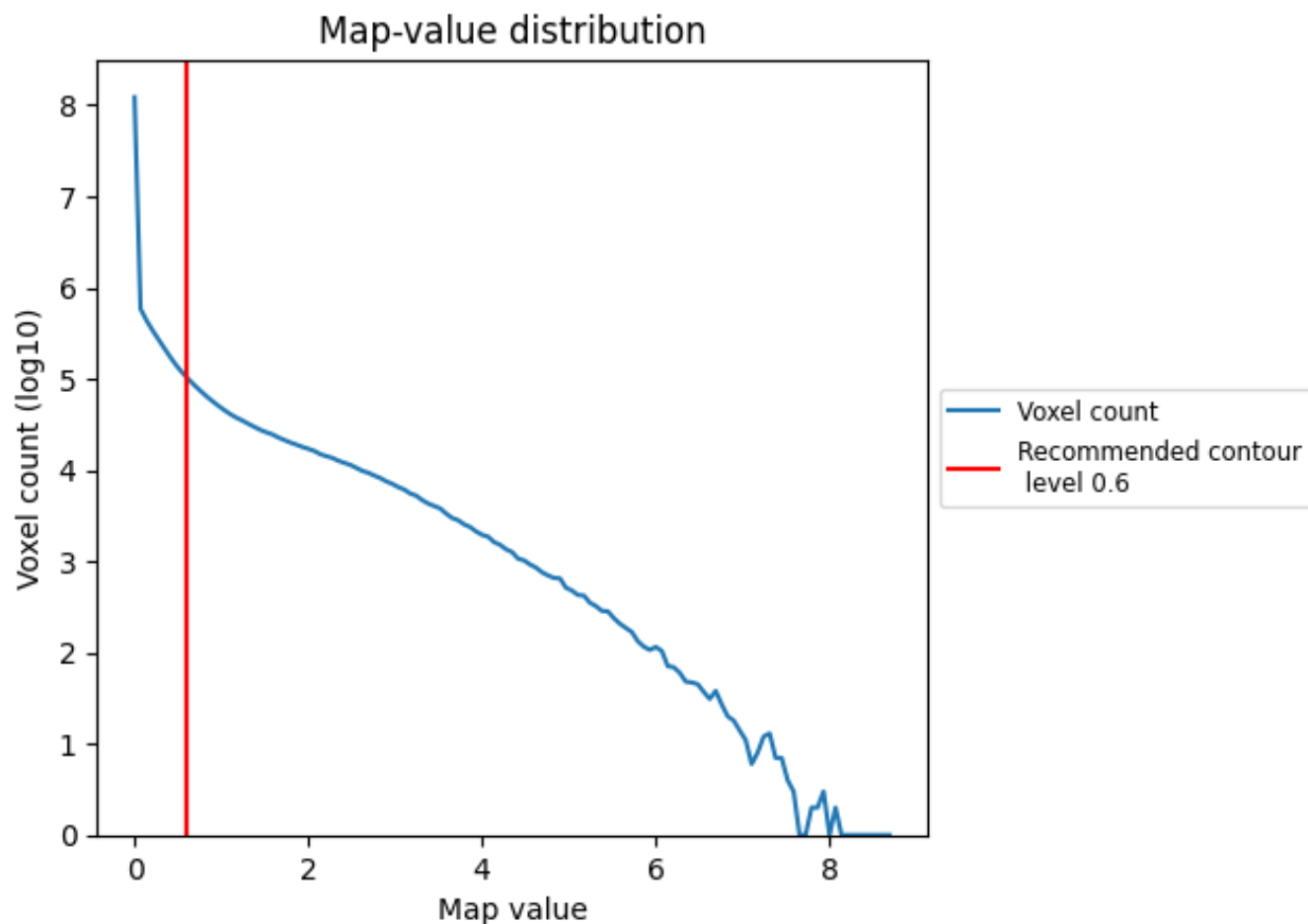
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

