



# Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 01:27 PM EDT

PDB ID : 8FLB / pdb\_00008flb  
EMDB ID : EMD-29273  
Title : Human nuclear pre-60S ribosomal subunit (State K2)  
Authors : Vanden Broeck, A.; Klinge, S.  
Deposited on : 2022-12-21  
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:

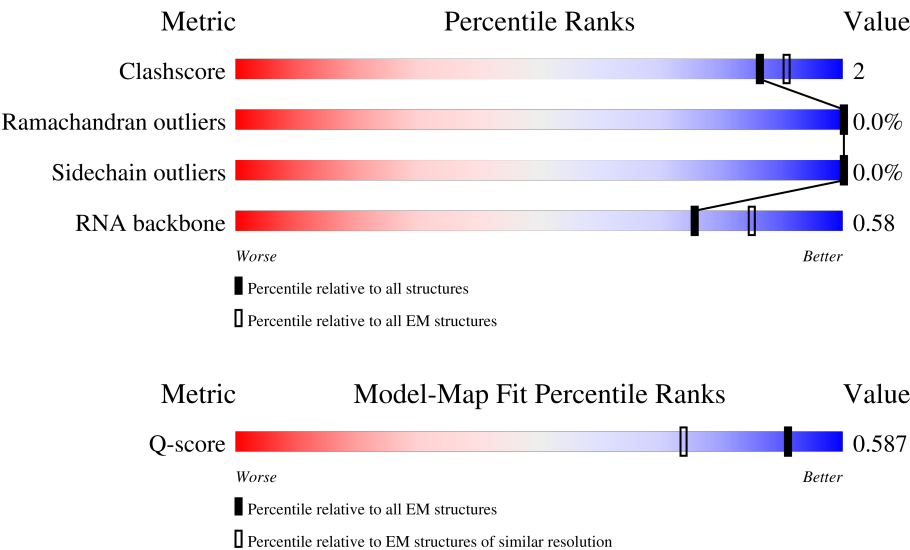
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

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.



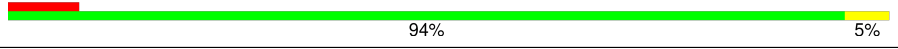
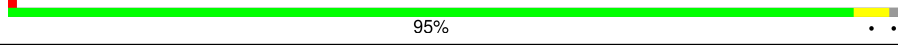
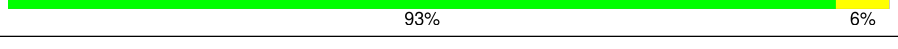
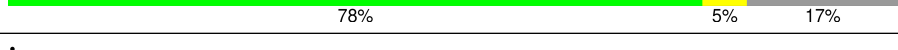
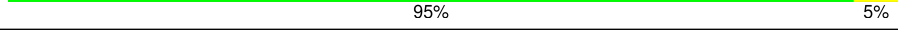
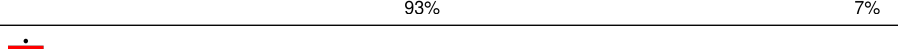
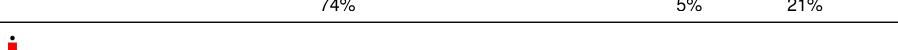
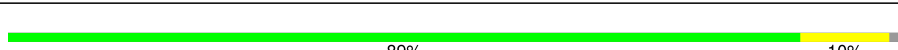
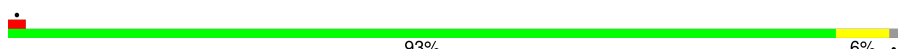
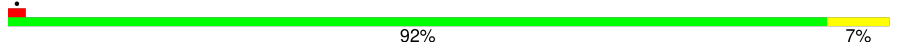
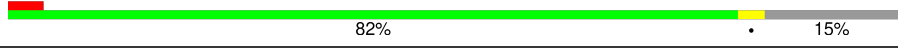
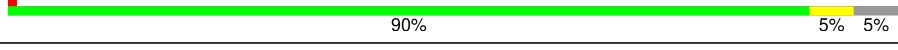
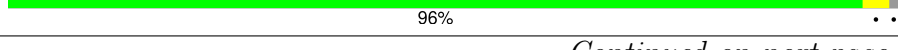
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 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   | BA    | 165    |                  |
| 2   | L1    | 157    |                  |
| 3   | L3    | 5070   |                  |

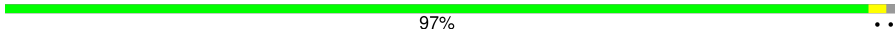
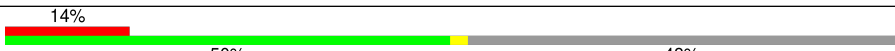
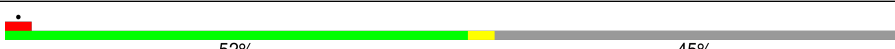
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | L4    | 121    |    |
| 5   | L5    | 178    |    |
| 6   | L6    | 211    |    |
| 7   | L7    | 203    |    |
| 8   | L8    | 215    |    |
| 9   | L9    | 204    |    |
| 10  | LA    | 184    |    |
| 11  | LB    | 188    |    |
| 12  | LC    | 176    |    |
| 13  | LD    | 196    |    |
| 14  | LE    | 160    |    |
| 15  | LF    | 128    |  |
| 16  | LG    | 140    |  |
| 17  | LH    | 156    |  |
| 18  | LI    | 145    |  |
| 19  | LJ    | 136    |  |
| 20  | LK    | 148    |  |
| 21  | LL    | 137    |  |
| 22  | LM    | 159    |  |
| 23  | LN    | 403    |  |
| 24  | LO    | 115    |  |
| 25  | LP    | 125    |  |
| 26  | LQ    | 135    |  |
| 27  | LR    | 117    |  |
| 28  | LS    | 123    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | LT    | 110    |    |
| 30  | LU    | 105    |    |
| 31  | LV    | 106    |    |
| 32  | LW    | 97     |    |
| 33  | LX    | 92     |    |
| 34  | LY    | 70     |    |
| 35  | LZ    | 51     |    |
| 36  | NK    | 129    |    |
| 37  | NL    | 478    |    |
| 38  | NP    | 134    |    |
| 39  | NR    | 203    |    |
| 40  | SA    | 427    |    |
| 41  | SB    | 297    |  |
| 42  | SC    | 288    |  |
| 43  | SD    | 248    |  |
| 44  | SE    | 266    |  |
| 45  | SF    | 257    |  |
| 46  | SG    | 192    |  |
| 47  | SH    | 293    |  |
| 48  | SI    | 255    |  |
| 49  | SK    | 245    |  |
| 50  | SM    | 588    |  |
| 51  | SQ    | 239    |  |
| 52  | SR    | 634    |  |
| 53  | SV    | 163    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | VB    | 99     |                  |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149034 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1   | BA    | 91       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 449   | 267 | 91 | 91 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 2   | L1    | 154      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3278  | 1463 | 581 | 1080 | 154 |         |       |

- Molecule 3 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 3   | L3    | 3420     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 73423 | 32721 | 13453 | 23829 | 3420 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4   | L4    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2561  | 1141 | 456 | 844 | 120 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | L5    | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1349  | 853 | 251 | 239 | 6 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | L6    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1064 | 352 | 281 | 4 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | L7    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1063 | 321 | 261 | 5 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | L8    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 713 | 213 | 178 | 7 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | L9    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | LA    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | LB    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1512  | 944 | 314 | 249 | 5 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 12  | LC    | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1461  | 930 | 284 | 236 | 11 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | LD    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1289  | 805 | 277 | 198 | 9 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | LE    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1264  | 803 | 246 | 210 | 5 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | LF    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 842   | 538 | 148 | 154 | 2 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | LG    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 648 | 199 | 182 | 5 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | LH    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1156  | 740 | 220 | 195 | 1 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | LI    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | LJ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | LK    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | LL    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | LM    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 751   | 469 | 165 | 113 | 4 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | LN    | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3239  | 2061 | 608 | 556 | 14 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | LO    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 468 | 131 | 133 | 6 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | LP    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 879   | 555 | 170 | 152 | 2 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LQ    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LR    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 555 | 183 | 144 | 6 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LS    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | LT    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | LU    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | LV    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 851   | 533 | 174 | 138 | 6 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | LW    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | LX    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 34  | LY    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | LZ    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 36 is a protein called Protein LLP homolog.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 36  | NK    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 581   | 363 | 128 | 88 | 2 |         |       |

- Molecule 37 is a protein called Ribosome biogenesis protein NOP53.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37  | NL    | 263      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1347 | 433 | 393 | 2 |         |       |

- Molecule 38 is a protein called Zinc finger protein 593.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | NP    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 847   | 520 | 178 | 145 | 4 |         |       |

- Molecule 39 is a protein called Translation machinery-associated protein 16.

| Mol | Chain | Residues | Atoms |     |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|
| 39  | NR    | 152      | Total | C   | N   | O   | P S | 1       | 0     |
|     |       |          | 1299  | 809 | 249 | 235 | 1 5 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40  | SA    | 358      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2853  | 1797 | 570 | 473 | 13 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41  | SB    | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2243  | 1419 | 406 | 404 | 14 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 42  | SC    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1747  | 1124 | 332 | 287 | 4 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 43  | SD    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1202 | 358 | 301 | 9 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44  | SE    | 231      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1869  | 1191 | 361 | 313 | 4 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45  | SF    | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1876  | 1177 | 383 | 310 | 6 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | SG    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 47 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | SH    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 501 | 130 | 139 | 3 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L7-like 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48  | SI    | 234      | Total | C    | N   | O   | S | 3       | 0     |
|     |       |          | 1952  | 1267 | 365 | 316 | 4 |         |       |

- Molecule 49 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49  | SK    | 244      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1852  | 1149 | 318 | 372 | 13 |         |       |

- Molecule 50 is a protein called Pescadillo homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | SM    | 399      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3278  | 2120 | 576 | 571 | 11 |         |       |

- Molecule 51 is a protein called mRNA turnover protein 4 homolog.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 51  | SQ    | 127      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 650   | 388 | 132 | 130 |  |         |       |

- Molecule 52 is a protein called GTP-binding protein 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | SR    | 601      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4932  | 3105 | 899 | 902 | 26 |         |       |

- Molecule 53 is a protein called Probable ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 53  | SV    | 139      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1184  | 754 | 229 | 191 | 10 |         |       |

- Molecule 54 is a protein called Leydig cell tumor 10 kDa protein homolog.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | VB    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 285 | 95 | 74 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 55  | L1    | 4        | Total | Mg | 0       |
|     |       |          | 4     | 4  |         |
| 55  | L3    | 74       | Total | Mg | 0       |
|     |       |          | 74    | 74 |         |
| 55  | L4    | 3        | Total | Mg | 0       |
|     |       |          | 3     | 3  |         |

*Continued on next page...*

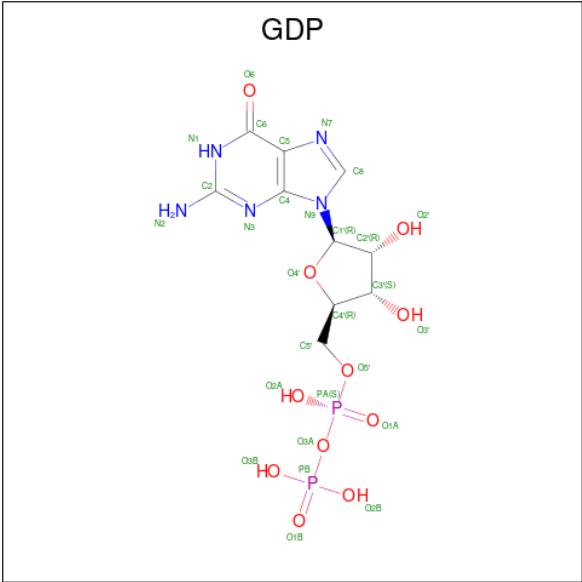
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 55  | LG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 55  | LN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 55  | LQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 55  | LR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 55  | LT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 55  | SF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 55  | SR    | 1        | Total<br>1 | Mg<br>1 | 0       |

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

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 56  | LR    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 56  | LV    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 56  | LW    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 56  | LX    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 56  | NP    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 56  | SV    | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 57 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 57  | SR    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

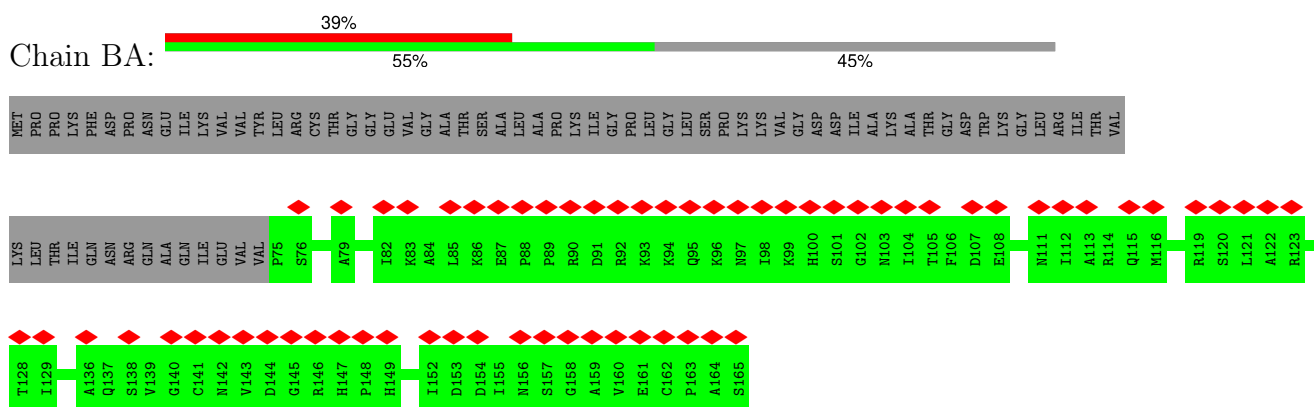
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 58  | SR    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

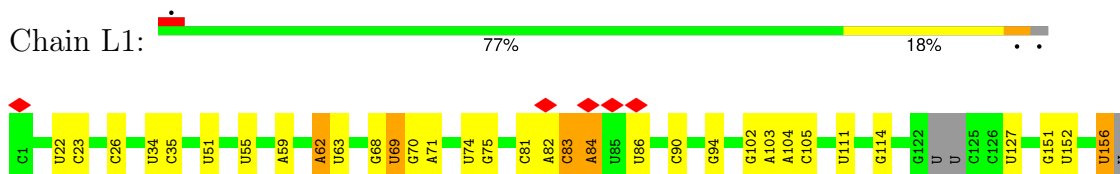
### 3 Residue-property plots

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

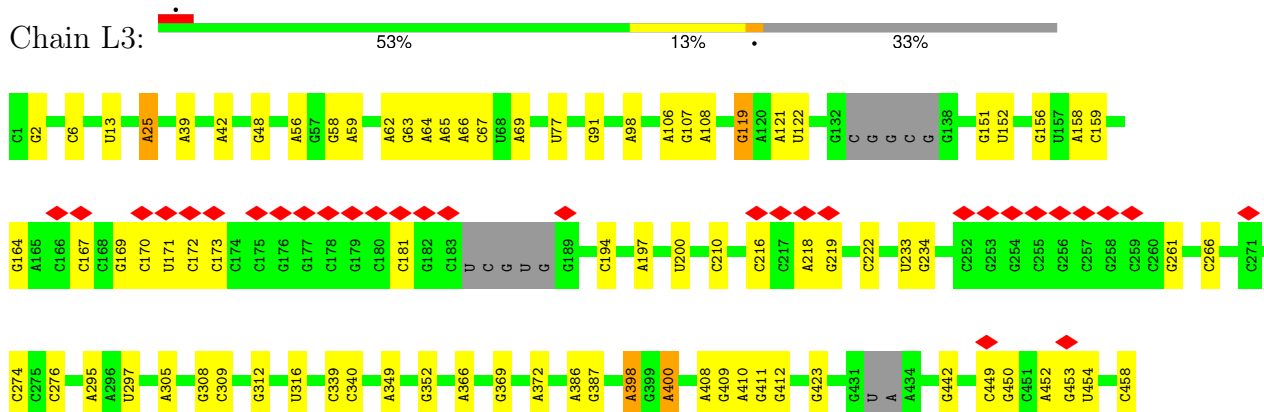
#### • Molecule 1: 60S ribosomal protein L12

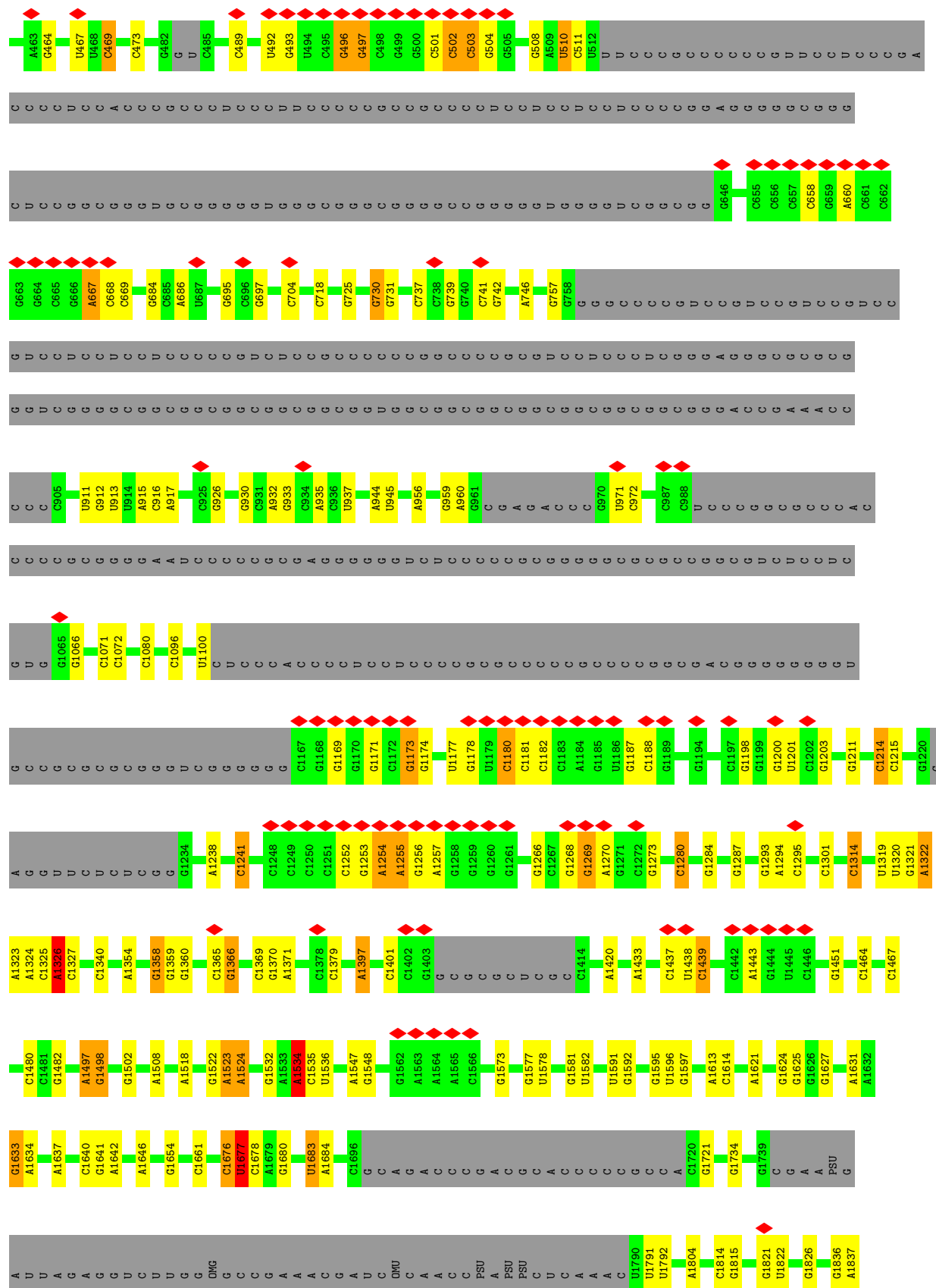


#### • Molecule 2: 5.8S rRNA



#### • Molecule 3: 28S rRNA





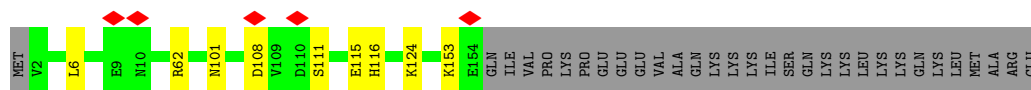




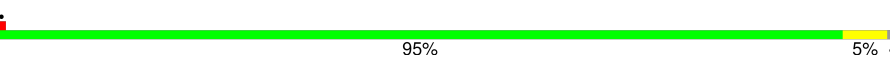


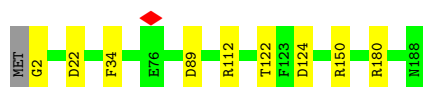
- Molecule 10: 60S ribosomal protein L17

Chain LA:  78% 5% 17%



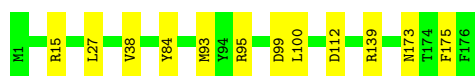
- Molecule 11: 60S ribosomal protein L18

Chain LB:  95% 5%



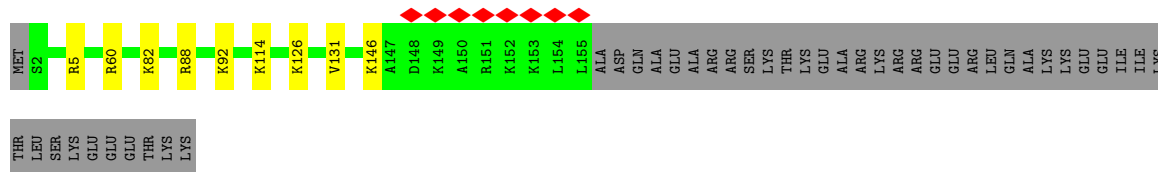
- Molecule 12: 60S ribosomal protein L18a

Chain LC:  93% 7%

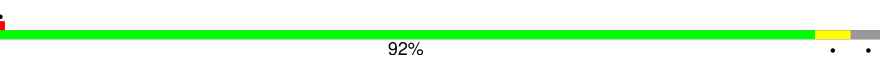


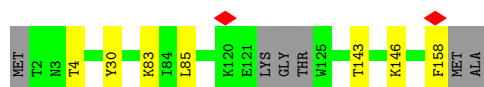
- Molecule 13: 60S ribosomal protein L19

Chain LD:  74% 5% 21%



- Molecule 14: 60S ribosomal protein L21

Chain LE:  92% 5% 3%

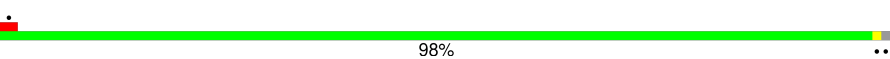


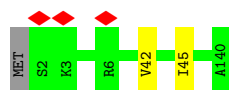
- Molecule 15: 60S ribosomal protein L22

Chain LF:  73% 7% 20%

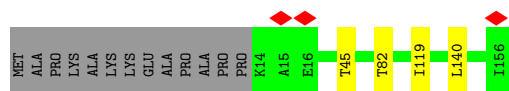


- Molecule 16: 60S ribosomal protein L23

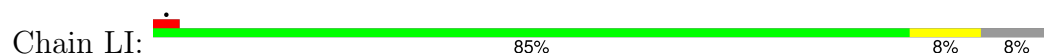
Chain LG:  98% 1% 1%



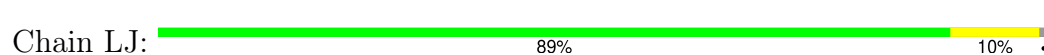
- Molecule 17: 60S ribosomal protein L23a



- Molecule 18: 60S ribosomal protein L26



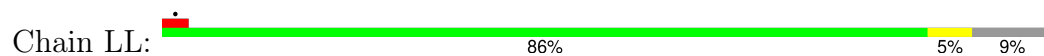
- Molecule 19: 60S ribosomal protein L27



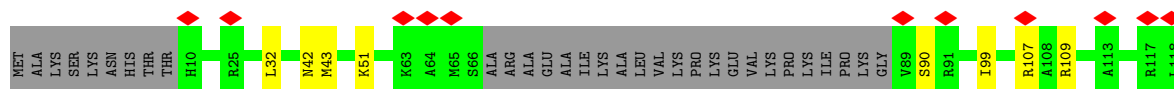
- Molecule 20: 60S ribosomal protein L27a



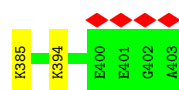
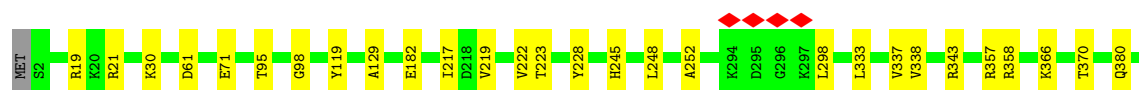
- Molecule 21: 60S ribosomal protein L28



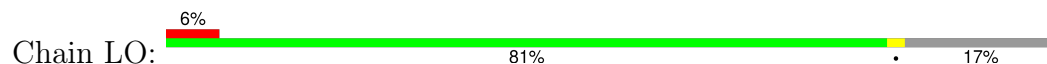
- Molecule 22: 60S ribosomal protein L29



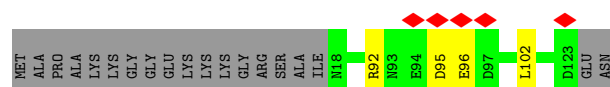
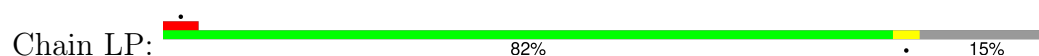
- Molecule 23: 60S ribosomal protein L3



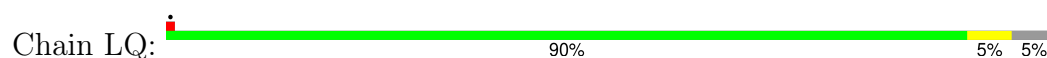
- Molecule 24: 60S ribosomal protein L30



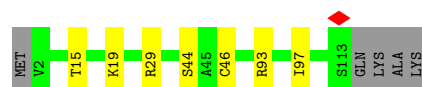
- Molecule 25: 60S ribosomal protein L31



- Molecule 26: 60S ribosomal protein L32



- Molecule 27: 60S ribosomal protein L34



- Molecule 28: 60S ribosomal protein L35





- Molecule 29: 60S ribosomal protein L35a

Chain LT: 97% ..



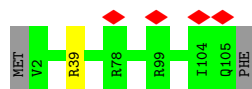
- Molecule 30: 60S ribosomal protein L36

Chain LU: 7% 90% 7% .



- Molecule 31: 60S ribosomal protein L36a

Chain LV: 97% ..



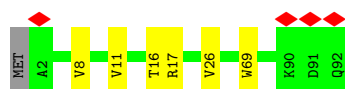
- Molecule 32: 60S ribosomal protein L37

Chain LW: 81% 7% 11%



- Molecule 33: 60S ribosomal protein L37a

Chain LX: 92% 7% .

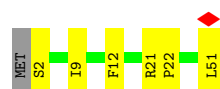


- Molecule 34: 60S ribosomal protein L38

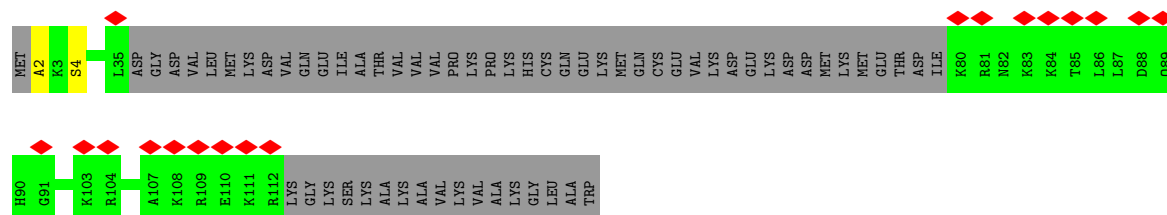
Chain LY: 6% 90% 9% .



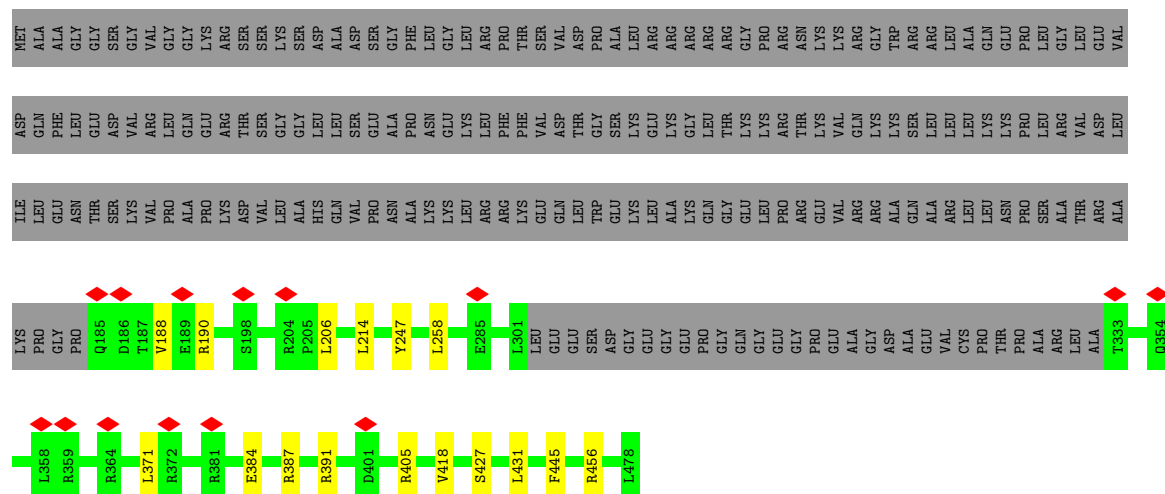
- Molecule 35: 60S ribosomal protein L39



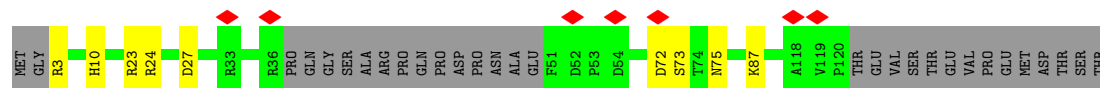
Chain NK: 



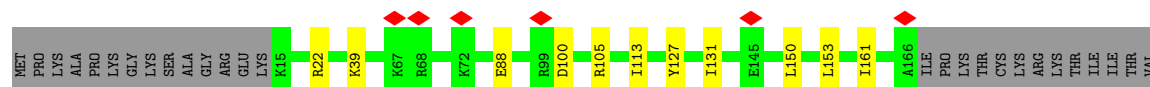
Chain NL: 



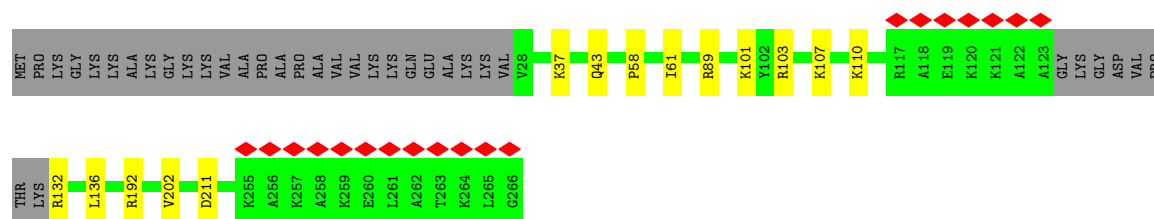
Chain NP: 



Chain NR: 







• Molecule 45: 60S ribosomal protein L8

Chain SF: 88% 7% 5%



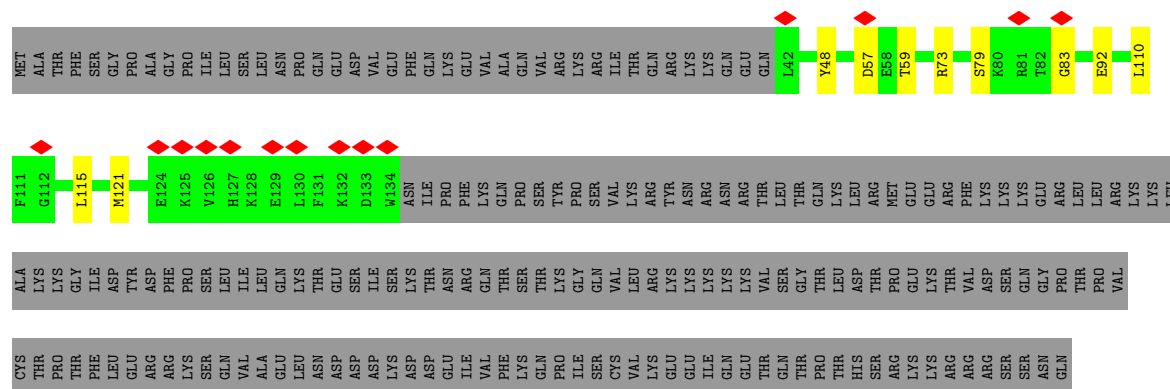
• Molecule 46: 60S ribosomal protein L9

Chain SG: 91% 8%



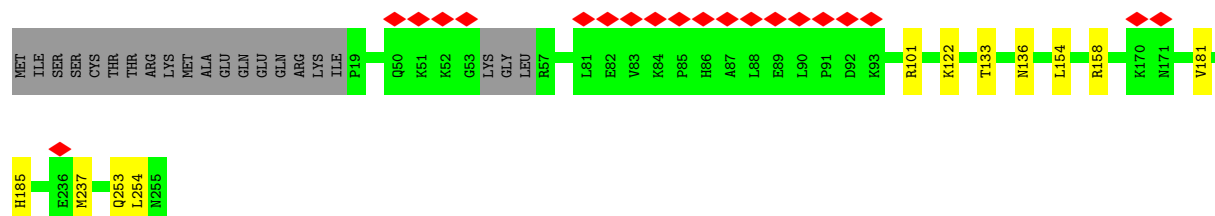
• Molecule 47: MKI67 FHA domain-interacting nucleolar phosphoprotein

