



Full wwPDB EM Validation Report ⓘ

May 28, 2026 – 11:33 am BST

PDB ID : 9RU8 / pdb_00009ru8
EMDB ID : EMD-54266
Title : WT-HEK 80S ribosome bound to TISU mRNA (WT-TISU)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 3.00 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

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>.

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

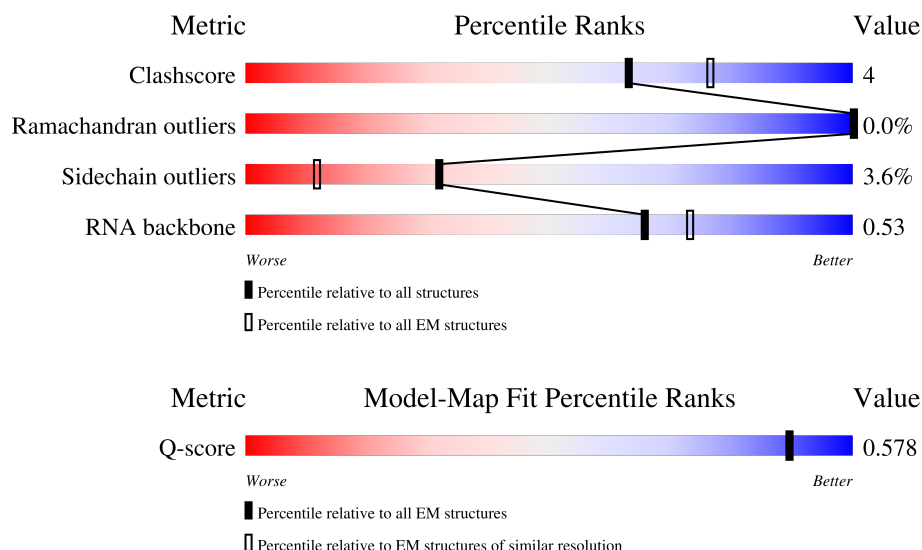
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.








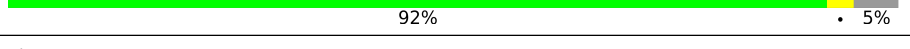
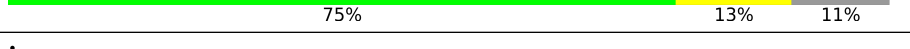
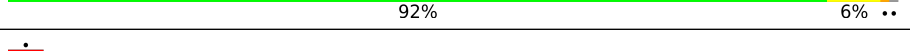
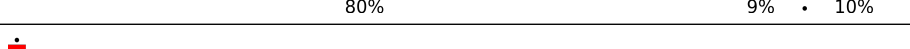
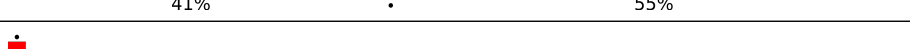
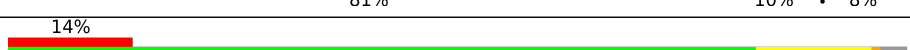

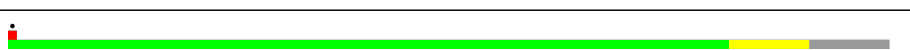







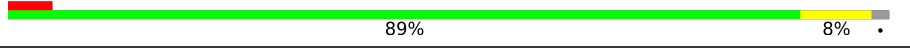
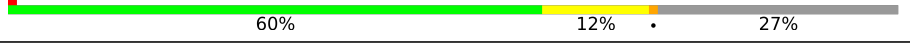



| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| RNA backbone | 8273 | 3508 | - |
| Q-score | - | 25397 | 14081 (2.50 - 3.50) |

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 ≥ 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 | Lm | 128 | |
| 2 | Ll | 51 | |
| 3 | Lo | 106 | |







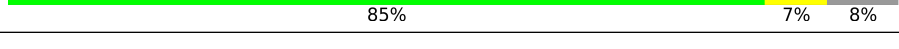
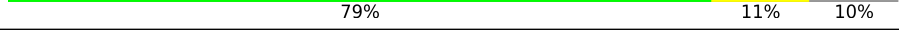
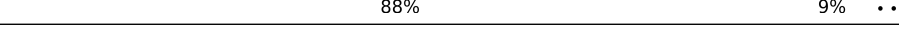
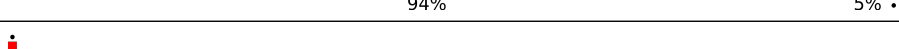
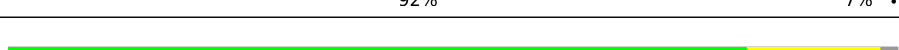

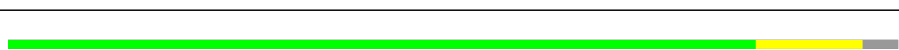

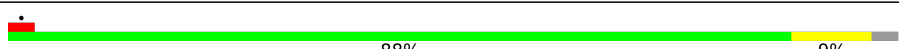





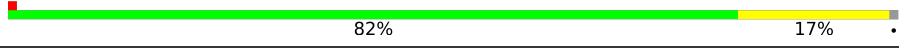
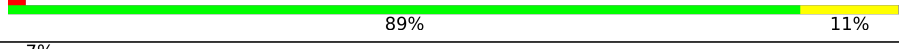



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | SY | 133 |  |
| 5 | SX | 143 |  |
| 6 | SW | 130 |  |
| 7 | SV | 83 |  |
| 8 | SR | 135 |  |
| 9 | SQ | 146 |  |
| 10 | SO | 151 |  |
| 11 | SN | 151 |  |
| 12 | SL | 158 |  |
| 13 | SK | 165 |  |
| 14 | SJ | 194 |  |
| 15 | SH | 194 |  |
| 16 | Sg | 317 |  |
| 17 | SF | 204 |  |
| 18 | SE | 263 |  |
| 19 | Se | 133 |  |
| 20 | SD | 243 |  |
| 21 | Sd | 56 |  |
| 22 | SC | 293 |  |
| 23 | Sc | 69 |  |
| 24 | SB | 264 |  |
| 25 | Sb | 84 |  |
| 26 | SA | 295 |  |
| 27 | LZ | 136 |  |
| 28 | LY | 145 |  |
























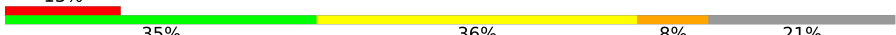

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 29 | LX | 156 |  |
| 30 | LW | 157 |  |
| 31 | LV | 140 |  |
| 32 | LU | 128 |  |
| 33 | LT | 160 |  |
| 34 | LS | 176 |  |
| 35 | LR | 196 |  |
| 36 | Lr | 137 |  |
| 37 | LQ | 188 |  |
| 38 | LP | 154 |  |
| 39 | Lp | 91 |  |
| 40 | LO | 203 |  |
| 41 | LN | 204 |  |
| 42 | Ln | 25 |  |
| 43 | LM | 215 |  |
| 44 | LL | 211 |  |
| 45 | Lk | 70 |  |
| 46 | LJ | 178 |  |
| 47 | Lj | 97 |  |
| 48 | LI | 214 |  |
| 49 | Li | 105 |  |
| 50 | LH | 192 |  |
| 51 | Lh | 123 |  |
| 52 | LG | 266 |  |
| 53 | Lg | 112 |  |



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 54 | LF | 248 |  |
| 55 | Lf | 111 |  |
| 56 | LE | 288 |  |
| 57 | Le | 135 |  |
| 58 | LD | 297 |  |
| 59 | Ld | 125 |  |
| 60 | LC | 427 |  |
| 61 | Lc | 115 |  |
| 62 | LB | 397 |  |
| 63 | Lb | 159 |  |
| 64 | LA | 257 |  |
| 65 | La | 148 |  |
| 66 | L7 | 119 |  |
| 67 | Pt | 77 |  |
| 68 | Sa | 115 |  |
| 69 | L8 | 156 |  |
| 70 | L5 | 5069 |  |
| 71 | SZ | 125 |  |
| 72 | ST | 145 |  |
| 73 | SP | 145 |  |
| 74 | S2 | 1869 |  |
| 75 | SG | 249 |  |
| 76 | SI | 208 |  |
| 77 | S6 | 75 |  |
| 78 | SS | 152 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 79 | mR | 27 |  11% 15% 74% |
| 80 | SU | 119 |  15% 68% 13% 16% |

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 201487 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 Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1 | Lm | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 407 | 251 | 87 | 63 | 6 | | |
| | | | | | | | | | |

- Molecule 2 is a protein called Large ribosomal subunit protein eL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2 | Ll | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 434 | 275 | 94 | 64 | 1 | | |
| | | | | | | | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Ll | 34 | ILE | LYS | conflict | UNP P62891 |

- Molecule 3 is a protein called Large ribosomal subunit protein eL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | Lo | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 822 | 516 | 166 | 134 | 6 | | |
| | | | | | | | | | |

- Molecule 4 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | SY | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 900 | 565 | 181 | 151 | 3 | | |
| | | | | | | | | | |

- Molecule 5 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | SX | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1060 | 669 | 214 | 174 | 3 | | |
| | | | | | | | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| SX | 62 | HIS | PRO | conflict | UNP P62266 |

- Molecule 6 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | SW | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1023 | 653 | 192 | 172 | 6 | | |

- Molecule 7 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | SV | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 623 | 388 | 117 | 113 | 5 | | |

- Molecule 8 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | SR | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 936 | 591 | 173 | 169 | 3 | | |

- Molecule 9 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | SQ | 139 | Total | C | N | O | S | 0 | 0 |
| | | | 918 | 570 | 181 | 166 | 1 | | |

- Molecule 10 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | SO | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 977 | 600 | 196 | 175 | 6 | | |

- Molecule 11 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | SN | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1186 | 761 | 221 | 203 | 1 | | |

- Molecule 12 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | SL | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1158 | 737 | 218 | 197 | 6 | | |

- Molecule 13 is a protein called Small ribosomal subunit protein eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13 | SK | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 468 | 302 | 86 | 79 | 1 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| SK | 68 | PHE | TYR | conflict | UNP P46783 |

- Molecule 14 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | SJ | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1430 | 915 | 285 | 228 | 2 | | |

- Molecule 15 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | SH | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1408 | 905 | 263 | 239 | 1 | | |

- Molecule 16 is a protein called Small ribosomal subunit protein RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | Sg | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1259 | 757 | 255 | 247 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Sg | 155 | PHE | ARG | conflict | UNP P63244 |

- Molecule 17 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | SF | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1327 | 835 | 251 | 238 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| SF | 15 | LYS | PRO | conflict | UNP P46782 |

- Molecule 18 is a protein called Small ribosomal subunit protein eS4, X isoform.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18 | SE | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2037 | 1304 | 383 | 342 | 8 | | |

- Molecule 19 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19 | Se | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 399 | 243 | 90 | 65 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | SD | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1094 | 689 | 201 | 201 | 3 | | |

- Molecule 21 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 21 | Sd | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 430 | 270 | 87 | 68 | 5 | | |

- Molecule 22 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22 | SC | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1694 | 1097 | 292 | 295 | 10 | | |

- Molecule 23 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23 | Sc | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 434 | 264 | 87 | 81 | 2 | | |

- Molecule 24 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24 | SB | 212 | Total | C | N | O | S | 1 | 0 |
| | | | 1694 | 1078 | 306 | 295 | 15 | | |

- Molecule 25 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | Sb | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 613 | 383 | 113 | 110 | 7 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26 | SA | 215 | Total | C | N | O | S | 0 | 0 |
| | | | 1658 | 1056 | 292 | 303 | 7 | | |

- Molecule 27 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | LZ | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1095 | 709 | 207 | 176 | 3 | | |

- Molecule 28 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | LY | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1060 | 666 | 215 | 176 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| LY | 52 | LYS | ASP | conflict | UNP P61254 |

- Molecule 29 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | LX | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 976 | 624 | 183 | 168 | 1 | | |

- Molecule 30 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 30 | LW | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 519 | 332 | 101 | 83 | 3 | | |

- Molecule 31 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | LV | 131 | Total | C | N | O | S | 1 | 0 |
| | | | 987 | 623 | 187 | 172 | 5 | | |

- Molecule 32 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | LU | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 800 | 513 | 140 | 145 | 2 | | |

- Molecule 33 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | LT | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1297 | 823 | 252 | 216 | 6 | | |

- Molecule 34 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 34 | LS | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1456 | 927 | 283 | 235 | 11 | | |

- Molecule 35 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | LR | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1458 | 903 | 312 | 234 | 9 | | |

- Molecule 36 is a protein called Large ribosomal subunit protein eL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | Lr | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 987 | 612 | 205 | 166 | 4 | | |

- Molecule 37 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | LQ | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1505 | 940 | 312 | 248 | 5 | | |

- Molecule 38 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | LP | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1230 | 769 | 240 | 212 | 9 | | |

- Molecule 39 is a protein called Large ribosomal subunit protein eL43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | Lp | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 695 | 439 | 134 | 115 | 7 | | |

- Molecule 40 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40 | LO | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1620 | 1044 | 318 | 253 | 5 | | |

- Molecule 41 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41 | LN | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1694 | 1069 | 356 | 265 | 4 | | |

- Molecule 42 is a protein called Small ribosomal subunit protein eS32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42 | Ln | 24 | Total | C | N | O | S | 0 | 0 |
| | | | 235 | 142 | 65 | 25 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Ln | 24 | ARG | SER | conflict | UNP P62945 |

- Molecule 43 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | LM | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1116 | 716 | 214 | 179 | 7 | | |

- Molecule 44 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44 | LL | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1638 | 1026 | 342 | 266 | 4 | | |

- Molecule 45 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 45 | Lk | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 557 | 358 | 101 | 97 | 1 | | |

- Molecule 46 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | LJ | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1329 | 843 | 246 | 234 | 6 | | |

- Molecule 47 is a protein called Large ribosomal subunit protein eL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | Lj | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 701 | 432 | 154 | 110 | 5 | | |

- Molecule 48 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48 | LI | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1632 | 1038 | 314 | 267 | 13 | | |

- Molecule 49 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | Li | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 812 | 509 | 171 | 127 | 5 | | |

- Molecule 50 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | LH | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1499 | 946 | 281 | 266 | 6 | | |

- Molecule 51 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | Lh | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 1010 | 638 | 204 | 167 | 1 | | |

- Molecule 52 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52 | LG | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1791 | 1142 | 346 | 299 | 4 | | |

- Molecule 53 is a protein called Large ribosomal subunit protein eL34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | Lg | 110 | Total | C | N | O | S | 1 | 0 |
| | | | 871 | 545 | 181 | 139 | 6 | | |

- Molecule 54 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54 | LF | 225 | Total | C | N | O | S | 0 | 0 |
| | | | 1835 | 1178 | 350 | 298 | 9 | | |

- Molecule 55 is a protein called Large ribosomal subunit protein eL33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55 | Lf | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 868 | 549 | 173 | 143 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Lf | 111 | LYS | - | expression tag | UNP P18077 |

- Molecule 56 is a protein called Large ribosomal subunit protein eL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56 | LE | 217 | Total | C | N | O | S | 1 | 0 |
| | | | 1721 | 1108 | 327 | 282 | 4 | | |

- Molecule 57 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57 | Le | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1044 | 660 | 215 | 164 | 5 | | |

- Molecule 58 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58 | LD | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2354 | 1487 | 429 | 424 | 14 | | |

- Molecule 59 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59 | Ld | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 840 | 534 | 165 | 139 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 60 | LC | 359 | Total | C | N | O | S | 0 | 0 |
| | | | 2862 | 1802 | 572 | 475 | 13 | | |

- Molecule 61 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61 | Lc | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 760 | 482 | 134 | 138 | 6 | | |

- Molecule 62 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 62 | LB | 396 | Total | C | N | O | S | 0 | 0 |
| | | | 3174 | 2022 | 597 | 542 | 13 | | |

- Molecule 63 is a protein called Large ribosomal subunit protein eL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63 | Lb | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 815 | 506 | 178 | 127 | 4 | | |

- Molecule 64 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 64 | LA | 248 | Total | C | N | O | S | 1 | 0 |
| | | | 1899 | 1190 | 389 | 314 | 6 | | |

- Molecule 65 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65 | La | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1157 | 732 | 236 | 186 | 3 | | |

- Molecule 66 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 66 | L7 | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2542 | 1132 | 454 | 837 | 119 | | |

- Molecule 67 is a RNA chain called P site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 67 | Pt | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1645 | 734 | 298 | 535 | 77 | 1 | | |

- Molecule 68 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68 | Sa | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 775 | 484 | 159 | 128 | 4 | | |

- Molecule 69 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 69 | L8 | 153 | Total | C | N | O | P | 0 | 0 |
| | | | 3256 | 1453 | 574 | 1076 | 153 | | |

- Molecule 70 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 70 | L5 | 3446 | Total | C | N | O | P | 1 | 0 |
| | | | 73960 | 32974 | 13527 | 24012 | 3447 | | |

- Molecule 71 is a protein called Small ribosomal subunit protein eS25.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 71 | SZ | 63 | Total | C | N | O | 0 | 0 |
| | | | 383 | 245 | 69 | 69 | | |

- Molecule 72 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72 | ST | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 837 | 529 | 163 | 143 | 2 | | |

- Molecule 73 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73 | SP | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 806 | 504 | 155 | 144 | 3 | | |

- Molecule 74 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 74 | S2 | 1569 | Total | C | N | O | P | 0 | 0 |
| | | | 33557 | 15003 | 6040 | 10945 | 1569 | | |

- Molecule 75 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 75 | SG | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1663 | 1043 | 329 | 284 | 7 | | |

- Molecule 76 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 76 | SI | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1648 | 1035 | 326 | 282 | 5 | | |

- Molecule 77 is a RNA chain called E site tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 77 | S6 | 59 | Total | C | N | O | P | 0 | 0 |
| | | | 1263 | 565 | 238 | 402 | 58 | | |

- Molecule 78 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 78 | SS | 138 | Total | C | N | O | | 0 | 0 |
| | | | 903 | 565 | 178 | 160 | | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| SS | 115 | ILE | LYS | conflict | UNP P62269 |
| SS | 117 | ALA | ILE | conflict | UNP P62269 |
| SS | 119 | PHE | ALA | conflict | UNP P62269 |

- Molecule 79 is a RNA chain called TISU mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 79 | mR | 7 | Total | C | N | O | P | 0 | 0 |
| | | | 152 | 68 | 30 | 47 | 7 | | |

- Molecule 80 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80 | SU | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 795 | 498 | 152 | 141 | 4 | | |

- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 81 | Lm | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 81 | Lo | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 81 | Sd | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 81 | Lp | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 81 | Lg | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 82 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 82 | SQ | 1 | Total K 1 1 | 0 |
| 82 | Lf | 1 | Total K 1 1 | 0 |
| 82 | LC | 1 | Total K 1 1 | 0 |
| 82 | LB | 1 | Total K 1 1 | 0 |
| 82 | L8 | 1 | Total K 1 1 | 0 |
| 82 | L5 | 60 | Total K 60 60 | 0 |
| 82 | S2 | 11 | Total K 11 11 | 0 |

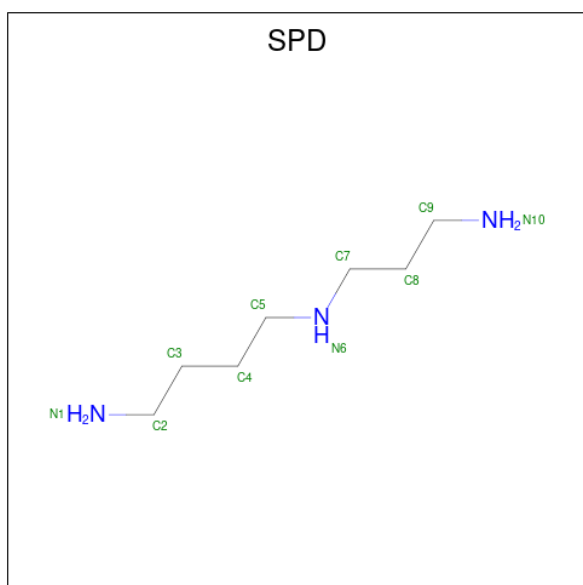
- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-------------------|---------|
| 83 | Sd | 1 | Total Mg 1 1 | 0 |
| 83 | LV | 1 | Total Mg 1 1 | 0 |
| 83 | LS | 1 | Total Mg 1 1 | 0 |
| 83 | LP | 1 | Total Mg 1 1 | 0 |
| 83 | LM | 1 | Total Mg 1 1 | 0 |
| 83 | LI | 2 | Total Mg 2 2 | 0 |
| 83 | Le | 1 | Total Mg 1 1 | 0 |
| 83 | LB | 1 | Total Mg 1 1 | 0 |
| 83 | L7 | 5 | Total Mg 5 5 | 0 |
| 83 | Pt | 1 | Total Mg 1 1 | 0 |
| 83 | L8 | 3 | Total Mg 3 3 | 0 |
| 83 | L5 | 81 | Total Mg 81 81 | 0 |
| 83 | S2 | 21 | Total Mg 21 21 | 0 |

- Molecule 84 is SODIUM ION (CCD ID: NA) (formula: Na).

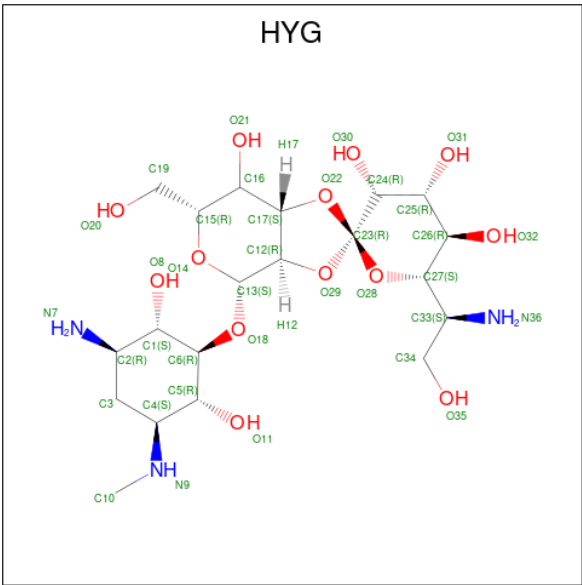
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 84 | LN | 1 | Total | Na | 0 |
| | | | 1 | 1 | |
| 84 | Le | 1 | Total | Na | 0 |
| | | | 1 | 1 | |
| 84 | LB | 1 | Total | Na | 0 |
| | | | 1 | 1 | |
| 84 | L5 | 46 | Total | Na | 0 |
| | | | 46 | 46 | |
| 84 | S2 | 12 | Total | Na | 0 |
| | | | 12 | 12 | |

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 85 | L5 | 1 | Total | C | N | 0 |
| | | | 10 | 7 | 3 | |
| 85 | L5 | 1 | Total | C | N | 0 |
| | | | 10 | 7 | 3 | |
| 85 | L5 | 1 | Total | C | N | 0 |
| | | | 10 | 7 | 3 | |

- Molecule 86 is HYGROMYCIN B (CCD ID: HYG) (formula: C₂₀H₃₇N₃O₁₃).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 86 | S2 | 1 | Total | C | N | O | 0 |
| | | | 36 | 20 | 3 | 13 | |

- Molecule 87 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 87 | Ll | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 87 | Lo | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 87 | SN | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 87 | SL | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 87 | SF | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 87 | LW | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 87 | LV | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 87 | LT | 4 | Total | O | 0 |
| | | | 4 | 4 | |
| 87 | LS | 5 | Total | O | 0 |
| | | | 5 | 5 | |
| 87 | LR | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 87 | LQ | 3 | Total | O | 0 |
| | | | 3 | 3 | |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 87 | LP | 3 | Total 3 | O 3 | 0 |
| 87 | Lp | 1 | Total 1 | O 1 | 0 |
| 87 | LN | 5 | Total 5 | O 5 | 0 |
| 87 | Ln | 2 | Total 2 | O 2 | 0 |
| 87 | LM | 1 | Total 1 | O 1 | 0 |
| 87 | LL | 2 | Total 2 | O 2 | 0 |
| 87 | Lj | 2 | Total 2 | O 2 | 0 |
| 87 | LI | 1 | Total 1 | O 1 | 0 |
| 87 | LH | 1 | Total 1 | O 1 | 0 |
| 87 | Lh | 2 | Total 2 | O 2 | 0 |
| 87 | LG | 1 | Total 1 | O 1 | 0 |
| 87 | Lg | 3 | Total 3 | O 3 | 0 |
| 87 | LF | 3 | Total 3 | O 3 | 0 |
| 87 | Le | 3 | Total 3 | O 3 | 0 |
| 87 | LD | 1 | Total 1 | O 1 | 0 |
| 87 | LC | 1 | Total 1 | O 1 | 0 |
| 87 | Lc | 2 | Total 2 | O 2 | 0 |
| 87 | LB | 7 | Total 7 | O 7 | 0 |
| 87 | Lb | 4 | Total 4 | O 4 | 0 |
| 87 | LA | 4 | Total 4 | O 4 | 0 |
| 87 | La | 3 | Total 3 | O 3 | 0 |

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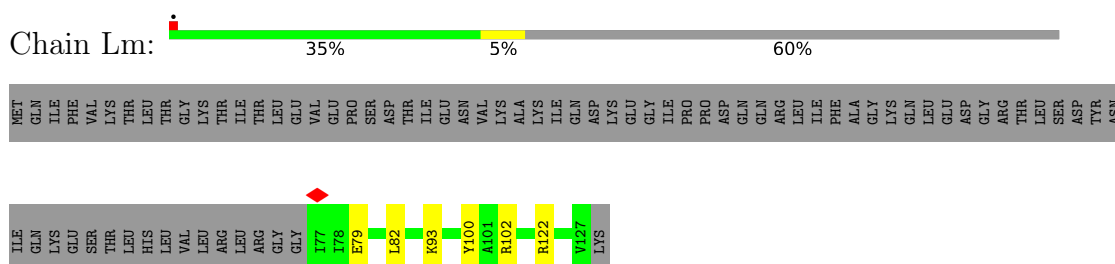
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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 87 | L7 | 9 | Total 9 | O 9 | 0 |
| 87 | Pt | 1 | Total 1 | O 1 | 0 |
| 87 | Sa | 1 | Total 1 | O 1 | 0 |
| 87 | L8 | 16 | Total 16 | O 16 | 0 |
| 87 | L5 | 473 | Total 473 | O 473 | 0 |
| 87 | S2 | 101 | Total 101 | O 101 | 0 |
| 87 | SI | 5 | Total 5 | O 5 | 0 |
| 87 | SS | 2 | Total 2 | O 2 | 0 |

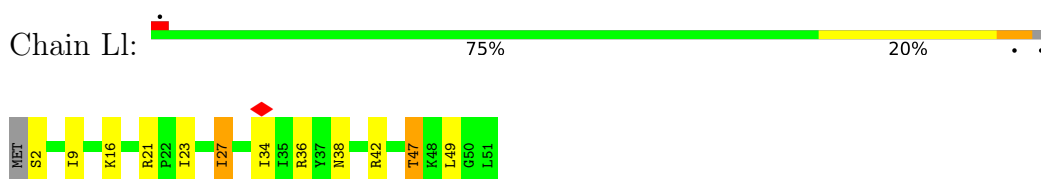
3 Residue-property plots [i](#)

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.

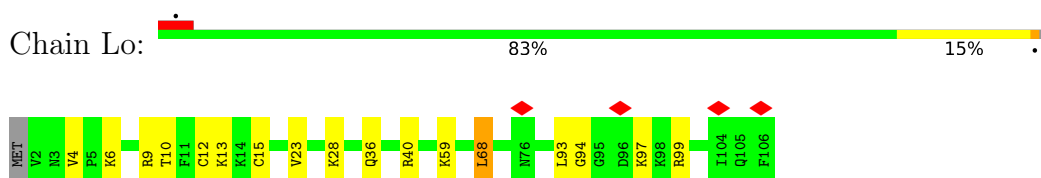
- Molecule 1: Ubiquitin-60S ribosomal protein L40



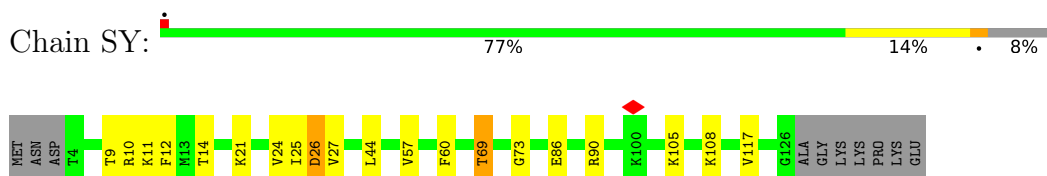
- Molecule 2: Large ribosomal subunit protein eL39



- Molecule 3: Large ribosomal subunit protein eL42



- Molecule 4: 40S ribosomal protein S24



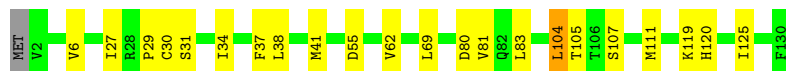
- Molecule 5: Small ribosomal subunit protein uS12





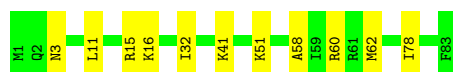
- Molecule 6: 40S ribosomal protein S15a

Chain SW: 82% 16% ..



- Molecule 7: 40S ribosomal protein S21

Chain SV: 87% 13%



- Molecule 8: 40S ribosomal protein S17

Chain SR: 85% 11% ..



- Molecule 9: 40S ribosomal protein S16

Chain SQ: 92% 5%



- Molecule 10: 40S ribosomal protein S14

Chain SO: 75% 13% 11%




- Molecule 11: 40S ribosomal protein S13

Chain SN: 92% 6% ..



- Molecule 12: Small ribosomal subunit protein uS17

Chain SF:  81% 9% 9%



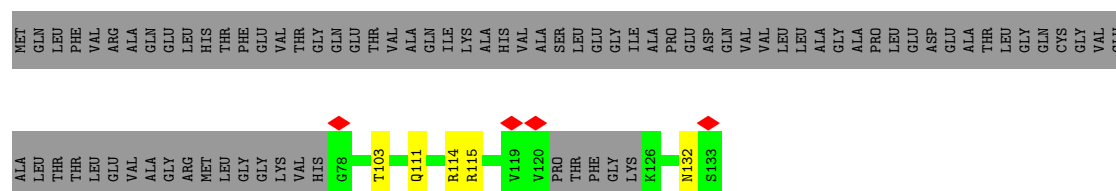
- Molecule 18: Small ribosomal subunit protein eS4, X isoform

Chain SE:  90% 8%



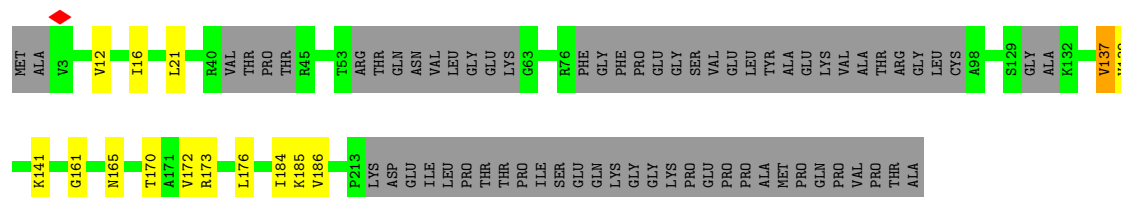
- Molecule 19: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se:  35% 62%



- Molecule 20: 40S ribosomal protein S3

Chain SD:  66% 6% 28%



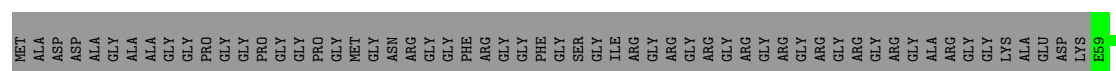
- Molecule 21: 40S ribosomal protein S29

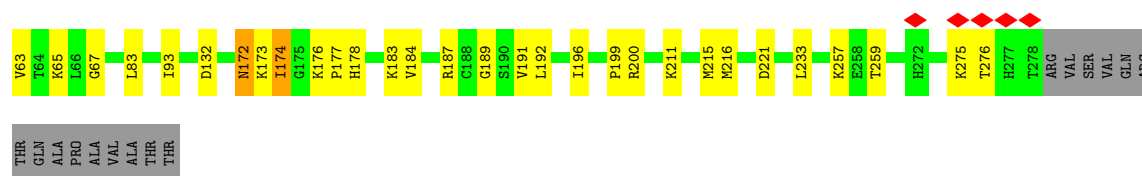
Chain Sd:  71% 27%



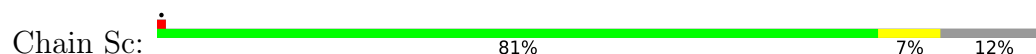
- Molecule 22: 40S ribosomal protein S2

Chain SC:  65% 10% 25%

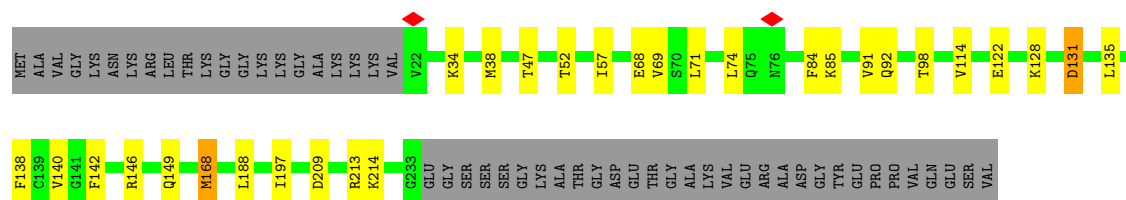




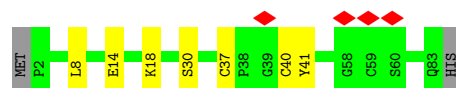
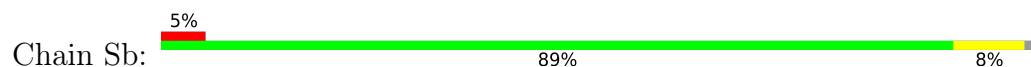
- Molecule 23: 40S ribosomal protein S28



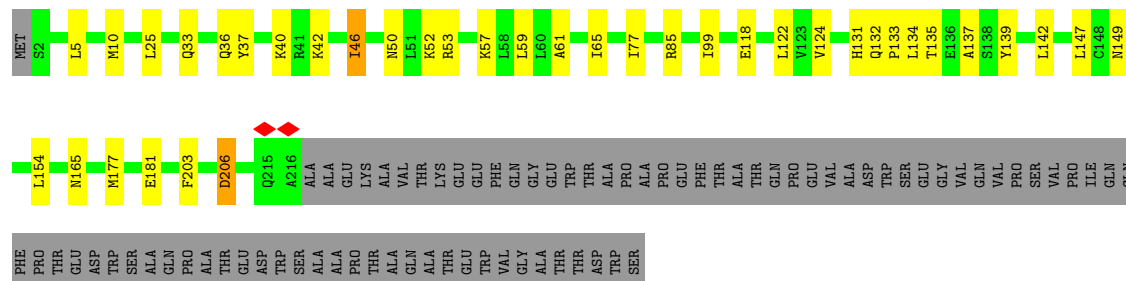
- Molecule 24: 40S ribosomal protein S3a



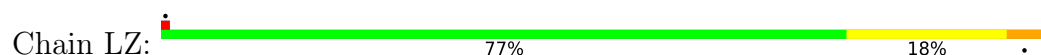
- Molecule 25: 40S ribosomal protein S27



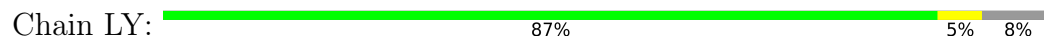
- Molecule 26: 40S ribosomal protein SA



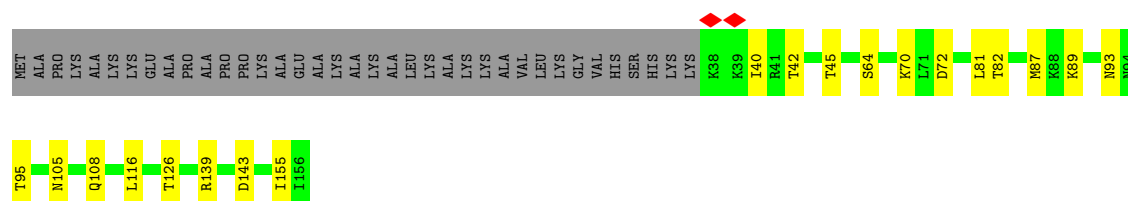
- Molecule 27: 60S ribosomal protein L27



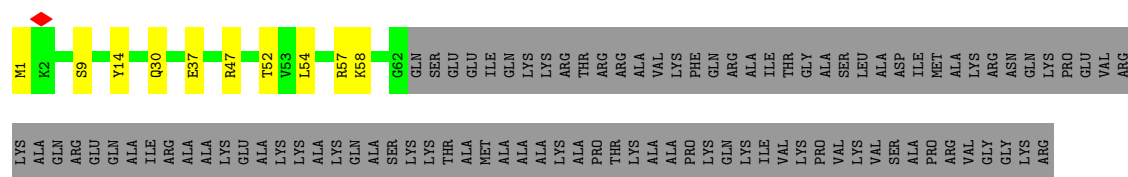
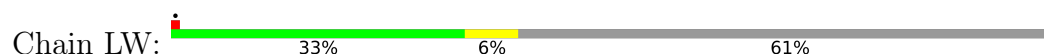
- Molecule 28: Large ribosomal subunit protein uL24



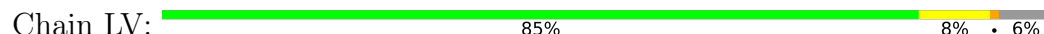
- Molecule 29: 60S ribosomal protein L23a



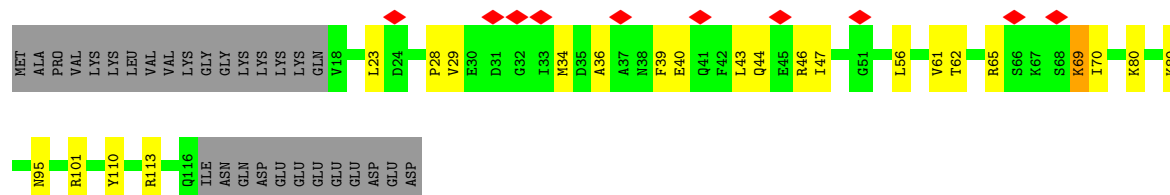
- Molecule 30: 60S ribosomal protein L24



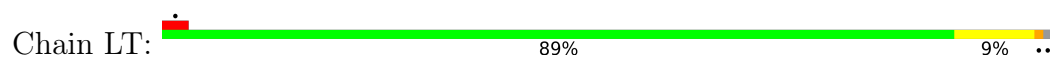
- Molecule 31: 60S ribosomal protein L23



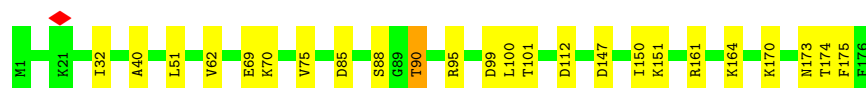
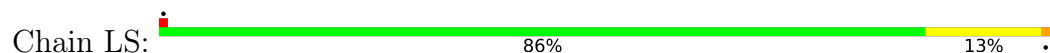
- Molecule 32: 60S ribosomal protein L22



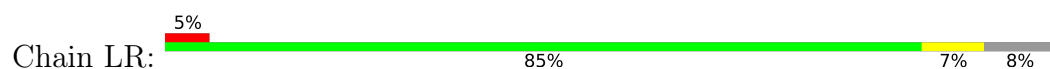
- Molecule 33: 60S ribosomal protein L21



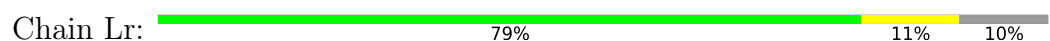
- Molecule 34: 60S ribosomal protein L18a



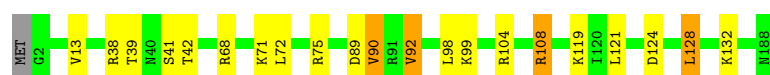
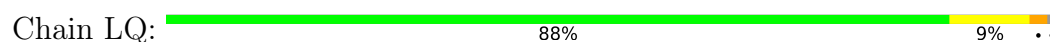
- Molecule 35: 60S ribosomal protein L19



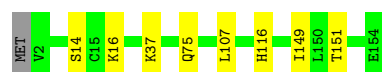
- Molecule 36: Large ribosomal subunit protein eL28



- Molecule 37: 60S ribosomal protein L18



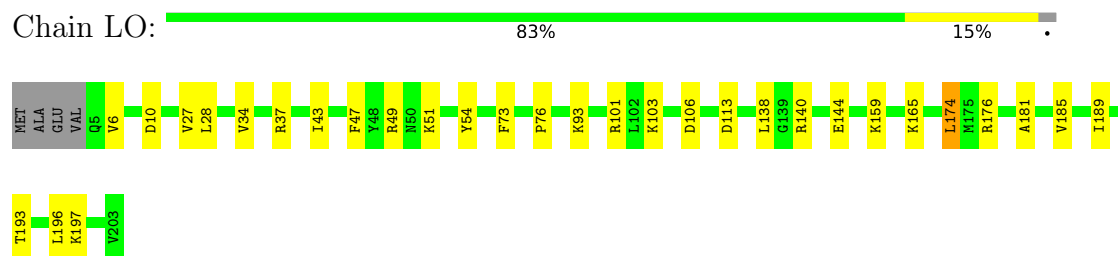
- Molecule 38: Large ribosomal subunit protein uL22



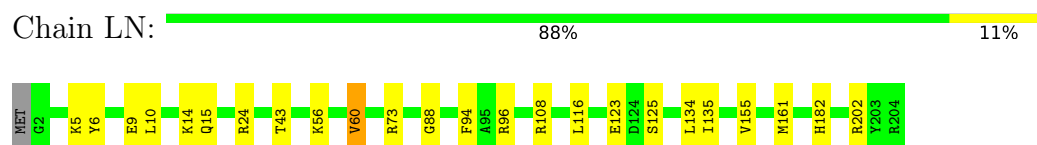
- Molecule 39: Large ribosomal subunit protein eL43



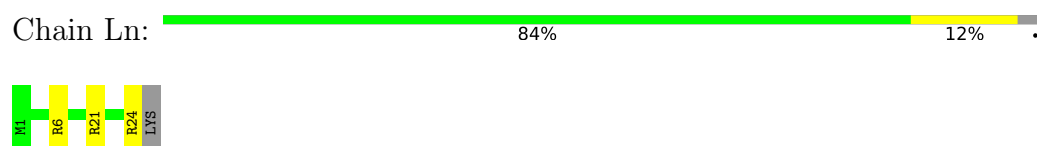
• Molecule 40: 60S ribosomal protein L13a



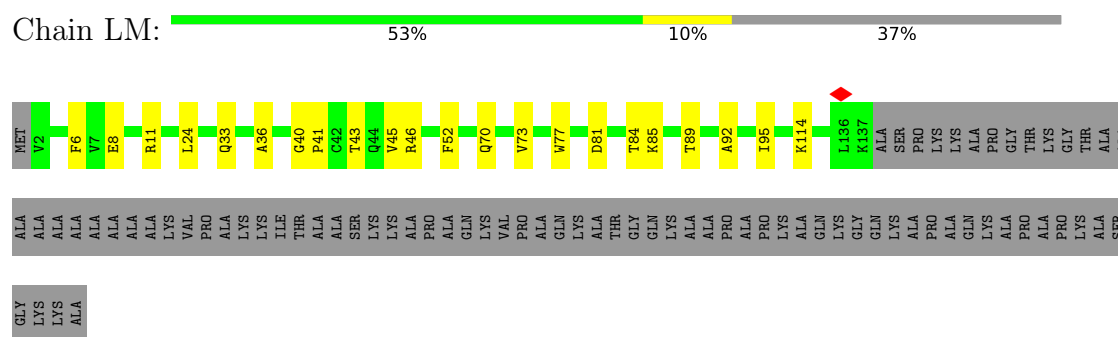
• Molecule 41: 60S ribosomal protein L15



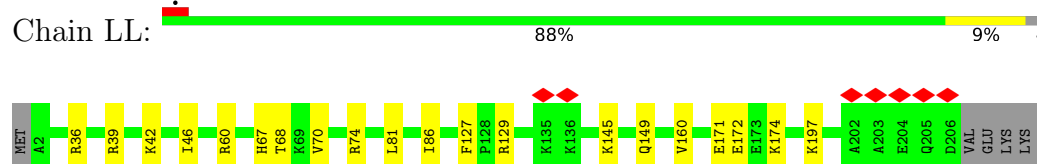
• Molecule 42: Small ribosomal subunit protein eS32



• Molecule 43: 60S ribosomal protein L14

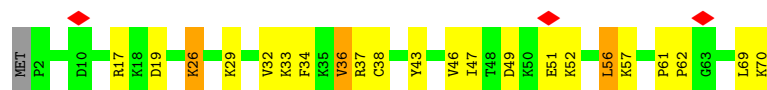


• Molecule 44: 60S ribosomal protein L13

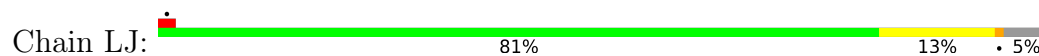


• Molecule 45: 60S ribosomal protein L38

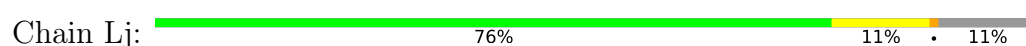




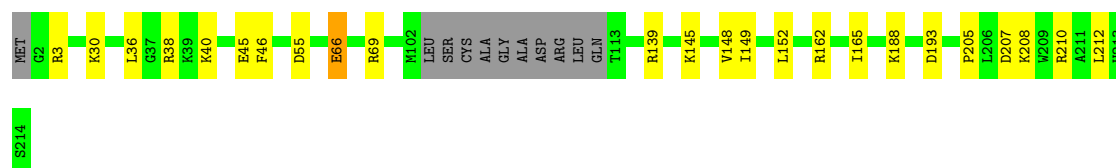
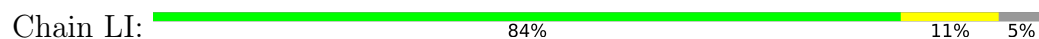
- Molecule 46: 60S ribosomal protein L11



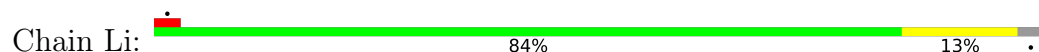
- Molecule 47: Large ribosomal subunit protein eL37



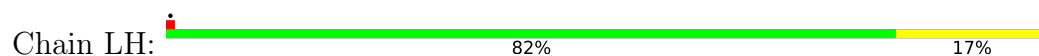
- Molecule 48: 60S ribosomal protein L10



- Molecule 49: 60S ribosomal protein L36

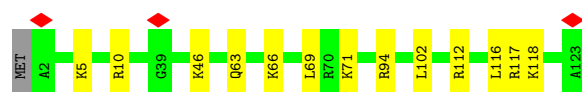


- Molecule 50: 60S ribosomal protein L9

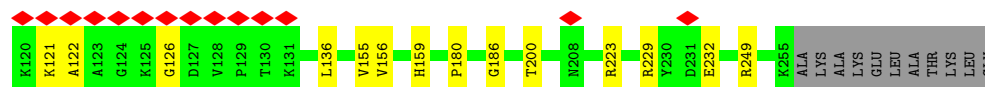
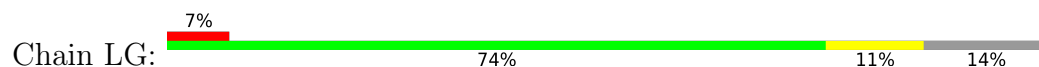


- Molecule 51: 60S ribosomal protein L35

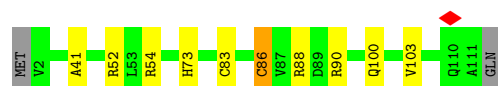




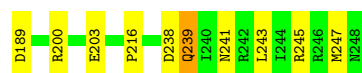
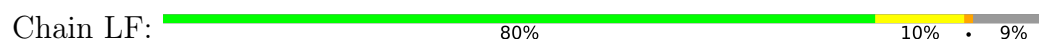
- Molecule 52: 60S ribosomal protein L7a



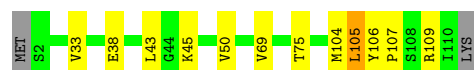
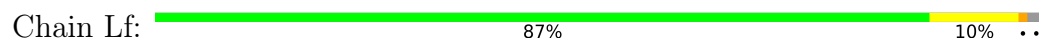
- Molecule 53: Large ribosomal subunit protein eL34



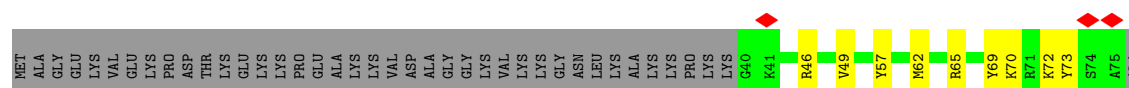
- Molecule 54: Large ribosomal subunit protein uL30

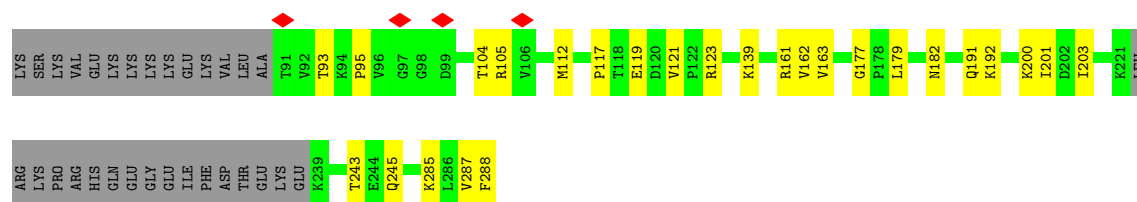


- Molecule 55: Large ribosomal subunit protein eL33



- Molecule 56: Large ribosomal subunit protein eL6





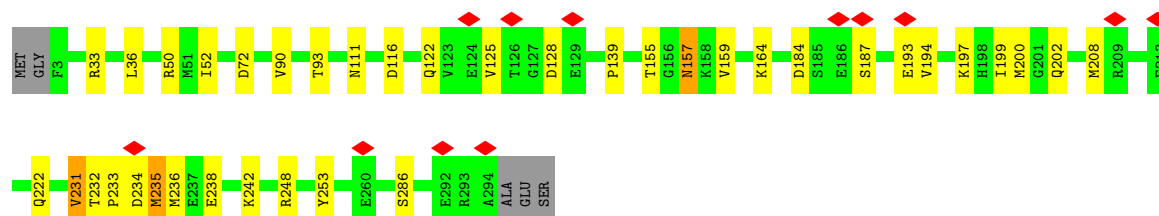
• Molecule 57: 60S ribosomal protein L32

Chain Le: 86% 8% 6%



• Molecule 58: 60S ribosomal protein L5

Chain LD: 86% 12% ..



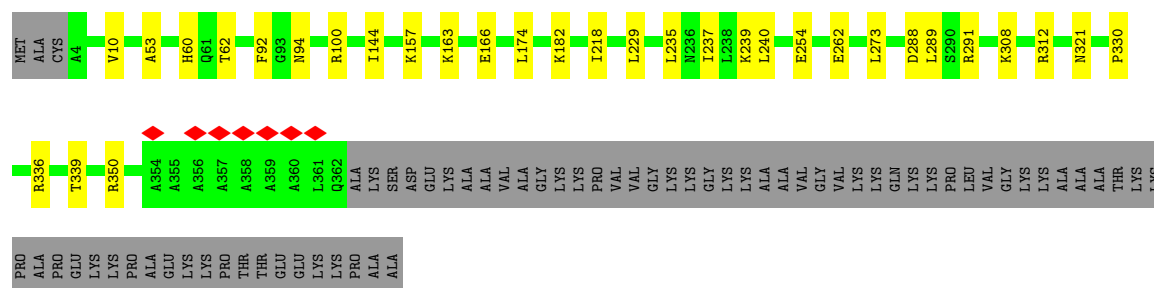
• Molecule 59: 60S ribosomal protein L31

Chain Ld: 74% 10% 15%



• Molecule 60: 60S ribosomal protein L4

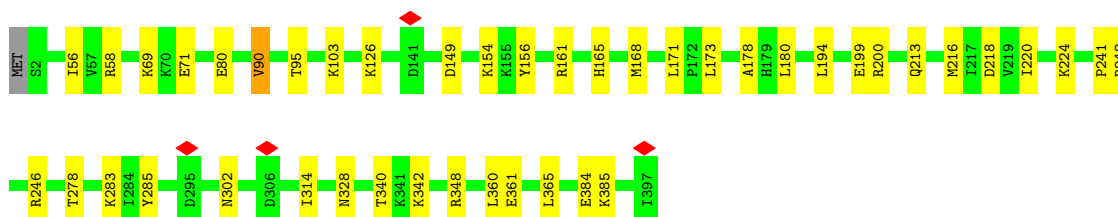
Chain LC: 77% 7% 16%



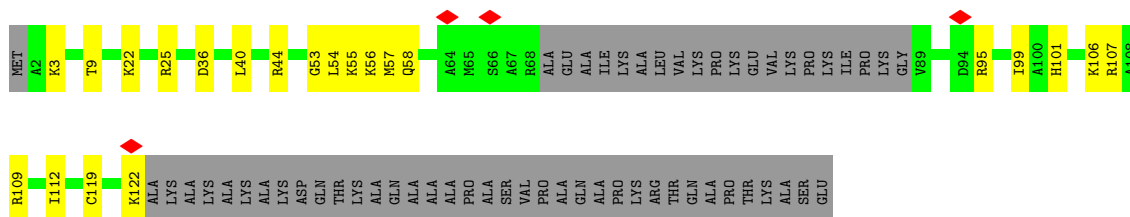
• Molecule 61: 60S ribosomal protein L30

Chain Lc: 73% 11% 15%

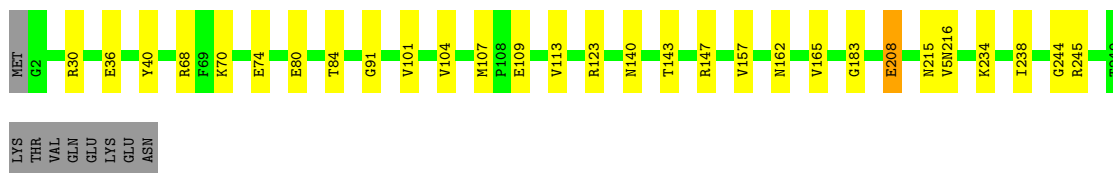
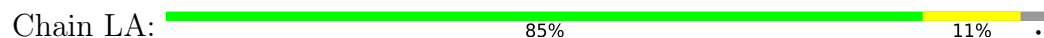
- Molecule 62: Large ribosomal subunit protein uL3



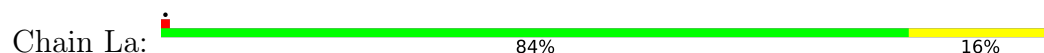
- Molecule 63: Large ribosomal subunit protein eL29



- Molecule 64: Large ribosomal subunit protein uL2



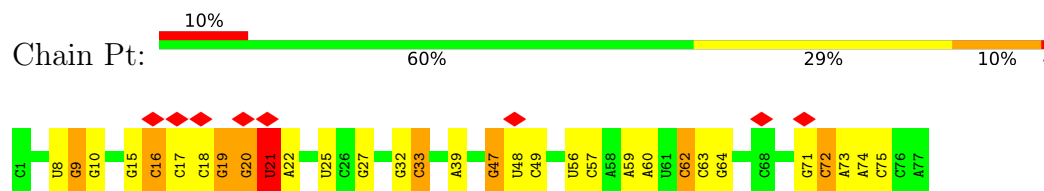
- Molecule 65: Large ribosomal subunit protein uL15



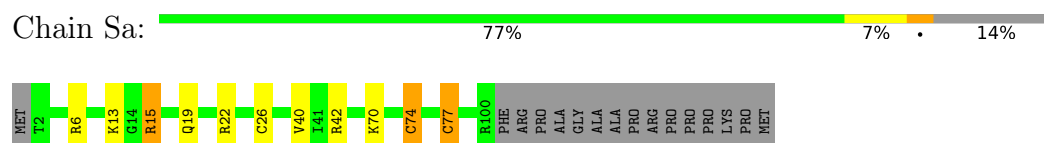
- Molecule 66: 5S rRNA



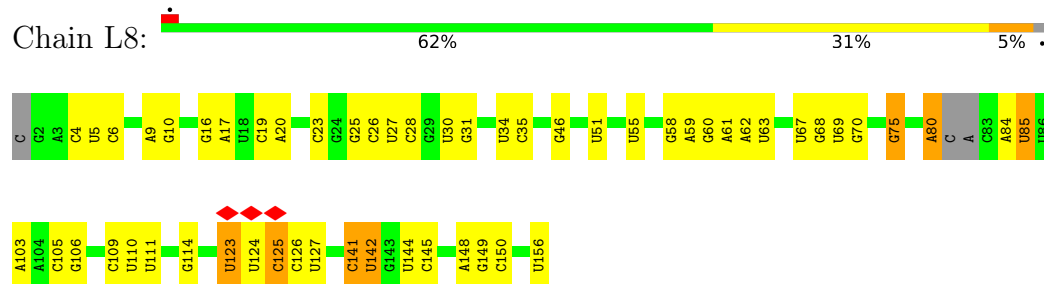
- Molecule 67: P site tRNA



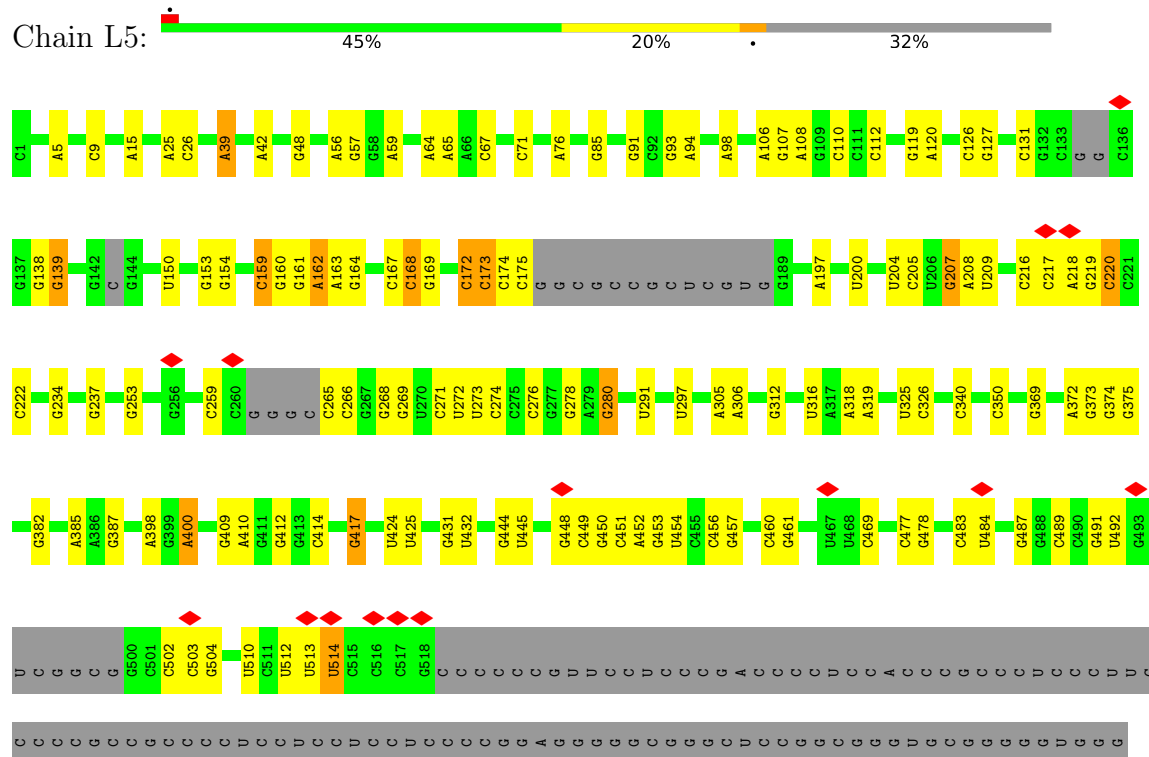
- Molecule 68: 40S ribosomal protein S26



- Molecule 69: 5.8S rRNA



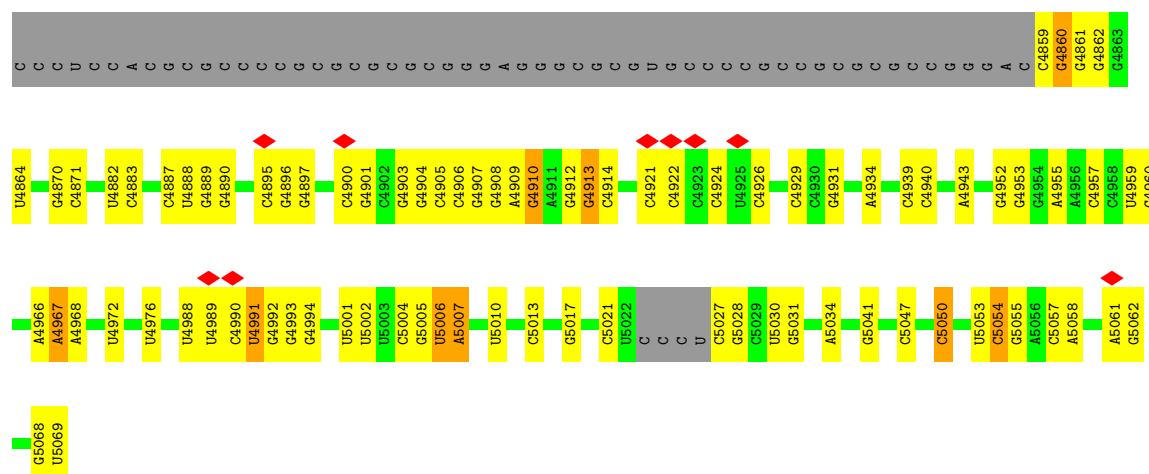
- Molecule 70: 28S rRNA



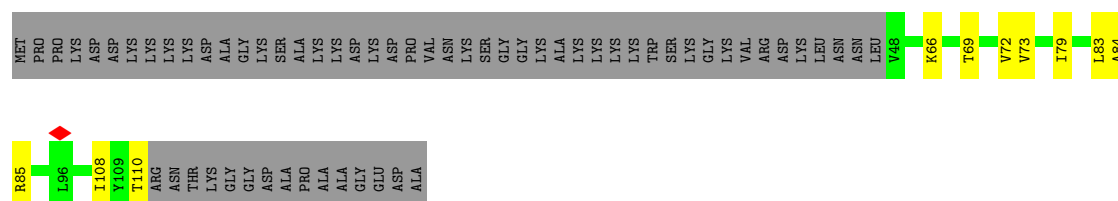




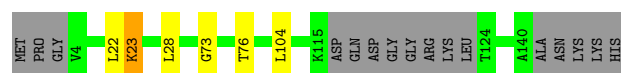
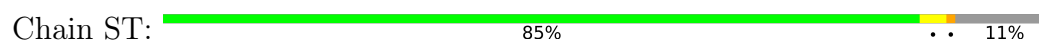




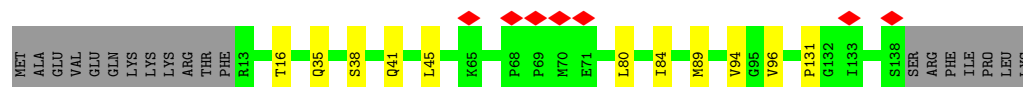
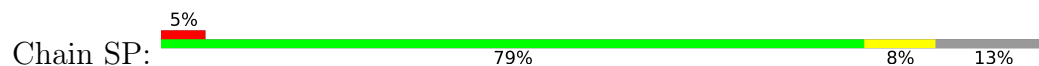
- Molecule 71: Small ribosomal subunit protein eS25



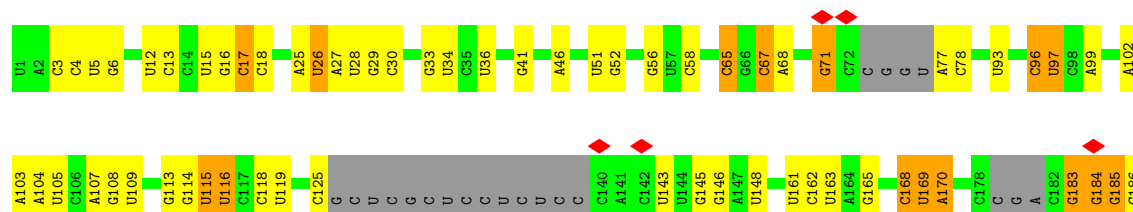
- Molecule 72: 40S ribosomal protein S19



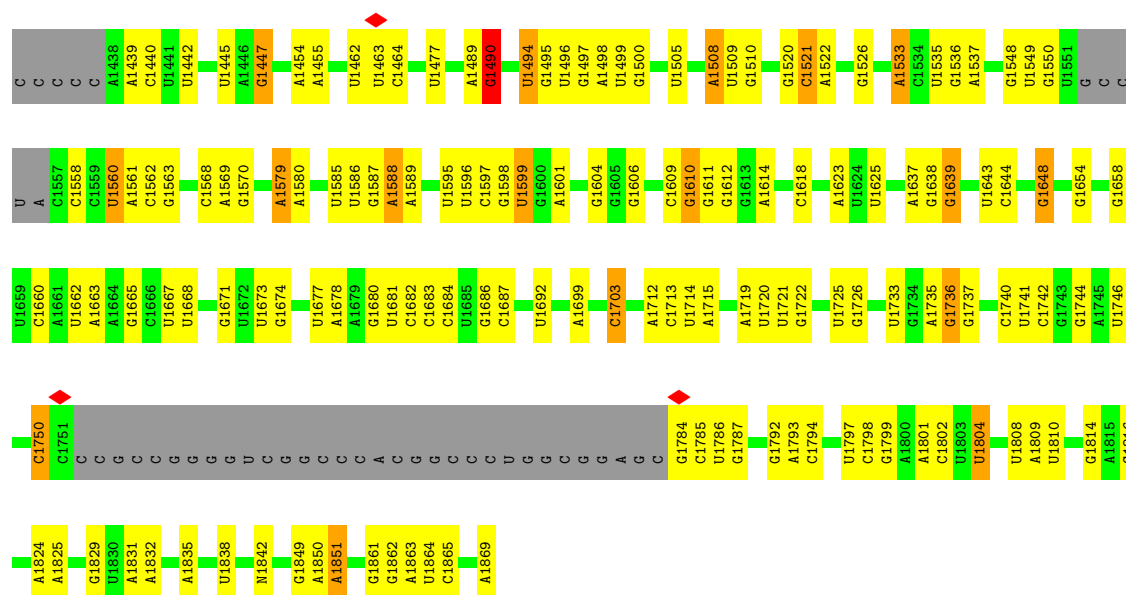
- Molecule 73: 40S ribosomal protein S15