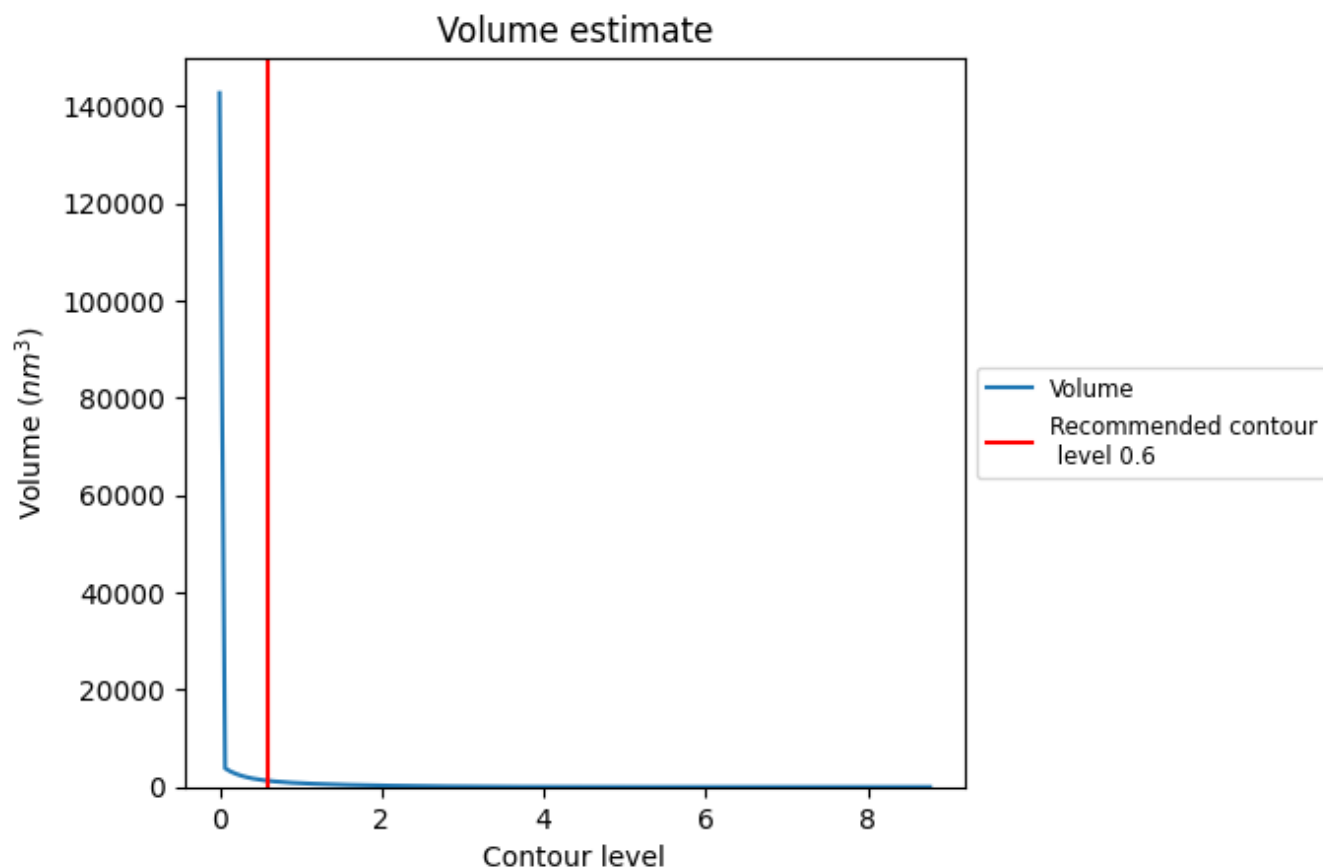
This section contains the results of statistical analysis of the map.