Chain SH: 28% 5% 68%

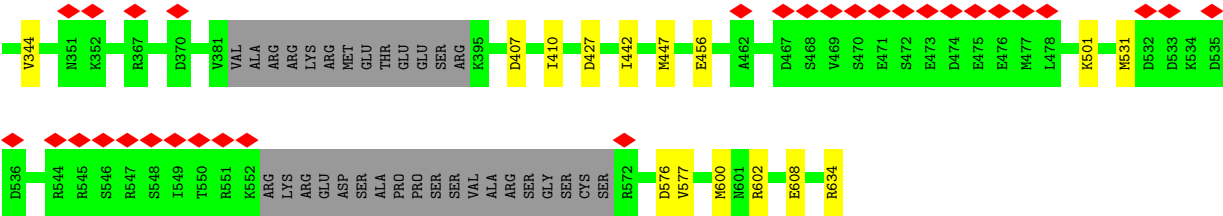


• Molecule 48: 60S ribosomal protein L7-like 1

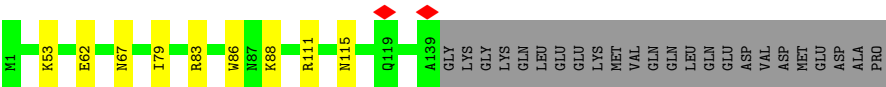
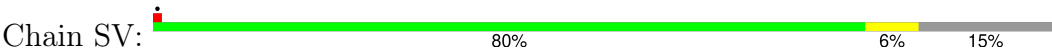
Chain SI: 87% 8% 8%



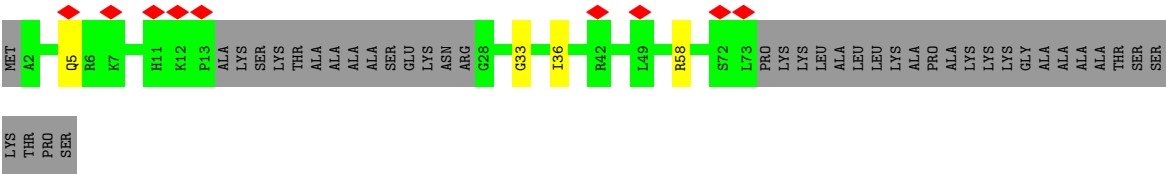
-



• Molecule 53: Probable ribosome biogenesis protein RLP24



• Molecule 54: Leydig cell tumor 10 kDa protein homolog



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 66157                                   | 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 ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 64000                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 10.877                                  | Depositor |
| Minimum map value                    | -0.003                                  | Depositor |
| Average map value                    | 0.055                                   | Depositor |
| Map value standard deviation         | 0.194                                   | Depositor |
| Recommended contour level            | 0.85                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 514.56, 514.56, 514.56                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.072, 1.072, 1.072                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, HIC, A2M, PTR, OMG, OMU, 1MA, 6MZ, UR3, GDP, ZN, MG, K, PSU

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   | BA    | 0.11         | 0/448       | 0.26        | 0/622       |
| 2   | L1    | 0.20         | 0/3589      | 0.26        | 0/5589      |
| 3   | L3    | 0.20         | 0/79642     | 0.28        | 0/124218    |
| 4   | L4    | 0.24         | 0/2861      | 0.29        | 0/4459      |
| 5   | L5    | 0.16         | 0/1372      | 0.29        | 0/1836      |
| 6   | L6    | 0.15         | 0/1732      | 0.28        | 0/2315      |
| 7   | L7    | 0.17         | 0/1682      | 0.30        | 0/2250      |
| 8   | L8    | 0.15         | 0/1133      | 0.27        | 0/1516      |
| 9   | L9    | 0.18         | 0/1746      | 0.31        | 0/2338      |
| 10  | LA    | 0.15         | 0/1268      | 0.32        | 0/1701      |
| 11  | LB    | 0.18         | 0/1536      | 0.33        | 0/2052      |
| 12  | LC    | 0.18         | 0/1501      | 0.32        | 0/2013      |
| 13  | LD    | 0.14         | 0/1305      | 0.24        | 0/1727      |
| 14  | LE    | 0.20         | 0/1291      | 0.34        | 0/1724      |
| 15  | LF    | 0.13         | 0/856       | 0.28        | 0/1149      |
| 16  | LG    | 0.17         | 0/1048      | 0.31        | 0/1402      |
| 17  | LH    | 0.14         | 0/1175      | 0.28        | 0/1572      |
| 18  | LI    | 0.16         | 0/1132      | 0.29        | 0/1504      |
| 19  | LJ    | 0.16         | 0/1130      | 0.26        | 0/1507      |
| 20  | LK    | 0.16         | 0/1191      | 0.29        | 0/1591      |
| 21  | LL    | 0.15         | 0/1017      | 0.28        | 0/1364      |
| 22  | LM    | 0.16         | 0/763       | 0.30        | 0/1005      |
| 23  | LN    | 0.16         | 0/3294      | 0.31        | 0/4406      |
| 24  | LO    | 0.11         | 0/748       | 0.23        | 0/1004      |
| 25  | LP    | 0.17         | 0/894       | 0.30        | 0/1204      |
| 26  | LQ    | 0.16         | 0/1071      | 0.28        | 0/1429      |
| 27  | LR    | 0.15         | 0/898       | 0.29        | 0/1197      |
| 28  | LS    | 0.13         | 0/1023      | 0.24        | 0/1351      |
| 29  | LT    | 0.16         | 0/895       | 0.30        | 0/1198      |
| 30  | LU    | 0.13         | 0/843       | 0.29        | 0/1115      |
| 31  | LV    | 0.18         | 0/864       | 0.33        | 0/1140      |
| 32  | LW    | 0.17         | 0/720       | 0.37        | 0/952       |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 33  | LX    | 0.13         | 0/718    | 0.28        | 0/953    |
| 34  | LY    | 0.12         | 0/575    | 0.24        | 0/761    |
| 35  | LZ    | 0.17         | 0/454    | 0.29        | 0/599    |
| 36  | NK    | 0.12         | 0/587    | 0.25        | 0/767    |
| 37  | NL    | 0.12         | 0/2207   | 0.25        | 0/2955   |
| 38  | NP    | 0.14         | 0/864    | 0.29        | 0/1154   |
| 39  | NR    | 0.12         | 0/1306   | 0.26        | 0/1740   |
| 40  | SA    | 0.17         | 0/2907   | 0.30        | 0/3905   |
| 41  | SB    | 0.17         | 0/2287   | 0.30        | 0/3065   |
| 42  | SC    | 0.14         | 0/1781   | 0.28        | 0/2388   |
| 43  | SD    | 0.16         | 0/1905   | 0.29        | 0/2539   |
| 44  | SE    | 0.16         | 0/1903   | 0.31        | 0/2559   |
| 45  | SF    | 0.16         | 0/1914   | 0.31        | 0/2567   |
| 46  | SG    | 0.15         | 0/1537   | 0.28        | 0/2066   |
| 47  | SH    | 0.12         | 0/794    | 0.26        | 0/1071   |
| 48  | SI    | 0.13         | 0/2003   | 0.26        | 0/2688   |
| 49  | SK    | 0.14         | 0/1877   | 0.31        | 0/2554   |
| 50  | SM    | 0.15         | 0/3357   | 0.27        | 0/4529   |
| 51  | SQ    | 0.11         | 0/648    | 0.29        | 0/894    |
| 52  | SR    | 0.14         | 0/5014   | 0.29        | 0/6727   |
| 53  | SV    | 0.18         | 0/1207   | 0.31        | 0/1600   |
| 54  | VB    | 0.11         | 0/459    | 0.28        | 0/605    |
| All | All   | 0.18         | 0/156972 | 0.28        | 0/229136 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | BA    | 449   | 0        | 207      | 0       | 0            |
| 2   | L1    | 3278  | 0        | 1665     | 17      | 0            |
| 3   | L3    | 73423 | 0        | 37192    | 281     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | L4    | 2561  | 0        | 1295     | 7       | 0            |
| 5   | L5    | 1349  | 0        | 1383     | 6       | 0            |
| 6   | L6    | 1701  | 0        | 1818     | 12      | 0            |
| 7   | L7    | 1650  | 0        | 1794     | 7       | 0            |
| 8   | L8    | 1111  | 0        | 1174     | 8       | 0            |
| 9   | L9    | 1701  | 0        | 1749     | 10      | 0            |
| 10  | LA    | 1242  | 0        | 1269     | 7       | 0            |
| 11  | LB    | 1512  | 0        | 1628     | 7       | 0            |
| 12  | LC    | 1461  | 0        | 1502     | 8       | 0            |
| 13  | LD    | 1289  | 0        | 1429     | 8       | 0            |
| 14  | LE    | 1264  | 0        | 1328     | 6       | 0            |
| 15  | LF    | 842   | 0        | 864      | 5       | 0            |
| 16  | LG    | 1034  | 0        | 1097     | 3       | 0            |
| 17  | LH    | 1156  | 0        | 1268     | 5       | 0            |
| 18  | LI    | 1115  | 0        | 1205     | 10      | 0            |
| 19  | LJ    | 1107  | 0        | 1182     | 8       | 0            |
| 20  | LK    | 1162  | 0        | 1213     | 7       | 0            |
| 21  | LL    | 1002  | 0        | 1068     | 6       | 0            |
| 22  | LM    | 751   | 0        | 820      | 8       | 0            |
| 23  | LN    | 3239  | 0        | 3377     | 24      | 0            |
| 24  | LO    | 738   | 0        | 774      | 1       | 0            |
| 25  | LP    | 879   | 0        | 924      | 2       | 0            |
| 26  | LQ    | 1053  | 0        | 1147     | 6       | 0            |
| 27  | LR    | 888   | 0        | 977      | 4       | 0            |
| 28  | LS    | 1015  | 0        | 1148     | 4       | 0            |
| 29  | LT    | 876   | 0        | 912      | 2       | 0            |
| 30  | LU    | 832   | 0        | 917      | 7       | 0            |
| 31  | LV    | 851   | 0        | 920      | 1       | 0            |
| 32  | LW    | 705   | 0        | 737      | 5       | 0            |
| 33  | LX    | 708   | 0        | 756      | 6       | 0            |
| 34  | LY    | 569   | 0        | 637      | 4       | 0            |
| 35  | LZ    | 444   | 0        | 483      | 5       | 0            |
| 36  | NK    | 581   | 0        | 656      | 2       | 0            |
| 37  | NL    | 2175  | 0        | 2235     | 14      | 0            |
| 38  | NP    | 847   | 0        | 854      | 7       | 0            |
| 39  | NR    | 1299  | 0        | 1318     | 7       | 0            |
| 40  | SA    | 2853  | 0        | 3028     | 24      | 0            |
| 41  | SB    | 2243  | 0        | 2268     | 9       | 0            |
| 42  | SC    | 1747  | 0        | 1897     | 17      | 0            |
| 43  | SD    | 1870  | 0        | 1996     | 8       | 0            |
| 44  | SE    | 1869  | 0        | 2014     | 11      | 0            |
| 45  | SF    | 1876  | 0        | 1970     | 14      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 46  | SG    | 1518   | 0        | 1601     | 10      | 0            |
| 47  | SH    | 773    | 0        | 755      | 5       | 0            |
| 48  | SI    | 1952   | 0        | 2086     | 7       | 0            |
| 49  | SK    | 1852   | 0        | 1828     | 11      | 0            |
| 50  | SM    | 3278   | 0        | 3332     | 20      | 0            |
| 51  | SQ    | 650    | 0        | 308      | 1       | 0            |
| 52  | SR    | 4932   | 0        | 5071     | 26      | 0            |
| 53  | SV    | 1184   | 0        | 1248     | 8       | 0            |
| 54  | VB    | 455    | 0        | 504      | 4       | 0            |
| 55  | L1    | 4      | 0        | 0        | 0       | 0            |
| 55  | L3    | 74     | 0        | 0        | 0       | 0            |
| 55  | L4    | 3      | 0        | 0        | 0       | 0            |
| 55  | LG    | 1      | 0        | 0        | 0       | 0            |
| 55  | LN    | 1      | 0        | 0        | 0       | 0            |
| 55  | LQ    | 1      | 0        | 0        | 0       | 0            |
| 55  | LR    | 1      | 0        | 0        | 0       | 0            |
| 55  | LT    | 1      | 0        | 0        | 0       | 0            |
| 55  | SF    | 1      | 0        | 0        | 0       | 0            |
| 55  | SR    | 1      | 0        | 0        | 0       | 0            |
| 56  | LR    | 1      | 0        | 0        | 0       | 0            |
| 56  | LV    | 1      | 0        | 0        | 0       | 0            |
| 56  | LW    | 1      | 0        | 0        | 0       | 0            |
| 56  | LX    | 1      | 0        | 0        | 0       | 0            |
| 56  | NP    | 1      | 0        | 0        | 0       | 0            |
| 56  | SV    | 1      | 0        | 0        | 0       | 0            |
| 57  | SR    | 28     | 0        | 12       | 0       | 0            |
| 58  | SR    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 149034 | 0        | 112840   | 529     | 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 2.