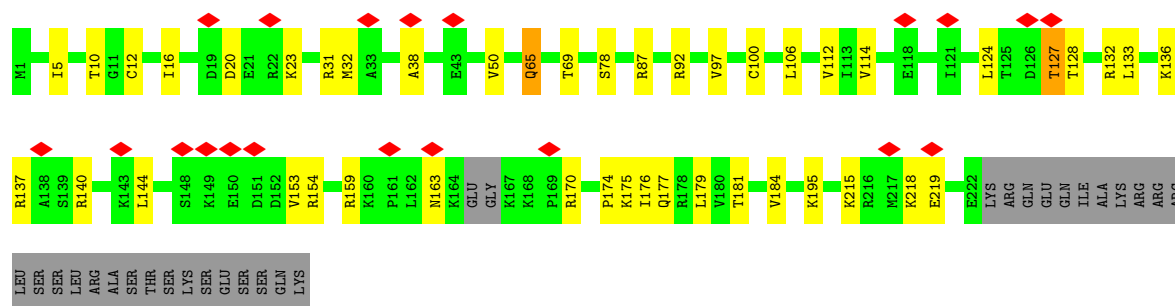
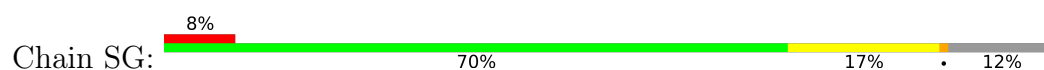
- Molecule 74: 18S rRNA



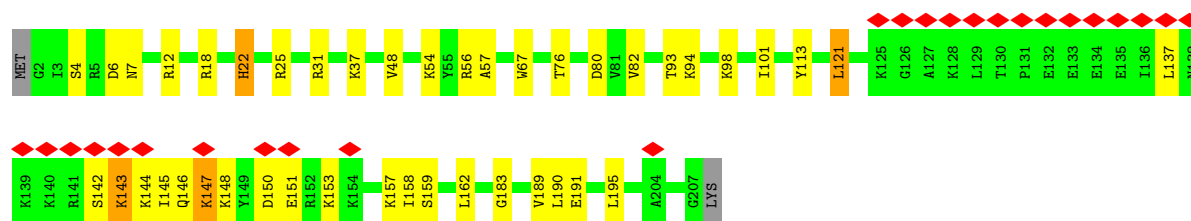
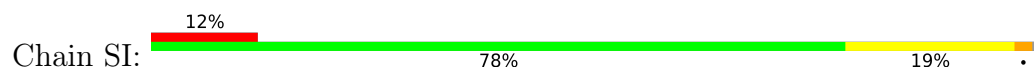




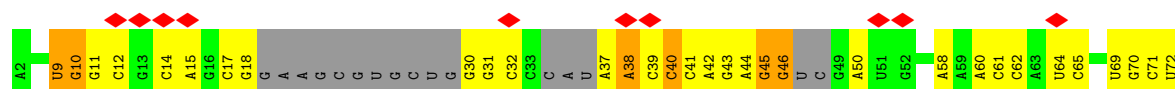
• Molecule 75: 40S ribosomal protein S6



• Molecule 76: 40S ribosomal protein S8



• Molecule 77: E site tRNA





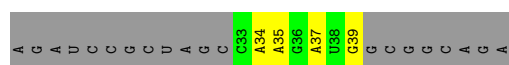
- Molecule 78: Small ribosomal subunit protein uS13

Chain SS: 83% 7% 9%



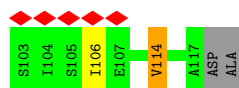
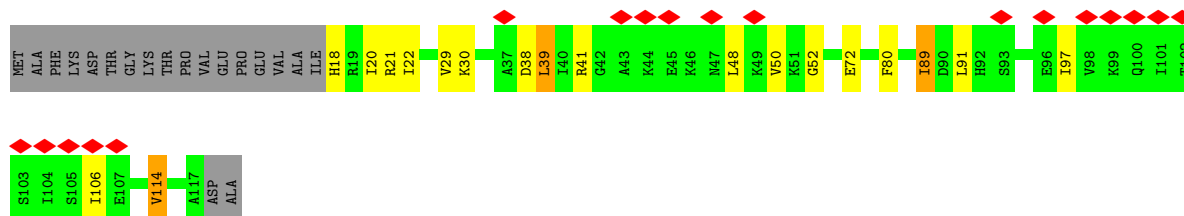
- Molecule 79: TISU mRNA

Chain mR: 11% 15% 74%



- Molecule 80: 40S ribosomal protein S20

Chain SU: 15% 68% 13% 16%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 74646 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 1500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.077 | Depositor |
| Minimum map value | -0.034 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.005 | Depositor |
| Map size (Å) | 404.16, 404.16, 404.16 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.842, 0.842, 0.842 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, K, 6MZ, 4AC, MG, G7M, HYG, OMG, SPD, 1MA, MA6, A2M, H2U, OMC, V5N, 5MC, NA, PSU, UR3, MLZ, B8N, 4SU, ZN

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 | Lm | 0.15 | 0/413 | 0.33 | 0/549 |
| 2 | Ll | 0.17 | 0/444 | 0.33 | 0/588 |
| 3 | Lo | 0.15 | 0/823 | 0.31 | 0/1088 |
| 4 | SY | 0.15 | 0/917 | 0.33 | 0/1234 |
| 5 | SX | 0.15 | 0/1077 | 0.33 | 0/1441 |
| 6 | SW | 0.17 | 0/1040 | 0.30 | 0/1393 |
| 7 | SV | 0.14 | 0/630 | 0.32 | 0/843 |
| 8 | SR | 0.15 | 0/950 | 0.35 | 0/1291 |
| 9 | SQ | 0.15 | 0/927 | 0.32 | 0/1258 |
| 10 | SO | 0.18 | 0/990 | 0.37 | 0/1330 |
| 11 | SN | 0.17 | 0/1210 | 0.32 | 0/1633 |
| 12 | SL | 0.15 | 0/1178 | 0.28 | 0/1578 |
| 13 | SK | 0.14 | 0/481 | 0.29 | 0/662 |
| 14 | SJ | 0.15 | 0/1455 | 0.30 | 0/1954 |
| 15 | SH | 0.15 | 0/1429 | 0.33 | 0/1929 |
| 16 | Sg | 0.14 | 0/1259 | 0.38 | 0/1730 |
| 17 | SF | 0.15 | 0/1345 | 0.33 | 0/1827 |
| 18 | SE | 0.14 | 0/2079 | 0.32 | 0/2801 |
| 19 | Se | 0.13 | 0/401 | 0.33 | 0/524 |
| 20 | SD | 0.14 | 0/1103 | 0.29 | 0/1505 |
| 21 | Sd | 0.15 | 0/441 | 0.28 | 0/589 |
| 22 | SC | 0.16 | 0/1731 | 0.34 | 0/2341 |
| 23 | Sc | 0.14 | 0/435 | 0.26 | 0/587 |
| 24 | SB | 0.16 | 0/1721 | 0.34 | 0/2304 |
| 25 | Sb | 0.14 | 0/625 | 0.31 | 0/842 |
| 26 | SA | 0.16 | 0/1695 | 0.31 | 0/2310 |
| 27 | LZ | 0.15 | 0/1118 | 0.30 | 0/1494 |
| 28 | LY | 0.15 | 0/1077 | 0.32 | 0/1440 |
| 29 | LX | 0.17 | 0/993 | 0.34 | 0/1334 |
| 30 | LW | 0.15 | 0/532 | 0.30 | 0/708 |
| 31 | LV | 0.15 | 0/1004 | 0.31 | 0/1346 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | LU | 0.15 | 0/814 | 0.38 | 0/1094 |
| 33 | LT | 0.15 | 0/1325 | 0.27 | 0/1770 |
| 34 | LS | 0.16 | 0/1496 | 0.30 | 0/2009 |
| 35 | LR | 0.18 | 0/1474 | 0.32 | 0/1957 |
| 36 | Lr | 0.19 | 0/1002 | 0.35 | 0/1344 |
| 37 | LQ | 0.17 | 0/1529 | 0.33 | 0/2044 |
| 38 | LP | 0.16 | 0/1256 | 0.33 | 0/1687 |
| 39 | Lp | 0.17 | 0/705 | 0.34 | 0/937 |
| 40 | LO | 0.18 | 0/1652 | 0.30 | 0/2211 |
| 41 | LN | 0.17 | 0/1739 | 0.34 | 0/2331 |
| 42 | Ln | 0.21 | 0/236 | 0.32 | 0/300 |
| 43 | LM | 0.17 | 0/1138 | 0.34 | 0/1523 |
| 44 | LL | 0.15 | 0/1669 | 0.29 | 0/2237 |
| 45 | Lk | 0.17 | 0/563 | 0.37 | 0/748 |
| 46 | LJ | 0.15 | 0/1352 | 0.32 | 0/1812 |
| 47 | Lj | 0.15 | 0/716 | 0.32 | 0/947 |
| 48 | LI | 0.16 | 0/1670 | 0.29 | 0/2230 |
| 49 | Li | 0.14 | 0/823 | 0.31 | 0/1092 |
| 50 | LH | 0.16 | 0/1518 | 0.31 | 0/2043 |
| 51 | Lh | 0.17 | 0/1018 | 0.34 | 0/1347 |
| 52 | LG | 0.16 | 0/1824 | 0.33 | 0/2465 |
| 53 | Lg | 0.19 | 0/884 | 0.35 | 0/1179 |
| 54 | LF | 0.18 | 0/1869 | 0.33 | 0/2498 |
| 55 | Lf | 0.17 | 0/887 | 0.33 | 0/1190 |
| 56 | LE | 0.14 | 0/1758 | 0.29 | 0/2360 |
| 57 | Le | 0.17 | 0/1062 | 0.31 | 0/1416 |
| 58 | LD | 0.14 | 0/2400 | 0.33 | 0/3220 |
| 59 | Ld | 0.16 | 0/854 | 0.34 | 0/1153 |
| 60 | LC | 0.16 | 0/2916 | 0.31 | 0/3917 |
| 61 | Lc | 0.18 | 0/770 | 0.36 | 0/1034 |
| 62 | LB | 0.15 | 0/3242 | 0.32 | 0/4343 |
| 63 | Lb | 0.17 | 0/817 | 0.37 | 0/1080 |
| 64 | LA | 0.16 | 0/1927 | 0.33 | 0/2582 |
| 65 | La | 0.16 | 0/1173 | 0.32 | 0/1566 |
| 66 | L7 | 0.16 | 0/2840 | 0.26 | 0/4425 |
| 67 | Pt | 0.23 | 0/1721 | 0.31 | 0/2679 |
| 68 | Sa | 0.21 | 0/788 | 0.44 | 1/1059 (0.1%) |
| 69 | L8 | 0.17 | 0/3564 | 0.30 | 0/5550 |
| 70 | L5 | 0.19 | 3/79828 (0.0%) | 0.30 | 0/124490 |
| 71 | SZ | 0.18 | 0/385 | 0.33 | 0/530 |
| 72 | ST | 0.15 | 0/851 | 0.28 | 0/1157 |
| 73 | SP | 0.14 | 0/814 | 0.34 | 0/1109 |
| 74 | S2 | 0.21 | 2/35763 (0.0%) | 0.31 | 0/55704 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 75 | SG | 0.13 | 0/1683 | 0.29 | 0/2261 |
| 76 | SI | 0.17 | 0/1677 | 0.33 | 0/2243 |
| 77 | S6 | 0.14 | 0/1411 | 0.32 | 0/2192 |
| 78 | SS | 0.14 | 0/916 | 0.32 | 0/1256 |
| 79 | mR | 0.30 | 0/170 | 0.66 | 0/263 |
| 80 | SU | 0.21 | 0/805 | 0.43 | 0/1081 |
| All | All | 0.18 | 5/210817 (0.0%) | 0.31 | 1/310118 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 26 | SA | 0 | 1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 70 | L5 | 3830 | A2M | O3'-P | 5.09 | 1.61 | 1.56 |
| 70 | L5 | 4523 | A2M | O3'-P | 5.06 | 1.61 | 1.56 |
| 74 | S2 | 668 | A2M | O3'-P | 5.05 | 1.61 | 1.56 |
| 70 | L5 | 3785 | A2M | O3'-P | 5.02 | 1.61 | 1.56 |
| 74 | S2 | 512 | A2M | O3'-P | 5.00 | 1.61 | 1.56 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 68 | Sa | 77 | CYS | CA-CB-SG | 5.08 | 126.08 | 114.40 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 26 | SA | 147 | LEU | Peptide |

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | Lm | 407 | 0 | 423 | 4 | 0 |
| 2 | Ll | 434 | 0 | 461 | 6 | 0 |
| 3 | Lo | 822 | 0 | 856 | 8 | 0 |
| 4 | SY | 900 | 0 | 831 | 15 | 0 |
| 5 | SX | 1060 | 0 | 1087 | 5 | 0 |
| 6 | SW | 1023 | 0 | 1063 | 11 | 0 |
| 7 | SV | 623 | 0 | 627 | 8 | 0 |
| 8 | SR | 936 | 0 | 866 | 8 | 0 |
| 9 | SQ | 918 | 0 | 804 | 4 | 0 |
| 10 | SO | 977 | 0 | 994 | 10 | 0 |
| 11 | SN | 1186 | 0 | 1247 | 8 | 0 |
| 12 | SL | 1158 | 0 | 1214 | 8 | 0 |
| 13 | SK | 468 | 0 | 317 | 4 | 0 |
| 14 | SJ | 1430 | 0 | 1498 | 13 | 0 |
| 15 | SH | 1408 | 0 | 1432 | 12 | 0 |
| 16 | Sg | 1259 | 0 | 646 | 6 | 0 |
| 17 | SF | 1327 | 0 | 1251 | 12 | 0 |
| 18 | SE | 2037 | 0 | 2131 | 11 | 0 |
| 19 | Se | 399 | 0 | 433 | 2 | 0 |
| 20 | SD | 1094 | 0 | 910 | 6 | 0 |
| 21 | Sd | 430 | 0 | 397 | 9 | 0 |
| 22 | SC | 1694 | 0 | 1769 | 17 | 0 |
| 23 | Sc | 434 | 0 | 419 | 3 | 0 |
| 24 | SB | 1694 | 0 | 1744 | 17 | 0 |
| 25 | Sb | 613 | 0 | 614 | 4 | 0 |
| 26 | SA | 1658 | 0 | 1630 | 23 | 0 |
| 27 | LZ | 1095 | 0 | 1164 | 16 | 0 |
| 28 | LY | 1060 | 0 | 1101 | 5 | 0 |
| 29 | LX | 976 | 0 | 1053 | 11 | 0 |
| 30 | LW | 519 | 0 | 533 | 6 | 0 |
| 31 | LV | 987 | 0 | 1052 | 5 | 0 |
| 32 | LU | 800 | 0 | 816 | 13 | 0 |
| 33 | LT | 1297 | 0 | 1366 | 9 | 0 |
| 34 | LS | 1456 | 0 | 1491 | 16 | 0 |
| 35 | LR | 1458 | 0 | 1555 | 8 | 0 |
| 36 | Lr | 987 | 0 | 1050 | 8 | 0 |
| 37 | LQ | 1505 | 0 | 1613 | 14 | 0 |
| 38 | LP | 1230 | 0 | 1250 | 4 | 0 |
| 39 | Lp | 695 | 0 | 746 | 3 | 0 |
| 40 | LO | 1620 | 0 | 1753 | 19 | 0 |
| 41 | LN | 1694 | 0 | 1738 | 16 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 42 | Ln | 235 | 0 | 284 | 2 | 0 |
| 43 | LM | 1116 | 0 | 1176 | 15 | 0 |
| 44 | LL | 1638 | 0 | 1737 | 14 | 0 |
| 45 | Lk | 557 | 0 | 611 | 14 | 0 |
| 46 | LJ | 1329 | 0 | 1346 | 13 | 0 |
| 47 | Lj | 701 | 0 | 735 | 9 | 0 |
| 48 | LI | 1632 | 0 | 1675 | 15 | 0 |
| 49 | Li | 812 | 0 | 870 | 12 | 0 |
| 50 | LH | 1499 | 0 | 1572 | 20 | 0 |
| 51 | Lh | 1010 | 0 | 1137 | 10 | 0 |
| 52 | LG | 1791 | 0 | 1883 | 19 | 0 |
| 53 | Lg | 871 | 0 | 953 | 5 | 0 |
| 54 | LF | 1835 | 0 | 1926 | 19 | 0 |
| 55 | Lf | 868 | 0 | 892 | 9 | 0 |
| 56 | LE | 1721 | 0 | 1839 | 22 | 0 |
| 57 | Le | 1044 | 0 | 1132 | 6 | 0 |
| 58 | LD | 2354 | 0 | 2345 | 21 | 0 |
| 59 | Ld | 840 | 0 | 859 | 8 | 0 |
| 60 | LC | 2862 | 0 | 3036 | 19 | 0 |
| 61 | Lc | 760 | 0 | 793 | 6 | 0 |
| 62 | LB | 3174 | 0 | 3294 | 27 | 0 |
| 63 | Lb | 815 | 0 | 869 | 13 | 0 |
| 64 | LA | 1899 | 0 | 1983 | 20 | 0 |
| 65 | La | 1157 | 0 | 1190 | 14 | 0 |
| 66 | L7 | 2542 | 0 | 1284 | 14 | 0 |
| 67 | Pt | 1645 | 0 | 844 | 15 | 0 |
| 68 | Sa | 775 | 0 | 813 | 10 | 0 |
| 69 | L8 | 3256 | 0 | 1652 | 30 | 0 |
| 70 | L5 | 73960 | 0 | 37478 | 514 | 0 |
| 71 | SZ | 383 | 0 | 313 | 7 | 0 |
| 72 | ST | 837 | 0 | 694 | 3 | 0 |
| 73 | SP | 806 | 0 | 652 | 3 | 0 |
| 74 | S2 | 33557 | 0 | 16987 | 250 | 0 |
| 75 | SG | 1663 | 0 | 1701 | 25 | 0 |
| 76 | SI | 1648 | 0 | 1700 | 28 | 0 |
| 77 | S6 | 1263 | 0 | 647 | 15 | 0 |
| 78 | SS | 903 | 0 | 728 | 7 | 0 |
| 79 | mR | 152 | 0 | 77 | 2 | 0 |
| 80 | SU | 795 | 0 | 862 | 13 | 0 |
| 81 | Lg | 1 | 0 | 0 | 0 | 0 |
| 81 | Lm | 1 | 0 | 0 | 0 | 0 |
| 81 | Lo | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 81 | Lp | 1 | 0 | 0 | 0 | 0 |
| 81 | Sd | 1 | 0 | 0 | 0 | 0 |
| 82 | L5 | 60 | 0 | 0 | 0 | 0 |
| 82 | L8 | 1 | 0 | 0 | 0 | 0 |
| 82 | LB | 1 | 0 | 0 | 0 | 0 |
| 82 | LC | 1 | 0 | 0 | 0 | 0 |
| 82 | Lf | 1 | 0 | 0 | 0 | 0 |
| 82 | S2 | 11 | 0 | 0 | 0 | 0 |
| 82 | SQ | 1 | 0 | 0 | 0 | 0 |
| 83 | L5 | 81 | 0 | 0 | 0 | 0 |
| 83 | L7 | 5 | 0 | 0 | 0 | 0 |
| 83 | L8 | 3 | 0 | 0 | 0 | 0 |
| 83 | LB | 1 | 0 | 0 | 0 | 0 |
| 83 | LI | 2 | 0 | 0 | 0 | 0 |
| 83 | LM | 1 | 0 | 0 | 0 | 0 |
| 83 | LP | 1 | 0 | 0 | 0 | 0 |
| 83 | LS | 1 | 0 | 0 | 0 | 0 |
| 83 | LV | 1 | 0 | 0 | 0 | 0 |
| 83 | Le | 1 | 0 | 0 | 0 | 0 |
| 83 | Pt | 1 | 0 | 0 | 0 | 0 |
| 83 | S2 | 21 | 0 | 0 | 0 | 0 |
| 83 | Sd | 1 | 0 | 0 | 0 | 0 |
| 84 | L5 | 46 | 0 | 0 | 0 | 0 |
| 84 | LB | 1 | 0 | 0 | 0 | 0 |
| 84 | LN | 1 | 0 | 0 | 0 | 0 |
| 84 | Le | 1 | 0 | 0 | 0 | 0 |
| 84 | S2 | 12 | 0 | 0 | 0 | 0 |
| 85 | L5 | 30 | 0 | 55 | 4 | 0 |
| 86 | S2 | 36 | 0 | 37 | 0 | 0 |
| 87 | L5 | 473 | 0 | 0 | 9 | 0 |
| 87 | L7 | 9 | 0 | 0 | 0 | 0 |
| 87 | L8 | 16 | 0 | 0 | 0 | 0 |
| 87 | LA | 4 | 0 | 0 | 0 | 0 |
| 87 | LB | 7 | 0 | 0 | 0 | 0 |
| 87 | LC | 1 | 0 | 0 | 0 | 0 |
| 87 | LD | 1 | 0 | 0 | 0 | 0 |
| 87 | LF | 3 | 0 | 0 | 0 | 0 |
| 87 | LG | 1 | 0 | 0 | 0 | 0 |
| 87 | LH | 1 | 0 | 0 | 0 | 0 |
| 87 | LI | 1 | 0 | 0 | 0 | 0 |
| 87 | LL | 2 | 0 | 0 | 0 | 0 |
| 87 | LM | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 87 | LN | 5 | 0 | 0 | 0 | 0 |
| 87 | LP | 3 | 0 | 0 | 0 | 0 |
| 87 | LQ | 3 | 0 | 0 | 0 | 0 |
| 87 | LR | 3 | 0 | 0 | 1 | 0 |
| 87 | LS | 5 | 0 | 0 | 0 | 0 |
| 87 | LT | 4 | 0 | 0 | 0 | 0 |
| 87 | LV | 2 | 0 | 0 | 0 | 0 |
| 87 | LW | 1 | 0 | 0 | 0 | 0 |
| 87 | La | 3 | 0 | 0 | 0 | 0 |
| 87 | Lb | 4 | 0 | 0 | 0 | 0 |
| 87 | Lc | 2 | 0 | 0 | 1 | 0 |
| 87 | Le | 3 | 0 | 0 | 0 | 0 |
| 87 | Lg | 3 | 0 | 0 | 0 | 0 |
| 87 | Lh | 2 | 0 | 0 | 0 | 0 |
| 87 | Lj | 2 | 0 | 0 | 0 | 0 |
| 87 | Ll | 2 | 0 | 0 | 0 | 0 |
| 87 | Ln | 2 | 0 | 0 | 0 | 0 |
| 87 | Lo | 1 | 0 | 0 | 0 | 0 |
| 87 | Lp | 1 | 0 | 0 | 0 | 0 |
| 87 | Pt | 1 | 0 | 0 | 0 | 0 |
| 87 | S2 | 101 | 0 | 0 | 1 | 0 |
| 87 | SF | 1 | 0 | 0 | 0 | 0 |
| 87 | SI | 5 | 0 | 0 | 0 | 0 |
| 87 | SL | 1 | 0 | 0 | 0 | 0 |
| 87 | SN | 3 | 0 | 0 | 0 | 0 |
| 87 | SS | 2 | 0 | 0 | 0 | 0 |
| 87 | Sa | 1 | 0 | 0 | 1 | 0 |
| All | All | 201487 | 0 | 144606 | 1404 | 0 |