### 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.

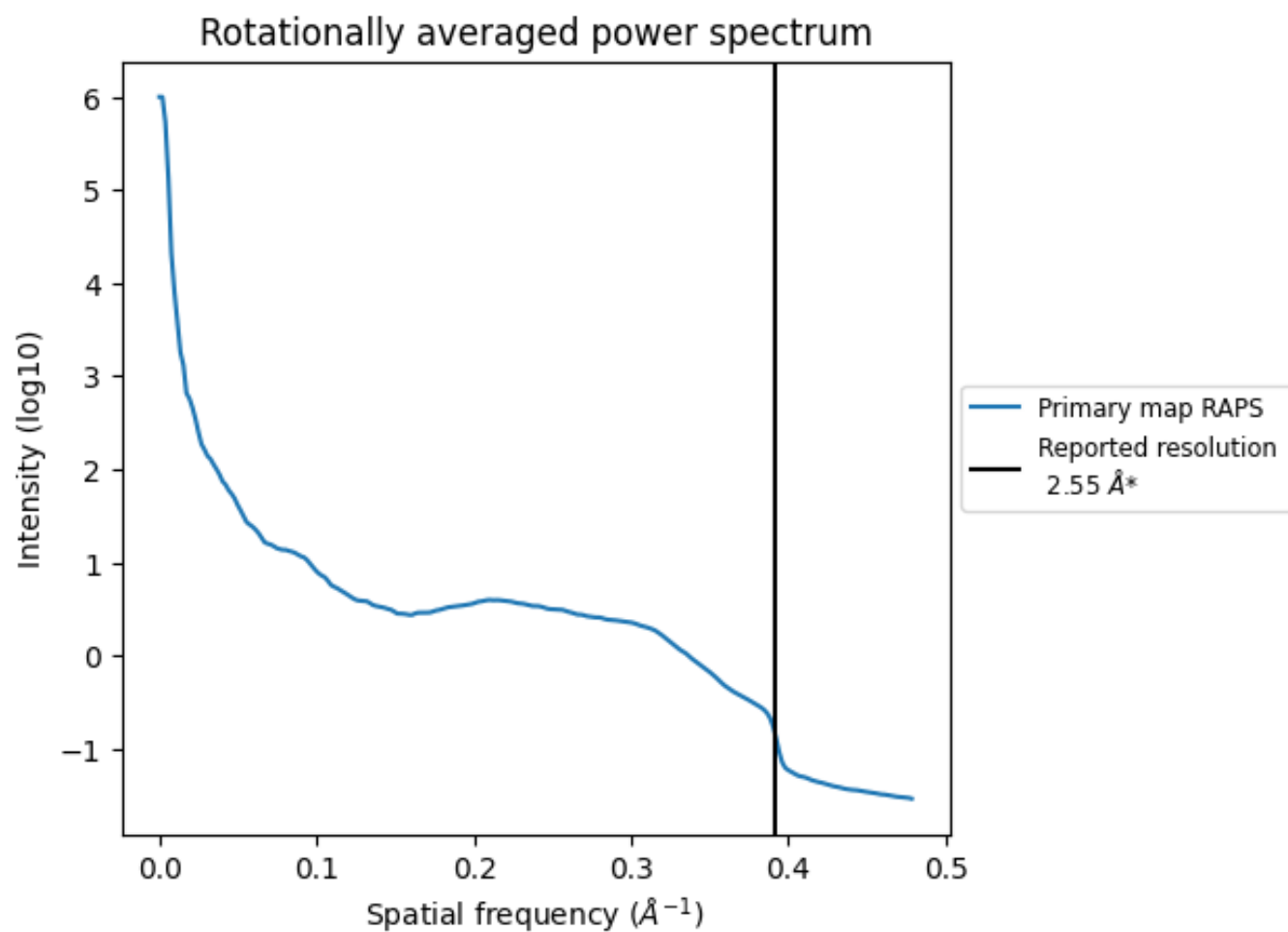
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1273  $\text{nm}^3$ ; this corresponds to an approximate mass of 1150 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 0.392 Å<sup>-1</sup>

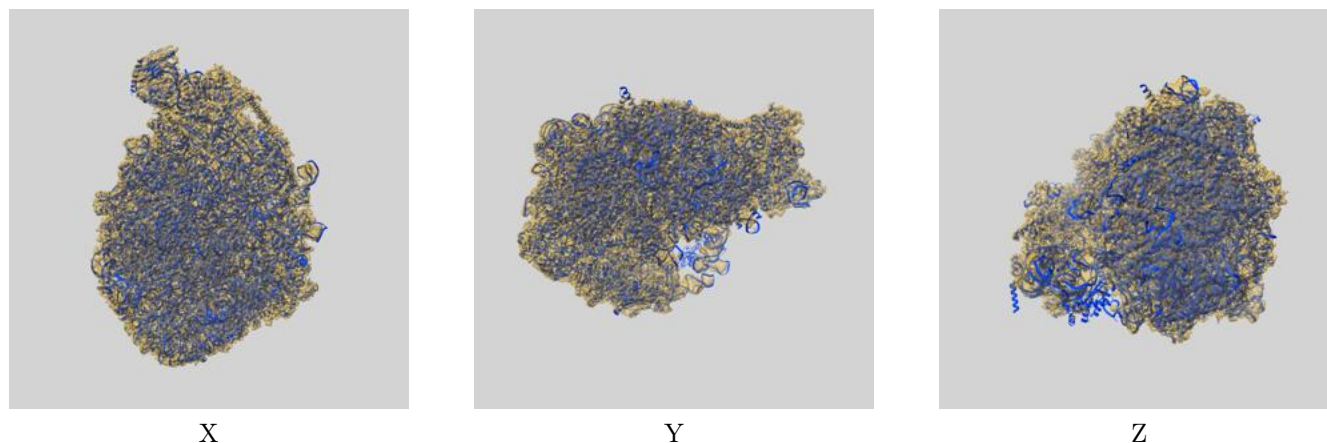
## 8 Fourier-Shell correlation

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

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

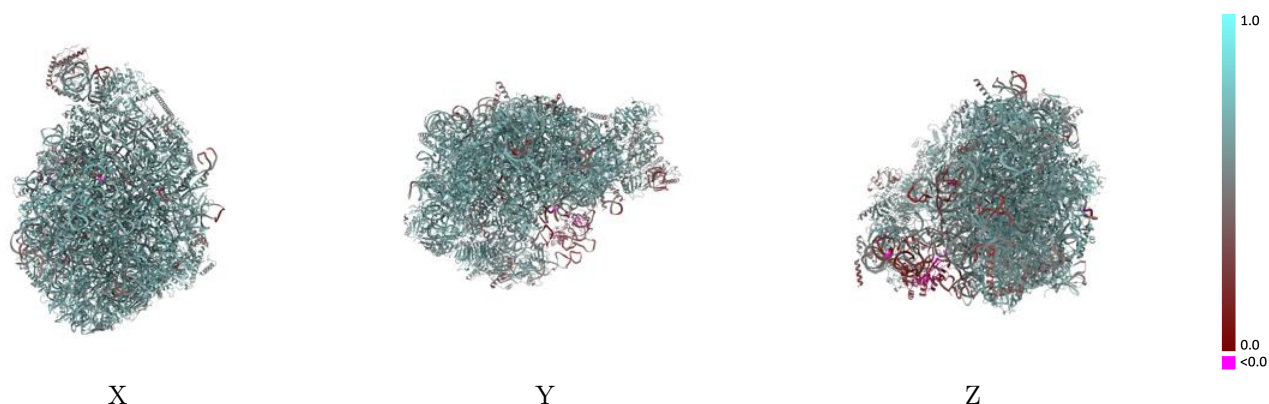
This section contains information regarding the fit between EMDB map EMD-17969 and PDB model 8PVK. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



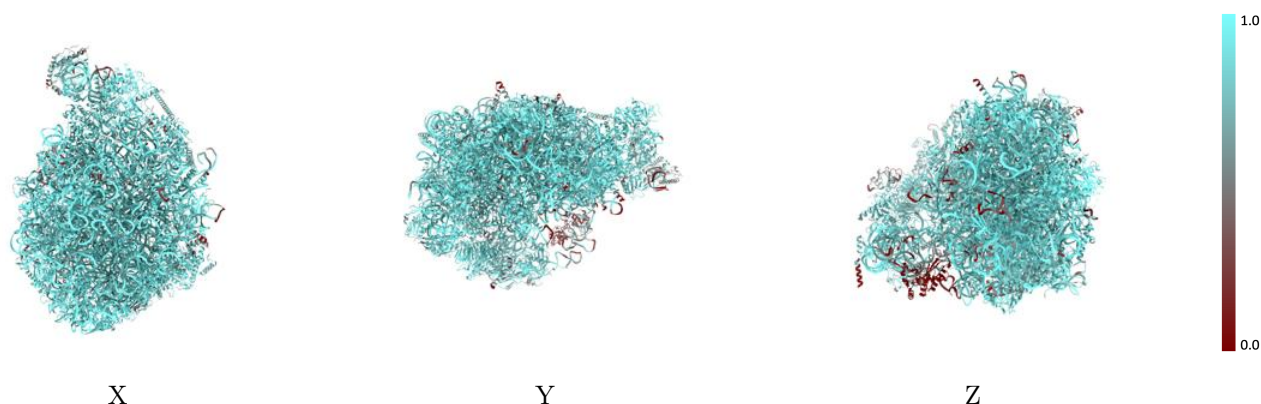