All (529) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:SA:109:ARG:O   | 40:SA:109:ARG:HG2 | 1.76                     | 0.86              |
| 3:L3:4156:G:OP2   | 3:L3:4157:A:O2'   | 1.97                     | 0.82              |
| 3:L3:1322:1MA:O2' | 3:L3:1323:A:O4'   | 1.94                     | 0.82              |
| 3:L3:1480:C:O2'   | 3:L3:1482:G:OP2   | 1.98                     | 0.81              |
| 4:L4:40:U:O2      | 5:L5:75:ARG:NH1   | 2.13                     | 0.81              |
| 3:L3:1931:C:N4    | 3:L3:2039:G:OP2   | 2.15                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L3:4768:G:OP1   | 7:L7:168:TYR:OH   | 2.00                     | 0.80              |
| 52:SR:600:MET:HE1 | 52:SR:608:GLU:HA  | 1.64                     | 0.79              |
| 2:L1:51:U:OP2     | 35:LZ:21:ARG:NH2  | 2.16                     | 0.79              |
| 3:L3:2520:C:O2    | 3:L3:2640:G:N2    | 2.15                     | 0.79              |
| 52:SR:456:GLU:OE1 | 53:SV:67:ASN:ND2  | 2.17                     | 0.78              |
| 3:L3:2848:G:O2'   | 3:L3:3838:U:O4    | 2.02                     | 0.78              |
| 3:L3:1397:A:O2'   | 3:L3:1467:C:O2'   | 2.02                     | 0.77              |
| 3:L3:1214:C:N4    | 22:LM:90:SER:O    | 2.18                     | 0.77              |
| 3:L3:2263:A:OP1   | 21:LL:107:ARG:NH2 | 2.18                     | 0.77              |
| 3:L3:4617:G:OP2   | 23:LN:358:ARG:NH2 | 2.18                     | 0.76              |
| 3:L3:2262:G:OP2   | 21:LL:98:ARG:NH1  | 2.17                     | 0.76              |
| 3:L3:4927:G:OP2   | 3:L3:4927:G:N2    | 2.16                     | 0.76              |
| 3:L3:2763:U:O2'   | 37:NL:391:ARG:NH2 | 2.19                     | 0.76              |
| 5:L5:120:ASP:OD2  | 5:L5:122:SER:OG   | 2.01                     | 0.76              |
| 3:L3:502:C:O2'    | 3:L3:503:C:OP1    | 2.03                     | 0.76              |
| 10:LA:115:GLU:OE2 | 10:LA:153:LYS:NZ  | 2.20                     | 0.75              |
| 3:L3:695:G:O2'    | 3:L3:697:G:OP2    | 2.04                     | 0.75              |
| 3:L3:222:C:OP2    | 40:SA:165:LYS:NZ  | 2.17                     | 0.75              |
| 3:L3:194:C:O2     | 18:LI:121:ARG:NH2 | 2.20                     | 0.75              |
| 3:L3:1853:G:O2'   | 3:L3:1854:G:OP2   | 2.04                     | 0.75              |
| 3:L3:2884:G:O2'   | 38:NP:75:ASN:ND2  | 2.18                     | 0.75              |
| 3:L3:1280:C:O2'   | 40:SA:321:ASN:OD1 | 2.04                     | 0.74              |
| 21:LL:66:ARG:NH1  | 21:LL:75:THR:O    | 2.20                     | 0.74              |
| 3:L3:2725:A:N6    | 13:LD:88:ARG:O    | 2.20                     | 0.74              |
| 14:LE:143:THR:OG1 | 14:LE:146:LYS:O   | 2.06                     | 0.74              |
| 3:L3:1177:U:OP2   | 3:L3:1180:C:N4    | 2.20                     | 0.74              |
| 19:LJ:30:ASP:O    | 19:LJ:39:SER:OG   | 2.04                     | 0.73              |
| 34:LY:27:LYS:NZ   | 34:LY:68:GLU:OE2  | 2.20                     | 0.73              |
| 3:L3:2545:U:O2'   | 3:L3:2547:G:N7    | 2.22                     | 0.73              |
| 7:L7:182:GLU:OE2  | 8:L8:119:ARG:NH2  | 2.22                     | 0.72              |
| 3:L3:4449:A:OP1   | 52:SR:118:LYS:NZ  | 2.21                     | 0.72              |
| 2:L1:75:OMG:OP2   | 18:LI:74:TYR:OH   | 2.06                     | 0.72              |
| 3:L3:1595:G:N2    | 52:SR:634:ARG:OXT | 2.19                     | 0.72              |
| 3:L3:1268:G:OP1   | 22:LM:107:ARG:NH1 | 2.23                     | 0.71              |
| 3:L3:935:A:O2'    | 8:L8:46:ARG:NH1   | 2.23                     | 0.71              |
| 3:L3:4691:A:OP1   | 46:SG:71:ARG:NH1  | 2.23                     | 0.71              |
| 48:SI:133:THR:OG1 | 48:SI:136:ASN:OD1 | 2.08                     | 0.71              |
| 3:L3:151:G:OP1    | 9:L9:49:ARG:NH2   | 2.24                     | 0.70              |
| 47:SH:73:ARG:NE   | 47:SH:92:GLU:OE1  | 2.24                     | 0.70              |
| 3:L3:295:A:OP2    | 31:LV:39:ARG:NH1  | 2.25                     | 0.70              |
| 3:L3:1508:A:OP1   | 40:SA:110:ARG:NH2 | 2.25                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L3:1880:G:OP1   | 3:L3:1882:U:O2'   | 2.09                     | 0.70              |
| 3:L3:4633:G:O2'   | 3:L3:4635:A:OP2   | 2.05                     | 0.70              |
| 3:L3:2843:U:O2'   | 3:L3:4632:U:OP1   | 2.10                     | 0.70              |
| 3:L3:1187:G:OP2   | 3:L3:1187:G:N2    | 2.24                     | 0.70              |
| 23:LN:357:ARG:NE  | 52:SR:407:ASP:OD1 | 2.24                     | 0.69              |
| 3:L3:1881:C:O2'   | 3:L3:1882:U:OP2   | 2.10                     | 0.69              |
| 3:L3:1518:A:OP1   | 20:LK:27:LYS:NZ   | 2.22                     | 0.69              |
| 3:L3:4471:PSU:OP1 | 46:SG:168:LYS:NZ  | 2.20                     | 0.69              |
| 20:LK:77:LYS:O    | 20:LK:80:THR:OG1  | 2.10                     | 0.68              |
| 3:L3:3838:U:OP2   | 38:NP:23:ARG:NH2  | 2.25                     | 0.68              |
| 42:SC:145:THR:OG1 | 42:SC:200:LYS:NZ  | 2.23                     | 0.68              |
| 3:L3:4717:A:OP2   | 23:LN:30:LYS:NZ   | 2.26                     | 0.68              |
| 3:L3:1889:U:OP1   | 29:LT:19:ARG:NH1  | 2.26                     | 0.68              |
| 37:NL:384:GLU:OE1 | 37:NL:387:ARG:NH2 | 2.26                     | 0.68              |
| 9:L9:17:ASP:OD1   | 9:L9:20:ARG:NH2   | 2.26                     | 0.68              |
| 3:L3:3614:G:O6    | 38:NP:87:LYS:NZ   | 2.27                     | 0.67              |
| 16:LG:42:VAL:CG1  | 16:LG:45:ILE:HD12 | 2.24                     | 0.67              |
| 3:L3:3718:A2M:H2  | 3:L3:3934:G:O4'   | 1.95                     | 0.67              |
| 3:L3:4476:C:O2'   | 46:SG:173:ARG:NH2 | 2.28                     | 0.67              |
| 3:L3:151:G:OP2    | 9:L9:4:TYR:OH     | 2.12                     | 0.67              |
| 24:LO:50:ASN:ND2  | 24:LO:75:SER:O    | 2.27                     | 0.67              |
| 4:L4:12:U:O3'     | 4:L4:109:U:O2'    | 2.09                     | 0.66              |
| 3:L3:4765:G:OP1   | 46:SG:23:ARG:NE   | 2.28                     | 0.66              |
| 49:SK:99:GLU:OE1  | 49:SK:125:THR:OG1 | 2.06                     | 0.66              |
| 3:L3:1814:C:O2'   | 22:LM:42:ASN:OD1  | 2.08                     | 0.66              |
| 3:L3:2522:G:OP2   | 27:LR:29:ARG:NH2  | 2.28                     | 0.66              |
| 3:L3:453:G:H1     | 3:L3:1293:G:H22   | 1.41                     | 0.66              |
| 15:LF:74:SER:OG   | 15:LF:76:VAL:O    | 2.14                     | 0.66              |
| 3:L3:4546:A:N7    | 45:SF:215:ASN:ND2 | 2.44                     | 0.66              |
| 4:L4:117:G:OP1    | 41:SB:253:TYR:OH  | 2.09                     | 0.66              |
| 3:L3:2487:G:OP1   | 37:NL:456:ARG:NH2 | 2.29                     | 0.66              |
| 7:L7:189:ILE:HD11 | 8:L8:119:ARG:HG3  | 1.77                     | 0.66              |
| 3:L3:67:C:OP2     | 3:L3:312:G:N2     | 2.28                     | 0.66              |
| 30:LU:50:PHE:O    | 30:LU:55:ARG:NH1  | 2.28                     | 0.66              |
| 44:SE:101:LYS:NZ  | 44:SE:211:ASP:OD1 | 2.24                     | 0.66              |
| 3:L3:4435:U:OP2   | 3:L3:4436:U:O2'   | 2.08                     | 0.65              |
| 3:L3:508:G:O2'    | 3:L3:510:U:OP2    | 2.06                     | 0.65              |
| 3:L3:2841:G:OP1   | 38:NP:10:HIS:NE2  | 2.30                     | 0.65              |
| 19:LJ:5:MET:HE3   | 19:LJ:25:ILE:HD11 | 1.79                     | 0.65              |
| 3:L3:2480:G:OP1   | 50:SM:22:LYS:NZ   | 2.29                     | 0.65              |
| 2:L1:62:A:OP1     | 28:LS:52:LYS:NZ   | 2.29                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:LK:38:LEU:O     | 20:LK:42:ARG:NH1   | 2.29                     | 0.65              |
| 12:LC:84:TYR:CE1   | 12:LC:93:MET:HE3   | 2.32                     | 0.65              |
| 3:L3:4117:U:O4'    | 44:SE:43:GLN:NE2   | 2.30                     | 0.65              |
| 3:L3:4305:G:O2'    | 3:L3:4306:OMU:O5'  | 2.15                     | 0.64              |
| 3:L3:725:G:OP2     | 40:SA:350:ARG:NH2  | 2.31                     | 0.64              |
| 3:L3:1238:A:O2'    | 43:SD:52:GLU:OE2   | 2.15                     | 0.64              |
| 3:L3:1621:A:OP2    | 32:LW:30:GLN:NE2   | 2.30                     | 0.64              |
| 50:SM:337:GLU:OE1  | 50:SM:380:ARG:NH2  | 2.29                     | 0.64              |
| 3:L3:369:G:N2      | 3:L3:372:A:OP2     | 2.27                     | 0.64              |
| 3:L3:121:A:OP1     | 44:SE:110:LYS:NZ   | 2.26                     | 0.64              |
| 11:LB:122:THR:OG1  | 11:LB:124:ASP:OD1  | 2.15                     | 0.64              |
| 3:L3:119:G:O4'     | 44:SE:132:ARG:NH1  | 2.30                     | 0.64              |
| 3:L3:4688:C:O2'    | 46:SG:155:SER:OG   | 2.03                     | 0.64              |
| 49:SK:95:ARG:HG3   | 49:SK:132:VAL:HG21 | 1.79                     | 0.64              |
| 3:L3:408:A:O2'     | 3:L3:411:G:OP2     | 2.16                     | 0.63              |
| 3:L3:1433:A:N6     | 3:L3:1451:G:O2'    | 2.32                     | 0.63              |
| 3:L3:4536:OMC:HM22 | 3:L3:4537:C:O4'    | 1.98                     | 0.63              |
| 3:L3:1071:C:O2     | 42:SC:70:LYS:NZ    | 2.27                     | 0.63              |
| 3:L3:1573:G:OP1    | 13:LD:92:LYS:NZ    | 2.30                     | 0.63              |
| 3:L3:3776:G:OP2    | 3:L3:3776:G:N2     | 2.26                     | 0.63              |
| 3:L3:4620:OMU:OP2  | 3:L3:4670:C:N4     | 2.32                     | 0.63              |
| 3:L3:489:C:O2'     | 3:L3:667:A:N6      | 2.31                     | 0.63              |
| 3:L3:1957:U:OP2    | 39:NR:105:ARG:NH2  | 2.31                     | 0.63              |
| 49:SK:121:LEU:O    | 49:SK:139:ARG:NH1  | 2.32                     | 0.63              |
| 12:LC:84:TYR:HE1   | 12:LC:93:MET:HE3   | 1.63                     | 0.63              |
| 7:L7:202:LEU:O     | 7:L7:202:LEU:HD23  | 1.98                     | 0.63              |
| 8:L8:135:LEU:HD12  | 8:L8:136:LEU:HD12  | 1.80                     | 0.62              |
| 3:L3:2318:G:N2     | 3:L3:2321:G:OP2    | 2.24                     | 0.62              |
| 3:L3:4220:6MZ:O2'  | 3:L3:4222:G:OP1    | 2.09                     | 0.62              |
| 46:SG:103:VAL:HG11 | 46:SG:144:LEU:HD21 | 1.80                     | 0.62              |
| 50:SM:33:ASP:OD1   | 50:SM:36:ARG:NH2   | 2.32                     | 0.62              |
| 3:L3:4524:G:C2     | 23:LN:252:ALA:HB1  | 2.35                     | 0.62              |
| 41:SB:76:CYS:SG    | 41:SB:112:ARG:NH1  | 2.72                     | 0.62              |
| 10:LA:124:LYS:O    | 52:SR:602:ARG:NH1  | 2.33                     | 0.62              |
| 3:L3:62:A:OP1      | 9:L9:169:ARG:NH1   | 2.32                     | 0.61              |
| 3:L3:1255:A:OP1    | 3:L3:1257:A:N6     | 2.33                     | 0.61              |
| 3:L3:3700:C:O2'    | 3:L3:3774:A:N3     | 2.32                     | 0.61              |
| 6:L6:129:ARG:NH1   | 28:LS:116:LEU:O    | 2.34                     | 0.61              |
| 16:LG:42:VAL:HG13  | 16:LG:45:ILE:HD12  | 1.82                     | 0.61              |
| 3:L3:2414:G:O2'    | 3:L3:2415:OMU:H5'' | 2.01                     | 0.61              |
| 4:L4:6:C:O2'       | 41:SB:50:ARG:NH2   | 2.33                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L3:458:C:OP2     | 42:SC:114:ARG:NH1  | 2.34                     | 0.61              |
| 23:LN:71:GLU:OE2   | 23:LN:366:LYS:NZ   | 2.29                     | 0.60              |
| 23:LN:219:VAL:HG11 | 23:LN:337:VAL:HG21 | 1.83                     | 0.60              |
| 37:NL:427:SER:OG   | 50:SM:379:ASP:OD1  | 2.19                     | 0.60              |
| 42:SC:281:ILE:CG2  | 42:SC:286:LEU:HD11 | 2.31                     | 0.60              |
| 42:SC:161:ARG:O    | 42:SC:182:ASN:ND2  | 2.34                     | 0.60              |
| 3:L3:1369:C:OP2    | 3:L3:1370:G:O2'    | 2.09                     | 0.60              |
| 3:L3:4623:OMG:OP1  | 23:LN:19:ARG:NH2   | 2.34                     | 0.60              |
| 52:SR:176:TYR:CE1  | 52:SR:271:LEU:HD22 | 2.37                     | 0.60              |
| 3:L3:122:U:O4      | 44:SE:107:LYS:NZ   | 2.28                     | 0.60              |
| 45:SF:107:MET:HB3  | 45:SF:111:THR:HG21 | 1.82                     | 0.60              |
| 3:L3:2258:C:N3     | 42:SC:90:ALA:N     | 2.50                     | 0.60              |
| 39:NR:131:ILE:HG21 | 39:NR:161:ILE:HD12 | 1.82                     | 0.60              |
| 3:L3:2876:OMG:HM22 | 3:L3:2877:G:H5'    | 1.84                     | 0.59              |
| 3:L3:5002:U:OP2    | 23:LN:385:LYS:NZ   | 2.24                     | 0.59              |
| 3:L3:2616:C:OP1    | 13:LD:60:ARG:NH1   | 2.35                     | 0.59              |
| 3:L3:2695:A:OP1    | 34:LY:35:LYS:NZ    | 2.36                     | 0.59              |
| 23:LN:219:VAL:HG11 | 23:LN:337:VAL:CG2  | 2.33                     | 0.59              |
| 3:L3:4580:U:O2'    | 23:LN:182:GLU:OE2  | 2.18                     | 0.58              |
| 50:SM:383:GLN:NE2  | 50:SM:384:GLN:O    | 2.37                     | 0.58              |
| 3:L3:4220:6MZ:OP2  | 3:L3:4220:6MZ:H8   | 2.03                     | 0.58              |
| 6:L6:62:PRO:O      | 6:L6:63:THR:OG1    | 2.18                     | 0.58              |
| 3:L3:4124:G:N2     | 44:SE:43:GLN:O     | 2.36                     | 0.58              |
| 23:LN:217:ILE:HD11 | 23:LN:333:LEU:HD21 | 1.84                     | 0.58              |
| 3:L3:2922:G:O2'    | 3:L3:3275:A:N6     | 2.37                     | 0.58              |
| 3:L3:1269:G:OP2    | 22:LM:107:ARG:NH2  | 2.36                     | 0.57              |
| 3:L3:1497:A:N7     | 11:LB:180:ARG:NH1  | 2.51                     | 0.57              |
| 2:L1:83:C:H42      | 18:LI:50:ARG:NE    | 2.02                     | 0.57              |
| 23:LN:95:THR:OG1   | 23:LN:98:GLY:O     | 2.19                     | 0.57              |
| 50:SM:267:LEU:O    | 50:SM:271:SER:N    | 2.38                     | 0.57              |
| 3:L3:1241:C:OP2    | 42:SC:72:LYS:NZ    | 2.37                     | 0.57              |
| 3:L3:1534:A2M:HM'3 | 3:L3:1637:A:C4     | 2.40                     | 0.57              |
| 41:SB:119:TYR:OH   | 41:SB:139:PRO:O    | 2.18                     | 0.57              |
| 3:L3:63:G:OP2      | 9:L9:169:ARG:NH2   | 2.35                     | 0.56              |
| 48:SI:253:GLN:O    | 50:SM:149:ARG:NH1  | 2.37                     | 0.56              |
| 37:NL:445:PHE:HD2  | 50:SM:220:MET:HE1  | 1.71                     | 0.56              |
| 47:SH:48:TYR:HB2   | 47:SH:121:MET:HE3  | 1.87                     | 0.56              |
| 3:L3:1498:G:OP1    | 11:LB:150:ARG:NH1  | 2.38                     | 0.56              |
| 6:L6:7:GLY:O       | 20:LK:49:HIS:NE2   | 2.36                     | 0.56              |
| 3:L3:442:G:OP1     | 29:LT:68:ARG:NH1   | 2.38                     | 0.56              |
| 3:L3:4635:A:H3'    | 3:L3:4636:PSU:H4'  | 1.87                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:SG:87:GLY:O     | 46:SG:186:THR:OG1  | 2.17                     | 0.56              |
| 48:SI:158:ARG:NH2  | 50:SM:360:LEU:O    | 2.39                     | 0.55              |
| 3:L3:2579:G:N2     | 3:L3:2582:A:OP2    | 2.31                     | 0.55              |
| 51:SQ:121:GLU:O    | 51:SQ:200:PHE:N    | 2.39                     | 0.55              |
| 3:L3:4500:PSU:H2'  | 3:L3:4501:U:C6     | 2.41                     | 0.55              |
| 3:L3:1238:A:OP2    | 42:SC:60:SER:OG    | 2.12                     | 0.55              |
| 3:L3:1577:G:OP1    | 33:LX:17:ARG:NH2   | 2.40                     | 0.55              |
| 46:SG:41:ILE:HG22  | 46:SG:43:VAL:HG13  | 1.88                     | 0.55              |
| 23:LN:223:THR:HG22 | 23:LN:338:VAL:HG13 | 1.88                     | 0.55              |
| 2:L1:156:U:OP2     | 44:SE:89:ARG:NH2   | 2.39                     | 0.55              |
| 3:L3:496:G:O2'     | 3:L3:497:G:OP1     | 2.24                     | 0.55              |
| 52:SR:233:ARG:HB2  | 52:SR:238:MET:HE3  | 1.89                     | 0.55              |
| 52:SR:427:ASP:OD2  | 53:SV:83:ARG:NH1   | 2.40                     | 0.55              |
| 3:L3:2351:OMC:HM22 | 3:L3:2352:U:H5'    | 1.89                     | 0.54              |
| 3:L3:156:G:OP2     | 28:LS:109:ARG:NH2  | 2.40                     | 0.54              |
| 33:LX:26:VAL:HG21  | 45:SF:180:LEU:HD11 | 1.88                     | 0.54              |
| 53:SV:53:LYS:NZ    | 53:SV:62:GLU:OE1   | 2.35                     | 0.54              |
| 37:NL:258:LEU:HD23 | 37:NL:418:VAL:HG11 | 1.89                     | 0.54              |
| 40:SA:109:ARG:O    | 40:SA:109:ARG:CG   | 2.54                     | 0.54              |
| 3:L3:1943:A:C2     | 54:VB:36:ILE:HD12  | 2.42                     | 0.54              |
| 3:L3:5022:U:HO2'   | 3:L3:5023:C:P      | 2.31                     | 0.54              |
| 21:LL:20:ARG:NH1   | 26:LQ:78:LEU:O     | 2.41                     | 0.54              |
| 3:L3:5000:G:OP1    | 23:LN:394:LYS:NZ   | 2.36                     | 0.54              |
| 17:LH:119:ILE:HD12 | 17:LH:140:LEU:CD2  | 2.39                     | 0.53              |
| 3:L3:2351:OMC:HM23 | 40:SA:95:MET:HG3   | 1.90                     | 0.53              |
| 3:L3:2562:G:O2'    | 3:L3:2565:A:N6     | 2.42                     | 0.53              |
| 3:L3:4587:G:OP1    | 7:L7:61:ARG:NH1    | 2.41                     | 0.53              |
| 17:LH:82:THR:O     | 17:LH:82:THR:HG22  | 2.08                     | 0.53              |
| 3:L3:3868:G:O2'    | 3:L3:3869:OMC:H5'' | 2.09                     | 0.53              |
| 33:LX:8:VAL:O      | 33:LX:11:VAL:HG22  | 2.09                     | 0.53              |
| 40:SA:193:LYS:HD2  | 40:SA:196:MET:HE2  | 1.89                     | 0.53              |
| 3:L3:309:C:OP2     | 30:LU:32:ARG:NH1   | 2.42                     | 0.53              |
| 40:SA:325:MET:HE1  | 43:SD:155:TYR:CZ   | 2.44                     | 0.53              |
| 3:L3:1437:C:O2'    | 3:L3:1438:U:O4'    | 2.25                     | 0.53              |
| 3:L3:4126:C:OP1    | 44:SE:37:LYS:NZ    | 2.29                     | 0.53              |
| 3:L3:4591:U:OP1    | 36:NK:4:SER:OG     | 2.22                     | 0.53              |
| 41:SB:191:ASN:OD1  | 41:SB:194:VAL:HG23 | 2.09                     | 0.53              |
| 3:L3:3717:A:N3     | 3:L3:4178:A:O2'    | 2.39                     | 0.53              |
| 3:L3:3734:PSU:H2'  | 3:L3:3735:G:O4'    | 2.09                     | 0.53              |
| 50:SM:189:TYR:CZ   | 50:SM:202:ILE:HD12 | 2.44                     | 0.53              |
| 45:SF:65:ASP:OD2   | 45:SF:72:ARG:NE    | 2.41                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:SR:447:MET:HE3  | 53:SV:88:LYS:HG3   | 1.91                     | 0.52              |
| 3:L3:158:A:N1      | 3:L3:276:C:O2'     | 2.37                     | 0.52              |
| 3:L3:1321:G:O2'    | 3:L3:1322:1MA:H5'  | 2.09                     | 0.52              |
| 3:L3:3715:PSU:H2'  | 3:L3:3716:C:O4'    | 2.08                     | 0.52              |
| 16:LG:42:VAL:HG11  | 16:LG:45:ILE:HD12  | 1.90                     | 0.52              |
| 40:SA:193:LYS:CD   | 40:SA:196:MET:HE2  | 2.38                     | 0.52              |
| 48:SI:181:VAL:O    | 48:SI:185:HIS:ND1  | 2.42                     | 0.52              |
| 3:L3:4088:C:OP1    | 45:SF:37:ARG:NH2   | 2.41                     | 0.52              |
| 37:NL:445:PHE:CD2  | 50:SM:220:MET:HE1  | 2.45                     | 0.52              |
| 42:SC:91:THR:OG1   | 42:SC:106:VAL:HG22 | 2.09                     | 0.52              |
| 54:VB:5:GLN:OE1    | 54:VB:5:GLN:N      | 2.40                     | 0.52              |
| 3:L3:400:A2M:H1'   | 10:LA:101:ASN:ND2  | 2.25                     | 0.52              |
| 3:L3:937:U:OP1     | 8:L8:46:ARG:NH1    | 2.43                     | 0.52              |
| 3:L3:2363:A2M:H2'  | 3:L3:2364:OMG:O4'  | 2.09                     | 0.52              |
| 3:L3:4593:C:OP2    | 36:NK:2:ALA:N      | 2.43                     | 0.52              |
| 11:LB:22:ASP:OD2   | 40:SA:283:LYS:NZ   | 2.34                     | 0.52              |
| 52:SR:174:CYS:SG   | 52:SR:244:LEU:HD21 | 2.50                     | 0.52              |
| 18:LI:34:LEU:HD22  | 18:LI:44:VAL:HG23  | 1.92                     | 0.52              |
| 3:L3:1548:G:O2'    | 3:L3:2812:A:N3     | 2.36                     | 0.52              |
| 4:L4:55:A:O2'      | 5:L5:151:ILE:O     | 2.22                     | 0.52              |
| 33:LX:69:TRP:NE1   | 45:SF:173:GLY:O    | 2.41                     | 0.52              |
| 38:NP:72:ASP:OD1   | 38:NP:73:SER:N     | 2.40                     | 0.51              |
| 2:L1:83:C:N3       | 18:LI:50:ARG:NH2   | 2.57                     | 0.51              |
| 3:L3:5039:U:O2'    | 53:SV:115:ASN:OD1  | 2.26                     | 0.51              |
| 3:L3:4208:U:OP1    | 3:L3:4334:U:O2'    | 2.24                     | 0.51              |
| 14:LE:83:LYS:HE2   | 14:LE:85:LEU:HD21  | 1.93                     | 0.51              |
| 3:L3:4296:PSU:H2'  | 3:L3:4297:G:O4'    | 2.11                     | 0.51              |
| 52:SR:269:LEU:HD22 | 52:SR:306:ILE:HG23 | 1.93                     | 0.51              |
| 3:L3:5047:C:O2'    | 3:L3:5050:C:OP2    | 2.23                     | 0.51              |
| 15:LF:67:LYS:O     | 15:LF:68:SER:OG    | 2.27                     | 0.51              |
| 52:SR:39:GLN:OE1   | 52:SR:41:HIS:NE2   | 2.36                     | 0.51              |
| 3:L3:1173:G:N2     | 3:L3:1188:C:N3     | 2.59                     | 0.51              |
| 3:L3:2043:A:N1     | 3:L3:4515:G:O2'    | 2.44                     | 0.51              |
| 6:L6:146:LEU:HD12  | 6:L6:146:LEU:O     | 2.11                     | 0.51              |
| 7:L7:190:ASP:OD1   | 7:L7:191:LYS:N     | 2.44                     | 0.51              |
| 26:LQ:26:ASP:OD1   | 26:LQ:27:ARG:N     | 2.44                     | 0.51              |
| 3:L3:4515:G:OP1    | 52:SR:49:ARG:NH1   | 2.43                     | 0.50              |
| 11:LB:89:ASP:O     | 11:LB:112:ARG:NH1  | 2.44                     | 0.50              |
| 3:L3:2815:A2M:H2'  | 3:L3:2816:G:C8     | 2.46                     | 0.50              |
| 13:LD:126:LYS:O    | 13:LD:131:VAL:HG12 | 2.12                     | 0.50              |
| 9:L9:126:THR:HG23  | 9:L9:127:TYR:CD2   | 2.46                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:LM:99:ILE:O    | 22:LM:109:ARG:NH1  | 2.44                     | 0.50              |
| 2:L1:74:U:O4      | 18:LI:72:GLN:NE2   | 2.42                     | 0.50              |
| 3:L3:2626:U:OP2   | 52:SR:501:LYS:NZ   | 2.38                     | 0.50              |
| 3:L3:5022:U:O2'   | 3:L3:5023:C:OP2    | 2.26                     | 0.50              |
| 42:SC:99:ASP:OD1  | 42:SC:100:LYS:N    | 2.44                     | 0.50              |
| 48:SI:101:ARG:NH1 | 48:SI:122:LYS:O    | 2.44                     | 0.50              |
| 3:L3:3887:OMC:H6  | 3:L3:3887:OMC:H5'  | 1.77                     | 0.50              |
| 50:SM:59:THR:HG22 | 50:SM:59:THR:O     | 2.12                     | 0.49              |
| 2:L1:152:U:OP1    | 3:L3:4162:C:N4     | 2.45                     | 0.49              |
| 3:L3:2407:G:O6    | 35:LZ:2:SER:N      | 2.45                     | 0.49              |
| 34:LY:17:ARG:NH2  | 34:LY:19:ASP:OD2   | 2.42                     | 0.49              |
| 15:LF:33:ILE:HG22 | 52:SR:531:MET:HE1  | 1.93                     | 0.49              |
| 3:L3:62:A:N3      | 3:L3:77:U:O2'      | 2.39                     | 0.49              |
| 3:L3:2380:G:N2    | 3:L3:2424:OMG:H5'' | 2.28                     | 0.49              |
| 3:L3:3938:G:N2    | 3:L3:4171:C:OP2    | 2.39                     | 0.49              |
| 50:SM:274:GLU:HB3 | 50:SM:362:ILE:HD12 | 1.94                     | 0.49              |
| 3:L3:216:C:OP1    | 3:L3:219:G:O2'     | 2.25                     | 0.49              |
| 3:L3:1314:C:O2'   | 26:LQ:24:GLN:NE2   | 2.46                     | 0.49              |
| 3:L3:2876:OMG:C8  | 33:LX:16:THR:HG22  | 2.47                     | 0.49              |
| 19:LJ:29:ILE:O    | 19:LJ:31:ASP:N     | 2.45                     | 0.49              |
| 27:LR:15:THR:O    | 27:LR:19:LYS:NZ    | 2.46                     | 0.49              |
| 42:SC:244:GLU:O   | 42:SC:248:ILE:HD12 | 2.13                     | 0.49              |
| 3:L3:2438:A:O2'   | 3:L3:2440:U:OP2    | 2.28                     | 0.49              |
| 3:L3:3920:PSU:H2' | 3:L3:3921:U:C6     | 2.48                     | 0.49              |
| 3:L3:1677:PSU:H4' | 3:L3:1680:G:C2     | 2.48                     | 0.49              |
| 6:L6:63:THR:HG21  | 20:LK:66:ASN:HB3   | 1.94                     | 0.49              |
| 3:L3:1523:A:O2'   | 3:L3:1524:A2M:H5'  | 2.13                     | 0.48              |
| 3:L3:2487:G:OP2   | 50:SM:152:LYS:NZ   | 2.36                     | 0.48              |
| 3:L3:4252:C:OP2   | 3:L3:4253:A:O2'    | 2.23                     | 0.48              |
| 3:L3:2758:G:OP1   | 37:NL:405:ARG:NH2  | 2.46                     | 0.48              |
| 3:L3:5023:C:OP2   | 3:L3:5025:C:N4     | 2.47                     | 0.48              |
| 9:L9:115:VAL:HG22 | 9:L9:134:LEU:CD2   | 2.43                     | 0.48              |
| 32:LW:48:ASN:OD1  | 32:LW:54:LYS:NZ    | 2.30                     | 0.48              |
| 35:LZ:9:ILE:HG23  | 35:LZ:51:LEU:HD21  | 1.95                     | 0.48              |
| 39:NR:150:LEU:HA  | 39:NR:153:LEU:HD13 | 1.95                     | 0.48              |
| 2:L1:69:PSU:H2'   | 2:L1:70:G:O4'      | 2.13                     | 0.48              |
| 3:L3:1627:G:O6    | 45:SF:3:ARG:NH2    | 2.46                     | 0.48              |
| 3:L3:2296:G:O2'   | 40:SA:242:PRO:O    | 2.31                     | 0.48              |
| 6:L6:100:PRO:O    | 30:LU:25:ARG:NH2   | 2.45                     | 0.48              |
| 13:LD:114:LYS:O   | 13:LD:146:LYS:NZ   | 2.46                     | 0.48              |
| 3:L3:3641:U:OP2   | 3:L3:3646:A:N6     | 2.40                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:LC:173:ASN:ND2  | 12:LC:175:PHE:O    | 2.47                     | 0.48              |
| 37:NL:190:ARG:NH2  | 50:SM:117:ASP:OD1  | 2.45                     | 0.48              |
| 11:LB:34:PHE:CD2   | 40:SA:293:LEU:HD22 | 2.48                     | 0.48              |
| 46:SG:113:GLU:OE1  | 46:SG:115:ARG:NH2  | 2.46                     | 0.48              |
| 2:L1:71:A:N1       | 2:L1:81:C:O2'      | 2.47                     | 0.48              |
| 12:LC:15:ARG:HB3   | 12:LC:27:LEU:HD23  | 1.95                     | 0.48              |
| 52:SR:128:GLN:OE1  | 54:VB:58:ARG:NE    | 2.42                     | 0.48              |
| 3:L3:1952:G:OP1    | 12:LC:139:ARG:NE   | 2.47                     | 0.48              |
| 3:L3:4670:C:O2'    | 3:L3:4672:A:OP2    | 2.30                     | 0.48              |
| 9:L9:124:ASP:OD1   | 9:L9:125:SER:N     | 2.44                     | 0.48              |
| 41:SB:62:CYS:HB3   | 41:SB:105:LEU:HD22 | 1.96                     | 0.48              |
| 52:SR:257:LEU:O    | 52:SR:294:LYS:NZ   | 2.44                     | 0.48              |
| 3:L3:2809:G:O2'    | 3:L3:4644:G:OP1    | 2.30                     | 0.47              |
| 46:SG:12:ILE:HG12  | 46:SG:18:ILE:HD12  | 1.94                     | 0.47              |
| 3:L3:366:A:N1      | 40:SA:84:THR:HG22  | 2.29                     | 0.47              |
| 3:L3:2590:G:O2'    | 3:L3:2755:A:N6     | 2.43                     | 0.47              |
| 50:SM:265:TYR:HB3  | 50:SM:362:ILE:HD11 | 1.97                     | 0.47              |
| 3:L3:4139:G:H21    | 3:L3:4140:C:N4     | 2.12                     | 0.47              |
| 3:L3:2303:C:OP1    | 26:LQ:107:ASN:ND2  | 2.47                     | 0.47              |
| 42:SC:180:VAL:HG23 | 42:SC:181:LEU:HD12 | 1.97                     | 0.47              |
| 3:L3:398:A2M:O5'   | 3:L3:398:A2M:H8    | 2.15                     | 0.47              |
| 25:LP:95:ASP:OD1   | 25:LP:96:GLU:N     | 2.47                     | 0.47              |
| 3:L3:305:A:OP1     | 30:LU:76:ARG:NH1   | 2.48                     | 0.47              |
| 3:L3:352:G:C6      | 40:SA:196:MET:HE3  | 2.50                     | 0.47              |
| 3:L3:2562:G:N2     | 3:L3:2565:A:OP2    | 2.44                     | 0.47              |
| 3:L3:2639:U:O2'    | 3:L3:2694:G:O6     | 2.27                     | 0.47              |
| 3:L3:4085:A:OP2    | 17:LH:45:THR:HG22  | 2.14                     | 0.47              |
| 12:LC:95:ARG:NH2   | 12:LC:112:ASP:OD2  | 2.41                     | 0.47              |
| 19:LJ:5:MET:HE3    | 19:LJ:25:ILE:CD1   | 2.45                     | 0.47              |
| 2:L1:84:A:N7       | 18:LI:113:LYS:NZ   | 2.53                     | 0.47              |
| 3:L3:1895:G:OP1    | 43:SD:96:ARG:NH2   | 2.48                     | 0.47              |
| 10:LA:6:LEU:HD12   | 10:LA:116:HIS:CD2  | 2.50                     | 0.47              |
| 3:L3:25:A:N3       | 3:L3:339:C:O2'     | 2.46                     | 0.47              |
| 3:L3:1646:A:O2'    | 32:LW:49:TRP:O     | 2.27                     | 0.47              |
| 8:L8:11:ARG:NH1    | 8:L8:58:THR:O      | 2.47                     | 0.47              |
| 3:L3:400:A2M:HM'3  | 10:LA:101:ASN:HD22 | 1.80                     | 0.46              |
| 52:SR:341:ALA:O    | 52:SR:344:VAL:HG22 | 2.15                     | 0.46              |
| 3:L3:4745:G:H22    | 3:L3:4955:A:H2     | 1.62                     | 0.46              |
| 18:LI:18:HIS:O     | 18:LI:78:TYR:OH    | 2.29                     | 0.46              |
| 3:L3:4227:OMU:HM23 | 3:L3:4227:OMU:H1'  | 1.64                     | 0.46              |
| 3:L3:737:C:OP2     | 8:L8:71:LYS:NZ     | 2.45                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L3:3620:G:OP1    | 3:L3:3622:C:N4     | 2.49                     | 0.46              |
| 3:L3:3830:A2M:HM'3 | 3:L3:3830:A2M:H1'  | 1.67                     | 0.46              |
| 47:SH:110:LEU:HD12 | 47:SH:115:LEU:HD21 | 1.97                     | 0.46              |
| 23:LN:248:LEU:HD23 | 23:LN:248:LEU:H    | 1.81                     | 0.46              |
| 3:L3:2368:A:N6     | 3:L3:2827:G:O2'    | 2.49                     | 0.46              |
| 17:LH:119:ILE:HD12 | 17:LH:140:LEU:HD22 | 1.97                     | 0.46              |
| 3:L3:386:A:OP2     | 18:LI:89:LYS:NZ    | 2.45                     | 0.46              |
| 37:NL:206:LEU:HD22 | 37:NL:214:LEU:HD22 | 1.98                     | 0.46              |
| 37:NL:456:ARG:NH1  | 50:SM:213:THR:O    | 2.46                     | 0.46              |
| 2:L1:75:OMG:H1'    | 2:L1:75:OMG:HM23   | 1.51                     | 0.46              |
| 3:L3:4288:C:O2'    | 3:L3:4321:U:OP1    | 2.29                     | 0.46              |
| 8:L8:135:LEU:CD1   | 8:L8:136:LEU:HD12  | 2.46                     | 0.46              |
| 23:LN:61:ASP:OD2   | 52:SR:410:ILE:HG23 | 2.16                     | 0.46              |
| 2:L1:26:C:O2'      | 40:SA:53:ALA:O     | 2.32                     | 0.46              |
| 23:LN:222:VAL:O    | 23:LN:343:ARG:NH1  | 2.49                     | 0.46              |
| 3:L3:152:U:OP1     | 9:L9:49:ARG:NH1    | 2.49                     | 0.46              |
| 3:L3:3939:G:O2'    | 3:L3:4076:G:N2     | 2.43                     | 0.46              |
| 3:L3:4618:OMG:H1'  | 3:L3:4618:OMG:HM23 | 1.70                     | 0.46              |
| 6:L6:17:ASP:OD2    | 6:L6:20:ARG:NH1    | 2.49                     | 0.46              |
| 3:L3:4392:OMG:HM23 | 3:L3:4392:OMG:H1'  | 1.65                     | 0.45              |
| 3:L3:1522:OMG:H4'  | 40:SA:75:ARG:O     | 2.15                     | 0.45              |
| 3:L3:2824:OMC:HM23 | 3:L3:2824:OMC:H1'  | 1.82                     | 0.45              |
| 44:SE:103:ARG:NH2  | 44:SE:192:ARG:O    | 2.49                     | 0.45              |
| 3:L3:3723:A:H2'    | 3:L3:3724:A2M:H8   | 1.99                     | 0.45              |
| 3:L3:4437:U:O4     | 52:SR:143:ARG:NH1  | 2.50                     | 0.45              |
| 30:LU:63:VAL:HG12  | 30:LU:63:VAL:O     | 2.16                     | 0.45              |
| 23:LN:370:THR:O    | 23:LN:370:THR:HG22 | 2.16                     | 0.45              |
| 28:LS:37:THR:O     | 28:LS:37:THR:HG22  | 2.15                     | 0.45              |
| 37:NL:247:TYR:HB2  | 37:NL:431:LEU:HD13 | 1.98                     | 0.45              |
| 49:SK:85:ARG:NH2   | 49:SK:89:PRO:O     | 2.49                     | 0.45              |
| 48:SI:154:LEU:HD12 | 50:SM:265:TYR:CD1  | 2.52                     | 0.45              |
| 3:L3:3841:OMC:HM23 | 3:L3:3841:OMC:H1'  | 1.63                     | 0.45              |
| 42:SC:95:PRO:HA    | 42:SC:104:THR:HG22 | 1.98                     | 0.45              |
| 3:L3:2588:C:OP1    | 3:L3:2768:C:O2'    | 2.20                     | 0.45              |
| 3:L3:3925:OMU:HM23 | 3:L3:3925:OMU:H1'  | 1.54                     | 0.45              |
| 49:SK:44:ASP:OD1   | 49:SK:45:THR:N     | 2.50                     | 0.45              |
| 3:L3:469:C:OP2     | 3:L3:684:G:N1      | 2.46                     | 0.45              |
| 3:L3:2632:PSU:H2'  | 3:L3:2633:U:C6     | 2.51                     | 0.45              |
| 3:L3:4156:G:P      | 3:L3:4157:A:HO2'   | 2.31                     | 0.45              |
| 3:L3:4220:6MZ:H2'  | 3:L3:4222:G:H5''   | 1.98                     | 0.45              |
| 3:L3:4361:PSU:H2'  | 3:L3:4362:A:O4'    | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:LL:64:ILE:HD11  | 21:LL:96:MET:HE2   | 1.99                     | 0.45              |
| 3:L3:3899:OMG:HM23 | 3:L3:3899:OMG:H1'  | 1.75                     | 0.45              |
| 3:L3:4571:A2M:H1'  | 3:L3:4571:A2M:HM'3 | 1.52                     | 0.45              |
| 3:L3:4637:OMG:H2'  | 3:L3:4638:U:C6     | 2.52                     | 0.45              |
| 4:L4:12:U:OP2      | 4:L4:67:C:O2'      | 2.33                     | 0.45              |
| 3:L3:1326:A2M:H1'  | 3:L3:1326:A2M:HM'3 | 1.57                     | 0.45              |
| 3:L3:1534:A2M:HM'2 | 3:L3:1535:C:H6     | 1.82                     | 0.45              |
| 3:L3:4201:G:O2'    | 3:L3:4202:U:OP2    | 2.32                     | 0.45              |
| 3:L3:4457:PSU:H1'  | 23:LN:252:ALA:HB3  | 1.98                     | 0.45              |
| 10:LA:108:ASP:OD1  | 10:LA:111:SER:OG   | 2.34                     | 0.45              |
| 3:L3:308:G:OP2     | 3:L3:308:G:N2      | 2.33                     | 0.44              |
| 3:L3:1401:C:OP2    | 22:LM:51:LYS:NZ    | 2.48                     | 0.44              |
| 3:L3:3893:C:O2'    | 3:L3:4979:A:N1     | 2.47                     | 0.44              |
| 27:LR:93:ARG:HG2   | 27:LR:97:ILE:HD12  | 1.98                     | 0.44              |
| 45:SF:142:GLU:O    | 45:SF:143:THR:OG1  | 2.21                     | 0.44              |
| 49:SK:6:SER:HA     | 49:SK:13:ILE:HD11  | 2.00                     | 0.44              |
| 3:L3:1438:U:O2'    | 3:L3:1439:C:OP1    | 2.34                     | 0.44              |
| 40:SA:56:GLU:OE2   | 40:SA:106:LYS:NZ   | 2.38                     | 0.44              |
| 42:SC:250:GLN:NE2  | 42:SC:254:ASP:OD2  | 2.47                     | 0.44              |
| 2:L1:68:G:O2'      | 2:L1:69:PSU:H5''   | 2.17                     | 0.44              |
| 3:L3:930:G:OP1     | 40:SA:353:LYS:NZ   | 2.46                     | 0.44              |
| 3:L3:1340:OMC:HM23 | 3:L3:1340:OMC:H1'  | 1.52                     | 0.44              |
| 3:L3:4405:G:O2'    | 54:VB:33:GLY:O     | 2.30                     | 0.44              |
| 4:L4:7:G:OP1       | 41:SB:33:ARG:NH1   | 2.50                     | 0.44              |
| 3:L3:718:C:OP1     | 43:SD:217:ARG:NH1  | 2.47                     | 0.44              |
| 3:L3:1532:G:OP2    | 32:LW:31:LYS:NZ    | 2.47                     | 0.44              |
| 3:L3:2427:G:OP1    | 13:LD:5:ARG:NH2    | 2.51                     | 0.44              |
| 3:L3:4478:G:N2     | 3:L3:4608:G:O2'    | 2.51                     | 0.44              |
| 44:SE:58:PRO:HD2   | 44:SE:61:ILE:HD12  | 1.99                     | 0.44              |
| 47:SH:57:ASP:OD1   | 47:SH:59:THR:OG1   | 2.25                     | 0.44              |
| 3:L3:1633:G:O6     | 3:L3:3918:G:O2'    | 2.34                     | 0.44              |
| 3:L3:2097:U:O3'    | 3:L3:2098:G:H4'    | 2.18                     | 0.44              |
| 3:L3:2835:A:O2'    | 23:LN:228:TYR:O    | 2.35                     | 0.44              |
| 3:L3:5039:U:OP1    | 53:SV:111:ARG:NH1  | 2.51                     | 0.44              |
| 12:LC:38:VAL:HG13  | 43:SD:237:GLU:OE1  | 2.18                     | 0.44              |
| 40:SA:137:VAL:HG21 | 40:SA:150:LEU:HD21 | 1.99                     | 0.44              |
| 3:L3:1676:C:OP2    | 3:L3:1677:PSU:N1   | 2.49                     | 0.44              |
| 3:L3:1826:G:H4'    | 22:LM:43:MET:HE3   | 1.99                     | 0.44              |
| 14:LE:30:TYR:HB2   | 41:SB:38:ILE:HD12  | 2.00                     | 0.44              |
| 3:L3:1464:C:H5''   | 22:LM:32:LEU:HD12  | 2.00                     | 0.43              |
| 3:L3:4498:OMU:HM23 | 3:L3:4498:OMU:H1'  | 1.47                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:LY:56:LEU:HD21  | 37:NL:371:LEU:HD21 | 2.00                     | 0.43              |
| 3:L3:3681:G:OP2    | 45:SF:128:ARG:NH2  | 2.50                     | 0.43              |
| 3:L3:3849:A:N3     | 38:NP:3:ARG:NH1    | 2.67                     | 0.43              |
| 3:L3:5001:PSU:H2'  | 3:L3:5002:U:O4'    | 2.18                     | 0.43              |
| 5:L5:127:GLY:C     | 5:L5:128:LEU:HD12  | 2.43                     | 0.43              |
| 48:SI:237:MET:HE1  | 48:SI:254:LEU:HD21 | 2.01                     | 0.43              |
| 52:SR:442:ILE:HD11 | 53:SV:86:TRP:CD1   | 2.53                     | 0.43              |
| 3:L3:3867:A2M:HM'3 | 3:L3:3867:A2M:H1'  | 1.75                     | 0.43              |
| 3:L3:4311:A:O2'    | 3:L3:4312:PSU:H5'' | 2.17                     | 0.43              |
| 49:SK:21:ASN:ND2   | 49:SK:112:ASP:OD2  | 2.50                     | 0.43              |
| 49:SK:76:THR:O     | 49:SK:96:ARG:NH1   | 2.50                     | 0.43              |
| 3:L3:1983:A:O2'    | 3:L3:2011:C:OP1    | 2.36                     | 0.43              |
| 3:L3:3744:OMG:HM23 | 3:L3:3744:OMG:H1'  | 1.78                     | 0.43              |
| 2:L1:90:C:O2'      | 18:LI:24:HIS:ND1   | 2.43                     | 0.43              |
| 2:L1:102:G:OP2     | 2:L1:104:A:O2'     | 2.36                     | 0.43              |
| 3:L3:1366:G:C2     | 6:L6:33:ILE:HD13   | 2.54                     | 0.43              |
| 50:SM:170:HIS:HB3  | 50:SM:283:LEU:HD11 | 2.01                     | 0.43              |
| 3:L3:1096:C:O2     | 3:L3:1200:G:N2     | 2.52                     | 0.43              |
| 3:L3:1931:C:N4     | 3:L3:2041:A:OP1    | 2.52                     | 0.43              |
| 33:LX:26:VAL:HG22  | 45:SF:178:PRO:HD2  | 2.01                     | 0.43              |
| 44:SE:136:LEU:HD22 | 44:SE:202:VAL:CG1  | 2.49                     | 0.43              |
| 3:L3:2363:A2M:H1'  | 3:L3:2363:A2M:HM'3 | 1.77                     | 0.43              |
| 9:L9:165:THR:HG23  | 9:L9:168:GLY:H     | 1.84                     | 0.43              |
| 12:LC:99:ASP:OD1   | 12:LC:100:LEU:N    | 2.50                     | 0.43              |
| 3:L3:398:A2M:HM'3  | 3:L3:398:A2M:H1'   | 1.74                     | 0.43              |
| 3:L3:1897:A:OP1    | 11:LB:2:GLY:N      | 2.51                     | 0.43              |
| 7:L7:186:GLU:HA    | 7:L7:189:ILE:HG22  | 2.01                     | 0.43              |
| 47:SH:79:SER:O     | 47:SH:83:GLY:N     | 2.47                     | 0.43              |
| 3:L3:2306:G:OP1    | 26:LQ:128:ARG:NH1  | 2.52                     | 0.43              |
| 3:L3:2434:G:O2'    | 3:L3:2527:A:N1     | 2.45                     | 0.43              |
| 3:L3:4208:U:OP2    | 14:LE:4:THR:HG23   | 2.19                     | 0.43              |
| 43:SD:171:ASP:OD1  | 43:SD:172:ASN:N    | 2.52                     | 0.43              |
| 45:SF:101:VAL:C    | 45:SF:102:LEU:HD12 | 2.44                     | 0.43              |
| 52:SR:258:SER:OG   | 52:SR:293:VAL:HG11 | 2.18                     | 0.43              |
| 3:L3:3717:A:H2'    | 3:L3:3718:A2M:H8   | 2.01                     | 0.43              |
| 45:SF:129:ALA:O    | 45:SF:169:VAL:HG11 | 2.18                     | 0.43              |
| 3:L3:2837:OMU:HM23 | 3:L3:2837:OMU:H1'  | 1.67                     | 0.42              |
| 3:L3:4568:A:O3'    | 23:LN:21:ARG:NH1   | 2.52                     | 0.42              |
| 3:L3:423:G:OP1     | 10:LA:62:ARG:NH1   | 2.51                     | 0.42              |
| 3:L3:911:U:H2'     | 3:L3:912:G:O4'     | 2.20                     | 0.42              |
| 6:L6:63:THR:HG22   | 6:L6:64:VAL:N      | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:L6:185:ALA:HB2   | 30:LU:7:MET:HE1    | 2.01                     | 0.42              |
| 3:L3:1326:A2M:H2'  | 3:L3:1327:C:C6     | 2.54                     | 0.42              |
| 3:L3:2863:G:O2'    | 13:LD:82:LYS:O     | 2.37                     | 0.42              |
| 19:LJ:10:VAL:HG11  | 19:LJ:129:TRP:HZ3  | 1.83                     | 0.42              |
| 42:SC:145:THR:HG1  | 42:SC:200:LYS:HZ3  | 1.53                     | 0.42              |
| 52:SR:442:ILE:CG2  | 53:SV:79:ILE:HD11  | 2.48                     | 0.42              |
| 52:SR:576:ASP:OD1  | 52:SR:577:VAL:N    | 2.53                     | 0.42              |
| 3:L3:1881:C:HO2'   | 3:L3:1882:U:P      | 2.37                     | 0.42              |
| 15:LF:28:PRO:HB3   | 15:LF:100:LEU:HD11 | 2.02                     | 0.42              |
| 3:L3:1534:A2M:HM'2 | 3:L3:1535:C:C6     | 2.55                     | 0.42              |
| 5:L5:22:LEU:HD22   | 5:L5:130:PHE:CE1   | 2.54                     | 0.42              |
| 49:SK:142:VAL:HG23 | 49:SK:142:VAL:O    | 2.19                     | 0.42              |
| 49:SK:174:SER:O    | 49:SK:178:GLN:N    | 2.49                     | 0.42              |
| 2:L1:22:U:H5       | 40:SA:196:MET:HE1  | 1.85                     | 0.42              |
| 3:L3:4305:G:H4'    | 3:L3:4306:OMU:OP1  | 2.20                     | 0.42              |
| 14:LE:30:TYR:O     | 41:SB:41:LYS:NZ    | 2.41                     | 0.42              |
| 3:L3:1591:U:OP2    | 3:L3:2856:C:O2'    | 2.32                     | 0.42              |
| 3:L3:2322:G:OP2    | 26:LQ:34:ASN:ND2   | 2.49                     | 0.42              |
| 21:LL:64:ILE:CD1   | 21:LL:96:MET:HE2   | 2.50                     | 0.42              |
| 25:LP:92:ARG:HA    | 25:LP:102:LEU:HD23 | 2.02                     | 0.42              |
| 39:NR:88:GLU:OE1   | 39:NR:113:ILE:HD11 | 2.20                     | 0.42              |
| 49:SK:49:VAL:HG12  | 49:SK:50:HIS:O     | 2.19                     | 0.42              |
| 6:L6:63:THR:HG21   | 20:LK:66:ASN:CB    | 2.50                     | 0.42              |
| 17:LH:119:ILE:HD12 | 17:LH:140:LEU:HD21 | 2.01                     | 0.42              |
| 37:NL:188:VAL:O    | 50:SM:163:ARG:NH1  | 2.53                     | 0.42              |
| 3:L3:730:G:OP2     | 43:SD:76:ARG:NE    | 2.53                     | 0.41              |
| 3:L3:1366:G:N2     | 3:L3:1371:A:OP2    | 2.52                     | 0.41              |
| 14:LE:158:PHE:O    | 39:NR:39:LYS:NZ    | 2.47                     | 0.41              |
| 43:SD:225:THR:HG22 | 43:SD:226:HIS:N    | 2.35                     | 0.41              |
| 3:L3:2859:G:H21    | 3:L3:3837:C:H1'    | 1.85                     | 0.41              |
| 3:L3:4934:A:O2'    | 3:L3:4935:C:OP2    | 2.33                     | 0.41              |
| 42:SC:50:LEU:HD23  | 42:SC:50:LEU:H     | 1.84                     | 0.41              |
| 42:SC:145:THR:HG1  | 42:SC:200:LYS:NZ   | 2.14                     | 0.41              |
| 3:L3:1959:U:O2'    | 39:NR:100:ASP:OD2  | 2.36                     | 0.41              |
| 3:L3:3659:G:OP1    | 45:SF:241:ARG:NH1  | 2.53                     | 0.41              |
| 3:L3:1677:PSU:H4'  | 3:L3:1680:G:N1     | 2.35                     | 0.41              |
| 20:LK:15:VAL:HG23  | 20:LK:16:SER:N     | 2.36                     | 0.41              |
| 27:LR:44:SER:OG    | 27:LR:46:CYS:SG    | 2.77                     | 0.41              |
| 3:L3:1358:G:O2'    | 3:L3:1360:G:O6     | 2.17                     | 0.41              |
| 3:L3:1864:G:O6     | 39:NR:22:ARG:NH2   | 2.54                     | 0.41              |
| 3:L3:1888:A:O2'    | 3:L3:3883:U:O2'    | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:LJ:33:THR:HG23  | 19:LJ:36:ARG:H     | 1.84                     | 0.41              |
| 3:L3:2334:C:C5     | 40:SA:191:ALA:HB2  | 2.56                     | 0.41              |
| 3:L3:3607:U:OP1    | 13:LD:88:ARG:NH1   | 2.54                     | 0.41              |
| 3:L3:2362:U:H2'    | 3:L3:2363:A2M:H8   | 2.03                     | 0.41              |
| 3:L3:4638:U:OP1    | 3:L3:5044:A:O2'    | 2.36                     | 0.41              |
| 6:L6:185:ALA:CB    | 30:LU:7:MET:HE1    | 2.50                     | 0.41              |
| 3:L3:3724:A2M:HM'3 | 3:L3:3724:A2M:H1'  | 1.64                     | 0.41              |
| 3:L3:2691:U:C2     | 3:L3:2692:U:C5     | 3.08                     | 0.41              |
| 3:L3:4494:OMG:H8   | 3:L3:4494:OMG:O5'  | 2.04                     | 0.41              |
| 19:LJ:100:VAL:HG13 | 19:LJ:107:LYS:HA   | 2.02                     | 0.41              |
| 32:LW:21:ARG:NH2   | 32:LW:41:ALA:O     | 2.43                     | 0.41              |
| 38:NP:24:ARG:NH2   | 38:NP:27:ASP:OD2   | 2.49                     | 0.41              |
| 40:SA:94:ASN:OD1   | 40:SA:94:ASN:N     | 2.54                     | 0.41              |
| 40:SA:211:TYR:OH   | 40:SA:218:ILE:HD11 | 2.21                     | 0.41              |
| 3:L3:1523:A:N3     | 3:L3:4389:C:O2'    | 2.46                     | 0.41              |
| 35:LZ:12:PHE:CD2   | 35:LZ:51:LEU:HD22  | 2.56                     | 0.41              |
| 35:LZ:21:ARG:NH1   | 35:LZ:22:PRO:O     | 2.51                     | 0.41              |
| 3:L3:1252:C:O2     | 3:L3:1254:A:N6     | 2.49                     | 0.40              |
| 3:L3:1321:G:C2'    | 3:L3:1322:1MA:H5'  | 2.51                     | 0.40              |
| 3:L3:3701:OMC:H4'  | 3:L3:3702:A:H5''   | 2.03                     | 0.40              |
| 15:LF:49:VAL:HG12  | 15:LF:50:ASN:OD1   | 2.21                     | 0.40              |
| 3:L3:2861:OMC:H1'  | 3:L3:2861:OMC:HM23 | 1.50                     | 0.40              |
| 19:LJ:74:VAL:HG23  | 19:LJ:101:PHE:CE2  | 2.57                     | 0.40              |
| 23:LN:119:TYR:OH   | 23:LN:129:ALA:N    | 2.53                     | 0.40              |
| 3:L3:1683:PSU:H2'  | 3:L3:1684:A:C8     | 2.56                     | 0.40              |
| 23:LN:298:LEU:HD23 | 23:LN:298:LEU:H    | 1.86                     | 0.40              |
| 23:LN:370:THR:N    | 23:LN:380:GLN:OE1  | 2.48                     | 0.40              |
| 45:SF:102:LEU:HB2  | 45:SF:107:MET:HE2  | 2.03                     | 0.40              |
| 52:SR:102:ALA:O    | 52:SR:106:VAL:HG23 | 2.20                     | 0.40              |
| 3:L3:106:A:H2'     | 3:L3:107:G:O4'     | 2.22                     | 0.40              |
| 5:L5:10:ASN:OD1    | 5:L5:11:PRO:HD2    | 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 |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | BA    | 89/165 (54%)  | 89 (100%)  | 0       | 0        | 100         | 100 |
| 5   | L5    | 166/178 (93%) | 165 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 6   | L6    | 208/211 (99%) | 203 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 7   | L7    | 199/203 (98%) | 196 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 8   | L8    | 133/215 (62%) | 130 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 9   | L9    | 201/204 (98%) | 198 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 10  | LA    | 151/184 (82%) | 147 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 11  | LB    | 185/188 (98%) | 180 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 12  | LC    | 174/176 (99%) | 172 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 13  | LD    | 152/196 (78%) | 150 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 14  | LE    | 150/160 (94%) | 145 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 15  | LF    | 101/128 (79%) | 99 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 16  | LG    | 137/140 (98%) | 135 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 17  | LH    | 141/156 (90%) | 141 (100%) | 0       | 0        | 100         | 100 |
| 18  | LI    | 132/145 (91%) | 130 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 19  | LJ    | 133/136 (98%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 20  | LK    | 145/148 (98%) | 143 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 21  | LL    | 123/137 (90%) | 122 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 22  | LM    | 87/159 (55%)  | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 23  | LN    | 399/403 (99%) | 391 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 24  | LO    | 93/115 (81%)  | 93 (100%)  | 0       | 0        | 100         | 100 |
| 25  | LP    | 104/125 (83%) | 102 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 26  | LQ    | 126/135 (93%) | 125 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 27  | LR    | 110/117 (94%) | 110 (100%) | 0       | 0        | 100         | 100 |
| 28  | LS    | 120/123 (98%) | 118 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 29  | LT    | 107/110 (97%) | 106 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 30  | LU    | 100/105 (95%) | 100 (100%) | 0       | 0        | 100         | 100 |
| 31  | LV    | 102/106 (96%) | 100 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 32  | LW    | 84/97 (87%)   | 83 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 33  | LX    | 89/92 (97%)   | 86 (97%)   | 3 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 34  | LY    | 67/70 (96%)      | 67 (100%)  | 0        | 0        | 100         | 100 |
| 35  | LZ    | 48/51 (94%)      | 47 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 36  | NK    | 63/129 (49%)     | 62 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 37  | NL    | 259/478 (54%)    | 258 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 38  | NP    | 100/134 (75%)    | 100 (100%) | 0        | 0        | 100         | 100 |
| 39  | NR    | 150/203 (74%)    | 147 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 40  | SA    | 356/427 (83%)    | 352 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 41  | SB    | 273/297 (92%)    | 269 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 42  | SC    | 211/288 (73%)    | 204 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 43  | SD    | 223/248 (90%)    | 218 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 44  | SE    | 228/266 (86%)    | 226 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 45  | SF    | 243/257 (95%)    | 236 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 46  | SG    | 188/192 (98%)    | 187 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 47  | SH    | 91/293 (31%)     | 90 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 48  | SI    | 233/255 (91%)    | 230 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 49  | SK    | 242/245 (99%)    | 237 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 50  | SM    | 393/588 (67%)    | 388 (99%)  | 5 (1%)   | 0        | 100         | 100 |
| 51  | SQ    | 121/239 (51%)    | 119 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 52  | SR    | 595/634 (94%)    | 587 (99%)  | 7 (1%)   | 1 (0%)   | 43          | 56  |
| 53  | SV    | 137/163 (84%)    | 136 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 54  | VB    | 54/99 (54%)      | 54 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 8516/10313 (83%) | 8390 (98%) | 125 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | SR    | 88  | ASP  |