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

All (1404) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 70:L5:1100:U:H3 | 70:L5:1195:G:H1 | 1.22 | 0.87 |
| 74:S2:885:U:H3 | 74:S2:901:G:H1 | 1.21 | 0.85 |
| 70:L5:3634:G:H1 | 70:L5:3826:C:H5 | 1.31 | 0.77 |
| 52:LG:180:PRO:HG3 | 52:LG:223:ARG:HE | 1.51 | 0.76 |
| 52:LG:249:ARG:NH2 | 70:L5:4075:U:OP1 | 2.19 | 0.76 |
| 49:Li:29:ARG:HH12 | 70:L5:276:C:H2' | 1.51 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:L5:4745:G:H1 | 70:L5:4955:A:H61 | 1.34 | 0.76 |
| 68:Sa:74:CYS:HB2 | 68:Sa:77:CYS:H | 1.50 | 0.75 |
| 52:LG:40:GLY:HA3 | 70:L5:4116:C:H1' | 1.68 | 0.75 |
| 76:SI:80:ASP:HB2 | 76:SI:94:LYS:HZ1 | 1.52 | 0.73 |
| 56:LE:72:LYS:HB2 | 63:Lb:119:CYS:HB2 | 1.71 | 0.72 |
| 74:S2:125:C:O3' | 75:SG:195:LYS:NZ | 2.22 | 0.72 |
| 70:L5:1804:A:H4' | 70:L5:1805:A:H5'' | 1.72 | 0.72 |
| 45:Lk:70:LYS:NZ | 70:L5:2714:G:OP1 | 2.23 | 0.72 |
| 58:LD:232:THR:HG22 | 58:LD:234:ASP:H | 1.54 | 0.71 |
| 70:L5:512:U:H3 | 70:L5:647:G:H1 | 1.37 | 0.71 |
| 80:SU:20:ILE:HD11 | 80:SU:114:VAL:HG13 | 1.71 | 0.71 |
| 68:Sa:15:ARG:NH1 | 74:S2:993:G:N7 | 2.39 | 0.71 |
| 70:L5:2579:G:N2 | 70:L5:2582:A:OP2 | 2.23 | 0.71 |
| 58:LD:208:MET:HE2 | 58:LD:233:PRO:HG3 | 1.73 | 0.70 |
| 74:S2:535:G:H22 | 74:S2:551:U:H3 | 1.39 | 0.70 |
| 27:LZ:89:ILE:HD11 | 27:LZ:121:ARG:HG2 | 1.74 | 0.70 |
| 11:SN:64:ARG:NH2 | 74:S2:919:A:OP2 | 2.24 | 0.70 |
| 74:S2:878:G:O6 | 74:S2:908:A:N7 | 2.25 | 0.70 |
| 74:S2:191:A:H62 | 74:S2:208:G:H21 | 1.38 | 0.70 |
| 70:L5:4091:G:H1 | 70:L5:4158:C:H41 | 1.37 | 0.69 |
| 47:Lj:56:ARG:NH2 | 70:L5:374:G:OP2 | 2.24 | 0.69 |
| 54:LF:43:ARG:NH1 | 70:L5:1704:C:OP1 | 2.26 | 0.69 |
| 1:Lm:93:LYS:HG2 | 1:Lm:102:ARG:HG2 | 1.73 | 0.69 |
| 70:L5:4620:OMU:OP2 | 70:L5:4670:C:N4 | 2.25 | 0.69 |
| 77:S6:9:U:H2' | 77:S6:46:G:H21 | 1.57 | 0.69 |
| 63:Lb:99:ILE:HD11 | 70:L5:1266:G:H5'' | 1.73 | 0.69 |
| 74:S2:928:G:H1 | 74:S2:1013:U:H3 | 1.41 | 0.69 |
| 56:LE:105:ARG:NH1 | 70:L5:469:C:O2 | 2.24 | 0.69 |
| 70:L5:704:C:N4 | 70:L5:707:C:OP2 | 2.26 | 0.69 |
| 54:LF:76:ARG:NH1 | 70:L5:730:G:OP2 | 2.26 | 0.69 |
| 74:S2:534:G:H22 | 74:S2:552:G:H1 | 1.42 | 0.68 |
| 50:LH:114:ILE:HB | 50:LH:124:ARG:HG3 | 1.74 | 0.68 |
| 55:Lf:33:VAL:HG13 | 55:Lf:38:GLU:HB2 | 1.74 | 0.68 |
| 27:LZ:68:ILE:O | 27:LZ:115:LYS:NZ | 2.27 | 0.68 |
| 18:SE:137:PRO:HB2 | 18:SE:150:PRO:HD2 | 1.75 | 0.68 |
| 43:LM:41:PRO:HG3 | 43:LM:73:VAL:HG23 | 1.76 | 0.67 |
| 60:LC:163:LYS:HB2 | 60:LC:166:GLU:HG3 | 1.74 | 0.67 |
| 70:L5:2582:A:H8 | 70:L5:2681:G:H21 | 1.42 | 0.67 |
| 74:S2:1750:C:N4 | 74:S2:1784:G:N7 | 2.40 | 0.67 |
| 64:LA:215:ASN:ND2 | 70:L5:4546:A:N7 | 2.42 | 0.67 |
| 14:SJ:155:LYS:HG3 | 14:SJ:156:HIS:HD2 | 1.60 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:LJ:41:GLU:HG3 | 46:LJ:48:PRO:HD3 | 1.77 | 0.67 |
| 64:LA:104:VAL:HA | 64:LA:107:MET:HE2 | 1.77 | 0.67 |
| 54:LF:47:ARG:HH21 | 60:LC:330:PRO:HG3 | 1.60 | 0.66 |
| 52:LG:229:ARG:NH1 | 52:LG:232:GLU:OE2 | 2.28 | 0.66 |
| 70:L5:4090:G:H1 | 70:L5:4159:C:H5 | 1.42 | 0.66 |
| 74:S2:183:G:N7 | 74:S2:184:G:O2' | 2.27 | 0.66 |
| 29:LX:139:ARG:NH1 | 70:L5:2533:C:OP1 | 2.28 | 0.66 |
| 69:L8:123:U:O2' | 69:L8:125:C:OP1 | 2.14 | 0.66 |
| 70:L5:2094:G:N2 | 70:L5:2095:A:O2' | 2.28 | 0.66 |
| 74:S2:925:G:H1 | 74:S2:1017:U:H3 | 1.44 | 0.66 |
| 14:SJ:26:ASP:OD1 | 14:SJ:30:LYS:NZ | 2.29 | 0.66 |
| 44:LL:172:GLU:HG2 | 49:Li:2:ALA:HB1 | 1.78 | 0.66 |
| 52:LG:58:PRO:HD2 | 52:LG:61:ILE:HD12 | 1.77 | 0.65 |
| 72:ST:22:LEU:HG | 72:ST:28:LEU:HD11 | 1.77 | 0.65 |
| 64:LA:36:GLU:HG3 | 64:LA:91:GLY:HA2 | 1.78 | 0.65 |
| 74:S2:981:A:H2' | 74:S2:982:G:C8 | 2.32 | 0.65 |
| 14:SJ:18:ARG:NH1 | 74:S2:3:C:O2 | 2.30 | 0.64 |
| 70:L5:3717:A:H2' | 70:L5:3718:A2M:H8 | 1.78 | 0.64 |
| 15:SH:106:ARG:O | 74:S2:798:G:O2' | 2.16 | 0.64 |
| 70:L5:1100:U:O2 | 70:L5:1195:G:N2 | 2.25 | 0.64 |
| 80:SU:38:ASP:OD1 | 80:SU:41:ARG:NH2 | 2.30 | 0.64 |
| 25:Sb:40:CYS:SG | 25:Sb:41:TYR:N | 2.70 | 0.64 |
| 14:SJ:38:ARG:NH1 | 74:S2:643:A:OP1 | 2.31 | 0.64 |
| 26:SA:33:GLN:HB3 | 26:SA:154:LEU:HD12 | 1.81 | 0.63 |
| 37:LQ:99:LYS:HE2 | 37:LQ:121:LEU:HD11 | 1.80 | 0.63 |
| 76:SI:67:TRP:NE1 | 76:SI:191:GLU:OE2 | 2.28 | 0.63 |
| 18:SE:100:ARG:HH12 | 18:SE:122:LYS:HA | 1.64 | 0.63 |
| 70:L5:1203:G:H2' | 70:L5:1204:C:H6 | 1.64 | 0.63 |
| 77:S6:64:U:H2' | 77:S6:65:C:H6 | 1.64 | 0.63 |
| 59:Ld:24:GLU:HG3 | 59:Ld:87:ARG:HG3 | 1.81 | 0.63 |
| 21:Sd:52:PHE:HB3 | 80:SU:80:PHE:HB3 | 1.81 | 0.62 |
| 77:S6:10:G:H1' | 77:S6:45:G:H2' | 1.80 | 0.62 |
| 37:LQ:104:ARG:NH2 | 70:L5:1353:G:N7 | 2.47 | 0.62 |
| 61:Lc:34:THR:HG23 | 61:Lc:95:ALA:HB2 | 1.82 | 0.62 |
| 70:L5:4594:U:H2' | 70:L5:4595:G:H8 | 1.65 | 0.62 |
| 32:LU:28:PRO:HB2 | 32:LU:34:MET:HG2 | 1.82 | 0.62 |
| 57:Le:98:GLU:OE2 | 70:L5:2324:C:O2' | 2.17 | 0.62 |
| 70:L5:138:G:H2' | 70:L5:139:G:H8 | 1.64 | 0.62 |
| 70:L5:1870:C:H2' | 70:L5:1871:A2M:H8 | 1.80 | 0.62 |
| 70:L5:3689:G:O2' | 70:L5:3818:U:OP2 | 2.16 | 0.62 |
| 16:Sg:238:ALA:HB3 | 16:Sg:251:ALA:HB3 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 62:LB:168:MET:HG3 | 62:LB:178:ALA:HA | 1.82 | 0.62 |
| 70:L5:268:G:H2' | 70:L5:269:G:H8 | 1.64 | 0.61 |
| 38:LP:16:LYS:HG2 | 38:LP:149:ILE:HG12 | 1.82 | 0.61 |
| 42:Ln:6:ARG:NH2 | 74:S2:1169:G:OP1 | 2.32 | 0.61 |
| 70:L5:4091:G:H22 | 70:L5:4158:C:H5 | 1.48 | 0.61 |
| 74:S2:1265:A:H8 | 74:S2:1326:U:H5 | 1.49 | 0.61 |
| 34:LS:70:LYS:NZ | 70:L5:733:A:OP1 | 2.34 | 0.61 |
| 39:Lp:44:LYS:NZ | 70:L5:2672:C:OP1 | 2.34 | 0.61 |
| 52:LG:159:HIS:HD2 | 52:LG:186:GLY:H | 1.47 | 0.61 |
| 70:L5:2351:OMC:HM22 | 70:L5:2352:U:H5' | 1.81 | 0.61 |
| 74:S2:1326:U:H1' | 74:S2:1494:U:H5' | 1.83 | 0.61 |
| 27:LZ:103:ASP:N | 27:LZ:103:ASP:OD1 | 2.30 | 0.61 |
| 43:LM:46:ARG:NH1 | 70:L5:937:U:OP1 | 2.33 | 0.61 |
| 37:LQ:39:THR:HG22 | 37:LQ:41:SER:H | 1.66 | 0.61 |
| 32:LU:46:ARG:HH21 | 32:LU:89:LYS:HD3 | 1.66 | 0.61 |
| 70:L5:3945:A:H2' | 70:L5:3946:G:H8 | 1.65 | 0.60 |
| 77:S6:15:A:H61 | 77:S6:46:G:H1 | 1.49 | 0.60 |
| 74:S2:190:G:H5' | 76:SI:145:ILE:HD13 | 1.83 | 0.60 |
| 74:S2:942:G:H2' | 74:S2:943:U:C6 | 2.36 | 0.60 |
| 74:S2:1536:G:H2' | 74:S2:1537:A:C8 | 2.36 | 0.60 |
| 77:S6:40:C:H2' | 77:S6:41:C:C6 | 2.36 | 0.60 |
| 75:SG:32:MET:HG3 | 75:SG:100:CYS:HB2 | 1.82 | 0.60 |
| 20:SD:138:VAL:HG22 | 20:SD:184:ILE:HG22 | 1.84 | 0.60 |
| 70:L5:1833:G:O2' | 70:L5:1835:G:N2 | 2.34 | 0.60 |
| 21:Sd:13:LYS:NZ | 74:S2:1618:C:OP1 | 2.35 | 0.60 |
| 40:LO:47:PHE:HZ | 40:LO:144:GLU:HG3 | 1.66 | 0.60 |
| 68:Sa:26:CYS:N | 68:Sa:77:CYS:SG | 2.74 | 0.60 |
| 74:S2:145:G:H2' | 74:S2:146:G:C8 | 2.36 | 0.60 |
| 37:LQ:108:ARG:NH2 | 70:L5:1355:G:OP1 | 2.34 | 0.59 |
| 67:Pt:9:G:O2' | 67:Pt:10:G:N7 | 2.30 | 0.59 |
| 70:L5:1399:G:H2' | 70:L5:1400:G:C8 | 2.37 | 0.59 |
| 60:LC:62:THR:OG1 | 70:L5:375:G:OP1 | 2.19 | 0.59 |
| 63:Lb:101:HIS:O | 63:Lb:109:ARG:NH1 | 2.34 | 0.59 |
| 24:SB:214:LYS:NZ | 74:S2:943:U:OP1 | 2.35 | 0.59 |
| 62:LB:80:GLU:OE2 | 62:LB:328:ASN:ND2 | 2.33 | 0.59 |
| 77:S6:41:C:H2' | 77:S6:42:A:C8 | 2.37 | 0.59 |
| 34:LS:95:ARG:NH2 | 34:LS:112:ASP:OD1 | 2.36 | 0.59 |
| 70:L5:2378:G:N2 | 70:L5:2381:A:OP2 | 2.35 | 0.59 |
| 35:LR:38:ARG:NH2 | 70:L5:2527:A:OP1 | 2.32 | 0.59 |
| 70:L5:3598:C:H2' | 70:L5:3599:A:H8 | 1.66 | 0.59 |
| 6:SW:55:ASP:OD1 | 6:SW:55:ASP:N | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:LI:38:ARG:NH2 | 48:LI:45:GLU:OE1 | 2.35 | 0.59 |
| 52:LG:117:ARG:HE | 52:LG:121:LYS:HE2 | 1.68 | 0.59 |
| 58:LD:125:VAL:HG21 | 58:LD:200:MET:HE3 | 1.83 | 0.59 |
| 70:L5:369:G:N2 | 70:L5:372:A:OP2 | 2.31 | 0.59 |
| 74:S2:1140:G:HO2' | 74:S2:1151:G:HO2' | 1.51 | 0.59 |
| 74:S2:71:G:O6 | 75:SG:170:ARG:NH1 | 2.35 | 0.59 |
| 4:SY:9:THR:O | 74:S2:835:C:N4 | 2.34 | 0.59 |
| 24:SB:138:PHE:O | 24:SB:213:ARG:N | 2.36 | 0.59 |
| 26:SA:50:ASN:HB3 | 26:SA:53:ARG:HG2 | 1.84 | 0.58 |
| 34:LS:173:ASN:ND2 | 34:LS:175:PHE:O | 2.36 | 0.58 |
| 74:S2:874:G:H2' | 74:S2:875:A:H8 | 1.68 | 0.58 |
| 58:LD:231:VAL:HA | 58:LD:235:MET:HE1 | 1.84 | 0.58 |
| 70:L5:2809:G:O2' | 70:L5:4644:G:OP1 | 2.22 | 0.58 |
| 30:LW:14:TYR:OH | 62:LB:384:GLU:OE2 | 2.21 | 0.58 |
| 64:LA:208:GLU:OE1 | 70:L5:1629:G:N1 | 2.30 | 0.58 |
| 70:L5:740:G:H21 | 70:L5:741:C:H41 | 1.50 | 0.58 |
| 70:L5:1214:C:H5' | 70:L5:1215:C:H5'' | 1.85 | 0.58 |
| 50:LH:92:MET:HG2 | 50:LH:179:ILE:HG22 | 1.84 | 0.58 |
| 74:S2:203:G:OP2 | 76:SI:143:LYS:NZ | 2.32 | 0.58 |
| 1:Lm:100:TYR:O | 70:L5:4472:G:O2' | 2.20 | 0.58 |
| 15:SH:100:ILE:HG12 | 15:SH:125:VAL:HG11 | 1.84 | 0.58 |
| 70:L5:965:G:O2' | 70:L5:2256:C:N3 | 2.34 | 0.58 |
| 70:L5:4634:U:O4 | 87:L5:5301:HOH:O | 2.16 | 0.58 |
| 4:SY:27:VAL:HB | 4:SY:69:THR:HG23 | 1.86 | 0.58 |
| 33:LT:108:ARG:NH2 | 70:L5:1802:A:O2' | 2.37 | 0.58 |
| 62:LB:242:ARG:NH2 | 70:L5:2856:C:O2 | 2.35 | 0.58 |
| 58:LD:50:ARG:NH1 | 58:LD:72:ASP:OD2 | 2.31 | 0.58 |
| 66:L7:23:A:N3 | 66:L7:118:C:O2' | 2.33 | 0.58 |
| 75:SG:154:ARG:HH21 | 75:SG:179:LEU:HD21 | 1.68 | 0.58 |
| 61:Lc:48:LEU:HD11 | 61:Lc:60:ILE:HG21 | 1.85 | 0.58 |
| 70:L5:3722:G:H2' | 70:L5:3723:A:H8 | 1.69 | 0.58 |
| 19:Se:111:GLN:O | 19:Se:115:ARG:HG2 | 2.04 | 0.58 |
| 26:SA:36:GLN:O | 26:SA:53:ARG:NH1 | 2.36 | 0.58 |
| 74:S2:1536:G:H2' | 74:S2:1537:A:H8 | 1.68 | 0.58 |
| 74:S2:1265:A:O2' | 74:S2:1327:G:OP2 | 2.19 | 0.58 |
| 80:SU:20:ILE:HG21 | 80:SU:97:ILE:HD11 | 1.85 | 0.58 |
| 7:SV:15:ARG:NH1 | 22:SC:83:LEU:O | 2.37 | 0.57 |
| 55:Lf:45:LYS:HD2 | 55:Lf:105:LEU:HA | 1.86 | 0.57 |
| 70:L5:1202:C:H2' | 70:L5:1203:G:H8 | 1.69 | 0.57 |
| 70:L5:5021:C:N4 | 87:L5:5333:HOH:O | 2.33 | 0.57 |
| 62:LB:173:LEU:HD22 | 62:LB:342:LYS:HD3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 70:L5:1857:C:H2' | 70:L5:1858:A:H8 | 1.69 | 0.57 |
| 74:S2:527:C:H2' | 74:S2:528:A:H8 | 1.70 | 0.57 |
| 74:S2:1662:U:O4 | 74:S2:1663:A:N6 | 2.37 | 0.57 |
| 11:SN:55:ARG:HD3 | 74:S2:1017:U:H5' | 1.86 | 0.57 |
| 53:Lg:83:CYS:SG | 53:Lg:86:CYS:HB2 | 2.44 | 0.57 |
| 38:LP:116:HIS:HB3 | 38:LP:149:ILE:HB | 1.85 | 0.57 |
| 64:LA:123:ARG:NH1 | 70:L5:4083:U:OP1 | 2.38 | 0.57 |
| 70:L5:220:C:H5 | 70:L5:237:G:H1 | 1.51 | 0.57 |
| 70:L5:1245:C:H2' | 70:L5:1246:G:H8 | 1.70 | 0.57 |
| 80:SU:18:HIS:O | 80:SU:18:HIS:ND1 | 2.32 | 0.57 |
| 22:SC:67:GLY:HA2 | 22:SC:93:ILE:HD11 | 1.87 | 0.57 |
| 22:SC:211:LYS:O | 22:SC:215:MET:HG2 | 2.05 | 0.57 |
| 33:LT:75:VAL:HG12 | 33:LT:88:ARG:HG2 | 1.87 | 0.57 |
| 44:LL:39:ARG:NH2 | 70:L5:1362:G:OP1 | 2.37 | 0.57 |
| 62:LB:103:LYS:NZ | 70:L5:4725:C:OP1 | 2.38 | 0.57 |
| 70:L5:2611:A:H5' | 70:L5:2688:G:H4' | 1.87 | 0.57 |
| 74:S2:168:C:O2' | 75:SG:133:LEU:O | 2.22 | 0.57 |
| 48:LI:30:LYS:HG3 | 48:LI:66:GLU:HG3 | 1.86 | 0.57 |
| 74:S2:381:C:OP2 | 76:SI:54:LYS:NZ | 2.38 | 0.57 |
| 16:Sg:23:THR:HG21 | 16:Sg:31:ILE:HA | 1.86 | 0.56 |
| 45:Lk:36:VAL:HG23 | 45:Lk:43:TYR:HB2 | 1.87 | 0.56 |
| 64:LA:107:MET:HE1 | 64:LA:113:VAL:HG11 | 1.87 | 0.56 |
| 29:LX:42:THR:HG21 | 52:LG:48:LYS:HG3 | 1.86 | 0.56 |
| 70:L5:268:G:H2' | 70:L5:269:G:C8 | 2.40 | 0.56 |
| 15:SH:119:SER:O | 74:S2:913:A:N6 | 2.37 | 0.56 |
| 43:LM:46:ARG:NH1 | 70:L5:935:A:O2' | 2.38 | 0.56 |
| 44:LL:129:ARG:NH2 | 70:L5:173:C:O5' | 2.38 | 0.56 |
| 54:LF:131:ASN:ND2 | 70:L5:1727:U:OP1 | 2.37 | 0.56 |
| 56:LE:161:ARG:O | 56:LE:182:ASN:ND2 | 2.38 | 0.56 |
| 60:LC:53:ALA:O | 69:L8:26:C:O2' | 2.23 | 0.56 |
| 70:L5:1754:U:H3 | 70:L5:1776:A:H61 | 1.53 | 0.56 |
| 74:S2:928:G:H2' | 74:S2:929:G:C8 | 2.39 | 0.56 |
| 2:L1:2:SER:N | 70:L5:2407:G:O6 | 2.39 | 0.56 |
| 7:SV:58:ALA:O | 7:SV:62:MET:HG3 | 2.05 | 0.56 |
| 28:LY:74:TYR:OH | 69:L8:75:OMG:OP2 | 2.24 | 0.56 |
| 70:L5:1480:C:O2' | 70:L5:1482:G:OP2 | 2.23 | 0.56 |
| 58:LD:157:ASN:HB3 | 58:LD:159:VAL:HG22 | 1.86 | 0.56 |
| 70:L5:4173:G:H2' | 70:L5:4174:U:C6 | 2.40 | 0.56 |
| 70:L5:4993:G:H22 | 70:L5:5058:A:H2 | 1.53 | 0.56 |
| 37:LQ:68:ARG:HA | 37:LQ:71:LYS:HE3 | 1.87 | 0.56 |
| 43:LM:81:ASP:OD2 | 43:LM:84:THR:OG1 | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 69:L8:126:C:H42 | 70:L5:2543:A:H4' | 1.69 | 0.56 |
| 74:S2:165:G:OP2 | 74:S2:165:G:N2 | 2.33 | 0.56 |
| 31:LV:15:ARG:HB2 | 70:L5:4618:OMG:H5'' | 1.87 | 0.56 |
| 62:LB:168:MET:HA | 62:LB:171:LEU:HD12 | 1.87 | 0.56 |
| 65:La:47:LYS:NZ | 70:L5:1684:A:OP1 | 2.38 | 0.56 |
| 67:Pt:16:C:H5' | 67:Pt:60:A:H2 | 1.70 | 0.56 |
| 70:L5:711:A:H2' | 70:L5:712:C:C6 | 2.41 | 0.56 |
| 74:S2:1609:C:O2 | 74:S2:1610:G:N1 | 2.39 | 0.56 |
| 24:SB:146:ARG:HB2 | 24:SB:149:GLN:HG3 | 1.87 | 0.56 |
| 62:LB:213:GLN:NE2 | 62:LB:285:TYR:O | 2.39 | 0.56 |
| 74:S2:797:C:O2' | 74:S2:798:G:O4' | 2.20 | 0.56 |
| 4:SY:10:ARG:NH2 | 4:SY:26:ASP:OD1 | 2.36 | 0.56 |
| 26:SA:77:ILE:HG13 | 26:SA:122:LEU:HD11 | 1.88 | 0.56 |
| 35:LR:64:ARG:NH2 | 70:L5:2633:U:OP1 | 2.38 | 0.56 |
| 58:LD:116:ASP:OD1 | 58:LD:116:ASP:N | 2.39 | 0.56 |
| 70:L5:4939:C:H5'' | 70:L5:4940:C:H5' | 1.87 | 0.56 |
| 74:S2:1244:PSU:H2' | 74:S2:1245:G:H8 | 1.71 | 0.56 |
| 74:S2:1742:C:H5 | 74:S2:1792:G:H1 | 1.52 | 0.56 |
| 26:SA:42:LYS:HD3 | 26:SA:46:ILE:HG23 | 1.86 | 0.55 |
| 44:LL:127:PHE:O | 51:Lh:117:ARG:NH2 | 2.34 | 0.55 |
| 56:LE:139:LYS:O | 56:LE:191:GLN:NE2 | 2.35 | 0.55 |
| 27:LZ:100:VAL:HG13 | 27:LZ:106:LEU:HB3 | 1.88 | 0.55 |
| 31:LV:115:SER:O | 31:LV:135:ASN:ND2 | 2.38 | 0.55 |
| 41:LN:116:LEU:HD22 | 41:LN:135:ILE:HD11 | 1.88 | 0.55 |
| 60:LC:182:LYS:HE3 | 70:L5:2300:A:H5'' | 1.88 | 0.55 |
| 62:LB:126:LYS:NZ | 70:L5:4966:A:OP2 | 2.38 | 0.55 |
| 70:L5:1377:G:H21 | 70:L5:1380:G:H5' | 1.71 | 0.55 |
| 70:L5:4274:A:H2' | 70:L5:4275:G:C8 | 2.41 | 0.55 |
| 74:S2:1228:A:H2' | 74:S2:1229:G:C8 | 2.40 | 0.55 |
| 4:SY:105:LYS:NZ | 74:S2:52:G:O2' | 2.36 | 0.55 |
| 7:SV:41:LYS:HD2 | 26:SA:5:LEU:HD11 | 1.87 | 0.55 |
| 40:LO:106:ASP:O | 70:L5:4910:G:N2 | 2.40 | 0.55 |
| 76:SI:142:SER:O | 76:SI:146:GLN:HB2 | 2.06 | 0.55 |
| 41:LN:73:ARG:NH1 | 41:LN:88:GLY:O | 2.40 | 0.55 |
| 41:LN:182:HIS:NE2 | 70:L5:291:U:O2' | 2.33 | 0.55 |
| 56:LE:119:GLU:HG3 | 57:Le:7:LEU:HD11 | 1.88 | 0.55 |
| 70:L5:1273:G:H2' | 70:L5:1274:A:C8 | 2.41 | 0.55 |
| 30:LW:1:MET:HE2 | 62:LB:71:GLU:HB2 | 1.89 | 0.55 |
| 70:L5:67:C:OP2 | 70:L5:312:G:N2 | 2.40 | 0.55 |
| 70:L5:1094:G:H2' | 70:L5:1095:A:H8 | 1.72 | 0.55 |
| 7:SV:32:ILE:HG12 | 7:SV:60:ARG:HD3 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:LH:12:ILE:HD12 | 50:LH:53:LYS:HB3 | 1.89 | 0.55 |
| 54:LF:243:LEU:HD11 | 54:LF:247:MET:HE3 | 1.89 | 0.55 |
| 70:L5:1441:C:H2' | 70:L5:1442:C:H6 | 1.72 | 0.55 |
| 4:SY:14:THR:HG23 | 4:SY:21:LYS:HG2 | 1.89 | 0.55 |
| 7:SV:3:ASN:HA | 22:SC:173:LYS:HG2 | 1.89 | 0.55 |
| 10:SO:34:PHE:HB3 | 10:SO:41:PHE:HB2 | 1.89 | 0.55 |
| 36:Lr:112:ARG:NH1 | 56:LE:117:PRO:O | 2.38 | 0.55 |
| 70:L5:450:G:H1 | 70:L5:1297:U:H3 | 1.55 | 0.55 |
| 74:S2:1354:G:N2 | 74:S2:1357:A:OP2 | 2.31 | 0.55 |
| 10:SO:50:LYS:O | 74:S2:975:G:N2 | 2.35 | 0.54 |
| 10:SO:56:VAL:HG13 | 10:SO:60:MET:HE2 | 1.88 | 0.54 |
| 69:L8:67:U:H2' | 69:L8:68:G:H8 | 1.71 | 0.54 |
| 74:S2:885:U:O2 | 74:S2:901:G:N2 | 2.31 | 0.54 |
| 23:Sc:12:ALA:HB1 | 23:Sc:32:VAL:HB | 1.89 | 0.54 |
| 29:LX:93:ASN:ND2 | 70:L5:2532:C:O2' | 2.33 | 0.54 |
| 33:LT:111:GLU:O | 33:LT:115:LYS:HG2 | 2.08 | 0.54 |
| 53:Lg:41:ALA:O | 53:Lg:52:ARG:NH1 | 2.39 | 0.54 |
| 74:S2:1533:A:H2 | 74:S2:1536:G:N3 | 2.05 | 0.54 |
| 77:S6:64:U:H2' | 77:S6:65:C:C6 | 2.43 | 0.54 |
| 22:SC:183:LYS:HG2 | 22:SC:196:ILE:HG12 | 1.88 | 0.54 |
| 38:LP:37:LYS:NZ | 70:L5:425:U:OP1 | 2.40 | 0.54 |
| 70:L5:2745:A:H2' | 70:L5:2746:A:C8 | 2.42 | 0.54 |
| 73:SP:131:PRO:O | 74:S2:1236:G:O2' | 2.22 | 0.54 |
| 14:SJ:79:ARG:NH2 | 74:S2:819:G:OP1 | 2.40 | 0.54 |
| 8:SR:5:ARG:NH2 | 74:S2:1455:A:OP1 | 2.41 | 0.54 |
| 17:SF:125:SER:HB2 | 17:SF:136:ARG:HH21 | 1.73 | 0.54 |
| 56:LE:46:ARG:O | 56:LE:65:ARG:NH1 | 2.40 | 0.54 |
| 67:Pt:72:C:H2' | 67:Pt:73:A:H8 | 1.73 | 0.54 |
| 2:Ll:23:ILE:HD12 | 2:Ll:27:ILE:HD11 | 1.90 | 0.54 |
| 41:LN:14:LYS:HE2 | 70:L5:280:G:H5'' | 1.90 | 0.54 |
| 65:La:26:ARG:NH1 | 70:L5:1655:C:OP2 | 2.41 | 0.54 |
| 67:Pt:62:C:H2' | 67:Pt:63:C:H6 | 1.73 | 0.54 |
| 70:L5:2745:A:H2' | 70:L5:2746:A:H8 | 1.73 | 0.54 |
| 74:S2:1490:OMG:N2 | 80:SU:72:GLU:OE1 | 2.39 | 0.54 |
| 70:L5:662:C:H2' | 70:L5:663:G:H8 | 1.71 | 0.54 |
| 70:L5:4694:G:N2 | 70:L5:4694:G:OP1 | 2.41 | 0.54 |
| 36:Lr:90:LEU:HD22 | 36:Lr:111:ILE:HG23 | 1.89 | 0.54 |
| 54:LF:94:ARG:NH1 | 54:LF:114:LEU:O | 2.39 | 0.54 |
| 63:Lb:36:ASP:OD1 | 70:L5:4314:C:O2' | 2.25 | 0.54 |
| 70:L5:4924:C:O2 | 70:L5:4926:C:N4 | 2.28 | 0.54 |
| 74:S2:527:C:H2' | 74:S2:528:A:C8 | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 74:S2:1253:A:OP2 | 74:S2:1526:G:N2 | 2.37 | 0.54 |
| 54:LF:46:ARG:NH1 | 70:L5:1704:C:O3' | 2.41 | 0.54 |
| 70:L5:4734:A:H2' | 70:L5:4735:G:C8 | 2.43 | 0.53 |
| 56:LE:46:ARG:NH2 | 70:L5:1070:G:O6 | 2.42 | 0.53 |
| 64:LA:68:ARG:HH11 | 64:LA:70:LYS:HD2 | 1.72 | 0.53 |
| 70:L5:2588:C:OP1 | 70:L5:2768:C:O2' | 2.20 | 0.53 |
| 76:SI:150:ASP:HA | 76:SI:153:LYS:HG2 | 1.90 | 0.53 |
| 14:SJ:18:ARG:NH2 | 74:S2:4:C:O2' | 2.38 | 0.53 |
| 59:Ld:46:LEU:HD13 | 70:L5:2373:C:H5' | 1.90 | 0.53 |
| 70:L5:2362:U:H2' | 70:L5:2363:A2M:H8 | 1.89 | 0.53 |
| 70:L5:3598:C:H2' | 70:L5:3599:A:C8 | 2.44 | 0.53 |
| 74:S2:163:U:OP2 | 75:SG:87:ARG:NH2 | 2.40 | 0.53 |
| 79:mR:34:A:H2' | 79:mR:35:A:H8 | 1.72 | 0.53 |
| 29:LX:105:ASN:ND2 | 29:LX:108:GLN:OE1 | 2.42 | 0.53 |
| 70:L5:660:A:O2' | 70:L5:661:C:H5' | 2.09 | 0.53 |
| 33:LT:61:THR:HG21 | 70:L5:1799:G:H21 | 1.72 | 0.53 |
| 70:L5:4736:C:H2' | 70:L5:4737:G:H8 | 1.74 | 0.53 |
| 18:SE:45:ILE:HB | 18:SE:80:ILE:HG23 | 1.91 | 0.53 |
| 20:SD:161:GLY:HA3 | 74:S2:1388:A:H61 | 1.73 | 0.53 |
| 70:L5:4173:G:H2' | 70:L5:4174:U:H6 | 1.73 | 0.53 |
| 56:LE:123:ARG:HG2 | 70:L5:959:G:C8 | 2.44 | 0.53 |
| 70:L5:691:C:H2' | 70:L5:692:A:C8 | 2.44 | 0.53 |
| 70:L5:2902:G:O4' | 70:L5:3596:A:N6 | 2.41 | 0.53 |
| 74:S2:1521:C:OP2 | 78:SS:136:THR:OG1 | 2.22 | 0.53 |
| 76:SI:121:LEU:HD21 | 76:SI:158:ILE:HD11 | 1.91 | 0.53 |
| 66:L7:12:U:OP2 | 66:L7:67:C:O2' | 2.27 | 0.53 |
| 3:Lo:36:GLN:OE1 | 3:Lo:40:ARG:NH2 | 2.40 | 0.53 |
| 4:SY:108:LYS:NZ | 74:S2:506:G:OP1 | 2.42 | 0.53 |
| 17:SF:67:PRO:HG2 | 17:SF:70:GLU:HB2 | 1.90 | 0.53 |
| 30:LW:47:ARG:HH12 | 30:LW:54:LEU:HD13 | 1.73 | 0.53 |
| 70:L5:93:G:H2' | 70:L5:94:A:C8 | 2.44 | 0.53 |
| 70:L5:921:C:H2' | 70:L5:922:C:H6 | 1.73 | 0.53 |
| 70:L5:2866:C:O2' | 70:L5:2867:C:O5' | 2.21 | 0.53 |
| 74:S2:1228:A:H2' | 74:S2:1229:G:H8 | 1.73 | 0.53 |
| 63:Lb:122:LYS:HA | 70:L5:1242:G:H4' | 1.89 | 0.53 |
| 27:LZ:14:LEU:HB3 | 53:Lg:88:ARG:HG3 | 1.91 | 0.52 |
| 40:LO:34:VAL:HG12 | 40:LO:103:LYS:HB2 | 1.90 | 0.52 |
| 65:La:76:ASP:HB3 | 65:La:115:GLY:HA3 | 1.92 | 0.52 |
| 70:L5:4449:A:N6 | 87:L5:5379:HOH:O | 2.43 | 0.52 |
| 74:S2:104:A:OP1 | 76:SI:12:ARG:NH1 | 2.42 | 0.52 |
| 18:SE:44:LEU:HD13 | 18:SE:82:TYR:HB3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:LL:74:ARG:NH1 | 70:L5:76:A:OP2 | 2.42 | 0.52 |
| 62:LB:58:ARG:NH1 | 62:LB:361:GLU:OE2 | 2.39 | 0.52 |
| 74:S2:25:A:HO2' | 74:S2:26:U:H6 | 1.56 | 0.52 |
| 39:Lp:38:THR:HA | 39:Lp:45:THR:HA | 1.91 | 0.52 |
| 53:Lg:90:ARG:NH2 | 70:L5:4123:C:OP1 | 2.43 | 0.52 |
| 69:L8:144:U:H2' | 69:L8:145:C:C6 | 2.45 | 0.52 |
| 74:S2:520:A:O2' | 74:S2:825:A:N3 | 2.37 | 0.52 |
| 24:SB:168:MET:HE2 | 24:SB:197:ILE:HG21 | 1.92 | 0.52 |
| 47:Lj:63:ARG:NH2 | 69:L8:58:G:O6 | 2.42 | 0.52 |
| 50:LH:19:THR:HB | 50:LH:26:ILE:HG12 | 1.90 | 0.52 |
| 70:L5:1252:C:O2 | 70:L5:1254:A:N6 | 2.42 | 0.52 |
| 11:SN:120:SER:OG | 74:S2:677:G:OP1 | 2.27 | 0.52 |
| 17:SF:73:THR:HG21 | 17:SF:90:VAL:HG12 | 1.92 | 0.52 |
| 58:LD:33:ARG:NH1 | 66:L7:7:G:OP1 | 2.42 | 0.52 |
| 34:LS:151:LYS:HG3 | 43:LM:8:GLU:HB3 | 1.92 | 0.52 |
| 60:LC:262:GLU:HB3 | 60:LC:273:LEU:HG | 1.92 | 0.52 |
| 70:L5:908:G:H2' | 70:L5:909:A:H8 | 1.75 | 0.52 |
| 70:L5:1479:G:H2' | 70:L5:1480:C:C6 | 2.44 | 0.52 |
| 70:L5:4608:G:O2' | 70:L5:4609:G:O5' | 2.27 | 0.52 |
| 12:SL:79:LYS:HB2 | 12:SL:87:VAL:HG22 | 1.91 | 0.52 |
| 34:LS:95:ARG:NH1 | 70:L5:1951:G:O2' | 2.39 | 0.52 |
| 49:Li:25:ARG:HH21 | 70:L5:159:C:H5' | 1.75 | 0.52 |
| 56:LE:69:TYR:HA | 56:LE:72:LYS:HE3 | 1.92 | 0.52 |
| 70:L5:2658:G:O2' | 70:L5:2675:G:N2 | 2.43 | 0.52 |
| 70:L5:3684:G:H2' | 70:L5:3685:C:C6 | 2.45 | 0.52 |
| 70:L5:3945:A:H2' | 70:L5:3946:G:C8 | 2.45 | 0.52 |
| 74:S2:1447:G:H5' | 80:SU:29:VAL:HG11 | 1.92 | 0.52 |
| 3:Lo:9:ARG:NH1 | 70:L5:4290:U:OP1 | 2.43 | 0.52 |
| 70:L5:4860:G:H2' | 70:L5:4861:G:H8 | 1.74 | 0.52 |
| 74:S2:1401:A:H4' | 80:SU:52:GLY:HA3 | 1.90 | 0.52 |
| 10:SO:100:THR:HG21 | 10:SO:104:ARG:HE | 1.75 | 0.52 |
| 62:LB:154:LYS:HG3 | 62:LB:194:LEU:HD12 | 1.91 | 0.52 |
| 70:L5:963:G:O6 | 70:L5:2095:A:N1 | 2.43 | 0.52 |
| 70:L5:1604:G:H2' | 70:L5:1605:G:C8 | 2.45 | 0.52 |
| 70:L5:1772:C:H2' | 70:L5:1773:U:C6 | 2.45 | 0.52 |
| 73:SP:38:SER:OG | 73:SP:41:GLN:OE1 | 2.27 | 0.52 |
| 6:SW:6:VAL:HG13 | 6:SW:29:PRO:HD2 | 1.91 | 0.51 |
| 20:SD:176:LEU:HD13 | 74:S2:1499:U:H4' | 1.92 | 0.51 |
| 35:LR:133:LYS:NZ | 87:LR:201:HOH:O | 2.42 | 0.51 |
| 50:LH:128:MET:HE2 | 50:LH:134:CYS:HB2 | 1.92 | 0.51 |
| 67:Pt:72:C:H2' | 67:Pt:73:A:C8 | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:L5:2736:G:N7 | 87:L5:5342:HOH:O | 2.34 | 0.51 |
| 70:L5:4115:G:H8 | 70:L5:4116:C:H5 | 1.58 | 0.51 |
| 74:S2:534:G:H22 | 74:S2:552:G:H22 | 1.57 | 0.51 |
| 75:SG:132:ARG:HG2 | 75:SG:133:LEU:HG | 1.91 | 0.51 |
| 41:LN:60:VAL:HG22 | 41:LN:134:LEU:HB2 | 1.92 | 0.51 |
| 61:Lc:106:ARG:NH2 | 87:Lc:202:HOH:O | 2.43 | 0.51 |
| 70:L5:1326:A2M:OP2 | 70:L5:4445:U:O2' | 2.28 | 0.51 |
| 70:L5:2029:A:H2' | 70:L5:2030:A:C8 | 2.45 | 0.51 |
| 70:L5:3700:C:O2' | 70:L5:3774:A:N3 | 2.39 | 0.51 |
| 70:L5:3823:G:C6 | 85:L5:5102:SPD:H42 | 2.45 | 0.51 |
| 74:S2:433:A:H5'' | 76:SI:22:HIS:HB3 | 1.92 | 0.51 |
| 76:SI:144:LYS:O | 76:SI:147:LYS:HG3 | 2.10 | 0.51 |
| 80:SU:50:VAL:HG22 | 80:SU:91:LEU:HG | 1.92 | 0.51 |
| 14:SJ:107:GLU:HA | 14:SJ:112:THR:HG21 | 1.92 | 0.51 |
| 27:LZ:9:LYS:NZ | 27:LZ:83:THR:O | 2.43 | 0.51 |
| 74:S2:184:G:H5' | 74:S2:185:G:C8 | 2.46 | 0.51 |
| 75:SG:5:ILE:HD12 | 75:SG:124:LEU:HD11 | 1.91 | 0.51 |
| 22:SC:178:HIS:ND1 | 22:SC:221:ASP:OD2 | 2.43 | 0.51 |
| 29:LX:40:ILE:HD12 | 52:LG:50:ASP:HB2 | 1.91 | 0.51 |
| 58:LD:90:VAL:HG21 | 58:LD:231:VAL:HG21 | 1.92 | 0.51 |
| 70:L5:4188:U:H2' | 70:L5:4189:U:C6 | 2.45 | 0.51 |
| 74:S2:312:G:H1 | 74:S2:337:C:H5 | 1.57 | 0.51 |
| 74:S2:582:U:H2' | 74:S2:583:A:H8 | 1.75 | 0.51 |
| 74:S2:948:C:H2' | 74:S2:949:G:H8 | 1.76 | 0.51 |
| 51:Lh:10:ARG:NH2 | 51:Lh:63:GLN:OE1 | 2.44 | 0.51 |
| 70:L5:1441:C:H2' | 70:L5:1442:C:C6 | 2.45 | 0.51 |
| 70:L5:2407:G:OP2 | 70:L5:2407:G:N2 | 2.41 | 0.51 |
| 70:L5:4594:U:H2' | 70:L5:4595:G:C8 | 2.44 | 0.51 |
| 74:S2:107:A:H2' | 74:S2:108:G:C8 | 2.46 | 0.51 |
| 19:Se:114:ARG:NH2 | 74:S2:639:C:OP1 | 2.44 | 0.51 |
| 60:LC:321:ASN:OD1 | 70:L5:1280:C:O2' | 2.22 | 0.51 |
| 70:L5:1718:C:H2' | 70:L5:1719:A:C4 | 2.46 | 0.51 |
| 74:S2:528:A:H2' | 74:S2:529:A:C8 | 2.46 | 0.51 |
| 51:Lh:66:LYS:HG2 | 69:L8:96:C:H5'' | 1.93 | 0.51 |
| 70:L5:4750:G:H2' | 70:L5:4751:G:C8 | 2.45 | 0.51 |
| 28:LY:54:GLU:HB2 | 28:LY:108:ARG:HB2 | 1.93 | 0.51 |
| 70:L5:1094:G:H2' | 70:L5:1095:A:C8 | 2.46 | 0.51 |
| 74:S2:534:G:N2 | 74:S2:552:G:H22 | 2.08 | 0.51 |
| 74:S2:1279:C:H2' | 74:S2:1280:G:H8 | 1.76 | 0.51 |
| 70:L5:1703:C:OP2 | 70:L5:1704:C:N4 | 2.44 | 0.51 |
| 70:L5:2601:A:N6 | 70:L5:2744:A:OP2 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 70:L5:3736:A:H2' | 70:L5:3737:A:C8 | 2.46 | 0.51 |
| 18:SE:199:GLU:OE2 | 18:SE:209:HIS:NE2 | 2.43 | 0.50 |
| 24:SB:122:GLU:HG2 | 24:SB:140:VAL:HG23 | 1.93 | 0.50 |
| 26:SA:59:LEU:HD22 | 26:SA:181:GLU:HG2 | 1.93 | 0.50 |
| 56:LE:73:TYR:OH | 70:L5:982:U:OP1 | 2.24 | 0.50 |
| 70:L5:163:A:H2' | 70:L5:164:G:H8 | 1.76 | 0.50 |
| 70:L5:1576:G:O2' | 70:L5:1578:U:O2 | 2.20 | 0.50 |
| 70:L5:4541:G:N2 | 70:L5:4544:A:OP2 | 2.37 | 0.50 |
| 22:SC:187:ARG:NH2 | 22:SC:189:GLY:O | 2.43 | 0.50 |
| 33:LT:17:ARG:HG2 | 70:L5:4277:G:H5'' | 1.93 | 0.50 |
| 40:LO:49:ARG:NH1 | 70:L5:1930:U:OP2 | 2.37 | 0.50 |
| 54:LF:105:VAL:HG13 | 54:LF:136:VAL:HG12 | 1.93 | 0.50 |
| 70:L5:3717:A:H2' | 70:L5:3718:A2M:C8 | 2.40 | 0.50 |
| 4:SY:57:VAL:HB | 4:SY:60:PHE:HE1 | 1.75 | 0.50 |
| 8:SR:101:ASP:OD2 | 26:SA:40:LYS:NZ | 2.44 | 0.50 |
| 18:SE:43:PRO:HD2 | 18:SE:46:ILE:HD12 | 1.94 | 0.50 |
| 30:LW:9:SER:HA | 30:LW:52:THR:HG23 | 1.92 | 0.50 |
| 70:L5:2411:C:H2' | 70:L5:2412:A:H8 | 1.75 | 0.50 |
| 70:L5:3880:G:H2' | 70:L5:3881:G:C8 | 2.46 | 0.50 |
| 2:LI:42:ARG:HG3 | 2:LI:47:THR:HG23 | 1.93 | 0.50 |
| 54:LF:57:TYR:OH | 54:LF:189:ASP:OD1 | 2.22 | 0.50 |
| 56:LE:243:THR:HG22 | 56:LE:245:GLN:H | 1.75 | 0.50 |
| 67:Pt:39:A:O2' | 74:S2:1058:A:OP1 | 2.28 | 0.50 |
| 70:L5:1548:G:O2' | 70:L5:2812:A:N3 | 2.40 | 0.50 |
| 74:S2:17:C:O2' | 74:S2:1194:A:N1 | 2.43 | 0.50 |
| 74:S2:1220:A:N3 | 74:S2:1677:U:O2' | 2.43 | 0.50 |
| 74:S2:1714:U:H2' | 74:S2:1715:A:C8 | 2.46 | 0.50 |
| 17:SF:126:THR:OG1 | 23:Sc:26:GLN:NE2 | 2.40 | 0.50 |
| 48:LI:207:ASP:OD1 | 48:LI:210:ARG:NH1 | 2.43 | 0.50 |
| 70:L5:1933:G:H2' | 70:L5:1934:A:C8 | 2.47 | 0.50 |
| 70:L5:3692:A:OP2 | 85:L5:5102:SPD:N10 | 2.42 | 0.50 |
| 70:L5:5047:C:O2' | 70:L5:5050:C:OP2 | 2.27 | 0.50 |
| 73:SP:45:LEU:HD21 | 73:SP:84:ILE:HD11 | 1.94 | 0.50 |
| 74:S2:640:A:H2' | 74:S2:641:A:C8 | 2.47 | 0.50 |
| 74:S2:1144:A:H2' | 74:S2:1145:A:C8 | 2.47 | 0.50 |
| 12:SL:125:ILE:HG13 | 12:SL:146:THR:HB | 1.94 | 0.50 |
| 55:Lf:107:PRO:HA | 56:LE:192[A]:LYS:HG2 | 1.94 | 0.50 |
| 70:L5:2411:C:H2' | 70:L5:2412:A:C8 | 2.47 | 0.50 |
| 7:SV:16:LYS:NZ | 22:SC:257:LYS:O | 2.35 | 0.50 |
| 51:Lh:5:LYS:NZ | 69:L8:87:G:OP1 | 2.39 | 0.50 |
| 61:Lc:18:LEU:O | 61:Lc:22:MET:HG2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:L5:163:A:H2' | 70:L5:164:G:C8 | 2.46 | 0.50 |
| 70:L5:1396:G:HO2' | 70:L5:1468:C:HO2' | 1.57 | 0.50 |
| 70:L5:2765:A:H2' | 70:L5:2766:A:C8 | 2.47 | 0.50 |
| 74:S2:28:U:H2' | 74:S2:29:G:H8 | 1.77 | 0.50 |
| 74:S2:1588:A:H2' | 74:S2:1589:A:C8 | 2.47 | 0.50 |
| 15:SH:51:ILE:HG23 | 15:SH:179:LYS:HD3 | 1.93 | 0.50 |
| 29:LX:87:MET:HE1 | 29:LX:155:ILE:HG22 | 1.94 | 0.50 |
| 63:Lb:55:LYS:HA | 63:Lb:58:GLN:HG3 | 1.94 | 0.50 |
| 66:L7:103:A:O2' | 70:L5:1741:G:O6 | 2.27 | 0.50 |
| 74:S2:553:U:H2' | 74:S2:554:A:C8 | 2.47 | 0.50 |
| 59:Ld:20:VAL:HA | 59:Ld:90:ARG:O | 2.12 | 0.50 |
| 74:S2:191:A:H62 | 74:S2:208:G:N2 | 2.07 | 0.50 |
| 74:S2:377:G:H5' | 76:SI:98:LYS:HB3 | 1.93 | 0.50 |
| 74:S2:607:U:O2' | 74:S2:630:U:O4' | 2.30 | 0.50 |
| 75:SG:38:ALA:HB2 | 75:SG:50:VAL:HG13 | 1.94 | 0.50 |
| 39:Lp:63:THR:H | 64:LA:84:THR:HG22 | 1.76 | 0.49 |
| 70:L5:679:C:H2' | 70:L5:680:G:H8 | 1.77 | 0.49 |
| 70:L5:2497:C:H2' | 70:L5:2498:C:H6 | 1.77 | 0.49 |
| 74:S2:51:U:H2' | 74:S2:52:G:C8 | 2.47 | 0.49 |
| 74:S2:472:C:O2' | 74:S2:474:G:OP1 | 2.23 | 0.49 |
| 4:SY:12:PHE:HZ | 4:SY:21:LYS:HD2 | 1.77 | 0.49 |
| 5:SX:61:GLN:O | 5:SX:62:HIS:ND1 | 2.45 | 0.49 |
| 70:L5:4745:G:H1 | 70:L5:4955:A:N6 | 2.07 | 0.49 |
| 6:SW:6:VAL:HG12 | 6:SW:34:ILE:HD11 | 1.94 | 0.49 |
| 48:LI:66:GLU:OE2 | 48:LI:69:ARG:NH1 | 2.35 | 0.49 |
| 54:LF:241:ASN:O | 54:LF:245:ARG:HG2 | 2.13 | 0.49 |
| 70:L5:2467:U:H4' | 70:L5:2468:U:H5' | 1.93 | 0.49 |
| 70:L5:3710:G:O2' | 70:L5:3713:U:O4 | 2.31 | 0.49 |
| 70:L5:5068:G:N2 | 70:L5:5069:U:O4 | 2.36 | 0.49 |
| 74:S2:77:A:H2 | 75:SG:175:LYS:HG3 | 1.77 | 0.49 |
| 11:SN:83:ASP:OD1 | 11:SN:83:ASP:N | 2.42 | 0.49 |
| 12:SL:111:VAL:HG12 | 12:SL:140:PHE:HB2 | 1.92 | 0.49 |
| 62:LB:385:LYS:NZ | 70:L5:5002:U:OP2 | 2.39 | 0.49 |
| 70:L5:1339:U:H2' | 70:L5:1340:OMC:C6 | 2.47 | 0.49 |
| 70:L5:1558:A:H2' | 70:L5:1559:G:C8 | 2.48 | 0.49 |
| 70:L5:4093:G:O2' | 70:L5:4094:G:H8 | 1.95 | 0.49 |
| 70:L5:4861:G:H2' | 70:L5:4862:G:H8 | 1.76 | 0.49 |
| 70:L5:4991:U:H2' | 70:L5:4992:G:C8 | 2.46 | 0.49 |
| 74:S2:416:U:HO2' | 74:S2:652:U:HO2' | 1.58 | 0.49 |
| 76:SI:113:TYR:CG | 76:SI:121:LEU:HD12 | 2.48 | 0.49 |
| 5:SX:123:VAL:HG12 | 5:SX:124:LYS:HG3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:LY:27:ARG:CZ | 69:L8:70:G:H5'' | 2.43 | 0.49 |
| 52:LG:159:HIS:CD2 | 52:LG:186:GLY:H | 2.29 | 0.49 |
| 65:La:13:GLY:HA2 | 70:L5:1660:U:H3' | 1.94 | 0.49 |
| 70:L5:963:G:N2 | 87:L5:5390:HOH:O | 2.46 | 0.49 |
| 70:L5:4504:C:H2' | 70:L5:4505:C:C6 | 2.47 | 0.49 |
| 74:S2:494:C:N4 | 74:S2:509:OMG:HN22 | 2.11 | 0.49 |
| 10:SO:135:ILE:O | 74:S2:943:U:O2' | 2.29 | 0.49 |
| 43:LM:70:GLN:HA | 43:LM:73:VAL:HG22 | 1.95 | 0.49 |
| 60:LC:60:HIS:HA | 60:LC:92:PHE:HE1 | 1.77 | 0.49 |
| 65:La:132:ARG:NH1 | 70:L5:1468:C:OP1 | 2.45 | 0.49 |
| 70:L5:689:U:H2' | 70:L5:690:C:C6 | 2.48 | 0.49 |
| 70:L5:2848:G:O2' | 70:L5:3838:U:O4 | 2.24 | 0.49 |
| 74:S2:588:G:OP2 | 74:S2:588:G:N2 | 2.45 | 0.49 |
| 74:S2:851:C:H5'' | 74:S2:852:G:H5' | 1.94 | 0.49 |
| 76:SI:37:LYS:HE3 | 76:SI:93:THR:HG22 | 1.95 | 0.49 |
| 1:Lm:82:LEU:HB3 | 50:LH:95:VAL:HG22 | 1.93 | 0.49 |
| 13:SK:31:LYS:HA | 13:SK:41:PRO:HA | 1.93 | 0.49 |
| 18:SE:172:PHE:HE2 | 18:SE:174:LYS:HE3 | 1.77 | 0.49 |
| 44:LL:129:ARG:HD3 | 51:Lh:117:ARG:HD2 | 1.93 | 0.49 |
| 70:L5:920:C:H2' | 70:L5:921:C:H6 | 1.78 | 0.49 |
| 70:L5:4591:U:H2' | 70:L5:4592:C:C6 | 2.48 | 0.49 |
| 74:S2:562:U:H2' | 74:S2:563:G:C8 | 2.48 | 0.49 |
| 27:LZ:24:VAL:HG21 | 27:LZ:87:VAL:HG12 | 1.93 | 0.49 |
| 33:LT:45:MET:HE3 | 33:LT:47:THR:HB | 1.95 | 0.49 |
| 52:LG:46:GLN:OE1 | 52:LG:49:ARG:NH1 | 2.46 | 0.49 |
| 56:LE:162:VAL:HG12 | 56:LE:177:GLY:HA2 | 1.95 | 0.49 |
| 62:LB:246:ARG:NH1 | 70:L5:4558:U:OP2 | 2.43 | 0.49 |
| 74:S2:484:A2M:O5' | 74:S2:484:A2M:H8 | 2.13 | 0.49 |
| 31:LV:48:ARG:NH1 | 70:L5:4621:C:OP1 | 2.38 | 0.49 |
| 51:Lh:46:LYS:HE2 | 69:L8:80:A:H1' | 1.95 | 0.49 |
| 69:L8:16:G:H22 | 70:L5:417:G:H2' | 1.78 | 0.49 |
| 70:L5:1617:G:H1' | 70:L5:2513:A:N6 | 2.28 | 0.49 |
| 70:L5:4921:C:H2' | 70:L5:4922:C:H6 | 1.78 | 0.49 |
| 9:SQ:140:ARG:HB2 | 74:S2:1644:C:H4' | 1.95 | 0.49 |
| 41:LN:5:LYS:O | 41:LN:9:GLU:HG2 | 2.13 | 0.49 |
| 46:LJ:78:LYS:O | 46:LJ:82:ILE:HG12 | 2.13 | 0.49 |
| 55:Lf:50:VAL:HG22 | 55:Lf:69:VAL:HG22 | 1.95 | 0.49 |
| 68:Sa:13:LYS:O | 68:Sa:15:ARG:NH2 | 2.46 | 0.49 |
| 70:L5:1273:G:H2' | 70:L5:1274:A:H8 | 1.78 | 0.49 |
| 35:LR:138:LEU:O | 35:LR:142:ILE:HG12 | 2.13 | 0.48 |
| 47:Lj:57:ASN:O | 47:Lj:57:ASN:ND2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:LI:36:LEU:HD12 | 48:LI:69:ARG:HE | 1.77 | 0.48 |
| 48:LI:46:PHE:HB2 | 48:LI:139:ARG:HD2 | 1.93 | 0.48 |
| 70:L5:4903:G:H2' | 70:L5:4904:G:H8 | 1.78 | 0.48 |
| 45:Lk:34:PHE:HE2 | 45:Lk:56:LEU:HB3 | 1.77 | 0.48 |
| 50:LH:93:ARG:NH2 | 50:LH:141:LYS:O | 2.46 | 0.48 |
| 60:LC:235:LEU:HD22 | 60:LC:240:LEU:HD11 | 1.95 | 0.48 |
| 62:LB:302:ASN:OD1 | 62:LB:314:ILE:N | 2.45 | 0.48 |
| 74:S2:1203:G:H2' | 74:S2:1204:A:C8 | 2.47 | 0.48 |
| 74:S2:1786:U:H2' | 74:S2:1787:G:H8 | 1.78 | 0.48 |
| 11:SN:5:HIS:HB2 | 11:SN:121:ARG:HH21 | 1.79 | 0.48 |
| 14:SJ:58:ARG:HD3 | 22:SC:199:PRO:HG2 | 1.94 | 0.48 |
| 45:Lk:26:LYS:HG2 | 45:Lk:69:LEU:HD12 | 1.95 | 0.48 |
| 46:LJ:146:ARG:HH21 | 46:LJ:147:ARG:HH12 | 1.61 | 0.48 |
| 70:L5:2520:C:H2' | 70:L5:2521:G:H8 | 1.79 | 0.48 |
| 70:L5:4537:C:H2' | 70:L5:4538:G:C8 | 2.48 | 0.48 |
| 45:Lk:29:LYS:H | 45:Lk:29:LYS:HD2 | 1.79 | 0.48 |
| 70:L5:2318:G:N2 | 70:L5:2321:G:OP2 | 2.30 | 0.48 |
| 74:S2:559:G:O2' | 74:S2:560:A:O5' | 2.28 | 0.48 |
| 26:SA:85:ARG:NH1 | 26:SA:203:PHE:O | 2.46 | 0.48 |
| 47:Lj:20:ARG:NH2 | 69:L8:109:C:O2' | 2.36 | 0.48 |
| 70:L5:3861:A:H2' | 70:L5:3862:A:C8 | 2.48 | 0.48 |
| 26:SA:206:ASP:N | 26:SA:206:ASP:OD1 | 2.44 | 0.48 |
| 43:LM:92:ALA:HA | 43:LM:95:ILE:HG12 | 1.95 | 0.48 |
| 55:Lf:43:LEU:O | 55:Lf:109:ARG:NH1 | 2.46 | 0.48 |
| 34:LS:88:SER:HB2 | 48:LI:162:ARG:HH12 | 1.78 | 0.48 |
| 52:LG:37:LYS:NZ | 70:L5:4126:C:OP1 | 2.39 | 0.48 |
| 64:LA:234:LYS:HG2 | 64:LA:238:ILE:HG12 | 1.96 | 0.48 |
| 70:L5:1942:A:H2' | 70:L5:1943:A:C8 | 2.49 | 0.48 |
| 70:L5:3723:A:H2' | 70:L5:3724:A:H8 | 1.77 | 0.48 |
| 74:S2:627:OMU:H5'' | 74:S2:627:OMU:H6 | 1.94 | 0.48 |
| 74:S2:964:A:H2' | 74:S2:965:U:H6 | 1.79 | 0.48 |
| 74:S2:1414:A:H2' | 74:S2:1415:C:H6 | 1.78 | 0.48 |
| 26:SA:137:ALA:HB1 | 26:SA:142:LEU:HB3 | 1.96 | 0.48 |
| 34:LS:99:ASP:OD1 | 34:LS:100:LEU:N | 2.46 | 0.48 |
| 70:L5:4521:PSU:OP2 | 87:L5:5302:HOH:O | 2.20 | 0.48 |
| 74:S2:1098:C:H2' | 74:S2:1099:G:C8 | 2.48 | 0.48 |
| 17:SF:159:ARG:NH1 | 74:S2:1535:U:O4 | 2.45 | 0.48 |
| 26:SA:37:TYR:OH | 26:SA:57:LYS:NZ | 2.43 | 0.48 |
| 32:LU:29:VAL:HG11 | 32:LU:36:ALA:HB2 | 1.96 | 0.48 |
| 42:Ln:24:ARG:HH12 | 70:L5:2872:C:H5'' | 1.79 | 0.48 |
| 56:LE:112:MET:HE1 | 70:L5:2261:G:H5' | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:Le:10:PRO:HD2 | 57:Le:69:MET:HE1 | 1.96 | 0.48 |
| 59:Ld:36:VAL:HG21 | 59:Ld:44:ARG:HG2 | 1.95 | 0.48 |
| 69:L8:141:C:C2 | 69:L8:142:U:C5 | 3.01 | 0.48 |
| 70:L5:2543:A:H2 | 70:L5:2773:G:H22 | 1.60 | 0.48 |
| 74:S2:1323:U:H2' | 74:S2:1324:G:C8 | 2.49 | 0.48 |
| 50:LH:26:ILE:HG22 | 50:LH:35:ARG:HG2 | 1.96 | 0.48 |
| 70:L5:3722:G:H2' | 70:L5:3723:A:C8 | 2.48 | 0.48 |
| 77:S6:10:G:OP2 | 77:S6:14:C:N4 | 2.46 | 0.48 |
| 4:SY:10:ARG:HG3 | 4:SY:24:VAL:HG23 | 1.96 | 0.47 |
| 61:Lc:37:MET:SD | 61:Lc:42:LYS:NZ | 2.87 | 0.47 |
| 63:Lb:22:LYS:HD2 | 63:Lb:25:ARG:HH22 | 1.79 | 0.47 |
| 64:LA:101:VAL:HG22 | 64:LA:165:VAL:HG22 | 1.96 | 0.47 |
| 70:L5:956:A:O2' | 70:L5:2077:C:OP1 | 2.30 | 0.47 |
| 70:L5:1204:C:H2' | 70:L5:1205:G:H8 | 1.78 | 0.47 |
| 71:SZ:69:THR:H | 71:SZ:72:VAL:HG22 | 1.79 | 0.47 |
| 14:SJ:93:LYS:HG2 | 14:SJ:95:ASP:H | 1.80 | 0.47 |
| 27:LZ:83:THR:HG22 | 27:LZ:85:TYR:H | 1.79 | 0.47 |
| 41:LN:108:ARG:HB2 | 41:LN:161:MET:HE1 | 1.96 | 0.47 |
| 65:La:35:ALA:HB1 | 70:L5:39:A:H5'' | 1.96 | 0.47 |
| 68:Sa:6:ARG:NH1 | 74:S2:1147:C:OP1 | 2.47 | 0.47 |
| 69:L8:67:U:H2' | 69:L8:68:G:C8 | 2.48 | 0.47 |
| 74:S2:448:A:H5'' | 76:SI:25:ARG:HA | 1.95 | 0.47 |
| 74:S2:867:OMG:HM23 | 74:S2:867:OMG:H1' | 1.55 | 0.47 |
| 74:S2:1401:A:H2' | 74:S2:1402:A:C8 | 2.48 | 0.47 |
| 31:LV:83:ARG:NH1 | 31:LV:100:ASP:OD1 | 2.47 | 0.47 |
| 52:LG:95:LEU:HD11 | 52:LG:156:VAL:HG21 | 1.96 | 0.47 |
| 57:Le:67:LYS:O | 57:Le:75:ARG:NH2 | 2.46 | 0.47 |
| 67:Pt:63:C:H2' | 67:Pt:64:G:H8 | 1.79 | 0.47 |
| 69:L8:75:OMG:H1' | 69:L8:75:OMG:HM23 | 1.65 | 0.47 |
| 70:L5:1811:G:H2' | 70:L5:1812:C:H6 | 1.79 | 0.47 |
| 70:L5:4238:G:H2' | 70:L5:4239:A:H8 | 1.80 | 0.47 |
| 74:S2:901:G:H2' | 74:S2:902:G:C8 | 2.49 | 0.47 |
| 74:S2:1719:A:N6 | 74:S2:1814:G:O2' | 2.47 | 0.47 |
| 12:SL:84:ARG:HE | 12:SL:115:PRO:HG3 | 1.78 | 0.47 |
| 14:SJ:155:LYS:HG3 | 14:SJ:156:HIS:CD2 | 2.47 | 0.47 |
| 32:LU:47:ILE:HD11 | 32:LU:56:LEU:HG | 1.95 | 0.47 |
| 33:LT:133:ALA:HB3 | 54:LF:127:LYS:HB2 | 1.96 | 0.47 |
| 44:LL:60:ARG:NH2 | 44:LL:68:THR:O | 2.47 | 0.47 |
| 70:L5:1332:C:H2' | 70:L5:1333:A:H8 | 1.78 | 0.47 |
| 70:L5:4750:G:H2' | 70:L5:4751:G:H8 | 1.80 | 0.47 |
| 70:L5:4967:A:H2' | 70:L5:4968:A:H8 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 74:S2:833:C:H2' | 74:S2:834:C:C6 | 2.50 | 0.47 |
| 76:SI:157:LYS:HB3 | 76:SI:157:LYS:HE3 | 1.69 | 0.47 |
| 27:LZ:120:GLU:HG2 | 27:LZ:123:LYS:HE2 | 1.96 | 0.47 |
| 44:LL:42:LYS:HE3 | 44:LL:46:ILE:HD13 | 1.97 | 0.47 |
| 62:LB:224:LYS:HG2 | 62:LB:340:THR:HB | 1.95 | 0.47 |
| 70:L5:3861:A:H2' | 70:L5:3862:A:H8 | 1.79 | 0.47 |
| 74:S2:206:G:H2' | 74:S2:207:G:H8 | 1.79 | 0.47 |
| 74:S2:533:A:H2' | 74:S2:534:G:C8 | 2.48 | 0.47 |
| 75:SG:181:THR:H | 75:SG:184:VAL:HG22 | 1.79 | 0.47 |
| 9:SQ:19:ALA:HB2 | 9:SQ:75:GLY:HA3 | 1.96 | 0.47 |
| 24:SB:142:PHE:HD1 | 24:SB:209:ASP:HB2 | 1.80 | 0.47 |
| 70:L5:271:C:H2' | 70:L5:272:U:C6 | 2.49 | 0.47 |
| 70:L5:514:U:H5 | 70:L5:647:G:H21 | 1.61 | 0.47 |
| 70:L5:908:G:H2' | 70:L5:909:A:C8 | 2.49 | 0.47 |
| 70:L5:4537:C:H2' | 70:L5:4538:G:H8 | 1.79 | 0.47 |
| 7:SV:51:LYS:HG3 | 7:SV:78:ILE:HD11 | 1.96 | 0.47 |
| 12:SL:33:LEU:HD12 | 12:SL:34:PRO:HD2 | 1.97 | 0.47 |
| 14:SJ:54:ARG:NH1 | 22:SC:200:ARG:O | 2.38 | 0.47 |
| 14:SJ:137:VAL:HG12 | 14:SJ:138:ARG:HG3 | 1.96 | 0.47 |
| 18:SE:143:ASP:OD1 | 18:SE:143:ASP:N | 2.44 | 0.47 |
| 29:LX:70:LYS:NZ | 69:L8:60:G:OP1 | 2.46 | 0.47 |
| 40:LO:140:ARG:O | 40:LO:144:GLU:HG2 | 2.15 | 0.47 |
| 64:LA:245:ARG:NH1 | 70:L5:3657:U:OP1 | 2.47 | 0.47 |
| 66:L7:63:C:H5' | 66:L7:64:G:H5'' | 1.97 | 0.47 |
| 68:Sa:40:VAL:HG11 | 68:Sa:42:ARG:HH11 | 1.80 | 0.47 |
| 70:L5:1271:G:OP2 | 70:L5:1271:G:N2 | 2.38 | 0.47 |
| 70:L5:1758:G:N2 | 70:L5:1773:U:O2 | 2.48 | 0.47 |
| 70:L5:4174:U:H2' | 70:L5:4175:G:H8 | 1.80 | 0.47 |
| 70:L5:4608:G:O2' | 70:L5:4609:G:H8 | 1.98 | 0.47 |
| 70:L5:4967:A:H2' | 70:L5:4968:A:C8 | 2.50 | 0.47 |
| 74:S2:78:C:OP1 | 75:SG:159:ARG:NH2 | 2.41 | 0.47 |
| 74:S2:656:G:N2 | 74:S2:663:C:H5'' | 2.30 | 0.47 |
| 76:SI:57:ALA:HB2 | 76:SI:183:GLY:HA2 | 1.95 | 0.47 |
| 34:LS:69:GLU:HB2 | 34:LS:101:THR:HG23 | 1.95 | 0.47 |
| 70:L5:1846:G:H2' | 70:L5:1847:C:C6 | 2.50 | 0.47 |
| 70:L5:2368:A:N6 | 70:L5:2827:G:O2' | 2.47 | 0.47 |
| 74:S2:17:C:H2' | 74:S2:18:C:C6 | 2.50 | 0.47 |
| 74:S2:1611:G:H8 | 74:S2:1612:G:C8 | 2.32 | 0.47 |
| 74:S2:1797:U:H2' | 74:S2:1798:C:C6 | 2.49 | 0.47 |
| 5:SX:68:LYS:HD2 | 5:SX:91:LEU:HD22 | 1.96 | 0.47 |
| 8:SR:105:MET:O | 8:SR:109:LEU:HG | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:SK:25:LYS:NZ | 74:S2:1497:G:O6 | 2.47 | 0.47 |
| 41:LN:202:ARG:NH2 | 70:L5:1372:A:OP1 | 2.48 | 0.47 |
| 59:Ld:39:LYS:NZ | 70:L5:2370:A:N7 | 2.55 | 0.47 |
| 62:LB:56:ILE:HD13 | 62:LB:365:LEU:HD22 | 1.97 | 0.47 |
| 70:L5:4991:U:H2' | 70:L5:4992:G:H8 | 1.79 | 0.47 |
| 74:S2:1505:U:H4' | 74:S2:1508:A:H1' | 1.97 | 0.47 |
| 45:Lk:17:ARG:NH2 | 45:Lk:19:ASP:OD2 | 2.48 | 0.47 |
| 50:LH:111:LEU:HD21 | 50:LH:125:ARG:HG2 | 1.96 | 0.47 |
| 44:LL:36:ARG:NH1 | 70:L5:1366:G:OP2 | 2.44 | 0.46 |
| 60:LC:350:ARG:HD2 | 70:L5:724:C:OP1 | 2.15 | 0.46 |
| 63:Lb:95:ARG:O | 63:Lb:99:ILE:HG12 | 2.14 | 0.46 |
| 67:Pt:20:G:H3' | 67:Pt:21:H2U:H52 | 1.96 | 0.46 |
| 70:L5:162:A:H2' | 70:L5:163:A:C8 | 2.50 | 0.46 |
| 70:L5:654:C:H2' | 70:L5:655:C:C6 | 2.50 | 0.46 |
| 70:L5:2091:C:O2 | 70:L5:2094:G:O2' | 2.22 | 0.46 |
| 74:S2:1562:C:H2' | 74:S2:1563:G:H8 | 1.79 | 0.46 |
| 76:SI:4:SER:OG | 76:SI:6:ASP:OD2 | 2.27 | 0.46 |
| 69:L8:148:A:H2' | 69:L8:149:G:C8 | 2.51 | 0.46 |
| 70:L5:4740:G:C4 | 70:L5:4742:G:H1' | 2.50 | 0.46 |
| 74:S2:5:U:H2' | 74:S2:6:G:H8 | 1.80 | 0.46 |
| 74:S2:211:G:H2' | 74:S2:212:C:C6 | 2.50 | 0.46 |
| 74:S2:212:C:H2' | 74:S2:213:G:C8 | 2.51 | 0.46 |
| 74:S2:1808:U:H2' | 74:S2:1809:A:C8 | 2.51 | 0.46 |
| 2:Ll:16:LYS:HD2 | 2:Ll:49:LEU:HD22 | 1.97 | 0.46 |
| 37:LQ:89:ASP:HB3 | 37:LQ:92:VAL:HG12 | 1.98 | 0.46 |
| 55:Lf:38:GLU:OE1 | 56:LE:285:LYS:NZ | 2.49 | 0.46 |
| 56:LE:95:PRO:HA | 56:LE:104:THR:HA | 1.96 | 0.46 |
| 58:LD:122:GLN:O | 58:LD:248:ARG:NH2 | 2.48 | 0.46 |
| 70:L5:382:G:N1 | 70:L5:385:A:OP2 | 2.40 | 0.46 |
| 70:L5:1307:A:H2' | 70:L5:1308:C:C6 | 2.50 | 0.46 |
| 70:L5:2092:G:H4' | 70:L5:2093:A:H5'' | 1.97 | 0.46 |
| 70:L5:2539:C:H2' | 70:L5:2540:C:C6 | 2.50 | 0.46 |
| 58:LD:52:ILE:HD13 | 66:L7:6:C:H4' | 1.96 | 0.46 |
| 70:L5:162:A:H2' | 70:L5:163:A:H8 | 1.80 | 0.46 |
| 70:L5:1203:G:H2' | 70:L5:1204:C:C6 | 2.45 | 0.46 |
| 76:SI:148:LYS:O | 76:SI:151:GLU:HG3 | 2.16 | 0.46 |
| 60:LC:157:LYS:HE2 | 60:LC:157:LYS:HB3 | 1.73 | 0.46 |
| 70:L5:1754:U:H2' | 70:L5:1755:C:C5 | 2.50 | 0.46 |
| 74:S2:455:A:H2' | 74:S2:456:C:C6 | 2.51 | 0.46 |
| 48:LI:55:ASP:HB2 | 48:LI:162:ARG:O | 2.16 | 0.46 |
| 60:LC:218:ILE:HA | 60:LC:229:LEU:HD13 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 68:Sa:74:CYS:SG | 87:Sa:201:HOH:O | 2.60 | 0.46 |
| 70:L5:4219:A:H2' | 70:L5:4220:6MZ:C8 | 2.46 | 0.46 |
| 74:S2:12:U:H2' | 74:S2:13:C:C6 | 2.51 | 0.46 |
| 74:S2:1804:OMU:H1' | 74:S2:1804:OMU:HM23 | 1.69 | 0.46 |
| 2:L1:21:ARG:O | 2:L1:38:ASN:ND2 | 2.49 | 0.46 |
| 22:SC:275:LYS:HD2 | 22:SC:276:THR:HG23 | 1.97 | 0.46 |
| 36:Lr:97:ILE:HD13 | 36:Lr:107:ARG:HA | 1.98 | 0.46 |
| 64:LA:40:TYR:OH | 70:L5:4117:U:O2' | 2.16 | 0.46 |
| 70:L5:2529:A:O2' | 70:L5:2531:C:OP2 | 2.33 | 0.46 |
| 8:SR:74:GLN:HA | 8:SR:77:GLU:HG3 | 1.97 | 0.46 |
| 21:Sd:10:HIS:NE2 | 74:S2:1261:C:O2 | 2.35 | 0.46 |
| 49:Li:76:ARG:HA | 49:Li:76:ARG:HD3 | 1.75 | 0.46 |
| 50:LH:165:THR:HG21 | 50:LH:179:ILE:HG13 | 1.97 | 0.46 |
| 62:LB:200:ARG:HA | 62:LB:200:ARG:HD3 | 1.72 | 0.46 |
| 65:La:89:ASN:HA | 65:La:92:LYS:HG2 | 1.97 | 0.46 |
| 65:La:91:ALA:HB2 | 65:La:120:GLN:HE21 | 1.81 | 0.46 |
| 70:L5:3873:G:H2' | 70:L5:3874:G:C8 | 2.51 | 0.46 |
| 70:L5:4069:U:H2' | 70:L5:4070:U:C6 | 2.51 | 0.46 |
| 70:L5:5027:C:H4' | 70:L5:5028:G:H5' | 1.97 | 0.46 |
| 74:S2:1403:C:H41 | 74:S2:1404:U:H5 | 1.63 | 0.46 |
| 77:S6:71:C:H2' | 77:S6:72:U:H6 | 1.81 | 0.46 |
| 7:SV:41:LYS:HE2 | 7:SV:41:LYS:HB3 | 1.87 | 0.46 |
| 50:LH:71:ARG:HH11 | 70:L5:4691:A:H5' | 1.80 | 0.46 |
| 52:LG:122:ALA:HA | 52:LG:126:GLY:HA2 | 1.97 | 0.46 |
| 58:LD:193:GLU:O | 58:LD:197:LYS:HG2 | 2.15 | 0.46 |
| 66:L7:38:U:N3 | 66:L7:41:G:OP2 | 2.39 | 0.46 |
| 70:L5:3917:A:H2' | 70:L5:3918:G:H8 | 1.80 | 0.46 |
| 71:SZ:79:ILE:HB | 71:SZ:83:LEU:HD23 | 1.97 | 0.46 |
| 75:SG:32:MET:HE2 | 75:SG:65:GLN:HB2 | 1.98 | 0.46 |
| 18:SE:100:ARG:HB2 | 18:SE:114:ILE:HD13 | 1.98 | 0.46 |
| 40:LO:176:ARG:HD2 | 70:L5:4769:G:H5'' | 1.97 | 0.46 |
| 48:LI:193:ASP:OD1 | 48:LI:193:ASP:N | 2.49 | 0.46 |
| 64:LA:147:ARG:HG3 | 64:LA:157:VAL:HG22 | 1.98 | 0.46 |
| 70:L5:3664:G:H2' | 70:L5:3665:G:H8 | 1.81 | 0.46 |
| 10:SO:134:PRO:HB3 | 74:S2:944:A:H5'' | 1.98 | 0.45 |
| 32:LU:40:GLU:O | 32:LU:44:GLN:NE2 | 2.46 | 0.45 |
| 36:Lr:67:ARG:NH2 | 70:L5:666:G:OP2 | 2.49 | 0.45 |
| 54:LF:184:ILE:HG23 | 54:LF:189:ASP:HB3 | 1.98 | 0.45 |
| 60:LC:94:ASN:ND2 | 87:L5:5359:HOH:O | 2.47 | 0.45 |
| 61:Lc:28:VAL:HG21 | 61:Lc:37:MET:HG3 | 1.97 | 0.45 |
| 70:L5:3893:C:H2' | 70:L5:3894:A:C8 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 74:S2:1798:C:H2' | 74:S2:1799:G:O4' | 2.16 | 0.45 |
| 36:Lr:6:GLN:O | 36:Lr:10:VAL:HG22 | 2.15 | 0.45 |
| 70:L5:444:G:H2' | 70:L5:445:U:C6 | 2.51 | 0.45 |
| 70:L5:699:C:H2' | 70:L5:700:G:H8 | 1.81 | 0.45 |
| 70:L5:907:C:H2' | 70:L5:908:G:H8 | 1.80 | 0.45 |
| 70:L5:3893:C:H2' | 70:L5:3894:A:H8 | 1.80 | 0.45 |
| 2:Ll:23:ILE:HG23 | 2:Ll:38:ASN:HB2 | 1.98 | 0.45 |
| 37:LQ:38:ARG:NH1 | 70:L5:2088:A:OP1 | 2.50 | 0.45 |
| 40:LO:193:THR:HG22 | 40:LO:197:LYS:HD3 | 1.99 | 0.45 |
| 48:LI:188:LYS:HD3 | 48:LI:212:LEU:HG | 1.98 | 0.45 |
| 69:L8:46:G:O2' | 69:L8:61:A:N1 | 2.48 | 0.45 |
| 70:L5:1202:C:H2' | 70:L5:1203:G:C8 | 2.51 | 0.45 |
| 74:S2:96:C:O2 | 74:S2:473:A:O2' | 2.33 | 0.45 |
| 74:S2:848:U:H2' | 74:S2:849:A:H8 | 1.82 | 0.45 |
| 74:S2:1801:A:H2' | 74:S2:1802:C:C6 | 2.52 | 0.45 |
| 8:SR:116:ASN:OD1 | 8:SR:116:ASN:N | 2.40 | 0.45 |
| 17:SF:166:ILE:HG12 | 74:S2:1599:U:C5 | 2.52 | 0.45 |
| 20:SD:12:VAL:O | 20:SD:16:ILE:HG12 | 2.16 | 0.45 |
| 20:SD:172:VAL:O | 20:SD:173:ARG:NE | 2.50 | 0.45 |
| 32:LU:80:LYS:HG2 | 32:LU:110:TYR:CE2 | 2.51 | 0.45 |
| 37:LQ:72:LEU:HB2 | 37:LQ:75:ARG:HD2 | 1.99 | 0.45 |
| 64:LA:109:GLU:CD | 64:LA:109:GLU:H | 2.24 | 0.45 |
| 67:Pt:19:G:N2 | 67:Pt:59:A:O5' | 2.49 | 0.45 |
| 74:S2:367:U:H4' | 74:S2:371:A:C8 | 2.52 | 0.45 |
| 74:S2:1740:C:H2' | 74:S2:1741:U:C6 | 2.50 | 0.45 |
| 76:SI:48:VAL:HG11 | 76:SI:54:LYS:HG3 | 1.98 | 0.45 |
| 17:SF:71:ARG:NH2 | 17:SF:148:ASN:OD1 | 2.50 | 0.45 |
| 38:LP:14:SER:HB3 | 38:LP:151:THR:HG22 | 1.98 | 0.45 |
| 52:LG:200:THR:OG1 | 70:L5:150:U:OP2 | 2.32 | 0.45 |
| 62:LB:216:MET:HE3 | 62:LB:283:LYS:HB2 | 1.98 | 0.45 |
| 62:LB:241:PRO:HD3 | 70:L5:4456:OMC:HM21 | 1.99 | 0.45 |
| 70:L5:1662:C:H2' | 70:L5:1663:C:C6 | 2.51 | 0.45 |
| 70:L5:4238:G:H2' | 70:L5:4239:A:C8 | 2.52 | 0.45 |
| 70:L5:4608:G:HO2' | 70:L5:4609:G:H8 | 1.61 | 0.45 |
| 70:L5:4906:C:H2' | 70:L5:4907:G:H8 | 1.81 | 0.45 |
| 74:S2:1007:C:H2' | 74:S2:1008:A:C8 | 2.52 | 0.45 |
| 74:S2:1226:G:N1 | 74:S2:1639:G7M:OP2 | 2.39 | 0.45 |
| 24:SB:69:VAL:HG11 | 24:SB:74:LEU:HD13 | 1.97 | 0.45 |
| 26:SA:25:LEU:HB3 | 26:SA:46:ILE:HD11 | 1.98 | 0.45 |
| 46:LJ:40:LEU:HD12 | 46:LJ:40:LEU:HA | 1.80 | 0.45 |
| 54:LF:182:TYR:HB3 | 54:LF:200:ARG:HG3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:La:84:GLU:O | 65:La:88:VAL:HG22 | 2.16 | 0.45 |
| 70:L5:4861:G:H2' | 70:L5:4862:G:C8 | 2.52 | 0.45 |
| 77:S6:30:G:H2' | 77:S6:31:G:C8 | 2.52 | 0.45 |
| 20:SD:137:VAL:HG13 | 20:SD:185:LYS:HB2 | 1.98 | 0.45 |