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



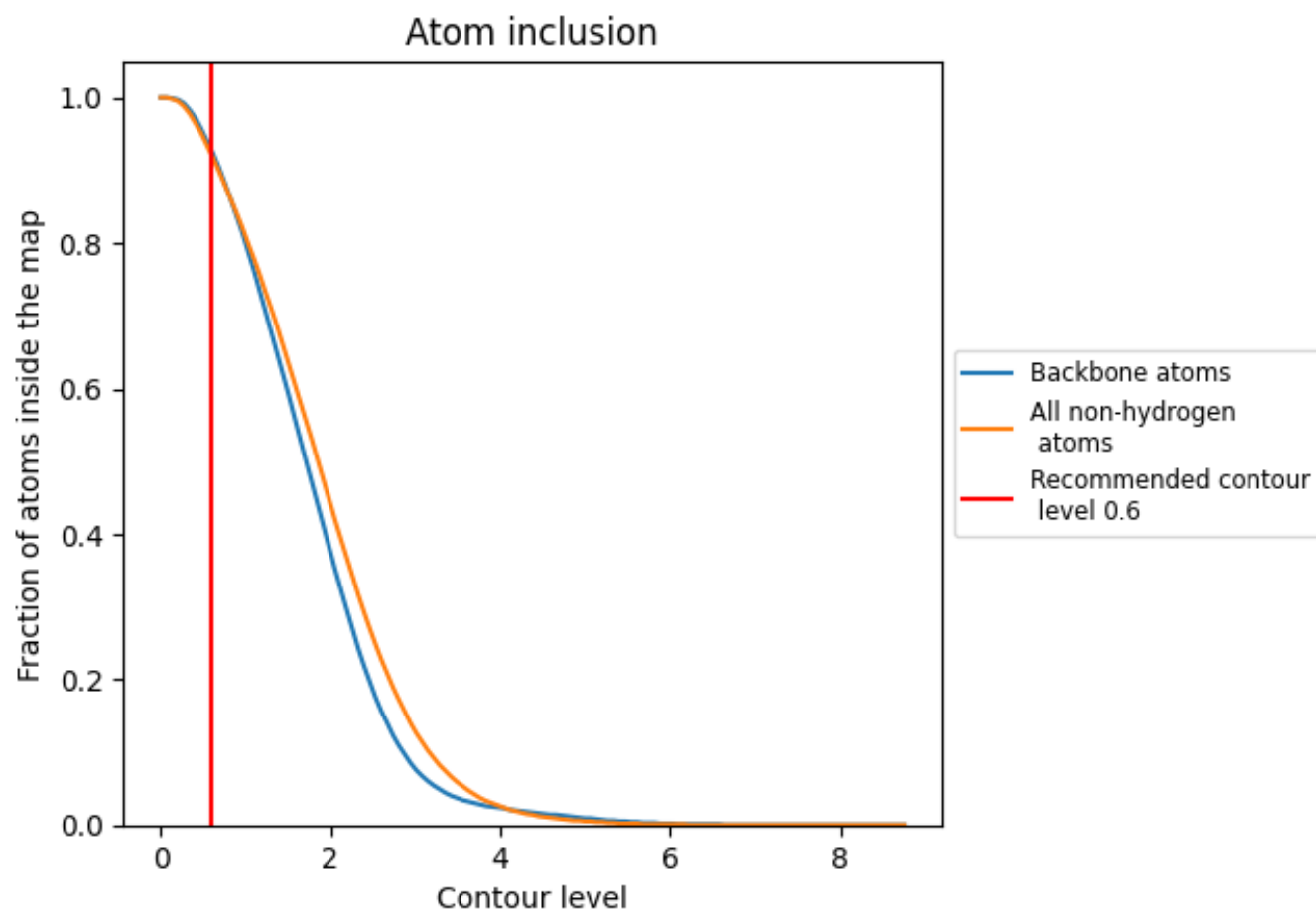
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9220   |  0.6060   |
| C1    |  0.9550   |  0.6080   |
| C2    |  0.9690   |  0.6450   |
| C3    |  0.7300   |  0.4480   |
| C4    |  0.9180   |  0.5110   |
| CB    |  0.7580   |  0.5000   |
| CF    |  0.8970   |  0.5920   |
| CH    |  0.8990   |  0.6180   |
| CI    |  0.8100   |  0.5130   |
| CJ    |  0.9510   |  0.6240   |
| CK    |  0.9640   |  0.6650   |
| CL    |  0.8570   |  0.5710   |
| CM    |  0.8750   |  0.5730   |
| CN    |  0.9440   |  0.6480   |
| CO    |  0.8860  |  0.6390  |
| CQ    |  0.8610 |  0.6100 |
| Cb    |  0.9430 |  0.6410 |