### 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   | L5    | 142/149 (95%)  | 142 (100%) | 0        | 100         | 100 |
| 6   | L6    | 176/177 (99%)  | 176 (100%) | 0        | 100         | 100 |
| 7   | L7    | 173/174 (99%)  | 173 (100%) | 0        | 100         | 100 |
| 8   | L8    | 115/161 (71%)  | 115 (100%) | 0        | 100         | 100 |
| 9   | L9    | 171/172 (99%)  | 171 (100%) | 0        | 100         | 100 |
| 10  | LA    | 134/163 (82%)  | 134 (100%) | 0        | 100         | 100 |
| 11  | LB    | 164/165 (99%)  | 164 (100%) | 0        | 100         | 100 |
| 12  | LC    | 157/157 (100%) | 157 (100%) | 0        | 100         | 100 |
| 13  | LD    | 138/175 (79%)  | 138 (100%) | 0        | 100         | 100 |
| 14  | LE    | 136/140 (97%)  | 136 (100%) | 0        | 100         | 100 |
| 15  | LF    | 93/115 (81%)   | 93 (100%)  | 0        | 100         | 100 |
| 16  | LG    | 106/107 (99%)  | 106 (100%) | 0        | 100         | 100 |
| 17  | LH    | 124/133 (93%)  | 124 (100%) | 0        | 100         | 100 |
| 18  | LI    | 124/135 (92%)  | 124 (100%) | 0        | 100         | 100 |
| 19  | LJ    | 117/118 (99%)  | 117 (100%) | 0        | 100         | 100 |
| 20  | LK    | 120/121 (99%)  | 120 (100%) | 0        | 100         | 100 |
| 21  | LL    | 109/121 (90%)  | 109 (100%) | 0        | 100         | 100 |
| 22  | LM    | 77/126 (61%)   | 77 (100%)  | 0        | 100         | 100 |
| 23  | LN    | 347/348 (100%) | 347 (100%) | 0        | 100         | 100 |
| 24  | LO    | 80/97 (82%)    | 80 (100%)  | 0        | 100         | 100 |
| 25  | LP    | 97/110 (88%)   | 97 (100%)  | 0        | 100         | 100 |
| 26  | LQ    | 114/121 (94%)  | 114 (100%) | 0        | 100         | 100 |
| 27  | LR    | 96/100 (96%)   | 96 (100%)  | 0        | 100         | 100 |
| 28  | LS    | 109/110 (99%)  | 109 (100%) | 0        | 100         | 100 |
| 29  | LT    | 88/89 (99%)    | 88 (100%)  | 0        | 100         | 100 |
| 30  | LU    | 86/89 (97%)    | 86 (100%)  | 0        | 100         | 100 |
| 31  | LV    | 92/94 (98%)    | 92 (100%)  | 0        | 100         | 100 |
| 32  | LW    | 73/80 (91%)    | 73 (100%)  | 0        | 100         | 100 |
| 33  | LX    | 74/75 (99%)    | 74 (100%)  | 0        | 100         | 100 |
| 34  | LY    | 64/65 (98%)    | 64 (100%)  | 0        | 100         | 100 |
| 35  | LZ    | 47/48 (98%)    | 47 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 36  | NK    | 61/115 (53%)    | 61 (100%)   | 0        | 100         | 100 |
| 37  | NL    | 227/402 (56%)   | 227 (100%)  | 0        | 100         | 100 |
| 38  | NP    | 88/114 (77%)    | 88 (100%)   | 0        | 100         | 100 |
| 39  | NR    | 140/183 (76%)   | 140 (100%)  | 0        | 100         | 100 |
| 40  | SA    | 298/348 (86%)   | 297 (100%)  | 1 (0%)   | 86          | 92  |
| 41  | SB    | 234/250 (94%)   | 234 (100%)  | 0        | 100         | 100 |
| 42  | SC    | 192/252 (76%)   | 192 (100%)  | 0        | 100         | 100 |
| 43  | SD    | 194/215 (90%)   | 194 (100%)  | 0        | 100         | 100 |
| 44  | SE    | 198/223 (89%)   | 198 (100%)  | 0        | 100         | 100 |
| 45  | SF    | 188/199 (94%)   | 188 (100%)  | 0        | 100         | 100 |
| 46  | SG    | 169/171 (99%)   | 169 (100%)  | 0        | 100         | 100 |
| 47  | SH    | 85/274 (31%)    | 85 (100%)   | 0        | 100         | 100 |
| 48  | SI    | 212/228 (93%)   | 212 (100%)  | 0        | 100         | 100 |
| 49  | SK    | 212/213 (100%)  | 212 (100%)  | 0        | 100         | 100 |
| 50  | SM    | 354/509 (70%)   | 354 (100%)  | 0        | 100         | 100 |
| 51  | SQ    | 6/214 (3%)      | 6 (100%)    | 0        | 100         | 100 |
| 52  | SR    | 545/574 (95%)   | 545 (100%)  | 0        | 100         | 100 |
| 53  | SV    | 128/149 (86%)   | 128 (100%)  | 0        | 100         | 100 |
| 54  | VB    | 48/76 (63%)     | 48 (100%)   | 0        | 100         | 100 |
| All | All   | 7322/8744 (84%) | 7321 (100%) | 1 (0%)   | 100         | 100 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | SA    | 109 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | L7    | 96  | GLN  |
| 8   | L8    | 34  | ASN  |
| 8   | L8    | 69  | HIS  |
| 9   | L9    | 109 | HIS  |
| 10  | LA    | 93  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | LA    | 97  | ASN  |
| 10  | LA    | 101 | ASN  |
| 10  | LA    | 116 | HIS  |
| 11  | LB    | 7   | HIS  |
| 11  | LB    | 160 | HIS  |
| 12  | LC    | 122 | HIS  |
| 13  | LD    | 40  | GLN  |
| 13  | LD    | 118 | HIS  |
| 13  | LD    | 141 | HIS  |
| 14  | LE    | 22  | HIS  |
| 14  | LE    | 58  | HIS  |
| 15  | LF    | 41  | GLN  |
| 17  | LH    | 93  | ASN  |
| 20  | LK    | 19  | HIS  |
| 21  | LL    | 21  | ASN  |
| 21  | LL    | 23  | GLN  |
| 23  | LN    | 123 | HIS  |
| 24  | LO    | 40  | GLN  |
| 25  | LP    | 69  | ASN  |
| 26  | LQ    | 126 | ASN  |
| 29  | LT    | 20  | ASN  |
| 29  | LT    | 21  | GLN  |
| 29  | LT    | 56  | ASN  |
| 29  | LT    | 99  | HIS  |
| 30  | LU    | 26  | HIS  |
| 33  | LX    | 56  | HIS  |
| 34  | LY    | 58  | GLN  |
| 35  | LZ    | 25  | GLN  |
| 35  | LZ    | 33  | ASN  |
| 37  | NL    | 365 | HIS  |
| 39  | NR    | 102 | GLN  |
| 39  | NR    | 155 | ASN  |
| 40  | SA    | 43  | ASN  |
| 40  | SA    | 198 | ASN  |
| 40  | SA    | 329 | ASN  |
| 42  | SC    | 190 | HIS  |
| 42  | SC    | 245 | GLN  |
| 42  | SC    | 268 | GLN  |
| 43  | SD    | 80  | ASN  |
| 43  | SD    | 239 | GLN  |
| 44  | SE    | 82  | GLN  |
| 44  | SE    | 141 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | SE    | 149 | ASN  |
| 45  | SF    | 22  | HIS  |
| 45  | SF    | 97  | ASN  |
| 46  | SG    | 40  | HIS  |
| 46  | SG    | 169 | ASN  |
| 48  | SI    | 225 | HIS  |
| 49  | SK    | 68  | HIS  |
| 50  | SM    | 50  | HIS  |
| 50  | SM    | 211 | HIS  |
| 50  | SM    | 245 | HIS  |
| 52  | SR    | 100 | ASN  |
| 52  | SR    | 157 | HIS  |
| 52  | SR    | 209 | HIS  |
| 53  | SV    | 39  | ASN  |
| 53  | SV    | 87  | ASN  |
| 53  | SV    | 132 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2   | L1    | 152/157 (96%)   | 18 (11%)          | 0               |
| 3   | L3    | 3390/5070 (66%) | 431 (12%)         | 8 (0%)          |
| 4   | L4    | 119/121 (98%)   | 10 (8%)           | 0               |
| All | All   | 3661/5348 (68%) | 459 (12%)         | 8 (0%)          |

All (459) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L1    | 23  | C    |
| 2   | L1    | 34  | U    |
| 2   | L1    | 35  | C    |
| 2   | L1    | 59  | A    |
| 2   | L1    | 62  | A    |
| 2   | L1    | 63  | U    |
| 2   | L1    | 82  | A    |
| 2   | L1    | 83  | C    |
| 2   | L1    | 84  | A    |
| 2   | L1    | 86  | U    |
| 2   | L1    | 94  | G    |
| 2   | L1    | 103 | A    |
| 2   | L1    | 105 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L1    | 111 | U    |
| 2   | L1    | 114 | G    |
| 2   | L1    | 127 | U    |
| 2   | L1    | 151 | G    |
| 2   | L1    | 156 | U    |
| 3   | L3    | 2   | G    |
| 3   | L3    | 6   | C    |
| 3   | L3    | 13  | U    |
| 3   | L3    | 25  | A    |
| 3   | L3    | 39  | A    |
| 3   | L3    | 42  | A    |
| 3   | L3    | 48  | G    |
| 3   | L3    | 56  | A    |
| 3   | L3    | 58  | G    |
| 3   | L3    | 59  | A    |
| 3   | L3    | 64  | A    |
| 3   | L3    | 65  | A    |
| 3   | L3    | 66  | A    |
| 3   | L3    | 69  | A    |
| 3   | L3    | 91  | G    |
| 3   | L3    | 98  | A    |
| 3   | L3    | 108 | A    |
| 3   | L3    | 119 | G    |
| 3   | L3    | 159 | C    |
| 3   | L3    | 164 | G    |
| 3   | L3    | 167 | C    |
| 3   | L3    | 169 | G    |
| 3   | L3    | 170 | C    |
| 3   | L3    | 171 | U    |
| 3   | L3    | 172 | C    |
| 3   | L3    | 173 | C    |
| 3   | L3    | 181 | C    |
| 3   | L3    | 197 | A    |
| 3   | L3    | 200 | U    |
| 3   | L3    | 210 | C    |
| 3   | L3    | 218 | A    |
| 3   | L3    | 233 | U    |
| 3   | L3    | 234 | G    |
| 3   | L3    | 261 | G    |
| 3   | L3    | 266 | C    |
| 3   | L3    | 274 | C    |
| 3   | L3    | 297 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L3    | 316 | U    |
| 3   | L3    | 340 | C    |
| 3   | L3    | 349 | A    |
| 3   | L3    | 387 | G    |
| 3   | L3    | 409 | G    |
| 3   | L3    | 410 | A    |
| 3   | L3    | 412 | G    |
| 3   | L3    | 449 | C    |
| 3   | L3    | 450 | G    |
| 3   | L3    | 452 | A    |
| 3   | L3    | 454 | U    |
| 3   | L3    | 464 | G    |
| 3   | L3    | 467 | U    |
| 3   | L3    | 469 | C    |
| 3   | L3    | 473 | C    |
| 3   | L3    | 492 | U    |
| 3   | L3    | 493 | G    |
| 3   | L3    | 496 | G    |
| 3   | L3    | 497 | G    |
| 3   | L3    | 501 | C    |
| 3   | L3    | 502 | C    |
| 3   | L3    | 503 | C    |
| 3   | L3    | 504 | G    |
| 3   | L3    | 510 | U    |
| 3   | L3    | 511 | C    |
| 3   | L3    | 658 | C    |
| 3   | L3    | 660 | A    |
| 3   | L3    | 667 | A    |
| 3   | L3    | 668 | C    |
| 3   | L3    | 669 | C    |
| 3   | L3    | 686 | A    |
| 3   | L3    | 704 | C    |
| 3   | L3    | 730 | G    |
| 3   | L3    | 731 | G    |
| 3   | L3    | 739 | G    |
| 3   | L3    | 741 | C    |
| 3   | L3    | 742 | G    |
| 3   | L3    | 746 | A    |
| 3   | L3    | 757 | G    |
| 3   | L3    | 913 | U    |
| 3   | L3    | 915 | A    |
| 3   | L3    | 916 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 917  | A    |
| 3   | L3    | 926  | G    |
| 3   | L3    | 932  | A    |
| 3   | L3    | 933  | G    |
| 3   | L3    | 944  | A    |
| 3   | L3    | 945  | U    |
| 3   | L3    | 956  | A    |
| 3   | L3    | 959  | G    |
| 3   | L3    | 960  | A    |
| 3   | L3    | 971  | U    |
| 3   | L3    | 972  | C    |
| 3   | L3    | 1066 | G    |
| 3   | L3    | 1072 | C    |
| 3   | L3    | 1080 | C    |
| 3   | L3    | 1100 | U    |
| 3   | L3    | 1169 | G    |
| 3   | L3    | 1171 | G    |
| 3   | L3    | 1173 | G    |
| 3   | L3    | 1174 | G    |
| 3   | L3    | 1178 | G    |
| 3   | L3    | 1180 | C    |
| 3   | L3    | 1181 | C    |
| 3   | L3    | 1182 | C    |
| 3   | L3    | 1198 | G    |
| 3   | L3    | 1201 | U    |
| 3   | L3    | 1203 | G    |
| 3   | L3    | 1211 | G    |
| 3   | L3    | 1214 | C    |
| 3   | L3    | 1215 | C    |
| 3   | L3    | 1241 | C    |
| 3   | L3    | 1253 | G    |
| 3   | L3    | 1254 | A    |
| 3   | L3    | 1255 | A    |
| 3   | L3    | 1256 | G    |
| 3   | L3    | 1266 | G    |
| 3   | L3    | 1269 | G    |
| 3   | L3    | 1270 | A    |
| 3   | L3    | 1273 | G    |
| 3   | L3    | 1280 | C    |
| 3   | L3    | 1284 | G    |
| 3   | L3    | 1287 | G    |
| 3   | L3    | 1294 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 1295 | C    |
| 3   | L3    | 1301 | C    |
| 3   | L3    | 1314 | C    |
| 3   | L3    | 1319 | U    |
| 3   | L3    | 1320 | U    |
| 3   | L3    | 1325 | C    |
| 3   | L3    | 1326 | A2M  |
| 3   | L3    | 1354 | A    |
| 3   | L3    | 1358 | G    |
| 3   | L3    | 1359 | G    |
| 3   | L3    | 1365 | C    |
| 3   | L3    | 1366 | G    |
| 3   | L3    | 1379 | C    |
| 3   | L3    | 1397 | A    |
| 3   | L3    | 1420 | A    |
| 3   | L3    | 1439 | C    |
| 3   | L3    | 1443 | A    |
| 3   | L3    | 1497 | A    |
| 3   | L3    | 1498 | G    |
| 3   | L3    | 1502 | G    |
| 3   | L3    | 1523 | A    |
| 3   | L3    | 1534 | A2M  |
| 3   | L3    | 1547 | A    |
| 3   | L3    | 1578 | U    |
| 3   | L3    | 1581 | G    |
| 3   | L3    | 1592 | G    |
| 3   | L3    | 1596 | U    |
| 3   | L3    | 1597 | G    |
| 3   | L3    | 1613 | A    |
| 3   | L3    | 1614 | C    |
| 3   | L3    | 1624 | G    |
| 3   | L3    | 1625 | OMG  |
| 3   | L3    | 1631 | A    |
| 3   | L3    | 1633 | G    |
| 3   | L3    | 1634 | A    |
| 3   | L3    | 1640 | C    |
| 3   | L3    | 1641 | G    |
| 3   | L3    | 1642 | A    |
| 3   | L3    | 1654 | G    |
| 3   | L3    | 1661 | C    |
| 3   | L3    | 1676 | C    |
| 3   | L3    | 1677 | PSU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 1678 | C    |
| 3   | L3    | 1721 | G    |
| 3   | L3    | 1734 | G    |
| 3   | L3    | 1791 | U    |
| 3   | L3    | 1804 | A    |
| 3   | L3    | 1815 | G    |
| 3   | L3    | 1821 | G    |
| 3   | L3    | 1822 | U    |
| 3   | L3    | 1836 | G    |
| 3   | L3    | 1837 | A    |
| 3   | L3    | 1842 | G    |
| 3   | L3    | 1850 | A    |
| 3   | L3    | 1854 | G    |
| 3   | L3    | 1855 | G    |
| 3   | L3    | 1860 | PSU  |
| 3   | L3    | 1866 | U    |
| 3   | L3    | 1869 | G    |
| 3   | L3    | 1880 | G    |
| 3   | L3    | 1881 | C    |
| 3   | L3    | 1882 | U    |
| 3   | L3    | 1883 | G    |
| 3   | L3    | 1887 | G    |
| 3   | L3    | 1888 | A    |
| 3   | L3    | 1891 | A    |
| 3   | L3    | 1897 | A    |
| 3   | L3    | 1910 | G    |
| 3   | L3    | 1919 | G    |
| 3   | L3    | 1921 | C    |
| 3   | L3    | 1922 | G    |
| 3   | L3    | 1925 | G    |
| 3   | L3    | 1936 | C    |
| 3   | L3    | 1960 | A    |
| 3   | L3    | 1974 | U    |
| 3   | L3    | 1984 | A    |
| 3   | L3    | 2002 | A    |
| 3   | L3    | 2016 | C    |
| 3   | L3    | 2021 | G    |
| 3   | L3    | 2026 | A    |
| 3   | L3    | 2044 | U    |
| 3   | L3    | 2046 | G    |
| 3   | L3    | 2055 | G    |
| 3   | L3    | 2056 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 2069 | A    |
| 3   | L3    | 2084 | C    |
| 3   | L3    | 2092 | G    |
| 3   | L3    | 2093 | A    |
| 3   | L3    | 2094 | G    |
| 3   | L3    | 2095 | A    |
| 3   | L3    | 2096 | G    |
| 3   | L3    | 2097 | U    |
| 3   | L3    | 2098 | G    |
| 3   | L3    | 2099 | G    |
| 3   | L3    | 2109 | G    |
| 3   | L3    | 2110 | C    |
| 3   | L3    | 2111 | G    |
| 3   | L3    | 2289 | C    |
| 3   | L3    | 2300 | A    |
| 3   | L3    | 2301 | G    |
| 3   | L3    | 2313 | A    |
| 3   | L3    | 2348 | G    |
| 3   | L3    | 2351 | OMC  |
| 3   | L3    | 2395 | A    |
| 3   | L3    | 2417 | A    |
| 3   | L3    | 2422 | OMC  |
| 3   | L3    | 2425 | U    |
| 3   | L3    | 2429 | A    |
| 3   | L3    | 2450 | G    |
| 3   | L3    | 2453 | A    |
| 3   | L3    | 2470 | C    |
| 3   | L3    | 2471 | G    |
| 3   | L3    | 2475 | G    |
| 3   | L3    | 2476 | G    |
| 3   | L3    | 2477 | A    |
| 3   | L3    | 2478 | C    |
| 3   | L3    | 2486 | G    |
| 3   | L3    | 2487 | G    |
| 3   | L3    | 2488 | C    |
| 3   | L3    | 2489 | C    |
| 3   | L3    | 2492 | C    |
| 3   | L3    | 2493 | G    |
| 3   | L3    | 2512 | A    |
| 3   | L3    | 2513 | A    |
| 3   | L3    | 2519 | U    |
| 3   | L3    | 2544 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 2545 | U    |
| 3   | L3    | 2548 | C    |
| 3   | L3    | 2554 | U    |
| 3   | L3    | 2587 | A    |
| 3   | L3    | 2601 | A    |
| 3   | L3    | 2627 | C    |
| 3   | L3    | 2638 | G    |
| 3   | L3    | 2653 | C    |
| 3   | L3    | 2669 | C    |
| 3   | L3    | 2687 | U    |
| 3   | L3    | 2694 | G    |
| 3   | L3    | 2695 | A    |
| 3   | L3    | 2696 | A    |
| 3   | L3    | 2711 | G    |
| 3   | L3    | 2743 | A    |
| 3   | L3    | 2760 | G    |
| 3   | L3    | 2764 | A    |
| 3   | L3    | 2769 | U    |
| 3   | L3    | 2772 | C    |
| 3   | L3    | 2787 | A2M  |
| 3   | L3    | 2788 | U    |
| 3   | L3    | 2790 | U    |
| 3   | L3    | 2814 | C    |
| 3   | L3    | 2826 | U    |
| 3   | L3    | 2827 | G    |
| 3   | L3    | 2855 | G    |
| 3   | L3    | 2877 | G    |
| 3   | L3    | 2902 | G    |
| 3   | L3    | 2917 | G    |
| 3   | L3    | 2918 | G    |
| 3   | L3    | 3271 | G    |
| 3   | L3    | 3585 | G    |
| 3   | L3    | 3593 | C    |
| 3   | L3    | 3595 | U    |
| 3   | L3    | 3597 | G    |
| 3   | L3    | 3617 | G    |
| 3   | L3    | 3626 | G    |
| 3   | L3    | 3635 | A    |
| 3   | L3    | 3644 | U    |
| 3   | L3    | 3653 | A    |
| 3   | L3    | 3662 | A    |
| 3   | L3    | 3696 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 3697 | U    |
| 3   | L3    | 3775 | A    |
| 3   | L3    | 3838 | U    |
| 3   | L3    | 3840 | U    |
| 3   | L3    | 3868 | G    |
| 3   | L3    | 3872 | A    |
| 3   | L3    | 3875 | G    |
| 3   | L3    | 3876 | A    |
| 3   | L3    | 3877 | A    |
| 3   | L3    | 3885 | G    |
| 3   | L3    | 3887 | OMC  |
| 3   | L3    | 3897 | G    |
| 3   | L3    | 3905 | A    |
| 3   | L3    | 3915 | U    |
| 3   | L3    | 3923 | A    |
| 3   | L3    | 4069 | U    |
| 3   | L3    | 4076 | G    |
| 3   | L3    | 4084 | G    |
| 3   | L3    | 4085 | A    |
| 3   | L3    | 4118 | U    |
| 3   | L3    | 4119 | C    |
| 3   | L3    | 4122 | G    |
| 3   | L3    | 4127 | A    |
| 3   | L3    | 4133 | C    |
| 3   | L3    | 4139 | G    |
| 3   | L3    | 4140 | C    |
| 3   | L3    | 4142 | C    |
| 3   | L3    | 4143 | G    |
| 3   | L3    | 4144 | C    |
| 3   | L3    | 4145 | C    |
| 3   | L3    | 4147 | G    |
| 3   | L3    | 4150 | G    |
| 3   | L3    | 4154 | G    |
| 3   | L3    | 4162 | C    |
| 3   | L3    | 4170 | A    |
| 3   | L3    | 4183 | G    |
| 3   | L3    | 4184 | G    |
| 3   | L3    | 4191 | G    |
| 3   | L3    | 4194 | U    |
| 3   | L3    | 4202 | U    |
| 3   | L3    | 4205 | A    |
| 3   | L3    | 4220 | 6MZ  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 4225 | G    |
| 3   | L3    | 4228 | OMG  |
| 3   | L3    | 4229 | U    |
| 3   | L3    | 4233 | A    |
| 3   | L3    | 4251 | A    |
| 3   | L3    | 4254 | G    |
| 3   | L3    | 4266 | G    |
| 3   | L3    | 4268 | A    |
| 3   | L3    | 4273 | A    |
| 3   | L3    | 4281 | A    |
| 3   | L3    | 4305 | G    |
| 3   | L3    | 4306 | OMU  |
| 3   | L3    | 4329 | G    |
| 3   | L3    | 4330 | G    |
| 3   | L3    | 4332 | C    |
| 3   | L3    | 4373 | G    |
| 3   | L3    | 4376 | A    |
| 3   | L3    | 4377 | G    |
| 3   | L3    | 4378 | A    |
| 3   | L3    | 4387 | C    |
| 3   | L3    | 4391 | G    |
| 3   | L3    | 4415 | A    |
| 3   | L3    | 4418 | G    |
| 3   | L3    | 4437 | U    |
| 3   | L3    | 4438 | U    |
| 3   | L3    | 4439 | U    |
| 3   | L3    | 4453 | C    |
| 3   | L3    | 4464 | A    |
| 3   | L3    | 4466 | C    |
| 3   | L3    | 4475 | G    |
| 3   | L3    | 4491 | G    |
| 3   | L3    | 4498 | OMU  |
| 3   | L3    | 4512 | U    |
| 3   | L3    | 4513 | A    |
| 3   | L3    | 4518 | A    |
| 3   | L3    | 4523 | A2M  |
| 3   | L3    | 4524 | G    |
| 3   | L3    | 4532 | PSU  |
| 3   | L3    | 4545 | G    |
| 3   | L3    | 4548 | A    |
| 3   | L3    | 4549 | G    |
| 3   | L3    | 4555 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 4556 | U    |
| 3   | L3    | 4557 | U    |
| 3   | L3    | 4558 | U    |
| 3   | L3    | 4560 | C    |
| 3   | L3    | 4567 | G    |
| 3   | L3    | 4584 | A    |
| 3   | L3    | 4590 | A2M  |
| 3   | L3    | 4608 | G    |
| 3   | L3    | 4618 | OMG  |
| 3   | L3    | 4636 | PSU  |
| 3   | L3    | 4637 | OMG  |
| 3   | L3    | 4656 | A    |
| 3   | L3    | 4670 | C    |
| 3   | L3    | 4672 | A    |
| 3   | L3    | 4678 | G    |
| 3   | L3    | 4679 | G    |
| 3   | L3    | 4701 | A    |
| 3   | L3    | 4708 | A    |
| 3   | L3    | 4709 | U    |
| 3   | L3    | 4719 | G    |
| 3   | L3    | 4720 | C    |
| 3   | L3    | 4740 | G    |
| 3   | L3    | 4741 | C    |
| 3   | L3    | 4742 | G    |
| 3   | L3    | 4750 | G    |
| 3   | L3    | 4751 | G    |
| 3   | L3    | 4754 | G    |
| 3   | L3    | 4757 | C    |
| 3   | L3    | 4759 | C    |
| 3   | L3    | 4765 | G    |
| 3   | L3    | 4772 | C    |
| 3   | L3    | 4773 | C    |
| 3   | L3    | 4870 | G    |
| 3   | L3    | 4871 | C    |
| 3   | L3    | 4882 | U    |
| 3   | L3    | 4883 | C    |
| 3   | L3    | 4900 | C    |
| 3   | L3    | 4901 | G    |
| 3   | L3    | 4910 | G    |
| 3   | L3    | 4911 | A    |
| 3   | L3    | 4914 | C    |
| 3   | L3    | 4916 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 4937 | C    |
| 3   | L3    | 4943 | A    |
| 3   | L3    | 4976 | U    |
| 3   | L3    | 5014 | A    |
| 3   | L3    | 5022 | U    |
| 3   | L3    | 5023 | C    |
| 3   | L3    | 5026 | U    |
| 3   | L3    | 5027 | C    |
| 3   | L3    | 5031 | G    |
| 3   | L3    | 5041 | G    |
| 3   | L3    | 5050 | C    |
| 3   | L3    | 5054 | C    |
| 3   | L3    | 5055 | G    |
| 3   | L3    | 5061 | A    |
| 3   | L3    | 5062 | G    |
| 3   | L3    | 5069 | U    |
| 4   | L4    | 7    | G    |
| 4   | L4    | 49   | A    |
| 4   | L4    | 53   | U    |
| 4   | L4    | 54   | A    |
| 4   | L4    | 64   | G    |
| 4   | L4    | 66   | G    |
| 4   | L4    | 97   | G    |
| 4   | L4    | 110  | G    |
| 4   | L4    | 111  | C    |
| 4   | L4    | 120  | U    |