| 29:LX:72:ASP:OD1 | 29:LX:72:ASP:N | 2.48 | 0.45 |
| 32:LU:101:ARG:HG2 | 32:LU:113:ARG:HG3 | 1.99 | 0.45 |
| 65:La:75:LEU:HB3 | 65:La:117:LEU:HD13 | 1.99 | 0.45 |
| 70:L5:3707:U:H2' | 70:L5:3708:C:C6 | 2.51 | 0.45 |
| 70:L5:4260:U:H2' | 70:L5:4261:C:H6 | 1.82 | 0.45 |
| 70:L5:4458:C:H2' | 70:L5:4459:U:C6 | 2.52 | 0.45 |
| 70:L5:4584:A:H2' | 70:L5:4585:U:O4' | 2.16 | 0.45 |
| 70:L5:4908:G:N2 | 70:L5:4913:G:OP1 | 2.50 | 0.45 |
| 74:S2:511:U:H2' | 74:S2:512:A2M:H8 | 1.99 | 0.45 |
| 10:SO:49:GLY:O | 74:S2:975:G:O2' | 2.31 | 0.45 |
| 21:Sd:21:CYS:HB3 | 21:Sd:26:ASN:H | 1.81 | 0.45 |
| 40:LO:10:ASP:OD2 | 40:LO:37:ARG:NH2 | 2.48 | 0.45 |
| 70:L5:2498:C:H2' | 70:L5:2499:C:H6 | 1.81 | 0.45 |
| 70:L5:4252:C:OP2 | 70:L5:4253:A:O2' | 2.29 | 0.45 |
| 70:L5:4575:G:N2 | 87:L5:5402:HOH:O | 2.48 | 0.45 |
| 74:S2:934:G:H22 | 74:S2:1008:A:H2 | 1.65 | 0.45 |
| 74:S2:1244:PSU:H2' | 74:S2:1245:G:C8 | 2.51 | 0.45 |
| 74:S2:1667:U:H2' | 74:S2:1668:U:C6 | 2.52 | 0.45 |
| 9:SQ:47:LEU:HA | 17:SF:49:LEU:HD11 | 1.98 | 0.45 |
| 16:Sg:251:ALA:HA | 16:Sg:256:ILE:HA | 1.98 | 0.45 |
| 46:LJ:119:TYR:CZ | 46:LJ:121:PRO:HA | 2.52 | 0.45 |
| 54:LF:200:ARG:HD2 | 54:LF:203:GLU:OE1 | 2.17 | 0.45 |
| 70:L5:676:C:H2' | 70:L5:677:G:H8 | 1.82 | 0.45 |
| 70:L5:1320:U:O2' | 70:L5:1891:A:N1 | 2.47 | 0.45 |
| 70:L5:4992:G:H2' | 70:L5:4993:G:C8 | 2.51 | 0.45 |
| 74:S2:656:G:H5' | 74:S2:662:G:N2 | 2.31 | 0.45 |
| 74:S2:1025:U:OP1 | 74:S2:1090:C:O2' | 2.33 | 0.45 |
| 24:SB:146:ARG:NE | 74:S2:1122:A:N3 | 2.65 | 0.45 |
| 33:LT:104:SER:HA | 33:LT:107:LYS:HE3 | 1.99 | 0.45 |
| 41:LN:6:TYR:HD2 | 49:Li:44:ILE:HD11 | 1.82 | 0.45 |
| 43:LM:114:LYS:HD2 | 70:L5:4929:C:H5'' | 1.99 | 0.45 |
| 46:LJ:56:THR:HG22 | 46:LJ:64:ARG:N | 2.32 | 0.45 |
| 53:Lg:100:GLN:HA | 53:Lg:103:VAL:HG22 | 1.99 | 0.45 |
| 54:LF:34:ARG:HD2 | 70:L5:1272:C:H5' | 1.98 | 0.45 |
| 59:Ld:65:ASP:OD2 | 59:Ld:67:ARG:NH1 | 2.50 | 0.45 |
| 69:L8:17:A:H61 | 70:L5:417:G:H1' | 1.82 | 0.45 |
| 70:L5:138:G:H2' | 70:L5:139:G:C8 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 70:L5:325:U:H2' | 70:L5:326:C:C6 | 2.51 | 0.45 |
| 70:L5:460:C:H2' | 70:L5:461:G:H8 | 1.82 | 0.45 |
| 70:L5:2811:G:N1 | 70:L5:2814:C:OP2 | 2.45 | 0.45 |
| 70:L5:4089:G:H2' | 70:L5:4090:G:C8 | 2.52 | 0.45 |
| 70:L5:4239:A:H2' | 70:L5:4240:G:C8 | 2.52 | 0.45 |
| 70:L5:4274:A:H2' | 70:L5:4275:G:H8 | 1.80 | 0.45 |
| 74:S2:952:G:H2' | 74:S2:953:C:C6 | 2.52 | 0.45 |
| 79:mR:34:A:H2' | 79:mR:35:A:C8 | 2.50 | 0.45 |
| 35:LR:4:LEU:HD22 | 35:LR:7:GLN:HG3 | 1.97 | 0.44 |
| 70:L5:2724:G:O2' | 70:L5:2726:G:OP2 | 2.35 | 0.44 |
| 70:L5:2744:A:H2' | 70:L5:2745:A:C8 | 2.52 | 0.44 |
| 70:L5:4623:OMG:H1' | 70:L5:4623:OMG:HM23 | 1.68 | 0.44 |
| 71:SZ:66:LYS:O | 71:SZ:110:THR:OG1 | 2.28 | 0.44 |
| 71:SZ:73:VAL:HG23 | 71:SZ:84:ALA:HB1 | 1.99 | 0.44 |
| 74:S2:1568:C:H2' | 74:S2:1569:A:C8 | 2.52 | 0.44 |
| 6:SW:111:MET:HE1 | 6:SW:119:LYS:HE2 | 1.98 | 0.44 |
| 12:SL:128:VAL:HG12 | 12:SL:142:VAL:HA | 1.98 | 0.44 |
| 26:SA:77:ILE:HD13 | 26:SA:99:ILE:HB | 2.00 | 0.44 |
| 27:LZ:95:VAL:HG21 | 27:LZ:109:LYS:HG2 | 1.98 | 0.44 |
| 45:Lk:37:ARG:HD3 | 45:Lk:38:CYS:O | 2.17 | 0.44 |
| 69:L8:9:A:H2' | 69:L8:10:G:H8 | 1.82 | 0.44 |
| 70:L5:956:A:H1' | 70:L5:2076:G:H5'' | 1.98 | 0.44 |
| 70:L5:1082:C:H2' | 70:L5:1083:U:O4' | 2.17 | 0.44 |
| 70:L5:2519:U:O2' | 70:L5:2530:U:O2 | 2.35 | 0.44 |
| 70:L5:2845:A:H61 | 70:L5:3843:C:H42 | 1.65 | 0.44 |
| 70:L5:3692:A:N7 | 85:L5:5102:SPD:H82 | 2.32 | 0.44 |
| 70:L5:3871:A:H2' | 70:L5:3872:A:C8 | 2.52 | 0.44 |
| 75:SG:20:ASP:OD1 | 75:SG:23:LYS:N | 2.40 | 0.44 |
| 78:SS:16:LEU:HB3 | 78:SS:17:ASN:H | 1.58 | 0.44 |
| 62:LB:165:HIS:HB3 | 62:LB:180:LEU:HD12 | 1.99 | 0.44 |
| 66:L7:82:G:H2' | 66:L7:83:A:C8 | 2.53 | 0.44 |
| 70:L5:3641:U:OP2 | 70:L5:3646:A:N6 | 2.44 | 0.44 |
| 74:S2:116:OMU:H6 | 74:S2:116:OMU:O5' | 2.17 | 0.44 |
| 74:S2:1101:U:H2' | 74:S2:1102:G:C8 | 2.52 | 0.44 |
| 76:SI:67:TRP:HA | 76:SI:189:VAL:HG22 | 2.00 | 0.44 |
| 77:S6:69:U:H2' | 77:S6:70:G:H8 | 1.83 | 0.44 |
| 6:SW:37:PHE:HD1 | 6:SW:41:MET:HE2 | 1.82 | 0.44 |
| 9:SQ:17:LYS:HE3 | 74:S2:1648:G:N7 | 2.33 | 0.44 |
| 21:Sd:39:CYS:HB2 | 21:Sd:42:CYS:SG | 2.58 | 0.44 |
| 32:LU:69:LYS:HE2 | 32:LU:69:LYS:HB3 | 1.84 | 0.44 |
| 37:LQ:90:VAL:HG13 | 65:La:80:THR:HG21 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 43:LM:40:GLY:HA3 | 43:LM:45:VAL:HB | 1.99 | 0.44 |
| 47:Lj:49:TRP:O | 70:L5:1646:A:O2' | 2.35 | 0.44 |
| 48:LI:40:LYS:HB3 | 48:LI:40:LYS:HE2 | 1.80 | 0.44 |
| 58:LD:184:ASP:OD2 | 58:LD:187:SER:OG | 2.35 | 0.44 |
| 70:L5:1186:U:H2' | 70:L5:1187:G:N3 | 2.33 | 0.44 |
| 70:L5:3599:A:H2' | 70:L5:3600:G:H8 | 1.82 | 0.44 |
| 70:L5:4620:OMU:H1' | 70:L5:4620:OMU:HM23 | 1.65 | 0.44 |
| 10:SO:145:GLY:O | 68:Sa:22:ARG:NH2 | 2.50 | 0.44 |
| 30:LW:52:THR:HG22 | 30:LW:54:LEU:H | 1.83 | 0.44 |
| 50:LH:4:ILE:HG12 | 50:LH:61:TRP:CH2 | 2.53 | 0.44 |
| 50:LH:85:THR:HG22 | 50:LH:86:LEU:HD13 | 2.00 | 0.44 |
| 66:L7:110:G:H2' | 66:L7:111:C:C6 | 2.53 | 0.44 |
| 70:L5:1332:C:H2' | 70:L5:1333:A:C8 | 2.52 | 0.44 |
| 70:L5:3710:G:H1' | 70:L5:3712:A:N6 | 2.32 | 0.44 |
| 74:S2:17:C:H2' | 74:S2:18:C:H6 | 1.82 | 0.44 |
| 4:SY:60:PHE:O | 74:S2:571:U:O2' | 2.32 | 0.44 |
| 6:SW:107:SER:HB3 | 74:S2:860:G:H21 | 1.83 | 0.44 |
| 46:LJ:44:THR:HG21 | 46:LJ:72:CYS:SG | 2.58 | 0.44 |
| 54:LF:66:ARG:NH2 | 70:L5:1210:C:O2' | 2.51 | 0.44 |
| 64:LA:30:ARG:HG3 | 64:LA:74:GLU:HG2 | 1.99 | 0.44 |
| 70:L5:456:C:H2' | 70:L5:457:G:C8 | 2.53 | 0.44 |
| 70:L5:2640:G:H2' | 70:L5:2641:A:C8 | 2.52 | 0.44 |
| 70:L5:4723:A:H2' | 70:L5:4724:A:C8 | 2.53 | 0.44 |
| 74:S2:1030:A:H2' | 74:S2:1031:A2M:H8 | 2.00 | 0.44 |
| 26:SA:131:HIS:O | 26:SA:135:THR:HG23 | 2.18 | 0.44 |
| 41:LN:24:ARG:NH2 | 41:LN:123:GLU:O | 2.50 | 0.44 |
| 46:LJ:52:LYS:HE3 | 46:LJ:52:LYS:HB3 | 1.84 | 0.44 |
| 50:LH:64:ARG:NH2 | 70:L5:4693:C:OP1 | 2.47 | 0.44 |
| 52:LG:48:LYS:HA | 52:LG:48:LYS:HD2 | 1.74 | 0.44 |
| 62:LB:194:LEU:HD23 | 62:LB:194:LEU:HA | 1.84 | 0.44 |
| 70:L5:4905:C:H2' | 70:L5:4906:C:H6 | 1.83 | 0.44 |
| 70:L5:4959:U:H2' | 70:L5:4960:G:C8 | 2.53 | 0.44 |
| 74:S2:453:C:O2' | 75:SG:92:ARG:O | 2.28 | 0.44 |
| 80:SU:39:LEU:HD13 | 80:SU:89:ILE:HD12 | 1.99 | 0.44 |
| 24:SB:34:LYS:O | 24:SB:98:THR:OG1 | 2.35 | 0.44 |
| 24:SB:131:ASP:OD1 | 24:SB:131:ASP:N | 2.50 | 0.44 |
| 32:LU:101:ARG:NH2 | 70:L5:2623:A:OP1 | 2.49 | 0.44 |
| 34:LS:32:ILE:HG21 | 34:LS:40:ALA:HA | 2.00 | 0.44 |
| 49:Li:51:ALA:HB3 | 49:Li:54:GLU:HG3 | 1.99 | 0.44 |
| 70:L5:456:C:H2' | 70:L5:457:G:H8 | 1.83 | 0.44 |
| 70:L5:3880:G:N7 | 87:L5:5351:HOH:O | 2.36 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 70:L5:4260:U:H2' | 70:L5:4261:C:C6 | 2.52 | 0.44 |
| 3:Lo:59:LYS:NZ | 70:L5:4371:G:OP1 | 2.50 | 0.44 |
| 18:SE:182:MET:HE2 | 18:SE:228:ILE:HD13 | 1.99 | 0.44 |
| 45:Lk:33:LYS:HG2 | 45:Lk:46:VAL:HG22 | 1.99 | 0.44 |
| 58:LD:233:PRO:HA | 58:LD:236:MET:HE3 | 2.00 | 0.44 |
| 62:LB:90:VAL:HG13 | 62:LB:161:ARG:HB2 | 1.99 | 0.44 |
| 70:L5:1308:C:H2' | 70:L5:1309:C:C6 | 2.53 | 0.44 |
| 70:L5:4905:C:H2' | 70:L5:4906:C:C6 | 2.52 | 0.44 |
| 74:S2:118:C:H1' | 74:S2:445:A:C5 | 2.52 | 0.44 |
| 74:S2:1101:U:H2' | 74:S2:1102:G:H8 | 1.83 | 0.44 |
| 74:S2:1113:A:H2' | 74:S2:1114:U:C6 | 2.53 | 0.44 |
| 16:Sg:59:LEU:HD22 | 16:Sg:95:GLY:HA2 | 1.99 | 0.43 |
| 24:SB:142:PHE:CD1 | 24:SB:209:ASP:HB2 | 2.53 | 0.43 |
| 41:LN:15:GLN:NE2 | 70:L5:305:A:OP2 | 2.49 | 0.43 |
| 46:LJ:56:THR:HG22 | 46:LJ:64:ARG:H | 1.83 | 0.43 |
| 57:Le:33:ARG:NH1 | 70:L5:1303:A:N7 | 2.66 | 0.43 |
| 64:LA:104:VAL:N | 64:LA:162:ASN:O | 2.45 | 0.43 |
| 70:L5:2483:G:H2' | 70:L5:2484:A:C8 | 2.53 | 0.43 |
| 74:S2:115:U:H2' | 74:S2:116:OMU:C6 | 2.48 | 0.43 |
| 74:S2:215:G:H2' | 74:S2:216:C:H6 | 1.82 | 0.43 |
| 74:S2:380:G:OP2 | 76:SI:56:ARG:NH2 | 2.48 | 0.43 |
| 4:SY:11:LYS:HB2 | 4:SY:24:VAL:HG22 | 2.00 | 0.43 |
| 27:LZ:57:MET:HB3 | 27:LZ:61:LYS:HB3 | 1.99 | 0.43 |
| 40:LO:54:TYR:OH | 40:LO:73:PHE:O | 2.31 | 0.43 |
| 45:Lk:57:LYS:HE2 | 45:Lk:57:LYS:HB2 | 1.81 | 0.43 |
| 51:Lh:118:LYS:HB2 | 51:Lh:118:LYS:HE3 | 1.79 | 0.43 |
| 70:L5:676:C:H2' | 70:L5:677:G:C8 | 2.52 | 0.43 |
| 70:L5:733:A:H2' | 70:L5:734:G:O4' | 2.18 | 0.43 |
| 70:L5:1415:G:H2' | 70:L5:1416:G:C8 | 2.53 | 0.43 |
| 70:L5:1416:G:H2' | 70:L5:1417:C:C6 | 2.53 | 0.43 |
| 70:L5:1558:A:H2' | 70:L5:1559:G:H8 | 1.83 | 0.43 |
| 70:L5:2815:A2M:H2' | 70:L5:2816:G:C8 | 2.53 | 0.43 |
| 70:L5:3925:OMU:HM23 | 70:L5:3925:OMU:H1' | 1.72 | 0.43 |
| 74:S2:1324:G:O2' | 74:S2:1510:G:O2' | 2.34 | 0.43 |
| 74:S2:1725:U:H2' | 74:S2:1726:G:H8 | 1.83 | 0.43 |
| 12:SL:3:ASP:N | 12:SL:3:ASP:OD1 | 2.51 | 0.43 |
| 21:Sd:22:ARG:HB3 | 21:Sd:38:MET:HG2 | 1.99 | 0.43 |
| 35:LR:105:LEU:HD12 | 35:LR:135:LYS:HE3 | 1.99 | 0.43 |
| 40:LO:181:ALA:O | 40:LO:185:VAL:HG22 | 2.18 | 0.43 |
| 46:LJ:108:GLY:HA3 | 70:L5:4251:A:H5'' | 1.99 | 0.43 |
| 47:Lj:46:LYS:HB2 | 47:Lj:46:LYS:HE3 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:Lf:104:MET:HG2 | 55:Lf:106:TYR:CZ | 2.53 | 0.43 |
| 67:Pt:25:U:O2' | 70:L5:3770:PSU:OP1 | 2.36 | 0.43 |
| 70:L5:2257:C:O2' | 70:L5:2259:G:OP1 | 2.27 | 0.43 |
| 70:L5:2654:C:H2' | 70:L5:2655:C:H6 | 1.82 | 0.43 |
| 74:S2:1057:C:O2' | 74:S2:1059:G:N7 | 2.46 | 0.43 |
| 34:LS:147:ASP:O | 70:L5:748:G:N2 | 2.51 | 0.43 |
| 44:LL:174:LYS:O | 65:La:138:LYS:NZ | 2.39 | 0.43 |
| 65:La:79:TRP:HH2 | 65:La:99:PRO:HG2 | 1.83 | 0.43 |
| 74:S2:1025:U:H2' | 74:S2:1026:C:O4' | 2.19 | 0.43 |
| 12:SL:98:LYS:HG3 | 74:S2:421:G:H5' | 1.99 | 0.43 |
| 31:LV:21:PRO:HA | 31:LV:54:ALA:HA | 2.01 | 0.43 |
| 40:LO:174:LEU:HD13 | 40:LO:174:LEU:HA | 1.83 | 0.43 |
| 54:LF:238:ASP:OD1 | 54:LF:239:GLN:NE2 | 2.51 | 0.43 |
| 60:LC:336:ARG:HA | 60:LC:339:THR:HG22 | 2.01 | 0.43 |
| 70:L5:1399:G:O2' | 70:L5:1400:G:OP1 | 2.29 | 0.43 |
| 70:L5:1662:C:H2' | 70:L5:1663:C:H6 | 1.82 | 0.43 |
| 72:ST:73:GLY:O | 72:ST:76:THR:OG1 | 2.27 | 0.43 |
| 22:SC:172:ASN:HB3 | 22:SC:174:ILE:HG22 | 2.00 | 0.43 |
| 34:LS:161:ARG:HD2 | 34:LS:164:LYS:HB3 | 2.01 | 0.43 |
| 52:LG:121:LYS:O | 52:LG:126:GLY:N | 2.52 | 0.43 |
| 56:LE:200:LYS:HE3 | 56:LE:200:LYS:HB2 | 1.90 | 0.43 |
| 62:LB:156:TYR:OH | 70:L5:4909:A:OP2 | 2.31 | 0.43 |
| 70:L5:167:C:O2' | 70:L5:168:C:H5' | 2.19 | 0.43 |
| 70:L5:1333:A:H2' | 70:L5:1334:A:C8 | 2.53 | 0.43 |
| 70:L5:1426:G:N1 | 70:L5:1458:C:OP2 | 2.32 | 0.43 |
| 70:L5:1473:U:H2' | 70:L5:1474:C:C6 | 2.54 | 0.43 |
| 70:L5:1577:G:O2' | 70:L5:1612:G:H4' | 2.19 | 0.43 |
| 70:L5:4651:A:H2' | 70:L5:4652:G:O4' | 2.19 | 0.43 |
| 70:L5:4685:U:H2' | 70:L5:4686:G:C8 | 2.53 | 0.43 |
| 70:L5:4896:G:H2' | 70:L5:4897:G:C8 | 2.54 | 0.43 |
| 74:S2:1144:A:H5' | 74:S2:1355:C:H41 | 1.83 | 0.43 |
| 74:S2:1686:G:H2' | 74:S2:1687:C:H6 | 1.83 | 0.43 |
| 75:SG:78:SER:HB3 | 75:SG:92:ARG:HG2 | 2.00 | 0.43 |
| 13:SK:7:ASN:O | 13:SK:11:ILE:HG12 | 2.19 | 0.43 |
| 46:LJ:37:ALA:HB2 | 46:LJ:70:VAL:HG11 | 2.00 | 0.43 |
| 49:Li:40:VAL:O | 49:Li:44:ILE:HG12 | 2.18 | 0.43 |
| 70:L5:1440:U:H2' | 70:L5:1441:C:C6 | 2.54 | 0.43 |
| 70:L5:5057:C:H2' | 70:L5:5058:A:C8 | 2.54 | 0.43 |
| 71:SZ:85:ARG:NH1 | 74:S2:1597:C:OP2 | 2.44 | 0.43 |
| 74:S2:1560:U:H2' | 74:S2:1561:A:H8 | 1.84 | 0.43 |
| 74:S2:1681:U:H2' | 74:S2:1682:C:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 6:SW:62:VAL:HG11 | 25:Sb:8:LEU:HG | 2.01 | 0.43 |
| 15:SH:117:PRO:HG2 | 15:SH:120:ARG:HD3 | 2.00 | 0.43 |
| 17:SF:50:PRO:O | 17:SF:70:GLU:HG2 | 2.18 | 0.43 |
| 40:LO:165:LYS:HD2 | 40:LO:165:LYS:HA | 1.79 | 0.43 |
| 56:LE:201:ILE:HG23 | 56:LE:203:ILE:HG23 | 2.00 | 0.43 |
| 66:L7:3:C:H2' | 66:L7:4:U:C6 | 2.54 | 0.43 |
| 70:L5:197:A:N3 | 70:L5:222:C:O2' | 2.46 | 0.43 |
| 70:L5:1257:A:H3' | 70:L5:1258:G:H8 | 1.84 | 0.43 |
| 70:L5:4196:OMG:HM23 | 70:L5:4196:OMG:H1' | 1.59 | 0.43 |
| 70:L5:5053:U:O2' | 70:L5:5054:C:OP1 | 2.36 | 0.43 |
| 74:S2:96:C:H2' | 74:S2:97:U:C6 | 2.53 | 0.43 |
| 74:S2:1079:C:OP2 | 87:S2:2001:HOH:O | 2.20 | 0.43 |
| 74:S2:1232:PSU:H2' | 74:S2:1233:G:C8 | 2.52 | 0.43 |
| 78:SS:111:LEU:HD13 | 78:SS:111:LEU:HA | 1.81 | 0.43 |
| 80:SU:30:LYS:HD2 | 80:SU:30:LYS:HA | 1.63 | 0.43 |
| 60:LC:312:ARG:NH2 | 70:L5:2275:G:OP2 | 2.51 | 0.43 |
| 69:L8:16:G:N2 | 70:L5:417:G:H2' | 2.33 | 0.43 |
| 70:L5:1278:C:H2' | 70:L5:1279:A:O4' | 2.18 | 0.43 |
| 70:L5:1645:C:H2' | 70:L5:1646:A:C8 | 2.53 | 0.43 |
| 74:S2:169:U:O2' | 74:S2:170:A:OP1 | 2.34 | 0.43 |
| 3:Lo:68:LEU:HA | 3:Lo:68:LEU:HD12 | 1.84 | 0.43 |
| 6:SW:30:CYS:SG | 6:SW:31:SER:N | 2.92 | 0.43 |
| 26:SA:61:ALA:O | 26:SA:65:ILE:HG22 | 2.19 | 0.43 |
| 26:SA:149:ASN:HB2 | 26:SA:165:ASN:OD1 | 2.19 | 0.43 |
| 41:LN:155:VAL:HG12 | 70:L5:57:G:H4' | 2.01 | 0.43 |
| 47:Lj:36:LYS:HD3 | 70:L5:372:A:H5'' | 2.00 | 0.43 |
| 50:LH:71:ARG:NH1 | 70:L5:4691:A:H5' | 2.33 | 0.43 |
| 50:LH:129:ARG:HH21 | 70:L5:4704:C:H4' | 1.83 | 0.43 |
| 70:L5:1247:U:H2' | 70:L5:1248:C:C6 | 2.54 | 0.43 |
| 70:L5:1625:OMG:H4' | 70:L5:1626:G:O5' | 2.18 | 0.43 |
| 70:L5:2107:C:H2' | 70:L5:2108:G:C8 | 2.54 | 0.43 |
| 17:SF:99:ILE:HD11 | 71:SZ:108:ILE:HG12 | 2.01 | 0.42 |
| 22:SC:216:MET:HE2 | 22:SC:216:MET:HB3 | 1.89 | 0.42 |
| 27:LZ:92:ASP:OD2 | 27:LZ:94:THR:OG1 | 2.32 | 0.42 |
| 35:LR:39:GLN:NE2 | 70:L5:2711:G:OP2 | 2.52 | 0.42 |
| 44:LL:81:LEU:HD22 | 44:LL:86:ILE:HB | 2.01 | 0.42 |
| 63:Lb:53:GLY:HA2 | 63:Lb:56:LYS:HD2 | 2.01 | 0.42 |
| 67:Pt:16:C:H5' | 67:Pt:60:A:C2 | 2.52 | 0.42 |
| 67:Pt:33:OMC:H1' | 67:Pt:33:OMC:HM23 | 1.72 | 0.42 |
| 70:L5:25:A:H2' | 70:L5:26:C:H6 | 1.84 | 0.42 |
| 70:L5:1322:1MA:H8 | 70:L5:1322:1MA:H2' | 1.43 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 70:L5:1719:A:H1' | 70:L5:1721:G:N7 | 2.34 | 0.42 |
| 70:L5:2884:G:H2' | 70:L5:2885:A:H8 | 1.84 | 0.42 |
| 70:L5:4906:C:H2' | 70:L5:4907:G:C8 | 2.54 | 0.42 |
| 74:S2:16:G:H2' | 74:S2:17:C:C6 | 2.53 | 0.42 |
| 77:S6:37:A:H3' | 77:S6:38:A:H2' | 2.01 | 0.42 |
| 1:Lm:122:ARG:NH2 | 70:L5:4473:A:O2' | 2.52 | 0.42 |
| 3:Lo:6:LYS:HG3 | 3:Lo:94:GLY:HA3 | 2.01 | 0.42 |
| 6:SW:38:LEU:HD23 | 6:SW:41:MET:HE3 | 1.99 | 0.42 |
| 40:LO:27:VAL:O | 40:LO:101:ARG:NH1 | 2.52 | 0.42 |
| 48:LI:152:LEU:HB3 | 48:LI:165:ILE:HD12 | 1.99 | 0.42 |
| 66:L7:57:C:H2' | 66:L7:58:A:H8 | 1.84 | 0.42 |
| 68:Sa:74:CYS:HB2 | 68:Sa:77:CYS:N | 2.27 | 0.42 |
| 69:L8:19:C:H2' | 69:L8:20:A:C8 | 2.54 | 0.42 |
| 70:L5:1196:G:H2' | 70:L5:1197:C:H6 | 1.84 | 0.42 |
| 70:L5:1477:C:HO2' | 70:L5:1478:C:H6 | 1.65 | 0.42 |
| 70:L5:1806:G:H2' | 70:L5:1807:C:C6 | 2.53 | 0.42 |
| 70:L5:3599:A:H2' | 70:L5:3600:G:C8 | 2.53 | 0.42 |
| 70:L5:3732:A:H3' | 70:L5:3733:A:H8 | 1.84 | 0.42 |
| 74:S2:67:C:H41 | 75:SG:163:ASN:HA | 1.83 | 0.42 |
| 74:S2:880:G:H3' | 74:S2:881:G:H8 | 1.84 | 0.42 |
| 74:S2:1315:U:H2' | 74:S2:1316:C:C6 | 2.54 | 0.42 |
| 74:S2:1325:G:H5' | 74:S2:1326:U:OP1 | 2.19 | 0.42 |
| 74:S2:1405:A:H2' | 74:S2:1406:G:O4' | 2.19 | 0.42 |
| 74:S2:1609:C:H3' | 78:SS:132:ARG:NH1 | 2.34 | 0.42 |
| 6:SW:104:LEU:HB3 | 6:SW:125:ILE:HA | 2.01 | 0.42 |
| 8:SR:109:LEU:HD22 | 26:SA:52:LYS:HG3 | 1.99 | 0.42 |
| 22:SC:65:LYS:HE2 | 26:SA:118:GLU:HB3 | 1.99 | 0.42 |
| 28:LY:28:LYS:HE3 | 28:LY:28:LYS:HB3 | 1.87 | 0.42 |
| 29:LX:64:SER:HB3 | 51:Lh:69:LEU:HD13 | 2.02 | 0.42 |
| 32:LU:95:ASN:O | 32:LU:95:ASN:ND2 | 2.52 | 0.42 |
| 41:LN:9:GLU:HB2 | 49:Li:44:ILE:HG13 | 2.01 | 0.42 |
| 56:LE:69:TYR:CD1 | 56:LE:70:LYS:HG3 | 2.55 | 0.42 |
| 58:LD:238:GLU:O | 58:LD:242:LYS:HD3 | 2.19 | 0.42 |
| 59:Ld:29:ILE:O | 59:Ld:33:ILE:HG12 | 2.20 | 0.42 |
| 60:LC:60:HIS:NE2 | 60:LC:100:ARG:HD3 | 2.34 | 0.42 |
| 70:L5:2261:G:H2' | 70:L5:2262:G:C4 | 2.54 | 0.42 |
| 70:L5:4088:C:H2' | 70:L5:4089:G:C8 | 2.55 | 0.42 |
| 74:S2:1550:G:H3' | 74:S2:1579:A:H61 | 1.85 | 0.42 |
| 75:SG:127:THR:OG1 | 75:SG:128:THR:N | 2.52 | 0.42 |
| 27:LZ:25:ILE:HA | 27:LZ:43:VAL:HG12 | 2.00 | 0.42 |
| 37:LQ:132:LYS:NZ | 70:L5:1449:C:OP1 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:LA:140:ASN:OD1 | 64:LA:143:THR:OG1 | 2.33 | 0.42 |
| 70:L5:1490:G:H2' | 70:L5:1491:A:C8 | 2.53 | 0.42 |
| 74:S2:558:G:H2' | 74:S2:559:G:C8 | 2.54 | 0.42 |
| 74:S2:912:C:H4' | 74:S2:913:A:OP2 | 2.18 | 0.42 |
| 74:S2:1725:U:H2' | 74:S2:1726:G:C8 | 2.54 | 0.42 |
| 3:Lo:13:LYS:HE3 | 3:Lo:13:LYS:HB3 | 1.89 | 0.42 |
| 4:SY:86:GLU:OE2 | 4:SY:90:ARG:NH1 | 2.38 | 0.42 |
| 10:SO:136:PRO:HG3 | 10:SO:139:SER:HB3 | 2.00 | 0.42 |
| 32:LU:113:ARG:NH1 | 70:L5:2703:G:OP1 | 2.53 | 0.42 |
| 40:LO:93:LYS:HE2 | 40:LO:93:LYS:HB2 | 1.71 | 0.42 |
| 40:LO:113:ASP:OD1 | 40:LO:113:ASP:N | 2.53 | 0.42 |
| 43:LM:6:PHE:H | 43:LM:11:ARG:HH21 | 1.68 | 0.42 |
| 45:Lk:51:GLU:HG2 | 45:Lk:52:LYS:H | 1.85 | 0.42 |
| 46:LJ:64:ARG:HH21 | 67:Pt:57:C:H4' | 1.85 | 0.42 |
| 52:LG:99:ALA:HB1 | 52:LG:136:LEU:HD11 | 2.01 | 0.42 |
| 62:LB:95:THR:HG22 | 70:L5:4910:G:H4' | 2.01 | 0.42 |
| 70:L5:1271:G:H21 | 70:L5:1271:G:P | 2.41 | 0.42 |
| 70:L5:1346:C:H2' | 70:L5:1347:G:H8 | 1.83 | 0.42 |
| 70:L5:4859:C:O2' | 70:L5:4860:G:N7 | 2.49 | 0.42 |
| 74:S2:573:PSU:O4 | 74:S2:576:A2M:H8 | 2.19 | 0.42 |
| 74:S2:639:C:H2' | 74:S2:640:A:H8 | 1.84 | 0.42 |
| 74:S2:1595:U:H2' | 74:S2:1596:U:C6 | 2.54 | 0.42 |
| 76:SI:142:SER:HB3 | 76:SI:145:ILE:HG13 | 2.00 | 0.42 |
| 11:SN:136:PRO:HG2 | 11:SN:139:TRP:HB2 | 2.01 | 0.42 |
| 32:LU:23:LEU:HD11 | 32:LU:39:PHE:HE2 | 1.83 | 0.42 |
| 58:LD:197:LYS:HE2 | 58:LD:202:GLN:HG3 | 2.01 | 0.42 |
| 58:LD:253:TYR:OH | 66:L7:117:G:OP1 | 2.29 | 0.42 |
| 60:LC:237:ILE:HD12 | 60:LC:237:ILE:HA | 1.85 | 0.42 |
| 67:Pt:10:G:N2 | 67:Pt:27:G:H1' | 2.35 | 0.42 |
| 68:Sa:70:LYS:HE3 | 68:Sa:70:LYS:HB3 | 1.91 | 0.42 |
| 70:L5:2358:G:H2' | 70:L5:2359:U:O4' | 2.20 | 0.42 |
| 70:L5:4921:C:C2 | 70:L5:4922:C:C5 | 3.07 | 0.42 |
| 70:L5:5030:U:H2' | 70:L5:5031:G:H8 | 1.85 | 0.42 |
| 74:S2:215:G:H2' | 74:S2:216:C:C6 | 2.54 | 0.42 |
| 76:SI:31:ARG:HH12 | 76:SI:48:VAL:HG12 | 1.84 | 0.42 |
| 21:Sd:34:TYR:OH | 74:S2:1549:U:OP1 | 2.30 | 0.42 |
| 24:SB:114:VAL:O | 74:S2:1869:A:N6 | 2.53 | 0.42 |
| 26:SA:77:ILE:HB | 26:SA:124:VAL:HG12 | 2.02 | 0.42 |
| 47:Lj:16:HIS:O | 47:Lj:25:LYS:NZ | 2.50 | 0.42 |
| 64:LA:40:TYR:HA | 64:LA:91:GLY:HA3 | 2.02 | 0.42 |
| 70:L5:1672:U:H2' | 70:L5:1673:U:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 70:L5:2555:G:H2' | 70:L5:2556:G:C8 | 2.54 | 0.42 |
| 70:L5:4896:G:H2' | 70:L5:4897:G:H8 | 1.83 | 0.42 |
| 74:S2:639:C:H2' | 74:S2:640:A:C8 | 2.55 | 0.42 |
| 32:LU:65:ARG:HG2 | 32:LU:70:ILE:HG12 | 2.02 | 0.42 |
| 40:LO:51:LYS:HE3 | 40:LO:144:GLU:HB3 | 2.02 | 0.42 |
| 41:LN:56:LYS:NZ | 70:L5:153:G:OP1 | 2.41 | 0.42 |
| 44:LL:145:LYS:HB3 | 44:LL:145:LYS:HE2 | 1.77 | 0.42 |
| 50:LH:41:ILE:HG22 | 50:LH:43:VAL:HG13 | 2.01 | 0.42 |
| 50:LH:177:ASP:OD1 | 50:LH:177:ASP:N | 2.53 | 0.42 |
| 57:Le:5:ARG:HE | 70:L5:454:U:H1' | 1.85 | 0.42 |
| 59:Ld:46:LEU:HD23 | 59:Ld:46:LEU:HA | 1.88 | 0.42 |
| 70:L5:172:C:N4 | 70:L5:265:C:N3 | 2.49 | 0.42 |
| 70:L5:417:G:OP1 | 70:L5:2329:U:O2' | 2.37 | 0.42 |
| 70:L5:4460:U:H2' | 70:L5:4461:C:C6 | 2.55 | 0.42 |
| 74:S2:1793:A:H2' | 74:S2:1794:C:H6 | 1.85 | 0.42 |
| 75:SG:218:LYS:HB2 | 75:SG:218:LYS:HE3 | 1.81 | 0.42 |
| 26:SA:139:TYR:OH | 74:S2:1353:A:OP1 | 2.35 | 0.42 |
| 37:LQ:13:VAL:HG12 | 70:L5:1691:G:H5'' | 2.02 | 0.42 |
| 43:LM:24:LEU:HB3 | 43:LM:77:TRP:HH2 | 1.84 | 0.42 |
| 63:Lb:54:LEU:HA | 63:Lb:57:MET:HG2 | 2.02 | 0.42 |
| 69:L8:144:U:H2' | 69:L8:145:C:H6 | 1.85 | 0.42 |
| 70:L5:674:G:H2' | 70:L5:675:C:C6 | 2.55 | 0.42 |
| 70:L5:1607:C:H5'' | 85:L5:5101:SPD:H91 | 2.02 | 0.42 |
| 70:L5:1927:U:OP1 | 70:L5:1949:U:O2' | 2.30 | 0.42 |
| 70:L5:2418:A:N1 | 70:L5:2429:A:O2' | 2.49 | 0.42 |
| 70:L5:3930:U:H2' | 70:L5:3931:C:C6 | 2.55 | 0.42 |
| 70:L5:4523:A2M:H5'' | 70:L5:4524:G:H5' | 2.01 | 0.42 |
| 74:S2:51:U:H2' | 74:S2:52:G:H8 | 1.84 | 0.42 |
| 74:S2:628:A:N6 | 74:S2:1500:G:O2' | 2.53 | 0.42 |
| 15:SH:22:GLY:O | 15:SH:25:GLN:HG2 | 2.20 | 0.42 |
| 16:Sg:56:GLN:HG3 | 16:Sg:57:ARG:H | 1.84 | 0.42 |
| 62:LB:103:LYS:HD2 | 62:LB:103:LYS:HA | 1.88 | 0.42 |
| 70:L5:207:G:H2' | 70:L5:208:A:C8 | 2.55 | 0.42 |
| 70:L5:1806:G:H2' | 70:L5:1807:C:H6 | 1.85 | 0.42 |
| 74:S2:1673:U:H2' | 74:S2:1674:G:O4' | 2.20 | 0.42 |
| 74:S2:1703:OMC:HM23 | 74:S2:1703:OMC:H1' | 1.85 | 0.42 |
| 78:SS:106:LYS:HD3 | 78:SS:106:LYS:HA | 1.83 | 0.42 |
| 3:Lo:97:LYS:HD2 | 70:L5:4233:A:OP2 | 2.19 | 0.41 |
| 6:SW:31:SER:HB3 | 6:SW:34:ILE:HG13 | 2.01 | 0.41 |
| 17:SF:59:LYS:HG2 | 17:SF:62:ARG:HH21 | 1.85 | 0.41 |
| 55:Lf:106:TYR:HB2 | 55:Lf:107:PRO:HD3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 70:L5:1757:U:H3 | 70:L5:1774:C:N4 | 2.18 | 0.41 |
| 70:L5:3656:A:H2' | 70:L5:3657:U:H6 | 1.85 | 0.41 |
| 70:L5:4080:C:H2' | 70:L5:4081:G:H8 | 1.85 | 0.41 |
| 70:L5:4174:U:H2' | 70:L5:4175:G:C8 | 2.55 | 0.41 |
| 70:L5:4481:U:H2' | 70:L5:4482:U:H6 | 1.85 | 0.41 |
| 70:L5:4578:G:H2' | 70:L5:4579:PSU:C6 | 2.55 | 0.41 |
| 76:SI:159:SER:HB2 | 76:SI:162:LEU:HD12 | 2.01 | 0.41 |
| 4:SY:44:LEU:HD23 | 4:SY:44:LEU:HA | 1.89 | 0.41 |
| 15:SH:43:LEU:HD13 | 15:SH:72:PHE:CZ | 2.55 | 0.41 |
| 15:SH:49:LYS:HB3 | 15:SH:49:LYS:HE3 | 1.81 | 0.41 |
| 24:SB:71:LEU:HD22 | 24:SB:84:PHE:HE2 | 1.85 | 0.41 |
| 24:SB:74:LEU:HD12 | 24:SB:74:LEU:HA | 1.92 | 0.41 |
| 45:Lk:51:GLU:OE1 | 45:Lk:51:GLU:N | 2.52 | 0.41 |
| 70:L5:1274:A:H2' | 70:L5:1275:G:O4' | 2.20 | 0.41 |
| 70:L5:1345:A:H2' | 70:L5:1346:C:C6 | 2.55 | 0.41 |
| 70:L5:1942:A:H2' | 70:L5:1943:A:H8 | 1.85 | 0.41 |
| 70:L5:4637:OMG:H1' | 70:L5:4637:OMG:HM23 | 1.86 | 0.41 |
| 70:L5:4699:U:H1' | 70:L5:4700:A:H5'' | 2.02 | 0.41 |
| 74:S2:96:C:H2' | 74:S2:97:U:H6 | 1.84 | 0.41 |
| 76:SI:101:ILE:HD12 | 76:SI:190:LEU:HD11 | 2.01 | 0.41 |
| 25:Sb:30:SER:OG | 74:S2:1016:U:OP1 | 2.34 | 0.41 |
| 41:LN:125:SER:HB3 | 70:L5:3937:C:H1' | 2.02 | 0.41 |
| 44:LL:127:PHE:HB2 | 51:Lh:118:LYS:HG3 | 2.02 | 0.41 |
| 45:Lk:61:PRO:HA | 45:Lk:62:PRO:HD3 | 1.91 | 0.41 |
| 46:LJ:75:ARG:NH2 | 66:L7:40:U:O2 | 2.45 | 0.41 |
| 64:LA:244:GLY:HA3 | 70:L5:3746:A:H5'' | 2.01 | 0.41 |
| 70:L5:750:U:H1' | 70:L5:917:A:C8 | 2.55 | 0.41 |
| 70:L5:1528:U:H2' | 70:L5:1529:G:C8 | 2.56 | 0.41 |
| 70:L5:1811:G:H2' | 70:L5:1812:C:C6 | 2.55 | 0.41 |
| 70:L5:2520:C:H2' | 70:L5:2521:G:C8 | 2.55 | 0.41 |
| 70:L5:2601:A:N6 | 70:L5:2743:A:H3' | 2.36 | 0.41 |
| 70:L5:4952:G:H2' | 70:L5:4953:G:O4' | 2.19 | 0.41 |
| 71:SZ:69:THR:O | 71:SZ:73:VAL:HG22 | 2.20 | 0.41 |
| 74:S2:29:G:H2' | 74:S2:30:C:C6 | 2.55 | 0.41 |
| 74:S2:102:A:H4' | 74:S2:104:A:C8 | 2.56 | 0.41 |
| 74:S2:910:G:OP2 | 74:S2:910:G:N2 | 2.42 | 0.41 |
| 74:S2:1189:A:H2' | 74:S2:1190:A:C8 | 2.55 | 0.41 |
| 74:S2:1255:G:OP1 | 74:S2:1256:G:O2' | 2.31 | 0.41 |
| 77:S6:70:G:H2' | 77:S6:71:C:C6 | 2.55 | 0.41 |
| 5:SX:68:LYS:HB3 | 5:SX:91:LEU:HD13 | 2.01 | 0.41 |
| 8:SR:96:ILE:HB | 8:SR:117:LEU:HD23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:SE:172:PHE:CE2 | 18:SE:174:LYS:HE3 | 2.56 | 0.41 |
| 21:Sd:24:CYS:HB2 | 74:S2:1496:U:H4' | 2.02 | 0.41 |
| 22:SC:257:LYS:HE3 | 22:SC:257:LYS:HB2 | 1.88 | 0.41 |
| 34:LS:95:ARG:HH12 | 70:L5:1951:G:HO2' | 1.66 | 0.41 |
| 34:LS:151:LYS:HG2 | 43:LM:6:PHE:HB3 | 2.02 | 0.41 |
| 70:L5:153:G:H2' | 70:L5:154:G:H8 | 1.85 | 0.41 |
| 70:L5:424:U:H2' | 70:L5:425:U:C6 | 2.55 | 0.41 |
| 70:L5:1818:G:OP2 | 70:L5:1818:G:N2 | 2.37 | 0.41 |
| 70:L5:4156:G:OP2 | 70:L5:4157:A:O2' | 2.30 | 0.41 |
| 21:Sd:33:LYS:HE2 | 21:Sd:34:TYR:CZ | 2.56 | 0.41 |
| 24:SB:149:GLN:HG2 | 74:S2:1123:C:H4' | 2.03 | 0.41 |
| 34:LS:70:LYS:HD2 | 34:LS:70:LYS:HA | 1.83 | 0.41 |
| 35:LR:151:ARG:O | 35:LR:154:LEU:HG | 2.21 | 0.41 |
| 40:LO:28:LEU:HD23 | 40:LO:28:LEU:HA | 1.93 | 0.41 |
| 43:LM:6:PHE:H | 43:LM:11:ARG:NH2 | 2.18 | 0.41 |
| 43:LM:85:LYS:O | 43:LM:89:THR:HG23 | 2.21 | 0.41 |
| 44:LL:36:ARG:NH2 | 70:L5:1364:U:OP2 | 2.32 | 0.41 |
| 45:Lk:47:ILE:HG22 | 45:Lk:49:ASP:H | 1.86 | 0.41 |
| 48:LI:3:ARG:HH12 | 70:L5:4430:G:H5' | 1.86 | 0.41 |
| 63:Lb:3:LYS:HD3 | 70:L5:4194:U:H3' | 2.01 | 0.41 |
| 67:Pt:74:A:H5'' | 67:Pt:75:C:H5' | 2.01 | 0.41 |
| 70:L5:271:C:H2' | 70:L5:272:U:H6 | 1.86 | 0.41 |
| 70:L5:699:C:H2' | 70:L5:700:G:C8 | 2.56 | 0.41 |
| 70:L5:1487:G:H2' | 70:L5:1488:G:C8 | 2.55 | 0.41 |
| 70:L5:2611:A:H2' | 70:L5:2612:G:C8 | 2.55 | 0.41 |
| 70:L5:3684:G:H2' | 70:L5:3685:C:H6 | 1.85 | 0.41 |
| 74:S2:206:G:H2' | 74:S2:207:G:C8 | 2.56 | 0.41 |
| 74:S2:1201:U:H2' | 74:S2:1202:U:C6 | 2.56 | 0.41 |
| 77:S6:69:U:H2' | 77:S6:70:G:C8 | 2.56 | 0.41 |
| 15:SH:63:PHE:HB3 | 15:SH:97:GLN:HG2 | 2.00 | 0.41 |
| 33:LT:99:SER:HG | 33:LT:101:SER:HG | 1.68 | 0.41 |
| 36:Lr:37:SER:OG | 70:L5:2267:U:OP1 | 2.31 | 0.41 |
| 40:LO:76:PRO:HB3 | 40:LO:138:LEU:HG | 2.02 | 0.41 |
| 49:Li:38:LYS:HE3 | 49:Li:38:LYS:HB3 | 1.85 | 0.41 |
| 58:LD:199:ILE:HG22 | 58:LD:200:MET:HE2 | 2.02 | 0.41 |
| 69:L8:26:C:H2' | 69:L8:27:U:C6 | 2.56 | 0.41 |
| 69:L8:27:U:H2' | 69:L8:28:C:C6 | 2.55 | 0.41 |
| 70:L5:400:A2M:HM'3 | 70:L5:400:A2M:H1' | 1.81 | 0.41 |
| 70:L5:2743:A:H2' | 70:L5:2744:A:C8 | 2.56 | 0.41 |
| 70:L5:3870:C:H2' | 70:L5:3871:A:H8 | 1.85 | 0.41 |
| 74:S2:441:C:H2' | 74:S2:442:C:C6 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 74:S2:1013:U:OP1 | 74:S2:1129:G:O2' | 2.38 | 0.41 |
| 74:S2:1610:G:OP2 | 78:SS:132:ARG:NH1 | 2.51 | 0.41 |
| 74:S2:1712:A:H2' | 74:S2:1713:C:C6 | 2.55 | 0.41 |
| 76:SI:195:LEU:HD12 | 76:SI:195:LEU:HA | 1.90 | 0.41 |
| 37:LQ:124:ASP:OD1 | 37:LQ:124:ASP:N | 2.52 | 0.41 |
| 40:LO:185:VAL:O | 40:LO:189:ILE:HG12 | 2.21 | 0.41 |
| 54:LF:216:PRO:HD3 | 54:LF:247:MET:HE2 | 2.02 | 0.41 |
| 70:L5:106:A:H2' | 70:L5:107:G:O4' | 2.20 | 0.41 |
| 70:L5:1189:G:H2' | 70:L5:1190:C:C6 | 2.56 | 0.41 |
| 70:L5:1545:G:H2' | 70:L5:1546:C:C6 | 2.56 | 0.41 |
| 70:L5:1563:A:H2' | 70:L5:1564:A:C8 | 2.55 | 0.41 |
| 70:L5:2448:G:H2' | 70:L5:2449:A:C8 | 2.56 | 0.41 |
| 70:L5:3661:G:H4' | 70:L5:3662:A:H5' | 2.02 | 0.41 |
| 70:L5:3867:A2M:HM'3 | 70:L5:3880:G:N2 | 2.36 | 0.41 |
| 70:L5:3932:U:H2' | 70:L5:3933:G:H8 | 1.86 | 0.41 |
| 70:L5:4481:U:H2' | 70:L5:4482:U:C6 | 2.56 | 0.41 |
| 70:L5:5004:C:H2' | 70:L5:5005:G:O4' | 2.20 | 0.41 |
| 72:ST:23:LYS:HD2 | 72:ST:23:LYS:HA | 1.90 | 0.41 |
| 74:S2:1183:A:H2' | 74:S2:1184:G:H8 | 1.86 | 0.41 |
| 77:S6:31:G:H2' | 77:S6:32:C:C6 | 2.56 | 0.41 |
| 15:SH:73:GLN:HB3 | 15:SH:135:PHE:CE1 | 2.56 | 0.41 |
| 49:Li:60:LEU:HD23 | 49:Li:60:LEU:HA | 1.94 | 0.41 |
| 54:LF:47:ARG:O | 54:LF:50:ILE:HG13 | 2.21 | 0.41 |
| 69:L8:5:U:H2' | 69:L8:6:C:H6 | 1.86 | 0.41 |
| 70:L5:1098:G:H2' | 70:L5:1099:C:C6 | 2.56 | 0.41 |
| 70:L5:2758:G:O2' | 70:L5:2765:A:N3 | 2.46 | 0.41 |
| 70:L5:3932:U:H2' | 70:L5:3933:G:C8 | 2.55 | 0.41 |
| 70:L5:4254:G:N3 | 70:L5:4254:G:H2' | 2.34 | 0.41 |
| 70:L5:4324:A:H2' | 70:L5:4325:A:C8 | 2.55 | 0.41 |
| 74:S2:416:U:H2' | 74:S2:417:C:O4' | 2.20 | 0.41 |
| 74:S2:455:A:H2' | 74:S2:456:C:H6 | 1.85 | 0.41 |
| 74:S2:509:OMG:H1' | 74:S2:509:OMG:HM23 | 1.72 | 0.41 |
| 74:S2:1683:C:H2' | 74:S2:1684:C:H6 | 1.86 | 0.41 |
| 75:SG:10:THR:HG23 | 75:SG:12:CYS:H | 1.86 | 0.41 |
| 78:SS:12:ILE:HD13 | 78:SS:21:ASP:HA | 2.02 | 0.41 |
| 80:SU:21:ARG:NH1 | 80:SU:21:ARG:HB2 | 2.36 | 0.41 |
| 11:SN:88:LEU:HD13 | 11:SN:125:LEU:HB3 | 2.03 | 0.41 |
| 16:Sg:125:ARG:HA | 16:Sg:125:ARG:HD3 | 1.89 | 0.41 |
| 17:SF:126:THR:HG21 | 23:Sc:27:CYS:SG | 2.60 | 0.41 |
| 25:Sb:14:GLU:O | 25:Sb:18:LYS:HG3 | 2.21 | 0.41 |
| 26:SA:132:GLN:HB3 | 26:SA:133:PRO:HD3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:LZ:58:GLY:O | 27:LZ:62:ILE:HG12 | 2.20 | 0.41 |
| 29:LX:89:LYS:HG3 | 29:LX:95:THR:HB | 2.02 | 0.41 |
| 29:LX:143:ASP:OD1 | 29:LX:143:ASP:N | 2.52 | 0.41 |
| 36:Lr:28:GLU:OE2 | 36:Lr:31:ASN:ND2 | 2.54 | 0.41 |
| 37:LQ:119:LYS:HE2 | 37:LQ:119:LYS:HB3 | 1.78 | 0.41 |
| 37:LQ:128:LEU:HA | 37:LQ:128:LEU:HD13 | 1.85 | 0.41 |
| 49:Li:65:LYS:HE2 | 49:Li:65:LYS:HB3 | 1.87 | 0.41 |
| 52:LG:33:GLU:O | 70:L5:4128:A:O2' | 2.34 | 0.41 |
| 56:LE:62:MET:HE1 | 56:LE:65:ARG:HH11 | 1.85 | 0.41 |
| 58:LD:128:ASP:O | 58:LD:164:LYS:NZ | 2.41 | 0.41 |
| 58:LD:139:PRO:HB3 | 70:L5:1820:C:H5' | 2.03 | 0.41 |
| 60:LC:239:LYS:H | 60:LC:239:LYS:HG2 | 1.71 | 0.41 |
| 69:L8:4:C:H2' | 69:L8:5:U:H6 | 1.86 | 0.41 |
| 70:L5:318:A:H2' | 70:L5:319:A:H8 | 1.86 | 0.41 |
| 70:L5:732:A:H2' | 70:L5:733:A:O4' | 2.21 | 0.41 |
| 70:L5:1260:G:H2' | 70:L5:1261:G:O4' | 2.21 | 0.41 |
| 70:L5:1857:C:H2' | 70:L5:1858:A:C8 | 2.52 | 0.41 |
| 70:L5:1965:G:H5' | 70:L5:4695:C:H1' | 2.03 | 0.41 |
| 70:L5:2079:G:H2' | 70:L5:2080:U:C6 | 2.56 | 0.41 |
| 70:L5:2730:U:H2' | 70:L5:2731:C:C6 | 2.56 | 0.41 |
| 70:L5:3602:C:H2' | 70:L5:3603:G:H8 | 1.86 | 0.41 |
| 70:L5:3633:C:H2' | 70:L5:3634:G:C8 | 2.56 | 0.41 |
| 70:L5:4186:A:H2' | 70:L5:4187:G:C8 | 2.55 | 0.41 |
| 70:L5:4522:G:O2' | 70:L5:4525:C:OP2 | 2.32 | 0.41 |
| 70:L5:4551:U:H2' | 70:L5:4552:PSU:C6 | 2.56 | 0.41 |
| 70:L5:4604:G:N2 | 70:L5:4607:A:OP2 | 2.37 | 0.41 |
| 70:L5:4903:G:H2' | 70:L5:4904:G:C8 | 2.54 | 0.41 |
| 74:S2:65:C:C6 | 75:SG:174:PRO:HB3 | 2.55 | 0.41 |
| 74:S2:553:U:H2' | 74:S2:554:A:H8 | 1.84 | 0.41 |
| 74:S2:948:C:H2' | 74:S2:949:G:C8 | 2.55 | 0.41 |
| 74:S2:1217:A:H2' | 74:S2:1218:C:C6 | 2.55 | 0.41 |
| 74:S2:1417:C:H2' | 74:S2:1418:C:C6 | 2.55 | 0.41 |
| 74:S2:1658:G:OP2 | 74:S2:1660:C:N4 | 2.51 | 0.41 |
| 74:S2:1809:A:H2' | 74:S2:1810:U:C6 | 2.56 | 0.41 |
| 75:SG:215:LYS:O | 75:SG:219:GLU:HG2 | 2.21 | 0.41 |
| 5:SX:67:ARG:HD2 | 5:SX:115:ILE:HG12 | 2.02 | 0.41 |
| 13:SK:24:LYS:O | 13:SK:42:ASN:ND2 | 2.54 | 0.41 |
| 15:SH:51:ILE:HD12 | 15:SH:179:LYS:HE2 | 2.02 | 0.41 |
| 22:SC:132:ASP:OD1 | 22:SC:132:ASP:N | 2.52 | 0.41 |
| 56:LE:57:TYR:HB2 | 56:LE:62:MET:HE3 | 2.04 | 0.41 |
| 63:Lb:40:LEU:O | 63:Lb:44:ARG:HG3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 70:L5:980:U:H2' | 70:L5:981:C:C6 | 2.56 | 0.41 |
| 70:L5:1514:U:H2' | 70:L5:1515:A:C8 | 2.56 | 0.41 |
| 70:L5:1749:A:H2' | 70:L5:1750:G:C8 | 2.55 | 0.41 |
| 70:L5:4704:C:H2' | 70:L5:4705:A:C8 | 2.55 | 0.41 |
| 74:S2:5:U:H2' | 74:S2:6:G:C8 | 2.55 | 0.41 |
| 74:S2:380:G:P | 76:SI:56:ARG:HH22 | 2.43 | 0.41 |
| 74:S2:1741:U:H2' | 74:S2:1742:C:O4' | 2.21 | 0.41 |
| 27:LZ:10:VAL:O | 27:LZ:83:THR:HB | 2.22 | 0.40 |
| 34:LS:174:THR:OG1 | 70:L5:4763:U:O2' | 2.30 | 0.40 |
| 41:LN:94:PHE:CE2 | 41:LN:96:ARG:HB2 | 2.56 | 0.40 |
| 48:LI:205:PRO:HD2 | 48:LI:208:LYS:HG3 | 2.02 | 0.40 |
| 70:L5:664:G:N2 | 70:L5:667:A:H62 | 2.20 | 0.40 |
| 70:L5:1207:C:H2' | 70:L5:1208:G:H8 | 1.86 | 0.40 |
| 70:L5:1564:A:H2' | 70:L5:1565:A:C8 | 2.55 | 0.40 |
| 70:L5:2335:C:H2' | 70:L5:2336:G:H8 | 1.86 | 0.40 |
| 70:L5:2412:A:H2' | 70:L5:2413:U:C6 | 2.56 | 0.40 |
| 70:L5:2497:C:H2' | 70:L5:2498:C:C6 | 2.56 | 0.40 |
| 70:L5:3736:A:H2' | 70:L5:3737:A:H8 | 1.84 | 0.40 |
| 70:L5:3829:G:H2' | 70:L5:3830:A2M:H8 | 2.03 | 0.40 |
| 70:L5:3923:A:H2' | 70:L5:3924:C:C6 | 2.56 | 0.40 |
| 70:L5:4887:C:H2' | 70:L5:4888:U:O4' | 2.21 | 0.40 |
| 74:S2:15:U:H2' | 74:S2:16:G:O4' | 2.21 | 0.40 |
| 74:S2:1390:U:H2' | 74:S2:1391:OMC:C6 | 2.57 | 0.40 |
| 75:SG:137:ARG:HB3 | 75:SG:140:ARG:HB2 | 2.02 | 0.40 |
| 4:SY:57:VAL:HB | 4:SY:60:PHE:CE1 | 2.56 | 0.40 |
| 30:LW:47:ARG:HG3 | 30:LW:58:LYS:HD3 | 2.03 | 0.40 |
| 43:LM:36:ALA:HB2 | 43:LM:52:PHE:CZ | 2.56 | 0.40 |
| 49:Li:25:ARG:HE | 70:L5:159:C:H5'' | 1.86 | 0.40 |
| 50:LH:92:MET:HG3 | 50:LH:180:TYR:C | 2.46 | 0.40 |
| 55:Lf:75:THR:HG22 | 70:L5:952:G:H4' | 2.02 | 0.40 |
| 70:L5:204:U:H2' | 70:L5:205:C:C6 | 2.56 | 0.40 |
| 70:L5:477:C:H2' | 70:L5:478:G:C8 | 2.56 | 0.40 |
| 70:L5:2424:OMG:H1' | 70:L5:2424:OMG:HM23 | 1.80 | 0.40 |
| 70:L5:2837:OMU:H1' | 70:L5:2837:OMU:HM23 | 1.88 | 0.40 |
| 74:S2:996:A:H2' | 74:S2:997:A:C8 | 2.56 | 0.40 |
| 74:S2:1010:G:H2' | 74:S2:1011:A:H8 | 1.85 | 0.40 |
| 74:S2:1374:C:H2' | 74:S2:1375:G:O4' | 2.21 | 0.40 |
| 74:S2:1395:C:H2' | 74:S2:1396:A:N3 | 2.37 | 0.40 |
| 74:S2:1736:G:H2' | 74:S2:1737:G:C8 | 2.56 | 0.40 |
| 3:Lo:12:CYS:HB3 | 3:Lo:15:CYS:HB2 | 2.03 | 0.40 |
| 4:SY:25:ILE:HD11 | 4:SY:73:GLY:HA3 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:SO:61:LYS:HD2 | 10:SO:76:LEU:HB3 | 2.02 | 0.40 |
| 26:SA:10:MET:HE3 | 26:SA:10:MET:HB2 | 1.86 | 0.40 |
| 34:LS:85:ASP:OD1 | 34:LS:90:THR:HB | 2.21 | 0.40 |
| 48:LI:145:LYS:O | 48:LI:149:ILE:HG12 | 2.20 | 0.40 |
| 50:LH:115:ARG:HG3 | 50:LH:123:ILE:HG23 | 2.03 | 0.40 |
| 51:Lh:102:LEU:HD23 | 51:Lh:102:LEU:HA | 1.94 | 0.40 |
| 63:Lb:54:LEU:O | 63:Lb:57:MET:HB2 | 2.21 | 0.40 |
| 70:L5:1730:U:H2' | 70:L5:1731:C:C6 | 2.57 | 0.40 |
| 70:L5:2555:G:H2' | 70:L5:2556:G:H8 | 1.85 | 0.40 |
| 70:L5:4696:C:H2' | 70:L5:4697:U:O4' | 2.21 | 0.40 |
| 74:S2:436:OMG:HM23 | 74:S2:436:OMG:H1' | 1.83 | 0.40 |
| 74:S2:1746:U:OP1 | 75:SG:31:ARG:NH2 | 2.55 | 0.40 |
| 80:SU:20:ILE:HG23 | 80:SU:91:LEU:HB2 | 2.02 | 0.40 |
| 14:SJ:60:LEU:HA | 14:SJ:60:LEU:HD23 | 1.87 | 0.40 |
| 22:SC:176:LYS:HG3 | 22:SC:177:PRO:HD2 | 2.04 | 0.40 |
| 60:LC:288:ASP:HB3 | 60:LC:291:ARG:HB2 | 2.03 | 0.40 |
| 62:LB:220:ILE:HG12 | 62:LB:278:THR:HG23 | 2.03 | 0.40 |
| 66:L7:28:C:H1' | 66:L7:54:A:H61 | 1.86 | 0.40 |
| 69:L8:30:U:H2' | 69:L8:31:G:H8 | 1.86 | 0.40 |
| 70:L5:126:C:H2' | 70:L5:127:G:H8 | 1.86 | 0.40 |
| 70:L5:749:G:N2 | 70:L5:912:G:O2' | 2.51 | 0.40 |
| 70:L5:956:A:H8 | 70:L5:957:G:C8 | 2.39 | 0.40 |
| 70:L5:963:G:N7 | 70:L5:964:A:N6 | 2.69 | 0.40 |
| 70:L5:1683:PSU:H2' | 70:L5:1684:A:C8 | 2.56 | 0.40 |
| 70:L5:3770:PSU:H2' | 70:L5:3771:C:C6 | 2.55 | 0.40 |
| 70:L5:4088:C:H2' | 70:L5:4089:G:H8 | 1.85 | 0.40 |
| 70:L5:5006:U:H4' | 70:L5:5007:A:H5' | 2.03 | 0.40 |
| 74:S2:1019:C:H2' | 74:S2:1020:A:O4' | 2.21 | 0.40 |
| 8:SR:74:GLN:O | 8:SR:78:ARG:HG2 | 2.21 | 0.40 |
| 11:SN:121:ARG:HA | 11:SN:124:ARG:HG2 | 2.04 | 0.40 |
| 15:SH:5:SER:OG | 15:SH:6:ALA:N | 2.51 | 0.40 |
| 24:SB:38:MET:H | 24:SB:38:MET:HG2 | 1.73 | 0.40 |
| 24:SB:68:GLU:HG3 | 24:SB:85:LYS:HG2 | 2.04 | 0.40 |
| 27:LZ:127:ASN:OD1 | 27:LZ:127:ASN:N | 2.54 | 0.40 |
| 28:LY:50:ARG:NH2 | 69:L8:85:U:O4 | 2.54 | 0.40 |
| 36:Lr:119:ARG:HA | 36:Lr:119:ARG:HD3 | 1.97 | 0.40 |
| 45:Lk:51:GLU:H | 45:Lk:51:GLU:CD | 2.27 | 0.40 |
| 47:Lj:67:LEU:HD23 | 47:Lj:67:LEU:HA | 1.89 | 0.40 |
| 58:LD:286:SER:OG | 70:L5:1178:G:O2' | 2.35 | 0.40 |
| 64:LA:183:GLY:HA2 | 70:L5:1613:A:H5' | 2.04 | 0.40 |
| 65:La:132:ARG:HH21 | 70:L5:1396:G:H5'' | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:L5:512:U:O4 | 70:L5:647:G:O6 | 2.40 | 0.40 |
| 70:L5:714:G:H2' | 70:L5:715:G:H8 | 1.86 | 0.40 |
| 70:L5:1207:C:C2 | 70:L5:1208:G:C8 | 3.10 | 0.40 |
| 75:SG:153:VAL:HG23 | 75:SG:176:ILE:HD13 | 2.02 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 1 | Lm | 49/128 (38%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 2 | Ll | 48/51 (94%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 3 | Lo | 102/106 (96%) | 99 (97%) | 3 (3%) | 0 | 100 | 100 |
| 4 | SY | 121/133 (91%) | 118 (98%) | 3 (2%) | 0 | 100 | 100 |
| 5 | SX | 139/143 (97%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 6 | SW | 127/130 (98%) | 124 (98%) | 3 (2%) | 0 | 100 | 100 |
| 7 | SV | 81/83 (98%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 8 | SR | 130/135 (96%) | 125 (96%) | 5 (4%) | 0 | 100 | 100 |
| 9 | SQ | 137/146 (94%) | 127 (93%) | 10 (7%) | 0 | 100 | 100 |
| 10 | SO | 132/151 (87%) | 125 (95%) | 7 (5%) | 0 | 100 | 100 |
| 11 | SN | 148/151 (98%) | 148 (100%) | 0 | 0 | 100 | 100 |
| 12 | SL | 138/158 (87%) | 135 (98%) | 3 (2%) | 0 | 100 | 100 |
| 13 | SK | 70/165 (42%) | 69 (99%) | 1 (1%) | 0 | 100 | 100 |
| 14 | SJ | 176/194 (91%) | 168 (96%) | 8 (4%) | 0 | 100 | 100 |
| 15 | SH | 187/194 (96%) | 181 (97%) | 6 (3%) | 0 | 100 | 100 |
| 16 | Sg | 221/317 (70%) | 180 (81%) | 39 (18%) | 2 (1%) | 14 | 48 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 17 | SF | 181/204 (89%) | 173 (96%) | 8 (4%) | 0 | 100 | 100 |
| 18 | SE | 258/263 (98%) | 251 (97%) | 7 (3%) | 0 | 100 | 100 |
| 19 | Se | 47/133 (35%) | 47 (100%) | 0 | 0 | 100 | 100 |
| 20 | SD | 165/243 (68%) | 161 (98%) | 4 (2%) | 0 | 100 | 100 |
| 21 | Sd | 53/56 (95%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 22 | SC | 218/293 (74%) | 211 (97%) | 7 (3%) | 0 | 100 | 100 |
| 23 | Sc | 59/69 (86%) | 55 (93%) | 4 (7%) | 0 | 100 | 100 |
| 24 | SB | 211/264 (80%) | 205 (97%) | 6 (3%) | 0 | 100 | 100 |
| 25 | Sb | 80/84 (95%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 26 | SA | 213/295 (72%) | 206 (97%) | 7 (3%) | 0 | 100 | 100 |
| 27 | LZ | 133/136 (98%) | 128 (96%) | 5 (4%) | 0 | 100 | 100 |
| 28 | LY | 131/145 (90%) | 128 (98%) | 3 (2%) | 0 | 100 | 100 |
| 29 | LX | 117/156 (75%) | 114 (97%) | 3 (3%) | 0 | 100 | 100 |
| 30 | LW | 60/157 (38%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 31 | LV | 130/140 (93%) | 128 (98%) | 2 (2%) | 0 | 100 | 100 |
| 32 | LU | 97/128 (76%) | 91 (94%) | 6 (6%) | 0 | 100 | 100 |
| 33 | LT | 157/160 (98%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 34 | LS | 174/176 (99%) | 172 (99%) | 2 (1%) | 0 | 100 | 100 |
| 35 | LR | 179/196 (91%) | 173 (97%) | 6 (3%) | 0 | 100 | 100 |
| 36 | Lr | 121/137 (88%) | 118 (98%) | 3 (2%) | 0 | 100 | 100 |
| 37 | LQ | 185/188 (98%) | 179 (97%) | 6 (3%) | 0 | 100 | 100 |
| 38 | LP | 151/154 (98%) | 148 (98%) | 3 (2%) | 0 | 100 | 100 |
| 39 | Lp | 88/91 (97%) | 85 (97%) | 3 (3%) | 0 | 100 | 100 |
| 40 | LO | 197/203 (97%) | 193 (98%) | 4 (2%) | 0 | 100 | 100 |
| 41 | LN | 201/204 (98%) | 197 (98%) | 4 (2%) | 0 | 100 | 100 |
| 42 | Ln | 22/25 (88%) | 22 (100%) | 0 | 0 | 100 | 100 |
| 43 | LM | 134/215 (62%) | 133 (99%) | 1 (1%) | 0 | 100 | 100 |
| 44 | LL | 203/211 (96%) | 196 (97%) | 7 (3%) | 0 | 100 | 100 |
| 45 | Lk | 67/70 (96%) | 65 (97%) | 2 (3%) | 0 | 100 | 100 |
| 46 | LJ | 167/178 (94%) | 162 (97%) | 5 (3%) | 0 | 100 | 100 |
| 47 | Lj | 84/97 (87%) | 84 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 48 | LI | 199/214 (93%) | 197 (99%) | 2 (1%) | 0 | 100 | 100 |
| 49 | Li | 100/105 (95%) | 98 (98%) | 2 (2%) | 0 | 100 | 100 |
| 50 | LH | 188/192 (98%) | 185 (98%) | 3 (2%) | 0 | 100 | 100 |
| 51 | Lh | 120/123 (98%) | 115 (96%) | 5 (4%) | 0 | 100 | 100 |
| 52 | LG | 226/266 (85%) | 217 (96%) | 9 (4%) | 0 | 100 | 100 |
| 53 | Lg | 109/112 (97%) | 107 (98%) | 2 (2%) | 0 | 100 | 100 |
| 54 | LF | 223/248 (90%) | 216 (97%) | 7 (3%) | 0 | 100 | 100 |
| 55 | Lf | 107/111 (96%) | 106 (99%) | 1 (1%) | 0 | 100 | 100 |
| 56 | LE | 212/288 (74%) | 205 (97%) | 7 (3%) | 0 | 100 | 100 |
| 57 | Le | 125/135 (93%) | 122 (98%) | 3 (2%) | 0 | 100 | 100 |
| 58 | LD | 290/297 (98%) | 285 (98%) | 5 (2%) | 0 | 100 | 100 |
| 59 | Ld | 104/125 (83%) | 103 (99%) | 1 (1%) | 0 | 100 | 100 |
| 60 | LC | 357/427 (84%) | 346 (97%) | 11 (3%) | 0 | 100 | 100 |
| 61 | Lc | 96/115 (84%) | 91 (95%) | 5 (5%) | 0 | 100 | 100 |
| 62 | LB | 394/397 (99%) | 383 (97%) | 11 (3%) | 0 | 100 | 100 |
| 63 | Lb | 96/159 (60%) | 92 (96%) | 4 (4%) | 0 | 100 | 100 |
| 64 | LA | 246/257 (96%) | 238 (97%) | 8 (3%) | 0 | 100 | 100 |
| 65 | La | 144/148 (97%) | 137 (95%) | 7 (5%) | 0 | 100 | 100 |
| 68 | Sa | 97/115 (84%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 71 | SZ | 61/125 (49%) | 56 (92%) | 5 (8%) | 0 | 100 | 100 |
| 72 | ST | 125/145 (86%) | 122 (98%) | 3 (2%) | 0 | 100 | 100 |
| 73 | SP | 124/145 (86%) | 117 (94%) | 7 (6%) | 0 | 100 | 100 |
| 75 | SG | 216/249 (87%) | 210 (97%) | 6 (3%) | 0 | 100 | 100 |
| 76 | SI | 204/208 (98%) | 199 (98%) | 5 (2%) | 0 | 100 | 100 |
| 78 | SS | 136/152 (90%) | 124 (91%) | 11 (8%) | 1 (1%) | 18 | 53 |
| 80 | SU | 98/119 (82%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| All | All | 10686/12433 (86%) | 10331 (97%) | 352 (3%) | 3 (0%) | 100 | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78 | SS | 119 | PHE |
| 16 | Sg | 236 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | Sg | 282 | GLU |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 1 | Lm | 43/116 (37%) | 42 (98%) | 1 (2%) | 44 | 74 |
| 2 | Ll | 45/48 (94%) | 40 (89%) | 5 (11%) | 6 | 25 |
| 3 | Lo | 82/93 (88%) | 75 (92%) | 7 (8%) | 10 | 36 |
| 4 | SY | 75/115 (65%) | 72 (96%) | 3 (4%) | 28 | 62 |
| 5 | SX | 101/115 (88%) | 96 (95%) | 5 (5%) | 22 | 56 |
| 6 | SW | 109/113 (96%) | 101 (93%) | 8 (7%) | 13 | 42 |
| 7 | SV | 63/67 (94%) | 62 (98%) | 1 (2%) | 55 | 79 |
| 8 | SR | 83/122 (68%) | 74 (89%) | 9 (11%) | 6 | 26 |
| 9 | SQ | 66/121 (54%) | 66 (100%) | 0 | 100 | 100 |
| 10 | SO | 97/119 (82%) | 92 (95%) | 5 (5%) | 21 | 55 |
| 11 | SN | 125/131 (95%) | 123 (98%) | 2 (2%) | 55 | 79 |
| 12 | SL | 127/142 (89%) | 125 (98%) | 2 (2%) | 55 | 79 |
| 13 | SK | 24/136 (18%) | 24 (100%) | 0 | 100 | 100 |
| 14 | SJ | 145/168 (86%) | 140 (97%) | 5 (3%) | 32 | 66 |
| 15 | SH | 139/174 (80%) | 131 (94%) | 8 (6%) | 18 | 51 |
| 16 | Sg | 17/275 (6%) | 17 (100%) | 0 | 100 | 100 |
| 17 | SF | 117/170 (69%) | 114 (97%) | 3 (3%) | 40 | 72 |
| 18 | SE | 215/225 (96%) | 210 (98%) | 5 (2%) | 44 | 74 |
| 19 | Se | 39/104 (38%) | 37 (95%) | 2 (5%) | 21 | 55 |
| 20 | SD | 74/202 (37%) | 68 (92%) | 6 (8%) | 11 | 38 |
| 21 | Sd | 41/49 (84%) | 38 (93%) | 3 (7%) | 13 | 42 |
| 22 | SC | 182/225 (81%) | 174 (96%) | 8 (4%) | 25 | 60 |
| 23 | Sc | 42/62 (68%) | 41 (98%) | 1 (2%) | 43 | 73 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 24 | SB | 183/231 (79%) | 173 (94%) | 10 (6%) | 19 | 53 |
| 25 | Sb | 68/76 (90%) | 67 (98%) | 1 (2%) | 57 | 80 |
| 26 | SA | 169/243 (70%) | 165 (98%) | 4 (2%) | 43 | 73 |
| 27 | LZ | 113/118 (96%) | 105 (93%) | 8 (7%) | 13 | 43 |
| 28 | LY | 111/135 (82%) | 110 (99%) | 1 (1%) | 70 | 85 |
| 29 | LX | 107/133 (80%) | 102 (95%) | 5 (5%) | 23 | 58 |
| 30 | LW | 54/126 (43%) | 51 (94%) | 3 (6%) | 19 | 52 |
| 31 | LV | 102/107 (95%) | 97 (95%) | 5 (5%) | 22 | 56 |
| 32 | LU | 87/115 (76%) | 83 (95%) | 4 (5%) | 24 | 58 |
| 33 | LT | 139/140 (99%) | 136 (98%) | 3 (2%) | 45 | 74 |
| 34 | LS | 156/157 (99%) | 150 (96%) | 6 (4%) | 29 | 63 |
| 35 | LR | 147/175 (84%) | 145 (99%) | 2 (1%) | 59 | 80 |
| 36 | Lr | 107/121 (88%) | 104 (97%) | 3 (3%) | 38 | 70 |
| 37 | LQ | 162/165 (98%) | 156 (96%) | 6 (4%) | 30 | 64 |
| 38 | LP | 131/135 (97%) | 129 (98%) | 2 (2%) | 57 | 80 |
| 39 | Lp | 72/74 (97%) | 70 (97%) | 2 (3%) | 38 | 70 |
| 40 | LO | 167/174 (96%) | 162 (97%) | 5 (3%) | 36 | 69 |
| 41 | LN | 170/172 (99%) | 167 (98%) | 3 (2%) | 51 | 77 |
| 42 | Ln | 23/24 (96%) | 22 (96%) | 1 (4%) | 26 | 60 |
| 43 | LM | 115/161 (71%) | 113 (98%) | 2 (2%) | 53 | 78 |
| 44 | LL | 166/177 (94%) | 160 (96%) | 6 (4%) | 31 | 65 |
| 45 | Lk | 61/65 (94%) | 57 (93%) | 4 (7%) | 15 | 46 |
| 46 | LJ | 136/149 (91%) | 129 (95%) | 7 (5%) | 21 | 55 |
| 47 | Lj | 72/80 (90%) | 69 (96%) | 3 (4%) | 26 | 61 |
| 48 | LI | 170/181 (94%) | 168 (99%) | 2 (1%) | 63 | 82 |
| 49 | Li | 80/89 (90%) | 77 (96%) | 3 (4%) | 29 | 63 |
| 50 | LH | 164/171 (96%) | 162 (99%) | 2 (1%) | 63 | 82 |
| 51 | Lh | 108/110 (98%) | 104 (96%) | 4 (4%) | 30 | 64 |
| 52 | LG | 184/223 (82%) | 179 (97%) | 5 (3%) | 39 | 71 |
| 53 | Lg | 92/96 (96%) | 88 (96%) | 4 (4%) | 26 | 60 |
| 54 | LF | 186/215 (86%) | 183 (98%) | 3 (2%) | 55 | 79 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 55 | Lf | 86/90 (96%) | 85 (99%) | 1 (1%) | 63 | 82 |
| 56 | LE | 184/252 (73%) | 177 (96%) | 7 (4%) | 29 | 63 |
| 57 | Le | 113/121 (93%) | 110 (97%) | 3 (3%) | 39 | 71 |
| 58 | LD | 239/250 (96%) | 230 (96%) | 9 (4%) | 29 | 63 |
| 59 | Ld | 85/110 (77%) | 83 (98%) | 2 (2%) | 43 | 73 |
| 60 | LC | 299/348 (86%) | 293 (98%) | 6 (2%) | 48 | 76 |
| 61 | Lc | 82/97 (84%) | 77 (94%) | 5 (6%) | 17 | 49 |
| 62 | LB | 339/346 (98%) | 332 (98%) | 7 (2%) | 47 | 75 |
| 63 | Lb | 81/125 (65%) | 77 (95%) | 4 (5%) | 22 | 56 |
| 64 | LA | 188/198 (95%) | 186 (99%) | 2 (1%) | 65 | 83 |
| 65 | La | 117/120 (98%) | 114 (97%) | 3 (3%) | 40 | 72 |
| 68 | Sa | 82/98 (84%) | 79 (96%) | 3 (4%) | 30 | 64 |
| 71 | SZ | 22/103 (21%) | 22 (100%) | 0 | 100 | 100 |
| 72 | ST | 52/115 (45%) | 50 (96%) | 2 (4%) | 29 | 63 |
| 73 | SP | 51/130 (39%) | 45 (88%) | 6 (12%) | 5 | 22 |
| 75 | SG | 163/218 (75%) | 152 (93%) | 11 (7%) | 15 | 46 |
| 76 | SI | 168/180 (93%) | 159 (95%) | 9 (5%) | 20 | 53 |
| 78 | SS | 59/132 (45%) | 54 (92%) | 5 (8%) | 10 | 36 |
| 80 | SU | 92/107 (86%) | 86 (94%) | 6 (6%) | 15 | 47 |
| All | All | 8355/10570 (79%) | 8056 (96%) | 299 (4%) | 32 | 65 |