| Cd    |  0.9490 |  0.6360 |
| Ce    |  0.8150 |  0.5550 |
| Cf    |  0.9210 |  0.5690 |
| Cg    |  0.9030 |  0.5700 |
| Ch    |  0.8730 |  0.5910 |
| Cz    |  0.7990 |  0.5320 |
| LA    |  0.9700 |  0.6550 |
| LB    |  0.9680 |  0.6780 |
| LC    |  0.9690 |  0.6690 |
| LD    |  0.8850 |  0.5800 |
| LE    |  0.9110 |  0.6200 |
| LF    |  0.9510 |  0.6470 |
| LG    |  0.9420 |  0.6310 |
| LH    |  0.9420 |  0.6490 |
| LJ    |  0.8340 |  0.5000 |
| LK    |  0.8410 |  0.5490 |
| LL    |  0.9350 |  0.6400 |
| LM    |  0.9520 |  0.6370 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| LN    |  0.9910   |  0.6760   |
| LO    |  0.9760   |  0.6770   |
| LP    |  0.9750   |  0.6720   |
| LQ    |  0.9310   |  0.6420   |
| LR    |  0.9450   |  0.6560   |
| LS    |  0.9610   |  0.6490   |
| LT    |  0.8200   |  0.5330   |
| LU    |  0.8900   |  0.5980   |
| LV    |  0.9750   |  0.6750   |
| LX    |  0.9340   |  0.6300   |
| LY    |  0.9390   |  0.6390   |
| LZ    |  0.9450   |  0.6390   |
| La    |  0.9500   |  0.6430   |
| Lc    |  0.9020   |  0.6170   |
| Ld    |  0.9300   |  0.6560   |
| Le    |  0.9810   |  0.6760   |
| Lf    |  0.9830   |  0.6880   |
| Lg    |  0.9160   |  0.6430   |
| Lh    |  0.9070   |  0.5950   |
| Li    |  0.9500  |  0.6030  |
| Lj    |  0.9900 |  0.6940 |
| Lk    |  0.8830 |  0.6050 |
| Ll    |  1.0000 |  0.7020 |
| Lp    |  0.9150 |  0.6290 |
| Lq    |  0.9490 |  0.6390 |
| Lr    |  0.0380 |  0.1190 |