All (8) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 496  | G    |
| 3   | L3    | 502  | C    |
| 3   | L3    | 503  | C    |
| 3   | L3    | 1324 | A    |
| 3   | L3    | 1625 | OMG  |
| 3   | L3    | 1853 | G    |
| 3   | L3    | 2095 | A    |
| 3   | L3    | 3616 | U    |

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

109 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$ |
| 3   | A2M  | L3    | 1326 | 3    | 22,25,26     | 0.89 | 0           | 30,36,39    | 2.04 | 7 (23%)     |
| 3   | PSU  | L3    | 4576 | 3    | 18,21,22     | 1.09 | 1 (5%)      | 21,30,33    | 1.92 | 6 (28%)     |
| 3   | OMG  | L3    | 4228 | 3    | 23,26,27     | 0.56 | 0           | 32,38,41    | 0.59 | 0           |
| 3   | PSU  | L3    | 4299 | 3    | 18,21,22     | 1.03 | 2 (11%)     | 21,30,33    | 2.04 | 5 (23%)     |
| 3   | OMU  | L3    | 3925 | 3    | 19,22,23     | 1.99 | 6 (31%)     | 25,31,34    | 1.89 | 5 (20%)     |
| 3   | PSU  | L3    | 4500 | 3    | 18,21,22     | 1.03 | 1 (5%)      | 21,30,33    | 1.98 | 5 (23%)     |
| 3   | PSU  | L3    | 4673 | 3    | 18,21,22     | 1.10 | 2 (11%)     | 21,30,33    | 1.95 | 4 (19%)     |
| 3   | A2M  | L3    | 1524 | 3    | 22,25,26     | 0.87 | 0           | 30,36,39    | 2.16 | 8 (26%)     |
| 3   | PSU  | L3    | 3851 | 3    | 18,21,22     | 1.10 | 1 (5%)      | 21,30,33    | 1.95 | 4 (19%)     |
| 3   | PSU  | L3    | 4403 | 3    | 18,21,22     | 1.09 | 1 (5%)      | 21,30,33    | 1.95 | 6 (28%)     |
| 3   | OMG  | L3    | 4499 | 3    | 23,26,27     | 0.46 | 0           | 32,38,41    | 0.46 | 0           |
| 3   | PSU  | L3    | 4293 | 3    | 18,21,22     | 1.01 | 1 (5%)      | 21,30,33    | 1.79 | 4 (19%)     |
| 3   | A2M  | L3    | 3867 | 3    | 22,25,26     | 0.87 | 0           | 30,36,39    | 2.08 | 7 (23%)     |
| 3   | PSU  | L3    | 4361 | 3    | 18,21,22     | 1.05 | 2 (11%)     | 21,30,33    | 2.00 | 4 (19%)     |
| 3   | PSU  | L3    | 4353 | 3    | 18,21,22     | 1.07 | 1 (5%)      | 21,30,33    | 2.05 | 6 (28%)     |
| 3   | A2M  | L3    | 2401 | 3    | 22,25,26     | 0.88 | 0           | 30,36,39    | 2.12 | 8 (26%)     |
| 3   | OMC  | L3    | 4456 | 3    | 19,22,23     | 0.54 | 0           | 25,31,34    | 0.66 | 0           |
| 3   | PSU  | L3    | 3637 | 3    | 18,21,22     | 1.05 | 1 (5%)      | 21,30,33    | 1.98 | 5 (23%)     |
| 3   | PSU  | L3    | 4493 | 3    | 18,21,22     | 1.07 | 1 (5%)      | 21,30,33    | 1.94 | 4 (19%)     |
| 3   | A2M  | L3    | 398  | 3    | 22,25,26     | 0.89 | 0           | 30,36,39    | 2.10 | 8 (26%)     |
| 3   | PSU  | L3    | 3734 | 3    | 18,21,22     | 1.11 | 1 (5%)      | 21,30,33    | 1.96 | 6 (28%)     |
| 2   | PSU  | L1    | 55   | 2    | 18,21,22     | 1.09 | 2 (11%)     | 21,30,33    | 1.92 | 5 (23%)     |
| 3   | PSU  | L3    | 2632 | 3    | 18,21,22     | 1.08 | 1 (5%)      | 21,30,33    | 1.90 | 4 (19%)     |
| 3   | A2M  | L3    | 2787 | 3    | 22,25,26     | 0.90 | 1 (4%)      | 30,36,39    | 2.10 | 7 (23%)     |
| 3   | OMC  | L3    | 2824 | 3    | 19,22,23     | 0.56 | 0           | 25,31,34    | 0.70 | 0           |
| 3   | OMG  | L3    | 3899 | 3    | 23,26,27     | 0.54 | 0           | 32,38,41    | 0.54 | 0           |
| 3   | OMC  | L3    | 2351 | 55,3 | 19,22,23     | 0.64 | 0           | 25,31,34    | 0.88 | 2 (8%)      |
| 3   | OMG  | L3    | 4618 | 3    | 23,26,27     | 0.51 | 0           | 32,38,41    | 0.52 | 0           |
| 3   | OMC  | L3    | 3701 | 3    | 19,22,23     | 0.52 | 0           | 25,31,34    | 0.57 | 0           |
| 39  | PTR  | NR    | 127  | 39   | 15,16,17     | 1.25 | 1 (6%)      | 17,22,24    | 0.61 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | L3    | 4471 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.98 | 5 (23%)  |
| 3   | OMC  | L3    | 3887 | 3    | 19,22,23     | 0.55 | 0        | 25,31,34    | 0.65 | 0        |
| 3   | PSU  | L3    | 3695 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.94 | 5 (23%)  |
| 2   | OMG  | L1    | 75   | 2    | 23,26,27     | 0.50 | 0        | 32,38,41    | 0.47 | 0        |
| 3   | PSU  | L3    | 3884 | 3    | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.88 | 4 (19%)  |
| 3   | OMG  | L3    | 1316 | 3    | 23,26,27     | 0.53 | 0        | 32,38,41    | 0.50 | 0        |
| 3   | PSU  | L3    | 1677 | 3    | 18,21,22     | 1.01 | 1 (5%)   | 21,30,33    | 1.89 | 5 (23%)  |
| 3   | PSU  | L3    | 4972 | 3    | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | OMC  | L3    | 3869 | 3    | 19,22,23     | 0.58 | 0        | 25,31,34    | 0.68 | 0        |
| 3   | PSU  | L3    | 4431 | 3    | 18,21,22     | 1.15 | 1 (5%)   | 21,30,33    | 1.94 | 5 (23%)  |
| 3   | OMG  | L3    | 2364 | 3    | 23,26,27     | 0.51 | 0        | 32,38,41    | 0.50 | 0        |
| 3   | PSU  | L3    | 3822 | 3    | 18,21,22     | 1.15 | 1 (5%)   | 21,30,33    | 1.94 | 5 (23%)  |
| 3   | PSU  | L3    | 1860 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.97 | 5 (23%)  |
| 3   | A2M  | L3    | 1534 | 55,3 | 22,25,26     | 0.92 | 1 (4%)   | 30,36,39    | 2.05 | 7 (23%)  |
| 3   | OMG  | L3    | 1522 | 3    | 23,26,27     | 0.53 | 0        | 32,38,41    | 0.61 | 0        |
| 3   | OMC  | L3    | 3841 | 3    | 19,22,23     | 0.55 | 0        | 25,31,34    | 0.64 | 0        |
| 3   | PSU  | L3    | 4532 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 2.00 | 5 (23%)  |
| 3   | OMC  | L3    | 4536 | 3    | 19,22,23     | 0.57 | 0        | 25,31,34    | 0.67 | 0        |
| 3   | OMG  | L3    | 4637 | 3    | 23,26,27     | 0.51 | 0        | 32,38,41    | 0.49 | 0        |
| 3   | A2M  | L3    | 4590 | 3    | 22,25,26     | 0.91 | 0        | 30,36,39    | 2.01 | 8 (26%)  |
| 3   | 1MA  | L3    | 1322 | 3    | 21,25,26     | 0.49 | 0        | 30,37,40    | 0.84 | 1 (3%)   |
| 3   | OMG  | L3    | 4392 | 3    | 23,26,27     | 0.53 | 0        | 32,38,41    | 0.49 | 0        |
| 3   | PSU  | L3    | 4689 | 3    | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.97 | 5 (23%)  |
| 3   | OMU  | L3    | 2415 | 3    | 19,22,23     | 2.04 | 7 (36%)  | 25,31,34    | 1.84 | 5 (20%)  |
| 3   | A2M  | L3    | 4523 | 3    | 22,25,26     | 0.88 | 0        | 30,36,39    | 2.08 | 7 (23%)  |
| 3   | A2M  | L3    | 1871 | 3    | 22,25,26     | 0.86 | 0        | 30,36,39    | 2.18 | 8 (26%)  |
| 3   | OMU  | L3    | 2837 | 3    | 19,22,23     | 2.05 | 7 (36%)  | 25,31,34    | 1.89 | 5 (20%)  |
| 3   | PSU  | L3    | 3920 | 55,3 | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 1.90 | 5 (23%)  |
| 3   | OMG  | L3    | 4370 | 3    | 23,26,27     | 0.56 | 0        | 32,38,41    | 0.55 | 0        |
| 3   | A2M  | L3    | 2815 | 3    | 22,25,26     | 0.89 | 0        | 30,36,39    | 2.10 | 7 (23%)  |
| 3   | OMG  | L3    | 3744 | 3    | 23,26,27     | 0.48 | 0        | 32,38,41    | 0.48 | 0        |
| 3   | PSU  | L3    | 4296 | 3    | 18,21,22     | 1.07 | 2 (11%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 3   | PSU  | L3    | 4457 | 3    | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 1.91 | 4 (19%)  |
| 3   | OMG  | L3    | 4494 | 3    | 23,26,27     | 0.53 | 0        | 32,38,41    | 0.52 | 0        |
| 2   | PSU  | L1    | 69   | 2    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 2.01 | 6 (28%)  |
| 3   | A2M  | L3    | 3718 | 3    | 22,25,26     | 0.93 | 1 (4%)   | 30,36,39    | 1.95 | 7 (23%)  |
| 3   | PSU  | L3    | 4636 | 3    | 18,21,22     | 1.11 | 1 (5%)   | 21,30,33    | 2.06 | 6 (28%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | OMC  | L3    | 2365 | 3    | 19,22,23     | 0.55 | 0        | 25,31,34    | 0.71 | 0        |
| 3   | PSU  | L3    | 5010 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.92 | 5 (23%)  |
| 3   | OMC  | L3    | 1340 | 3    | 19,22,23     | 0.60 | 0        | 25,31,34    | 0.74 | 0        |
| 3   | PSU  | L3    | 4552 | 3    | 18,21,22     | 1.05 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | PSU  | L3    | 1683 | 3    | 18,21,22     | 1.07 | 2 (11%)  | 21,30,33    | 2.04 | 5 (23%)  |
| 3   | A2M  | L3    | 2363 | 55,3 | 22,25,26     | 0.89 | 1 (4%)   | 30,36,39    | 2.01 | 7 (23%)  |
| 3   | PSU  | L3    | 4628 | 3    | 18,21,22     | 1.06 | 2 (11%)  | 21,30,33    | 1.93 | 6 (28%)  |
| 3   | OMU  | L3    | 4498 | 3    | 19,22,23     | 2.11 | 7 (36%)  | 25,31,34    | 1.79 | 5 (20%)  |
| 3   | OMC  | L3    | 2861 | 3    | 19,22,23     | 0.54 | 0        | 25,31,34    | 0.69 | 1 (4%)   |
| 3   | OMG  | L3    | 2424 | 3    | 23,26,27     | 0.52 | 0        | 32,38,41    | 0.44 | 0        |
| 3   | PSU  | L3    | 3715 | 3    | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 1.97 | 6 (28%)  |
| 3   | PSU  | L3    | 3844 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.97 | 5 (23%)  |
| 3   | OMU  | L3    | 4227 | 3    | 19,22,23     | 1.99 | 6 (31%)  | 25,31,34    | 1.86 | 4 (16%)  |
| 3   | A2M  | L3    | 3830 | 3    | 22,25,26     | 0.89 | 0        | 30,36,39    | 2.06 | 7 (23%)  |
| 3   | A2M  | L3    | 400  | 3    | 22,25,26     | 0.86 | 0        | 30,36,39    | 2.04 | 7 (23%)  |
| 3   | A2M  | L3    | 3825 | 3    | 22,25,26     | 0.88 | 0        | 30,36,39    | 2.10 | 7 (23%)  |
| 3   | PSU  | L3    | 4579 | 3    | 18,21,22     | 1.05 | 1 (5%)   | 21,30,33    | 1.90 | 4 (19%)  |
| 3   | OMU  | L3    | 4306 | 3    | 19,22,23     | 2.00 | 6 (31%)  | 25,31,34    | 1.91 | 4 (16%)  |
| 3   | OMC  | L3    | 2804 | 3    | 19,22,23     | 0.58 | 0        | 25,31,34    | 0.66 | 0        |
| 3   | PSU  | L3    | 1862 | 3    | 18,21,22     | 1.10 | 2 (11%)  | 21,30,33    | 1.98 | 5 (23%)  |
| 3   | PSU  | L3    | 3639 | 3    | 18,21,22     | 1.05 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 23  | HIC  | LN    | 245  | 23   | 10,11,12     | 1.49 | 1 (10%)  | 9,14,16     | 1.22 | 1 (11%)  |
| 3   | A2M  | L3    | 3724 | 3    | 22,25,26     | 0.88 | 0        | 30,36,39    | 2.05 | 7 (23%)  |
| 3   | A2M  | L3    | 4571 | 3    | 22,25,26     | 0.86 | 0        | 30,36,39    | 2.00 | 7 (23%)  |
| 3   | PSU  | L3    | 4521 | 3    | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.94 | 4 (19%)  |
| 3   | OMG  | L3    | 3627 | 3    | 23,26,27     | 0.50 | 0        | 32,38,41    | 0.58 | 0        |
| 3   | PSU  | L3    | 3730 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.93 | 4 (19%)  |
| 3   | PSU  | L3    | 1792 | 3    | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.92 | 5 (23%)  |
| 3   | OMG  | L3    | 1625 | 3    | 23,26,27     | 0.52 | 0        | 32,38,41    | 0.48 | 0        |
| 3   | OMG  | L3    | 2876 | 3    | 23,26,27     | 0.48 | 0        | 32,38,41    | 0.45 | 0        |
| 3   | OMC  | L3    | 2422 | 55,3 | 19,22,23     | 0.55 | 0        | 25,31,34    | 0.68 | 0        |
| 3   | UR3  | L3    | 4530 | 3    | 19,22,23     | 1.15 | 3 (15%)  | 26,32,35    | 1.53 | 2 (7%)   |
| 3   | PSU  | L3    | 1536 | 3    | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.94 | 4 (19%)  |
| 3   | 6MZ  | L3    | 4220 | 3    | 22,25,26     | 1.17 | 2 (9%)   | 29,36,39    | 2.19 | 9 (31%)  |
| 3   | PSU  | L3    | 3853 | 3    | 18,21,22     | 1.04 | 1 (5%)   | 21,30,33    | 1.88 | 4 (19%)  |
| 3   | PSU  | L3    | 2508 | 3    | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.88 | 4 (19%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | L3    | 1582 | 3    | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 2.00 | 5 (23%)  |
| 3   | PSU  | L3    | 2839 | 3    | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.89 | 4 (19%)  |
| 3   | OMU  | L3    | 4620 | 3    | 19,22,23     | 1.95 | 6 (31%)  | 25,31,34    | 1.64 | 4 (16%)  |
| 3   | PSU  | L3    | 4312 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.97 | 5 (23%)  |
| 3   | PSU  | L3    | 5001 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.87 | 4 (19%)  |
| 3   | OMG  | L3    | 4623 | 3    | 23,26,27     | 0.49 | 0        | 32,38,41    | 0.56 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | A2M  | L3    | 1326 | 3    | -       | 3/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4576 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 4228 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4299 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | L3    | 3925 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 4500 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 4673 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 1524 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3851 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 4403 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 4499 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4293 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 3867 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4361 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 4353 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 2401 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 4456 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 3637 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 4493 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 398  | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3734 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | PSU  | L1    | 55   | 2    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 2632 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 2787 | 3    | -       | 5/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 2824 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | OMG  | L3    | 3899 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 2351 | 55,3 | -       | 2/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | OMG  | L3    | 4618 | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L3    | 3701 | 3    | -       | 7/9/27/28  | 0/2/2/2 |
| 39  | PTR  | NR    | 127  | 39   | -       | 1/10/11/13 | 0/1/1/1 |
| 3   | PSU  | L3    | 4471 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L3    | 3887 | 3    | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L3    | 3695 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | OMG  | L1    | 75   | 2    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 3884 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L3    | 1316 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 1677 | 3    | -       | 3/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 4972 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L3    | 3869 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L3    | 4431 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L3    | 2364 | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 3822 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 1860 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L3    | 1534 | 55,3 | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L3    | 1522 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L3    | 3841 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L3    | 4532 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L3    | 4536 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMG  | L3    | 4637 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L3    | 4590 | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | 1MA  | L3    | 1322 | 3    | -       | 0/7/25/26  | 0/3/3/3 |
| 3   | OMG  | L3    | 4392 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 4689 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMU  | L3    | 2415 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | A2M  | L3    | 4523 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L3    | 1871 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMU  | L3    | 2837 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L3    | 3920 | 55,3 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L3    | 4370 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L3    | 2815 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L3    | 3744 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 4296 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 4457 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L3    | 4494 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L1    | 69   | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L3    | 3718 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 4636 | 3    | -       | 1/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | OMC  | L3    | 2365 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 5010 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L3    | 1340 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 4552 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 1683 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 2363 | 55,3 | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4628 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | L3    | 4498 | 3    | -       | 2/9/27/28 | 0/2/2/2 |
| 3   | OMC  | L3    | 2861 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | OMG  | L3    | 2424 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3715 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 3844 | 3    | -       | 1/7/25/26 | 0/2/2/2 |
| 3   | OMU  | L3    | 4227 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | A2M  | L3    | 3830 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L3    | 400  | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L3    | 3825 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4579 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | L3    | 4306 | 3    | -       | 4/9/27/28 | 0/2/2/2 |
| 3   | OMC  | L3    | 2804 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 1862 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 3639 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 23  | HIC  | LN    | 245  | 23   | -       | 2/5/6/8   | 0/1/1/1 |
| 3   | A2M  | L3    | 3724 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L3    | 4571 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4521 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 3627 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3730 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 1792 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 1625 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | OMG  | L3    | 2876 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 2422 | 55,3 | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | UR3  | L3    | 4530 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 1536 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | 6MZ  | L3    | 4220 | 3    | -       | 3/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3853 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 2508 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 1582 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 2839 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | L3    | 4620 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 4312 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 5001 | 3    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | OMG  | L3    | 4623 | 3    | -       | 0/9/27/28 | 0/3/3/3 |

All (113) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | L3    | 4498 | OMU  | C6-N1 | 4.88  | 1.49        | 1.38     |
| 3   | L3    | 2415 | OMU  | C6-N1 | 4.66  | 1.49        | 1.38     |
| 3   | L3    | 2837 | OMU  | C6-N1 | 4.66  | 1.49        | 1.38     |
| 3   | L3    | 4306 | OMU  | C6-N1 | 4.64  | 1.49        | 1.38     |
| 3   | L3    | 4620 | OMU  | C6-N1 | 4.57  | 1.49        | 1.38     |
| 3   | L3    | 4227 | OMU  | C6-N1 | 4.54  | 1.48        | 1.38     |
| 39  | NR    | 127  | PTR  | OH-CZ | -4.53 | 1.30        | 1.40     |
| 3   | L3    | 3925 | OMU  | C6-N1 | 4.51  | 1.48        | 1.38     |
| 3   | L3    | 4498 | OMU  | C2-N1 | 4.36  | 1.45        | 1.38     |
| 3   | L3    | 2837 | OMU  | C2-N1 | 4.18  | 1.45        | 1.38     |
| 3   | L3    | 4498 | OMU  | C5-C4 | 4.18  | 1.52        | 1.43     |
| 3   | L3    | 4306 | OMU  | C2-N1 | 4.16  | 1.45        | 1.38     |
| 3   | L3    | 2415 | OMU  | C2-N1 | 4.13  | 1.44        | 1.38     |
| 3   | L3    | 3925 | OMU  | C2-N1 | 4.09  | 1.44        | 1.38     |
| 3   | L3    | 4620 | OMU  | C2-N1 | 4.05  | 1.44        | 1.38     |
| 3   | L3    | 2837 | OMU  | C5-C4 | 4.04  | 1.52        | 1.43     |
| 3   | L3    | 4227 | OMU  | C2-N1 | 4.03  | 1.44        | 1.38     |
| 3   | L3    | 2415 | OMU  | C5-C4 | 4.00  | 1.52        | 1.43     |
| 3   | L3    | 4220 | 6MZ  | C6-N6 | 3.99  | 1.38        | 1.34     |
| 3   | L3    | 3925 | OMU  | C5-C4 | 3.88  | 1.52        | 1.43     |
| 3   | L3    | 4227 | OMU  | C5-C4 | 3.87  | 1.52        | 1.43     |
| 3   | L3    | 3822 | PSU  | C6-C5 | 3.80  | 1.39        | 1.35     |
| 3   | L3    | 4431 | PSU  | C6-C5 | 3.75  | 1.39        | 1.35     |
| 3   | L3    | 4306 | OMU  | C5-C4 | 3.67  | 1.51        | 1.43     |
| 3   | L3    | 5001 | PSU  | C6-C5 | 3.65  | 1.39        | 1.35     |
| 3   | L3    | 3715 | PSU  | C6-C5 | 3.60  | 1.39        | 1.35     |
| 3   | L3    | 4620 | OMU  | C5-C4 | 3.60  | 1.51        | 1.43     |
| 3   | L3    | 4636 | PSU  | C6-C5 | 3.58  | 1.39        | 1.35     |
| 3   | L3    | 1860 | PSU  | C6-C5 | 3.52  | 1.39        | 1.35     |
| 3   | L3    | 3734 | PSU  | C6-C5 | 3.51  | 1.39        | 1.35     |
| 3   | L3    | 3695 | PSU  | C6-C5 | 3.48  | 1.39        | 1.35     |
| 3   | L3    | 3730 | PSU  | C6-C5 | 3.48  | 1.39        | 1.35     |
| 3   | L3    | 4457 | PSU  | C6-C5 | 3.48  | 1.39        | 1.35     |
| 3   | L3    | 4403 | PSU  | C6-C5 | 3.48  | 1.39        | 1.35     |
| 3   | L3    | 5010 | PSU  | C6-C5 | 3.47  | 1.39        | 1.35     |
| 3   | L3    | 4972 | PSU  | C6-C5 | 3.47  | 1.39        | 1.35     |
| 3   | L3    | 4673 | PSU  | C6-C5 | 3.46  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | L3    | 4532 | PSU  | C6-C5  | 3.46  | 1.39        | 1.35     |
| 3   | L3    | 3844 | PSU  | C6-C5  | 3.45  | 1.39        | 1.35     |
| 3   | L3    | 2508 | PSU  | C6-C5  | 3.44  | 1.39        | 1.35     |
| 3   | L3    | 3851 | PSU  | C6-C5  | 3.44  | 1.39        | 1.35     |
| 3   | L3    | 1862 | PSU  | C6-C5  | 3.43  | 1.39        | 1.35     |
| 3   | L3    | 2632 | PSU  | C6-C5  | 3.43  | 1.39        | 1.35     |
| 3   | L3    | 2839 | PSU  | C6-C5  | 3.40  | 1.39        | 1.35     |
| 3   | L3    | 4521 | PSU  | C6-C5  | 3.38  | 1.39        | 1.35     |
| 2   | L1    | 69   | PSU  | C6-C5  | 3.37  | 1.39        | 1.35     |
| 3   | L3    | 3884 | PSU  | C6-C5  | 3.37  | 1.39        | 1.35     |
| 3   | L3    | 4576 | PSU  | C6-C5  | 3.36  | 1.39        | 1.35     |
| 3   | L3    | 4353 | PSU  | C6-C5  | 3.35  | 1.39        | 1.35     |
| 2   | L1    | 55   | PSU  | C6-C5  | 3.34  | 1.39        | 1.35     |
| 3   | L3    | 4493 | PSU  | C6-C5  | 3.34  | 1.39        | 1.35     |
| 3   | L3    | 4312 | PSU  | C6-C5  | 3.32  | 1.39        | 1.35     |
| 3   | L3    | 1792 | PSU  | C6-C5  | 3.32  | 1.39        | 1.35     |
| 3   | L3    | 4471 | PSU  | C6-C5  | 3.31  | 1.39        | 1.35     |
| 3   | L3    | 3637 | PSU  | C6-C5  | 3.31  | 1.39        | 1.35     |
| 3   | L3    | 1536 | PSU  | C6-C5  | 3.31  | 1.39        | 1.35     |
| 3   | L3    | 4552 | PSU  | C6-C5  | 3.30  | 1.38        | 1.35     |
| 3   | L3    | 3853 | PSU  | C6-C5  | 3.29  | 1.38        | 1.35     |
| 3   | L3    | 3920 | PSU  | C6-C5  | 3.24  | 1.38        | 1.35     |
| 3   | L3    | 1582 | PSU  | C6-C5  | 3.23  | 1.38        | 1.35     |
| 3   | L3    | 4500 | PSU  | C6-C5  | 3.22  | 1.38        | 1.35     |
| 3   | L3    | 4579 | PSU  | C6-C5  | 3.21  | 1.38        | 1.35     |
| 3   | L3    | 4296 | PSU  | C6-C5  | 3.20  | 1.38        | 1.35     |
| 3   | L3    | 3639 | PSU  | C6-C5  | 3.19  | 1.38        | 1.35     |
| 3   | L3    | 1683 | PSU  | C6-C5  | 3.14  | 1.38        | 1.35     |
| 3   | L3    | 4628 | PSU  | C6-C5  | 3.13  | 1.38        | 1.35     |
| 3   | L3    | 4689 | PSU  | C6-C5  | 3.13  | 1.38        | 1.35     |
| 3   | L3    | 4361 | PSU  | C6-C5  | 3.10  | 1.38        | 1.35     |
| 3   | L3    | 4530 | UR3  | C2-N1  | -3.04 | 1.34        | 1.38     |
| 3   | L3    | 4306 | OMU  | O4-C4  | -3.01 | 1.18        | 1.24     |
| 23  | LN    | 245  | HIC  | CD2-CG | 3.00  | 1.41        | 1.36     |
| 3   | L3    | 4293 | PSU  | C6-C5  | 2.96  | 1.38        | 1.35     |
| 3   | L3    | 4299 | PSU  | C6-C5  | 2.90  | 1.38        | 1.35     |
| 3   | L3    | 4227 | OMU  | O4-C4  | -2.89 | 1.18        | 1.24     |
| 3   | L3    | 4620 | OMU  | O4-C4  | -2.89 | 1.18        | 1.24     |
| 3   | L3    | 4530 | UR3  | C4-N3  | -2.88 | 1.34        | 1.40     |
| 3   | L3    | 3925 | OMU  | O4-C4  | -2.82 | 1.19        | 1.24     |
| 3   | L3    | 2415 | OMU  | O4-C4  | -2.80 | 1.19        | 1.24     |
| 3   | L3    | 2837 | OMU  | O4-C4  | -2.79 | 1.19        | 1.24     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | L3    | 1677 | PSU  | C6-C5 | 2.76  | 1.38        | 1.35     |
| 3   | L3    | 4498 | OMU  | O4-C4 | -2.71 | 1.19        | 1.24     |
| 3   | L3    | 4498 | OMU  | C2-N3 | 2.64  | 1.42        | 1.38     |
| 3   | L3    | 4306 | OMU  | O2-C2 | -2.56 | 1.18        | 1.23     |
| 3   | L3    | 2837 | OMU  | C2-N3 | 2.54  | 1.42        | 1.38     |
| 3   | L3    | 4227 | OMU  | O2-C2 | -2.52 | 1.18        | 1.23     |
| 3   | L3    | 2415 | OMU  | C2-N3 | 2.43  | 1.42        | 1.38     |
| 3   | L3    | 2415 | OMU  | O2-C2 | -2.40 | 1.18        | 1.23     |
| 3   | L3    | 3925 | OMU  | O2-C2 | -2.32 | 1.19        | 1.23     |
| 3   | L3    | 4620 | OMU  | O2-C2 | -2.27 | 1.19        | 1.23     |
| 3   | L3    | 2837 | OMU  | O2-C2 | -2.27 | 1.19        | 1.23     |
| 3   | L3    | 3925 | OMU  | C2-N3 | 2.26  | 1.41        | 1.38     |
| 3   | L3    | 4530 | UR3  | C2-N3 | -2.21 | 1.34        | 1.39     |
| 3   | L3    | 2787 | A2M  | C5-N7 | -2.20 | 1.35        | 1.39     |
| 3   | L3    | 4306 | OMU  | C2-N3 | 2.19  | 1.41        | 1.38     |
| 3   | L3    | 3718 | A2M  | C5-N7 | -2.18 | 1.35        | 1.39     |
| 3   | L3    | 4220 | 6MZ  | C5-N7 | -2.17 | 1.35        | 1.39     |
| 3   | L3    | 1534 | A2M  | C5-N7 | -2.14 | 1.35        | 1.39     |
| 3   | L3    | 4227 | OMU  | C2-N3 | 2.14  | 1.41        | 1.38     |
| 3   | L3    | 4498 | OMU  | O2-C2 | -2.13 | 1.19        | 1.23     |
| 3   | L3    | 4620 | OMU  | C2-N3 | 2.13  | 1.41        | 1.38     |
| 2   | L1    | 55   | PSU  | C4-C5 | -2.09 | 1.38        | 1.44     |
| 3   | L3    | 4299 | PSU  | C4-C5 | -2.09 | 1.38        | 1.44     |
| 3   | L3    | 1683 | PSU  | C4-C5 | -2.07 | 1.38        | 1.44     |
| 3   | L3    | 4498 | OMU  | C4-N3 | 2.07  | 1.42        | 1.38     |
| 3   | L3    | 3920 | PSU  | C4-C5 | -2.06 | 1.38        | 1.44     |
| 3   | L3    | 4628 | PSU  | C4-C5 | -2.06 | 1.38        | 1.44     |
| 3   | L3    | 2363 | A2M  | C5-N7 | -2.06 | 1.35        | 1.39     |
| 3   | L3    | 4673 | PSU  | C4-C5 | -2.05 | 1.38        | 1.44     |
| 3   | L3    | 4361 | PSU  | C4-C5 | -2.04 | 1.38        | 1.44     |
| 3   | L3    | 2415 | OMU  | C4-N3 | 2.03  | 1.42        | 1.38     |
| 3   | L3    | 2837 | OMU  | C4-N3 | 2.02  | 1.42        | 1.38     |
| 3   | L3    | 4296 | PSU  | C4-C5 | -2.02 | 1.38        | 1.44     |
| 3   | L3    | 1862 | PSU  | C4-C5 | -2.01 | 1.38        | 1.44     |