All (299) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Lm | 79 | GLU |
| 2 | Ll | 9 | ILE |
| 2 | Ll | 27 | ILE |
| 2 | Ll | 34 | ILE |
| 2 | Ll | 36 | ARG |
| 2 | Ll | 47 | THR |
| 3 | Lo | 4 | VAL |
| 3 | Lo | 10 | THR |
| 3 | Lo | 23 | VAL |
| 3 | Lo | 28 | LYS |
| 3 | Lo | 68 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | Lo | 93 | LEU |
| 3 | Lo | 99 | ARG |
| 4 | SY | 26 | ASP |
| 4 | SY | 69 | THR |
| 4 | SY | 117 | VAL |
| 5 | SX | 7 | LEU |
| 5 | SX | 19 | ASP |
| 5 | SX | 66 | ILE |
| 5 | SX | 82 | THR |
| 5 | SX | 105 | PHE |
| 6 | SW | 27 | ILE |
| 6 | SW | 69 | LEU |
| 6 | SW | 80 | ASP |
| 6 | SW | 81 | VAL |
| 6 | SW | 83 | LEU |
| 6 | SW | 104 | LEU |
| 6 | SW | 105 | THR |
| 6 | SW | 120 | HIS |
| 7 | SV | 11 | LEU |
| 8 | SR | 22 | THR |
| 8 | SR | 24 | LEU |
| 8 | SR | 30 | THR |
| 8 | SR | 85 | VAL |
| 8 | SR | 87 | GLU |
| 8 | SR | 91 | LEU |
| 8 | SR | 105 | MET |
| 8 | SR | 116 | ASN |
| 8 | SR | 124 | VAL |
| 10 | SO | 46 | ASP |
| 10 | SO | 88 | LEU |
| 10 | SO | 97 | LEU |
| 10 | SO | 116 | LEU |
| 10 | SO | 151 | LEU |
| 11 | SN | 83 | ASP |
| 11 | SN | 125 | LEU |
| 12 | SL | 18 | GLN |
| 12 | SL | 125 | ILE |
| 14 | SJ | 15 | THR |
| 14 | SJ | 25 | LEU |
| 14 | SJ | 26 | ASP |
| 14 | SJ | 50 | LEU |
| 14 | SJ | 92 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | SH | 20 | GLU |
| 15 | SH | 30 | LEU |
| 15 | SH | 43 | LEU |
| 15 | SH | 60 | ILE |
| 15 | SH | 69 | LEU |
| 15 | SH | 80 | VAL |
| 15 | SH | 92 | VAL |
| 15 | SH | 153 | LEU |
| 17 | SF | 19 | LEU |
| 17 | SF | 76 | MET |
| 17 | SF | 124 | ASP |
| 18 | SE | 12 | VAL |
| 18 | SE | 80 | ILE |
| 18 | SE | 102 | ILE |
| 18 | SE | 133 | THR |
| 18 | SE | 173 | ILE |
| 19 | Se | 103 | THR |
| 19 | Se | 132 | ASN |
| 20 | SD | 21 | LEU |
| 20 | SD | 137 | VAL |
| 20 | SD | 141 | LYS |
| 20 | SD | 165 | ASN |
| 20 | SD | 170 | THR |
| 20 | SD | 186 | VAL |
| 21 | Sd | 30 | LEU |
| 21 | Sd | 36 | LEU |
| 21 | Sd | 53 | ILE |
| 22 | SC | 63 | VAL |
| 22 | SC | 172 | ASN |
| 22 | SC | 174 | ILE |
| 22 | SC | 184 | VAL |
| 22 | SC | 191 | VAL |
| 22 | SC | 192 | LEU |
| 22 | SC | 233 | LEU |
| 22 | SC | 259 | THR |
| 23 | Sc | 51 | ARG |
| 24 | SB | 47 | THR |
| 24 | SB | 52 | THR |
| 24 | SB | 57 | ILE |
| 24 | SB | 91 | VAL |
| 24 | SB | 92 | GLN |
| 24 | SB | 128 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | SB | 131 | ASP |
| 24 | SB | 135 | LEU |
| 24 | SB | 168 | MET |
| 24 | SB | 188 | LEU |
| 25 | Sb | 37 | CYS |
| 26 | SA | 46 | ILE |
| 26 | SA | 134 | LEU |
| 26 | SA | 177 | MET |
| 26 | SA | 206 | ASP |
| 27 | LZ | 10 | VAL |
| 27 | LZ | 27 | LYS |
| 27 | LZ | 53 | VAL |
| 27 | LZ | 87 | VAL |
| 27 | LZ | 89 | ILE |
| 27 | LZ | 103 | ASP |
| 27 | LZ | 106 | LEU |
| 27 | LZ | 113 | GLU |
| 28 | LY | 87 | ARG |
| 29 | LX | 45 | THR |
| 29 | LX | 81 | LEU |
| 29 | LX | 82 | THR |
| 29 | LX | 116 | LEU |
| 29 | LX | 126 | THR |
| 30 | LW | 30 | GLN |
| 30 | LW | 37 | GLU |
| 30 | LW | 57 | ARG |
| 31 | LV | 15 | ARG |
| 31 | LV | 28 | CYS |
| 31 | LV | 57 | VAL |
| 31 | LV | 71 | GLU |
| 31 | LV | 128 | LEU |
| 32 | LU | 43 | LEU |
| 32 | LU | 61 | VAL |
| 32 | LU | 62 | THR |
| 32 | LU | 69 | LYS |
| 33 | LT | 38 | ASP |
| 33 | LT | 111 | GLU |
| 33 | LT | 124 | THR |
| 34 | LS | 51 | LEU |
| 34 | LS | 62 | VAL |
| 34 | LS | 75 | VAL |
| 34 | LS | 90 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | LS | 150 | ILE |
| 34 | LS | 170 | LYS |
| 35 | LR | 3 | MET |
| 35 | LR | 27 | ASN |
| 36 | Lr | 5 | LEU |
| 36 | Lr | 99 | LYS |
| 36 | Lr | 124 | VAL |
| 37 | LQ | 42 | THR |
| 37 | LQ | 90 | VAL |
| 37 | LQ | 92 | VAL |
| 37 | LQ | 98 | LEU |
| 37 | LQ | 108 | ARG |
| 37 | LQ | 128 | LEU |
| 38 | LP | 75 | GLN |
| 38 | LP | 107 | LEU |
| 39 | Lp | 22 | LEU |
| 39 | Lp | 74 | THR |
| 40 | LO | 6 | VAL |
| 40 | LO | 43 | ILE |
| 40 | LO | 159 | LYS |
| 40 | LO | 174 | LEU |
| 40 | LO | 196 | LEU |
| 41 | LN | 10 | LEU |
| 41 | LN | 43 | THR |
| 41 | LN | 60 | VAL |
| 42 | Ln | 21 | ARG |
| 43 | LM | 33 | GLN |
| 43 | LM | 43 | THR |
| 44 | LL | 67 | HIS |
| 44 | LL | 70 | VAL |
| 44 | LL | 149 | GLN |
| 44 | LL | 160 | VAL |
| 44 | LL | 171 | GLU |
| 44 | LL | 197 | LYS |
| 45 | Lk | 26 | LYS |
| 45 | Lk | 32 | VAL |
| 45 | Lk | 36 | VAL |
| 45 | Lk | 56 | LEU |
| 46 | LJ | 17 | ILE |
| 46 | LJ | 49 | VAL |
| 46 | LJ | 56 | THR |
| 46 | LJ | 95 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 46 | LJ | 110 | GLN |
| 46 | LJ | 112 | HIS |
| 46 | LJ | 150 | CYS |
| 47 | Lj | 33 | THR |
| 47 | Lj | 57 | ASN |
| 47 | Lj | 69 | ILE |
| 48 | LI | 66 | GLU |
| 48 | LI | 148 | VAL |
| 49 | Li | 43 | MET |
| 49 | Li | 79 | THR |
| 49 | Li | 85 | ARG |
| 50 | LH | 135 | SER |
| 50 | LH | 163 | GLN |
| 51 | Lh | 71 | LYS |
| 51 | Lh | 94 | ARG |
| 51 | Lh | 112 | ARG |
| 51 | Lh | 116 | LEU |
| 52 | LG | 97 | LYS |
| 52 | LG | 108 | GLN |
| 52 | LG | 113 | ARG |
| 52 | LG | 114 | LEU |
| 52 | LG | 155 | VAL |
| 53 | Lg | 54[A] | ARG |
| 53 | Lg | 54[B] | ARG |
| 53 | Lg | 73 | HIS |
| 53 | Lg | 86 | CYS |
| 54 | LF | 50 | ILE |
| 54 | LF | 187 | MET |
| 54 | LF | 239 | GLN |
| 55 | Lf | 105 | LEU |
| 56 | LE | 49 | VAL |
| 56 | LE | 93 | THR |
| 56 | LE | 121 | VAL |
| 56 | LE | 163 | VAL |
| 56 | LE | 179 | LEU |
| 56 | LE | 287 | VAL |
| 56 | LE | 288 | PHE |
| 57 | Le | 26 | ASP |
| 57 | Le | 78 | LEU |
| 57 | Le | 94 | SER |
| 58 | LD | 36 | LEU |
| 58 | LD | 93 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58 | LD | 111 | ASN |
| 58 | LD | 155 | THR |
| 58 | LD | 157 | ASN |
| 58 | LD | 194 | VAL |
| 58 | LD | 222 | GLN |
| 58 | LD | 231 | VAL |
| 58 | LD | 235 | MET |
| 59 | Ld | 20 | VAL |
| 59 | Ld | 122 | VAL |
| 60 | LC | 10 | VAL |
| 60 | LC | 144 | ILE |
| 60 | LC | 174 | LEU |
| 60 | LC | 254 | GLU |
| 60 | LC | 289 | LEU |
| 60 | LC | 308 | LYS |
| 61 | Lc | 18 | LEU |
| 61 | Lc | 55 | LEU |
| 61 | Lc | 68 | LYS |
| 61 | Lc | 93 | THR |
| 61 | Lc | 94 | LEU |
| 62 | LB | 69 | LYS |
| 62 | LB | 90 | VAL |
| 62 | LB | 149 | ASP |
| 62 | LB | 199 | GLU |
| 62 | LB | 218 | ASP |
| 62 | LB | 348 | ARG |
| 62 | LB | 360 | LEU |
| 63 | Lb | 9 | THR |
| 63 | Lb | 106 | LYS |
| 63 | Lb | 107 | ARG |
| 63 | Lb | 112 | ILE |
| 64 | LA | 80 | GLU |
| 64 | LA | 208 | GLU |
| 65 | La | 8 | THR |
| 65 | La | 15 | VAL |
| 65 | La | 125 | LYS |
| 68 | Sa | 15 | ARG |
| 68 | Sa | 19 | GLN |
| 68 | Sa | 74 | CYS |
| 72 | ST | 23 | LYS |
| 72 | ST | 104 | LEU |
| 73 | SP | 16 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 73 | SP | 35 | GLN |
| 73 | SP | 80 | LEU |
| 73 | SP | 89 | MET |
| 73 | SP | 94 | VAL |
| 73 | SP | 96 | VAL |
| 75 | SG | 16 | ILE |
| 75 | SG | 65 | GLN |
| 75 | SG | 69 | THR |
| 75 | SG | 97 | VAL |
| 75 | SG | 106 | LEU |
| 75 | SG | 112 | VAL |
| 75 | SG | 114 | VAL |
| 75 | SG | 127 | THR |
| 75 | SG | 136 | LYS |
| 75 | SG | 144 | LEU |
| 75 | SG | 177 | GLN |
| 76 | SI | 7 | ASN |
| 76 | SI | 18 | ARG |
| 76 | SI | 22 | HIS |
| 76 | SI | 76 | THR |
| 76 | SI | 82 | VAL |
| 76 | SI | 121 | LEU |
| 76 | SI | 137 | LEU |
| 76 | SI | 143 | LYS |
| 76 | SI | 147 | LYS |
| 78 | SS | 13 | LEU |
| 78 | SS | 16 | LEU |
| 78 | SS | 83 | PHE |
| 78 | SS | 111 | LEU |
| 78 | SS | 139 | THR |
| 80 | SU | 22 | ILE |
| 80 | SU | 39 | LEU |
| 80 | SU | 48 | LEU |
| 80 | SU | 89 | ILE |
| 80 | SU | 106 | ILE |
| 80 | SU | 114 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | Ll | 4 | HIS |
| 3 | Lo | 25 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | SY | 22 | GLN |
| 5 | SX | 16 | HIS |
| 5 | SX | 31 | HIS |
| 5 | SX | 63 | ASN |
| 7 | SV | 33 | GLN |
| 8 | SR | 29 | HIS |
| 11 | SN | 49 | GLN |
| 11 | SN | 105 | ASN |
| 12 | SL | 11 | GLN |
| 12 | SL | 94 | HIS |
| 12 | SL | 112 | HIS |
| 12 | SL | 141 | ASN |
| 13 | SK | 28 | HIS |
| 13 | SK | 32 | HIS |
| 14 | SJ | 75 | ASN |
| 14 | SJ | 113 | GLN |
| 14 | SJ | 154 | GLN |
| 17 | SF | 36 | GLN |
| 18 | SE | 17 | HIS |
| 18 | SE | 36 | HIS |
| 18 | SE | 138 | HIS |
| 20 | SD | 159 | HIS |
| 21 | Sd | 3 | HIS |
| 25 | Sb | 9 | HIS |
| 25 | Sb | 51 | GLN |
| 26 | SA | 9 | GLN |
| 27 | LZ | 132 | GLN |
| 28 | LY | 20 | ASN |
| 29 | LX | 105 | ASN |
| 29 | LX | 111 | GLN |
| 32 | LU | 94 | ASN |
| 33 | LT | 66 | ASN |
| 33 | LT | 131 | GLN |
| 33 | LT | 144 | ASN |
| 34 | LS | 108 | GLN |
| 36 | Lr | 4 | HIS |
| 36 | Lr | 6 | GLN |
| 36 | Lr | 31 | ASN |
| 36 | Lr | 41 | ASN |
| 37 | LQ | 7 | HIS |
| 37 | LQ | 162 | HIS |
| 38 | LP | 97 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | LP | 133 | HIS |
| 40 | LO | 63 | ASN |
| 40 | LO | 180 | GLN |
| 41 | LN | 32 | GLN |
| 41 | LN | 109 | HIS |
| 43 | LM | 33 | GLN |
| 43 | LM | 66 | HIS |
| 43 | LM | 70 | GLN |
| 44 | LL | 104 | ASN |
| 44 | LL | 175 | ASN |
| 44 | LL | 188 | ASN |
| 46 | LJ | 71 | HIS |
| 47 | Lj | 13 | ASN |
| 50 | LH | 140 | GLN |
| 50 | LH | 163 | GLN |
| 50 | LH | 188 | GLN |
| 52 | LG | 38 | ASN |
| 52 | LG | 225 | ASN |
| 53 | Lg | 100 | GLN |
| 54 | LF | 80 | ASN |
| 54 | LF | 99 | ASN |
| 54 | LF | 119 | ASN |
| 54 | LF | 126 | ASN |
| 55 | Lf | 99 | HIS |
| 56 | LE | 157 | HIS |
| 57 | Le | 52 | GLN |
| 57 | Le | 81 | ASN |
| 58 | LD | 131 | ASN |
| 58 | LD | 267 | ASN |
| 58 | LD | 282 | GLN |
| 59 | Ld | 34 | HIS |
| 60 | LC | 116 | ASN |
| 60 | LC | 142 | HIS |
| 60 | LC | 212 | ASN |
| 60 | LC | 362 | GLN |
| 62 | LB | 123 | HIS |
| 62 | LB | 138 | GLN |
| 62 | LB | 203 | GLN |
| 63 | Lb | 11 | ASN |
| 63 | Lb | 60 | ASN |
| 64 | LA | 86 | GLN |
| 65 | La | 120 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68 | Sa | 17 | HIS |
| 72 | ST | 11 | GLN |
| 76 | SI | 167 | GLN |
| 78 | SS | 135 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 66 | L7 | 118/119 (99%) | 11 (9%) | 0 |
| 67 | Pt | 76/77 (98%) | 16 (21%) | 0 |
| 69 | L8 | 151/156 (96%) | 26 (17%) | 0 |
| 70 | L5 | 3414/5069 (67%) | 552 (16%) | 10 (0%) |
| 74 | S2 | 1550/1869 (82%) | 269 (17%) | 6 (0%) |
| 77 | S6 | 55/75 (73%) | 18 (32%) | 1 (1%) |
| 79 | mR | 6/27 (22%) | 2 (33%) | 0 |
| All | All | 5370/7392 (72%) | 894 (16%) | 17 (0%) |