All (411) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L3    | 4220 | 6MZ  | C5-C4-N3 | -5.86 | 118.65      | 126.72   |
| 3   | L3    | 2815 | A2M  | C5-C4-N3 | -5.77 | 118.77      | 126.72   |
| 3   | L3    | 3825 | A2M  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 3   | L3    | 3925 | OMU  | C4-N3-C2 | -5.69 | 119.55      | 126.61   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L3    | 2787 | A2M  | C5-C4-N3 | -5.66 | 118.92      | 126.72   |
| 3   | L3    | 3718 | A2M  | C5-C4-N3 | -5.63 | 118.96      | 126.72   |
| 3   | L3    | 4227 | OMU  | C4-N3-C2 | -5.62 | 119.63      | 126.61   |
| 3   | L3    | 4306 | OMU  | C4-N3-C2 | -5.58 | 119.69      | 126.61   |
| 3   | L3    | 2837 | OMU  | C4-N3-C2 | -5.56 | 119.70      | 126.61   |
| 3   | L3    | 1534 | A2M  | C5-C4-N3 | -5.54 | 119.08      | 126.72   |
| 3   | L3    | 4523 | A2M  | C5-C4-N3 | -5.53 | 119.11      | 126.72   |
| 3   | L3    | 1326 | A2M  | C5-C4-N3 | -5.52 | 119.11      | 126.72   |
| 3   | L3    | 1524 | A2M  | C5-C4-N3 | -5.52 | 119.12      | 126.72   |
| 3   | L3    | 4530 | UR3  | C4-N3-C2 | -5.52 | 120.14      | 124.58   |
| 3   | L3    | 4571 | A2M  | C5-C4-N3 | -5.48 | 119.17      | 126.72   |
| 3   | L3    | 3867 | A2M  | C5-C4-N3 | -5.45 | 119.21      | 126.72   |
| 3   | L3    | 2415 | OMU  | C4-N3-C2 | -5.44 | 119.86      | 126.61   |
| 3   | L3    | 3830 | A2M  | C5-C4-N3 | -5.43 | 119.24      | 126.72   |
| 3   | L3    | 2363 | A2M  | C5-C4-N3 | -5.42 | 119.25      | 126.72   |
| 3   | L3    | 4498 | OMU  | C4-N3-C2 | -5.42 | 119.89      | 126.61   |
| 3   | L3    | 398  | A2M  | C5-C4-N3 | -5.36 | 119.34      | 126.72   |
| 3   | L3    | 2401 | A2M  | C5-C4-N3 | -5.26 | 119.47      | 126.72   |
| 3   | L3    | 3724 | A2M  | C5-C4-N3 | -5.23 | 119.52      | 126.72   |
| 3   | L3    | 400  | A2M  | C5-C4-N3 | -5.22 | 119.53      | 126.72   |
| 3   | L3    | 1871 | A2M  | C5-C4-N3 | -5.20 | 119.56      | 126.72   |
| 3   | L3    | 4353 | PSU  | N1-C2-N3 | 5.19  | 120.64      | 115.17   |
| 3   | L3    | 4636 | PSU  | C4-N3-C2 | -5.18 | 119.24      | 126.37   |
| 3   | L3    | 4299 | PSU  | C4-N3-C2 | -5.16 | 119.27      | 126.37   |
| 3   | L3    | 4636 | PSU  | N1-C2-N3 | 5.15  | 120.60      | 115.17   |
| 3   | L3    | 1683 | PSU  | N1-C2-N3 | 5.13  | 120.58      | 115.17   |
| 3   | L3    | 1582 | PSU  | C4-N3-C2 | -5.10 | 119.34      | 126.37   |
| 3   | L3    | 4353 | PSU  | C4-N3-C2 | -5.09 | 119.36      | 126.37   |
| 3   | L3    | 3637 | PSU  | C4-N3-C2 | -5.07 | 119.39      | 126.37   |
| 3   | L3    | 4299 | PSU  | N1-C2-N3 | 5.06  | 120.50      | 115.17   |
| 3   | L3    | 3637 | PSU  | N1-C2-N3 | 5.03  | 120.48      | 115.17   |
| 3   | L3    | 4361 | PSU  | N1-C2-N3 | 5.03  | 120.47      | 115.17   |
| 3   | L3    | 4312 | PSU  | N1-C2-N3 | 5.01  | 120.45      | 115.17   |
| 3   | L3    | 4296 | PSU  | C4-N3-C2 | -5.01 | 119.47      | 126.37   |
| 3   | L3    | 4532 | PSU  | C4-N3-C2 | -4.98 | 119.51      | 126.37   |
| 3   | L3    | 4493 | PSU  | C4-N3-C2 | -4.97 | 119.52      | 126.37   |
| 3   | L3    | 4532 | PSU  | N1-C2-N3 | 4.97  | 120.41      | 115.17   |
| 3   | L3    | 4689 | PSU  | N1-C2-N3 | 4.97  | 120.41      | 115.17   |
| 3   | L3    | 1683 | PSU  | C4-N3-C2 | -4.96 | 119.54      | 126.37   |
| 3   | L3    | 4500 | PSU  | C4-N3-C2 | -4.96 | 119.54      | 126.37   |
| 3   | L3    | 4361 | PSU  | C4-N3-C2 | -4.95 | 119.55      | 126.37   |
| 3   | L3    | 1582 | PSU  | N1-C2-N3 | 4.94  | 120.38      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L3    | 4521 | PSU  | N1-C2-N3 | 4.93  | 120.37      | 115.17   |
| 3   | L3    | 4471 | PSU  | N1-C2-N3 | 4.93  | 120.36      | 115.17   |
| 2   | L1    | 69   | PSU  | N1-C2-N3 | 4.92  | 120.36      | 115.17   |
| 3   | L3    | 1677 | PSU  | C4-N3-C2 | -4.92 | 119.59      | 126.37   |
| 3   | L3    | 4552 | PSU  | N1-C2-N3 | 4.92  | 120.36      | 115.17   |
| 3   | L3    | 4500 | PSU  | N1-C2-N3 | 4.91  | 120.35      | 115.17   |
| 3   | L3    | 3851 | PSU  | N1-C2-N3 | 4.91  | 120.34      | 115.17   |
| 3   | L3    | 1862 | PSU  | C4-N3-C2 | -4.90 | 119.61      | 126.37   |
| 3   | L3    | 3851 | PSU  | C4-N3-C2 | -4.90 | 119.61      | 126.37   |
| 3   | L3    | 3695 | PSU  | C4-N3-C2 | -4.90 | 119.62      | 126.37   |
| 3   | L3    | 4471 | PSU  | C4-N3-C2 | -4.90 | 119.62      | 126.37   |
| 3   | L3    | 1860 | PSU  | N1-C2-N3 | 4.90  | 120.34      | 115.17   |
| 3   | L3    | 3844 | PSU  | N1-C2-N3 | 4.90  | 120.33      | 115.17   |
| 3   | L3    | 3844 | PSU  | C4-N3-C2 | -4.89 | 119.63      | 126.37   |
| 3   | L3    | 4972 | PSU  | C4-N3-C2 | -4.89 | 119.63      | 126.37   |
| 3   | L3    | 4673 | PSU  | N1-C2-N3 | 4.89  | 120.32      | 115.17   |
| 3   | L3    | 4493 | PSU  | N1-C2-N3 | 4.88  | 120.31      | 115.17   |
| 2   | L1    | 69   | PSU  | C4-N3-C2 | -4.88 | 119.65      | 126.37   |
| 3   | L3    | 4972 | PSU  | N1-C2-N3 | 4.87  | 120.31      | 115.17   |
| 3   | L3    | 3715 | PSU  | N1-C2-N3 | 4.87  | 120.31      | 115.17   |
| 3   | L3    | 3734 | PSU  | C4-N3-C2 | -4.87 | 119.67      | 126.37   |
| 3   | L3    | 1862 | PSU  | N1-C2-N3 | 4.87  | 120.30      | 115.17   |
| 3   | L3    | 1860 | PSU  | C4-N3-C2 | -4.87 | 119.67      | 126.37   |
| 3   | L3    | 4521 | PSU  | C4-N3-C2 | -4.86 | 119.67      | 126.37   |
| 3   | L3    | 1536 | PSU  | C4-N3-C2 | -4.86 | 119.68      | 126.37   |
| 3   | L3    | 3639 | PSU  | C4-N3-C2 | -4.86 | 119.68      | 126.37   |
| 3   | L3    | 4296 | PSU  | N1-C2-N3 | 4.85  | 120.28      | 115.17   |
| 3   | L3    | 4312 | PSU  | C4-N3-C2 | -4.85 | 119.69      | 126.37   |
| 3   | L3    | 4403 | PSU  | N1-C2-N3 | 4.84  | 120.28      | 115.17   |
| 3   | L3    | 2632 | PSU  | C4-N3-C2 | -4.84 | 119.70      | 126.37   |
| 3   | L3    | 4403 | PSU  | C4-N3-C2 | -4.84 | 119.70      | 126.37   |
| 3   | L3    | 2508 | PSU  | C4-N3-C2 | -4.84 | 119.70      | 126.37   |
| 3   | L3    | 4431 | PSU  | C4-N3-C2 | -4.84 | 119.70      | 126.37   |
| 3   | L3    | 4689 | PSU  | C4-N3-C2 | -4.83 | 119.71      | 126.37   |
| 3   | L3    | 3730 | PSU  | C4-N3-C2 | -4.83 | 119.72      | 126.37   |
| 3   | L3    | 3822 | PSU  | N1-C2-N3 | 4.83  | 120.26      | 115.17   |
| 3   | L3    | 4552 | PSU  | C4-N3-C2 | -4.82 | 119.72      | 126.37   |
| 3   | L3    | 4457 | PSU  | N1-C2-N3 | 4.82  | 120.25      | 115.17   |
| 3   | L3    | 1792 | PSU  | N1-C2-N3 | 4.81  | 120.25      | 115.17   |
| 3   | L3    | 3825 | A2M  | N3-C4-N9 | 4.80  | 135.34      | 127.17   |
| 3   | L3    | 4673 | PSU  | C4-N3-C2 | -4.80 | 119.75      | 126.37   |
| 3   | L3    | 4590 | A2M  | C5-C4-N3 | -4.80 | 120.11      | 126.72   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L3    | 1792 | PSU  | C4-N3-C2 | -4.80 | 119.77      | 126.37   |
| 3   | L3    | 1536 | PSU  | N1-C2-N3 | 4.80  | 120.23      | 115.17   |
| 2   | L1    | 55   | PSU  | C4-N3-C2 | -4.79 | 119.77      | 126.37   |
| 3   | L3    | 3639 | PSU  | N1-C2-N3 | 4.79  | 120.22      | 115.17   |
| 3   | L3    | 3884 | PSU  | N1-C2-N3 | 4.78  | 120.21      | 115.17   |
| 3   | L3    | 5010 | PSU  | N1-C2-N3 | 4.78  | 120.21      | 115.17   |
| 3   | L3    | 4576 | PSU  | C4-N3-C2 | -4.77 | 119.80      | 126.37   |
| 3   | L3    | 3715 | PSU  | C4-N3-C2 | -4.77 | 119.80      | 126.37   |
| 3   | L3    | 2839 | PSU  | N1-C2-N3 | 4.76  | 120.19      | 115.17   |
| 3   | L3    | 3730 | PSU  | N1-C2-N3 | 4.76  | 120.19      | 115.17   |
| 3   | L3    | 3734 | PSU  | N1-C2-N3 | 4.75  | 120.18      | 115.17   |
| 3   | L3    | 4431 | PSU  | N1-C2-N3 | 4.75  | 120.18      | 115.17   |
| 3   | L3    | 4576 | PSU  | N1-C2-N3 | 4.75  | 120.18      | 115.17   |
| 3   | L3    | 5001 | PSU  | N1-C2-N3 | 4.75  | 120.17      | 115.17   |
| 3   | L3    | 1677 | PSU  | N1-C2-N3 | 4.73  | 120.16      | 115.17   |
| 3   | L3    | 3695 | PSU  | N1-C2-N3 | 4.73  | 120.16      | 115.17   |
| 3   | L3    | 3920 | PSU  | C4-N3-C2 | -4.73 | 119.85      | 126.37   |
| 3   | L3    | 4457 | PSU  | C4-N3-C2 | -4.73 | 119.86      | 126.37   |
| 3   | L3    | 4628 | PSU  | C4-N3-C2 | -4.73 | 119.86      | 126.37   |
| 3   | L3    | 2632 | PSU  | N1-C2-N3 | 4.73  | 120.15      | 115.17   |
| 3   | L3    | 5010 | PSU  | C4-N3-C2 | -4.72 | 119.86      | 126.37   |
| 3   | L3    | 4628 | PSU  | N1-C2-N3 | 4.72  | 120.14      | 115.17   |
| 3   | L3    | 4220 | 6MZ  | N3-C4-N9 | 4.71  | 135.18      | 127.17   |
| 3   | L3    | 3853 | PSU  | C4-N3-C2 | -4.71 | 119.89      | 126.37   |
| 3   | L3    | 4579 | PSU  | N1-C2-N3 | 4.70  | 120.13      | 115.17   |
| 3   | L3    | 3920 | PSU  | N1-C2-N3 | 4.68  | 120.10      | 115.17   |
| 3   | L3    | 2815 | A2M  | N3-C4-N9 | 4.67  | 135.11      | 127.17   |
| 3   | L3    | 3822 | PSU  | C4-N3-C2 | -4.65 | 119.96      | 126.37   |
| 3   | L3    | 2508 | PSU  | N1-C2-N3 | 4.64  | 120.06      | 115.17   |
| 3   | L3    | 4579 | PSU  | C4-N3-C2 | -4.64 | 119.98      | 126.37   |
| 3   | L3    | 2839 | PSU  | C4-N3-C2 | -4.63 | 120.00      | 126.37   |
| 3   | L3    | 3718 | A2M  | N3-C4-N9 | 4.63  | 135.04      | 127.17   |
| 3   | L3    | 3853 | PSU  | N1-C2-N3 | 4.62  | 120.04      | 115.17   |
| 3   | L3    | 3867 | A2M  | N3-C4-N9 | 4.62  | 135.02      | 127.17   |
| 3   | L3    | 3884 | PSU  | C4-N3-C2 | -4.62 | 120.01      | 126.37   |
| 2   | L1    | 55   | PSU  | N1-C2-N3 | 4.61  | 120.03      | 115.17   |
| 3   | L3    | 5001 | PSU  | C4-N3-C2 | -4.61 | 120.02      | 126.37   |
| 3   | L3    | 2787 | A2M  | N3-C4-N9 | 4.59  | 134.98      | 127.17   |
| 3   | L3    | 4523 | A2M  | N3-C4-N9 | 4.58  | 134.95      | 127.17   |
| 3   | L3    | 4293 | PSU  | C4-N3-C2 | -4.55 | 120.10      | 126.37   |
| 3   | L3    | 1524 | A2M  | N3-C4-N9 | 4.54  | 134.88      | 127.17   |
| 3   | L3    | 2363 | A2M  | N3-C4-N9 | 4.52  | 134.85      | 127.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L3    | 4293 | PSU  | N1-C2-N3 | 4.50  | 119.92      | 115.17   |
| 3   | L3    | 4571 | A2M  | N3-C4-N9 | 4.49  | 134.81      | 127.17   |
| 3   | L3    | 398  | A2M  | N3-C4-N9 | 4.47  | 134.77      | 127.17   |
| 3   | L3    | 1534 | A2M  | N3-C4-N9 | 4.46  | 134.75      | 127.17   |
| 3   | L3    | 3830 | A2M  | N3-C4-N9 | 4.46  | 134.75      | 127.17   |
| 3   | L3    | 4306 | OMU  | N3-C2-N1 | 4.44  | 120.67      | 114.89   |
| 3   | L3    | 1326 | A2M  | N3-C4-N9 | 4.43  | 134.71      | 127.17   |
| 3   | L3    | 4590 | A2M  | N3-C2-N1 | -4.41 | 121.91      | 128.58   |
| 3   | L3    | 3724 | A2M  | N3-C4-N9 | 4.39  | 134.63      | 127.17   |
| 3   | L3    | 1871 | A2M  | N3-C4-N9 | 4.37  | 134.60      | 127.17   |
| 3   | L3    | 3724 | A2M  | N3-C2-N1 | -4.36 | 121.98      | 128.58   |
| 3   | L3    | 4620 | OMU  | C4-N3-C2 | -4.34 | 121.23      | 126.61   |
| 3   | L3    | 2401 | A2M  | N3-C4-N9 | 4.33  | 134.52      | 127.17   |
| 3   | L3    | 400  | A2M  | N3-C4-N9 | 4.33  | 134.52      | 127.17   |
| 3   | L3    | 1871 | A2M  | N3-C2-N1 | -4.30 | 122.07      | 128.58   |
| 3   | L3    | 2401 | A2M  | N3-C2-N1 | -4.24 | 122.17      | 128.58   |
| 3   | L3    | 1524 | A2M  | N3-C2-N1 | -4.23 | 122.18      | 128.58   |
| 3   | L3    | 400  | A2M  | N3-C2-N1 | -4.22 | 122.19      | 128.58   |
| 3   | L3    | 398  | A2M  | N3-C2-N1 | -4.20 | 122.23      | 128.58   |
| 3   | L3    | 2415 | OMU  | N3-C2-N1 | 4.19  | 120.34      | 114.89   |
| 3   | L3    | 2837 | OMU  | N3-C2-N1 | 4.18  | 120.33      | 114.89   |
| 3   | L3    | 2363 | A2M  | N3-C2-N1 | -4.14 | 122.31      | 128.58   |
| 3   | L3    | 1326 | A2M  | N3-C2-N1 | -4.14 | 122.31      | 128.58   |
| 3   | L3    | 3925 | OMU  | N3-C2-N1 | 4.14  | 120.28      | 114.89   |
| 3   | L3    | 4523 | A2M  | N3-C2-N1 | -4.13 | 122.32      | 128.58   |
| 3   | L3    | 3830 | A2M  | N3-C2-N1 | -4.13 | 122.33      | 128.58   |
| 3   | L3    | 2787 | A2M  | N3-C2-N1 | -4.09 | 122.39      | 128.58   |
| 3   | L3    | 4227 | OMU  | C5-C4-N3 | 4.09  | 120.53      | 114.80   |
| 3   | L3    | 3867 | A2M  | N3-C2-N1 | -4.09 | 122.39      | 128.58   |
| 3   | L3    | 2815 | A2M  | N3-C2-N1 | -4.08 | 122.40      | 128.58   |
| 3   | L3    | 4498 | OMU  | N3-C2-N1 | 4.07  | 120.19      | 114.89   |
| 3   | L3    | 3825 | A2M  | N3-C2-N1 | -4.04 | 122.47      | 128.58   |
| 3   | L3    | 4571 | A2M  | N3-C2-N1 | -4.03 | 122.48      | 128.58   |
| 3   | L3    | 1534 | A2M  | N3-C2-N1 | -3.98 | 122.55      | 128.58   |
| 3   | L3    | 3925 | OMU  | C5-C4-N3 | 3.95  | 120.34      | 114.80   |
| 3   | L3    | 4227 | OMU  | N3-C2-N1 | 3.90  | 119.97      | 114.89   |
| 3   | L3    | 4220 | 6MZ  | N1-C2-N3 | -3.88 | 122.70      | 128.58   |
| 3   | L3    | 4220 | 6MZ  | C5-N7-C8 | 3.84  | 109.48      | 103.45   |
| 3   | L3    | 2815 | A2M  | C5-N7-C8 | 3.80  | 109.42      | 103.45   |
| 3   | L3    | 4590 | A2M  | N3-C4-N9 | 3.78  | 133.59      | 127.17   |
| 3   | L3    | 4306 | OMU  | C5-C4-N3 | 3.78  | 120.09      | 114.80   |
| 3   | L3    | 3825 | A2M  | C5-N7-C8 | 3.78  | 109.39      | 103.45   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | L3    | 2401 | A2M  | C5-N7-C8   | 3.76  | 109.36      | 103.45   |
| 3   | L3    | 1524 | A2M  | C5-N7-C8   | 3.76  | 109.36      | 103.45   |
| 3   | L3    | 3867 | A2M  | C5-N7-C8   | 3.75  | 109.35      | 103.45   |
| 3   | L3    | 400  | A2M  | C5-N7-C8   | 3.74  | 109.33      | 103.45   |
| 3   | L3    | 2815 | A2M  | C2-N3-C4   | 3.73  | 120.95      | 111.83   |
| 3   | L3    | 4523 | A2M  | C5-N7-C8   | 3.73  | 109.31      | 103.45   |
| 3   | L3    | 2787 | A2M  | C5-N7-C8   | 3.73  | 109.31      | 103.45   |
| 3   | L3    | 3830 | A2M  | C5-N7-C8   | 3.72  | 109.30      | 103.45   |
| 3   | L3    | 4590 | A2M  | C5-N7-C8   | 3.72  | 109.30      | 103.45   |
| 3   | L3    | 1326 | A2M  | C5-N7-C8   | 3.72  | 109.30      | 103.45   |
| 3   | L3    | 1871 | A2M  | C5-N7-C8   | 3.72  | 109.29      | 103.45   |
| 3   | L3    | 1534 | A2M  | C5-N7-C8   | 3.72  | 109.29      | 103.45   |
| 3   | L3    | 4498 | OMU  | C5-C4-N3   | 3.71  | 120.00      | 114.80   |
| 3   | L3    | 1524 | A2M  | C2-N3-C4   | 3.71  | 120.89      | 111.83   |
| 3   | L3    | 398  | A2M  | C5-N7-C8   | 3.68  | 109.24      | 103.45   |
| 3   | L3    | 3825 | A2M  | C2-N3-C4   | 3.67  | 120.80      | 111.83   |
| 3   | L3    | 1326 | A2M  | C2-N3-C4   | 3.67  | 120.78      | 111.83   |
| 3   | L3    | 2837 | OMU  | C5-C4-N3   | 3.66  | 119.93      | 114.80   |
| 3   | L3    | 2415 | OMU  | C5-C4-N3   | 3.65  | 119.91      | 114.80   |
| 3   | L3    | 3724 | A2M  | C5-N7-C8   | 3.64  | 109.17      | 103.45   |
| 3   | L3    | 4220 | 6MZ  | C2-N3-C4   | 3.64  | 120.71      | 111.83   |
| 3   | L3    | 4523 | A2M  | C2-N3-C4   | 3.62  | 120.67      | 111.83   |
| 3   | L3    | 2787 | A2M  | C2-N3-C4   | 3.62  | 120.66      | 111.83   |
| 3   | L3    | 2363 | A2M  | C5-N7-C8   | 3.61  | 109.12      | 103.45   |
| 3   | L3    | 1534 | A2M  | C2-N3-C4   | 3.60  | 120.62      | 111.83   |
| 3   | L3    | 2401 | A2M  | C2-N3-C4   | 3.60  | 120.62      | 111.83   |
| 3   | L3    | 3718 | A2M  | N3-C2-N1   | -3.59 | 123.15      | 128.58   |
| 3   | L3    | 4571 | A2M  | C2-N3-C4   | 3.58  | 120.57      | 111.83   |
| 3   | L3    | 4571 | A2M  | C5-N7-C8   | 3.57  | 109.07      | 103.45   |
| 3   | L3    | 3830 | A2M  | C2-N3-C4   | 3.57  | 120.56      | 111.83   |
| 3   | L3    | 3724 | A2M  | C2-N3-C4   | 3.56  | 120.53      | 111.83   |
| 3   | L3    | 398  | A2M  | C2-N3-C4   | 3.56  | 120.53      | 111.83   |
| 3   | L3    | 400  | A2M  | C2-N3-C4   | 3.56  | 120.52      | 111.83   |
| 3   | L3    | 3867 | A2M  | C2-N3-C4   | 3.55  | 120.51      | 111.83   |
| 3   | L3    | 1871 | A2M  | C2-N3-C4   | 3.55  | 120.50      | 111.83   |
| 3   | L3    | 2363 | A2M  | C2-N3-C4   | 3.55  | 120.50      | 111.83   |
| 3   | L3    | 1871 | A2M  | C2'-C1'-N9 | -3.53 | 107.94      | 113.75   |
| 3   | L3    | 4620 | OMU  | C5-C4-N3   | 3.46  | 119.64      | 114.80   |
| 3   | L3    | 4590 | A2M  | C2-N3-C4   | 3.45  | 120.26      | 111.83   |
| 3   | L3    | 4530 | UR3  | C5-C4-N3   | 3.44  | 119.58      | 115.04   |
| 3   | L3    | 4620 | OMU  | N3-C2-N1   | 3.43  | 119.36      | 114.89   |
| 3   | L3    | 3718 | A2M  | C2-N3-C4   | 3.38  | 120.08      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L3    | 3718 | A2M  | C5-N7-C8    | 3.34  | 108.71      | 103.45   |
| 3   | L3    | 4227 | OMU  | O4-C4-C5    | -3.30 | 119.48      | 125.16   |
| 3   | L3    | 3853 | PSU  | O2-C2-N1    | -3.24 | 119.45      | 122.79   |
| 3   | L3    | 4590 | A2M  | C4-C5-N7    | -3.19 | 106.94      | 110.58   |
| 3   | L3    | 2401 | A2M  | C2'-C1'-N9  | -3.16 | 108.54      | 113.75   |
| 3   | L3    | 4500 | PSU  | O2-C2-N1    | -3.16 | 119.53      | 122.79   |
| 3   | L3    | 1683 | PSU  | O2-C2-N1    | -3.16 | 119.53      | 122.79   |
| 3   | L3    | 4220 | 6MZ  | C4-C5-N7    | -3.15 | 106.97      | 110.58   |
| 3   | L3    | 2837 | OMU  | O4-C4-C5    | -3.13 | 119.76      | 125.16   |
| 3   | L3    | 1677 | PSU  | O2-C2-N1    | -3.11 | 119.58      | 122.79   |
| 3   | L3    | 1534 | A2M  | C4-C5-N7    | -3.11 | 107.03      | 110.58   |
| 3   | L3    | 4532 | PSU  | O2-C2-N1    | -3.09 | 119.60      | 122.79   |
| 3   | L3    | 3925 | OMU  | O4-C4-C5    | -3.08 | 119.85      | 125.16   |
| 3   | L3    | 1326 | A2M  | C4-C5-N7    | -3.07 | 107.07      | 110.58   |
| 3   | L3    | 4579 | PSU  | O2-C2-N1    | -3.07 | 119.62      | 122.79   |
| 3   | L3    | 3822 | PSU  | O2-C2-N1    | -3.07 | 119.62      | 122.79   |
| 3   | L3    | 2815 | A2M  | C4-C5-N7    | -3.06 | 107.08      | 110.58   |
| 2   | L1    | 69   | PSU  | O2-C2-N1    | -3.04 | 119.66      | 122.79   |
| 3   | L3    | 4523 | A2M  | C4-C5-N7    | -3.01 | 107.14      | 110.58   |
| 3   | L3    | 4361 | PSU  | O2-C2-N1    | -3.00 | 119.69      | 122.79   |
| 3   | L3    | 4353 | PSU  | O2-C2-N1    | -3.00 | 119.69      | 122.79   |
| 3   | L3    | 2415 | OMU  | O4-C4-C5    | -2.99 | 120.00      | 125.16   |
| 23  | LN    | 245  | HIC  | NE2-CE1-ND1 | -2.97 | 111.53      | 112.66   |
| 3   | L3    | 4628 | PSU  | O2-C2-N1    | -2.97 | 119.73      | 122.79   |
| 3   | L3    | 1524 | A2M  | C4-C5-N7    | -2.96 | 107.19      | 110.58   |
| 3   | L3    | 4306 | OMU  | O4-C4-C5    | -2.96 | 120.05      | 125.16   |
| 3   | L3    | 3830 | A2M  | C4-C5-N7    | -2.95 | 107.21      | 110.58   |
| 3   | L3    | 4620 | OMU  | O4-C4-C5    | -2.94 | 120.09      | 125.16   |
| 3   | L3    | 400  | A2M  | C4-C5-N7    | -2.94 | 107.22      | 110.58   |
| 3   | L3    | 3639 | PSU  | O2-C2-N1    | -2.93 | 119.76      | 122.79   |
| 3   | L3    | 1536 | PSU  | O2-C2-N1    | -2.93 | 119.76      | 122.79   |
| 3   | L3    | 2401 | A2M  | C4-C5-N7    | -2.93 | 107.23      | 110.58   |
| 3   | L3    | 3730 | PSU  | O2-C2-N1    | -2.93 | 119.77      | 122.79   |
| 3   | L3    | 1862 | PSU  | O2-C2-N1    | -2.91 | 119.79      | 122.79   |
| 3   | L3    | 4571 | A2M  | C4-C5-N7    | -2.90 | 107.26      | 110.58   |
| 2   | L1    | 55   | PSU  | O2-C2-N1    | -2.90 | 119.80      | 122.79   |
| 3   | L3    | 398  | A2M  | C4-C5-N7    | -2.90 | 107.27      | 110.58   |
| 3   | L3    | 2787 | A2M  | C4-C5-N7    | -2.88 | 107.28      | 110.58   |
| 3   | L3    | 2401 | A2M  | N9-C8-N7    | -2.87 | 109.86      | 113.94   |
| 3   | L3    | 1871 | A2M  | C4-C5-N7    | -2.87 | 107.30      | 110.58   |
| 3   | L3    | 2363 | A2M  | C4-C5-N7    | -2.87 | 107.30      | 110.58   |
| 3   | L3    | 3844 | PSU  | O2-C2-N1    | -2.86 | 119.83      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | L3    | 3724 | A2M  | C4-C5-N7   | -2.86 | 107.31      | 110.58   |
| 3   | L3    | 2839 | PSU  | O2-C2-N1   | -2.86 | 119.84      | 122.79   |
| 3   | L3    | 3884 | PSU  | C6-N1-C2   | -2.86 | 120.04      | 122.69   |
| 3   | L3    | 4220 | 6MZ  | C9-N6-C6   | -2.86 | 120.20      | 122.85   |
| 3   | L3    | 3825 | A2M  | N9-C8-N7   | -2.85 | 109.89      | 113.94   |
| 3   | L3    | 3825 | A2M  | C4-C5-N7   | -2.84 | 107.33      | 110.58   |
| 3   | L3    | 1871 | A2M  | N9-C8-N7   | -2.83 | 109.91      | 113.94   |
| 3   | L3    | 3867 | A2M  | N9-C8-N7   | -2.83 | 109.93      | 113.94   |
| 3   | L3    | 400  | A2M  | N9-C8-N7   | -2.83 | 109.93      | 113.94   |
| 3   | L3    | 3867 | A2M  | C4-C5-N7   | -2.82 | 107.35      | 110.58   |
| 3   | L3    | 4498 | OMU  | O4-C4-C5   | -2.82 | 120.30      | 125.16   |
| 3   | L3    | 1860 | PSU  | O2-C2-N1   | -2.81 | 119.89      | 122.79   |
| 3   | L3    | 1524 | A2M  | N9-C8-N7   | -2.80 | 109.97      | 113.94   |
| 3   | L3    | 3884 | PSU  | O2-C2-N1   | -2.78 | 119.92      | 122.79   |
| 3   | L3    | 4972 | PSU  | O2-C2-N1   | -2.78 | 119.92      | 122.79   |
| 3   | L3    | 3715 | PSU  | O2-C2-N1   | -2.78 | 119.92      | 122.79   |
| 3   | L3    | 4403 | PSU  | O2-C2-N1   | -2.78 | 119.93      | 122.79   |
| 3   | L3    | 1524 | A2M  | C2'-C1'-N9 | -2.77 | 109.19      | 113.75   |
| 3   | L3    | 3851 | PSU  | O2-C2-N1   | -2.77 | 119.93      | 122.79   |
| 3   | L3    | 2839 | PSU  | C6-N1-C2   | -2.77 | 120.12      | 122.69   |
| 3   | L3    | 4579 | PSU  | C6-N1-C2   | -2.76 | 120.13      | 122.69   |
| 3   | L3    | 398  | A2M  | C2'-C1'-N9 | -2.76 | 109.21      | 113.75   |
| 3   | L3    | 4457 | PSU  | O2-C2-N1   | -2.76 | 119.94      | 122.79   |
| 3   | L3    | 4431 | PSU  | O2-C2-N1   | -2.76 | 119.95      | 122.79   |
| 3   | L3    | 3718 | A2M  | C4-C5-N7   | -2.75 | 107.44      | 110.58   |
| 3   | L3    | 3830 | A2M  | N9-C8-N7   | -2.75 | 110.03      | 113.94   |
| 3   | L3    | 4673 | PSU  | C6-N1-C2   | -2.75 | 120.14      | 122.69   |
| 3   | L3    | 4299 | PSU  | O2-C2-N1   | -2.74 | 119.97      | 122.79   |
| 3   | L3    | 4312 | PSU  | O2-C2-N1   | -2.73 | 119.97      | 122.79   |
| 3   | L3    | 3734 | PSU  | O2-C2-N1   | -2.72 | 119.98      | 122.79   |
| 3   | L3    | 4590 | A2M  | N9-C8-N7   | -2.72 | 110.08      | 113.94   |
| 3   | L3    | 4523 | A2M  | N9-C8-N7   | -2.72 | 110.08      | 113.94   |
| 3   | L3    | 3724 | A2M  | N9-C8-N7   | -2.71 | 110.09      | 113.94   |
| 3   | L3    | 1683 | PSU  | C6-N1-C2   | -2.71 | 120.17      | 122.69   |
| 3   | L3    | 4689 | PSU  | C6-N1-C2   | -2.71 | 120.18      | 122.69   |
| 3   | L3    | 1326 | A2M  | N9-C8-N7   | -2.70 | 110.10      | 113.94   |
| 3   | L3    | 4521 | PSU  | O2-C2-N1   | -2.70 | 120.00      | 122.79   |
| 3   | L3    | 5001 | PSU  | C6-N1-C2   | -2.70 | 120.19      | 122.69   |
| 3   | L3    | 2508 | PSU  | O2-C2-N1   | -2.69 | 120.01      | 122.79   |
| 3   | L3    | 2632 | PSU  | O2-C2-N1   | -2.69 | 120.02      | 122.79   |
| 3   | L3    | 4471 | PSU  | O2-C2-N1   | -2.67 | 120.03      | 122.79   |
| 3   | L3    | 1792 | PSU  | O2-C2-N1   | -2.67 | 120.04      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L3    | 4636 | PSU  | O2-C2-N1 | -2.66 | 120.04      | 122.79   |
| 3   | L3    | 1582 | PSU  | O2-C2-N1 | -2.66 | 120.04      | 122.79   |
| 3   | L3    | 4457 | PSU  | C6-N1-C2 | -2.66 | 120.22      | 122.69   |
| 3   | L3    | 398  | A2M  | N9-C8-N7 | -2.66 | 110.17      | 113.94   |
| 3   | L3    | 4296 | PSU  | O2-C2-N1 | -2.63 | 120.07      | 122.79   |
| 3   | L3    | 2815 | A2M  | N9-C8-N7 | -2.63 | 110.20      | 113.94   |
| 3   | L3    | 5010 | PSU  | C6-N1-C2 | -2.62 | 120.26      | 122.69   |
| 3   | L3    | 5010 | PSU  | O2-C2-N1 | -2.62 | 120.09      | 122.79   |
| 3   | L3    | 2787 | A2M  | N9-C8-N7 | -2.61 | 110.24      | 113.94   |
| 3   | L3    | 4361 | PSU  | C6-N1-C2 | -2.61 | 120.27      | 122.69   |
| 3   | L3    | 5001 | PSU  | O2-C2-N1 | -2.60 | 120.10      | 122.79   |
| 3   | L3    | 4312 | PSU  | C6-N1-C2 | -2.60 | 120.28      | 122.69   |
| 3   | L3    | 4673 | PSU  | O2-C2-N1 | -2.59 | 120.11      | 122.79   |
| 3   | L3    | 4636 | PSU  | C6-C5-C4 | 2.59  | 119.92      | 118.17   |
| 3   | L3    | 3695 | PSU  | O2-C2-N1 | -2.59 | 120.12      | 122.79   |
| 3   | L3    | 3822 | PSU  | C6-N1-C2 | -2.59 | 120.29      | 122.69   |
| 3   | L3    | 4493 | PSU  | O2-C2-N1 | -2.58 | 120.12      | 122.79   |
| 2   | L1    | 69   | PSU  | C6-N1-C2 | -2.58 | 120.30      | 122.69   |
| 3   | L3    | 4689 | PSU  | O2-C2-N1 | -2.57 | 120.14      | 122.79   |
| 3   | L3    | 4571 | A2M  | N9-C8-N7 | -2.55 | 110.32      | 113.94   |
| 3   | L3    | 3715 | PSU  | C6-N1-C2 | -2.54 | 120.33      | 122.69   |
| 3   | L3    | 4576 | PSU  | O2-C2-N1 | -2.53 | 120.18      | 122.79   |
| 3   | L3    | 1534 | A2M  | N9-C8-N7 | -2.53 | 110.34      | 113.94   |
| 3   | L3    | 4353 | PSU  | C6-N1-C2 | -2.53 | 120.34      | 122.69   |
| 3   | L3    | 4552 | PSU  | C6-N1-C2 | -2.53 | 120.35      | 122.69   |
| 3   | L3    | 4293 | PSU  | C6-N1-C2 | -2.52 | 120.35      | 122.69   |
| 3   | L3    | 4628 | PSU  | C6-N1-C2 | -2.51 | 120.36      | 122.69   |
| 3   | L3    | 2363 | A2M  | N9-C8-N7 | -2.51 | 110.37      | 113.94   |
| 3   | L3    | 4552 | PSU  | O2-C2-N1 | -2.51 | 120.20      | 122.79   |
| 3   | L3    | 3734 | PSU  | C6-C5-C4 | 2.49  | 119.86      | 118.17   |
| 3   | L3    | 4471 | PSU  | C6-C5-C4 | 2.49  | 119.86      | 118.17   |
| 3   | L3    | 3730 | PSU  | C6-N1-C2 | -2.49 | 120.38      | 122.69   |
| 3   | L3    | 4500 | PSU  | C6-N1-C2 | -2.49 | 120.38      | 122.69   |
| 3   | L3    | 1536 | PSU  | C6-N1-C2 | -2.48 | 120.39      | 122.69   |
| 3   | L3    | 1860 | PSU  | C6-N1-C2 | -2.48 | 120.39      | 122.69   |
| 3   | L3    | 4403 | PSU  | C6-N1-C2 | -2.48 | 120.39      | 122.69   |
| 3   | L3    | 3844 | PSU  | C6-N1-C2 | -2.47 | 120.40      | 122.69   |
| 3   | L3    | 1862 | PSU  | C6-N1-C2 | -2.47 | 120.40      | 122.69   |
| 3   | L3    | 4576 | PSU  | C6-N1-C2 | -2.47 | 120.40      | 122.69   |
| 3   | L3    | 4972 | PSU  | C6-N1-C2 | -2.46 | 120.41      | 122.69   |
| 3   | L3    | 3920 | PSU  | C6-N1-C2 | -2.45 | 120.42      | 122.69   |
| 3   | L3    | 4293 | PSU  | O2-C2-N1 | -2.45 | 120.27      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L3    | 1582 | PSU  | C6-C5-C4    | 2.44  | 119.82      | 118.17   |
| 3   | L3    | 4299 | PSU  | C6-C5-C4    | 2.43  | 119.82      | 118.17   |
| 3   | L3    | 2351 | OMC  | C1'-N1-C2   | 2.42  | 123.78      | 118.44   |
| 3   | L3    | 1862 | PSU  | C6-C5-C4    | 2.42  | 119.80      | 118.17   |
| 3   | L3    | 4521 | PSU  | C6-N1-C2    | -2.41 | 120.45      | 122.69   |
| 3   | L3    | 4220 | 6MZ  | N9-C8-N7    | -2.41 | 110.52      | 113.94   |
| 3   | L3    | 4431 | PSU  | C6-N1-C2    | -2.40 | 120.46      | 122.69   |
| 3   | L3    | 4471 | PSU  | C6-N1-C2    | -2.40 | 120.47      | 122.69   |
| 3   | L3    | 3920 | PSU  | O2-C2-N1    | -2.39 | 120.32      | 122.79   |
| 3   | L3    | 3637 | PSU  | C6-C5-C4    | 2.39  | 119.79      | 118.17   |
| 3   | L3    | 1322 | 1MA  | N1-C6-N6    | 2.39  | 125.72      | 119.71   |
| 3   | L3    | 3822 | PSU  | C6-C5-C4    | 2.37  | 119.78      | 118.17   |
| 2   | L1    | 69   | PSU  | O4'-C1'-C2' | 2.37  | 108.44      | 105.15   |
| 3   | L3    | 4532 | PSU  | C6-C5-C4    | 2.37  | 119.77      | 118.17   |
| 3   | L3    | 3853 | PSU  | C6-N1-C2    | -2.37 | 120.49      | 122.69   |
| 3   | L3    | 3637 | PSU  | O2-C2-N1    | -2.36 | 120.35      | 122.79   |
| 3   | L3    | 3715 | PSU  | O4'-C1'-C2' | 2.36  | 108.42      | 105.15   |
| 3   | L3    | 4299 | PSU  | C6-N1-C2    | -2.36 | 120.50      | 122.69   |
| 3   | L3    | 4431 | PSU  | C6-C5-C4    | 2.34  | 119.76      | 118.17   |
| 3   | L3    | 3844 | PSU  | C6-C5-C4    | 2.34  | 119.75      | 118.17   |
| 3   | L3    | 2632 | PSU  | C6-N1-C2    | -2.34 | 120.52      | 122.69   |
| 3   | L3    | 3695 | PSU  | C6-C5-C4    | 2.33  | 119.75      | 118.17   |
| 3   | L3    | 1792 | PSU  | C6-C5-C4    | 2.33  | 119.74      | 118.17   |
| 2   | L1    | 55   | PSU  | C6-N1-C2    | -2.32 | 120.53      | 122.69   |
| 3   | L3    | 4493 | PSU  | C6-N1-C2    | -2.31 | 120.54      | 122.69   |
| 3   | L3    | 3851 | PSU  | C6-N1-C2    | -2.31 | 120.55      | 122.69   |
| 3   | L3    | 4296 | PSU  | C6-C5-C4    | 2.29  | 119.72      | 118.17   |
| 3   | L3    | 4296 | PSU  | C6-N1-C2    | -2.29 | 120.56      | 122.69   |
| 3   | L3    | 2837 | OMU  | O2-C2-N1    | -2.28 | 119.83      | 122.80   |
| 3   | L3    | 1677 | PSU  | C6-C5-C4    | 2.28  | 119.71      | 118.17   |
| 3   | L3    | 3734 | PSU  | C6-N1-C2    | -2.27 | 120.59      | 122.69   |
| 3   | L3    | 3695 | PSU  | C6-N1-C2    | -2.26 | 120.59      | 122.69   |
| 3   | L3    | 4532 | PSU  | C6-N1-C2    | -2.26 | 120.59      | 122.69   |
| 3   | L3    | 3639 | PSU  | C6-N1-C2    | -2.25 | 120.60      | 122.69   |
| 3   | L3    | 4576 | PSU  | C6-C5-C4    | 2.25  | 119.69      | 118.17   |
| 3   | L3    | 1792 | PSU  | C6-N1-C2    | -2.25 | 120.61      | 122.69   |
| 3   | L3    | 4628 | PSU  | C6-C5-C4    | 2.23  | 119.68      | 118.17   |
| 3   | L3    | 1683 | PSU  | C6-C5-C4    | 2.23  | 119.68      | 118.17   |
| 3   | L3    | 3715 | PSU  | C6-C5-C4    | 2.23  | 119.68      | 118.17   |
| 3   | L3    | 2508 | PSU  | C6-N1-C2    | -2.22 | 120.63      | 122.69   |
| 3   | L3    | 3637 | PSU  | C6-N1-C2    | -2.22 | 120.63      | 122.69   |
| 3   | L3    | 2415 | OMU  | O2-C2-N1    | -2.22 | 119.91      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L3    | 4220 | 6MZ  | C4-C5-C6    | 2.22  | 118.62      | 116.78   |
| 3   | L3    | 4636 | PSU  | C6-N1-C2    | -2.21 | 120.64      | 122.69   |
| 2   | L1    | 55   | PSU  | C6-C5-C4    | 2.21  | 119.67      | 118.17   |
| 3   | L3    | 4590 | A2M  | C2-N1-C6    | 2.21  | 122.36      | 118.73   |
| 3   | L3    | 1677 | PSU  | C6-N1-C2    | -2.21 | 120.64      | 122.69   |
| 3   | L3    | 4689 | PSU  | C6-C5-C4    | 2.19  | 119.65      | 118.17   |
| 3   | L3    | 3639 | PSU  | C6-C5-C4    | 2.19  | 119.65      | 118.17   |
| 3   | L3    | 1860 | PSU  | C6-C5-C4    | 2.18  | 119.64      | 118.17   |
| 3   | L3    | 3920 | PSU  | C6-C5-C4    | 2.17  | 119.64      | 118.17   |
| 3   | L3    | 1582 | PSU  | C6-N1-C2    | -2.16 | 120.68      | 122.69   |
| 3   | L3    | 5010 | PSU  | C6-C5-C4    | 2.15  | 119.63      | 118.17   |
| 3   | L3    | 4403 | PSU  | C6-C5-C4    | 2.14  | 119.62      | 118.17   |
| 2   | L1    | 69   | PSU  | C6-C5-C4    | 2.14  | 119.62      | 118.17   |
| 3   | L3    | 4628 | PSU  | O4'-C1'-C2' | 2.09  | 108.04      | 105.15   |
| 3   | L3    | 4636 | PSU  | O4'-C1'-C2' | 2.09  | 108.04      | 105.15   |
| 3   | L3    | 3734 | PSU  | O4'-C1'-C2' | 2.09  | 108.04      | 105.15   |
| 3   | L3    | 3718 | A2M  | N9-C8-N7    | -2.08 | 110.98      | 113.94   |
| 3   | L3    | 3925 | OMU  | O2-C2-N1    | -2.08 | 120.09      | 122.80   |
| 3   | L3    | 4353 | PSU  | O4'-C1'-C2' | 2.08  | 108.03      | 105.15   |
| 3   | L3    | 4353 | PSU  | C6-C5-C4    | 2.08  | 119.58      | 118.17   |
| 3   | L3    | 4403 | PSU  | O4'-C1'-C2' | 2.07  | 108.02      | 105.15   |
| 3   | L3    | 4552 | PSU  | C6-C5-C4    | 2.07  | 119.57      | 118.17   |
| 3   | L3    | 4972 | PSU  | C6-C5-C4    | 2.05  | 119.56      | 118.17   |
| 3   | L3    | 4312 | PSU  | C6-C5-C4    | 2.05  | 119.55      | 118.17   |
| 3   | L3    | 4498 | OMU  | O2-C2-N1    | -2.04 | 120.14      | 122.80   |
| 3   | L3    | 4500 | PSU  | C6-C5-C4    | 2.04  | 119.55      | 118.17   |
| 3   | L3    | 4576 | PSU  | O4'-C1'-C2' | 2.03  | 107.96      | 105.15   |
| 3   | L3    | 2351 | OMC  | C1'-N1-C6   | -2.01 | 116.48      | 120.78   |
| 3   | L3    | 2861 | OMC  | C1'-N1-C2   | 2.01  | 122.87      | 118.44   |

There are no chirality outliers.

All (84) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | L1    | 75   | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 398  | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 1316 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 1326 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L3    | 1326 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L3    | 1326 | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 1340 | OMC  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 1860 | PSU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | L3    | 2363 | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 2364 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 2815 | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 2837 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 2861 | OMC  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 3701 | OMC  | C2'-C1'-N1-C2   |
| 3   | L3    | 3701 | OMC  | C2'-C1'-N1-C6   |
| 3   | L3    | 3718 | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 3724 | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 3830 | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 3841 | OMC  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 3867 | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 3869 | OMC  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 3887 | OMC  | C3'-C4'-C5'-O5' |
| 3   | L3    | 3899 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 3925 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 4227 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 4392 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 4498 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 4571 | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 4590 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L3    | 4618 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 4637 | OMG  | O4'-C4'-C5'-O5' |
| 39  | NR    | 127  | PTR  | O-C-CA-CB       |
| 3   | L3    | 1860 | PSU  | C3'-C4'-C5'-O5' |
| 3   | L3    | 2787 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L3    | 4220 | 6MZ  | O4'-C4'-C5'-O5' |
| 3   | L3    | 4306 | OMU  | C3'-C4'-C5'-O5' |
| 3   | L3    | 4523 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L3    | 4523 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L3    | 4618 | OMG  | O4'-C4'-C5'-O5' |
| 3   | L3    | 1677 | PSU  | C3'-C4'-C5'-O5' |
| 3   | L3    | 1677 | PSU  | O4'-C4'-C5'-O5' |
| 3   | L3    | 2364 | OMG  | O4'-C4'-C5'-O5' |
| 3   | L3    | 3887 | OMC  | O4'-C4'-C5'-O5' |
| 3   | L3    | 4306 | OMU  | O4'-C4'-C5'-O5' |
| 3   | L3    | 4590 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L3    | 4637 | OMG  | C3'-C4'-C5'-O5' |
| 3   | L3    | 2401 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L3    | 2787 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L3    | 4220 | 6MZ  | C3'-C4'-C5'-O5' |
| 3   | L3    | 4618 | OMG  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | LN    | 245  | HIC  | CA-CB-CG-ND1    |
| 3   | L3    | 4590 | A2M  | C4'-C5'-O5'-P   |
| 23  | LN    | 245  | HIC  | CA-CB-CG-CD2    |
| 3   | L3    | 3701 | OMC  | O4'-C4'-C5'-O5' |
| 3   | L3    | 400  | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 3701 | OMC  | C3'-C4'-C5'-O5' |
| 3   | L3    | 2787 | A2M  | C2'-C1'-N9-C8   |
| 3   | L3    | 1625 | OMG  | C3'-C2'-O2'-CM2 |
| 3   | L3    | 1625 | OMG  | C3'-C4'-C5'-O5' |
| 3   | L3    | 2401 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L3    | 1534 | A2M  | C4'-C5'-O5'-P   |
| 3   | L3    | 4306 | OMU  | C4'-C5'-O5'-P   |
| 3   | L3    | 4228 | OMG  | O4'-C4'-C5'-O5' |
| 3   | L3    | 2351 | OMC  | C3'-C2'-O2'-CM2 |
| 3   | L3    | 2876 | OMG  | C3'-C2'-O2'-CM2 |
| 3   | L3    | 2787 | A2M  | C2'-C1'-N9-C4   |
| 3   | L3    | 4228 | OMG  | C3'-C4'-C5'-O5' |
| 3   | L3    | 4220 | 6MZ  | C4'-C5'-O5'-P   |
| 3   | L3    | 3701 | OMC  | O4'-C1'-N1-C6   |
| 3   | L3    | 3844 | PSU  | C4'-C5'-O5'-P   |
| 3   | L3    | 2364 | OMG  | C3'-C4'-C5'-O5' |
| 3   | L3    | 2787 | A2M  | O4'-C1'-N9-C8   |
| 3   | L3    | 1871 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L3    | 2351 | OMC  | C2'-C1'-N1-C6   |
| 3   | L3    | 2876 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 3744 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 3701 | OMC  | O4'-C1'-N1-C2   |
| 3   | L3    | 1677 | PSU  | C2'-C1'-C5-C6   |
| 3   | L3    | 4636 | PSU  | C4'-C5'-O5'-P   |
| 3   | L3    | 1316 | OMG  | C3'-C2'-O2'-CM2 |
| 3   | L3    | 1524 | A2M  | O4'-C1'-N9-C8   |
| 3   | L3    | 3701 | OMC  | C4'-C5'-O5'-P   |
| 3   | L3    | 4498 | OMU  | C4'-C5'-O5'-P   |
| 3   | L3    | 4306 | OMU  | C2'-C1'-N1-C2   |

There are no ring outliers.

57 monomers are involved in 76 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | L3    | 1326 | A2M  | 2       | 0            |
| 3   | L3    | 3925 | OMU  | 1       | 0            |
| 3   | L3    | 4500 | PSU  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | L3    | 1524 | A2M  | 1       | 0            |
| 3   | L3    | 3867 | A2M  | 1       | 0            |
| 3   | L3    | 4361 | PSU  | 1       | 0            |
| 3   | L3    | 398  | A2M  | 2       | 0            |
| 3   | L3    | 3734 | PSU  | 1       | 0            |
| 3   | L3    | 2632 | PSU  | 1       | 0            |
| 3   | L3    | 2824 | OMC  | 1       | 0            |
| 3   | L3    | 3899 | OMG  | 1       | 0            |
| 3   | L3    | 2351 | OMC  | 2       | 0            |
| 3   | L3    | 4618 | OMG  | 1       | 0            |
| 3   | L3    | 3701 | OMC  | 1       | 0            |
| 3   | L3    | 4471 | PSU  | 1       | 0            |
| 3   | L3    | 3887 | OMC  | 1       | 0            |
| 2   | L1    | 75   | OMG  | 2       | 0            |
| 3   | L3    | 1677 | PSU  | 3       | 0            |
| 3   | L3    | 3869 | OMC  | 1       | 0            |
| 3   | L3    | 2364 | OMG  | 1       | 0            |
| 3   | L3    | 1534 | A2M  | 3       | 0            |
| 3   | L3    | 1522 | OMG  | 1       | 0            |
| 3   | L3    | 3841 | OMC  | 1       | 0            |
| 3   | L3    | 4536 | OMC  | 1       | 0            |
| 3   | L3    | 4637 | OMG  | 1       | 0            |
| 3   | L3    | 1322 | 1MA  | 3       | 0            |
| 3   | L3    | 4392 | OMG  | 1       | 0            |
| 3   | L3    | 2415 | OMU  | 1       | 0            |
| 3   | L3    | 2837 | OMU  | 1       | 0            |
| 3   | L3    | 3920 | PSU  | 1       | 0            |
| 3   | L3    | 2815 | A2M  | 1       | 0            |
| 3   | L3    | 3744 | OMG  | 1       | 0            |
| 3   | L3    | 4296 | PSU  | 1       | 0            |
| 3   | L3    | 4457 | PSU  | 1       | 0            |
| 3   | L3    | 4494 | OMG  | 1       | 0            |
| 2   | L1    | 69   | PSU  | 2       | 0            |
| 3   | L3    | 3718 | A2M  | 2       | 0            |
| 3   | L3    | 4636 | PSU  | 1       | 0            |
| 3   | L3    | 1340 | OMC  | 1       | 0            |
| 3   | L3    | 1683 | PSU  | 1       | 0            |
| 3   | L3    | 2363 | A2M  | 3       | 0            |
| 3   | L3    | 4498 | OMU  | 1       | 0            |
| 3   | L3    | 2861 | OMC  | 1       | 0            |
| 3   | L3    | 2424 | OMG  | 1       | 0            |
| 3   | L3    | 3715 | PSU  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | L3    | 4227 | OMU  | 1       | 0            |
| 3   | L3    | 3830 | A2M  | 1       | 0            |
| 3   | L3    | 400  | A2M  | 2       | 0            |
| 3   | L3    | 4306 | OMU  | 2       | 0            |
| 3   | L3    | 3724 | A2M  | 2       | 0            |
| 3   | L3    | 4571 | A2M  | 1       | 0            |
| 3   | L3    | 2876 | OMG  | 2       | 0            |
| 3   | L3    | 4220 | 6MZ  | 3       | 0            |
| 3   | L3    | 4620 | OMU  | 1       | 0            |
| 3   | L3    | 4312 | PSU  | 1       | 0            |
| 3   | L3    | 5001 | PSU  | 1       | 0            |
| 3   | L3    | 4623 | OMG  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 95 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 57  | GDP  | SR    | 1001 | 58,55 | 29,30,30     | 3.03 | 12 (41%)    | 45,47,47    | 2.70 | 17 (37%)    |

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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 57  | GDP  | SR    | 1001 | 58,55 | -       | 0/16/32/32 | 0/3/3/3 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 57  | SR    | 1001 | GDP  | O6-C6   | 8.79  | 1.40        | 1.23     |
| 57  | SR    | 1001 | GDP  | C5-N7   | 6.54  | 1.52        | 1.39     |
| 57  | SR    | 1001 | GDP  | PA-O3A  | 4.98  | 1.64        | 1.59     |
| 57  | SR    | 1001 | GDP  | C2-N2   | 4.84  | 1.45        | 1.34     |
| 57  | SR    | 1001 | GDP  | C8-N9   | -4.04 | 1.28        | 1.37     |
| 57  | SR    | 1001 | GDP  | C4-N9   | -3.81 | 1.28        | 1.38     |
| 57  | SR    | 1001 | GDP  | C5-C4   | 3.80  | 1.49        | 1.38     |
| 57  | SR    | 1001 | GDP  | C4-N3   | 2.83  | 1.40        | 1.34     |
| 57  | SR    | 1001 | GDP  | PB-O2B  | -2.35 | 1.46        | 1.54     |
| 57  | SR    | 1001 | GDP  | PB-O3B  | -2.28 | 1.46        | 1.54     |
| 57  | SR    | 1001 | GDP  | O4'-C1' | 2.27  | 1.47        | 1.42     |
| 57  | SR    | 1001 | GDP  | C2'-C3' | -2.03 | 1.47        | 1.53     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | SR    | 1001 | GDP  | C8-N9-C4    | 7.78  | 120.61      | 106.03   |
| 57  | SR    | 1001 | GDP  | C5-C4-N3    | -6.77 | 117.61      | 128.39   |
| 57  | SR    | 1001 | GDP  | N9-C4-N3    | 6.71  | 139.36      | 125.95   |
| 57  | SR    | 1001 | GDP  | C2-N3-C4    | 5.38  | 121.56      | 112.30   |
| 57  | SR    | 1001 | GDP  | C6-C5-N7    | 4.82  | 139.06      | 130.29   |
| 57  | SR    | 1001 | GDP  | C4-C5-N7    | -4.69 | 103.24      | 110.67   |
| 57  | SR    | 1001 | GDP  | C3'-C2'-C1' | 3.09  | 107.31      | 101.46   |
| 57  | SR    | 1001 | GDP  | N9-C8-N7    | -3.04 | 107.77      | 113.40   |
| 57  | SR    | 1001 | GDP  | C2-N1-C6    | -2.98 | 119.71      | 125.11   |
| 57  | SR    | 1001 | GDP  | O2B-PB-O3A  | 2.96  | 114.56      | 104.64   |
| 57  | SR    | 1001 | GDP  | O3B-PB-O3A  | 2.81  | 114.05      | 104.64   |
| 57  | SR    | 1001 | GDP  | C2'-C3'-C4' | 2.76  | 107.94      | 102.61   |
| 57  | SR    | 1001 | GDP  | C1'-N9-C4   | -2.67 | 118.59      | 126.49   |
| 57  | SR    | 1001 | GDP  | C5-C6-N1    | 2.60  | 119.88      | 113.25   |
| 57  | SR    | 1001 | GDP  | O2A-PA-O1A  | -2.51 | 100.75      | 112.44   |
| 57  | SR    | 1001 | GDP  | O6-C6-C5    | -2.44 | 120.10      | 126.53   |
| 57  | SR    | 1001 | GDP  | C1'-N9-C8   | -2.10 | 120.77      | 126.73   |

There are no chirality outliers.

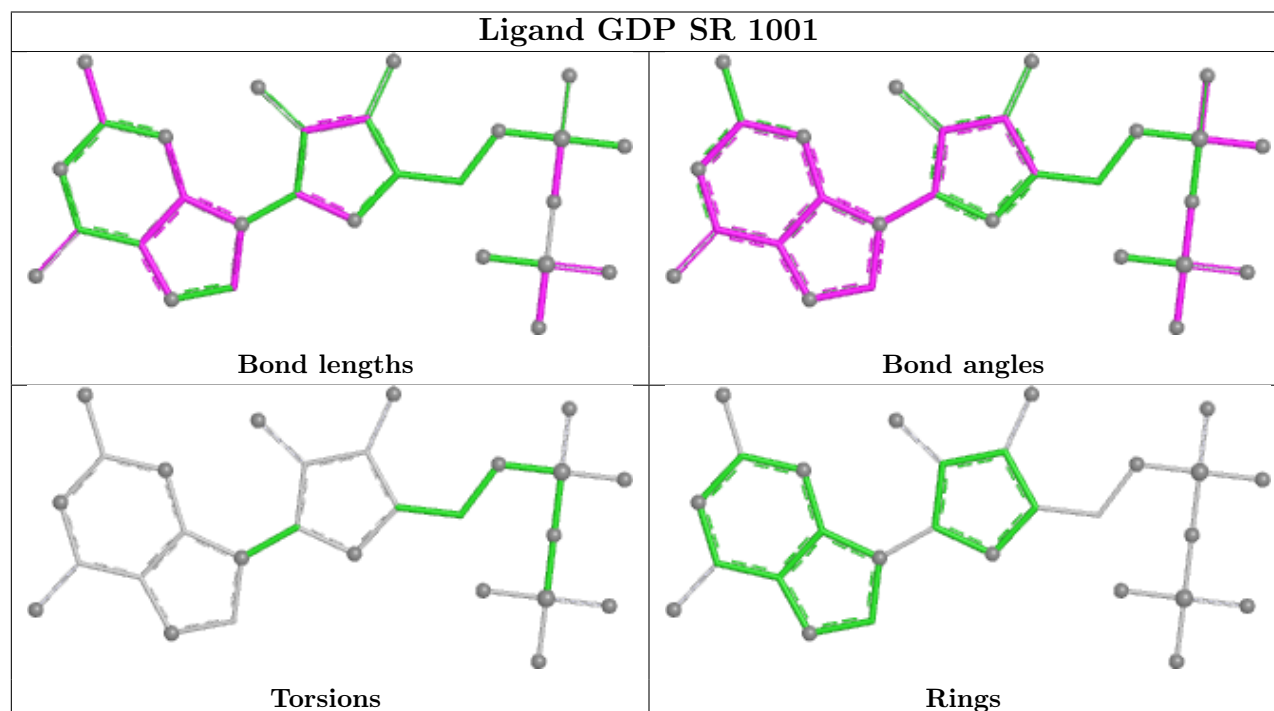
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

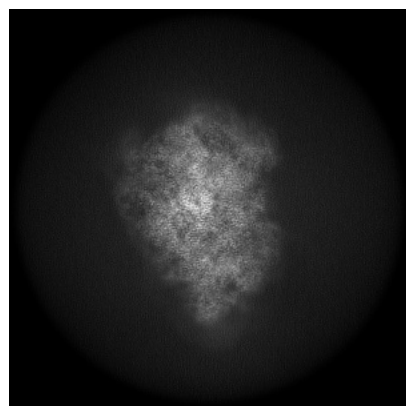
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29273. These allow visual inspection of the internal detail of the map and identification of artifacts.

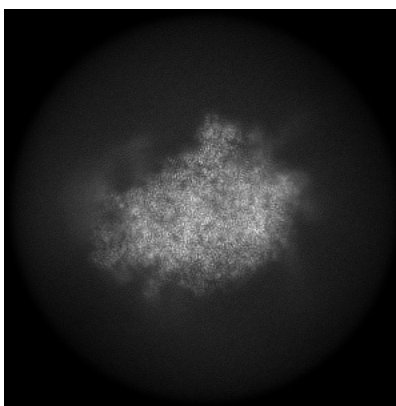
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

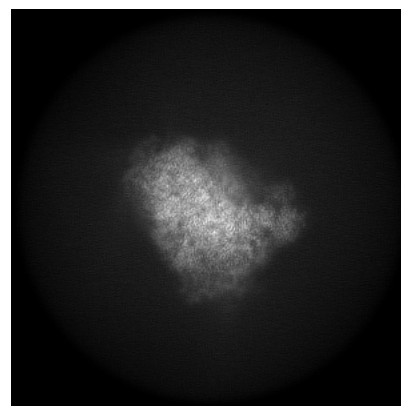
#### 6.1.1 Primary map



X

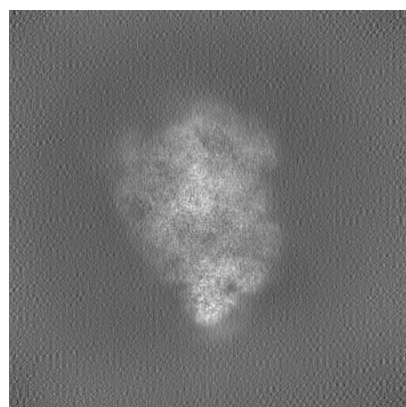


Y

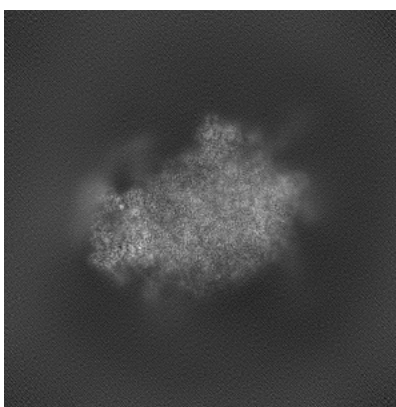


Z

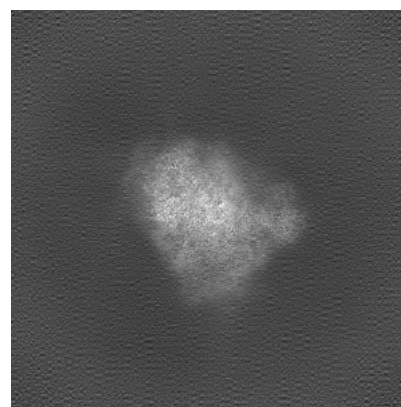
#### 6.1.2 Raw map



X



Y

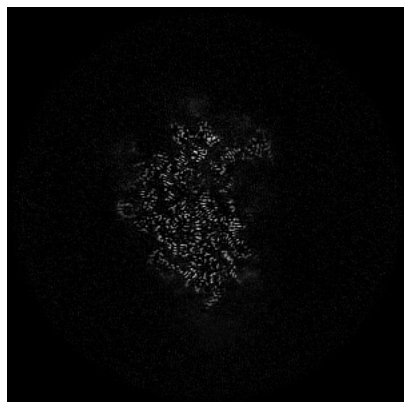


Z

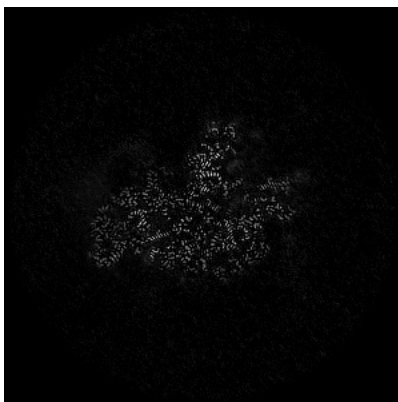
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

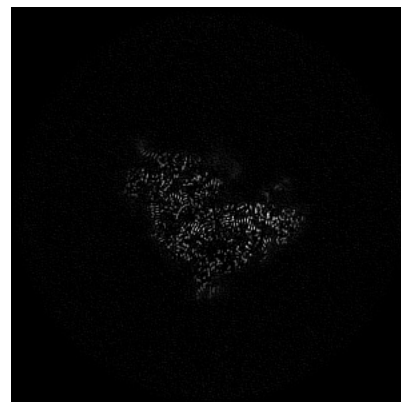
### 6.2.1 Primary map



X Index: 240

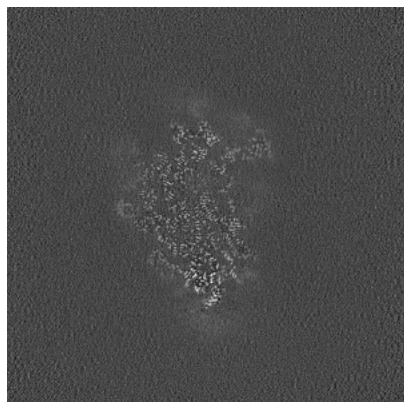


Y Index: 240

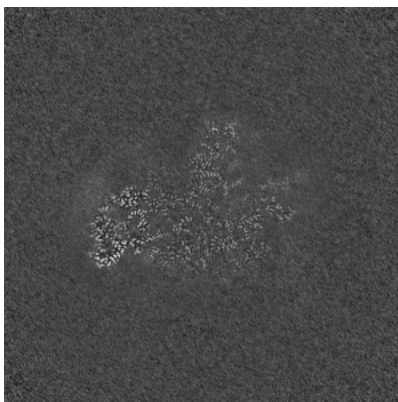


Z Index: 240

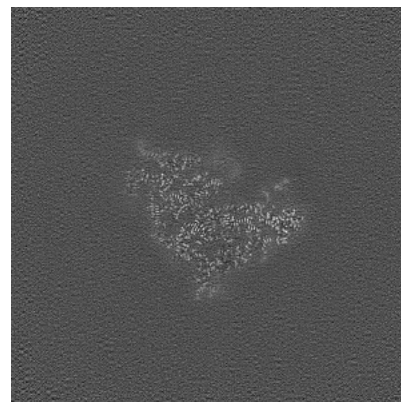
### 6.2.2 Raw map



X Index: 240



Y Index: 240

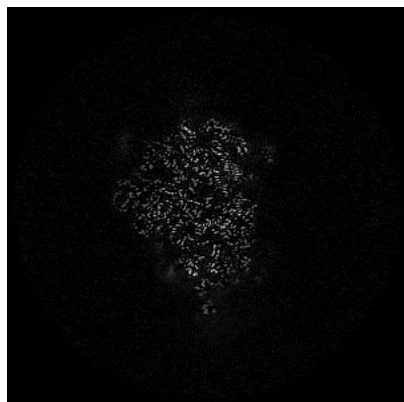


Z Index: 240

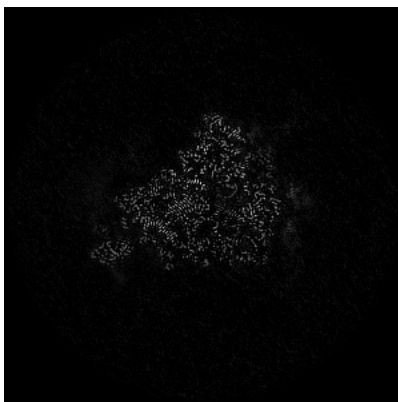
The images above show central slices of the map in three orthogonal directions.

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

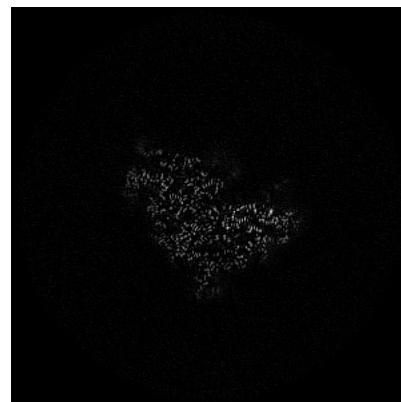
### 6.3.1 Primary map



X Index: 226

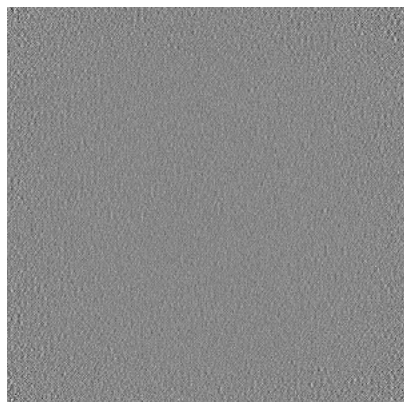


Y Index: 227

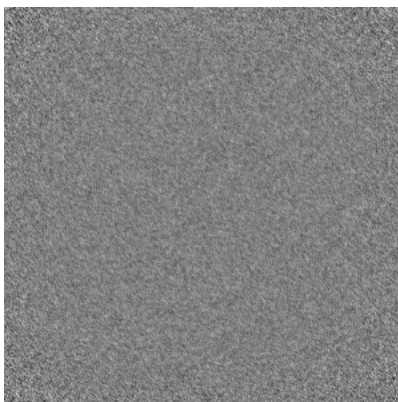


Z Index: 239

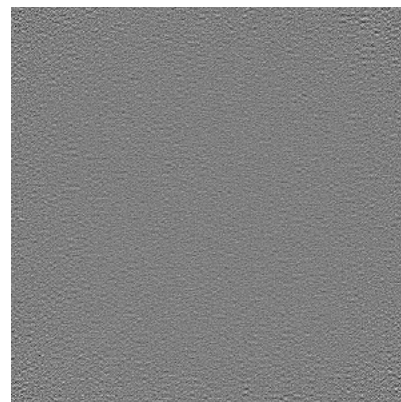
### 6.3.2 Raw map



X Index: 0



Y Index: 0

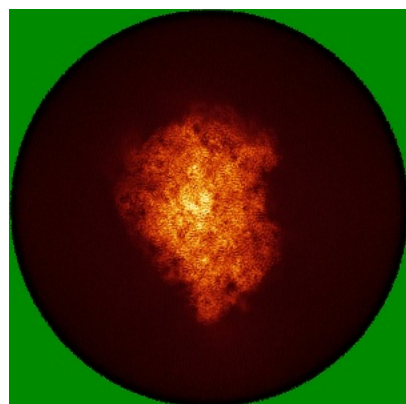


Z Index: 0

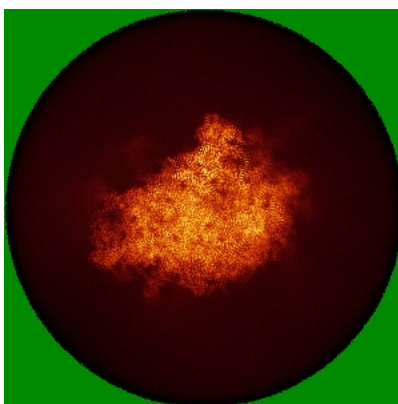
The images above show the largest variance slices of the map in three orthogonal directions.