All (894) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66 | L7 | 7 | G |
| 66 | L7 | 25 | G |
| 66 | L7 | 31 | G |
| 66 | L7 | 33 | U |
| 66 | L7 | 53 | U |
| 66 | L7 | 54 | A |
| 66 | L7 | 64 | G |
| 66 | L7 | 97 | G |
| 66 | L7 | 100 | A |
| 66 | L7 | 102 | U |
| 66 | L7 | 110 | G |
| 67 | Pt | 9 | G |
| 67 | Pt | 15 | G |
| 67 | Pt | 16 | C |
| 67 | Pt | 17 | C |
| 67 | Pt | 18 | C |
| 67 | Pt | 19 | G |
| 67 | Pt | 20 | G |
| 67 | Pt | 21 | H2U |
| 67 | Pt | 22 | A |
| 67 | Pt | 32 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 67 | Pt | 47 | G7M |
| 67 | Pt | 48 | U |
| 67 | Pt | 49 | C |
| 67 | Pt | 62 | C |
| 67 | Pt | 71 | G |
| 67 | Pt | 72 | C |
| 69 | L8 | 23 | C |
| 69 | L8 | 25 | G |
| 69 | L8 | 34 | U |
| 69 | L8 | 35 | C |
| 69 | L8 | 51 | U |
| 69 | L8 | 59 | A |
| 69 | L8 | 62 | A |
| 69 | L8 | 63 | U |
| 69 | L8 | 80 | A |
| 69 | L8 | 84 | A |
| 69 | L8 | 85 | U |
| 69 | L8 | 87 | G |
| 69 | L8 | 103 | A |
| 69 | L8 | 105 | C |
| 69 | L8 | 106 | G |
| 69 | L8 | 110 | U |
| 69 | L8 | 111 | U |
| 69 | L8 | 114 | G |
| 69 | L8 | 123 | U |
| 69 | L8 | 124 | U |
| 69 | L8 | 125 | C |
| 69 | L8 | 127 | U |
| 69 | L8 | 141 | C |
| 69 | L8 | 142 | U |
| 69 | L8 | 150 | C |
| 69 | L8 | 156 | U |
| 70 | L5 | 5 | A |
| 70 | L5 | 9 | C |
| 70 | L5 | 15 | A |
| 70 | L5 | 39 | A |
| 70 | L5 | 42 | A |
| 70 | L5 | 48 | G |
| 70 | L5 | 56 | A |
| 70 | L5 | 59 | A |
| 70 | L5 | 64 | A |
| 70 | L5 | 65 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 70 | L5 | 71 | C |
| 70 | L5 | 85 | G |
| 70 | L5 | 91 | G |
| 70 | L5 | 98 | A |
| 70 | L5 | 108 | A |
| 70 | L5 | 110 | C |
| 70 | L5 | 112 | C |
| 70 | L5 | 119 | G |
| 70 | L5 | 120 | A |
| 70 | L5 | 131 | C |
| 70 | L5 | 139 | G |
| 70 | L5 | 159 | C |
| 70 | L5 | 160 | G |
| 70 | L5 | 161 | G |
| 70 | L5 | 162 | A |
| 70 | L5 | 168 | C |
| 70 | L5 | 169 | G |
| 70 | L5 | 172 | C |
| 70 | L5 | 173 | C |
| 70 | L5 | 174 | C |
| 70 | L5 | 175 | C |
| 70 | L5 | 200 | U |
| 70 | L5 | 207 | G |
| 70 | L5 | 209 | U |
| 70 | L5 | 216 | C |
| 70 | L5 | 217 | C |
| 70 | L5 | 218 | A |
| 70 | L5 | 219 | G |
| 70 | L5 | 220 | C |
| 70 | L5 | 234 | G |
| 70 | L5 | 253 | G |
| 70 | L5 | 259 | C |
| 70 | L5 | 266 | C |
| 70 | L5 | 273 | U |
| 70 | L5 | 274 | C |
| 70 | L5 | 278 | G |
| 70 | L5 | 280 | G |
| 70 | L5 | 297 | U |
| 70 | L5 | 306 | A |
| 70 | L5 | 316 | U |
| 70 | L5 | 340 | C |
| 70 | L5 | 350 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 70 | L5 | 373 | G |
| 70 | L5 | 387 | G |
| 70 | L5 | 409 | G |
| 70 | L5 | 410 | A |
| 70 | L5 | 412 | G |
| 70 | L5 | 414 | C |
| 70 | L5 | 417 | G |
| 70 | L5 | 431 | G |
| 70 | L5 | 432 | U |
| 70 | L5 | 448 | G |
| 70 | L5 | 449 | C |
| 70 | L5 | 451 | C |
| 70 | L5 | 452 | A |
| 70 | L5 | 453 | G |
| 70 | L5 | 483 | C |
| 70 | L5 | 484 | U |
| 70 | L5 | 487 | G |
| 70 | L5 | 489 | C |
| 70 | L5 | 491 | G |
| 70 | L5 | 492 | U |
| 70 | L5 | 502 | C |
| 70 | L5 | 503 | C |
| 70 | L5 | 504 | G |
| 70 | L5 | 510 | U |
| 70 | L5 | 513 | U |
| 70 | L5 | 514 | U |
| 70 | L5 | 644 | G |
| 70 | L5 | 647 | G |
| 70 | L5 | 648 | G |
| 70 | L5 | 661 | C |
| 70 | L5 | 665 | C |
| 70 | L5 | 666 | G |
| 70 | L5 | 667 | A |
| 70 | L5 | 669 | C |
| 70 | L5 | 685 | C |
| 70 | L5 | 696 | C |
| 70 | L5 | 704 | C |
| 70 | L5 | 705 | G |
| 70 | L5 | 731 | G |
| 70 | L5 | 738 | C |
| 70 | L5 | 739 | G |
| 70 | L5 | 740 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 742 | G |
| 70 | L5 | 746 | A |
| 70 | L5 | 760 | G |
| 70 | L5 | 904 | C |
| 70 | L5 | 913 | U |
| 70 | L5 | 914 | U |
| 70 | L5 | 915 | A |
| 70 | L5 | 916 | C |
| 70 | L5 | 917 | A |
| 70 | L5 | 918 | G |
| 70 | L5 | 925 | C |
| 70 | L5 | 926 | G |
| 70 | L5 | 932 | A |
| 70 | L5 | 933 | G |
| 70 | L5 | 935 | A |
| 70 | L5 | 944 | A |
| 70 | L5 | 958 | G |
| 70 | L5 | 959 | G |
| 70 | L5 | 960 | A |
| 70 | L5 | 962 | C |
| 70 | L5 | 963 | G |
| 70 | L5 | 965 | G |
| 70 | L5 | 966 | A |
| 70 | L5 | 967 | C |
| 70 | L5 | 968 | C |
| 70 | L5 | 969 | C |
| 70 | L5 | 970 | G |
| 70 | L5 | 977 | C |
| 70 | L5 | 982 | U |
| 70 | L5 | 1070 | G |
| 70 | L5 | 1072 | C |
| 70 | L5 | 1084 | C |
| 70 | L5 | 1170 | G |
| 70 | L5 | 1181 | C |
| 70 | L5 | 1182 | C |
| 70 | L5 | 1183 | C |
| 70 | L5 | 1199 | G |
| 70 | L5 | 1200 | G |
| 70 | L5 | 1210 | C |
| 70 | L5 | 1211 | G |
| 70 | L5 | 1214 | C |
| 70 | L5 | 1215 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 1216 | C |
| 70 | L5 | 1220 | G |
| 70 | L5 | 1241 | C |
| 70 | L5 | 1254 | A |
| 70 | L5 | 1255 | A |
| 70 | L5 | 1258 | G |
| 70 | L5 | 1261 | G |
| 70 | L5 | 1266 | G |
| 70 | L5 | 1270 | A |
| 70 | L5 | 1271 | G |
| 70 | L5 | 1273 | G |
| 70 | L5 | 1276 | C |
| 70 | L5 | 1277 | G |
| 70 | L5 | 1284 | G |
| 70 | L5 | 1285 | U |
| 70 | L5 | 1287 | G |
| 70 | L5 | 1293 | G |
| 70 | L5 | 1295 | C |
| 70 | L5 | 1296 | G |
| 70 | L5 | 1301 | C |
| 70 | L5 | 1302 | U |
| 70 | L5 | 1303 | A |
| 70 | L5 | 1304 | C |
| 70 | L5 | 1326 | A2M |
| 70 | L5 | 1337 | A |
| 70 | L5 | 1354 | A |
| 70 | L5 | 1359 | G |
| 70 | L5 | 1366 | G |
| 70 | L5 | 1378 | C |
| 70 | L5 | 1379 | C |
| 70 | L5 | 1387 | A |
| 70 | L5 | 1397 | A |
| 70 | L5 | 1398 | A |
| 70 | L5 | 1400 | G |
| 70 | L5 | 1401 | C |
| 70 | L5 | 1402 | C |
| 70 | L5 | 1415 | G |
| 70 | L5 | 1427 | A |
| 70 | L5 | 1439 | C |
| 70 | L5 | 1443 | A |
| 70 | L5 | 1452 | A |
| 70 | L5 | 1454 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 1476 | C |
| 70 | L5 | 1477 | C |
| 70 | L5 | 1478 | C |
| 70 | L5 | 1479 | G |
| 70 | L5 | 1481 | C |
| 70 | L5 | 1483 | C |
| 70 | L5 | 1484 | G |
| 70 | L5 | 1485 | C |
| 70 | L5 | 1486 | C |
| 70 | L5 | 1498 | G |
| 70 | L5 | 1502 | G |
| 70 | L5 | 1523 | A |
| 70 | L5 | 1525 | A |
| 70 | L5 | 1534 | A2M |
| 70 | L5 | 1535 | C |
| 70 | L5 | 1547 | A |
| 70 | L5 | 1564 | A |
| 70 | L5 | 1566 | C |
| 70 | L5 | 1574 | G |
| 70 | L5 | 1578 | U |
| 70 | L5 | 1591 | U |
| 70 | L5 | 1596 | U |
| 70 | L5 | 1612 | G |
| 70 | L5 | 1614 | C |
| 70 | L5 | 1624 | G |
| 70 | L5 | 1625 | OMG |
| 70 | L5 | 1631 | A |
| 70 | L5 | 1633 | G |
| 70 | L5 | 1634 | A |
| 70 | L5 | 1640 | C |
| 70 | L5 | 1641 | G |
| 70 | L5 | 1654 | G |
| 70 | L5 | 1661 | C |
| 70 | L5 | 1676 | C |
| 70 | L5 | 1677 | PSU |
| 70 | L5 | 1678 | C |
| 70 | L5 | 1691 | G |
| 70 | L5 | 1697 | G |
| 70 | L5 | 1698 | C |
| 70 | L5 | 1703 | C |
| 70 | L5 | 1704 | C |
| 70 | L5 | 1720 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 1721 | G |
| 70 | L5 | 1734 | G |
| 70 | L5 | 1755 | C |
| 70 | L5 | 1757 | U |
| 70 | L5 | 1759 | G |
| 70 | L5 | 1773 | U |
| 70 | L5 | 1774 | C |
| 70 | L5 | 1776 | A |
| 70 | L5 | 1787 | A |
| 70 | L5 | 1794 | A |
| 70 | L5 | 1803 | G |
| 70 | L5 | 1804 | A |
| 70 | L5 | 1805 | A |
| 70 | L5 | 1806 | G |
| 70 | L5 | 1821 | G |
| 70 | L5 | 1836 | G |
| 70 | L5 | 1837 | A |
| 70 | L5 | 1842 | G |
| 70 | L5 | 1843 | A |
| 70 | L5 | 1855 | G |
| 70 | L5 | 1869 | G |
| 70 | L5 | 1889 | U |
| 70 | L5 | 1897 | A |
| 70 | L5 | 1915 | C |
| 70 | L5 | 1918 | U |
| 70 | L5 | 1919 | G |
| 70 | L5 | 1921 | C |
| 70 | L5 | 1922 | G |
| 70 | L5 | 1925 | G |
| 70 | L5 | 1931 | C |
| 70 | L5 | 1932 | A |
| 70 | L5 | 1940 | G |
| 70 | L5 | 1948 | G |
| 70 | L5 | 1951 | G |
| 70 | L5 | 1959 | U |
| 70 | L5 | 1969 | G |
| 70 | L5 | 2025 | A |
| 70 | L5 | 2026 | A |
| 70 | L5 | 2046 | G |
| 70 | L5 | 2048 | U |
| 70 | L5 | 2055 | G |
| 70 | L5 | 2056 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 2069 | A |
| 70 | L5 | 2084 | C |
| 70 | L5 | 2085 | G |
| 70 | L5 | 2092 | G |
| 70 | L5 | 2093 | A |
| 70 | L5 | 2095 | A |
| 70 | L5 | 2097 | U |
| 70 | L5 | 2098 | G |
| 70 | L5 | 2102 | G |
| 70 | L5 | 2108 | G |
| 70 | L5 | 2258 | C |
| 70 | L5 | 2260 | C |
| 70 | L5 | 2261 | G |
| 70 | L5 | 2279 | A |
| 70 | L5 | 2289 | C |
| 70 | L5 | 2300 | A |
| 70 | L5 | 2301 | G |
| 70 | L5 | 2306 | G |
| 70 | L5 | 2313 | A |
| 70 | L5 | 2331 | G |
| 70 | L5 | 2348 | G |
| 70 | L5 | 2351 | OMC |
| 70 | L5 | 2360 | A |
| 70 | L5 | 2381 | A |
| 70 | L5 | 2395 | A |
| 70 | L5 | 2397 | G |
| 70 | L5 | 2398 | U |
| 70 | L5 | 2417 | A |
| 70 | L5 | 2421 | G |
| 70 | L5 | 2425 | U |
| 70 | L5 | 2447 | U |
| 70 | L5 | 2450 | G |
| 70 | L5 | 2453 | A |
| 70 | L5 | 2469 | C |
| 70 | L5 | 2471 | G |
| 70 | L5 | 2474 | G |
| 70 | L5 | 2503 | G |
| 70 | L5 | 2513 | A |
| 70 | L5 | 2518 | G |
| 70 | L5 | 2519 | U |
| 70 | L5 | 2520 | C |
| 70 | L5 | 2529 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 2542 | G |
| 70 | L5 | 2554 | U |
| 70 | L5 | 2573 | A |
| 70 | L5 | 2577 | C |
| 70 | L5 | 2587 | A |
| 70 | L5 | 2589 | C |
| 70 | L5 | 2601 | A |
| 70 | L5 | 2602 | G |
| 70 | L5 | 2627 | C |
| 70 | L5 | 2653 | C |
| 70 | L5 | 2658 | G |
| 70 | L5 | 2659 | A |
| 70 | L5 | 2669 | C |
| 70 | L5 | 2681 | G |
| 70 | L5 | 2687 | U |
| 70 | L5 | 2688 | G |
| 70 | L5 | 2694 | G |
| 70 | L5 | 2695 | A |
| 70 | L5 | 2696 | A |
| 70 | L5 | 2711 | G |
| 70 | L5 | 2714 | G |
| 70 | L5 | 2724 | G |
| 70 | L5 | 2726 | G |
| 70 | L5 | 2743 | A |
| 70 | L5 | 2754 | G |
| 70 | L5 | 2760 | G |
| 70 | L5 | 2788 | U |
| 70 | L5 | 2790 | U |
| 70 | L5 | 2798 | A |
| 70 | L5 | 2814 | C |
| 70 | L5 | 2826 | U |
| 70 | L5 | 2827 | G |
| 70 | L5 | 2829 | U |
| 70 | L5 | 2855 | G |
| 70 | L5 | 2866 | C |
| 70 | L5 | 2867 | C |
| 70 | L5 | 2871 | A |
| 70 | L5 | 2902 | G |
| 70 | L5 | 3597 | G |
| 70 | L5 | 3604 | A |
| 70 | L5 | 3606 | U |
| 70 | L5 | 3615 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 3618 | C |
| 70 | L5 | 3619 | G |
| 70 | L5 | 3626 | G |
| 70 | L5 | 3635 | A |
| 70 | L5 | 3644 | U |
| 70 | L5 | 3646 | A |
| 70 | L5 | 3648 | A |
| 70 | L5 | 3662 | A |
| 70 | L5 | 3664 | G |
| 70 | L5 | 3673 | C |
| 70 | L5 | 3711 | A |
| 70 | L5 | 3712 | A |
| 70 | L5 | 3727 | A |
| 70 | L5 | 3729 | PSU |
| 70 | L5 | 3732 | A |
| 70 | L5 | 3733 | A |
| 70 | L5 | 3750 | G |
| 70 | L5 | 3753 | G |
| 70 | L5 | 3759 | A |
| 70 | L5 | 3760 | A2M |
| 70 | L5 | 3761 | C |
| 70 | L5 | 3762 | PSU |
| 70 | L5 | 3776 | G |
| 70 | L5 | 3777 | G |
| 70 | L5 | 3783 | A |
| 70 | L5 | 3784 | A |
| 70 | L5 | 3785 | A2M |
| 70 | L5 | 3786 | U |
| 70 | L5 | 3787 | G |
| 70 | L5 | 3791 | C |
| 70 | L5 | 3811 | G |
| 70 | L5 | 3812 | C |
| 70 | L5 | 3814 | U |
| 70 | L5 | 3816 | A |
| 70 | L5 | 3817 | A |
| 70 | L5 | 3818 | U |
| 70 | L5 | 3819 | G |
| 70 | L5 | 3824 | A |
| 70 | L5 | 3838 | U |
| 70 | L5 | 3839 | G |
| 70 | L5 | 3840 | U |
| 70 | L5 | 3844 | PSU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 3876 | A |
| 70 | L5 | 3877 | A |
| 70 | L5 | 3878 | C |
| 70 | L5 | 3879 | G |
| 70 | L5 | 3897 | G |
| 70 | L5 | 3901 | A |
| 70 | L5 | 3905 | A |
| 70 | L5 | 3906 | A |
| 70 | L5 | 3907 | G |
| 70 | L5 | 3908 | A |
| 70 | L5 | 3915 | U |
| 70 | L5 | 3948 | C |
| 70 | L5 | 3951 | G |
| 70 | L5 | 3952 | A |
| 70 | L5 | 4072 | C |
| 70 | L5 | 4076 | G |
| 70 | L5 | 4084 | G |
| 70 | L5 | 4093 | G |
| 70 | L5 | 4094 | G |
| 70 | L5 | 4095 | G |
| 70 | L5 | 4096 | C |
| 70 | L5 | 4097 | G |
| 70 | L5 | 4116 | C |
| 70 | L5 | 4118 | U |
| 70 | L5 | 4119 | C |
| 70 | L5 | 4121 | G |
| 70 | L5 | 4122 | G |
| 70 | L5 | 4127 | A |
| 70 | L5 | 4150 | G |
| 70 | L5 | 4162 | C |
| 70 | L5 | 4163 | U |
| 70 | L5 | 4170 | A |
| 70 | L5 | 4183 | G |
| 70 | L5 | 4184 | G |
| 70 | L5 | 4191 | G |
| 70 | L5 | 4196 | OMG |
| 70 | L5 | 4203 | A |
| 70 | L5 | 4222 | G |
| 70 | L5 | 4229 | U |
| 70 | L5 | 4233 | A |
| 70 | L5 | 4234 | A |
| 70 | L5 | 4251 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 4254 | G |
| 70 | L5 | 4266 | G |
| 70 | L5 | 4268 | A |
| 70 | L5 | 4273 | A |
| 70 | L5 | 4280 | A |
| 70 | L5 | 4281 | A |
| 70 | L5 | 4282 | A |
| 70 | L5 | 4291 | G |
| 70 | L5 | 4297 | G |
| 70 | L5 | 4304 | A |
| 70 | L5 | 4305 | G |
| 70 | L5 | 4314 | C |
| 70 | L5 | 4330 | G |
| 70 | L5 | 4332 | C |
| 70 | L5 | 4339 | A |
| 70 | L5 | 4349 | C |
| 70 | L5 | 4350 | C |
| 70 | L5 | 4354 | U |
| 70 | L5 | 4355 | G |
| 70 | L5 | 4373 | G |
| 70 | L5 | 4376 | A |
| 70 | L5 | 4377 | G |
| 70 | L5 | 4378 | A |
| 70 | L5 | 4379 | A |
| 70 | L5 | 4387 | C |
| 70 | L5 | 4391 | G |
| 70 | L5 | 4393 | G |
| 70 | L5 | 4394 | A |
| 70 | L5 | 4415 | A |
| 70 | L5 | 4420 | PSU |
| 70 | L5 | 4421 | C |
| 70 | L5 | 4440 | G |
| 70 | L5 | 4448 | G |
| 70 | L5 | 4449 | A |
| 70 | L5 | 4464 | A |
| 70 | L5 | 4465 | U |
| 70 | L5 | 4488 | A |
| 70 | L5 | 4512 | U |
| 70 | L5 | 4513 | A |
| 70 | L5 | 4515 | G |
| 70 | L5 | 4519 | C |
| 70 | L5 | 4524 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 4528 | G |
| 70 | L5 | 4529 | G |
| 70 | L5 | 4548 | A |
| 70 | L5 | 4560 | C |
| 70 | L5 | 4567 | G |
| 70 | L5 | 4570 | G |
| 70 | L5 | 4575 | G |
| 70 | L5 | 4584 | A |
| 70 | L5 | 4590 | A2M |
| 70 | L5 | 4600 | G |
| 70 | L5 | 4606 | G |
| 70 | L5 | 4609 | G |
| 70 | L5 | 4610 | A |
| 70 | L5 | 4636 | PSU |
| 70 | L5 | 4637 | OMG |
| 70 | L5 | 4639 | G |
| 70 | L5 | 4652 | G |
| 70 | L5 | 4656 | A |
| 70 | L5 | 4657 | U |
| 70 | L5 | 4670 | C |
| 70 | L5 | 4672 | A |
| 70 | L5 | 4695 | C |
| 70 | L5 | 4700 | A |
| 70 | L5 | 4703 | U |
| 70 | L5 | 4708 | A |
| 70 | L5 | 4709 | U |
| 70 | L5 | 4721 | G |
| 70 | L5 | 4739 | C |
| 70 | L5 | 4740 | G |
| 70 | L5 | 4741 | C |
| 70 | L5 | 4742 | G |
| 70 | L5 | 4743 | G |
| 70 | L5 | 4750 | G |
| 70 | L5 | 4754 | G |
| 70 | L5 | 4757 | C |
| 70 | L5 | 4759 | C |
| 70 | L5 | 4761 | G |
| 70 | L5 | 4765 | G |
| 70 | L5 | 4771 | C |
| 70 | L5 | 4772 | C |
| 70 | L5 | 4773 | C |
| 70 | L5 | 4775 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 4776 | G |
| 70 | L5 | 4860 | G |
| 70 | L5 | 4864 | U |
| 70 | L5 | 4870 | G |
| 70 | L5 | 4871 | C |
| 70 | L5 | 4882 | U |
| 70 | L5 | 4883 | C |
| 70 | L5 | 4889 | G |
| 70 | L5 | 4890 | G |
| 70 | L5 | 4895 | C |
| 70 | L5 | 4900 | C |
| 70 | L5 | 4901 | G |
| 70 | L5 | 4910 | G |
| 70 | L5 | 4912 | G |
| 70 | L5 | 4913 | G |
| 70 | L5 | 4914 | C |
| 70 | L5 | 4931 | G |
| 70 | L5 | 4934 | A |
| 70 | L5 | 4943 | A |
| 70 | L5 | 4957 | C |
| 70 | L5 | 4967 | A |
| 70 | L5 | 4976 | U |
| 70 | L5 | 4988 | U |
| 70 | L5 | 4989 | U |
| 70 | L5 | 4990 | C |
| 70 | L5 | 4991 | U |
| 70 | L5 | 4994 | G |
| 70 | L5 | 5006 | U |
| 70 | L5 | 5007 | A |
| 70 | L5 | 5013 | C |
| 70 | L5 | 5017 | G |
| 70 | L5 | 5034 | A |
| 70 | L5 | 5041 | G |
| 70 | L5 | 5050 | C |
| 70 | L5 | 5054 | C |
| 70 | L5 | 5055 | G |
| 70 | L5 | 5061 | A |
| 70 | L5 | 5062 | G |
| 74 | S2 | 17 | C |
| 74 | S2 | 26 | U |
| 74 | S2 | 33 | G |
| 74 | S2 | 41 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 74 | S2 | 46 | A |
| 74 | S2 | 56 | G |
| 74 | S2 | 58 | C |
| 74 | S2 | 65 | C |
| 74 | S2 | 67 | C |
| 74 | S2 | 68 | A |
| 74 | S2 | 71 | G |
| 74 | S2 | 97 | U |
| 74 | S2 | 103 | A |
| 74 | S2 | 113 | G |
| 74 | S2 | 114 | G |
| 74 | S2 | 115 | U |
| 74 | S2 | 143 | U |
| 74 | S2 | 148 | U |
| 74 | S2 | 161 | U |
| 74 | S2 | 162 | C |
| 74 | S2 | 168 | C |
| 74 | S2 | 170 | A |
| 74 | S2 | 183 | G |
| 74 | S2 | 184 | G |
| 74 | S2 | 185 | G |
| 74 | S2 | 186 | C |
| 74 | S2 | 187 | G |
| 74 | S2 | 190 | G |
| 74 | S2 | 191 | A |
| 74 | S2 | 192 | C |
| 74 | S2 | 208 | G |
| 74 | S2 | 214 | U |
| 74 | S2 | 292 | A |
| 74 | S2 | 295 | C |
| 74 | S2 | 298 | G |
| 74 | S2 | 305 | U |
| 74 | S2 | 306 | C |
| 74 | S2 | 307 | G |
| 74 | S2 | 308 | G |
| 74 | S2 | 309 | G |
| 74 | S2 | 312 | G |
| 74 | S2 | 319 | C |
| 74 | S2 | 320 | C |
| 74 | S2 | 321 | U |
| 74 | S2 | 332 | G |
| 74 | S2 | 339 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 74 | S2 | 340 | C |
| 74 | S2 | 362 | C |
| 74 | S2 | 364 | A |
| 74 | S2 | 369 | C |
| 74 | S2 | 370 | G |
| 74 | S2 | 385 | G |
| 74 | S2 | 386 | C |
| 74 | S2 | 407 | G |
| 74 | S2 | 409 | C |
| 74 | S2 | 421 | G |
| 74 | S2 | 448 | A |
| 74 | S2 | 449 | A |
| 74 | S2 | 450 | C |
| 74 | S2 | 452 | G |
| 74 | S2 | 464 | A |
| 74 | S2 | 465 | A |
| 74 | S2 | 466 | G |
| 74 | S2 | 471 | G |
| 74 | S2 | 472 | C |
| 74 | S2 | 473 | A |
| 74 | S2 | 474 | G |
| 74 | S2 | 482 | G |
| 74 | S2 | 487 | U |
| 74 | S2 | 488 | U |
| 74 | S2 | 492 | C |
| 74 | S2 | 493 | A |
| 74 | S2 | 496 | C |
| 74 | S2 | 502 | C |
| 74 | S2 | 507 | G |
| 74 | S2 | 508 | A |
| 74 | S2 | 516 | A |
| 74 | S2 | 525 | A |
| 74 | S2 | 533 | A |
| 74 | S2 | 554 | A |
| 74 | S2 | 556 | U |
| 74 | S2 | 559 | G |
| 74 | S2 | 560 | A |
| 74 | S2 | 563 | G |
| 74 | S2 | 564 | A |
| 74 | S2 | 568 | C |
| 74 | S2 | 576 | A2M |
| 74 | S2 | 589 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 74 | S2 | 590 | A2M |
| 74 | S2 | 591 | U |
| 74 | S2 | 604 | A |
| 74 | S2 | 607 | U |
| 74 | S2 | 614 | C |
| 74 | S2 | 626 | G |
| 74 | S2 | 627 | OMU |
| 74 | S2 | 628 | A |
| 74 | S2 | 643 | A |
| 74 | S2 | 644 | OMG |
| 74 | S2 | 655 | A |
| 74 | S2 | 659 | G |
| 74 | S2 | 660 | C |
| 74 | S2 | 668 | A2M |
| 74 | S2 | 669 | A |
| 74 | S2 | 671 | A |
| 74 | S2 | 672 | A |
| 74 | S2 | 673 | G |
| 74 | S2 | 688 | U |
| 74 | S2 | 690 | G |
| 74 | S2 | 797 | C |
| 74 | S2 | 799 | U |
| 74 | S2 | 821 | G |
| 74 | S2 | 822 | PSU |
| 74 | S2 | 845 | G |
| 74 | S2 | 847 | A |
| 74 | S2 | 861 | A |
| 74 | S2 | 869 | A |
| 74 | S2 | 870 | A |
| 74 | S2 | 876 | C |
| 74 | S2 | 877 | C |
| 74 | S2 | 878 | G |
| 74 | S2 | 879 | C |
| 74 | S2 | 881 | G |
| 74 | S2 | 883 | U |
| 74 | S2 | 908 | A |
| 74 | S2 | 913 | A |
| 74 | S2 | 914 | U |
| 74 | S2 | 920 | A |
| 74 | S2 | 922 | A |
| 74 | S2 | 933 | G |
| 74 | S2 | 934 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 74 | S2 | 943 | U |
| 74 | S2 | 971 | G |
| 74 | S2 | 990 | A |
| 74 | S2 | 992 | A |
| 74 | S2 | 997 | A |
| 74 | S2 | 999 | G |
| 74 | S2 | 1017 | U |
| 74 | S2 | 1023 | A |
| 74 | S2 | 1026 | C |
| 74 | S2 | 1027 | A |
| 74 | S2 | 1045 | U |
| 74 | S2 | 1049 | A |
| 74 | S2 | 1061 | U |
| 74 | S2 | 1062 | A |
| 74 | S2 | 1067 | C |
| 74 | S2 | 1080 | A |
| 74 | S2 | 1083 | A |
| 74 | S2 | 1085 | C |
| 74 | S2 | 1096 | G |
| 74 | S2 | 1109 | C |
| 74 | S2 | 1115 | U |
| 74 | S2 | 1119 | A |
| 74 | S2 | 1121 | G |
| 74 | S2 | 1138 | C |
| 74 | S2 | 1153 | C |
| 74 | S2 | 1154 | U |
| 74 | S2 | 1155 | U |
| 74 | S2 | 1157 | G |
| 74 | S2 | 1171 | G |
| 74 | S2 | 1188 | A |
| 74 | S2 | 1195 | A |
| 74 | S2 | 1207 | G |
| 74 | S2 | 1208 | A |
| 74 | S2 | 1215 | C |
| 74 | S2 | 1224 | G |
| 74 | S2 | 1242 | U |
| 74 | S2 | 1243 | PSU |
| 74 | S2 | 1245 | G |
| 74 | S2 | 1247 | C |
| 74 | S2 | 1251 | A |
| 74 | S2 | 1253 | A |
| 74 | S2 | 1256 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 74 | S2 | 1257 | G |
| 74 | S2 | 1258 | A |
| 74 | S2 | 1259 | A |
| 74 | S2 | 1262 | C |
| 74 | S2 | 1264 | C |
| 74 | S2 | 1271 | C |
| 74 | S2 | 1274 | G |
| 74 | S2 | 1275 | G |
| 74 | S2 | 1301 | A |
| 74 | S2 | 1302 | G |
| 74 | S2 | 1303 | C |
| 74 | S2 | 1305 | C |
| 74 | S2 | 1325 | G |
| 74 | S2 | 1326 | U |
| 74 | S2 | 1327 | G |
| 74 | S2 | 1330 | G |
| 74 | S2 | 1341 | C |
| 74 | S2 | 1342 | U |
| 74 | S2 | 1358 | U |
| 74 | S2 | 1371 | U |
| 74 | S2 | 1372 | U |
| 74 | S2 | 1373 | C |
| 74 | S2 | 1375 | G |
| 74 | S2 | 1378 | A |
| 74 | S2 | 1397 | U |
| 74 | S2 | 1403 | C |
| 74 | S2 | 1404 | U |
| 74 | S2 | 1405 | A |
| 74 | S2 | 1415 | C |
| 74 | S2 | 1439 | A |
| 74 | S2 | 1440 | C |
| 74 | S2 | 1442 | U |
| 74 | S2 | 1447 | G |
| 74 | S2 | 1454 | A |
| 74 | S2 | 1462 | U |
| 74 | S2 | 1463 | U |
| 74 | S2 | 1464 | C |
| 74 | S2 | 1477 | U |
| 74 | S2 | 1489 | A |
| 74 | S2 | 1490 | OMG |
| 74 | S2 | 1494 | U |
| 74 | S2 | 1495 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 74 | S2 | 1498 | A |
| 74 | S2 | 1509 | U |
| 74 | S2 | 1520 | G |
| 74 | S2 | 1521 | C |
| 74 | S2 | 1522 | A |
| 74 | S2 | 1533 | A |
| 74 | S2 | 1548 | G |
| 74 | S2 | 1558 | C |
| 74 | S2 | 1560 | U |
| 74 | S2 | 1570 | G |
| 74 | S2 | 1579 | A |
| 74 | S2 | 1580 | A |
| 74 | S2 | 1585 | U |
| 74 | S2 | 1586 | U |
| 74 | S2 | 1587 | G |
| 74 | S2 | 1588 | A |
| 74 | S2 | 1598 | G |
| 74 | S2 | 1599 | U |
| 74 | S2 | 1601 | A |
| 74 | S2 | 1604 | G |
| 74 | S2 | 1606 | G |
| 74 | S2 | 1610 | G |
| 74 | S2 | 1614 | A |
| 74 | S2 | 1623 | A |
| 74 | S2 | 1637 | A |
| 74 | S2 | 1638 | G |
| 74 | S2 | 1648 | G |
| 74 | S2 | 1654 | G |
| 74 | S2 | 1665 | G |
| 74 | S2 | 1671 | G |
| 74 | S2 | 1680 | G |
| 74 | S2 | 1699 | A |
| 74 | S2 | 1720 | U |
| 74 | S2 | 1721 | U |
| 74 | S2 | 1722 | G |
| 74 | S2 | 1733 | U |
| 74 | S2 | 1735 | A |
| 74 | S2 | 1736 | G |
| 74 | S2 | 1744 | G |
| 74 | S2 | 1750 | C |
| 74 | S2 | 1785 | C |
| 74 | S2 | 1816 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 74 | S2 | 1824 | A |
| 74 | S2 | 1825 | A |
| 74 | S2 | 1829 | G |
| 74 | S2 | 1831 | A |
| 74 | S2 | 1835 | A |
| 74 | S2 | 1838 | U |
| 74 | S2 | 1849 | G |
| 74 | S2 | 1851 | MA6 |
| 74 | S2 | 1861 | G |
| 74 | S2 | 1862 | G |
| 74 | S2 | 1863 | A |
| 74 | S2 | 1864 | U |
| 74 | S2 | 1865 | C |
| 77 | S6 | 9 | U |
| 77 | S6 | 10 | G |
| 77 | S6 | 11 | G |
| 77 | S6 | 12 | C |
| 77 | S6 | 17 | C |
| 77 | S6 | 18 | G |
| 77 | S6 | 38 | A |
| 77 | S6 | 39 | C |
| 77 | S6 | 40 | C |
| 77 | S6 | 43 | G |
| 77 | S6 | 44 | A |
| 77 | S6 | 45 | G |
| 77 | S6 | 46 | G |
| 77 | S6 | 50 | A |
| 77 | S6 | 58 | A |
| 77 | S6 | 61 | C |
| 77 | S6 | 62 | C |
| 77 | S6 | 76 | A |
| 79 | mR | 37 | A |
| 79 | mR | 39 | G |

All (17) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 491 | G |
| 70 | L5 | 934 | C |
| 70 | L5 | 1303 | A |
| 70 | L5 | 1399 | G |
| 70 | L5 | 1483 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 70 | L5 | 1563 | A |
| 70 | L5 | 1633 | G |
| 70 | L5 | 2541 | G |
| 70 | L5 | 4281 | A |
| 70 | L5 | 4699 | U |
| 74 | S2 | 96 | C |
| 74 | S2 | 169 | U |
| 74 | S2 | 912 | C |
| 74 | S2 | 1244 | PSU |
| 74 | S2 | 1508 | A |
| 74 | S2 | 1598 | G |
| 77 | S6 | 60 | A |

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

208 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 |
| 70 | PSU | L5 | 5010 | 70 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 70 | PSU | L5 | 2508 | 70 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.68 | 4 (18%) |
| 74 | OMG | S2 | 509 | 74 | 23,26,27 | 2.39 | 8 (34%) | 33,38,41 | 2.00 | 9 (27%) |
| 70 | A2M | L5 | 1871 | 70 | 22,25,26 | 3.48 | 9 (40%) | 31,36,39 | 2.39 | 10 (32%) |
| 74 | PSU | S2 | 651 | 74 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.71 | 4 (18%) |
| 70 | PSU | L5 | 2632 | 70 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.63 | 4 (18%) |
| 70 | OMG | L5 | 2424 | 70 | 23,26,27 | 2.43 | 8 (34%) | 33,38,41 | 2.03 | 9 (27%) |
| 67 | H2U | Pt | 21 | 67 | 18,21,22 | 3.04 | 5 (27%) | 21,30,33 | 1.93 | 4 (19%) |
| 70 | OMG | L5 | 1316 | 70 | 23,26,27 | 2.43 | 8 (34%) | 33,38,41 | 2.03 | 10 (30%) |
| 74 | PSU | S2 | 1177 | 74 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.68 | 4 (18%) |
| 74 | PSU | S2 | 1056 | 74 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 74 | PSU | S2 | 1136 | 74 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 70 | OMC | L5 | 3887 | 70 | 19,22,23 | 2.97 | 8 (42%) | 26,31,34 | 0.77 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 74 | PSU | S2 | 1232 | 74 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.72 | 4 (18%) |
| 74 | PSU | S2 | 1692 | 74 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.67 | 4 (18%) |
| 74 | A2M | S2 | 27 | 74,83 | 22,25,26 | 3.42 | 10 (45%) | 31,36,39 | 2.38 | 10 (32%) |
| 74 | PSU | S2 | 1238 | 74 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.77 | 4 (18%) |
| 70 | PSU | L5 | 4569 | 70 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.71 | 4 (18%) |
| 70 | OMG | L5 | 4499 | 70 | 23,26,27 | 2.43 | 8 (34%) | 33,38,41 | 2.04 | 10 (30%) |
| 65 | V5N | La | 39 | 65 | 9,11,12 | 2.68 | 2 (22%) | 9,14,16 | 1.27 | 1 (11%) |
| 70 | OMC | L5 | 3869 | 70 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 0.73 | 0 |
| 70 | PSU | L5 | 3768 | 70 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.73 | 4 (18%) |
| 70 | OMC | L5 | 1881 | 82,70 | 19,22,23 | 2.97 | 8 (42%) | 26,31,34 | 0.81 | 0 |
| 74 | OMU | S2 | 1804 | 74 | 19,22,23 | 3.04 | 8 (42%) | 26,31,34 | 1.70 | 4 (15%) |
| 74 | PSU | S2 | 1081 | 74 | 18,21,22 | 0.96 | 1 (5%) | 22,30,33 | 1.70 | 2 (9%) |
| 74 | A2M | S2 | 1383 | 74 | 22,25,26 | 3.42 | 9 (40%) | 31,36,39 | 2.38 | 9 (29%) |
| 74 | MA6 | S2 | 1850 | 74 | 23,26,27 | 1.38 | 4 (17%) | 34,38,41 | 3.66 | 11 (32%) |
| 70 | PSU | L5 | 4689 | 70 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.74 | 4 (18%) |
| 70 | A2M | L5 | 400 | 70 | 22,25,26 | 3.42 | 9 (40%) | 31,36,39 | 2.38 | 9 (29%) |
| 70 | A2M | L5 | 3830 | 70 | 22,25,26 | 3.40 | 9 (40%) | 31,36,39 | 2.43 | 11 (35%) |
| 74 | PSU | S2 | 1445 | 74 | 18,21,22 | 1.08 | 1 (5%) | 22,30,33 | 1.85 | 5 (22%) |
| 70 | OMU | L5 | 4227 | 70 | 19,22,23 | 2.95 | 8 (42%) | 26,31,34 | 1.72 | 4 (15%) |
| 70 | A2M | L5 | 2363 | 84,83,70 | 22,25,26 | 3.47 | 9 (40%) | 31,36,39 | 2.39 | 10 (32%) |
| 70 | PSU | L5 | 4442 | 70 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.73 | 5 (22%) |
| 70 | PSU | L5 | 4403 | 70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.80 | 5 (22%) |
| 70 | PSU | L5 | 4431 | 70 | 18,21,22 | 1.11 | 1 (5%) | 22,30,33 | 1.71 | 4 (18%) |
| 69 | PSU | L8 | 69 | 69 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.71 | 5 (22%) |
| 70 | OMG | L5 | 4392 | 70 | 23,26,27 | 2.40 | 8 (34%) | 33,38,41 | 2.06 | 10 (30%) |
| 70 | PSU | L5 | 4972 | 70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.74 | 4 (18%) |
| 74 | PSU | S2 | 649 | 74 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.77 | 4 (18%) |
| 70 | PSU | L5 | 1582 | 70 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.58 | 4 (18%) |
| 70 | PSU | L5 | 3695 | 70 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.78 | 5 (22%) |
| 70 | PSU | L5 | 4420 | 70 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.65 | 5 (22%) |
| 74 | A2M | S2 | 668 | 74,83 | 22,25,26 | 3.40 | 10 (45%) | 31,36,39 | 2.45 | 11 (35%) |
| 74 | PSU | S2 | 801 | 74 | 18,21,22 | 1.11 | 1 (5%) | 22,30,33 | 1.72 | 4 (18%) |
| 74 | PSU | S2 | 1174 | 74 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 74 | OMG | S2 | 1328 | 74 | 23,26,27 | 2.43 | 8 (34%) | 33,38,41 | 2.05 | 10 (30%) |
| 3 | MLZ | Lo | 53 | 3 | 8,9,10 | 0.73 | 0 | 4,9,11 | 0.61 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 70 | PSU | L5 | 1683 | 70 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.78 | 4 (18%) |
| 70 | OMC | L5 | 2422 | 84,70 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 0.78 | 0 |
| 70 | PSU | L5 | 4521 | 83,70 | 18,21,22 | 1.11 | 1 (5%) | 22,30,33 | 1.79 | 4 (18%) |
| 70 | UR3 | L5 | 4530 | 70 | 19,22,23 | 2.77 | 7 (36%) | 26,32,35 | 1.34 | 2 (7%) |
| 70 | PSU | L5 | 3762 | 70 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.63 | 4 (18%) |
| 67 | G7M | Pt | 47 | 67 | 23,26,27 | 2.63 | 9 (39%) | 35,39,42 | 2.46 | 11 (31%) |
| 70 | A2M | L5 | 3825 | 70 | 22,25,26 | 3.43 | 10 (45%) | 31,36,39 | 2.40 | 11 (35%) |
| 70 | PSU | L5 | 4532 | 70 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.68 | 4 (18%) |
| 70 | OMC | L5 | 3701 | 84,82,70 | 19,22,23 | 2.93 | 8 (42%) | 26,31,34 | 0.73 | 0 |
| 70 | A2M | L5 | 4523 | 83,70 | 22,25,26 | 3.42 | 9 (40%) | 31,36,39 | 2.35 | 9 (29%) |
| 70 | PSU | L5 | 3920 | 83,70 | 18,21,22 | 1.08 | 1 (5%) | 22,30,33 | 1.72 | 4 (18%) |
| 70 | OMG | L5 | 2876 | 70 | 23,26,27 | 2.44 | 8 (34%) | 33,38,41 | 2.10 | 10 (30%) |
| 70 | OMG | L5 | 4618 | 70 | 23,26,27 | 2.41 | 8 (34%) | 33,38,41 | 2.06 | 10 (30%) |
| 70 | OMC | L5 | 2861 | 70 | 19,22,23 | 2.98 | 8 (42%) | 26,31,34 | 0.78 | 0 |
| 74 | A2M | S2 | 484 | 74 | 22,25,26 | 3.42 | 9 (40%) | 31,36,39 | 2.37 | 9 (29%) |
| 74 | PSU | S2 | 36 | 74 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 74 | PSU | S2 | 109 | 74 | 18,21,22 | 1.11 | 1 (5%) | 22,30,33 | 1.78 | 4 (18%) |
| 70 | OMC | L5 | 1340 | 70 | 19,22,23 | 2.94 | 8 (42%) | 26,31,34 | 0.76 | 0 |
| 70 | PSU | L5 | 3729 | 70 | 18,21,22 | 1.10 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 70 | OMG | L5 | 4370 | 70 | 23,26,27 | 2.41 | 8 (34%) | 33,38,41 | 2.06 | 9 (27%) |
| 64 | V5N | LA | 216 | 64 | 9,11,12 | 2.65 | 2 (22%) | 9,14,16 | 1.18 | 1 (11%) |
| 70 | OMG | L5 | 3627 | 70 | 23,26,27 | 2.43 | 8 (34%) | 33,38,41 | 2.10 | 10 (30%) |
| 70 | PSU | L5 | 1782 | 70 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.69 | 3 (13%) |
| 70 | OMU | L5 | 4498 | 70 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 1.70 | 4 (15%) |
| 70 | PSU | L5 | 4579 | 70 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 74 | PSU | S2 | 573 | 74 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.72 | 3 (13%) |
| 74 | OMG | S2 | 683 | 74 | 23,26,27 | 2.44 | 8 (34%) | 33,38,41 | 2.03 | 10 (30%) |
| 74 | PSU | S2 | 119 | 74 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.58 | 4 (18%) |
| 74 | OMG | S2 | 867 | 74 | 23,26,27 | 2.41 | 8 (34%) | 33,38,41 | 2.07 | 10 (30%) |
| 74 | PSU | S2 | 681 | 74 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.71 | 4 (18%) |
| 74 | PSU | S2 | 814 | 74 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.61 | 4 (18%) |
| 70 | PSU | L5 | 4636 | 70 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.80 | 3 (13%) |
| 67 | OMC | Pt | 33 | 67 | 19,22,23 | 3.01 | 8 (42%) | 26,31,34 | 1.02 | 2 (7%) |
| 74 | A2M | S2 | 1031 | 74 | 22,25,26 | 3.46 | 9 (40%) | 31,36,39 | 2.41 | 11 (35%) |
| 74 | PSU | S2 | 1625 | 74 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.72 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 74 | PSU | S2 | 572 | 74 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.70 | 5 (22%) |
| 70 | OMC | L5 | 3841 | 70 | 19,22,23 | 2.97 | 8 (42%) | 26,31,34 | 0.80 | 0 |
| 74 | MA6 | S2 | 1851 | 74 | 23,26,27 | 1.37 | 4 (17%) | 34,38,41 | 3.78 | 11 (32%) |
| 74 | PSU | S2 | 686 | 74 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.79 | 4 (18%) |
| 74 | PSU | S2 | 1243 | 74 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.73 | 4 (18%) |
| 74 | A2M | S2 | 99 | 74,83 | 22,25,26 | 3.44 | 9 (40%) | 31,36,39 | 2.35 | 10 (32%) |
| 70 | PSU | L5 | 3884 | 70 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.77 | 4 (18%) |
| 74 | PSU | S2 | 406 | 74 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 70 | OMG | L5 | 2364 | 70 | 23,26,27 | 2.39 | 8 (34%) | 33,38,41 | 2.05 | 10 (30%) |
| 70 | 5MC | L5 | 3782 | 83,70 | 18,22,23 | 3.65 | 7 (38%) | 26,32,35 | 1.09 | 2 (7%) |
| 74 | A2M | S2 | 512 | 74 | 22,25,26 | 3.39 | 10 (45%) | 31,36,39 | 2.47 | 10 (32%) |
| 70 | PSU | L5 | 4361 | 70 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.73 | 4 (18%) |
| 70 | PSU | L5 | 1792 | 82,70 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.61 | 4 (18%) |
| 74 | A2M | S2 | 576 | 74 | 22,25,26 | 3.40 | 9 (40%) | 31,36,39 | 2.31 | 9 (29%) |
| 70 | PSU | L5 | 4471 | 70 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.66 | 4 (18%) |
| 74 | PSU | S2 | 1004 | 74 | 18,21,22 | 1.08 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 70 | PSU | L5 | 4353 | 70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.73 | 4 (18%) |
| 74 | 6MZ | S2 | 1832 | 74,83 | 22,25,26 | 2.63 | 4 (18%) | 30,36,39 | 2.33 | 10 (33%) |
| 74 | PSU | S2 | 93 | 74 | 18,21,22 | 1.00 | 1 (5%) | 22,30,33 | 1.65 | 4 (18%) |
| 70 | A2M | L5 | 4571 | 70 | 22,25,26 | 3.45 | 9 (40%) | 31,36,39 | 2.32 | 10 (32%) |
| 70 | A2M | L5 | 1326 | 70 | 22,25,26 | 3.41 | 10 (45%) | 31,36,39 | 2.35 | 8 (25%) |
| 70 | PSU | L5 | 3844 | 70 | 18,21,22 | 1.00 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 74 | PSU | S2 | 918 | 74 | 18,21,22 | 1.12 | 2 (11%) | 22,30,33 | 1.83 | 5 (22%) |
| 74 | PSU | S2 | 1347 | 74 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.79 | 4 (18%) |
| 70 | PSU | L5 | 1779 | 70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 70 | PSU | L5 | 4576 | 70 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.70 | 4 (18%) |
| 74 | A2M | S2 | 1678 | 74 | 22,25,26 | 3.49 | 9 (40%) | 31,36,39 | 2.53 | 11 (35%) |
| 70 | OMG | L5 | 4196 | 70 | 23,26,27 | 2.43 | 8 (34%) | 33,38,41 | 2.02 | 10 (30%) |
| 70 | PSU | L5 | 4628 | 70 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.87 | 4 (18%) |
| 74 | OMU | S2 | 627 | 74 | 19,22,23 | 3.03 | 8 (42%) | 26,31,34 | 1.73 | 5 (19%) |
| 70 | PSU | L5 | 1536 | 70 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.68 | 4 (18%) |
| 74 | PSU | S2 | 822 | 74 | 18,21,22 | 1.12 | 2 (11%) | 22,30,33 | 1.83 | 5 (22%) |
| 70 | PSU | L5 | 4500 | 70 | 18,21,22 | 1.11 | 1 (5%) | 22,30,33 | 1.84 | 5 (22%) |
| 70 | 6MZ | L5 | 4220 | 70 | 22,25,26 | 2.62 | 4 (18%) | 30,36,39 | 2.30 | 11 (36%) |
| 70 | A2M | L5 | 1534 | 83,70 | 22,25,26 | 3.46 | 9 (40%) | 31,36,39 | 2.36 | 9 (29%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 70 | OMG | L5 | 4494 | 70 | 23,26,27 | 2.43 | 8 (34%) | 33,38,41 | 2.05 | 9 (27%) |
| 70 | PSU | L5 | 3637 | 70 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.79 | 4 (18%) |
| 67 | 4SU | Pt | 8 | 67 | 18,21,22 | 3.51 | 7 (38%) | 26,30,33 | 2.20 | 5 (19%) |
| 70 | A2M | L5 | 2401 | 70 | 22,25,26 | 3.41 | 10 (45%) | 31,36,39 | 2.38 | 10 (32%) |
| 74 | PSU | S2 | 1367 | 74 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.82 | 4 (18%) |
| 74 | PSU | S2 | 1643 | 74,83 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.73 | 4 (18%) |
| 74 | PSU | S2 | 34 | 74 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 74 | OMU | S2 | 116 | 74 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 1.66 | 5 (19%) |
| 63 | MLZ | Lb | 5 | 63 | 8,9,10 | 0.77 | 0 | 4,9,11 | 0.65 | 0 |
| 74 | OMG | S2 | 1490 | 74 | 23,26,27 | 2.41 | 8 (34%) | 33,38,41 | 2.02 | 10 (30%) |
| 70 | PSU | L5 | 1744 | 70 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.77 | 4 (18%) |
| 70 | PSU | L5 | 3770 | 70 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 70 | PSU | L5 | 4552 | 70 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.71 | 4 (18%) |
| 70 | PSU | L5 | 4423 | 70 | 18,21,22 | 1.08 | 1 (5%) | 22,30,33 | 1.74 | 4 (18%) |
| 74 | PSU | S2 | 296 | 74 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.73 | 4 (18%) |
| 70 | OMG | L5 | 3744 | 70 | 23,26,27 | 2.42 | 8 (34%) | 33,38,41 | 2.03 | 10 (30%) |
| 74 | OMG | S2 | 644 | 74 | 23,26,27 | 2.42 | 8 (34%) | 33,38,41 | 2.04 | 10 (30%) |
| 70 | OMC | L5 | 3808 | 70 | 19,22,23 | 2.94 | 8 (42%) | 26,31,34 | 0.85 | 0 |
| 70 | PSU | L5 | 3764 | 70 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 70 | OMC | L5 | 2365 | 83,70 | 19,22,23 | 2.94 | 8 (42%) | 26,31,34 | 0.68 | 0 |
| 74 | A2M | S2 | 590 | 74 | 22,25,26 | 3.41 | 9 (40%) | 31,36,39 | 2.54 | 11 (35%) |
| 70 | PSU | L5 | 3734 | 70 | 18,21,22 | 1.00 | 1 (5%) | 22,30,33 | 1.69 | 4 (18%) |
| 70 | OMG | L5 | 4623 | 70 | 23,26,27 | 2.43 | 8 (34%) | 33,38,41 | 2.05 | 10 (30%) |
| 70 | OMG | L5 | 1522 | 70 | 23,26,27 | 2.42 | 8 (34%) | 33,38,41 | 2.09 | 10 (30%) |
| 70 | OMC | L5 | 2804 | 70 | 19,22,23 | 2.96 | 8 (42%) | 26,31,34 | 0.66 | 0 |
| 70 | PSU | L5 | 4312 | 70 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 70 | PSU | L5 | 3851 | 70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.70 | 4 (18%) |
| 70 | PSU | L5 | 4673 | 70 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 70 | PSU | L5 | 4457 | 70 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.81 | 4 (18%) |
| 70 | OMC | L5 | 4456 | 70 | 19,22,23 | 2.94 | 8 (42%) | 26,31,34 | 0.84 | 1 (3%) |
| 70 | A2M | L5 | 398 | 70 | 22,25,26 | 3.42 | 9 (40%) | 31,36,39 | 2.37 | 11 (35%) |
| 74 | G7M | S2 | 1639 | 74,67 | 23,26,27 | 2.59 | 9 (39%) | 35,39,42 | 2.49 | 11 (31%) |
| 70 | PSU | L5 | 1862 | 70 | 18,21,22 | 1.01 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 70 | PSU | L5 | 1677 | 70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.74 | 4 (18%) |
| 70 | PSU | L5 | 2843 | 70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.86 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 69 | OMG | L8 | 75 | 69 | 23,26,27 | 2.44 | 8 (34%) | 33,38,41 | 2.04 | 10 (30%) |
| 70 | OMG | L5 | 3899 | 83,70 | 23,26,27 | 2.40 | 8 (34%) | 33,38,41 | 2.06 | 10 (30%) |
| 74 | OMG | S2 | 436 | 74 | 23,26,27 | 2.39 | 8 (34%) | 33,38,41 | 2.06 | 10 (30%) |
| 70 | OMG | L5 | 1625 | 70 | 23,26,27 | 2.44 | 8 (34%) | 33,38,41 | 2.03 | 10 (30%) |
| 74 | A2M | S2 | 468 | 74 | 22,25,26 | 3.43 | 9 (40%) | 31,36,39 | 2.32 | 10 (32%) |
| 74 | OMC | S2 | 462 | 74 | 19,22,23 | 3.00 | 8 (42%) | 26,31,34 | 0.78 | 0 |
| 70 | PSU | L5 | 1860 | 70 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.69 | 4 (18%) |
| 70 | A2M | L5 | 3718 | 70 | 22,25,26 | 3.42 | 9 (40%) | 31,36,39 | 2.36 | 9 (29%) |
| 70 | OMC | L5 | 2351 | 70 | 19,22,23 | 2.95 | 8 (42%) | 26,31,34 | 1.08 | 3 (11%) |
| 74 | PSU | S2 | 866 | 74 | 18,21,22 | 1.11 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 67 | PSU | Pt | 56 | 67 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.74 | 4 (18%) |
| 74 | PSU | S2 | 1239 | 74 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.74 | 3 (13%) |
| 74 | OMC | S2 | 1391 | 74 | 19,22,23 | 2.98 | 8 (42%) | 26,31,34 | 0.79 | 0 |
| 70 | A2M | L5 | 3867 | 70 | 22,25,26 | 3.43 | 9 (40%) | 31,36,39 | 2.43 | 10 (32%) |
| 70 | OMG | L5 | 4228 | 70 | 23,26,27 | 2.42 | 9 (39%) | 33,38,41 | 2.09 | 10 (30%) |
| 70 | PSU | L5 | 1781 | 70 | 18,21,22 | 1.08 | 1 (5%) | 22,30,33 | 1.64 | 4 (18%) |
| 70 | A2M | L5 | 4590 | 70 | 22,25,26 | 3.43 | 9 (40%) | 31,36,39 | 2.43 | 9 (29%) |
| 70 | OMG | L5 | 4637 | 70 | 23,26,27 | 2.40 | 8 (34%) | 33,38,41 | 2.07 | 10 (30%) |
| 70 | OMU | L5 | 2837 | 70 | 19,22,23 | 2.98 | 8 (42%) | 26,31,34 | 1.77 | 5 (19%) |
| 70 | PSU | L5 | 5001 | 70 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.77 | 4 (18%) |
| 70 | A2M | L5 | 3785 | 70 | 22,25,26 | 3.35 | 9 (40%) | 31,36,39 | 2.60 | 13 (41%) |
| 70 | PSU | L5 | 4293 | 70 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.78 | 4 (18%) |
| 74 | OMC | S2 | 1703 | 74 | 19,22,23 | 3.00 | 8 (42%) | 26,31,34 | 0.71 | 0 |
| 70 | PSU | L5 | 4531 | 70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.77 | 5 (22%) |
| 74 | PSU | S2 | 863 | 74 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.70 | 4 (18%) |
| 70 | OMG | L5 | 3792 | 70 | 23,26,27 | 2.41 | 8 (34%) | 33,38,41 | 2.05 | 9 (27%) |
| 70 | A2M | L5 | 3760 | 70 | 22,25,26 | 3.41 | 9 (40%) | 31,36,39 | 2.52 | 11 (35%) |
| 70 | OMU | L5 | 3925 | 70 | 19,22,23 | 2.96 | 8 (42%) | 26,31,34 | 1.72 | 5 (19%) |
| 70 | PSU | L5 | 4296 | 70 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.72 | 4 (18%) |
| 70 | OMU | L5 | 4620 | 70 | 19,22,23 | 2.93 | 8 (42%) | 26,31,34 | 1.67 | 4 (15%) |
| 70 | PSU | L5 | 3853 | 84,70 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.69 | 4 (18%) |
| 70 | PSU | L5 | 3715 | 70 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.67 | 4 (18%) |
| 74 | PSU | S2 | 105 | 74 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.71 | 4 (18%) |
| 74 | PSU | S2 | 815 | 74 | 18,21,22 | 0.98 | 1 (5%) | 22,30,33 | 1.65 | 4 (18%) |
| 70 | PSU | L5 | 2839 | 70 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.73 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 74 | B8N | S2 | 1248 | 74 | 24,29,30 | 3.16 | 8 (33%) | 29,42,45 | 1.79 | 7 (24%) |
| 70 | OMC | L5 | 2824 | 70 | 19,22,23 | 3.02 | 8 (42%) | 26,31,34 | 0.75 | 0 |
| 69 | PSU | L8 | 55 | 69 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.72 | 4 (18%) |
| 74 | PSU | S2 | 609 | 74 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.78 | 4 (18%) |
| 70 | PSU | L5 | 3758 | 84,70 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 70 | PSU | L5 | 4493 | 70 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.73 | 4 (18%) |
| 70 | OMC | L5 | 4536 | 70 | 19,22,23 | 2.98 | 8 (42%) | 26,31,34 | 0.78 | 0 |
| 70 | A2M | L5 | 1524 | 70 | 22,25,26 | 3.41 | 10 (45%) | 31,36,39 | 2.47 | 11 (35%) |
| 74 | PSU | S2 | 966 | 74 | 18,21,22 | 0.99 | 1 (5%) | 22,30,33 | 1.60 | 3 (13%) |
| 74 | 4AC | S2 | 1337 | 74 | 21,24,25 | 3.47 | 9 (42%) | 29,34,37 | 1.03 | 2 (6%) |
| 70 | 1MA | L5 | 1322 | 84,70 | 21,25,26 | 2.91 | 6 (28%) | 31,37,40 | 2.87 | 8 (25%) |
| 70 | PSU | L5 | 4299 | 70 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 74 | PSU | S2 | 218 | 74 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.74 | 5 (22%) |
| 74 | OMU | S2 | 428 | 74 | 19,22,23 | 2.98 | 8 (42%) | 26,31,34 | 1.73 | 4 (15%) |
| 74 | OMC | S2 | 517 | 74 | 19,22,23 | 3.00 | 8 (42%) | 26,31,34 | 0.77 | 0 |
| 70 | 5MC | L5 | 4447 | 70 | 18,22,23 | 3.66 | 7 (38%) | 26,32,35 | 1.08 | 1 (3%) |
| 74 | 4AC | S2 | 1842 | 74 | 21,24,25 | 3.34 | 9 (42%) | 29,34,37 | 1.06 | 3 (10%) |
| 74 | PSU | S2 | 1244 | 74 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.86 | 4 (18%) |
| 70 | PSU | L5 | 3639 | 70 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.77 | 4 (18%) |
| 70 | A2M | L5 | 2815 | 70 | 22,25,26 | 3.42 | 9 (40%) | 31,36,39 | 2.41 | 10 (32%) |