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

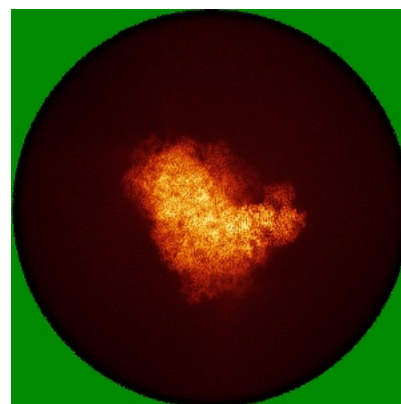
### 6.4.1 Primary map



X

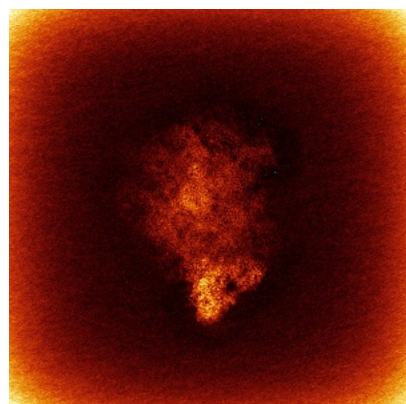


Y

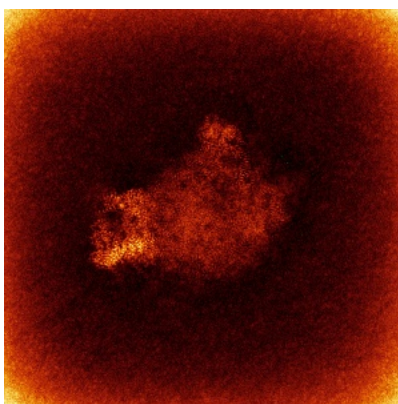


Z

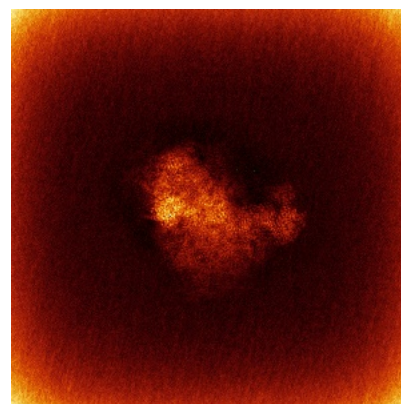
### 6.4.2 Raw map



X



Y



Z

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

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

### 6.5.1 Primary map



X



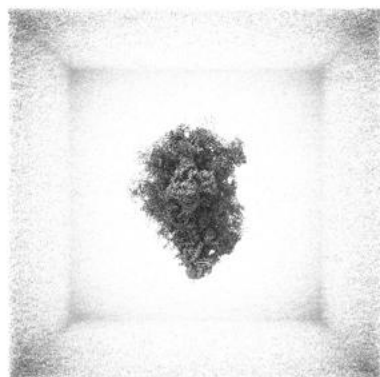
Y



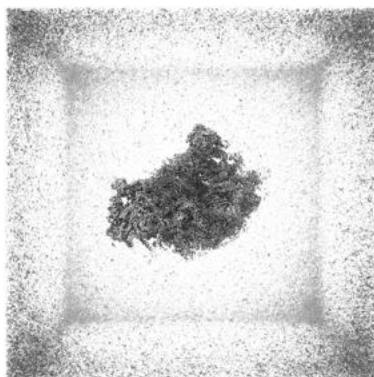
Z

The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

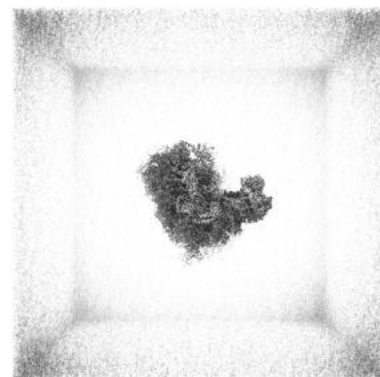
### 6.5.2 Raw map



X



Y



Z

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

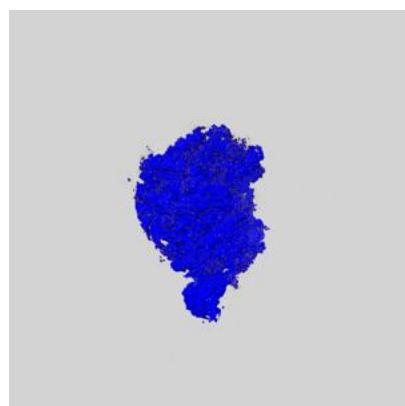
## 6.6 Mask visualisation [i](#)

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

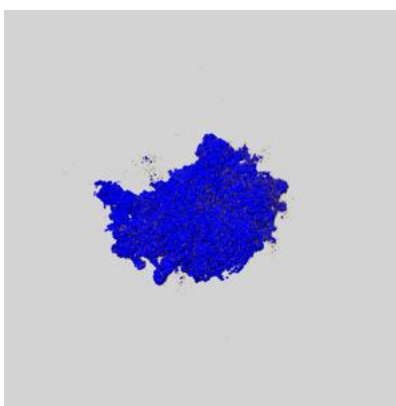
A mask typically either:

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

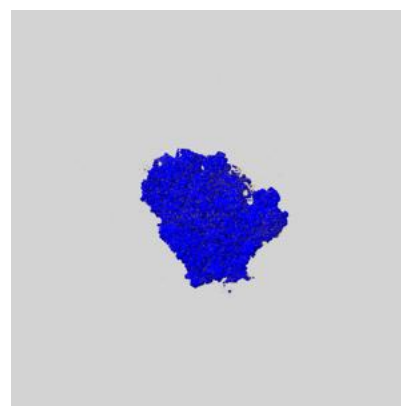
### 6.6.1 emd\_29273\_msk\_1.map [i](#)



X



Y

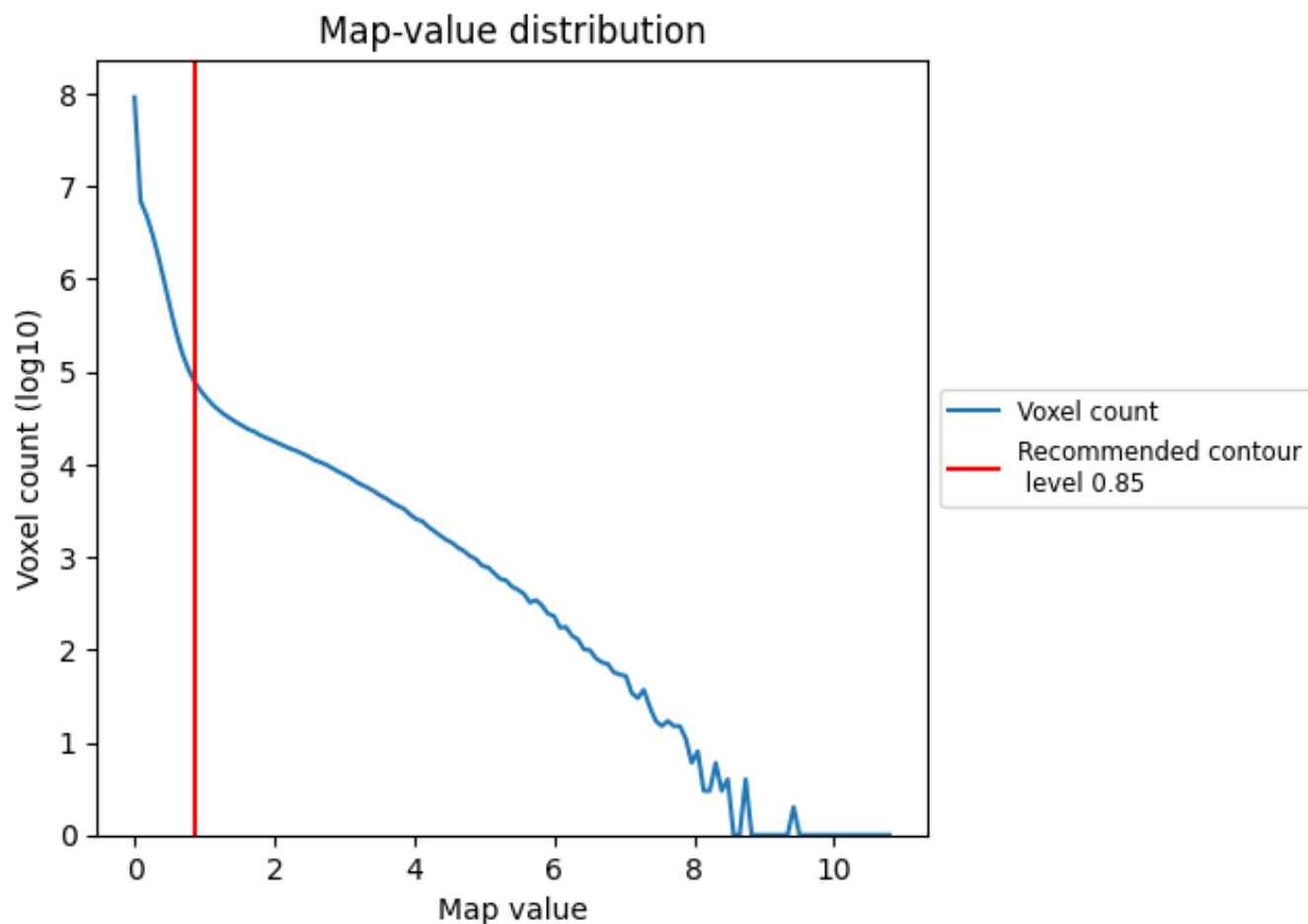


Z

## 7 Map analysis [i](#)

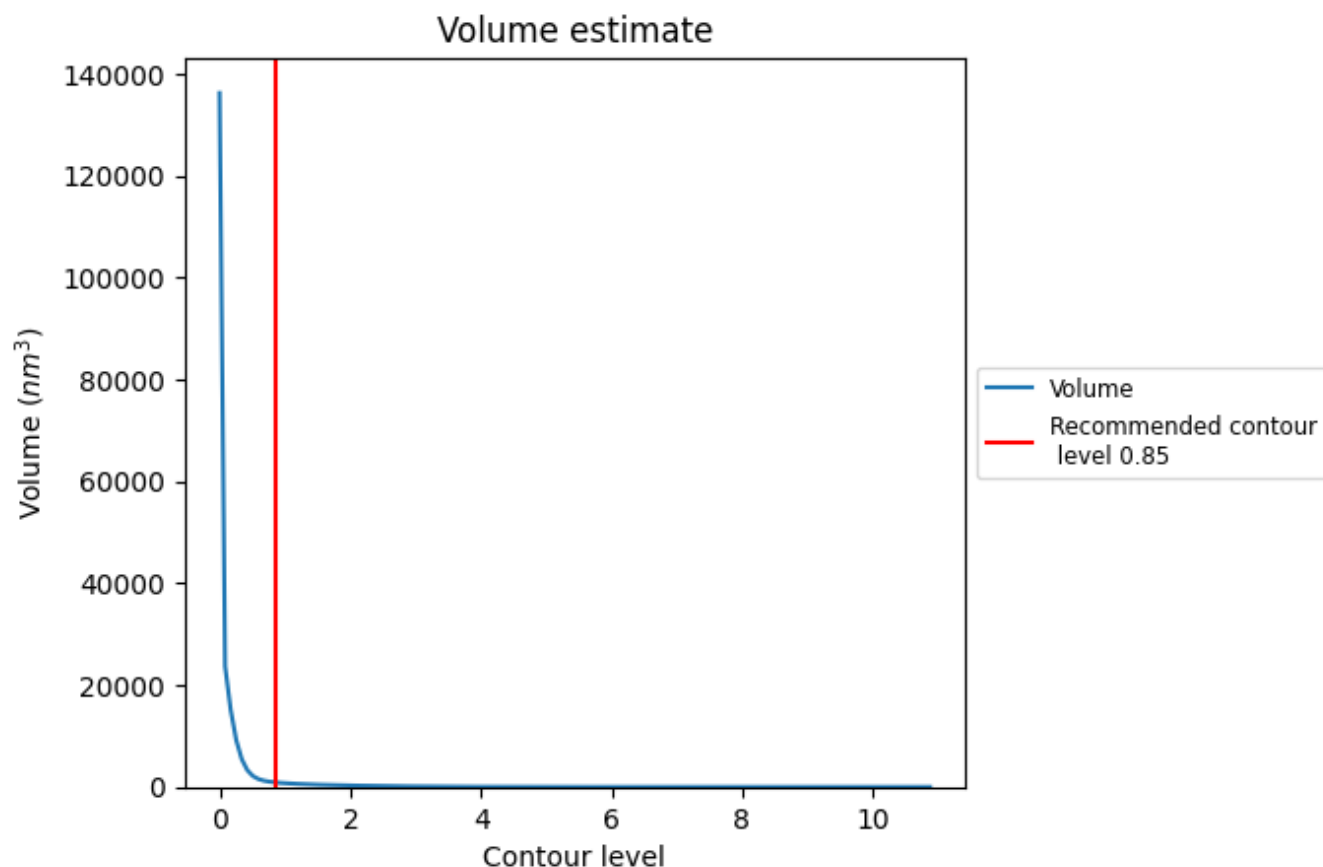
This section contains the results of statistical analysis of the map.

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



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

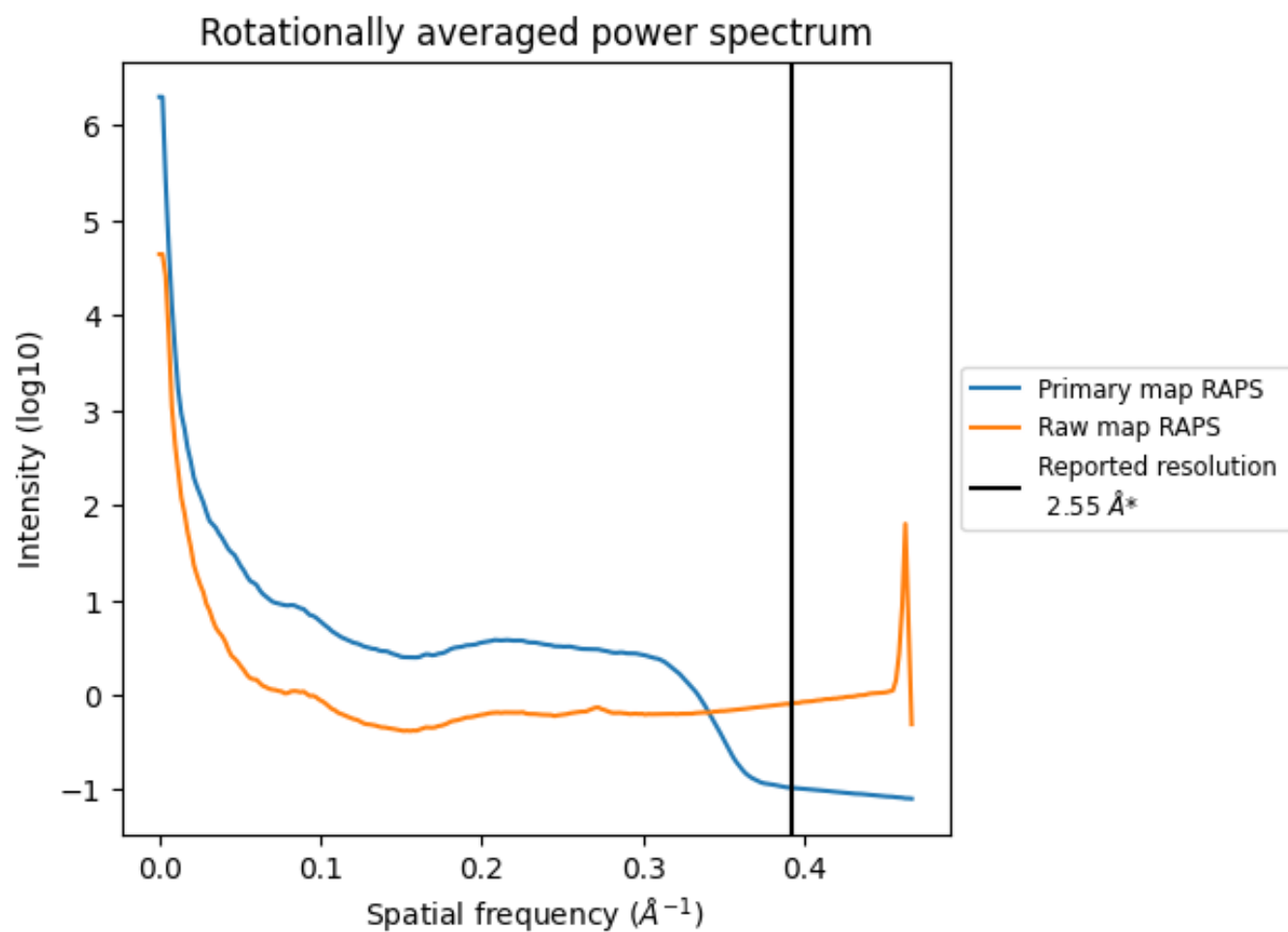
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 895  $\text{nm}^3$ ; this corresponds to an approximate mass of 809 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 ⓘ

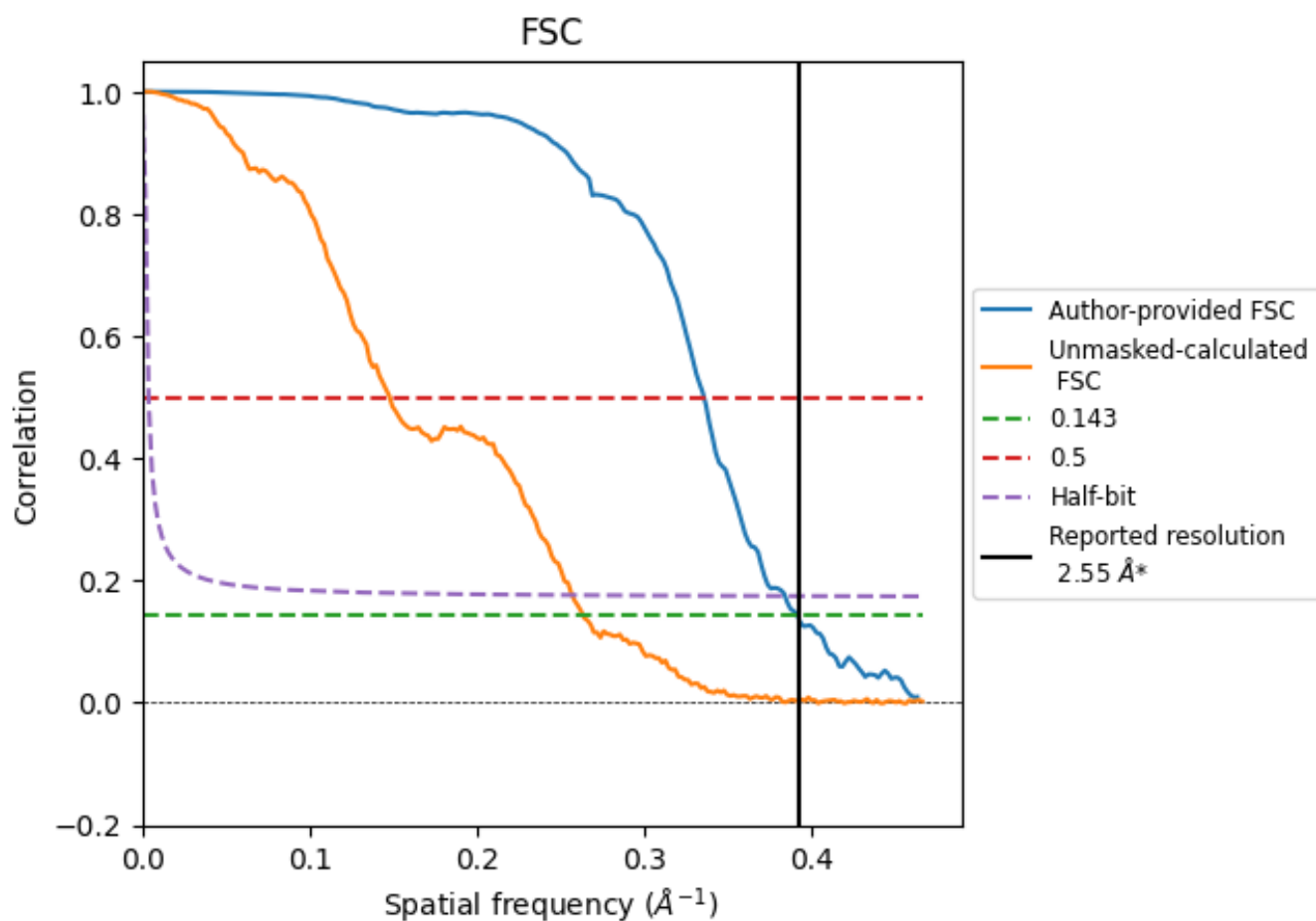


\*Reported resolution corresponds to spatial frequency of 0.392 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.392 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

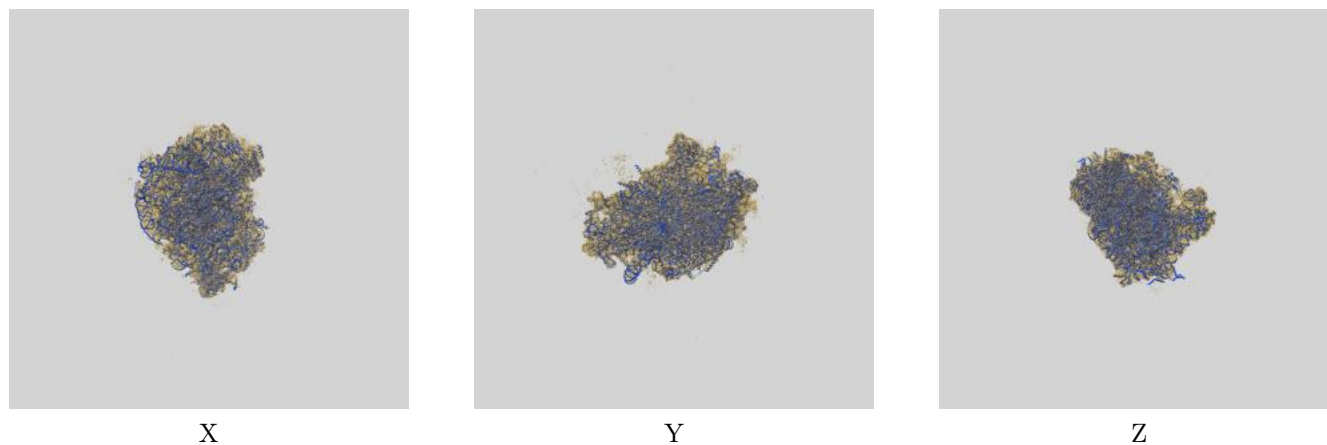
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.55                               | -    | -        |
| Author-provided FSC curve | 2.55                               | 2.98 | 2.60     |
| Unmasked-calculated*      | 3.79                               | 6.76 | 3.89     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 2.55 by more than 10 %

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

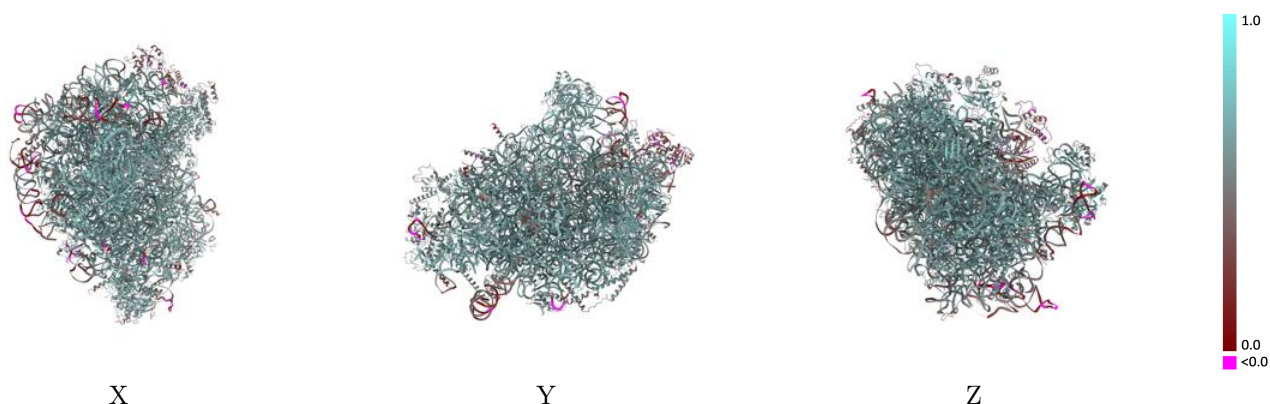
This section contains information regarding the fit between EMDB map EMD-29273 and PDB model 8FLB. Per-residue inclusion information can be found in section [3](#) on page [16](#).

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



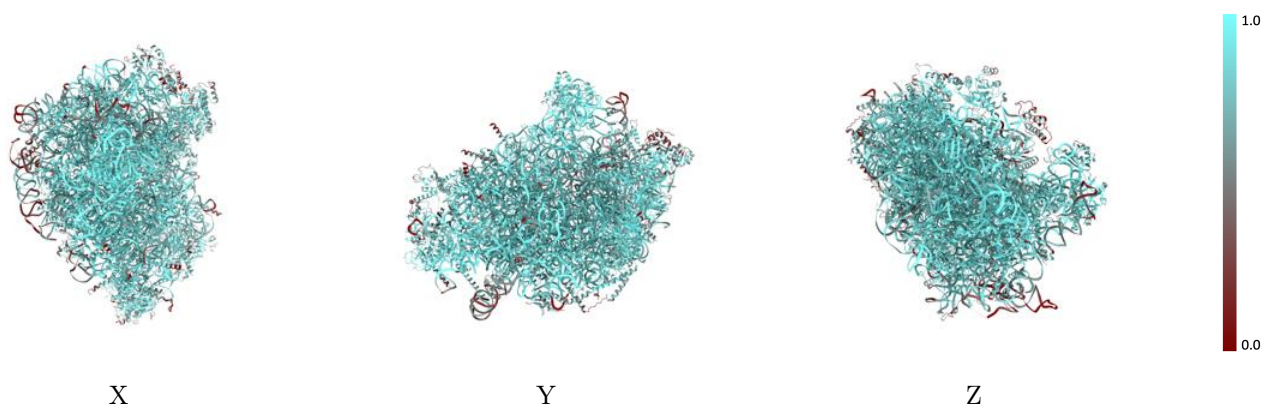
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



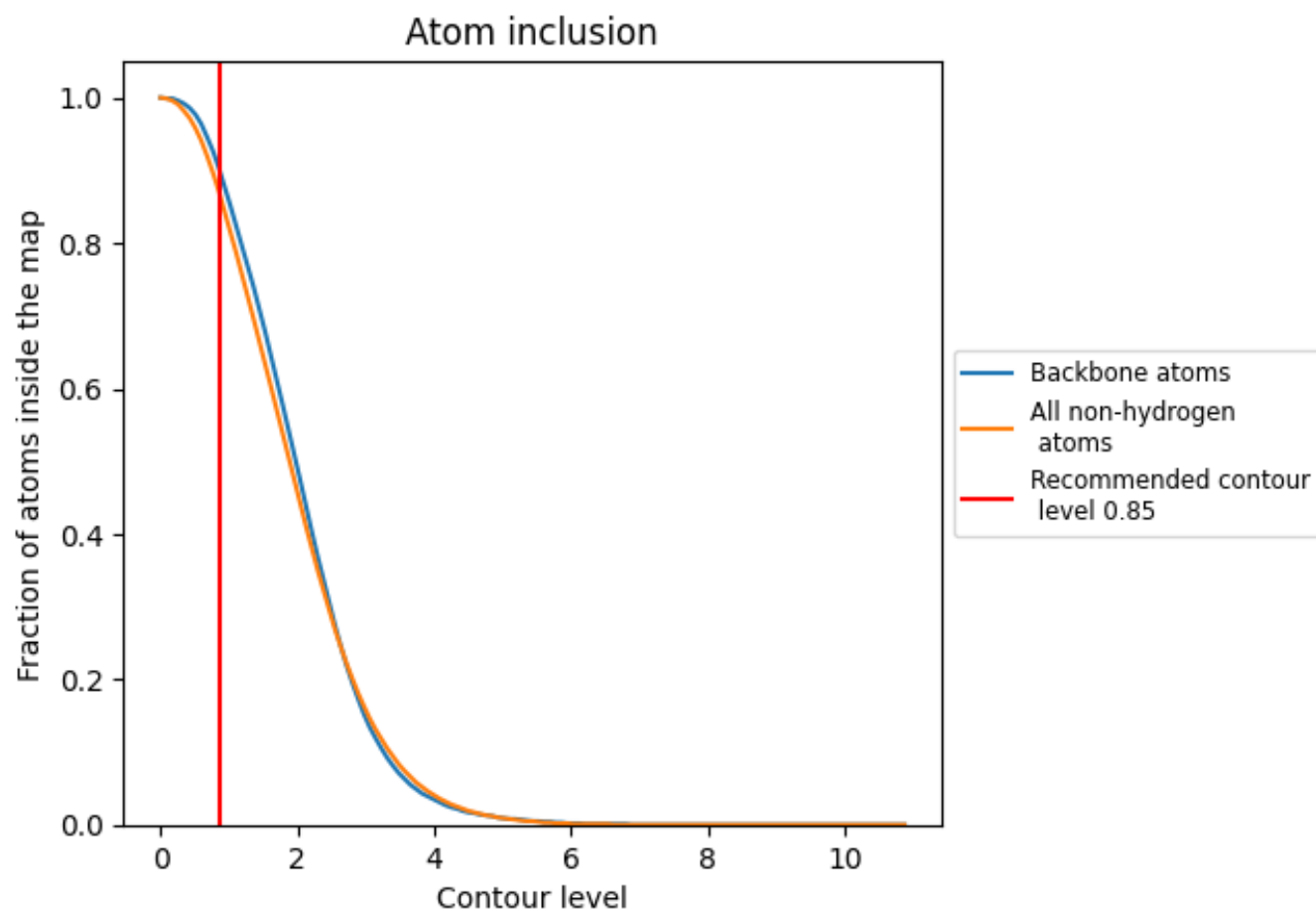
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.85).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.85) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8710   |  0.5870   |
| BA    |  0.3030   |  0.2780   |
| L1    |  0.9500   |  0.6260   |
| L3    |  0.8850   |  0.5750   |
| L4    |  0.9790   |  0.6330   |
| L5    |  0.8200   |  0.5590   |
| L6    |  0.8020   |  0.5790   |
| L7    |  0.9030   |  0.6290   |
| L8    |  0.8980   |  0.6220   |
| L9    |  0.9670   |  0.6580   |
| LA    |  0.8850   |  0.6160   |
| LB    |  0.9200   |  0.6320   |
| LC    |  0.9630   |  0.6630   |
| LD    |  0.8400   |  0.6000   |
| LE    |  0.8890  |  0.6040  |
| LF    |  0.7830 |  0.5740 |
| LG    |  0.9050 |  0.6230 |
| LH    |  0.8680 |  0.6240 |
| LI    |  0.8510 |  0.5950 |
| LJ    |  0.9210 |  0.6290 |
| LK    |  0.9230 |  0.6380 |
| LL    |  0.8790 |  0.6050 |
| LM    |  0.7290 |  0.5260 |
| LN    |  0.8920 |  0.6210 |
| LO    |  0.8040 |  0.5850 |
| LP    |  0.8400 |  0.6000 |
| LQ    |  0.8940 |  0.6210 |
| LR    |  0.9180 |  0.6230 |
| LS    |  0.8590 |  0.6110 |
| LT    |  0.9410 |  0.6420 |
| LU    |  0.7890 |  0.5700 |
| LV    |  0.8900 |  0.6120 |
| LW    |  0.9420 |  0.6400 |
| LX    |  0.8070 |  0.5880 |
| LY    |  0.7380 |  0.5760 |



*Continued on next page...*

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| LZ    |  0.9410   |  0.6340   |
| NK    |  0.6580   |  0.5260   |
| NL    |  0.8070   |  0.5740   |
| NP    |  0.8310   |  0.5860   |
| NR    |  0.7370   |  0.5440   |
| SA    |  0.8940   |  0.6190   |
| SB    |  0.8880   |  0.6060   |
| SC    |  0.7640   |  0.5620   |
| SD    |  0.8830   |  0.6170   |
| SE    |  0.8610   |  0.5990   |
| SF    |  0.9230   |  0.6360   |
| SG    |  0.9000   |  0.6130   |
| SH    |  0.6820   |  0.5050   |
| SI    |  0.7270   |  0.5360   |
| SK    |  0.8420   |  0.5870   |
| SM    |  0.9010   |  0.6190   |
| SQ    |  0.6030   |  0.3730   |
| SR    |  0.7780  |  0.5580  |
| SV    |  0.8330 |  0.5850 |
| VB    |  0.6450 |  0.5280 |