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 |
|-----|------|-------|------|------|---------|-----------|---------|
| 70 | PSU | L5 | 5010 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 2508 | 70 | - | 2/7/25/26 | 0/2/2/2 |
| 74 | OMG | S2 | 509 | 74 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | A2M | L5 | 1871 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 651 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 2632 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 2424 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 67 | H2U | Pt | 21 | 67 | - | 4/7/38/39 | 0/2/2/2 |
| 70 | OMG | L5 | 1316 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 1177 | 74 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|----------|---------|------------|---------|
| 74 | PSU | S2 | 1056 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 1136 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 3887 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 74 | PSU | S2 | 1232 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 1692 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | A2M | S2 | 27 | 74,83 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 1238 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4569 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 4499 | 70 | - | 2/9/27/28 | 0/3/3/3 |
| 65 | V5N | La | 39 | 65 | - | 0/9/10/12 | 0/1/1/1 |
| 70 | OMC | L5 | 3869 | 70 | - | 1/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 3768 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 1881 | 82,70 | - | 0/9/27/28 | 0/2/2/2 |
| 74 | OMU | S2 | 1804 | 74 | - | 1/9/27/28 | 0/2/2/2 |
| 74 | PSU | S2 | 1081 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | A2M | S2 | 1383 | 74 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | MA6 | S2 | 1850 | 74 | - | 0/11/29/30 | 0/3/3/3 |
| 70 | PSU | L5 | 4689 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | A2M | L5 | 400 | 70 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | A2M | L5 | 3830 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 1445 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMU | L5 | 4227 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | A2M | L5 | 2363 | 84,83,70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 4442 | 70 | - | 1/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4403 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4431 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 69 | PSU | L8 | 69 | 69 | - | 1/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 4392 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 4972 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 649 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 1582 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 3695 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4420 | 70 | - | 4/7/25/26 | 0/2/2/2 |
| 74 | A2M | S2 | 668 | 74,83 | - | 3/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 801 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 1174 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | OMG | S2 | 1328 | 74 | - | 1/9/27/28 | 0/3/3/3 |
| 3 | MLZ | Lo | 53 | 3 | - | 4/7/8/10 | - |
| 70 | PSU | L5 | 1683 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 2422 | 84,70 | - | 2/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 4521 | 83,70 | - | 1/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|----------|---------|------------|---------|
| 70 | UR3 | L5 | 4530 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 3762 | 70 | - | 2/7/25/26 | 0/2/2/2 |
| 67 | G7M | Pt | 47 | 67 | - | 1/7/25/26 | 0/3/3/3 |
| 70 | A2M | L5 | 3825 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 4532 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 3701 | 84,82,70 | - | 4/9/27/28 | 0/2/2/2 |
| 70 | A2M | L5 | 4523 | 83,70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 3920 | 83,70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 2876 | 70 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | OMG | L5 | 4618 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | OMC | L5 | 2861 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 74 | A2M | S2 | 484 | 74 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 36 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 109 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 1340 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 3729 | 70 | - | 2/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 4370 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 64 | V5N | LA | 216 | 64 | - | 1/9/10/12 | 0/1/1/1 |
| 70 | OMG | L5 | 3627 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 1782 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMU | L5 | 4498 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 4579 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 573 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | OMG | S2 | 683 | 74 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 119 | 74 | - | 1/7/25/26 | 0/2/2/2 |
| 74 | OMG | S2 | 867 | 74 | - | 1/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 681 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 814 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4636 | 70 | - | 4/7/25/26 | 0/2/2/2 |
| 67 | OMC | Pt | 33 | 67 | - | 2/9/27/28 | 0/2/2/2 |
| 74 | A2M | S2 | 1031 | 74 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 1625 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 572 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 3841 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 74 | MA6 | S2 | 1851 | 74 | - | 1/11/29/30 | 0/3/3/3 |
| 74 | PSU | S2 | 686 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 1243 | 74 | - | 2/7/25/26 | 0/2/2/2 |
| 74 | A2M | S2 | 99 | 74,83 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 3884 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 406 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 2364 | 70 | - | 0/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|-----------|---------|
| 70 | 5MC | L5 | 3782 | 83,70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | A2M | S2 | 512 | 74 | - | 2/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 4361 | 70 | - | 1/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 1792 | 82,70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | A2M | S2 | 576 | 74 | - | 2/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 4471 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 1004 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4353 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | 6MZ | S2 | 1832 | 74,83 | - | 2/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 93 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | A2M | L5 | 4571 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | A2M | L5 | 1326 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 3844 | 70 | - | 3/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 918 | 74 | - | 2/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 1347 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 1779 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4576 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | A2M | S2 | 1678 | 74 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | OMG | L5 | 4196 | 70 | - | 3/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 4628 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | OMU | S2 | 627 | 74 | - | 1/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 1536 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 822 | 74 | - | 2/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4500 | 70 | - | 1/7/25/26 | 0/2/2/2 |
| 70 | 6MZ | L5 | 4220 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | A2M | L5 | 1534 | 83,70 | - | 2/9/27/28 | 0/3/3/3 |
| 70 | OMG | L5 | 4494 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 3637 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 67 | 4SU | Pt | 8 | 67 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | A2M | L5 | 2401 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 1367 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 1643 | 74,83 | - | 1/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 34 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | OMU | S2 | 116 | 74 | - | 1/9/27/28 | 0/2/2/2 |
| 63 | MLZ | Lb | 5 | 63 | - | 5/7/8/10 | - |
| 74 | OMG | S2 | 1490 | 74 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 1744 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 3770 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4552 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4423 | 70 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|-----------|---------|
| 74 | PSU | S2 | 296 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 3744 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | OMG | S2 | 644 | 74 | - | 3/9/27/28 | 0/3/3/3 |
| 70 | OMC | L5 | 3808 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 3764 | 70 | - | 2/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 2365 | 83,70 | - | 0/9/27/28 | 0/2/2/2 |
| 74 | A2M | S2 | 590 | 74 | - | 3/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 3734 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 4623 | 70 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | OMG | L5 | 1522 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | OMC | L5 | 2804 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 4312 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 3851 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4673 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4457 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 4456 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | A2M | L5 | 398 | 70 | - | 1/9/27/28 | 0/3/3/3 |
| 74 | G7M | S2 | 1639 | 74,67 | - | 0/7/25/26 | 0/3/3/3 |
| 70 | PSU | L5 | 1862 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 1677 | 70 | - | 4/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 2843 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 69 | OMG | L8 | 75 | 69 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | OMG | L5 | 3899 | 83,70 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | OMG | S2 | 436 | 74 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | OMG | L5 | 1625 | 70 | - | 2/9/27/28 | 0/3/3/3 |
| 74 | A2M | S2 | 468 | 74 | - | 0/9/27/28 | 0/3/3/3 |
| 74 | OMC | S2 | 462 | 74 | - | 1/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 1860 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | A2M | L5 | 3718 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | OMC | L5 | 2351 | 70 | - | 3/9/27/28 | 0/2/2/2 |
| 74 | PSU | S2 | 866 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 67 | PSU | Pt | 56 | 67 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 1239 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | OMC | S2 | 1391 | 74 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | A2M | L5 | 3867 | 70 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | OMG | L5 | 4228 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 1781 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | A2M | L5 | 4590 | 70 | - | 2/9/27/28 | 0/3/3/3 |
| 70 | OMG | L5 | 4637 | 70 | - | 2/9/27/28 | 0/3/3/3 |
| 70 | OMU | L5 | 2837 | 70 | - | 0/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|------------|---------|
| 70 | PSU | L5 | 5001 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | A2M | L5 | 3785 | 70 | - | 1/9/27/28 | 0/3/3/3 |
| 70 | PSU | L5 | 4293 | 70 | - | 2/7/25/26 | 0/2/2/2 |
| 74 | OMC | S2 | 1703 | 74 | - | 1/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 4531 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 863 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMG | L5 | 3792 | 70 | - | 0/9/27/28 | 0/3/3/3 |
| 70 | A2M | L5 | 3760 | 70 | - | 3/9/27/28 | 0/3/3/3 |
| 70 | OMU | L5 | 3925 | 70 | - | 1/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 4296 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMU | L5 | 4620 | 70 | - | 1/9/27/28 | 0/2/2/2 |
| 70 | PSU | L5 | 3853 | 84,70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 3715 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 105 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 815 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 2839 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | B8N | S2 | 1248 | 74 | - | 4/16/34/35 | 0/2/2/2 |
| 70 | OMC | L5 | 2824 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 69 | PSU | L8 | 55 | 69 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 609 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 3758 | 84,70 | - | 1/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 4493 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | OMC | L5 | 4536 | 70 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | A2M | L5 | 1524 | 70 | - | 1/9/27/28 | 0/3/3/3 |
| 74 | PSU | S2 | 966 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | 4AC | S2 | 1337 | 74 | - | 0/11/29/30 | 0/2/2/2 |
| 70 | 1MA | L5 | 1322 | 84,70 | - | 0/7/25/26 | 0/3/3/3 |
| 70 | PSU | L5 | 4299 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | PSU | S2 | 218 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 74 | OMU | S2 | 428 | 74 | - | 6/9/27/28 | 0/2/2/2 |
| 74 | OMC | S2 | 517 | 74 | - | 0/9/27/28 | 0/2/2/2 |
| 70 | 5MC | L5 | 4447 | 70 | - | 4/7/25/26 | 0/2/2/2 |
| 74 | 4AC | S2 | 1842 | 74 | - | 0/11/29/30 | 0/2/2/2 |
| 74 | PSU | S2 | 1244 | 74 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | PSU | L5 | 3639 | 70 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | A2M | L5 | 2815 | 70 | - | 0/9/27/28 | 0/3/3/3 |

All (926) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 74 | S2 | 1832 | 6MZ | C6-N6 | 10.79 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 70 | L5 | 4220 | 6MZ | C6-N6 | 10.58 | 1.45 | 1.34 |
| 67 | Pt | 21 | H2U | C2-N1 | 9.64 | 1.49 | 1.35 |
| 70 | L5 | 4447 | 5MC | C6-C5 | 9.55 | 1.50 | 1.34 |
| 70 | L5 | 3782 | 5MC | C6-C5 | 9.33 | 1.49 | 1.34 |
| 74 | S2 | 1031 | A2M | C2'-C1' | -8.88 | 1.30 | 1.53 |
| 70 | L5 | 2363 | A2M | C2'-C1' | -8.86 | 1.30 | 1.53 |
| 74 | S2 | 1678 | A2M | C2'-C1' | -8.85 | 1.30 | 1.53 |
| 70 | L5 | 3867 | A2M | C2'-C1' | -8.85 | 1.30 | 1.53 |
| 70 | L5 | 1871 | A2M | C2'-C1' | -8.84 | 1.30 | 1.53 |
| 70 | L5 | 1534 | A2M | C2'-C1' | -8.82 | 1.30 | 1.53 |
| 74 | S2 | 1383 | A2M | O4'-C1' | 8.73 | 1.62 | 1.42 |
| 70 | L5 | 1326 | A2M | C2'-C1' | -8.69 | 1.30 | 1.53 |
| 74 | S2 | 468 | A2M | C2'-C1' | -8.67 | 1.30 | 1.53 |
| 74 | S2 | 99 | A2M | C2'-C1' | -8.67 | 1.30 | 1.53 |
| 70 | L5 | 4571 | A2M | C2'-C1' | -8.66 | 1.30 | 1.53 |
| 74 | S2 | 27 | A2M | C2'-C1' | -8.65 | 1.30 | 1.53 |
| 70 | L5 | 4590 | A2M | C2'-C1' | -8.64 | 1.30 | 1.53 |
| 70 | L5 | 1534 | A2M | O4'-C1' | 8.63 | 1.62 | 1.42 |
| 70 | L5 | 3830 | A2M | C2'-C1' | -8.63 | 1.30 | 1.53 |
| 70 | L5 | 4590 | A2M | O4'-C1' | 8.62 | 1.62 | 1.42 |
| 74 | S2 | 1383 | A2M | C2'-C1' | -8.62 | 1.30 | 1.53 |
| 74 | S2 | 1678 | A2M | O4'-C1' | 8.62 | 1.62 | 1.42 |
| 70 | L5 | 398 | A2M | C2'-C1' | -8.61 | 1.30 | 1.53 |
| 70 | L5 | 3825 | A2M | C2'-C1' | -8.61 | 1.30 | 1.53 |
| 70 | L5 | 1871 | A2M | O4'-C1' | 8.61 | 1.62 | 1.42 |
| 74 | S2 | 99 | A2M | O4'-C1' | 8.61 | 1.62 | 1.42 |
| 70 | L5 | 2401 | A2M | O4'-C1' | 8.60 | 1.62 | 1.42 |
| 70 | L5 | 398 | A2M | O4'-C1' | 8.60 | 1.62 | 1.42 |
| 70 | L5 | 2815 | A2M | C2'-C1' | -8.60 | 1.30 | 1.53 |
| 70 | L5 | 400 | A2M | C2'-C1' | -8.60 | 1.30 | 1.53 |
| 70 | L5 | 4523 | A2M | O4'-C1' | 8.58 | 1.62 | 1.42 |
| 70 | L5 | 3785 | A2M | C2'-C1' | -8.58 | 1.31 | 1.53 |
| 70 | L5 | 4523 | A2M | C2'-C1' | -8.58 | 1.31 | 1.53 |
| 70 | L5 | 3718 | A2M | C2'-C1' | -8.58 | 1.31 | 1.53 |
| 74 | S2 | 468 | A2M | O4'-C1' | 8.57 | 1.62 | 1.42 |
| 74 | S2 | 512 | A2M | O4'-C1' | 8.57 | 1.62 | 1.42 |
| 70 | L5 | 2363 | A2M | O4'-C1' | 8.57 | 1.62 | 1.42 |
| 70 | L5 | 2815 | A2M | O4'-C1' | 8.56 | 1.62 | 1.42 |
| 74 | S2 | 590 | A2M | O4'-C1' | 8.56 | 1.62 | 1.42 |
| 70 | L5 | 3718 | A2M | O4'-C1' | 8.56 | 1.62 | 1.42 |
| 74 | S2 | 484 | A2M | C2'-C1' | -8.55 | 1.31 | 1.53 |
| 70 | L5 | 3760 | A2M | C2'-C1' | -8.55 | 1.31 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 70 | L5 | 400 | A2M | O4'-C1' | 8.55 | 1.62 | 1.42 |
| 74 | S2 | 576 | A2M | C2'-C1' | -8.54 | 1.31 | 1.53 |
| 74 | S2 | 27 | A2M | O4'-C1' | 8.53 | 1.62 | 1.42 |
| 70 | L5 | 3825 | A2M | O4'-C1' | 8.51 | 1.62 | 1.42 |
| 70 | L5 | 2401 | A2M | C2'-C1' | -8.50 | 1.31 | 1.53 |
| 70 | L5 | 4571 | A2M | O4'-C1' | 8.50 | 1.62 | 1.42 |
| 70 | L5 | 3830 | A2M | O4'-C1' | 8.49 | 1.62 | 1.42 |
| 74 | S2 | 484 | A2M | O4'-C1' | 8.48 | 1.62 | 1.42 |
| 74 | S2 | 590 | A2M | C2'-C1' | -8.47 | 1.31 | 1.53 |
| 74 | S2 | 576 | A2M | O4'-C1' | 8.46 | 1.62 | 1.42 |
| 70 | L5 | 1524 | A2M | O4'-C1' | 8.46 | 1.62 | 1.42 |
| 70 | L5 | 3760 | A2M | O4'-C1' | 8.43 | 1.62 | 1.42 |
| 74 | S2 | 512 | A2M | C2'-C1' | -8.43 | 1.31 | 1.53 |
| 74 | S2 | 1031 | A2M | O4'-C1' | 8.41 | 1.61 | 1.42 |
| 74 | S2 | 668 | A2M | C2'-C1' | -8.40 | 1.31 | 1.53 |
| 70 | L5 | 1524 | A2M | C2'-C1' | -8.39 | 1.31 | 1.53 |
| 70 | L5 | 3867 | A2M | O4'-C1' | 8.37 | 1.61 | 1.42 |
| 70 | L5 | 1326 | A2M | O4'-C1' | 8.26 | 1.61 | 1.42 |
| 74 | S2 | 668 | A2M | O4'-C1' | 8.16 | 1.61 | 1.42 |
| 70 | L5 | 3785 | A2M | O4'-C1' | 7.99 | 1.60 | 1.42 |
| 70 | L5 | 1322 | 1MA | C2-N3 | 7.97 | 1.45 | 1.30 |
| 70 | L5 | 1322 | 1MA | C4-N3 | 7.80 | 1.51 | 1.35 |
| 74 | S2 | 1248 | B8N | C4-N3 | -7.72 | 1.26 | 1.40 |
| 74 | S2 | 1248 | B8N | C6-N1 | 7.69 | 1.55 | 1.36 |
| 67 | Pt | 8 | 4SU | C4-N3 | 7.62 | 1.45 | 1.37 |
| 74 | S2 | 1804 | OMU | C2-N1 | 7.13 | 1.49 | 1.38 |
| 70 | L5 | 4530 | UR3 | C2-N1 | 7.00 | 1.48 | 1.38 |
| 70 | L5 | 4498 | OMU | C2-N1 | 6.93 | 1.49 | 1.38 |
| 74 | S2 | 627 | OMU | C2-N1 | 6.92 | 1.49 | 1.38 |
| 74 | S2 | 428 | OMU | C2-N1 | 6.89 | 1.49 | 1.38 |
| 74 | S2 | 116 | OMU | C2-N1 | 6.88 | 1.49 | 1.38 |
| 74 | S2 | 627 | OMU | C2-N3 | 6.86 | 1.50 | 1.38 |
| 70 | L5 | 4227 | OMU | C2-N1 | 6.82 | 1.49 | 1.38 |
| 74 | S2 | 116 | OMU | C2-N3 | 6.81 | 1.50 | 1.38 |
| 70 | L5 | 3925 | OMU | C2-N1 | 6.79 | 1.49 | 1.38 |
| 74 | S2 | 1804 | OMU | C2-N3 | 6.78 | 1.50 | 1.38 |
| 70 | L5 | 2837 | OMU | C2-N3 | 6.78 | 1.50 | 1.38 |
| 74 | S2 | 1337 | 4AC | C4-N3 | 6.77 | 1.44 | 1.32 |
| 70 | L5 | 2837 | OMU | C2-N1 | 6.76 | 1.49 | 1.38 |
| 74 | S2 | 428 | OMU | C2-N3 | 6.76 | 1.50 | 1.38 |
| 74 | S2 | 668 | A2M | O4'-C4' | -6.70 | 1.30 | 1.45 |
| 70 | L5 | 4620 | OMU | C2-N1 | 6.69 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 70 | L5 | 3925 | OMU | C2-N3 | 6.65 | 1.49 | 1.38 |
| 70 | L5 | 4498 | OMU | C2-N3 | 6.62 | 1.49 | 1.38 |
| 70 | L5 | 4227 | OMU | C2-N3 | 6.60 | 1.49 | 1.38 |
| 70 | L5 | 4620 | OMU | C2-N3 | 6.58 | 1.49 | 1.38 |
| 70 | L5 | 1524 | A2M | O4'-C4' | -6.57 | 1.30 | 1.45 |
| 74 | S2 | 1678 | A2M | O4'-C4' | -6.56 | 1.30 | 1.45 |
| 74 | S2 | 1337 | 4AC | C6-C5 | 6.55 | 1.50 | 1.35 |
| 70 | L5 | 4571 | A2M | O4'-C4' | -6.53 | 1.30 | 1.45 |
| 70 | L5 | 3782 | 5MC | C4-N3 | 6.50 | 1.45 | 1.34 |
| 74 | S2 | 1842 | 4AC | C4-N3 | 6.50 | 1.44 | 1.32 |
| 74 | S2 | 590 | A2M | O4'-C4' | -6.49 | 1.30 | 1.45 |
| 67 | Pt | 47 | G7M | C4-N3 | 6.47 | 1.49 | 1.34 |
| 70 | L5 | 3760 | A2M | O4'-C4' | -6.46 | 1.30 | 1.45 |
| 74 | S2 | 683 | OMG | C4-N3 | 6.45 | 1.49 | 1.34 |
| 70 | L5 | 4196 | OMG | C4-N3 | 6.45 | 1.49 | 1.34 |
| 74 | S2 | 1328 | OMG | C4-N3 | 6.45 | 1.49 | 1.34 |
| 70 | L5 | 2363 | A2M | O4'-C4' | -6.45 | 1.30 | 1.45 |
| 70 | L5 | 400 | A2M | O4'-C4' | -6.44 | 1.30 | 1.45 |
| 70 | L5 | 4590 | A2M | O4'-C4' | -6.44 | 1.30 | 1.45 |
| 69 | L8 | 75 | OMG | C4-N3 | 6.43 | 1.49 | 1.34 |
| 70 | L5 | 1625 | OMG | C4-N3 | 6.43 | 1.49 | 1.34 |
| 70 | L5 | 1871 | A2M | O4'-C4' | -6.43 | 1.30 | 1.45 |
| 70 | L5 | 3792 | OMG | C4-N3 | 6.42 | 1.49 | 1.34 |
| 67 | Pt | 8 | 4SU | C2-N3 | 6.41 | 1.49 | 1.38 |
| 64 | LA | 216 | V5N | CG-ND1 | -6.41 | 1.31 | 1.37 |
| 70 | L5 | 2876 | OMG | C4-N3 | 6.41 | 1.49 | 1.34 |
| 74 | S2 | 1842 | 4AC | C6-C5 | 6.41 | 1.50 | 1.35 |
| 74 | S2 | 1031 | A2M | O4'-C4' | -6.40 | 1.30 | 1.45 |
| 67 | Pt | 8 | 4SU | C2-N1 | 6.40 | 1.48 | 1.38 |
| 74 | S2 | 484 | A2M | O4'-C4' | -6.40 | 1.30 | 1.45 |
| 70 | L5 | 4623 | OMG | C4-N3 | 6.39 | 1.49 | 1.34 |
| 70 | L5 | 1316 | OMG | C4-N3 | 6.39 | 1.49 | 1.34 |
| 70 | L5 | 4499 | OMG | C4-N3 | 6.39 | 1.49 | 1.34 |
| 70 | L5 | 3825 | A2M | O4'-C4' | -6.38 | 1.30 | 1.45 |
| 74 | S2 | 1248 | B8N | C6-C5 | 6.38 | 1.43 | 1.34 |
| 74 | S2 | 462 | OMC | C2-N3 | 6.37 | 1.49 | 1.36 |
| 70 | L5 | 4392 | OMG | C4-N3 | 6.37 | 1.49 | 1.34 |
| 70 | L5 | 3627 | OMG | C4-N3 | 6.36 | 1.49 | 1.34 |
| 65 | La | 39 | V5N | CG-ND1 | -6.36 | 1.31 | 1.37 |
| 70 | L5 | 4370 | OMG | C4-N3 | 6.36 | 1.49 | 1.34 |
| 70 | L5 | 1326 | A2M | O4'-C4' | -6.35 | 1.30 | 1.45 |
| 70 | L5 | 4523 | A2M | O4'-C4' | -6.35 | 1.30 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 74 | S2 | 644 | OMG | C4-N3 | 6.35 | 1.49 | 1.34 |
| 67 | Pt | 33 | OMC | C2-N3 | 6.35 | 1.49 | 1.36 |
| 70 | L5 | 3744 | OMG | C4-N3 | 6.35 | 1.49 | 1.34 |
| 74 | S2 | 99 | A2M | O4'-C4' | -6.35 | 1.30 | 1.45 |
| 70 | L5 | 1534 | A2M | O4'-C4' | -6.35 | 1.30 | 1.45 |
| 70 | L5 | 4494 | OMG | C4-N3 | 6.34 | 1.49 | 1.34 |
| 74 | S2 | 867 | OMG | C4-N3 | 6.33 | 1.49 | 1.34 |
| 74 | S2 | 509 | OMG | C4-N3 | 6.33 | 1.49 | 1.34 |
| 70 | L5 | 3867 | A2M | O4'-C4' | -6.32 | 1.30 | 1.45 |
| 70 | L5 | 2424 | OMG | C4-N3 | 6.32 | 1.49 | 1.34 |
| 74 | S2 | 1639 | G7M | C4-N3 | 6.32 | 1.49 | 1.34 |
| 74 | S2 | 1490 | OMG | C4-N3 | 6.32 | 1.49 | 1.34 |
| 70 | L5 | 4618 | OMG | C4-N3 | 6.31 | 1.49 | 1.34 |
| 74 | S2 | 27 | A2M | O4'-C4' | -6.31 | 1.30 | 1.45 |
| 70 | L5 | 3899 | OMG | C4-N3 | 6.31 | 1.49 | 1.34 |
| 70 | L5 | 1522 | OMG | C4-N3 | 6.31 | 1.49 | 1.34 |
| 74 | S2 | 517 | OMC | C2-N3 | 6.31 | 1.49 | 1.36 |
| 70 | L5 | 4637 | OMG | C4-N3 | 6.31 | 1.49 | 1.34 |
| 70 | L5 | 2364 | OMG | C4-N3 | 6.29 | 1.49 | 1.34 |
| 70 | L5 | 4228 | OMG | C4-N3 | 6.28 | 1.49 | 1.34 |
| 70 | L5 | 4536 | OMC | C2-N3 | 6.27 | 1.49 | 1.36 |
| 74 | S2 | 468 | A2M | O4'-C4' | -6.27 | 1.31 | 1.45 |
| 70 | L5 | 2815 | A2M | O4'-C4' | -6.27 | 1.31 | 1.45 |
| 70 | L5 | 2824 | OMC | C2-N3 | 6.27 | 1.49 | 1.36 |
| 74 | S2 | 1391 | OMC | C2-N3 | 6.27 | 1.49 | 1.36 |
| 70 | L5 | 3841 | OMC | C2-N3 | 6.26 | 1.49 | 1.36 |
| 70 | L5 | 398 | A2M | O4'-C4' | -6.25 | 1.31 | 1.45 |
| 70 | L5 | 3782 | 5MC | C2-N3 | 6.25 | 1.49 | 1.36 |
| 70 | L5 | 3869 | OMC | C2-N3 | 6.25 | 1.49 | 1.36 |
| 70 | L5 | 2861 | OMC | C2-N3 | 6.24 | 1.49 | 1.36 |
| 70 | L5 | 1340 | OMC | C2-N3 | 6.24 | 1.49 | 1.36 |
| 74 | S2 | 436 | OMG | C4-N3 | 6.24 | 1.49 | 1.34 |
| 70 | L5 | 2804 | OMC | C2-N3 | 6.23 | 1.49 | 1.36 |
| 70 | L5 | 3785 | A2M | O4'-C4' | -6.23 | 1.31 | 1.45 |
| 70 | L5 | 3718 | A2M | O4'-C4' | -6.23 | 1.31 | 1.45 |
| 74 | S2 | 576 | A2M | O4'-C4' | -6.23 | 1.31 | 1.45 |
| 74 | S2 | 1703 | OMC | C2-N3 | 6.22 | 1.49 | 1.36 |
| 70 | L5 | 4447 | 5MC | C4-N3 | 6.22 | 1.44 | 1.34 |
| 70 | L5 | 2401 | A2M | O4'-C4' | -6.20 | 1.31 | 1.45 |
| 74 | S2 | 512 | A2M | O4'-C4' | -6.19 | 1.31 | 1.45 |
| 70 | L5 | 3887 | OMC | C2-N3 | 6.18 | 1.48 | 1.36 |
| 74 | S2 | 1383 | A2M | O4'-C4' | -6.17 | 1.31 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 70 | L5 | 2422 | OMC | C2-N3 | 6.15 | 1.48 | 1.36 |
| 70 | L5 | 4530 | UR3 | C6-C5 | 6.15 | 1.49 | 1.35 |
| 70 | L5 | 2365 | OMC | C2-N3 | 6.15 | 1.48 | 1.36 |
| 70 | L5 | 4456 | OMC | C2-N3 | 6.14 | 1.48 | 1.36 |
| 70 | L5 | 3830 | A2M | O4'-C4' | -6.14 | 1.31 | 1.45 |
| 74 | S2 | 1337 | 4AC | C7-N4 | 6.14 | 1.48 | 1.37 |
| 67 | Pt | 21 | H2U | C2-N3 | 6.09 | 1.48 | 1.38 |
| 70 | L5 | 1881 | OMC | C6-C5 | 6.08 | 1.49 | 1.35 |
| 70 | L5 | 1881 | OMC | C2-N3 | 6.06 | 1.48 | 1.36 |
| 70 | L5 | 3808 | OMC | C2-N3 | 6.05 | 1.48 | 1.36 |
| 70 | L5 | 3701 | OMC | C2-N3 | 6.05 | 1.48 | 1.36 |
| 70 | L5 | 2351 | OMC | C2-N3 | 6.04 | 1.48 | 1.36 |
| 70 | L5 | 4447 | 5MC | C2-N3 | 6.04 | 1.48 | 1.36 |
| 74 | S2 | 1703 | OMC | C6-C5 | 6.04 | 1.49 | 1.35 |
| 70 | L5 | 2824 | OMC | C6-C5 | 6.02 | 1.49 | 1.35 |
| 74 | S2 | 1248 | B8N | C2-N1 | 6.00 | 1.57 | 1.39 |
| 70 | L5 | 3701 | OMC | C6-C5 | 5.98 | 1.49 | 1.35 |
| 70 | L5 | 2861 | OMC | C6-C5 | 5.98 | 1.48 | 1.35 |
| 70 | L5 | 4536 | OMC | C6-C5 | 5.97 | 1.48 | 1.35 |
| 74 | S2 | 517 | OMC | C6-C5 | 5.97 | 1.48 | 1.35 |
| 70 | L5 | 3887 | OMC | C6-C5 | 5.96 | 1.48 | 1.35 |
| 74 | S2 | 462 | OMC | C6-C5 | 5.96 | 1.48 | 1.35 |
| 70 | L5 | 2422 | OMC | C6-C5 | 5.96 | 1.48 | 1.35 |
| 70 | L5 | 2365 | OMC | C6-C5 | 5.94 | 1.48 | 1.35 |
| 74 | S2 | 1391 | OMC | C6-C5 | 5.94 | 1.48 | 1.35 |
| 70 | L5 | 3869 | OMC | C6-C5 | 5.94 | 1.48 | 1.35 |
| 70 | L5 | 2351 | OMC | C6-C5 | 5.93 | 1.48 | 1.35 |
| 70 | L5 | 2804 | OMC | C6-C5 | 5.93 | 1.48 | 1.35 |
| 67 | Pt | 33 | OMC | C6-C5 | 5.89 | 1.48 | 1.35 |
| 70 | L5 | 4456 | OMC | C6-C5 | 5.87 | 1.48 | 1.35 |
| 70 | L5 | 1340 | OMC | C6-C5 | 5.87 | 1.48 | 1.35 |
| 70 | L5 | 3841 | OMC | C6-C5 | 5.86 | 1.48 | 1.35 |
| 70 | L5 | 3808 | OMC | C6-C5 | 5.83 | 1.48 | 1.35 |
| 74 | S2 | 1337 | 4AC | C2-N3 | 5.79 | 1.48 | 1.36 |
| 74 | S2 | 1804 | OMU | C6-C5 | 5.73 | 1.48 | 1.35 |
| 74 | S2 | 627 | OMU | C6-C5 | 5.72 | 1.48 | 1.35 |
| 70 | L5 | 4498 | OMU | C6-C5 | 5.65 | 1.48 | 1.35 |
| 74 | S2 | 116 | OMU | C6-C5 | 5.64 | 1.48 | 1.35 |
| 70 | L5 | 1625 | OMG | C2-N3 | 5.63 | 1.46 | 1.33 |
| 70 | L5 | 2837 | OMU | C6-C5 | 5.61 | 1.48 | 1.35 |
| 74 | S2 | 1842 | 4AC | C7-N4 | 5.60 | 1.47 | 1.37 |
| 70 | L5 | 3925 | OMU | C6-C5 | 5.60 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 70 | L5 | 4620 | OMU | C6-C5 | 5.57 | 1.48 | 1.35 |
| 70 | L5 | 4227 | OMU | C6-C5 | 5.56 | 1.48 | 1.35 |
| 70 | L5 | 4499 | OMG | C2-N3 | 5.53 | 1.46 | 1.33 |
| 74 | S2 | 428 | OMU | C6-C5 | 5.52 | 1.47 | 1.35 |
| 74 | S2 | 1842 | 4AC | C2-N3 | 5.52 | 1.47 | 1.36 |
| 70 | L5 | 2876 | OMG | C2-N3 | 5.51 | 1.46 | 1.33 |
| 70 | L5 | 3627 | OMG | C2-N3 | 5.51 | 1.46 | 1.33 |
| 69 | L8 | 75 | OMG | C2-N3 | 5.50 | 1.46 | 1.33 |
| 70 | L5 | 2424 | OMG | C2-N3 | 5.50 | 1.46 | 1.33 |
| 70 | L5 | 4623 | OMG | C2-N3 | 5.49 | 1.46 | 1.33 |
| 74 | S2 | 644 | OMG | C2-N3 | 5.49 | 1.46 | 1.33 |
| 70 | L5 | 4637 | OMG | C2-N3 | 5.48 | 1.46 | 1.33 |
| 70 | L5 | 4494 | OMG | C2-N3 | 5.48 | 1.46 | 1.33 |
| 70 | L5 | 4196 | OMG | C2-N3 | 5.48 | 1.46 | 1.33 |
| 70 | L5 | 3744 | OMG | C2-N3 | 5.47 | 1.46 | 1.33 |
| 74 | S2 | 1328 | OMG | C2-N3 | 5.46 | 1.46 | 1.33 |
| 74 | S2 | 683 | OMG | C2-N3 | 5.45 | 1.46 | 1.33 |
| 67 | Pt | 8 | 4SU | C6-C5 | 5.45 | 1.47 | 1.35 |
| 70 | L5 | 4370 | OMG | C2-N3 | 5.44 | 1.46 | 1.33 |
| 74 | S2 | 509 | OMG | C2-N3 | 5.43 | 1.46 | 1.33 |
| 70 | L5 | 4618 | OMG | C2-N3 | 5.43 | 1.46 | 1.33 |
| 70 | L5 | 4228 | OMG | C2-N3 | 5.41 | 1.46 | 1.33 |
| 74 | S2 | 867 | OMG | C2-N3 | 5.41 | 1.46 | 1.33 |
| 70 | L5 | 4392 | OMG | C2-N3 | 5.40 | 1.46 | 1.33 |
| 70 | L5 | 1522 | OMG | C2-N3 | 5.40 | 1.46 | 1.33 |
| 70 | L5 | 1316 | OMG | C2-N3 | 5.39 | 1.46 | 1.33 |
| 74 | S2 | 1639 | G7M | C2-N3 | 5.37 | 1.46 | 1.33 |
| 74 | S2 | 1490 | OMG | C2-N3 | 5.36 | 1.46 | 1.33 |
| 70 | L5 | 3899 | OMG | C2-N3 | 5.36 | 1.46 | 1.33 |
| 70 | L5 | 2364 | OMG | C2-N3 | 5.32 | 1.46 | 1.33 |
| 67 | Pt | 47 | G7M | C2-N3 | 5.32 | 1.46 | 1.33 |
| 70 | L5 | 4530 | UR3 | C2-N3 | 5.32 | 1.49 | 1.39 |
| 74 | S2 | 436 | OMG | C2-N3 | 5.31 | 1.46 | 1.33 |
| 70 | L5 | 3792 | OMG | C2-N3 | 5.29 | 1.45 | 1.33 |
| 70 | L5 | 2824 | OMC | C4-N3 | 5.17 | 1.44 | 1.34 |
| 70 | L5 | 3869 | OMC | C4-N3 | 5.14 | 1.44 | 1.34 |
| 74 | S2 | 462 | OMC | C4-N3 | 5.13 | 1.44 | 1.34 |
| 74 | S2 | 1391 | OMC | C4-N3 | 5.10 | 1.44 | 1.34 |
| 74 | S2 | 517 | OMC | C4-N3 | 5.09 | 1.44 | 1.34 |
| 67 | Pt | 33 | OMC | C4-N3 | 5.07 | 1.44 | 1.34 |
| 70 | L5 | 3841 | OMC | C4-N3 | 5.06 | 1.44 | 1.34 |
| 74 | S2 | 1703 | OMC | C4-N3 | 5.05 | 1.44 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 70 | L5 | 2422 | OMC | C4-N3 | 5.04 | 1.44 | 1.34 |
| 70 | L5 | 4536 | OMC | C4-N3 | 5.04 | 1.44 | 1.34 |
| 67 | Pt | 33 | OMC | C4-N4 | 5.02 | 1.45 | 1.33 |
| 70 | L5 | 3808 | OMC | C4-N4 | 5.01 | 1.45 | 1.33 |
| 70 | L5 | 2804 | OMC | C4-N3 | 5.01 | 1.44 | 1.34 |
| 70 | L5 | 3887 | OMC | C4-N3 | 5.01 | 1.44 | 1.34 |
| 70 | L5 | 2365 | OMC | C4-N3 | 5.00 | 1.44 | 1.34 |
| 70 | L5 | 4447 | 5MC | C6-N1 | 4.97 | 1.46 | 1.38 |
| 74 | S2 | 462 | OMC | C4-N4 | 4.97 | 1.45 | 1.33 |
| 70 | L5 | 2861 | OMC | C4-N3 | 4.97 | 1.44 | 1.34 |
| 70 | L5 | 1340 | OMC | C4-N3 | 4.97 | 1.44 | 1.34 |
| 70 | L5 | 2422 | OMC | C4-N4 | 4.97 | 1.45 | 1.33 |
| 74 | S2 | 517 | OMC | C4-N4 | 4.94 | 1.45 | 1.33 |
| 70 | L5 | 3869 | OMC | C4-N4 | 4.94 | 1.45 | 1.33 |
| 74 | S2 | 1703 | OMC | C4-N4 | 4.94 | 1.45 | 1.33 |
| 70 | L5 | 3701 | OMC | C4-N3 | 4.93 | 1.44 | 1.34 |
| 70 | L5 | 2824 | OMC | C4-N4 | 4.93 | 1.45 | 1.33 |
| 70 | L5 | 3808 | OMC | C4-N3 | 4.92 | 1.44 | 1.34 |
| 70 | L5 | 3887 | OMC | C4-N4 | 4.92 | 1.45 | 1.33 |
| 70 | L5 | 2861 | OMC | C4-N4 | 4.91 | 1.45 | 1.33 |
| 70 | L5 | 4456 | OMC | C4-N4 | 4.90 | 1.45 | 1.33 |
| 70 | L5 | 1881 | OMC | C4-N3 | 4.89 | 1.44 | 1.34 |
| 70 | L5 | 3841 | OMC | C4-N4 | 4.89 | 1.45 | 1.33 |
| 70 | L5 | 2804 | OMC | C4-N4 | 4.89 | 1.45 | 1.33 |
| 74 | S2 | 1391 | OMC | C4-N4 | 4.89 | 1.45 | 1.33 |
| 70 | L5 | 4536 | OMC | C4-N4 | 4.89 | 1.45 | 1.33 |
| 70 | L5 | 1881 | OMC | C4-N4 | 4.88 | 1.45 | 1.33 |
| 70 | L5 | 3701 | OMC | C4-N4 | 4.87 | 1.45 | 1.33 |
| 67 | Pt | 47 | G7M | C2-N2 | 4.87 | 1.45 | 1.34 |
| 70 | L5 | 4456 | OMC | C4-N3 | 4.87 | 1.44 | 1.34 |
| 70 | L5 | 1340 | OMC | C4-N4 | 4.86 | 1.45 | 1.33 |
| 70 | L5 | 2351 | OMC | C4-N3 | 4.83 | 1.44 | 1.34 |
| 70 | L5 | 2351 | OMC | C4-N4 | 4.82 | 1.45 | 1.33 |
| 70 | L5 | 2365 | OMC | C4-N4 | 4.81 | 1.45 | 1.33 |
| 74 | S2 | 1639 | G7M | C2-N2 | 4.80 | 1.45 | 1.34 |
| 67 | Pt | 33 | OMC | C2-N1 | 4.80 | 1.50 | 1.40 |
| 67 | Pt | 21 | H2U | C4-N3 | 4.79 | 1.45 | 1.37 |
| 70 | L5 | 3627 | OMG | C2-N2 | 4.79 | 1.45 | 1.34 |
| 70 | L5 | 3782 | 5MC | C6-N1 | 4.78 | 1.46 | 1.38 |
| 67 | Pt | 8 | 4SU | C4-S4 | -4.76 | 1.59 | 1.68 |
| 70 | L5 | 2424 | OMG | C2-N2 | 4.75 | 1.45 | 1.34 |
| 70 | L5 | 1625 | OMG | C2-N2 | 4.75 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 69 | L8 | 75 | OMG | C2-N2 | 4.75 | 1.45 | 1.34 |
| 74 | S2 | 683 | OMG | C2-N2 | 4.74 | 1.45 | 1.34 |
| 74 | S2 | 867 | OMG | C2-N2 | 4.73 | 1.45 | 1.34 |
| 70 | L5 | 4499 | OMG | C2-N2 | 4.72 | 1.45 | 1.34 |
| 74 | S2 | 1328 | OMG | C2-N2 | 4.72 | 1.45 | 1.34 |
| 70 | L5 | 4370 | OMG | C2-N2 | 4.72 | 1.45 | 1.34 |
| 74 | S2 | 1490 | OMG | C2-N2 | 4.72 | 1.45 | 1.34 |
| 70 | L5 | 4618 | OMG | C2-N2 | 4.71 | 1.45 | 1.34 |
| 74 | S2 | 644 | OMG | C2-N2 | 4.71 | 1.45 | 1.34 |
| 70 | L5 | 3744 | OMG | C2-N2 | 4.70 | 1.45 | 1.34 |
| 70 | L5 | 4494 | OMG | C2-N2 | 4.70 | 1.45 | 1.34 |
| 70 | L5 | 2364 | OMG | C2-N2 | 4.68 | 1.45 | 1.34 |
| 70 | L5 | 2351 | OMC | C2-N1 | 4.68 | 1.50 | 1.40 |
| 70 | L5 | 3792 | OMG | C2-N2 | 4.67 | 1.45 | 1.34 |
| 70 | L5 | 4228 | OMG | C2-N2 | 4.67 | 1.45 | 1.34 |
| 70 | L5 | 2876 | OMG | C2-N2 | 4.67 | 1.45 | 1.34 |
| 70 | L5 | 3899 | OMG | C2-N2 | 4.65 | 1.45 | 1.34 |
| 70 | L5 | 4392 | OMG | C2-N2 | 4.64 | 1.45 | 1.34 |
| 70 | L5 | 1316 | OMG | C2-N2 | 4.63 | 1.45 | 1.34 |
| 74 | S2 | 1337 | 4AC | C5-C4 | 4.62 | 1.50 | 1.40 |
| 70 | L5 | 4623 | OMG | C2-N2 | 4.61 | 1.45 | 1.34 |
| 70 | L5 | 4571 | A2M | C6-N6 | 4.61 | 1.45 | 1.34 |
| 70 | L5 | 4196 | OMG | C2-N2 | 4.60 | 1.45 | 1.34 |
| 74 | S2 | 436 | OMG | C2-N2 | 4.60 | 1.45 | 1.34 |
| 70 | L5 | 1522 | OMG | C2-N2 | 4.60 | 1.45 | 1.34 |
| 74 | S2 | 509 | OMG | C2-N2 | 4.59 | 1.45 | 1.34 |
| 74 | S2 | 1639 | G7M | C5-N7 | -4.58 | 1.33 | 1.39 |
| 70 | L5 | 3808 | OMC | C2-N1 | 4.57 | 1.49 | 1.40 |
| 70 | L5 | 4637 | OMG | C2-N2 | 4.56 | 1.45 | 1.34 |
| 70 | L5 | 3760 | A2M | C6-N6 | 4.53 | 1.45 | 1.34 |
| 74 | S2 | 1842 | 4AC | O2-C2 | -4.52 | 1.15 | 1.23 |
| 70 | L5 | 2824 | OMC | C2-N1 | 4.51 | 1.49 | 1.40 |
| 74 | S2 | 468 | A2M | C6-N6 | 4.51 | 1.45 | 1.34 |
| 70 | L5 | 3841 | OMC | C2-N1 | 4.51 | 1.49 | 1.40 |
| 74 | S2 | 517 | OMC | C2-N1 | 4.51 | 1.49 | 1.40 |
| 70 | L5 | 4456 | OMC | C2-N1 | 4.50 | 1.49 | 1.40 |
| 70 | L5 | 1524 | A2M | C6-N6 | 4.50 | 1.45 | 1.34 |
| 74 | S2 | 1678 | A2M | C6-N6 | 4.49 | 1.45 | 1.34 |
| 74 | S2 | 462 | OMC | C2-N1 | 4.49 | 1.49 | 1.40 |
| 70 | L5 | 2815 | A2M | C6-N6 | 4.49 | 1.45 | 1.34 |
| 74 | S2 | 590 | A2M | C6-N6 | 4.48 | 1.45 | 1.34 |
| 70 | L5 | 2422 | OMC | C2-N1 | 4.48 | 1.49 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 74 | S2 | 1391 | OMC | C2-N1 | 4.47 | 1.49 | 1.40 |
| 70 | L5 | 4447 | 5MC | C4-N4 | 4.47 | 1.45 | 1.34 |
| 74 | S2 | 668 | A2M | C6-N6 | 4.47 | 1.45 | 1.34 |
| 70 | L5 | 1881 | OMC | C2-N1 | 4.46 | 1.49 | 1.40 |
| 70 | L5 | 1871 | A2M | C6-N6 | 4.46 | 1.45 | 1.34 |
| 70 | L5 | 4590 | A2M | C6-N6 | 4.46 | 1.45 | 1.34 |
| 70 | L5 | 3869 | OMC | C2-N1 | 4.45 | 1.49 | 1.40 |
| 74 | S2 | 512 | A2M | C6-N6 | 4.45 | 1.45 | 1.34 |
| 74 | S2 | 576 | A2M | C6-N6 | 4.45 | 1.45 | 1.34 |
| 67 | Pt | 47 | G7M | C5-N7 | -4.45 | 1.34 | 1.39 |
| 74 | S2 | 1703 | OMC | C2-N1 | 4.45 | 1.49 | 1.40 |
| 74 | S2 | 484 | A2M | C6-N6 | 4.45 | 1.45 | 1.34 |
| 70 | L5 | 398 | A2M | C6-N6 | 4.44 | 1.45 | 1.34 |
| 74 | S2 | 99 | A2M | C6-N6 | 4.44 | 1.45 | 1.34 |
| 70 | L5 | 3887 | OMC | C2-N1 | 4.43 | 1.49 | 1.40 |
| 70 | L5 | 2861 | OMC | C2-N1 | 4.43 | 1.49 | 1.40 |
| 70 | L5 | 4536 | OMC | C2-N1 | 4.43 | 1.49 | 1.40 |
| 70 | L5 | 3782 | 5MC | C4-N4 | 4.42 | 1.45 | 1.34 |
| 70 | L5 | 1534 | A2M | C6-N6 | 4.42 | 1.45 | 1.34 |
| 74 | S2 | 27 | A2M | C6-N6 | 4.41 | 1.45 | 1.34 |
| 70 | L5 | 4523 | A2M | C6-N6 | 4.40 | 1.45 | 1.34 |
| 70 | L5 | 2401 | A2M | C6-N6 | 4.40 | 1.45 | 1.34 |
| 70 | L5 | 400 | A2M | C6-N6 | 4.39 | 1.45 | 1.34 |
| 67 | Pt | 8 | 4SU | C5-C4 | 4.39 | 1.48 | 1.42 |
| 70 | L5 | 3718 | A2M | C6-N6 | 4.38 | 1.45 | 1.34 |
| 70 | L5 | 3867 | A2M | C6-N6 | 4.37 | 1.45 | 1.34 |
| 70 | L5 | 3825 | A2M | C6-N6 | 4.37 | 1.45 | 1.34 |
| 74 | S2 | 1842 | 4AC | C5-C4 | 4.35 | 1.50 | 1.40 |
| 74 | S2 | 1842 | 4AC | C2-N1 | 4.35 | 1.49 | 1.40 |
| 70 | L5 | 2363 | A2M | C6-N6 | 4.34 | 1.45 | 1.34 |
| 70 | L5 | 3782 | 5MC | C2-N1 | 4.33 | 1.49 | 1.40 |
| 70 | L5 | 3830 | A2M | C6-N6 | 4.33 | 1.45 | 1.34 |
| 70 | L5 | 1340 | OMC | C2-N1 | 4.33 | 1.49 | 1.40 |
| 74 | S2 | 1383 | A2M | C6-N6 | 4.33 | 1.45 | 1.34 |
| 74 | S2 | 1031 | A2M | C6-N6 | 4.29 | 1.44 | 1.34 |
| 70 | L5 | 1326 | A2M | C6-N6 | 4.29 | 1.44 | 1.34 |
| 74 | S2 | 1337 | 4AC | O2-C2 | -4.29 | 1.15 | 1.23 |
| 70 | L5 | 3701 | OMC | C2-N1 | 4.27 | 1.49 | 1.40 |
| 65 | La | 39 | V5N | CD2-NE2 | -4.22 | 1.31 | 1.37 |
| 70 | L5 | 3785 | A2M | C6-N6 | 4.22 | 1.44 | 1.34 |
| 74 | S2 | 1337 | 4AC | C2-N1 | 4.22 | 1.49 | 1.40 |
| 70 | L5 | 2804 | OMC | C2-N1 | 4.21 | 1.49 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 70 | L5 | 2365 | OMC | C2-N1 | 4.20 | 1.49 | 1.40 |
| 74 | S2 | 627 | OMU | C4-N3 | 4.18 | 1.46 | 1.38 |
| 74 | S2 | 1804 | OMU | C4-N3 | 4.11 | 1.45 | 1.38 |
| 74 | S2 | 1337 | 4AC | C4-N4 | 4.11 | 1.45 | 1.39 |
| 64 | LA | 216 | V5N | CD2-NE2 | -4.10 | 1.31 | 1.37 |
| 70 | L5 | 4447 | 5MC | C2-N1 | 4.07 | 1.48 | 1.40 |
| 74 | S2 | 428 | OMU | C4-N3 | 4.03 | 1.45 | 1.38 |
| 74 | S2 | 116 | OMU | C4-N3 | 4.01 | 1.45 | 1.38 |
| 70 | L5 | 4227 | OMU | C4-N3 | 3.99 | 1.45 | 1.38 |
| 70 | L5 | 4498 | OMU | C4-N3 | 3.93 | 1.45 | 1.38 |
| 70 | L5 | 1322 | 1MA | C2-N1 | 3.92 | 1.43 | 1.35 |
| 70 | L5 | 2837 | OMU | C4-N3 | 3.92 | 1.45 | 1.38 |
| 70 | L5 | 3925 | OMU | C4-N3 | 3.89 | 1.45 | 1.38 |
| 70 | L5 | 4620 | OMU | C4-N3 | 3.87 | 1.45 | 1.38 |
| 67 | Pt | 47 | G7M | C5-C6 | 3.84 | 1.54 | 1.43 |
| 74 | S2 | 1639 | G7M | C5-C6 | 3.82 | 1.54 | 1.43 |
| 70 | L5 | 1322 | 1MA | C5-C6 | 3.81 | 1.53 | 1.43 |
| 74 | S2 | 1851 | MA6 | C6-N6 | 3.79 | 1.48 | 1.36 |
| 74 | S2 | 1850 | MA6 | C6-N6 | 3.77 | 1.48 | 1.36 |
| 70 | L5 | 3762 | PSU | C6-C5 | 3.73 | 1.39 | 1.35 |
| 74 | S2 | 801 | PSU | C6-C5 | 3.70 | 1.39 | 1.35 |
| 70 | L5 | 4431 | PSU | C6-C5 | 3.63 | 1.39 | 1.35 |
| 70 | L5 | 3853 | PSU | C6-C5 | 3.62 | 1.39 | 1.35 |
| 70 | L5 | 1781 | PSU | C6-C5 | 3.62 | 1.39 | 1.35 |
| 70 | L5 | 4420 | PSU | C6-C5 | 3.61 | 1.39 | 1.35 |
| 74 | S2 | 866 | PSU | C6-C5 | 3.60 | 1.39 | 1.35 |
| 74 | S2 | 1842 | 4AC | C4-N4 | 3.60 | 1.45 | 1.39 |
| 74 | S2 | 1248 | B8N | C1'-C5 | 3.57 | 1.58 | 1.50 |
| 70 | L5 | 5010 | PSU | C6-C5 | 3.56 | 1.39 | 1.35 |
| 70 | L5 | 4532 | PSU | C6-C5 | 3.55 | 1.39 | 1.35 |
| 70 | L5 | 4500 | PSU | C6-C5 | 3.52 | 1.39 | 1.35 |
| 70 | L5 | 3729 | PSU | C6-C5 | 3.51 | 1.39 | 1.35 |
| 70 | L5 | 4423 | PSU | C6-C5 | 3.51 | 1.39 | 1.35 |
| 74 | S2 | 1004 | PSU | C6-C5 | 3.50 | 1.39 | 1.35 |
| 70 | L5 | 4673 | PSU | C6-C5 | 3.50 | 1.39 | 1.35 |
| 70 | L5 | 1683 | PSU | C6-C5 | 3.49 | 1.39 | 1.35 |
| 70 | L5 | 4471 | PSU | C6-C5 | 3.48 | 1.39 | 1.35 |
| 74 | S2 | 109 | PSU | C6-C5 | 3.48 | 1.39 | 1.35 |
| 74 | S2 | 105 | PSU | C6-C5 | 3.47 | 1.39 | 1.35 |
| 74 | S2 | 1243 | PSU | C6-C5 | 3.47 | 1.39 | 1.35 |
| 74 | S2 | 1232 | PSU | C6-C5 | 3.46 | 1.39 | 1.35 |
| 69 | L8 | 55 | PSU | C6-C5 | 3.46 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 70 | L5 | 4521 | PSU | C6-C5 | 3.46 | 1.39 | 1.35 |
| 67 | Pt | 56 | PSU | C6-C5 | 3.45 | 1.39 | 1.35 |
| 70 | L5 | 3884 | PSU | C6-C5 | 3.45 | 1.39 | 1.35 |
| 70 | L5 | 4293 | PSU | C6-C5 | 3.44 | 1.39 | 1.35 |
| 70 | L5 | 3920 | PSU | C6-C5 | 3.44 | 1.39 | 1.35 |
| 70 | L5 | 3637 | PSU | C6-C5 | 3.44 | 1.39 | 1.35 |
| 70 | L5 | 1860 | PSU | C6-C5 | 3.43 | 1.39 | 1.35 |
| 74 | S2 | 1244 | PSU | C6-C5 | 3.43 | 1.39 | 1.35 |
| 74 | S2 | 119 | PSU | C6-C5 | 3.42 | 1.39 | 1.35 |
| 74 | S2 | 918 | PSU | C6-C5 | 3.42 | 1.39 | 1.35 |
| 70 | L5 | 2632 | PSU | C6-C5 | 3.42 | 1.39 | 1.35 |
| 70 | L5 | 4493 | PSU | C6-C5 | 3.41 | 1.39 | 1.35 |
| 70 | L5 | 1792 | PSU | C6-C5 | 3.41 | 1.39 | 1.35 |
| 70 | L5 | 2839 | PSU | C6-C5 | 3.41 | 1.39 | 1.35 |
| 70 | L5 | 4636 | PSU | C6-C5 | 3.40 | 1.39 | 1.35 |
| 70 | L5 | 1316 | OMG | C5-N7 | -3.39 | 1.32 | 1.39 |
| 70 | L5 | 1536 | PSU | C6-C5 | 3.39 | 1.39 | 1.35 |
| 70 | L5 | 1744 | PSU | C6-C5 | 3.39 | 1.39 | 1.35 |
| 70 | L5 | 4689 | PSU | C6-C5 | 3.38 | 1.39 | 1.35 |
| 74 | S2 | 651 | PSU | C6-C5 | 3.38 | 1.39 | 1.35 |
| 74 | S2 | 1625 | PSU | C6-C5 | 3.38 | 1.39 | 1.35 |
| 74 | S2 | 1445 | PSU | C6-C5 | 3.38 | 1.39 | 1.35 |
| 70 | L5 | 4569 | PSU | C6-C5 | 3.37 | 1.39 | 1.35 |
| 74 | S2 | 1842 | 4AC | C6-N1 | 3.37 | 1.46 | 1.38 |
| 70 | L5 | 4972 | PSU | C6-C5 | 3.36 | 1.39 | 1.35 |
| 74 | S2 | 1174 | PSU | C6-C5 | 3.36 | 1.39 | 1.35 |
| 70 | L5 | 4196 | OMG | C5-N7 | -3.36 | 1.32 | 1.39 |
| 74 | S2 | 34 | PSU | C6-C5 | 3.36 | 1.39 | 1.35 |
| 70 | L5 | 3792 | OMG | C5-N7 | -3.35 | 1.32 | 1.39 |
| 74 | S2 | 1337 | 4AC | C6-N1 | 3.35 | 1.46 | 1.38 |
| 70 | L5 | 3715 | PSU | C6-C5 | 3.35 | 1.39 | 1.35 |
| 70 | L5 | 4299 | PSU | C6-C5 | 3.34 | 1.39 | 1.35 |
| 70 | L5 | 3695 | PSU | C6-C5 | 3.34 | 1.39 | 1.35 |
| 74 | S2 | 822 | PSU | C6-C5 | 3.33 | 1.39 | 1.35 |
| 70 | L5 | 4296 | PSU | C6-C5 | 3.33 | 1.39 | 1.35 |
| 70 | L5 | 4576 | PSU | C6-C5 | 3.33 | 1.39 | 1.35 |
| 70 | L5 | 1522 | OMG | C5-N7 | -3.33 | 1.32 | 1.39 |
| 70 | L5 | 4623 | OMG | C5-N7 | -3.33 | 1.32 | 1.39 |
| 70 | L5 | 1625 | OMG | C5-N7 | -3.33 | 1.32 | 1.39 |
| 74 | S2 | 1056 | PSU | C6-C5 | 3.33 | 1.39 | 1.35 |
| 74 | S2 | 218 | PSU | C6-C5 | 3.32 | 1.39 | 1.35 |
| 74 | S2 | 814 | PSU | C6-C5 | 3.32 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 74 | S2 | 649 | PSU | C6-C5 | 3.32 | 1.39 | 1.35 |
| 70 | L5 | 3851 | PSU | C6-C5 | 3.31 | 1.39 | 1.35 |
| 74 | S2 | 863 | PSU | C6-C5 | 3.31 | 1.39 | 1.35 |
| 70 | L5 | 4353 | PSU | C6-C5 | 3.31 | 1.39 | 1.35 |
| 70 | L5 | 4494 | OMG | C5-N7 | -3.31 | 1.32 | 1.39 |
| 70 | L5 | 2876 | OMG | C5-N7 | -3.30 | 1.32 | 1.39 |
| 70 | L5 | 4628 | PSU | C6-C5 | 3.30 | 1.39 | 1.35 |
| 70 | L5 | 2508 | PSU | C6-C5 | 3.30 | 1.39 | 1.35 |
| 70 | L5 | 2424 | OMG | C5-N7 | -3.30 | 1.32 | 1.39 |
| 70 | L5 | 4457 | PSU | C6-C5 | 3.30 | 1.39 | 1.35 |
| 70 | L5 | 4531 | PSU | C6-C5 | 3.30 | 1.39 | 1.35 |
| 74 | S2 | 1177 | PSU | C6-C5 | 3.30 | 1.39 | 1.35 |
| 74 | S2 | 1238 | PSU | C6-C5 | 3.29 | 1.39 | 1.35 |
| 74 | S2 | 509 | OMG | C5-N7 | -3.29 | 1.32 | 1.39 |
| 74 | S2 | 609 | PSU | C6-C5 | 3.29 | 1.39 | 1.35 |
| 74 | S2 | 1692 | PSU | C6-C5 | 3.29 | 1.39 | 1.35 |
| 74 | S2 | 1490 | OMG | C5-N7 | -3.28 | 1.32 | 1.39 |
| 70 | L5 | 3768 | PSU | C6-C5 | 3.28 | 1.39 | 1.35 |
| 74 | S2 | 1239 | PSU | C6-C5 | 3.27 | 1.39 | 1.35 |
| 70 | L5 | 3764 | PSU | C6-C5 | 3.27 | 1.39 | 1.35 |
| 70 | L5 | 4361 | PSU | C6-C5 | 3.27 | 1.39 | 1.35 |
| 70 | L5 | 2365 | OMC | C6-N1 | 3.26 | 1.45 | 1.38 |
| 74 | S2 | 436 | OMG | C5-N7 | -3.26 | 1.32 | 1.39 |
| 74 | S2 | 681 | PSU | C6-C5 | 3.26 | 1.39 | 1.35 |
| 70 | L5 | 1322 | 1MA | C5-N7 | -3.26 | 1.32 | 1.39 |
| 70 | L5 | 3627 | OMG | C5-N7 | -3.26 | 1.32 | 1.39 |
| 74 | S2 | 683 | OMG | C5-N7 | -3.26 | 1.32 | 1.39 |
| 70 | L5 | 3899 | OMG | C5-N7 | -3.25 | 1.32 | 1.39 |
| 70 | L5 | 1582 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 70 | L5 | 1779 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 70 | L5 | 1782 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 70 | L5 | 2804 | OMC | C6-N1 | 3.25 | 1.45 | 1.38 |
| 70 | L5 | 3887 | OMC | C6-N1 | 3.25 | 1.45 | 1.38 |
| 74 | S2 | 93 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 74 | S2 | 406 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 74 | S2 | 1643 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 74 | S2 | 1703 | OMC | C6-N1 | 3.24 | 1.45 | 1.38 |
| 70 | L5 | 4312 | PSU | C6-C5 | 3.24 | 1.39 | 1.35 |
| 74 | S2 | 644 | OMG | C5-N7 | -3.24 | 1.32 | 1.39 |
| 70 | L5 | 5001 | PSU | C6-C5 | 3.24 | 1.39 | 1.35 |
| 70 | L5 | 3758 | PSU | C6-C5 | 3.24 | 1.39 | 1.35 |
| 74 | S2 | 573 | PSU | C6-C5 | 3.24 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 74 | S2 | 1347 | PSU | C6-C5 | 3.23 | 1.39 | 1.35 |
| 70 | L5 | 2351 | OMC | C6-N1 | 3.23 | 1.45 | 1.38 |
| 70 | L5 | 4552 | PSU | C6-C5 | 3.23 | 1.39 | 1.35 |
| 70 | L5 | 3770 | PSU | C6-C5 | 3.22 | 1.39 | 1.35 |
| 70 | L5 | 2824 | OMC | C6-N1 | 3.22 | 1.45 | 1.38 |
| 70 | L5 | 3734 | PSU | C6-C5 | 3.22 | 1.39 | 1.35 |
| 70 | L5 | 3844 | PSU | C6-C5 | 3.22 | 1.39 | 1.35 |
| 69 | L8 | 69 | PSU | C6-C5 | 3.22 | 1.39 | 1.35 |
| 74 | S2 | 1367 | PSU | C6-C5 | 3.21 | 1.39 | 1.35 |
| 74 | S2 | 686 | PSU | C6-C5 | 3.21 | 1.39 | 1.35 |
| 70 | L5 | 1871 | A2M | O3'-C3' | -3.21 | 1.35 | 1.43 |
| 70 | L5 | 1881 | OMC | C6-N1 | 3.21 | 1.45 | 1.38 |
| 70 | L5 | 4579 | PSU | C6-C5 | 3.20 | 1.39 | 1.35 |
| 70 | L5 | 4618 | OMG | C5-N7 | -3.20 | 1.32 | 1.39 |
| 74 | S2 | 1136 | PSU | C6-C5 | 3.20 | 1.39 | 1.35 |
| 74 | S2 | 296 | PSU | C6-C5 | 3.20 | 1.39 | 1.35 |
| 70 | L5 | 3785 | A2M | C5-C4 | -3.19 | 1.33 | 1.39 |
| 70 | L5 | 1862 | PSU | C6-C5 | 3.19 | 1.39 | 1.35 |
| 70 | L5 | 2422 | OMC | C6-N1 | 3.19 | 1.45 | 1.38 |
| 70 | L5 | 3639 | PSU | C6-C5 | 3.19 | 1.39 | 1.35 |
| 70 | L5 | 2861 | OMC | C6-N1 | 3.19 | 1.45 | 1.38 |
| 74 | S2 | 572 | PSU | C6-C5 | 3.18 | 1.39 | 1.35 |
| 70 | L5 | 2843 | PSU | C6-C5 | 3.18 | 1.39 | 1.35 |
| 74 | S2 | 36 | PSU | C6-C5 | 3.18 | 1.39 | 1.35 |
| 70 | L5 | 3869 | OMC | C6-N1 | 3.17 | 1.45 | 1.38 |
| 74 | S2 | 517 | OMC | C6-N1 | 3.17 | 1.45 | 1.38 |
| 70 | L5 | 4370 | OMG | C5-N7 | -3.17 | 1.32 | 1.39 |
| 70 | L5 | 4392 | OMG | C5-N7 | -3.17 | 1.32 | 1.39 |
| 69 | L8 | 75 | OMG | C5-N7 | -3.16 | 1.32 | 1.39 |
| 70 | L5 | 4228 | OMG | C5-N7 | -3.16 | 1.32 | 1.39 |
| 70 | L5 | 4403 | PSU | C6-C5 | 3.16 | 1.39 | 1.35 |
| 70 | L5 | 2364 | OMG | C5-N7 | -3.16 | 1.33 | 1.39 |
| 70 | L5 | 3744 | OMG | C5-N7 | -3.15 | 1.33 | 1.39 |
| 70 | L5 | 4637 | OMG | C5-N7 | -3.15 | 1.33 | 1.39 |
| 74 | S2 | 1031 | A2M | C5-C4 | -3.14 | 1.33 | 1.39 |
| 70 | L5 | 3925 | OMU | O4-C4 | -3.14 | 1.18 | 1.24 |
| 70 | L5 | 4536 | OMC | C6-N1 | 3.14 | 1.45 | 1.38 |
| 74 | S2 | 966 | PSU | C6-C5 | 3.14 | 1.39 | 1.35 |
| 70 | L5 | 4499 | OMG | C5-N7 | -3.12 | 1.33 | 1.39 |
| 70 | L5 | 4442 | PSU | C6-C5 | 3.12 | 1.39 | 1.35 |
| 70 | L5 | 3841 | OMC | C6-N1 | 3.11 | 1.45 | 1.38 |
| 74 | S2 | 462 | OMC | C6-N1 | 3.11 | 1.45 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 74 | S2 | 1391 | OMC | C6-N1 | 3.11 | 1.45 | 1.38 |
| 70 | L5 | 1677 | PSU | C6-C5 | 3.10 | 1.38 | 1.35 |
| 70 | L5 | 3760 | A2M | O3'-C3' | -3.09 | 1.35 | 1.43 |
| 70 | L5 | 4530 | UR3 | C6-N1 | 3.09 | 1.45 | 1.38 |
| 70 | L5 | 2837 | OMU | O4-C4 | -3.09 | 1.18 | 1.24 |
| 70 | L5 | 3718 | A2M | O3'-C3' | -3.09 | 1.35 | 1.43 |
| 70 | L5 | 3701 | OMC | C6-N1 | 3.09 | 1.45 | 1.38 |
| 74 | S2 | 1328 | OMG | C5-N7 | -3.08 | 1.33 | 1.39 |
| 70 | L5 | 1326 | A2M | C5-C4 | -3.08 | 1.33 | 1.39 |
| 74 | S2 | 590 | A2M | O3'-C3' | -3.08 | 1.35 | 1.43 |
| 74 | S2 | 27 | A2M | O3'-C3' | -3.07 | 1.35 | 1.43 |
| 70 | L5 | 4456 | OMC | C6-N1 | 3.07 | 1.45 | 1.38 |
| 74 | S2 | 428 | OMU | O4-C4 | -3.06 | 1.18 | 1.24 |
| 70 | L5 | 3867 | A2M | O3'-C3' | -3.06 | 1.35 | 1.43 |
| 70 | L5 | 4571 | A2M | O3'-C3' | -3.06 | 1.35 | 1.43 |
| 70 | L5 | 1534 | A2M | O3'-C3' | -3.06 | 1.35 | 1.43 |
| 67 | Pt | 33 | OMC | C6-N1 | 3.05 | 1.45 | 1.38 |
| 70 | L5 | 4220 | 6MZ | C5-C4 | -3.05 | 1.33 | 1.39 |
| 74 | S2 | 815 | PSU | C6-C5 | 3.04 | 1.38 | 1.35 |
| 70 | L5 | 4498 | OMU | O4-C4 | -3.04 | 1.18 | 1.24 |
| 70 | L5 | 4620 | OMU | O4-C4 | -3.04 | 1.18 | 1.24 |
| 74 | S2 | 668 | A2M | C5-C4 | -3.03 | 1.33 | 1.39 |
| 70 | L5 | 3808 | OMC | C6-N1 | 3.03 | 1.45 | 1.38 |
| 70 | L5 | 1326 | A2M | O3'-C3' | -3.03 | 1.35 | 1.43 |
| 74 | S2 | 867 | OMG | C5-N7 | -3.03 | 1.33 | 1.39 |
| 74 | S2 | 1678 | A2M | O3'-C3' | -3.03 | 1.35 | 1.43 |
| 74 | S2 | 1031 | A2M | O3'-C3' | -3.02 | 1.35 | 1.43 |
| 70 | L5 | 4590 | A2M | O3'-C3' | -3.02 | 1.35 | 1.43 |
| 70 | L5 | 2363 | A2M | O3'-C3' | -3.02 | 1.35 | 1.43 |
| 70 | L5 | 400 | A2M | O3'-C3' | -3.02 | 1.35 | 1.43 |
| 74 | S2 | 468 | A2M | O3'-C3' | -3.01 | 1.35 | 1.43 |
| 70 | L5 | 3718 | A2M | C5-C4 | -3.00 | 1.33 | 1.39 |
| 70 | L5 | 1871 | A2M | C5-C4 | -3.00 | 1.33 | 1.39 |
| 74 | S2 | 1383 | A2M | O3'-C3' | -2.99 | 1.35 | 1.43 |
| 74 | S2 | 1678 | A2M | C5-C4 | -2.99 | 1.33 | 1.39 |
| 70 | L5 | 2363 | A2M | C5-C4 | -2.98 | 1.33 | 1.39 |
| 70 | L5 | 398 | A2M | O3'-C3' | -2.98 | 1.36 | 1.43 |
| 70 | L5 | 3825 | A2M | C5-C4 | -2.98 | 1.33 | 1.39 |
| 70 | L5 | 1340 | OMC | C6-N1 | 2.97 | 1.45 | 1.38 |
| 70 | L5 | 1524 | A2M | O3'-C3' | -2.97 | 1.36 | 1.43 |
| 70 | L5 | 3830 | A2M | C5-C4 | -2.97 | 1.33 | 1.39 |
| 70 | L5 | 3867 | A2M | C5-C4 | -2.96 | 1.33 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 70 | L5 | 3830 | A2M | O3'-C3' | -2.96 | 1.36 | 1.43 |
| 74 | S2 | 99 | A2M | O3'-C3' | -2.96 | 1.36 | 1.43 |
| 74 | S2 | 116 | OMU | O4-C4 | -2.95 | 1.18 | 1.24 |
| 74 | S2 | 484 | A2M | C5-C4 | -2.95 | 1.33 | 1.39 |
| 70 | L5 | 4227 | OMU | O4-C4 | -2.94 | 1.18 | 1.24 |
| 70 | L5 | 4220 | 6MZ | C5-N7 | -2.93 | 1.33 | 1.39 |
| 70 | L5 | 1534 | A2M | C5-C4 | -2.93 | 1.33 | 1.39 |
| 70 | L5 | 4523 | A2M | C5-C4 | -2.93 | 1.33 | 1.39 |
| 74 | S2 | 27 | A2M | C5-C4 | -2.92 | 1.33 | 1.39 |
| 74 | S2 | 468 | A2M | C5-C4 | -2.92 | 1.33 | 1.39 |
| 74 | S2 | 512 | A2M | C5-C4 | -2.92 | 1.33 | 1.39 |
| 70 | L5 | 1524 | A2M | C5-C4 | -2.91 | 1.33 | 1.39 |
| 70 | L5 | 2401 | A2M | O3'-C3' | -2.91 | 1.36 | 1.43 |
| 74 | S2 | 1804 | OMU | O4-C4 | -2.91 | 1.18 | 1.24 |
| 70 | L5 | 3825 | A2M | O3'-C3' | -2.91 | 1.36 | 1.43 |
| 70 | L5 | 2815 | A2M | O3'-C3' | -2.89 | 1.36 | 1.43 |
| 74 | S2 | 1804 | OMU | C6-N1 | 2.89 | 1.45 | 1.38 |
| 70 | L5 | 2815 | A2M | C5-C4 | -2.89 | 1.33 | 1.39 |
| 74 | S2 | 627 | OMU | O4-C4 | -2.88 | 1.18 | 1.24 |
| 74 | S2 | 576 | A2M | O3'-C3' | -2.88 | 1.36 | 1.43 |
| 74 | S2 | 668 | A2M | O2'-C2' | 2.88 | 1.50 | 1.42 |
| 70 | L5 | 400 | A2M | C5-C4 | -2.88 | 1.33 | 1.39 |
| 74 | S2 | 1031 | A2M | C5-N7 | -2.88 | 1.33 | 1.39 |
| 74 | S2 | 99 | A2M | C5-C4 | -2.88 | 1.33 | 1.39 |
| 70 | L5 | 2824 | OMC | O2-C2 | -2.88 | 1.18 | 1.23 |
| 70 | L5 | 1326 | A2M | O2'-C2' | 2.87 | 1.50 | 1.42 |
| 70 | L5 | 2401 | A2M | C5-C4 | -2.87 | 1.33 | 1.39 |
| 67 | Pt | 47 | G7M | C2-N1 | 2.87 | 1.44 | 1.37 |
| 74 | S2 | 512 | A2M | O3'-C3' | -2.87 | 1.36 | 1.43 |
| 70 | L5 | 4523 | A2M | O3'-C3' | -2.87 | 1.36 | 1.43 |
| 74 | S2 | 1678 | A2M | O2'-C2' | 2.86 | 1.50 | 1.42 |
| 74 | S2 | 1703 | OMC | O2-C2 | -2.86 | 1.18 | 1.23 |
| 70 | L5 | 398 | A2M | O2'-C2' | 2.85 | 1.49 | 1.42 |
| 74 | S2 | 1832 | 6MZ | C5-C4 | -2.85 | 1.33 | 1.39 |
| 74 | S2 | 576 | A2M | O2'-C2' | 2.85 | 1.49 | 1.42 |
| 74 | S2 | 627 | OMU | C6-N1 | 2.84 | 1.44 | 1.38 |
| 70 | L5 | 398 | A2M | C5-C4 | -2.84 | 1.33 | 1.39 |
| 70 | L5 | 4571 | A2M | C5-C4 | -2.84 | 1.33 | 1.39 |
| 74 | S2 | 668 | A2M | O3'-C3' | -2.83 | 1.36 | 1.43 |
| 74 | S2 | 1383 | A2M | C5-C4 | -2.83 | 1.33 | 1.39 |
| 70 | L5 | 2861 | OMC | O2-C2 | -2.83 | 1.18 | 1.23 |
| 70 | L5 | 4523 | A2M | C5-N7 | -2.83 | 1.33 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 70 | L5 | 3841 | OMC | O2-C2 | -2.82 | 1.18 | 1.23 |
| 74 | S2 | 484 | A2M | O3'-C3' | -2.82 | 1.36 | 1.43 |
| 70 | L5 | 2815 | A2M | O2'-C2' | 2.82 | 1.49 | 1.42 |
| 70 | L5 | 3701 | OMC | O2-C2 | -2.81 | 1.18 | 1.23 |
| 70 | L5 | 400 | A2M | O2'-C2' | 2.81 | 1.49 | 1.42 |
| 74 | S2 | 1383 | A2M | O2'-C2' | 2.81 | 1.49 | 1.42 |
| 74 | S2 | 512 | A2M | O2'-C2' | 2.81 | 1.49 | 1.42 |
| 70 | L5 | 4590 | A2M | C5-C4 | -2.81 | 1.33 | 1.39 |
| 70 | L5 | 3760 | A2M | O2'-C2' | 2.80 | 1.49 | 1.42 |
| 74 | S2 | 99 | A2M | O2'-C2' | 2.80 | 1.49 | 1.42 |
| 70 | L5 | 3825 | A2M | C5-N7 | -2.80 | 1.33 | 1.39 |
| 70 | L5 | 1881 | OMC | O2-C2 | -2.80 | 1.18 | 1.23 |
| 74 | S2 | 576 | A2M | C5-N7 | -2.79 | 1.33 | 1.39 |
| 74 | S2 | 484 | A2M | C5-N7 | -2.79 | 1.33 | 1.39 |
| 70 | L5 | 2815 | A2M | C5-N7 | -2.79 | 1.33 | 1.39 |
| 74 | S2 | 484 | A2M | O2'-C2' | 2.79 | 1.49 | 1.42 |
| 74 | S2 | 590 | A2M | O2'-C2' | 2.78 | 1.49 | 1.42 |
| 70 | L5 | 3869 | OMC | O2-C2 | -2.78 | 1.18 | 1.23 |
| 70 | L5 | 4498 | OMU | C6-N1 | 2.78 | 1.44 | 1.38 |
| 70 | L5 | 1534 | A2M | O2'-C2' | 2.78 | 1.49 | 1.42 |
| 70 | L5 | 3785 | A2M | O2'-C2' | 2.78 | 1.49 | 1.42 |
| 70 | L5 | 2804 | OMC | O2-C2 | -2.78 | 1.18 | 1.23 |
| 70 | L5 | 3760 | A2M | C5-C4 | -2.78 | 1.33 | 1.39 |
| 70 | L5 | 2365 | OMC | O2-C2 | -2.77 | 1.18 | 1.23 |
| 70 | L5 | 1340 | OMC | O2-C2 | -2.77 | 1.18 | 1.23 |
| 70 | L5 | 2422 | OMC | O2-C2 | -2.76 | 1.18 | 1.23 |
| 70 | L5 | 3867 | A2M | O2'-C2' | 2.76 | 1.49 | 1.42 |
| 70 | L5 | 2401 | A2M | C5-N7 | -2.76 | 1.33 | 1.39 |
| 70 | L5 | 3825 | A2M | O2'-C2' | 2.76 | 1.49 | 1.42 |
| 70 | L5 | 2363 | A2M | C5-N7 | -2.76 | 1.33 | 1.39 |
| 70 | L5 | 2401 | A2M | O2'-C2' | 2.76 | 1.49 | 1.42 |
| 70 | L5 | 4447 | 5MC | O2-C2 | -2.76 | 1.18 | 1.23 |
| 74 | S2 | 590 | A2M | C5-C4 | -2.75 | 1.33 | 1.39 |
| 74 | S2 | 512 | A2M | C5-N7 | -2.75 | 1.33 | 1.39 |
| 70 | L5 | 3925 | OMU | C6-N1 | 2.75 | 1.44 | 1.38 |
| 74 | S2 | 99 | A2M | C5-N7 | -2.74 | 1.33 | 1.39 |
| 70 | L5 | 4590 | A2M | O2'-C2' | 2.73 | 1.49 | 1.42 |
| 74 | S2 | 468 | A2M | O2'-C2' | 2.73 | 1.49 | 1.42 |
| 70 | L5 | 2351 | OMC | O2-C2 | -2.73 | 1.18 | 1.23 |
| 74 | S2 | 576 | A2M | C5-C4 | -2.73 | 1.33 | 1.39 |
| 74 | S2 | 1639 | G7M | C2-N1 | 2.73 | 1.44 | 1.37 |
| 70 | L5 | 3785 | A2M | O3'-C3' | -2.72 | 1.36 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 74 | S2 | 116 | OMU | C6-N1 | 2.72 | 1.44 | 1.38 |
| 70 | L5 | 4571 | A2M | O2'-C2' | 2.72 | 1.49 | 1.42 |
| 70 | L5 | 2837 | OMU | C6-N1 | 2.72 | 1.44 | 1.38 |
| 70 | L5 | 2363 | A2M | O2'-C2' | 2.72 | 1.49 | 1.42 |
| 70 | L5 | 4227 | OMU | C6-N1 | 2.72 | 1.44 | 1.38 |
| 74 | S2 | 517 | OMC | O2-C2 | -2.71 | 1.18 | 1.23 |
| 70 | L5 | 3830 | A2M | O2'-C2' | 2.71 | 1.49 | 1.42 |
| 70 | L5 | 1871 | A2M | O2'-C2' | 2.71 | 1.49 | 1.42 |
| 70 | L5 | 3718 | A2M | O2'-C2' | 2.71 | 1.49 | 1.42 |
| 70 | L5 | 4392 | OMG | O6-C6 | -2.71 | 1.18 | 1.23 |
| 70 | L5 | 1524 | A2M | C5-N7 | -2.71 | 1.33 | 1.39 |
| 70 | L5 | 3782 | 5MC | O2-C2 | -2.70 | 1.18 | 1.23 |
| 70 | L5 | 4523 | A2M | O2'-C2' | 2.70 | 1.49 | 1.42 |
| 70 | L5 | 1524 | A2M | O2'-C2' | 2.70 | 1.49 | 1.42 |
| 67 | Pt | 8 | 4SU | C6-N1 | 2.70 | 1.44 | 1.38 |
| 70 | L5 | 4456 | OMC | O2-C2 | -2.69 | 1.18 | 1.23 |
| 70 | L5 | 3808 | OMC | O2-C2 | -2.69 | 1.18 | 1.23 |
| 70 | L5 | 4571 | A2M | C5-N7 | -2.69 | 1.33 | 1.39 |
| 74 | S2 | 1391 | OMC | O2-C2 | -2.68 | 1.18 | 1.23 |
| 70 | L5 | 1316 | OMG | O6-C6 | -2.68 | 1.18 | 1.23 |
| 74 | S2 | 1383 | A2M | C5-N7 | -2.68 | 1.34 | 1.39 |
| 74 | S2 | 428 | OMU | C6-N1 | 2.68 | 1.44 | 1.38 |
| 70 | L5 | 1326 | A2M | C5-N7 | -2.68 | 1.34 | 1.39 |
| 70 | L5 | 3867 | A2M | C5-N7 | -2.67 | 1.34 | 1.39 |
| 74 | S2 | 436 | OMG | O6-C6 | -2.67 | 1.18 | 1.23 |
| 74 | S2 | 1850 | MA6 | C5-C4 | -2.67 | 1.34 | 1.39 |
| 74 | S2 | 1851 | MA6 | C5-C4 | -2.67 | 1.34 | 1.39 |
| 70 | L5 | 4196 | OMG | O6-C6 | -2.66 | 1.18 | 1.23 |
| 70 | L5 | 4536 | OMC | O2-C2 | -2.66 | 1.18 | 1.23 |
| 74 | S2 | 1081 | PSU | C6-C5 | 2.66 | 1.38 | 1.35 |
| 70 | L5 | 3785 | A2M | C5-N7 | -2.66 | 1.34 | 1.39 |
| 70 | L5 | 3887 | OMC | O2-C2 | -2.65 | 1.18 | 1.23 |
| 70 | L5 | 2424 | OMG | C2-N1 | 2.65 | 1.44 | 1.37 |
| 74 | S2 | 462 | OMC | O2-C2 | -2.65 | 1.18 | 1.23 |
| 70 | L5 | 4620 | OMU | C6-N1 | 2.64 | 1.44 | 1.38 |
| 74 | S2 | 27 | A2M | O2'-C2' | 2.64 | 1.49 | 1.42 |
| 74 | S2 | 867 | OMG | C2-N1 | 2.64 | 1.44 | 1.37 |
| 74 | S2 | 27 | A2M | C5-N7 | -2.64 | 1.34 | 1.39 |
| 70 | L5 | 1534 | A2M | C5-N7 | -2.64 | 1.34 | 1.39 |
| 70 | L5 | 2364 | OMG | O6-C6 | -2.63 | 1.18 | 1.23 |
| 70 | L5 | 1871 | A2M | C5-N7 | -2.63 | 1.34 | 1.39 |
| 70 | L5 | 2876 | OMG | O6-C6 | -2.63 | 1.18 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 70 | L5 | 4494 | OMG | O6-C6 | -2.63 | 1.18 | 1.23 |
| 70 | L5 | 4618 | OMG | O6-C6 | -2.63 | 1.18 | 1.23 |
| 70 | L5 | 3899 | OMG | O6-C6 | -2.63 | 1.18 | 1.23 |
| 70 | L5 | 3627 | OMG | O6-C6 | -2.62 | 1.18 | 1.23 |
| 70 | L5 | 2876 | OMG | C2-N1 | 2.62 | 1.44 | 1.37 |
| 70 | L5 | 3792 | OMG | O6-C6 | -2.62 | 1.18 | 1.23 |
| 67 | Pt | 33 | OMC | O2-C2 | -2.62 | 1.18 | 1.23 |
| 74 | S2 | 1678 | A2M | C5-N7 | -2.62 | 1.34 | 1.39 |
| 74 | S2 | 1832 | 6MZ | C5-N7 | -2.62 | 1.34 | 1.39 |
| 70 | L5 | 3744 | OMG | C2-N1 | 2.62 | 1.44 | 1.37 |
| 74 | S2 | 1328 | OMG | O6-C6 | -2.62 | 1.18 | 1.23 |
| 70 | L5 | 3760 | A2M | C5-N7 | -2.61 | 1.34 | 1.39 |
| 70 | L5 | 4494 | OMG | C2-N1 | 2.61 | 1.44 | 1.37 |
| 74 | S2 | 683 | OMG | C2-N1 | 2.61 | 1.44 | 1.37 |
| 70 | L5 | 4623 | OMG | O6-C6 | -2.61 | 1.18 | 1.23 |
| 70 | L5 | 4228 | OMG | O6-C6 | -2.60 | 1.18 | 1.23 |
| 74 | S2 | 644 | OMG | O6-C6 | -2.60 | 1.18 | 1.23 |
| 70 | L5 | 1522 | OMG | O6-C6 | -2.60 | 1.18 | 1.23 |
| 70 | L5 | 4590 | A2M | C5-N7 | -2.60 | 1.34 | 1.39 |
| 70 | L5 | 4499 | OMG | C2-N1 | 2.60 | 1.44 | 1.37 |
| 70 | L5 | 4637 | OMG | O6-C6 | -2.60 | 1.18 | 1.23 |
| 74 | S2 | 590 | A2M | C5-N7 | -2.60 | 1.34 | 1.39 |
| 69 | L8 | 75 | OMG | C2-N1 | 2.60 | 1.44 | 1.37 |
| 70 | L5 | 3718 | A2M | C5-N7 | -2.59 | 1.34 | 1.39 |
| 70 | L5 | 400 | A2M | C5-N7 | -2.59 | 1.34 | 1.39 |
| 70 | L5 | 3627 | OMG | C2-N1 | 2.59 | 1.44 | 1.37 |
| 74 | S2 | 1328 | OMG | C2-N1 | 2.59 | 1.44 | 1.37 |
| 70 | L5 | 4499 | OMG | O6-C6 | -2.59 | 1.18 | 1.23 |
| 74 | S2 | 683 | OMG | O6-C6 | -2.59 | 1.18 | 1.23 |
| 74 | S2 | 1851 | MA6 | C5-N7 | -2.59 | 1.34 | 1.39 |
| 70 | L5 | 4370 | OMG | O6-C6 | -2.59 | 1.18 | 1.23 |
| 74 | S2 | 509 | OMG | O6-C6 | -2.59 | 1.18 | 1.23 |
| 74 | S2 | 468 | A2M | C5-N7 | -2.59 | 1.34 | 1.39 |
| 70 | L5 | 1625 | OMG | C2-N1 | 2.58 | 1.44 | 1.37 |
| 70 | L5 | 3830 | A2M | C5-N7 | -2.58 | 1.34 | 1.39 |
| 67 | Pt | 47 | G7M | O6-C6 | -2.58 | 1.18 | 1.23 |
| 74 | S2 | 644 | OMG | C2-N1 | 2.58 | 1.44 | 1.37 |
| 70 | L5 | 4623 | OMG | C2-N1 | 2.58 | 1.44 | 1.37 |
| 74 | S2 | 1031 | A2M | O2'-C2' | 2.57 | 1.49 | 1.42 |
| 74 | S2 | 668 | A2M | C5-N7 | -2.57 | 1.34 | 1.39 |
| 70 | L5 | 1316 | OMG | C2-N1 | 2.57 | 1.44 | 1.37 |
| 70 | L5 | 4618 | OMG | C2-N1 | 2.57 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 74 | S2 | 1850 | MA6 | C5-N7 | -2.56 | 1.34 | 1.39 |
| 74 | S2 | 1490 | OMG | C2-N1 | 2.56 | 1.44 | 1.37 |
| 67 | Pt | 47 | G7M | C6-N1 | 2.56 | 1.43 | 1.38 |
| 70 | L5 | 4228 | OMG | C2-N1 | 2.55 | 1.44 | 1.37 |
| 70 | L5 | 1625 | OMG | O6-C6 | -2.55 | 1.18 | 1.23 |
| 74 | S2 | 1490 | OMG | O6-C6 | -2.55 | 1.18 | 1.23 |
| 70 | L5 | 3744 | OMG | O6-C6 | -2.55 | 1.18 | 1.23 |
| 74 | S2 | 436 | OMG | C2-N1 | 2.55 | 1.44 | 1.37 |
| 70 | L5 | 1522 | OMG | C2-N1 | 2.54 | 1.44 | 1.37 |
| 70 | L5 | 4370 | OMG | C2-N1 | 2.53 | 1.43 | 1.37 |
| 70 | L5 | 2364 | OMG | C2-N1 | 2.53 | 1.43 | 1.37 |
| 70 | L5 | 2424 | OMG | O6-C6 | -2.52 | 1.18 | 1.23 |
| 70 | L5 | 398 | A2M | C5-N7 | -2.52 | 1.34 | 1.39 |
| 74 | S2 | 1703 | OMC | C5-C4 | 2.52 | 1.48 | 1.42 |
| 70 | L5 | 4196 | OMG | C2-N1 | 2.52 | 1.43 | 1.37 |
| 70 | L5 | 4637 | OMG | C5-C6 | 2.51 | 1.53 | 1.44 |
| 70 | L5 | 3792 | OMG | C2-N1 | 2.51 | 1.43 | 1.37 |
| 74 | S2 | 867 | OMG | C5-C6 | 2.51 | 1.53 | 1.44 |
| 70 | L5 | 4637 | OMG | C2-N1 | 2.50 | 1.43 | 1.37 |
| 70 | L5 | 3899 | OMG | C2-N1 | 2.50 | 1.43 | 1.37 |
| 70 | L5 | 4228 | OMG | C5-C6 | 2.49 | 1.53 | 1.44 |
| 69 | L8 | 75 | OMG | O6-C6 | -2.49 | 1.18 | 1.23 |
| 70 | L5 | 2422 | OMC | C5-C4 | 2.49 | 1.48 | 1.42 |
| 70 | L5 | 1522 | OMG | C5-C6 | 2.48 | 1.53 | 1.44 |
| 74 | S2 | 1639 | G7M | O6-C6 | -2.47 | 1.18 | 1.23 |
| 74 | S2 | 867 | OMG | O6-C6 | -2.47 | 1.18 | 1.23 |
| 74 | S2 | 1639 | G7M | C6-N1 | 2.47 | 1.43 | 1.38 |
| 70 | L5 | 2824 | OMC | C5-C4 | 2.46 | 1.48 | 1.42 |
| 70 | L5 | 2876 | OMG | C5-C6 | 2.46 | 1.53 | 1.44 |
| 70 | L5 | 2424 | OMG | C5-C6 | 2.45 | 1.53 | 1.44 |
| 70 | L5 | 4498 | OMU | O2-C2 | -2.45 | 1.18 | 1.23 |
| 70 | L5 | 3701 | OMC | C5-C4 | 2.45 | 1.48 | 1.42 |
| 70 | L5 | 3925 | OMU | O2-C2 | -2.45 | 1.18 | 1.23 |
| 70 | L5 | 4620 | OMU | O2-C2 | -2.44 | 1.18 | 1.23 |
| 70 | L5 | 3744 | OMG | C5-C6 | 2.44 | 1.53 | 1.44 |
| 70 | L5 | 4392 | OMG | C5-C6 | 2.44 | 1.53 | 1.44 |
| 70 | L5 | 3825 | A2M | C8-N9 | -2.44 | 1.33 | 1.37 |
| 69 | L8 | 75 | OMG | C5-C6 | 2.44 | 1.53 | 1.44 |
| 70 | L5 | 4392 | OMG | C2-N1 | 2.43 | 1.43 | 1.37 |
| 74 | S2 | 517 | OMC | C5-C4 | 2.43 | 1.48 | 1.42 |
| 74 | S2 | 509 | OMG | C2-N1 | 2.43 | 1.43 | 1.37 |
| 70 | L5 | 1881 | OMC | C5-C4 | 2.43 | 1.48 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 74 | S2 | 1031 | A2M | C8-N9 | -2.42 | 1.33 | 1.37 |
| 70 | L5 | 2804 | OMC | C5-C4 | 2.42 | 1.48 | 1.42 |
| 74 | S2 | 116 | OMU | O2-C2 | -2.41 | 1.18 | 1.23 |
| 70 | L5 | 4227 | OMU | O2-C2 | -2.41 | 1.18 | 1.23 |
| 74 | S2 | 644 | OMG | C5-C6 | 2.41 | 1.53 | 1.44 |
| 74 | S2 | 1328 | OMG | C5-C6 | 2.41 | 1.53 | 1.44 |
| 70 | L5 | 4623 | OMG | C5-C6 | 2.41 | 1.53 | 1.44 |
| 74 | S2 | 1490 | OMG | C5-C6 | 2.41 | 1.53 | 1.44 |
| 74 | S2 | 867 | OMG | C6-N1 | 2.40 | 1.43 | 1.38 |
| 70 | L5 | 4499 | OMG | C5-C6 | 2.40 | 1.53 | 1.44 |
| 69 | L8 | 75 | OMG | C6-N1 | 2.40 | 1.43 | 1.38 |
| 70 | L5 | 2364 | OMG | C5-C6 | 2.39 | 1.53 | 1.44 |
| 70 | L5 | 2861 | OMC | C5-C4 | 2.39 | 1.48 | 1.42 |
| 70 | L5 | 3627 | OMG | C5-C6 | 2.39 | 1.53 | 1.44 |
| 70 | L5 | 2837 | OMU | O2-C2 | -2.38 | 1.18 | 1.23 |
| 70 | L5 | 1625 | OMG | C5-C6 | 2.38 | 1.53 | 1.44 |
| 70 | L5 | 2365 | OMC | C5-C4 | 2.37 | 1.48 | 1.42 |
| 74 | S2 | 462 | OMC | C5-C4 | 2.37 | 1.48 | 1.42 |
| 70 | L5 | 3899 | OMG | C5-C6 | 2.37 | 1.53 | 1.44 |
| 74 | S2 | 428 | OMU | O2-C2 | -2.37 | 1.18 | 1.23 |
| 70 | L5 | 1316 | OMG | C5-C6 | 2.36 | 1.53 | 1.44 |
| 74 | S2 | 1804 | OMU | O2-C2 | -2.36 | 1.18 | 1.23 |
| 70 | L5 | 4618 | OMG | C5-C6 | 2.36 | 1.53 | 1.44 |
| 70 | L5 | 3869 | OMC | C5-C4 | 2.35 | 1.48 | 1.42 |
| 70 | L5 | 3744 | OMG | C6-N1 | 2.35 | 1.43 | 1.38 |
| 74 | S2 | 627 | OMU | C5-C4 | 2.35 | 1.48 | 1.43 |
| 74 | S2 | 1248 | B8N | O2-C2 | -2.35 | 1.18 | 1.22 |
| 70 | L5 | 4196 | OMG | C5-C6 | 2.34 | 1.53 | 1.44 |
| 70 | L5 | 4370 | OMG | C5-C6 | 2.34 | 1.53 | 1.44 |
| 74 | S2 | 509 | OMG | C5-C6 | 2.34 | 1.53 | 1.44 |
| 74 | S2 | 683 | OMG | C6-N1 | 2.34 | 1.43 | 1.38 |
| 70 | L5 | 4536 | OMC | C5-C4 | 2.34 | 1.48 | 1.42 |
| 74 | S2 | 683 | OMG | C5-C6 | 2.34 | 1.53 | 1.44 |
| 74 | S2 | 436 | OMG | C5-C6 | 2.33 | 1.53 | 1.44 |
| 70 | L5 | 2424 | OMG | C6-N1 | 2.33 | 1.43 | 1.38 |
| 70 | L5 | 1522 | OMG | C6-N1 | 2.33 | 1.43 | 1.38 |
| 74 | S2 | 1248 | B8N | O4-C4 | -2.33 | 1.18 | 1.23 |
| 70 | L5 | 2876 | OMG | C6-N1 | 2.33 | 1.43 | 1.38 |
| 70 | L5 | 4530 | UR3 | C5-C4 | 2.33 | 1.49 | 1.43 |
| 70 | L5 | 4494 | OMG | C5-C6 | 2.32 | 1.53 | 1.44 |
| 70 | L5 | 4220 | 6MZ | C8-N9 | -2.31 | 1.33 | 1.37 |
| 70 | L5 | 3887 | OMC | C5-C4 | 2.31 | 1.48 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 70 | L5 | 4456 | OMC | C5-C4 | 2.31 | 1.48 | 1.42 |
| 70 | L5 | 4623 | OMG | C6-N1 | 2.31 | 1.43 | 1.38 |
| 70 | L5 | 3808 | OMC | C5-C4 | 2.30 | 1.48 | 1.42 |
| 74 | S2 | 627 | OMU | O2-C2 | -2.30 | 1.18 | 1.23 |
| 70 | L5 | 3792 | OMG | C5-C6 | 2.30 | 1.52 | 1.44 |
| 74 | S2 | 1804 | OMU | C5-C4 | 2.30 | 1.48 | 1.43 |
| 74 | S2 | 1678 | A2M | C8-N9 | -2.30 | 1.33 | 1.37 |
| 70 | L5 | 4499 | OMG | C6-N1 | 2.29 | 1.43 | 1.38 |
| 70 | L5 | 1340 | OMC | C5-C4 | 2.29 | 1.48 | 1.42 |
| 74 | S2 | 1328 | OMG | C6-N1 | 2.29 | 1.43 | 1.38 |
| 70 | L5 | 4618 | OMG | C6-N1 | 2.29 | 1.43 | 1.38 |
| 70 | L5 | 4228 | OMG | C6-N1 | 2.28 | 1.43 | 1.38 |
| 74 | S2 | 1391 | OMC | C5-C4 | 2.28 | 1.48 | 1.42 |
| 70 | L5 | 3841 | OMC | C5-C4 | 2.28 | 1.48 | 1.42 |
| 74 | S2 | 644 | OMG | C6-N1 | 2.27 | 1.43 | 1.38 |
| 70 | L5 | 4370 | OMG | C6-N1 | 2.27 | 1.43 | 1.38 |
| 70 | L5 | 1316 | OMG | C6-N1 | 2.27 | 1.43 | 1.38 |
| 70 | L5 | 1625 | OMG | C6-N1 | 2.27 | 1.43 | 1.38 |
| 74 | S2 | 484 | A2M | C8-N9 | -2.27 | 1.33 | 1.37 |
| 70 | L5 | 4227 | OMU | C5-C4 | 2.27 | 1.48 | 1.43 |
| 67 | Pt | 21 | H2U | O4-C4 | -2.26 | 1.18 | 1.23 |
| 70 | L5 | 4498 | OMU | C5-C4 | 2.26 | 1.48 | 1.43 |
| 70 | L5 | 3792 | OMG | C6-N1 | 2.26 | 1.43 | 1.38 |
| 70 | L5 | 1534 | A2M | C8-N9 | -2.26 | 1.33 | 1.37 |
| 70 | L5 | 4494 | OMG | C6-N1 | 2.26 | 1.43 | 1.38 |
| 70 | L5 | 1322 | 1MA | C4-N9 | -2.25 | 1.32 | 1.38 |
| 70 | L5 | 2363 | A2M | C8-N9 | -2.25 | 1.33 | 1.37 |
| 74 | S2 | 1490 | OMG | C6-N1 | 2.25 | 1.43 | 1.38 |
| 70 | L5 | 2364 | OMG | C6-N1 | 2.25 | 1.43 | 1.38 |
| 74 | S2 | 436 | OMG | C6-N1 | 2.24 | 1.43 | 1.38 |
| 70 | L5 | 2837 | OMU | C5-C4 | 2.23 | 1.48 | 1.43 |
| 67 | Pt | 21 | H2U | O2-C2 | -2.22 | 1.19 | 1.23 |
| 70 | L5 | 2351 | OMC | C5-C4 | 2.21 | 1.48 | 1.42 |
| 67 | Pt | 33 | OMC | C5-C4 | 2.21 | 1.48 | 1.42 |
| 70 | L5 | 2401 | A2M | C8-N9 | -2.21 | 1.33 | 1.37 |
| 70 | L5 | 4196 | OMG | C6-N1 | 2.21 | 1.42 | 1.38 |
| 70 | L5 | 3830 | A2M | C8-N9 | -2.21 | 1.33 | 1.37 |
| 70 | L5 | 3760 | A2M | C8-N9 | -2.20 | 1.33 | 1.37 |
| 74 | S2 | 116 | OMU | C5-C4 | 2.20 | 1.48 | 1.43 |
| 74 | S2 | 99 | A2M | C8-N9 | -2.20 | 1.33 | 1.37 |
| 70 | L5 | 4637 | OMG | C6-N1 | 2.20 | 1.42 | 1.38 |
| 70 | L5 | 3718 | A2M | C8-N9 | -2.19 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 74 | S2 | 590 | A2M | C8-N9 | -2.19 | 1.33 | 1.37 |
| 70 | L5 | 3867 | A2M | C8-N9 | -2.19 | 1.33 | 1.37 |
| 70 | L5 | 1524 | A2M | C8-N9 | -2.18 | 1.33 | 1.37 |
| 70 | L5 | 4523 | A2M | C8-N9 | -2.18 | 1.33 | 1.37 |
| 74 | S2 | 668 | A2M | C8-N9 | -2.18 | 1.33 | 1.37 |
| 70 | L5 | 3627 | OMG | C6-N1 | 2.17 | 1.42 | 1.38 |
| 74 | S2 | 27 | A2M | C8-N9 | -2.17 | 1.33 | 1.37 |
| 70 | L5 | 2815 | A2M | C8-N9 | -2.17 | 1.33 | 1.37 |
| 70 | L5 | 4620 | OMU | C5-C4 | 2.16 | 1.48 | 1.43 |
| 74 | S2 | 512 | A2M | C8-N9 | -2.16 | 1.33 | 1.37 |
| 70 | L5 | 3925 | OMU | C5-C4 | 2.16 | 1.48 | 1.43 |
| 74 | S2 | 1832 | 6MZ | C8-N9 | -2.16 | 1.33 | 1.37 |
| 74 | S2 | 1850 | MA6 | C8-N9 | -2.16 | 1.33 | 1.37 |
| 70 | L5 | 1871 | A2M | C8-N9 | -2.15 | 1.33 | 1.37 |
| 70 | L5 | 4590 | A2M | C8-N9 | -2.15 | 1.33 | 1.37 |
| 70 | L5 | 3785 | A2M | C8-N9 | -2.15 | 1.33 | 1.37 |
| 74 | S2 | 1851 | MA6 | C8-N9 | -2.15 | 1.33 | 1.37 |
| 67 | Pt | 47 | G7M | C4-N9 | -2.14 | 1.32 | 1.38 |
| 74 | S2 | 1248 | B8N | C2-N3 | 2.14 | 1.42 | 1.38 |
| 74 | S2 | 822 | PSU | O4'-C1' | -2.14 | 1.40 | 1.43 |
| 74 | S2 | 428 | OMU | C5-C4 | 2.14 | 1.48 | 1.43 |
| 70 | L5 | 1524 | A2M | O5'-C5' | -2.13 | 1.39 | 1.44 |
| 70 | L5 | 3899 | OMG | C6-N1 | 2.13 | 1.42 | 1.38 |
| 74 | S2 | 576 | A2M | C8-N9 | -2.13 | 1.33 | 1.37 |
| 74 | S2 | 509 | OMG | C6-N1 | 2.12 | 1.42 | 1.38 |
| 70 | L5 | 4571 | A2M | C8-N9 | -2.10 | 1.33 | 1.37 |
| 70 | L5 | 4392 | OMG | C6-N1 | 2.10 | 1.42 | 1.38 |
| 70 | L5 | 400 | A2M | C8-N9 | -2.09 | 1.33 | 1.37 |
| 70 | L5 | 398 | A2M | C8-N9 | -2.07 | 1.33 | 1.37 |
| 70 | L5 | 4530 | UR3 | O4-C4 | -2.07 | 1.19 | 1.23 |
| 74 | S2 | 1383 | A2M | O5'-C5' | -2.07 | 1.39 | 1.44 |
| 70 | L5 | 1326 | A2M | C8-N9 | -2.07 | 1.33 | 1.37 |
| 74 | S2 | 918 | PSU | O4'-C1' | -2.07 | 1.41 | 1.43 |
| 70 | L5 | 4530 | UR3 | O2-C2 | -2.07 | 1.18 | 1.22 |
| 74 | S2 | 668 | A2M | O5'-C5' | -2.06 | 1.39 | 1.44 |
| 70 | L5 | 4228 | OMG | C4-N9 | -2.05 | 1.32 | 1.38 |
| 70 | L5 | 1326 | A2M | O5'-C5' | -2.05 | 1.39 | 1.44 |
| 70 | L5 | 2401 | A2M | O5'-C5' | -2.03 | 1.39 | 1.44 |
| 70 | L5 | 3825 | A2M | O5'-C5' | -2.02 | 1.39 | 1.44 |
| 74 | S2 | 27 | A2M | O5'-C5' | -2.02 | 1.39 | 1.44 |
| 74 | S2 | 468 | A2M | C8-N9 | -2.01 | 1.33 | 1.37 |
| 74 | S2 | 512 | A2M | O5'-C5' | -2.01 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 74 | S2 | 1639 | G7M | C4-N9 | -2.01 | 1.32 | 1.38 |

All (1125) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 74 | S2 | 1851 | MA6 | N1-C6-N6 | -15.79 | 99.82 | 117.08 |
| 74 | S2 | 1850 | MA6 | N1-C6-N6 | -15.05 | 100.62 | 117.08 |
| 70 | L5 | 1322 | 1MA | C1'-N9-C8 | -9.09 | 100.81 | 126.70 |
| 74 | S2 | 1851 | MA6 | C5-C6-N6 | 8.87 | 140.75 | 125.30 |
| 70 | L5 | 1322 | 1MA | C1'-N9-C4 | 8.83 | 152.73 | 126.50 |
| 74 | S2 | 1850 | MA6 | C5-C6-N6 | 8.43 | 139.98 | 125.30 |
| 67 | Pt | 8 | 4SU | C4-N3-C2 | -7.71 | 119.85 | 127.34 |
| 74 | S2 | 1639 | G7M | C1'-N9-C4 | 7.34 | 148.29 | 126.50 |
| 67 | Pt | 47 | G7M | C1'-N9-C8 | -7.31 | 102.07 | 126.74 |
| 74 | S2 | 1639 | G7M | C1'-N9-C8 | -7.26 | 102.24 | 126.74 |
| 67 | Pt | 47 | G7M | C1'-N9-C4 | 7.04 | 147.42 | 126.50 |
| 67 | Pt | 21 | H2U | C4-N3-C2 | -6.56 | 120.35 | 125.79 |
| 74 | S2 | 590 | A2M | C5-C4-N3 | -6.02 | 118.90 | 126.75 |
| 70 | L5 | 2876 | OMG | C5-C4-N3 | -6.01 | 118.71 | 128.46 |
| 70 | L5 | 3830 | A2M | N3-C2-N1 | -5.83 | 119.48 | 128.60 |
| 74 | S2 | 512 | A2M | N3-C2-N1 | -5.79 | 119.54 | 128.60 |
| 70 | L5 | 4590 | A2M | N3-C2-N1 | -5.78 | 119.56 | 128.60 |
| 70 | L5 | 3760 | A2M | C5-C4-N3 | -5.77 | 119.22 | 126.75 |
| 70 | L5 | 1322 | 1MA | N1-C2-N3 | -5.75 | 119.16 | 126.00 |
| 74 | S2 | 512 | A2M | C5-C4-N3 | -5.75 | 119.25 | 126.75 |
| 74 | S2 | 1031 | A2M | N3-C2-N1 | -5.73 | 119.64 | 128.60 |
| 70 | L5 | 1871 | A2M | N3-C2-N1 | -5.69 | 119.70 | 128.60 |
| 70 | L5 | 1625 | OMG | C5-C4-N3 | -5.68 | 119.25 | 128.46 |
| 74 | S2 | 668 | A2M | N3-C2-N1 | -5.67 | 119.72 | 128.60 |
| 70 | L5 | 4637 | OMG | C5-C4-N3 | -5.67 | 119.26 | 128.46 |
| 70 | L5 | 1534 | A2M | N3-C2-N1 | -5.67 | 119.74 | 128.60 |
| 70 | L5 | 2815 | A2M | C5-C4-N3 | -5.67 | 119.36 | 126.75 |
| 74 | S2 | 1678 | A2M | C5-C4-N3 | -5.66 | 119.37 | 126.75 |
| 70 | L5 | 2363 | A2M | N3-C2-N1 | -5.64 | 119.78 | 128.60 |
| 74 | S2 | 1850 | MA6 | N1-C2-N3 | -5.62 | 119.81 | 128.60 |
| 70 | L5 | 400 | A2M | N3-C2-N1 | -5.59 | 119.85 | 128.60 |
| 74 | S2 | 1678 | A2M | N3-C2-N1 | -5.59 | 119.85 | 128.60 |
| 70 | L5 | 1326 | A2M | N3-C2-N1 | -5.59 | 119.86 | 128.60 |
| 74 | S2 | 683 | OMG | C5-C4-N3 | -5.58 | 119.40 | 128.46 |
| 70 | L5 | 2401 | A2M | C5-C4-N3 | -5.58 | 119.47 | 126.75 |
| 74 | S2 | 644 | OMG | C5-C4-N3 | -5.58 | 119.42 | 128.46 |
| 70 | L5 | 3792 | OMG | C5-C4-N3 | -5.57 | 119.42 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 74 | S2 | 468 | A2M | N3-C2-N1 | -5.56 | 119.90 | 128.60 |
| 74 | S2 | 484 | A2M | N3-C2-N1 | -5.56 | 119.90 | 128.60 |
| 74 | S2 | 590 | A2M | N3-C2-N1 | -5.56 | 119.91 | 128.60 |
| 67 | Pt | 8 | 4SU | C5-C4-N3 | 5.56 | 119.84 | 114.69 |
| 74 | S2 | 1383 | A2M | N3-C2-N1 | -5.56 | 119.91 | 128.60 |
| 70 | L5 | 4571 | A2M | N3-C2-N1 | -5.53 | 119.95 | 128.60 |
| 74 | S2 | 509 | OMG | C5-C4-N3 | -5.53 | 119.50 | 128.46 |
| 74 | S2 | 1851 | MA6 | N1-C2-N3 | -5.52 | 119.96 | 128.60 |
| 74 | S2 | 27 | A2M | N3-C2-N1 | -5.52 | 119.97 | 128.60 |
| 70 | L5 | 3760 | A2M | N3-C2-N1 | -5.51 | 119.97 | 128.60 |
| 74 | S2 | 1031 | A2M | C5-C4-N3 | -5.51 | 119.56 | 126.75 |
| 74 | S2 | 99 | A2M | N3-C2-N1 | -5.51 | 119.98 | 128.60 |
| 70 | L5 | 4618 | OMG | C5-C4-N3 | -5.51 | 119.52 | 128.46 |
| 70 | L5 | 3825 | A2M | C5-C4-N3 | -5.51 | 119.56 | 126.75 |
| 70 | L5 | 3718 | A2M | N3-C2-N1 | -5.50 | 120.00 | 128.60 |
| 70 | L5 | 3825 | A2M | N3-C2-N1 | -5.50 | 120.00 | 128.60 |
| 70 | L5 | 1524 | A2M | N3-C2-N1 | -5.48 | 120.03 | 128.60 |
| 70 | L5 | 4196 | OMG | C5-C4-N3 | -5.48 | 119.58 | 128.46 |
| 74 | S2 | 27 | A2M | C5-C4-N3 | -5.47 | 119.61 | 126.75 |
| 74 | S2 | 1851 | MA6 | C5-C4-N3 | -5.46 | 119.62 | 126.75 |
| 70 | L5 | 4523 | A2M | C5-C4-N3 | -5.46 | 119.62 | 126.75 |
| 70 | L5 | 2401 | A2M | N3-C2-N1 | -5.46 | 120.07 | 128.60 |
| 70 | L5 | 3830 | A2M | C5-C4-N3 | -5.45 | 119.64 | 126.75 |
| 70 | L5 | 4523 | A2M | N3-C2-N1 | -5.45 | 120.07 | 128.60 |
| 70 | L5 | 2815 | A2M | N3-C2-N1 | -5.45 | 120.08 | 128.60 |
| 70 | L5 | 4392 | OMG | C5-C4-N3 | -5.43 | 119.66 | 128.46 |
| 70 | L5 | 3785 | A2M | C5-C4-N3 | -5.42 | 119.68 | 126.75 |
| 70 | L5 | 2364 | OMG | C5-C4-N3 | -5.42 | 119.67 | 128.46 |
| 70 | L5 | 3785 | A2M | N3-C2-N1 | -5.42 | 120.13 | 128.60 |
| 70 | L5 | 4623 | OMG | C5-C4-N3 | -5.41 | 119.68 | 128.46 |
| 70 | L5 | 398 | A2M | N3-C2-N1 | -5.41 | 120.14 | 128.60 |
| 70 | L5 | 3867 | A2M | C5-C4-N3 | -5.40 | 119.70 | 126.75 |
| 74 | S2 | 99 | A2M | C5-C4-N3 | -5.39 | 119.71 | 126.75 |
| 70 | L5 | 3899 | OMG | C5-C4-N3 | -5.38 | 119.74 | 128.46 |
| 74 | S2 | 1383 | A2M | C5-C4-N3 | -5.37 | 119.74 | 126.75 |
| 70 | L5 | 4494 | OMG | C5-C4-N3 | -5.36 | 119.76 | 128.46 |
| 74 | S2 | 1490 | OMG | C5-C4-N3 | -5.36 | 119.76 | 128.46 |
| 74 | S2 | 484 | A2M | C5-C4-N3 | -5.36 | 119.76 | 126.75 |
| 70 | L5 | 3627 | OMG | C5-C4-N3 | -5.36 | 119.77 | 128.46 |
| 70 | L5 | 1524 | A2M | C5-C4-N3 | -5.36 | 119.76 | 126.75 |
| 74 | S2 | 576 | A2M | C5-C4-N3 | -5.35 | 119.77 | 126.75 |
| 70 | L5 | 400 | A2M | C5-C4-N3 | -5.35 | 119.78 | 126.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 70 | L5 | 3744 | OMG | C5-C4-N3 | -5.34 | 119.79 | 128.46 |
| 70 | L5 | 3718 | A2M | C5-C4-N3 | -5.34 | 119.78 | 126.75 |
| 70 | L5 | 2837 | OMU | C4-N3-C2 | -5.34 | 119.54 | 126.58 |
| 70 | L5 | 2424 | OMG | C5-C4-N3 | -5.34 | 119.80 | 128.46 |
| 70 | L5 | 398 | A2M | C5-C4-N3 | -5.33 | 119.79 | 126.75 |
| 70 | L5 | 4227 | OMU | C4-N3-C2 | -5.33 | 119.55 | 126.58 |
| 70 | L5 | 4498 | OMU | C4-N3-C2 | -5.32 | 119.56 | 126.58 |
| 70 | L5 | 4590 | A2M | C5-C4-N3 | -5.31 | 119.83 | 126.75 |
| 70 | L5 | 3867 | A2M | N3-C2-N1 | -5.30 | 120.31 | 128.60 |
| 70 | L5 | 3925 | OMU | C4-N3-C2 | -5.30 | 119.59 | 126.58 |
| 70 | L5 | 4220 | 6MZ | N1-C2-N3 | -5.30 | 120.31 | 128.60 |
| 74 | S2 | 627 | OMU | C4-N3-C2 | -5.30 | 119.59 | 126.58 |
| 74 | S2 | 428 | OMU | C4-N3-C2 | -5.30 | 119.59 | 126.58 |
| 74 | S2 | 576 | A2M | N3-C2-N1 | -5.29 | 120.33 | 128.60 |
| 70 | L5 | 4499 | OMG | C5-C4-N3 | -5.28 | 119.89 | 128.46 |
| 74 | S2 | 436 | OMG | C5-C4-N3 | -5.28 | 119.89 | 128.46 |
| 70 | L5 | 1316 | OMG | C5-C4-N3 | -5.27 | 119.91 | 128.46 |
| 74 | S2 | 1850 | MA6 | C5-C4-N3 | -5.27 | 119.88 | 126.75 |
| 70 | L5 | 1522 | OMG | C5-C4-N3 | -5.26 | 119.92 | 128.46 |
| 70 | L5 | 2363 | A2M | C5-C4-N3 | -5.26 | 119.89 | 126.75 |
| 74 | S2 | 1328 | OMG | C5-C4-N3 | -5.24 | 119.95 | 128.46 |
| 70 | L5 | 1326 | A2M | C5-C4-N3 | -5.24 | 119.91 | 126.75 |
| 74 | S2 | 668 | A2M | C5-C4-N3 | -5.24 | 119.92 | 126.75 |
| 69 | L8 | 75 | OMG | C5-C4-N3 | -5.23 | 119.97 | 128.46 |
| 70 | L5 | 1534 | A2M | C5-C4-N3 | -5.23 | 119.93 | 126.75 |
| 74 | S2 | 1832 | 6MZ | N1-C2-N3 | -5.22 | 120.43 | 128.60 |
| 74 | S2 | 468 | A2M | C5-C4-N3 | -5.21 | 119.96 | 126.75 |
| 70 | L5 | 4370 | OMG | C5-C4-N3 | -5.19 | 120.04 | 128.46 |
| 70 | L5 | 4571 | A2M | C5-C4-N3 | -5.18 | 119.99 | 126.75 |
| 74 | S2 | 1248 | B8N | C5-C4-N3 | 5.18 | 125.76 | 116.17 |
| 70 | L5 | 3867 | A2M | N6-C6-N1 | -5.17 | 107.03 | 118.35 |
| 74 | S2 | 1804 | OMU | C4-N3-C2 | -5.16 | 119.78 | 126.58 |
| 74 | S2 | 867 | OMG | C5-C4-N3 | -5.14 | 120.13 | 128.46 |
| 74 | S2 | 1678 | A2M | N6-C6-N1 | -5.13 | 107.12 | 118.35 |
| 74 | S2 | 512 | A2M | N6-C6-N1 | -5.08 | 107.22 | 118.35 |
| 70 | L5 | 1871 | A2M | C5-C4-N3 | -5.08 | 120.12 | 126.75 |
| 70 | L5 | 4590 | A2M | N6-C6-N1 | -5.08 | 107.23 | 118.35 |
| 74 | S2 | 1832 | 6MZ | N9-C8-N7 | -5.06 | 107.00 | 113.91 |
| 70 | L5 | 4228 | OMG | C5-C4-N3 | -5.06 | 120.26 | 128.46 |
| 74 | S2 | 590 | A2M | N6-C6-N1 | -5.04 | 107.32 | 118.35 |
| 70 | L5 | 3785 | A2M | N6-C6-N1 | -5.03 | 107.33 | 118.35 |
| 70 | L5 | 4620 | OMU | C4-N3-C2 | -5.02 | 119.96 | 126.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 70 | L5 | 2363 | A2M | N6-C6-N1 | -4.99 | 107.41 | 118.35 |
| 70 | L5 | 1524 | A2M | N6-C6-N1 | -4.98 | 107.44 | 118.35 |
| 70 | L5 | 3718 | A2M | N6-C6-N1 | -4.96 | 107.49 | 118.35 |
| 74 | S2 | 668 | A2M | N6-C6-N1 | -4.94 | 107.53 | 118.35 |
| 70 | L5 | 1534 | A2M | N6-C6-N1 | -4.92 | 107.57 | 118.35 |
| 70 | L5 | 4530 | UR3 | C4-N3-C2 | -4.92 | 119.93 | 124.56 |
| 70 | L5 | 398 | A2M | N6-C6-N1 | -4.91 | 107.59 | 118.35 |
| 70 | L5 | 3830 | A2M | N6-C6-N1 | -4.91 | 107.59 | 118.35 |
| 70 | L5 | 400 | A2M | N6-C6-N1 | -4.90 | 107.61 | 118.35 |
| 70 | L5 | 4628 | PSU | N1-C2-N3 | 4.90 | 120.69 | 115.13 |
| 74 | S2 | 116 | OMU | C4-N3-C2 | -4.90 | 120.11 | 126.58 |
| 70 | L5 | 2876 | OMG | C2-N3-C4 | 4.89 | 121.01 | 112.30 |
| 74 | S2 | 27 | A2M | N6-C6-N1 | -4.88 | 107.66 | 118.35 |
| 74 | S2 | 1832 | 6MZ | C5-C4-N3 | -4.85 | 120.43 | 126.75 |
| 70 | L5 | 1326 | A2M | N6-C6-N1 | -4.84 | 107.75 | 118.35 |
| 70 | L5 | 3637 | PSU | N1-C2-N3 | 4.83 | 120.61 | 115.13 |
| 70 | L5 | 3825 | A2M | N6-C6-N1 | -4.83 | 107.78 | 118.35 |
| 70 | L5 | 2843 | PSU | C4-N3-C2 | -4.83 | 119.39 | 126.34 |
| 74 | S2 | 1383 | A2M | N6-C6-N1 | -4.81 | 107.82 | 118.35 |
| 70 | L5 | 2815 | A2M | N6-C6-N1 | -4.80 | 107.85 | 118.35 |
| 70 | L5 | 1871 | A2M | N6-C6-N1 | -4.79 | 107.85 | 118.35 |
| 70 | L5 | 3760 | A2M | N6-C6-N1 | -4.79 | 107.86 | 118.35 |
| 70 | L5 | 2843 | PSU | N1-C2-N3 | 4.79 | 120.55 | 115.13 |
| 74 | S2 | 576 | A2M | N6-C6-N1 | -4.78 | 107.87 | 118.35 |
| 70 | L5 | 4636 | PSU | C4-N3-C2 | -4.77 | 119.46 | 126.34 |
| 74 | S2 | 484 | A2M | N6-C6-N1 | -4.77 | 107.89 | 118.35 |
| 70 | L5 | 3792 | OMG | C2-N3-C4 | 4.75 | 120.77 | 112.30 |
| 74 | S2 | 99 | A2M | N6-C6-N1 | -4.75 | 107.95 | 118.35 |
| 74 | S2 | 1031 | A2M | N6-C6-N1 | -4.74 | 107.97 | 118.35 |
| 74 | S2 | 1367 | PSU | C4-N3-C2 | -4.71 | 119.55 | 126.34 |
| 74 | S2 | 1239 | PSU | C4-N3-C2 | -4.71 | 119.55 | 126.34 |
| 70 | L5 | 4500 | PSU | N1-C2-N3 | 4.71 | 120.47 | 115.13 |
| 74 | S2 | 1445 | PSU | C4-N3-C2 | -4.71 | 119.56 | 126.34 |
| 74 | S2 | 1445 | PSU | N1-C2-N3 | 4.70 | 120.46 | 115.13 |
| 70 | L5 | 2401 | A2M | N6-C6-N1 | -4.70 | 108.06 | 118.35 |
| 70 | L5 | 4220 | 6MZ | N9-C8-N7 | -4.69 | 107.49 | 113.91 |
| 74 | S2 | 573 | PSU | C4-N3-C2 | -4.68 | 119.60 | 126.34 |
| 74 | S2 | 1136 | PSU | C4-N3-C2 | -4.68 | 119.60 | 126.34 |
| 70 | L5 | 1862 | PSU | C4-N3-C2 | -4.67 | 119.60 | 126.34 |
| 74 | S2 | 468 | A2M | N6-C6-N1 | -4.67 | 108.12 | 118.35 |
| 74 | S2 | 822 | PSU | N1-C2-N3 | 4.67 | 120.42 | 115.13 |
| 74 | S2 | 683 | OMG | C2-N3-C4 | 4.67 | 120.62 | 112.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 70 | L5 | 4521 | PSU | C4-N3-C2 | -4.67 | 119.61 | 126.34 |
| 74 | S2 | 649 | PSU | N1-C2-N3 | 4.67 | 120.42 | 115.13 |
| 70 | L5 | 2364 | OMG | C2-N3-C4 | 4.66 | 120.61 | 112.30 |
| 70 | L5 | 4457 | PSU | N1-C2-N3 | 4.65 | 120.40 | 115.13 |
| 70 | L5 | 5001 | PSU | N1-C2-N3 | 4.65 | 120.39 | 115.13 |
| 74 | S2 | 609 | PSU | C4-N3-C2 | -4.65 | 119.65 | 126.34 |
| 70 | L5 | 4457 | PSU | C4-N3-C2 | -4.64 | 119.65 | 126.34 |
| 74 | S2 | 918 | PSU | N1-C2-N3 | 4.64 | 120.39 | 115.13 |
| 70 | L5 | 4628 | PSU | C4-N3-C2 | -4.64 | 119.65 | 126.34 |
| 74 | S2 | 1081 | PSU | C4-N3-C2 | -4.63 | 119.67 | 126.34 |
| 74 | S2 | 1367 | PSU | N1-C2-N3 | 4.63 | 120.38 | 115.13 |
| 70 | L5 | 4637 | OMG | C2-N3-C4 | 4.62 | 120.54 | 112.30 |
| 70 | L5 | 4293 | PSU | N1-C2-N3 | 4.62 | 120.37 | 115.13 |
| 70 | L5 | 4523 | A2M | N6-C6-N1 | -4.62 | 108.22 | 118.35 |
| 74 | S2 | 1347 | PSU | C4-N3-C2 | -4.62 | 119.68 | 126.34 |
| 70 | L5 | 4500 | PSU | C4-N3-C2 | -4.62 | 119.68 | 126.34 |
| 70 | L5 | 3639 | PSU | C4-N3-C2 | -4.62 | 119.68 | 126.34 |
| 74 | S2 | 686 | PSU | C4-N3-C2 | -4.62 | 119.69 | 126.34 |
| 70 | L5 | 1677 | PSU | C4-N3-C2 | -4.62 | 119.69 | 126.34 |
| 74 | S2 | 1244 | PSU | C4-N3-C2 | -4.62 | 119.69 | 126.34 |
| 70 | L5 | 3695 | PSU | C4-N3-C2 | -4.61 | 119.69 | 126.34 |
| 70 | L5 | 4618 | OMG | C2-N3-C4 | 4.61 | 120.51 | 112.30 |
| 70 | L5 | 4531 | PSU | C4-N3-C2 | -4.61 | 119.70 | 126.34 |
| 70 | L5 | 3770 | PSU | N1-C2-N3 | 4.61 | 120.35 | 115.13 |
| 70 | L5 | 4673 | PSU | N1-C2-N3 | 4.60 | 120.35 | 115.13 |
| 70 | L5 | 1683 | PSU | N1-C2-N3 | 4.60 | 120.34 | 115.13 |
| 74 | S2 | 1056 | PSU | C4-N3-C2 | -4.60 | 119.71 | 126.34 |
| 70 | L5 | 1862 | PSU | N1-C2-N3 | 4.60 | 120.34 | 115.13 |
| 70 | L5 | 4571 | A2M | N6-C6-N1 | -4.60 | 108.28 | 118.35 |
| 70 | L5 | 3764 | PSU | N1-C2-N3 | 4.59 | 120.33 | 115.13 |
| 70 | L5 | 4353 | PSU | C4-N3-C2 | -4.59 | 119.73 | 126.34 |
| 74 | S2 | 36 | PSU | C4-N3-C2 | -4.58 | 119.73 | 126.34 |
| 74 | S2 | 406 | PSU | N1-C2-N3 | 4.58 | 120.32 | 115.13 |
| 74 | S2 | 109 | PSU | N1-C2-N3 | 4.58 | 120.32 | 115.13 |
| 74 | S2 | 1244 | PSU | N1-C2-N3 | 4.58 | 120.31 | 115.13 |
| 74 | S2 | 406 | PSU | C4-N3-C2 | -4.58 | 119.75 | 126.34 |
| 70 | L5 | 3695 | PSU | N1-C2-N3 | 4.57 | 120.31 | 115.13 |
| 70 | L5 | 4403 | PSU | C4-N3-C2 | -4.57 | 119.76 | 126.34 |
| 70 | L5 | 1782 | PSU | C4-N3-C2 | -4.57 | 119.76 | 126.34 |
| 70 | L5 | 3844 | PSU | C4-N3-C2 | -4.57 | 119.76 | 126.34 |
| 70 | L5 | 1779 | PSU | C4-N3-C2 | -4.56 | 119.76 | 126.34 |
| 70 | L5 | 1683 | PSU | C4-N3-C2 | -4.56 | 119.77 | 126.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 70 | L5 | 3770 | PSU | C4-N3-C2 | -4.56 | 119.77 | 126.34 |
| 74 | S2 | 644 | OMG | C2-N3-C4 | 4.56 | 120.42 | 112.30 |
| 70 | L5 | 1625 | OMG | C2-N3-C4 | 4.55 | 120.41 | 112.30 |
| 74 | S2 | 686 | PSU | N1-C2-N3 | 4.55 | 120.29 | 115.13 |
| 70 | L5 | 3758 | PSU | C4-N3-C2 | -4.55 | 119.78 | 126.34 |
| 70 | L5 | 3637 | PSU | C4-N3-C2 | -4.55 | 119.78 | 126.34 |
| 74 | S2 | 1490 | OMG | C2-N3-C4 | 4.55 | 120.40 | 112.30 |
| 74 | S2 | 1347 | PSU | N1-C2-N3 | 4.55 | 120.28 | 115.13 |
| 70 | L5 | 1779 | PSU | N1-C2-N3 | 4.54 | 120.28 | 115.13 |
| 70 | L5 | 3853 | PSU | N1-C2-N3 | 4.54 | 120.27 | 115.13 |
| 70 | L5 | 4636 | PSU | N1-C2-N3 | 4.54 | 120.27 | 115.13 |
| 70 | L5 | 3920 | PSU | N1-C2-N3 | 4.54 | 120.27 | 115.13 |
| 70 | L5 | 1744 | PSU | C4-N3-C2 | -4.54 | 119.80 | 126.34 |
| 70 | L5 | 4293 | PSU | C4-N3-C2 | -4.54 | 119.80 | 126.34 |
| 67 | Pt | 56 | PSU | C4-N3-C2 | -4.54 | 119.80 | 126.34 |
| 74 | S2 | 34 | PSU | N1-C2-N3 | 4.54 | 120.27 | 115.13 |
| 70 | L5 | 4361 | PSU | C4-N3-C2 | -4.54 | 119.80 | 126.34 |
| 70 | L5 | 4220 | 6MZ | C5-C4-N3 | -4.54 | 120.83 | 126.75 |
| 70 | L5 | 3884 | PSU | N1-C2-N3 | 4.53 | 120.26 | 115.13 |
| 74 | S2 | 1243 | PSU | N1-C2-N3 | 4.53 | 120.26 | 115.13 |
| 70 | L5 | 4299 | PSU | N1-C2-N3 | 4.53 | 120.26 | 115.13 |
| 70 | L5 | 4423 | PSU | N1-C2-N3 | 4.53 | 120.26 | 115.13 |
| 70 | L5 | 4689 | PSU | C4-N3-C2 | -4.52 | 119.82 | 126.34 |
| 74 | S2 | 1248 | B8N | C4-N3-C2 | -4.52 | 119.75 | 125.46 |
| 74 | S2 | 1004 | PSU | N1-C2-N3 | 4.52 | 120.25 | 115.13 |
| 70 | L5 | 4403 | PSU | N1-C2-N3 | 4.52 | 120.25 | 115.13 |
| 70 | L5 | 3744 | OMG | C2-N3-C4 | 4.52 | 120.35 | 112.30 |
| 74 | S2 | 918 | PSU | C4-N3-C2 | -4.52 | 119.83 | 126.34 |
| 70 | L5 | 3729 | PSU | N1-C2-N3 | 4.52 | 120.25 | 115.13 |
| 70 | L5 | 4521 | PSU | N1-C2-N3 | 4.51 | 120.25 | 115.13 |
| 74 | S2 | 1174 | PSU | C4-N3-C2 | -4.51 | 119.84 | 126.34 |
| 70 | L5 | 2839 | PSU | C4-N3-C2 | -4.51 | 119.84 | 126.34 |
| 74 | S2 | 1238 | PSU | C4-N3-C2 | -4.51 | 119.84 | 126.34 |
| 70 | L5 | 4392 | OMG | C2-N3-C4 | 4.51 | 120.33 | 112.30 |
| 74 | S2 | 866 | PSU | N1-C2-N3 | 4.51 | 120.24 | 115.13 |
| 74 | S2 | 609 | PSU | N1-C2-N3 | 4.51 | 120.23 | 115.13 |
| 70 | L5 | 5001 | PSU | C4-N3-C2 | -4.50 | 119.85 | 126.34 |
| 70 | L5 | 5010 | PSU | N1-C2-N3 | 4.50 | 120.23 | 115.13 |
| 74 | S2 | 109 | PSU | C4-N3-C2 | -4.50 | 119.85 | 126.34 |
| 70 | L5 | 4493 | PSU | C4-N3-C2 | -4.50 | 119.85 | 126.34 |
| 70 | L5 | 4972 | PSU | N1-C2-N3 | 4.50 | 120.22 | 115.13 |
| 70 | L5 | 3785 | A2M | N9-C8-N7 | -4.50 | 107.77 | 113.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 74 | S2 | 1678 | A2M | N9-C8-N7 | -4.50 | 107.77 | 113.91 |
| 70 | L5 | 1677 | PSU | N1-C2-N3 | 4.50 | 120.22 | 115.13 |
| 74 | S2 | 1238 | PSU | N1-C2-N3 | 4.49 | 120.22 | 115.13 |
| 70 | L5 | 3884 | PSU | C4-N3-C2 | -4.49 | 119.87 | 126.34 |
| 70 | L5 | 3844 | PSU | N1-C2-N3 | 4.49 | 120.22 | 115.13 |
| 74 | S2 | 866 | PSU | C4-N3-C2 | -4.49 | 119.87 | 126.34 |
| 70 | L5 | 1744 | PSU | N1-C2-N3 | 4.49 | 120.22 | 115.13 |
| 70 | L5 | 4361 | PSU | N1-C2-N3 | 4.49 | 120.22 | 115.13 |
| 70 | L5 | 3851 | PSU | C4-N3-C2 | -4.49 | 119.87 | 126.34 |
| 74 | S2 | 681 | PSU | C4-N3-C2 | -4.49 | 119.87 | 126.34 |
| 70 | L5 | 4228 | OMG | C1'-N9-C4 | -4.49 | 113.18 | 126.50 |
| 70 | L5 | 4493 | PSU | N1-C2-N3 | 4.48 | 120.21 | 115.13 |
| 70 | L5 | 4370 | OMG | C2-N3-C4 | 4.48 | 120.29 | 112.30 |
| 70 | L5 | 4531 | PSU | N1-C2-N3 | 4.48 | 120.21 | 115.13 |
| 74 | S2 | 1136 | PSU | N1-C2-N3 | 4.48 | 120.21 | 115.13 |
| 70 | L5 | 4312 | PSU | N1-C2-N3 | 4.48 | 120.20 | 115.13 |
| 74 | S2 | 218 | PSU | C4-N3-C2 | -4.48 | 119.89 | 126.34 |
| 70 | L5 | 1522 | OMG | C2-N3-C4 | 4.48 | 120.28 | 112.30 |
| 70 | L5 | 3729 | PSU | C4-N3-C2 | -4.47 | 119.89 | 126.34 |
| 70 | L5 | 3758 | PSU | N1-C2-N3 | 4.47 | 120.20 | 115.13 |
| 74 | S2 | 1232 | PSU | N1-C2-N3 | 4.47 | 120.19 | 115.13 |
| 74 | S2 | 1643 | PSU | N1-C2-N3 | 4.47 | 120.19 | 115.13 |
| 74 | S2 | 1832 | 6MZ | C5-N7-C8 | 4.47 | 109.86 | 103.51 |
| 70 | L5 | 3768 | PSU | C4-N3-C2 | -4.46 | 119.91 | 126.34 |
| 70 | L5 | 4196 | OMG | C2-N3-C4 | 4.46 | 120.25 | 112.30 |
| 70 | L5 | 3734 | PSU | C4-N3-C2 | -4.46 | 119.91 | 126.34 |
| 74 | S2 | 1232 | PSU | C4-N3-C2 | -4.46 | 119.91 | 126.34 |
| 74 | S2 | 801 | PSU | C4-N3-C2 | -4.46 | 119.91 | 126.34 |
| 70 | L5 | 4431 | PSU | N1-C2-N3 | 4.46 | 120.18 | 115.13 |
| 69 | L8 | 75 | OMG | C2-N3-C4 | 4.46 | 120.24 | 112.30 |
| 70 | L5 | 4499 | OMG | C2-N3-C4 | 4.46 | 120.24 | 112.30 |
| 70 | L5 | 3899 | OMG | C2-N3-C4 | 4.46 | 120.24 | 112.30 |
| 74 | S2 | 436 | OMG | C2-N3-C4 | 4.46 | 120.24 | 112.30 |
| 74 | S2 | 1056 | PSU | N1-C2-N3 | 4.45 | 120.18 | 115.13 |
| 70 | L5 | 4312 | PSU | C4-N3-C2 | -4.45 | 119.92 | 126.34 |
| 69 | L8 | 55 | PSU | C4-N3-C2 | -4.45 | 119.92 | 126.34 |
| 70 | L5 | 4423 | PSU | C4-N3-C2 | -4.45 | 119.93 | 126.34 |
| 70 | L5 | 1871 | A2M | N9-C8-N7 | -4.44 | 107.84 | 113.91 |
| 74 | S2 | 36 | PSU | N1-C2-N3 | 4.44 | 120.16 | 115.13 |
| 67 | Pt | 56 | PSU | N1-C2-N3 | 4.44 | 120.16 | 115.13 |
| 74 | S2 | 218 | PSU | N1-C2-N3 | 4.44 | 120.16 | 115.13 |
| 70 | L5 | 4673 | PSU | C4-N3-C2 | -4.44 | 119.94 | 126.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 74 | S2 | 668 | A2M | N9-C8-N7 | -4.44 | 107.84 | 113.91 |
| 74 | S2 | 34 | PSU | C4-N3-C2 | -4.44 | 119.94 | 126.34 |
| 70 | L5 | 3627 | OMG | C2-N3-C4 | 4.44 | 120.20 | 112.30 |
| 70 | L5 | 4569 | PSU | C4-N3-C2 | -4.44 | 119.95 | 126.34 |
| 70 | L5 | 3851 | PSU | N1-C2-N3 | 4.44 | 120.16 | 115.13 |
| 70 | L5 | 5010 | PSU | C4-N3-C2 | -4.44 | 119.95 | 126.34 |
| 70 | L5 | 4296 | PSU | N1-C2-N3 | 4.44 | 120.16 | 115.13 |
| 74 | S2 | 801 | PSU | N1-C2-N3 | 4.44 | 120.16 | 115.13 |
| 70 | L5 | 3768 | PSU | N1-C2-N3 | 4.43 | 120.15 | 115.13 |
| 70 | L5 | 4228 | OMG | C2-N3-C4 | 4.43 | 120.20 | 112.30 |
| 74 | S2 | 1692 | PSU | C4-N3-C2 | -4.43 | 119.95 | 126.34 |
| 70 | L5 | 4579 | PSU | N1-C2-N3 | 4.43 | 120.15 | 115.13 |
| 74 | S2 | 1328 | OMG | C2-N3-C4 | 4.43 | 120.19 | 112.30 |
| 70 | L5 | 1536 | PSU | C4-N3-C2 | -4.43 | 119.96 | 126.34 |
| 74 | S2 | 105 | PSU | C4-N3-C2 | -4.43 | 119.96 | 126.34 |
| 69 | L8 | 55 | PSU | N1-C2-N3 | 4.43 | 120.15 | 115.13 |
| 70 | L5 | 4689 | PSU | N1-C2-N3 | 4.43 | 120.14 | 115.13 |
| 70 | L5 | 4552 | PSU | N1-C2-N3 | 4.42 | 120.14 | 115.13 |
| 74 | S2 | 105 | PSU | N1-C2-N3 | 4.42 | 120.14 | 115.13 |
| 70 | L5 | 4442 | PSU | N1-C2-N3 | 4.42 | 120.14 | 115.13 |
| 70 | L5 | 4972 | PSU | C4-N3-C2 | -4.42 | 119.97 | 126.34 |
| 74 | S2 | 1625 | PSU | C4-N3-C2 | -4.42 | 119.97 | 126.34 |
| 70 | L5 | 4623 | OMG | C2-N3-C4 | 4.42 | 120.17 | 112.30 |
| 74 | S2 | 296 | PSU | C4-N3-C2 | -4.42 | 119.97 | 126.34 |
| 74 | S2 | 651 | PSU | N1-C2-N3 | 4.42 | 120.13 | 115.13 |
| 74 | S2 | 572 | PSU | C4-N3-C2 | -4.42 | 119.98 | 126.34 |
| 69 | L8 | 69 | PSU | N1-C2-N3 | 4.42 | 120.13 | 115.13 |
| 70 | L5 | 4494 | OMG | C2-N3-C4 | 4.42 | 120.17 | 112.30 |
| 70 | L5 | 4431 | PSU | C4-N3-C2 | -4.41 | 119.98 | 126.34 |
| 70 | L5 | 4296 | PSU | C4-N3-C2 | -4.41 | 119.98 | 126.34 |
| 70 | L5 | 3639 | PSU | N1-C2-N3 | 4.41 | 120.13 | 115.13 |
| 70 | L5 | 3764 | PSU | C4-N3-C2 | -4.41 | 119.98 | 126.34 |
| 70 | L5 | 4299 | PSU | C4-N3-C2 | -4.41 | 119.98 | 126.34 |
| 74 | S2 | 509 | OMG | C2-N3-C4 | 4.41 | 120.16 | 112.30 |
| 70 | L5 | 4471 | PSU | N1-C2-N3 | 4.41 | 120.13 | 115.13 |
| 70 | L5 | 2508 | PSU | N1-C2-N3 | 4.41 | 120.12 | 115.13 |
| 70 | L5 | 4569 | PSU | N1-C2-N3 | 4.40 | 120.12 | 115.13 |
| 70 | L5 | 1860 | PSU | C4-N3-C2 | -4.40 | 120.00 | 126.34 |
| 70 | L5 | 2839 | PSU | N1-C2-N3 | 4.40 | 120.12 | 115.13 |
| 70 | L5 | 4579 | PSU | C4-N3-C2 | -4.40 | 120.00 | 126.34 |
| 70 | L5 | 3920 | PSU | C4-N3-C2 | -4.40 | 120.00 | 126.34 |
| 74 | S2 | 1625 | PSU | N1-C2-N3 | 4.39 | 120.10 | 115.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 74 | S2 | 867 | OMG | C2-N3-C4 | 4.39 | 120.12 | 112.30 |
| 74 | S2 | 822 | PSU | C4-N3-C2 | -4.39 | 120.02 | 126.34 |
| 74 | S2 | 1177 | PSU | C4-N3-C2 | -4.38 | 120.03 | 126.34 |
| 70 | L5 | 4532 | PSU | N1-C2-N3 | 4.38 | 120.09 | 115.13 |
| 70 | L5 | 1316 | OMG | C2-N3-C4 | 4.38 | 120.10 | 112.30 |
| 74 | S2 | 1174 | PSU | N1-C2-N3 | 4.38 | 120.09 | 115.13 |
| 74 | S2 | 649 | PSU | C4-N3-C2 | -4.37 | 120.04 | 126.34 |
| 70 | L5 | 4353 | PSU | N1-C2-N3 | 4.37 | 120.08 | 115.13 |
| 74 | S2 | 681 | PSU | N1-C2-N3 | 4.37 | 120.08 | 115.13 |
| 74 | S2 | 1643 | PSU | C4-N3-C2 | -4.37 | 120.05 | 126.34 |
| 70 | L5 | 4552 | PSU | C4-N3-C2 | -4.36 | 120.05 | 126.34 |
| 70 | L5 | 4576 | PSU | N1-C2-N3 | 4.36 | 120.07 | 115.13 |
| 74 | S2 | 93 | PSU | C4-N3-C2 | -4.36 | 120.06 | 126.34 |
| 70 | L5 | 4590 | A2M | C5-C6-N6 | 4.36 | 132.91 | 123.43 |
| 69 | L8 | 69 | PSU | C4-N3-C2 | -4.36 | 120.06 | 126.34 |
| 70 | L5 | 4576 | PSU | C4-N3-C2 | -4.35 | 120.06 | 126.34 |
| 74 | S2 | 296 | PSU | N1-C2-N3 | 4.35 | 120.06 | 115.13 |
| 70 | L5 | 2424 | OMG | C2-N3-C4 | 4.35 | 120.06 | 112.30 |
| 74 | S2 | 1004 | PSU | C4-N3-C2 | -4.35 | 120.07 | 126.34 |
| 74 | S2 | 1239 | PSU | N1-C2-N3 | 4.35 | 120.06 | 115.13 |
| 74 | S2 | 1243 | PSU | C4-N3-C2 | -4.35 | 120.07 | 126.34 |
| 74 | S2 | 863 | PSU | N1-C2-N3 | 4.35 | 120.06 | 115.13 |
| 70 | L5 | 1860 | PSU | N1-C2-N3 | 4.35 | 120.06 | 115.13 |
| 74 | S2 | 572 | PSU | N1-C2-N3 | 4.33 | 120.04 | 115.13 |
| 70 | L5 | 3867 | A2M | C5-C6-N6 | 4.33 | 132.85 | 123.43 |
| 70 | L5 | 3734 | PSU | N1-C2-N3 | 4.33 | 120.03 | 115.13 |
| 74 | S2 | 651 | PSU | C4-N3-C2 | -4.33 | 120.11 | 126.34 |
| 70 | L5 | 4442 | PSU | C4-N3-C2 | -4.32 | 120.12 | 126.34 |
| 70 | L5 | 3760 | A2M | N9-C8-N7 | -4.31 | 108.01 | 113.91 |
| 70 | L5 | 3762 | PSU | N1-C2-N3 | 4.31 | 120.02 | 115.13 |
| 70 | L5 | 1781 | PSU | N1-C2-N3 | 4.31 | 120.01 | 115.13 |
| 74 | S2 | 1850 | MA6 | N9-C8-N7 | -4.31 | 108.02 | 113.91 |
| 74 | S2 | 867 | OMG | C1'-N9-C4 | -4.30 | 113.72 | 126.50 |
| 74 | S2 | 863 | PSU | C4-N3-C2 | -4.30 | 120.14 | 126.34 |
| 74 | S2 | 815 | PSU | N1-C2-N3 | 4.30 | 120.00 | 115.13 |
| 70 | L5 | 1536 | PSU | N1-C2-N3 | 4.30 | 120.00 | 115.13 |
| 74 | S2 | 93 | PSU | N1-C2-N3 | 4.30 | 120.00 | 115.13 |
| 74 | S2 | 1081 | PSU | N1-C2-N3 | 4.29 | 119.99 | 115.13 |
| 70 | L5 | 398 | A2M | N9-C8-N7 | -4.29 | 108.05 | 113.91 |
| 74 | S2 | 1678 | A2M | C5-C6-N6 | 4.28 | 132.75 | 123.43 |
| 70 | L5 | 2363 | A2M | N9-C8-N7 | -4.28 | 108.06 | 113.91 |
| 74 | S2 | 1031 | A2M | N9-C8-N7 | -4.28 | 108.06 | 113.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 70 | L5 | 3715 | PSU | C4-N3-C2 | -4.28 | 120.18 | 126.34 |
| 70 | L5 | 4420 | PSU | N1-C2-N3 | 4.27 | 119.97 | 115.13 |
| 70 | L5 | 3715 | PSU | N1-C2-N3 | 4.27 | 119.97 | 115.13 |
| 70 | L5 | 3830 | A2M | N9-C8-N7 | -4.26 | 108.08 | 113.91 |
| 70 | L5 | 4532 | PSU | C4-N3-C2 | -4.26 | 120.20 | 126.34 |
| 74 | S2 | 1692 | PSU | N1-C2-N3 | 4.25 | 119.95 | 115.13 |
| 70 | L5 | 1782 | PSU | N1-C2-N3 | 4.25 | 119.94 | 115.13 |
| 70 | L5 | 1524 | A2M | N9-C8-N7 | -4.25 | 108.11 | 113.91 |
| 74 | S2 | 1639 | G7M | C2-N3-C4 | 4.24 | 119.86 | 112.30 |
| 74 | S2 | 1177 | PSU | N1-C2-N3 | 4.24 | 119.93 | 115.13 |
| 70 | L5 | 1781 | PSU | C4-N3-C2 | -4.24 | 120.24 | 126.34 |
| 70 | L5 | 4228 | OMG | C1'-N9-C8 | 4.23 | 138.75 | 126.70 |
| 74 | S2 | 966 | PSU | C4-N3-C2 | -4.23 | 120.24 | 126.34 |
| 74 | S2 | 573 | PSU | N1-C2-N3 | 4.23 | 119.92 | 115.13 |
| 70 | L5 | 1792 | PSU | C4-N3-C2 | -4.23 | 120.25 | 126.34 |
| 74 | S2 | 814 | PSU | C4-N3-C2 | -4.22 | 120.26 | 126.34 |
| 70 | L5 | 3853 | PSU | C4-N3-C2 | -4.22 | 120.26 | 126.34 |
| 70 | L5 | 1524 | A2M | C5-C6-N6 | 4.22 | 132.60 | 123.43 |
| 70 | L5 | 2632 | PSU | C4-N3-C2 | -4.21 | 120.28 | 126.34 |
| 70 | L5 | 3825 | A2M | N9-C8-N7 | -4.19 | 108.18 | 113.91 |
| 74 | S2 | 1832 | 6MZ | C4-C5-C6 | 4.18 | 120.05 | 116.81 |
| 74 | S2 | 512 | A2M | C5-C6-N6 | 4.18 | 132.53 | 123.43 |
| 70 | L5 | 2508 | PSU | C4-N3-C2 | -4.18 | 120.32 | 126.34 |
| 70 | L5 | 4471 | PSU | C4-N3-C2 | -4.17 | 120.33 | 126.34 |
| 70 | L5 | 2632 | PSU | N1-C2-N3 | 4.17 | 119.85 | 115.13 |
| 74 | S2 | 668 | A2M | C5-C6-N6 | 4.17 | 132.50 | 123.43 |
| 70 | L5 | 1522 | OMG | C1'-N9-C4 | -4.16 | 114.13 | 126.50 |
| 67 | Pt | 47 | G7M | C2-N3-C4 | 4.16 | 119.72 | 112.30 |
| 70 | L5 | 1792 | PSU | N1-C2-N3 | 4.16 | 119.84 | 115.13 |
| 74 | S2 | 468 | A2M | N9-C8-N7 | -4.16 | 108.23 | 113.91 |
| 70 | L5 | 4590 | A2M | N9-C8-N7 | -4.15 | 108.24 | 113.91 |
| 74 | S2 | 815 | PSU | C4-N3-C2 | -4.15 | 120.36 | 126.34 |
| 70 | L5 | 2815 | A2M | N9-C8-N7 | -4.15 | 108.24 | 113.91 |
| 70 | L5 | 1582 | PSU | N1-C2-N3 | 4.15 | 119.83 | 115.13 |
| 74 | S2 | 814 | PSU | N1-C2-N3 | 4.14 | 119.81 | 115.13 |
| 70 | L5 | 400 | A2M | N9-C8-N7 | -4.13 | 108.26 | 113.91 |
| 70 | L5 | 3867 | A2M | N9-C8-N7 | -4.13 | 108.27 | 113.91 |
| 74 | S2 | 119 | PSU | N1-C2-N3 | 4.13 | 119.80 | 115.13 |
| 70 | L5 | 2401 | A2M | N9-C8-N7 | -4.12 | 108.27 | 113.91 |
| 74 | S2 | 1851 | MA6 | N9-C8-N7 | -4.12 | 108.28 | 113.91 |
| 70 | L5 | 3718 | A2M | C5-C6-N6 | 4.11 | 132.37 | 123.43 |
| 70 | L5 | 1534 | A2M | C5-C6-N6 | 4.11 | 132.37 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 70 | L5 | 4370 | OMG | C1'-N9-C4 | -4.10 | 114.31 | 126.50 |
| 70 | L5 | 1534 | A2M | N9-C8-N7 | -4.10 | 108.31 | 113.91 |
| 74 | S2 | 966 | PSU | N1-C2-N3 | 4.10 | 119.77 | 115.13 |
| 70 | L5 | 1326 | A2M | N9-C8-N7 | -4.10 | 108.31 | 113.91 |
| 74 | S2 | 99 | A2M | N9-C8-N7 | -4.10 | 108.31 | 113.91 |
| 70 | L5 | 1871 | A2M | C5-C6-N6 | 4.09 | 132.34 | 123.43 |
| 70 | L5 | 2363 | A2M | C5-C6-N6 | 4.09 | 132.34 | 123.43 |
| 74 | S2 | 590 | A2M | C5-C6-N6 | 4.09 | 132.34 | 123.43 |
| 74 | S2 | 590 | A2M | N9-C8-N7 | -4.08 | 108.33 | 113.91 |
| 70 | L5 | 4571 | A2M | N9-C8-N7 | -4.08 | 108.33 | 113.91 |
| 74 | S2 | 27 | A2M | N9-C8-N7 | -4.08 | 108.33 | 113.91 |
| 70 | L5 | 3830 | A2M | C5-C6-N6 | 4.08 | 132.31 | 123.43 |
| 74 | S2 | 1851 | MA6 | C4-C5-C6 | 4.07 | 120.44 | 115.88 |
| 70 | L5 | 4220 | 6MZ | C4-C5-C6 | 4.06 | 119.96 | 116.81 |
| 74 | S2 | 576 | A2M | C5-C6-N6 | 4.06 | 132.27 | 123.43 |
| 70 | L5 | 398 | A2M | C5-C6-N6 | 4.05 | 132.25 | 123.43 |
| 74 | S2 | 1850 | MA6 | C4-C5-C6 | 4.05 | 120.42 | 115.88 |
| 74 | S2 | 27 | A2M | C5-C6-N6 | 4.05 | 132.25 | 123.43 |
| 70 | L5 | 3762 | PSU | C4-N3-C2 | -4.05 | 120.51 | 126.34 |
| 74 | S2 | 1383 | A2M | N9-C8-N7 | -4.05 | 108.38 | 113.91 |
| 70 | L5 | 400 | A2M | C5-C6-N6 | 4.04 | 132.23 | 123.43 |
| 70 | L5 | 3825 | A2M | C5-C6-N6 | 4.04 | 132.23 | 123.43 |
| 70 | L5 | 3627 | OMG | C1'-N9-C4 | -4.04 | 114.50 | 126.50 |
| 70 | L5 | 1522 | OMG | C1'-N9-C8 | 4.02 | 138.13 | 126.70 |
| 74 | S2 | 1328 | OMG | C1'-N9-C4 | -4.02 | 114.57 | 126.50 |
| 70 | L5 | 1326 | A2M | C5-C6-N6 | 4.01 | 132.16 | 123.43 |
| 69 | L8 | 75 | OMG | C1'-N9-C4 | -4.01 | 114.60 | 126.50 |
| 70 | L5 | 4420 | PSU | C4-N3-C2 | -4.01 | 120.57 | 126.34 |
| 74 | S2 | 484 | A2M | N9-C8-N7 | -4.00 | 108.45 | 113.91 |
| 70 | L5 | 2815 | A2M | C5-C6-N6 | 3.99 | 132.12 | 123.43 |
| 74 | S2 | 512 | A2M | N9-C8-N7 | -3.99 | 108.45 | 113.91 |
| 74 | S2 | 867 | OMG | C1'-N9-C8 | 3.99 | 138.05 | 126.70 |
| 74 | S2 | 1031 | A2M | C5-C6-N6 | 3.98 | 132.09 | 123.43 |
| 74 | S2 | 99 | A2M | C5-C6-N6 | 3.98 | 132.09 | 123.43 |
| 70 | L5 | 4499 | OMG | C1'-N9-C4 | -3.98 | 114.69 | 126.50 |
| 70 | L5 | 3718 | A2M | N9-C8-N7 | -3.96 | 108.49 | 113.91 |
| 74 | S2 | 1383 | A2M | C5-C6-N6 | 3.96 | 132.05 | 123.43 |
| 70 | L5 | 3785 | A2M | C5-C6-N6 | 3.96 | 132.05 | 123.43 |
| 74 | S2 | 484 | A2M | C5-C6-N6 | 3.95 | 132.02 | 123.43 |
| 70 | L5 | 4392 | OMG | C1'-N9-C4 | -3.95 | 114.78 | 126.50 |
| 70 | L5 | 2424 | OMG | C1'-N9-C4 | -3.94 | 114.80 | 126.50 |
| 70 | L5 | 3899 | OMG | C1'-N9-C4 | -3.94 | 114.81 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 70 | L5 | 1322 | 1MA | C5-C4-N3 | -3.93 | 121.39 | 127.26 |
| 70 | L5 | 4523 | A2M | N9-C8-N7 | -3.92 | 108.55 | 113.91 |
| 70 | L5 | 4447 | 5MC | C5-C6-N1 | -3.92 | 119.31 | 123.34 |
| 70 | L5 | 3760 | A2M | C5-C6-N6 | 3.92 | 131.95 | 123.43 |
| 74 | S2 | 576 | A2M | N9-C8-N7 | -3.91 | 108.56 | 113.91 |
| 74 | S2 | 1804 | OMU | N3-C2-N1 | 3.90 | 120.07 | 114.89 |
| 67 | Pt | 47 | G7M | C5-C6-N1 | 3.89 | 119.92 | 111.79 |
| 74 | S2 | 1639 | G7M | C5-C6-N1 | 3.89 | 119.92 | 111.79 |
| 70 | L5 | 2401 | A2M | C5-C6-N6 | 3.89 | 131.90 | 123.43 |
| 74 | S2 | 468 | A2M | C5-C6-N6 | 3.89 | 131.90 | 123.43 |
| 74 | S2 | 436 | OMG | C1'-N9-C4 | -3.89 | 114.94 | 126.50 |
| 70 | L5 | 4370 | OMG | C1'-N9-C8 | 3.89 | 137.77 | 126.70 |
| 70 | L5 | 4523 | A2M | C5-C6-N6 | 3.88 | 131.88 | 123.43 |
| 70 | L5 | 3925 | OMU | N3-C2-N1 | 3.87 | 120.02 | 114.89 |
| 74 | S2 | 590 | A2M | C2-N3-C4 | 3.86 | 120.88 | 111.75 |
| 70 | L5 | 4571 | A2M | C5-C6-N6 | 3.86 | 131.83 | 123.43 |
| 70 | L5 | 2837 | OMU | N3-C2-N1 | 3.85 | 120.00 | 114.89 |
| 70 | L5 | 4220 | 6MZ | C5-N7-C8 | 3.85 | 108.98 | 103.51 |
| 70 | L5 | 2424 | OMG | C1'-N9-C8 | 3.85 | 137.66 | 126.70 |
| 70 | L5 | 3627 | OMG | C1'-N9-C8 | 3.84 | 137.64 | 126.70 |
| 74 | S2 | 512 | A2M | C2-N3-C4 | 3.84 | 120.83 | 111.75 |
| 70 | L5 | 3785 | A2M | C4'-O4'-C1' | -3.84 | 101.01 | 109.47 |
| 74 | S2 | 119 | PSU | C4-N3-C2 | -3.83 | 120.82 | 126.34 |
| 70 | L5 | 4494 | OMG | C1'-N9-C4 | -3.83 | 115.14 | 126.50 |
| 70 | L5 | 4227 | OMU | N3-C2-N1 | 3.82 | 119.96 | 114.89 |
| 74 | S2 | 590 | A2M | N3-C4-N9 | 3.81 | 133.37 | 127.08 |
| 70 | L5 | 1582 | PSU | C4-N3-C2 | -3.81 | 120.85 | 126.34 |
| 70 | L5 | 4392 | OMG | C1'-N9-C8 | 3.80 | 137.53 | 126.70 |
| 70 | L5 | 3744 | OMG | C1'-N9-C4 | -3.80 | 115.23 | 126.50 |
| 70 | L5 | 4623 | OMG | C1'-N9-C4 | -3.79 | 115.24 | 126.50 |
| 70 | L5 | 1322 | 1MA | C2-N3-C4 | 3.79 | 119.86 | 112.41 |
| 70 | L5 | 3760 | A2M | N3-C4-N9 | 3.79 | 133.33 | 127.08 |
| 74 | S2 | 1639 | G7M | C5-C4-N3 | -3.79 | 120.89 | 128.15 |
| 70 | L5 | 2364 | OMG | C1'-N9-C4 | -3.78 | 115.26 | 126.50 |
| 70 | L5 | 4620 | OMU | N3-C2-N1 | 3.78 | 119.91 | 114.89 |
| 74 | S2 | 627 | OMU | N3-C2-N1 | 3.78 | 119.91 | 114.89 |
| 74 | S2 | 1678 | A2M | C2-N3-C4 | 3.77 | 120.66 | 111.75 |
| 69 | L8 | 75 | OMG | C1'-N9-C8 | 3.77 | 137.43 | 126.70 |
| 70 | L5 | 4498 | OMU | N3-C2-N1 | 3.77 | 119.89 | 114.89 |
| 74 | S2 | 116 | OMU | N3-C2-N1 | 3.77 | 119.89 | 114.89 |
| 70 | L5 | 1316 | OMG | C1'-N9-C4 | -3.73 | 115.41 | 126.50 |
| 70 | L5 | 3760 | A2M | C2-N3-C4 | 3.73 | 120.56 | 111.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 70 | L5 | 4499 | OMG | C1'-N9-C8 | 3.72 | 137.30 | 126.70 |
| 74 | S2 | 1490 | OMG | C1'-N9-C4 | -3.71 | 115.48 | 126.50 |
| 70 | L5 | 3899 | OMG | C1'-N9-C8 | 3.71 | 137.25 | 126.70 |
| 70 | L5 | 2876 | OMG | N9-C4-N3 | 3.70 | 133.37 | 125.94 |
| 74 | S2 | 1850 | MA6 | C2-N1-C6 | 3.70 | 120.49 | 111.75 |
| 74 | S2 | 1328 | OMG | C1'-N9-C8 | 3.69 | 137.20 | 126.70 |
| 70 | L5 | 3830 | A2M | C2-N3-C4 | 3.68 | 120.44 | 111.75 |
| 70 | L5 | 4590 | A2M | C2-N3-C4 | 3.68 | 120.44 | 111.75 |
| 70 | L5 | 4494 | OMG | C1'-N9-C8 | 3.67 | 137.14 | 126.70 |
| 70 | L5 | 400 | A2M | C2-N3-C4 | 3.67 | 120.41 | 111.75 |
| 70 | L5 | 4618 | OMG | C1'-N9-C4 | -3.67 | 115.61 | 126.50 |
| 74 | S2 | 436 | OMG | C1'-N9-C8 | 3.66 | 137.13 | 126.70 |
| 70 | L5 | 2815 | A2M | C2-N3-C4 | 3.65 | 120.39 | 111.75 |
| 74 | S2 | 1851 | MA6 | C2-N1-C6 | 3.65 | 120.38 | 111.75 |
| 70 | L5 | 4623 | OMG | C1'-N9-C8 | 3.65 | 137.09 | 126.70 |
| 74 | S2 | 428 | OMU | N3-C2-N1 | 3.64 | 119.73 | 114.89 |
| 70 | L5 | 1534 | A2M | C2-N3-C4 | 3.64 | 120.34 | 111.75 |
| 74 | S2 | 668 | A2M | C2-N3-C4 | 3.63 | 120.34 | 111.75 |
| 70 | L5 | 1625 | OMG | N9-C4-N3 | 3.63 | 133.22 | 125.94 |
| 70 | L5 | 2364 | OMG | C1'-N9-C8 | 3.63 | 137.02 | 126.70 |
| 70 | L5 | 2363 | A2M | C2-N3-C4 | 3.62 | 120.31 | 111.75 |
| 70 | L5 | 3785 | A2M | C2-N3-C4 | 3.62 | 120.29 | 111.75 |
| 74 | S2 | 27 | A2M | C2-N3-C4 | 3.61 | 120.28 | 111.75 |
| 70 | L5 | 4196 | OMG | C1'-N9-C4 | -3.61 | 115.78 | 126.50 |
| 74 | S2 | 1031 | A2M | C2-N3-C4 | 3.61 | 120.28 | 111.75 |
| 70 | L5 | 2401 | A2M | C2-N3-C4 | 3.61 | 120.28 | 111.75 |
| 74 | S2 | 1383 | A2M | C2-N3-C4 | 3.60 | 120.26 | 111.75 |
| 74 | S2 | 99 | A2M | C2-N3-C4 | 3.60 | 120.25 | 111.75 |
| 70 | L5 | 3825 | A2M | C2-N3-C4 | 3.60 | 120.25 | 111.75 |
| 70 | L5 | 1524 | A2M | C2-N3-C4 | 3.60 | 120.25 | 111.75 |
| 74 | S2 | 484 | A2M | C2-N3-C4 | 3.60 | 120.25 | 111.75 |
| 67 | Pt | 8 | 4SU | N3-C2-N1 | 3.59 | 119.65 | 114.89 |
| 70 | L5 | 3744 | OMG | C1'-N9-C8 | 3.58 | 136.90 | 126.70 |
| 70 | L5 | 1326 | A2M | C2-N3-C4 | 3.58 | 120.21 | 111.75 |
| 74 | S2 | 1490 | OMG | C1'-N9-C8 | 3.58 | 136.88 | 126.70 |
| 70 | L5 | 3718 | A2M | C2-N3-C4 | 3.57 | 120.18 | 111.75 |
| 70 | L5 | 4523 | A2M | C2-N3-C4 | 3.57 | 120.18 | 111.75 |
| 70 | L5 | 4637 | OMG | C1'-N9-C4 | -3.57 | 115.91 | 126.50 |
| 74 | S2 | 1851 | MA6 | C2-N3-C4 | 3.57 | 120.17 | 111.75 |
| 67 | Pt | 47 | G7M | C5-C4-N3 | -3.56 | 121.32 | 128.15 |
| 70 | L5 | 4571 | A2M | C2-N3-C4 | 3.54 | 120.12 | 111.75 |
| 74 | S2 | 1678 | A2M | C5-N7-C8 | 3.54 | 108.54 | 103.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 74 | S2 | 1639 | G7M | CN7-N7-C5 | 3.54 | 131.16 | 126.77 |
| 74 | S2 | 644 | OMG | C1'-N9-C4 | -3.54 | 116.00 | 126.50 |
| 74 | S2 | 683 | OMG | N9-C4-N3 | 3.53 | 133.04 | 125.94 |
| 74 | S2 | 468 | A2M | C2-N3-C4 | 3.53 | 120.10 | 111.75 |
| 70 | L5 | 1871 | A2M | C2-N3-C4 | 3.53 | 120.09 | 111.75 |
| 70 | L5 | 3867 | A2M | C2-N3-C4 | 3.53 | 120.08 | 111.75 |
| 70 | L5 | 4498 | OMU | C5-C4-N3 | 3.51 | 120.09 | 114.84 |
| 70 | L5 | 2815 | A2M | N3-C4-N9 | 3.51 | 132.87 | 127.08 |
| 70 | L5 | 1316 | OMG | C1'-N9-C8 | 3.51 | 136.69 | 126.70 |
| 70 | L5 | 398 | A2M | C2-N3-C4 | 3.51 | 120.04 | 111.75 |
| 70 | L5 | 4618 | OMG | C1'-N9-C8 | 3.50 | 136.66 | 126.70 |
| 74 | S2 | 1850 | MA6 | C2-N3-C4 | 3.49 | 120.01 | 111.75 |
| 67 | Pt | 21 | H2U | N3-C2-N1 | 3.48 | 120.33 | 116.65 |
| 74 | S2 | 509 | OMG | C1'-N9-C4 | -3.48 | 116.17 | 126.50 |
| 74 | S2 | 428 | OMU | C5-C4-N3 | 3.47 | 120.03 | 114.84 |
| 70 | L5 | 2401 | A2M | N3-C4-N9 | 3.44 | 132.75 | 127.08 |
| 67 | Pt | 8 | 4SU | C5-C4-S4 | -3.44 | 120.04 | 124.47 |
| 70 | L5 | 3792 | OMG | N9-C4-N3 | 3.44 | 132.84 | 125.94 |
| 74 | S2 | 512 | A2M | N3-C4-N9 | 3.42 | 132.72 | 127.08 |
| 74 | S2 | 576 | A2M | C2-N3-C4 | 3.42 | 119.84 | 111.75 |
| 70 | L5 | 4227 | OMU | C5-C4-N3 | 3.42 | 119.95 | 114.84 |
| 70 | L5 | 4196 | OMG | C1'-N9-C8 | 3.41 | 136.40 | 126.70 |
| 67 | Pt | 47 | G7M | O6-C6-C5 | -3.41 | 120.37 | 128.06 |
| 70 | L5 | 3792 | OMG | C1'-N9-C4 | -3.40 | 116.39 | 126.50 |
| 70 | L5 | 3925 | OMU | C5-C4-N3 | 3.40 | 119.93 | 114.84 |
| 74 | S2 | 509 | OMG | C1'-N9-C8 | 3.40 | 136.37 | 126.70 |
| 70 | L5 | 4637 | OMG | C1'-N9-C8 | 3.40 | 136.37 | 126.70 |
| 74 | S2 | 644 | OMG | C1'-N9-C8 | 3.39 | 136.35 | 126.70 |
| 74 | S2 | 509 | OMG | N9-C4-N3 | 3.39 | 132.75 | 125.94 |
| 70 | L5 | 4637 | OMG | N9-C4-N3 | 3.38 | 132.73 | 125.94 |
| 70 | L5 | 3785 | A2M | O4'-C1'-N9 | 3.38 | 114.71 | 108.06 |
| 70 | L5 | 3830 | A2M | N3-C4-N9 | 3.38 | 132.64 | 127.08 |
| 74 | S2 | 1031 | A2M | N3-C4-N9 | 3.37 | 132.64 | 127.08 |
| 70 | L5 | 3825 | A2M | N3-C4-N9 | 3.37 | 132.63 | 127.08 |
| 74 | S2 | 644 | OMG | N9-C4-N3 | 3.36 | 132.69 | 125.94 |
| 70 | L5 | 2876 | OMG | C2-N1-C6 | -3.36 | 118.97 | 125.10 |
| 74 | S2 | 1850 | MA6 | N3-C4-N9 | 3.36 | 132.62 | 127.08 |
| 70 | L5 | 3760 | A2M | C5-N7-C8 | 3.35 | 108.27 | 103.51 |
| 74 | S2 | 627 | OMU | C5-C4-N3 | 3.34 | 119.84 | 114.84 |
| 74 | S2 | 1678 | A2M | N3-C4-N9 | 3.34 | 132.58 | 127.08 |
| 70 | L5 | 2837 | OMU | C5-C4-N3 | 3.33 | 119.83 | 114.84 |
| 70 | L5 | 4618 | OMG | N9-C4-N3 | 3.32 | 132.60 | 125.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 70 | L5 | 4196 | OMG | N9-C4-N3 | 3.32 | 132.60 | 125.94 |
| 74 | S2 | 27 | A2M | N3-C4-N9 | 3.31 | 132.54 | 127.08 |
| 74 | S2 | 683 | OMG | C1'-N9-C4 | -3.31 | 116.67 | 126.50 |
| 70 | L5 | 4523 | A2M | N3-C4-N9 | 3.31 | 132.53 | 127.08 |
| 74 | S2 | 1851 | MA6 | N3-C4-N9 | 3.27 | 132.47 | 127.08 |
| 74 | S2 | 1832 | 6MZ | C4-C5-N7 | -3.27 | 106.63 | 110.62 |
| 74 | S2 | 1832 | 6MZ | C2-N3-C4 | 3.27 | 119.48 | 111.75 |
| 70 | L5 | 4494 | OMG | N9-C4-N3 | 3.27 | 132.50 | 125.94 |
| 74 | S2 | 1804 | OMU | C5-C4-N3 | 3.26 | 119.72 | 114.84 |
| 70 | L5 | 1524 | A2M | C5-N7-C8 | 3.25 | 108.13 | 103.51 |
| 70 | L5 | 4620 | OMU | C5-C4-N3 | 3.25 | 119.71 | 114.84 |
| 70 | L5 | 4623 | OMG | N9-C4-N3 | 3.25 | 132.47 | 125.94 |
| 74 | S2 | 1031 | A2M | C5-N7-C8 | 3.24 | 108.12 | 103.51 |
| 70 | L5 | 2815 | A2M | C5-N7-C8 | 3.24 | 108.12 | 103.51 |
| 70 | L5 | 4637 | OMG | C2-N1-C6 | -3.24 | 119.19 | 125.10 |
| 74 | S2 | 668 | A2M | C5-N7-C8 | 3.24 | 108.11 | 103.51 |
| 70 | L5 | 1625 | OMG | C1'-N9-C4 | -3.23 | 116.90 | 126.50 |
| 70 | L5 | 1316 | OMG | N9-C4-N3 | 3.22 | 132.41 | 125.94 |
| 74 | S2 | 1328 | OMG | N9-C4-N3 | 3.22 | 132.40 | 125.94 |
| 70 | L5 | 3792 | OMG | C1'-N9-C8 | 3.21 | 135.84 | 126.70 |
| 70 | L5 | 4499 | OMG | N9-C4-N3 | 3.21 | 132.39 | 125.94 |
| 70 | L5 | 3825 | A2M | C5-N7-C8 | 3.21 | 108.07 | 103.51 |
| 70 | L5 | 3785 | A2M | C5-N7-C8 | 3.21 | 108.07 | 103.51 |
| 70 | L5 | 3782 | 5MC | C5-C6-N1 | -3.21 | 120.03 | 123.34 |
| 70 | L5 | 3627 | OMG | N9-C4-N3 | 3.21 | 132.38 | 125.94 |
| 70 | L5 | 3785 | A2M | N3-C4-N9 | 3.20 | 132.36 | 127.08 |
| 70 | L5 | 3830 | A2M | C5-N7-C8 | 3.20 | 108.06 | 103.51 |
| 74 | S2 | 99 | A2M | N3-C4-N9 | 3.20 | 132.36 | 127.08 |
| 74 | S2 | 1639 | G7M | O6-C6-C5 | -3.20 | 120.84 | 128.06 |
| 70 | L5 | 4571 | A2M | N3-C4-N9 | 3.20 | 132.35 | 127.08 |
| 74 | S2 | 644 | OMG | C2-N1-C6 | -3.20 | 119.27 | 125.10 |
| 70 | L5 | 400 | A2M | N3-C4-N9 | 3.19 | 132.34 | 127.08 |
| 70 | L5 | 3899 | OMG | N9-C4-N3 | 3.19 | 132.34 | 125.94 |
| 74 | S2 | 484 | A2M | N3-C4-N9 | 3.19 | 132.33 | 127.08 |
| 74 | S2 | 590 | A2M | C5-N7-C8 | 3.18 | 108.03 | 103.51 |
| 70 | L5 | 2363 | A2M | C5-N7-C8 | 3.18 | 108.03 | 103.51 |
| 70 | L5 | 4590 | A2M | C5-N7-C8 | 3.18 | 108.02 | 103.51 |
| 70 | L5 | 4392 | OMG | N9-C4-N3 | 3.17 | 132.31 | 125.94 |
| 74 | S2 | 1851 | MA6 | C5-N7-C8 | 3.17 | 108.01 | 103.51 |
| 70 | L5 | 2364 | OMG | N9-C4-N3 | 3.17 | 132.30 | 125.94 |
| 70 | L5 | 3744 | OMG | N9-C4-N3 | 3.17 | 132.30 | 125.94 |
| 70 | L5 | 3867 | A2M | N3-C4-N9 | 3.16 | 132.29 | 127.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 70 | L5 | 1871 | A2M | C5-N7-C8 | 3.16 | 108.00 | 103.51 |
| 70 | L5 | 1625 | OMG | C2-N1-C6 | -3.16 | 119.34 | 125.10 |
| 74 | S2 | 1383 | A2M | N3-C4-N9 | 3.16 | 132.29 | 127.08 |
| 74 | S2 | 512 | A2M | C5-N7-C8 | 3.15 | 107.99 | 103.51 |
| 70 | L5 | 3718 | A2M | N3-C4-N9 | 3.15 | 132.28 | 127.08 |
| 70 | L5 | 4220 | 6MZ | C2-N3-C4 | 3.15 | 119.19 | 111.75 |
| 74 | S2 | 1490 | OMG | N9-C4-N3 | 3.15 | 132.26 | 125.94 |
| 74 | S2 | 576 | A2M | N3-C4-N9 | 3.15 | 132.27 | 127.08 |
| 70 | L5 | 398 | A2M | C5-N7-C8 | 3.15 | 107.98 | 103.51 |
| 74 | S2 | 468 | A2M | N3-C4-N9 | 3.14 | 132.26 | 127.08 |
| 74 | S2 | 116 | OMU | C5-C4-N3 | 3.14 | 119.53 | 114.84 |
| 74 | S2 | 99 | A2M | C5-N7-C8 | 3.14 | 107.96 | 103.51 |
| 70 | L5 | 4618 | OMG | C2-N1-C6 | -3.13 | 119.38 | 125.10 |
| 70 | L5 | 2401 | A2M | C5-N7-C8 | 3.12 | 107.94 | 103.51 |
| 74 | S2 | 1850 | MA6 | C5-N7-C8 | 3.12 | 107.94 | 103.51 |
| 74 | S2 | 436 | OMG | N9-C4-N3 | 3.12 | 132.19 | 125.94 |
| 70 | L5 | 398 | A2M | N3-C4-N9 | 3.11 | 132.22 | 127.08 |
| 69 | L8 | 75 | OMG | N9-C4-N3 | 3.11 | 132.19 | 125.94 |
| 70 | L5 | 3867 | A2M | C5-N7-C8 | 3.11 | 107.92 | 103.51 |
| 70 | L5 | 4370 | OMG | N9-C4-N3 | 3.10 | 132.17 | 125.94 |
| 70 | L5 | 1524 | A2M | N3-C4-N9 | 3.10 | 132.20 | 127.08 |
| 70 | L5 | 2424 | OMG | N9-C4-N3 | 3.10 | 132.16 | 125.94 |
| 70 | L5 | 1871 | A2M | N3-C4-N9 | 3.09 | 132.18 | 127.08 |
| 74 | S2 | 683 | OMG | C1'-N9-C8 | 3.09 | 135.50 | 126.70 |
| 70 | L5 | 2363 | A2M | N3-C4-N9 | 3.09 | 132.18 | 127.08 |
| 70 | L5 | 1522 | OMG | C2-N1-C6 | -3.08 | 119.48 | 125.10 |
| 70 | L5 | 4220 | 6MZ | C9-N6-C6 | -3.08 | 120.22 | 122.87 |
| 74 | S2 | 683 | OMG | C2-N1-C6 | -3.08 | 119.48 | 125.10 |
| 70 | L5 | 2424 | OMG | C2-N1-C6 | -3.08 | 119.48 | 125.10 |
| 70 | L5 | 4623 | OMG | C2-N1-C6 | -3.08 | 119.49 | 125.10 |
| 74 | S2 | 509 | OMG | C2-N1-C6 | -3.07 | 119.50 | 125.10 |
| 70 | L5 | 1779 | PSU | O2-C2-N1 | -3.07 | 119.41 | 122.79 |
| 70 | L5 | 4494 | OMG | C2-N1-C6 | -3.07 | 119.51 | 125.10 |
| 74 | S2 | 867 | OMG | C2-N1-C6 | -3.06 | 119.51 | 125.10 |
| 74 | S2 | 27 | A2M | C5-N7-C8 | 3.06 | 107.86 | 103.51 |
| 70 | L5 | 3792 | OMG | C2-N1-C6 | -3.06 | 119.52 | 125.10 |
| 74 | S2 | 1383 | A2M | C5-N7-C8 | 3.06 | 107.85 | 103.51 |
| 74 | S2 | 822 | PSU | O2-C2-N1 | -3.06 | 119.42 | 122.79 |
| 70 | L5 | 4392 | OMG | C2-N1-C6 | -3.06 | 119.53 | 125.10 |
| 70 | L5 | 4590 | A2M | N3-C4-N9 | 3.05 | 132.12 | 127.08 |
| 74 | S2 | 428 | OMU | O4-C4-C5 | -3.05 | 119.80 | 125.16 |
| 70 | L5 | 400 | A2M | C5-N7-C8 | 3.05 | 107.84 | 103.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 70 | L5 | 1534 | A2M | N3-C4-N9 | 3.05 | 132.10 | 127.08 |
| 70 | L5 | 1326 | A2M | N3-C4-N9 | 3.04 | 132.10 | 127.08 |
| 70 | L5 | 4196 | OMG | C2-N1-C6 | -3.03 | 119.57 | 125.10 |
| 70 | L5 | 2837 | OMU | O4-C4-C5 | -3.03 | 119.82 | 125.16 |
| 74 | S2 | 436 | OMG | C2-N1-C6 | -3.03 | 119.58 | 125.10 |
| 74 | S2 | 1248 | B8N | N3-C2-N1 | 3.02 | 121.03 | 116.76 |
| 70 | L5 | 4523 | A2M | C5-N7-C8 | 3.02 | 107.80 | 103.51 |
| 70 | L5 | 2351 | OMC | O2-C2-N3 | -3.01 | 117.43 | 122.33 |
| 70 | L5 | 3627 | OMG | C2-N1-C6 | -3.01 | 119.62 | 125.10 |
| 70 | L5 | 1625 | OMG | C1'-N9-C8 | 3.00 | 135.25 | 126.70 |
| 70 | L5 | 2364 | OMG | C2-N1-C6 | -3.00 | 119.63 | 125.10 |
| 70 | L5 | 1534 | A2M | C5-N7-C8 | 3.00 | 107.77 | 103.51 |
| 74 | S2 | 668 | A2M | N3-C4-N9 | 2.99 | 132.01 | 127.08 |
| 74 | S2 | 1328 | OMG | C2-N1-C6 | -2.99 | 119.65 | 125.10 |
| 69 | L8 | 75 | OMG | C2-N1-C6 | -2.99 | 119.65 | 125.10 |
| 74 | S2 | 484 | A2M | C5-N7-C8 | 2.99 | 107.75 | 103.51 |
| 70 | L5 | 2876 | OMG | C1'-N9-C4 | -2.99 | 117.63 | 126.50 |
| 70 | L5 | 1326 | A2M | C5-N7-C8 | 2.98 | 107.74 | 103.51 |
| 70 | L5 | 1522 | OMG | N9-C4-N3 | 2.98 | 131.92 | 125.94 |
| 70 | L5 | 4370 | OMG | C2-N1-C6 | -2.97 | 119.68 | 125.10 |
| 70 | L5 | 1316 | OMG | C2-N1-C6 | -2.97 | 119.68 | 125.10 |
| 70 | L5 | 4499 | OMG | C2-N1-C6 | -2.97 | 119.68 | 125.10 |
| 70 | L5 | 4228 | OMG | C2-N1-C6 | -2.97 | 119.69 | 125.10 |
| 74 | S2 | 867 | OMG | N9-C4-N3 | 2.94 | 131.85 | 125.94 |
| 70 | L5 | 4571 | A2M | C5-N7-C8 | 2.94 | 107.68 | 103.51 |
| 74 | S2 | 468 | A2M | C5-N7-C8 | 2.94 | 107.68 | 103.51 |
| 70 | L5 | 3744 | OMG | C2-N1-C6 | -2.93 | 119.75 | 125.10 |
| 74 | S2 | 1639 | G7M | N9-C4-N3 | 2.93 | 131.82 | 125.94 |
| 74 | S2 | 576 | A2M | C5-N7-C8 | 2.93 | 107.67 | 103.51 |
| 70 | L5 | 3899 | OMG | C2-N1-C6 | -2.92 | 119.77 | 125.10 |
| 74 | S2 | 867 | OMG | N9-C8-N7 | -2.92 | 107.89 | 113.39 |
| 70 | L5 | 4227 | OMU | O4-C4-C5 | -2.92 | 120.03 | 125.16 |
| 67 | Pt | 47 | G7M | N9-C4-N3 | 2.92 | 131.80 | 125.94 |
| 74 | S2 | 1639 | G7M | CN7-N7-C8 | -2.90 | 120.36 | 124.84 |
| 74 | S2 | 1490 | OMG | C2-N1-C6 | -2.90 | 119.81 | 125.10 |
| 70 | L5 | 3718 | A2M | C5-N7-C8 | 2.89 | 107.62 | 103.51 |
| 74 | S2 | 627 | OMU | O4-C4-C5 | -2.89 | 120.08 | 125.16 |
| 70 | L5 | 4228 | OMG | N9-C8-N7 | -2.88 | 107.96 | 113.39 |
| 74 | S2 | 1238 | PSU | O2-C2-N1 | -2.88 | 119.62 | 122.79 |
| 70 | L5 | 2876 | OMG | C1'-N9-C8 | 2.88 | 134.90 | 126.70 |
| 70 | L5 | 3925 | OMU | O4-C4-C5 | -2.86 | 120.13 | 125.16 |
| 67 | Pt | 47 | G7M | CN7-N7-C5 | 2.85 | 130.31 | 126.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 74 | S2 | 1639 | G7M | C2-N1-C6 | -2.85 | 119.90 | 125.10 |
| 74 | S2 | 116 | OMU | O4-C4-C5 | -2.85 | 120.15 | 125.16 |
| 70 | L5 | 4228 | OMG | N9-C4-N3 | 2.83 | 131.63 | 125.94 |
| 74 | S2 | 1004 | PSU | O2-C2-N1 | -2.83 | 119.67 | 122.79 |
| 70 | L5 | 3899 | OMG | N9-C8-N7 | -2.83 | 108.06 | 113.39 |
| 74 | S2 | 1328 | OMG | N9-C8-N7 | -2.82 | 108.07 | 113.39 |
| 70 | L5 | 3627 | OMG | N9-C8-N7 | -2.82 | 108.08 | 113.39 |
| 70 | L5 | 1522 | OMG | N9-C8-N7 | -2.81 | 108.11 | 113.39 |
| 74 | S2 | 1804 | OMU | O4-C4-C5 | -2.80 | 120.24 | 125.16 |
| 70 | L5 | 2876 | OMG | C5-C6-N1 | 2.80 | 120.29 | 113.19 |
| 70 | L5 | 4531 | PSU | O2-C2-N1 | -2.79 | 119.71 | 122.79 |
| 70 | L5 | 3792 | OMG | C5-C6-N1 | 2.79 | 120.28 | 113.19 |
| 74 | S2 | 822 | PSU | C6-N1-C2 | -2.79 | 119.83 | 122.68 |
| 74 | S2 | 436 | OMG | N9-C8-N7 | -2.79 | 108.13 | 113.39 |
| 69 | L8 | 75 | OMG | N9-C8-N7 | -2.79 | 108.14 | 113.39 |
| 70 | L5 | 3770 | PSU | O2-C2-N1 | -2.79 | 119.72 | 122.79 |
| 70 | L5 | 4498 | OMU | O4-C4-C5 | -2.78 | 120.27 | 125.16 |
| 70 | L5 | 4620 | OMU | O4-C4-C5 | -2.77 | 120.29 | 125.16 |
| 74 | S2 | 1445 | PSU | O2-C2-N1 | -2.77 | 119.74 | 122.79 |
| 70 | L5 | 4499 | OMG | N9-C8-N7 | -2.77 | 108.18 | 113.39 |
| 74 | S2 | 683 | OMG | C5-C6-N1 | 2.77 | 120.22 | 113.19 |
| 70 | L5 | 1744 | PSU | O2-C2-N1 | -2.76 | 119.75 | 122.79 |
| 70 | L5 | 4370 | OMG | C5-C6-N1 | 2.76 | 120.21 | 113.19 |
| 70 | L5 | 4579 | PSU | O2-C2-N1 | -2.76 | 119.75 | 122.79 |
| 74 | S2 | 649 | PSU | O2-C2-N1 | -2.76 | 119.75 | 122.79 |
| 70 | L5 | 4618 | OMG | C5-C6-N1 | 2.75 | 120.18 | 113.19 |
| 70 | L5 | 4370 | OMG | N9-C8-N7 | -2.75 | 108.21 | 113.39 |
| 67 | Pt | 47 | G7M | C2-N1-C6 | -2.75 | 120.09 | 125.10 |
| 74 | S2 | 644 | OMG | C5-C6-N1 | 2.75 | 120.17 | 113.19 |
| 70 | L5 | 4392 | OMG | C5-C6-N1 | 2.74 | 120.16 | 113.19 |
| 70 | L5 | 3884 | PSU | O2-C2-N1 | -2.74 | 119.77 | 122.79 |
| 70 | L5 | 1316 | OMG | N9-C8-N7 | -2.74 | 108.23 | 113.39 |
| 70 | L5 | 4637 | OMG | N9-C8-N7 | -2.74 | 108.23 | 113.39 |
| 70 | L5 | 4312 | PSU | O2-C2-N1 | -2.74 | 119.78 | 122.79 |
| 74 | S2 | 1174 | PSU | O2-C2-N1 | -2.74 | 119.78 | 122.79 |
| 74 | S2 | 1328 | OMG | C5-C6-N1 | 2.74 | 120.14 | 113.19 |
| 70 | L5 | 4628 | PSU | O2-C2-N1 | -2.74 | 119.78 | 122.79 |
| 70 | L5 | 4637 | OMG | C5-C6-N1 | 2.73 | 120.14 | 113.19 |
| 70 | L5 | 1625 | OMG | C5-C6-N1 | 2.73 | 120.12 | 113.19 |
| 70 | L5 | 2839 | PSU | O2-C2-N1 | -2.73 | 119.79 | 122.79 |
| 70 | L5 | 4423 | PSU | O2-C2-N1 | -2.72 | 119.79 | 122.79 |
| 69 | L8 | 75 | OMG | C5-C6-N1 | 2.71 | 120.08 | 113.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 70 | L5 | 4499 | OMG | C5-C6-N1 | 2.71 | 120.07 | 113.19 |
| 70 | L5 | 4228 | OMG | C5-C6-N1 | 2.71 | 120.06 | 113.19 |
| 70 | L5 | 1677 | PSU | O2-C2-N1 | -2.71 | 119.81 | 122.79 |
| 70 | L5 | 3744 | OMG | N9-C8-N7 | -2.70 | 108.30 | 113.39 |
| 70 | L5 | 4196 | OMG | C5-C6-N1 | 2.70 | 120.06 | 113.19 |
| 70 | L5 | 4392 | OMG | N9-C8-N7 | -2.70 | 108.30 | 113.39 |
| 70 | L5 | 2364 | OMG | C5-C6-N1 | 2.70 | 120.05 | 113.19 |
| 74 | S2 | 1243 | PSU | O2-C2-N1 | -2.70 | 119.81 | 122.79 |
| 70 | L5 | 3792 | OMG | O6-C6-C5 | -2.70 | 119.44 | 126.60 |
| 74 | S2 | 406 | PSU | O2-C2-N1 | -2.70 | 119.82 | 122.79 |
| 74 | S2 | 686 | PSU | O2-C2-N1 | -2.70 | 119.82 | 122.79 |
| 70 | L5 | 4494 | OMG | C5-C6-N1 | 2.69 | 120.03 | 113.19 |
| 70 | L5 | 1522 | OMG | C5-C6-N1 | 2.69 | 120.03 | 113.19 |
| 74 | S2 | 649 | PSU | C6-N1-C2 | -2.69 | 119.93 | 122.68 |
| 70 | L5 | 2364 | OMG | N9-C8-N7 | -2.69 | 108.33 | 113.39 |
| 70 | L5 | 3627 | OMG | C5-C6-N1 | 2.69 | 120.02 | 113.19 |
| 70 | L5 | 4196 | OMG | N9-C8-N7 | -2.69 | 108.33 | 113.39 |
| 70 | L5 | 3758 | PSU | O2-C2-N1 | -2.68 | 119.84 | 122.79 |
| 74 | S2 | 1347 | PSU | O2-C2-N1 | -2.68 | 119.84 | 122.79 |
| 70 | L5 | 4623 | OMG | C5-C6-N1 | 2.68 | 119.99 | 113.19 |
| 70 | L5 | 1862 | PSU | O2-C2-N1 | -2.68 | 119.84 | 122.79 |
| 74 | S2 | 683 | OMG | O6-C6-C5 | -2.68 | 119.50 | 126.60 |
| 70 | L5 | 3764 | PSU | O2-C2-N1 | -2.68 | 119.84 | 122.79 |
| 74 | S2 | 436 | OMG | C5-C6-N1 | 2.67 | 119.98 | 113.19 |
| 74 | S2 | 867 | OMG | C5-C6-N1 | 2.67 | 119.98 | 113.19 |
| 70 | L5 | 4618 | OMG | N9-C8-N7 | -2.67 | 108.36 | 113.39 |
| 70 | L5 | 4500 | PSU | O2-C2-N1 | -2.67 | 119.85 | 122.79 |
| 74 | S2 | 1136 | PSU | O2-C2-N1 | -2.67 | 119.85 | 122.79 |
| 70 | L5 | 4494 | OMG | O6-C6-C5 | -2.67 | 119.52 | 126.60 |
| 67 | Pt | 56 | PSU | O2-C2-N1 | -2.67 | 119.85 | 122.79 |
| 74 | S2 | 509 | OMG | C5-C6-N1 | 2.67 | 119.97 | 113.19 |
| 74 | S2 | 866 | PSU | O2-C2-N1 | -2.67 | 119.85 | 122.79 |
| 74 | S2 | 609 | PSU | O2-C2-N1 | -2.66 | 119.86 | 122.79 |
| 70 | L5 | 1625 | OMG | N9-C8-N7 | -2.66 | 108.38 | 113.39 |
| 70 | L5 | 4623 | OMG | N9-C8-N7 | -2.66 | 108.38 | 113.39 |
| 74 | S2 | 119 | PSU | C6-N1-C2 | -2.66 | 119.97 | 122.68 |
| 70 | L5 | 1625 | OMG | O6-C6-C5 | -2.66 | 119.55 | 126.60 |
| 74 | S2 | 36 | PSU | O2-C2-N1 | -2.66 | 119.87 | 122.79 |
| 70 | L5 | 2508 | PSU | O2-C2-N1 | -2.65 | 119.87 | 122.79 |
| 74 | S2 | 1625 | PSU | O2-C2-N1 | -2.65 | 119.87 | 122.79 |
| 70 | L5 | 1316 | OMG | C5-C6-N1 | 2.64 | 119.90 | 113.19 |
| 74 | S2 | 683 | OMG | N9-C8-N7 | -2.64 | 108.42 | 113.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 70 | L5 | 2632 | PSU | O2-C2-N1 | -2.64 | 119.89 | 122.79 |
| 74 | S2 | 1248 | B8N | O4-C4-N3 | -2.63 | 115.51 | 119.98 |
| 74 | S2 | 34 | PSU | O2-C2-N1 | -2.63 | 119.89 | 122.79 |
| 70 | L5 | 3792 | OMG | N9-C8-N7 | -2.63 | 108.43 | 113.39 |
| 70 | L5 | 4532 | PSU | O2-C2-N1 | -2.63 | 119.89 | 122.79 |
| 70 | L5 | 3762 | PSU | O2-C2-N1 | -2.63 | 119.89 | 122.79 |
| 74 | S2 | 105 | PSU | O2-C2-N1 | -2.63 | 119.89 | 122.79 |
| 67 | Pt | 21 | H2U | C5-C4-N3 | 2.62 | 119.60 | 116.65 |
| 70 | L5 | 3744 | OMG | C5-C6-N1 | 2.62 | 119.84 | 113.19 |
| 74 | S2 | 1490 | OMG | N9-C8-N7 | -2.62 | 108.46 | 113.39 |
| 70 | L5 | 2424 | OMG | C5-C6-N1 | 2.62 | 119.83 | 113.19 |
| 70 | L5 | 2876 | OMG | O6-C6-C5 | -2.61 | 119.67 | 126.60 |
| 74 | S2 | 1490 | OMG | C5-C6-N1 | 2.61 | 119.83 | 113.19 |
| 70 | L5 | 2876 | OMG | N9-C8-N7 | -2.61 | 108.47 | 113.39 |
| 70 | L5 | 4628 | PSU | C6-N1-C2 | -2.61 | 120.02 | 122.68 |
| 70 | L5 | 4569 | PSU | O2-C2-N1 | -2.61 | 119.92 | 122.79 |
| 69 | L8 | 69 | PSU | O2-C2-N1 | -2.60 | 119.92 | 122.79 |
| 70 | L5 | 5010 | PSU | O2-C2-N1 | -2.60 | 119.92 | 122.79 |
| 70 | L5 | 3899 | OMG | C5-C6-N1 | 2.60 | 119.80 | 113.19 |
| 70 | L5 | 3768 | PSU | O2-C2-N1 | -2.60 | 119.93 | 122.79 |
| 67 | Pt | 21 | H2U | C5-C6-N1 | 2.60 | 120.17 | 111.61 |
| 74 | S2 | 644 | OMG | N9-C8-N7 | -2.60 | 108.50 | 113.39 |
| 74 | S2 | 1367 | PSU | O2-C2-N1 | -2.60 | 119.93 | 122.79 |
| 70 | L5 | 4220 | 6MZ | N3-C4-N9 | 2.59 | 131.36 | 127.08 |
| 70 | L5 | 4494 | OMG | N9-C8-N7 | -2.59 | 108.51 | 113.39 |
| 70 | L5 | 4972 | PSU | O2-C2-N1 | -2.59 | 119.94 | 122.79 |
| 70 | L5 | 4618 | OMG | O6-C6-C5 | -2.59 | 119.73 | 126.60 |
| 74 | S2 | 1328 | OMG | O6-C6-C5 | -2.58 | 119.75 | 126.60 |
| 70 | L5 | 4370 | OMG | O6-C6-C5 | -2.58 | 119.76 | 126.60 |
| 70 | L5 | 2424 | OMG | O6-C6-C5 | -2.58 | 119.77 | 126.60 |
| 74 | S2 | 436 | OMG | O6-C6-C5 | -2.57 | 119.77 | 126.60 |
| 74 | S2 | 644 | OMG | O6-C6-C5 | -2.57 | 119.77 | 126.60 |
| 70 | L5 | 4299 | PSU | O2-C2-N1 | -2.57 | 119.96 | 122.79 |
| 70 | L5 | 4457 | PSU | O2-C2-N1 | -2.57 | 119.96 | 122.79 |
| 70 | L5 | 4403 | PSU | O2-C2-N1 | -2.57 | 119.96 | 122.79 |
| 74 | S2 | 1244 | PSU | O2-C2-N1 | -2.57 | 119.97 | 122.79 |
| 67 | Pt | 47 | G7M | CN7-N7-C8 | -2.56 | 120.88 | 124.84 |
| 70 | L5 | 3762 | PSU | C6-N1-C2 | -2.56 | 120.06 | 122.68 |
| 70 | L5 | 3639 | PSU | O2-C2-N1 | -2.56 | 119.97 | 122.79 |
| 74 | S2 | 296 | PSU | O2-C2-N1 | -2.56 | 119.97 | 122.79 |
| 74 | S2 | 1643 | PSU | O2-C2-N1 | -2.56 | 119.98 | 122.79 |
| 74 | S2 | 572 | PSU | O2-C2-N1 | -2.56 | 119.98 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 70 | L5 | 4420 | PSU | C6-N1-C2 | -2.56 | 120.07 | 122.68 |
| 70 | L5 | 4636 | PSU | O2-C2-N1 | -2.55 | 119.98 | 122.79 |
| 70 | L5 | 4689 | PSU | O2-C2-N1 | -2.55 | 119.98 | 122.79 |
| 74 | S2 | 966 | PSU | O2-C2-N1 | -2.55 | 119.98 | 122.79 |
| 70 | L5 | 4623 | OMG | O6-C6-C5 | -2.55 | 119.84 | 126.60 |
| 74 | S2 | 1239 | PSU | O2-C2-N1 | -2.55 | 119.99 | 122.79 |
| 70 | L5 | 1683 | PSU | O2-C2-N1 | -2.54 | 119.99 | 122.79 |
| 70 | L5 | 4471 | PSU | O2-C2-N1 | -2.54 | 119.99 | 122.79 |
| 70 | L5 | 3729 | PSU | O2-C2-N1 | -2.54 | 119.99 | 122.79 |
| 70 | L5 | 4420 | PSU | O2-C2-N1 | -2.54 | 120.00 | 122.79 |
| 74 | S2 | 651 | PSU | O2-C2-N1 | -2.53 | 120.01 | 122.79 |
| 74 | S2 | 863 | PSU | O2-C2-N1 | -2.53 | 120.01 | 122.79 |
| 74 | S2 | 1832 | 6MZ | N3-C4-N9 | 2.52 | 131.24 | 127.08 |
| 70 | L5 | 2424 | OMG | N9-C8-N7 | -2.52 | 108.64 | 113.39 |
| 70 | L5 | 3785 | A2M | O4'-C1'-C2' | -2.52 | 102.15 | 106.57 |
| 70 | L5 | 1316 | OMG | O6-C6-C5 | -2.52 | 119.92 | 126.60 |
| 74 | S2 | 1177 | PSU | O2-C2-N1 | -2.51 | 120.02 | 122.79 |
| 69 | L8 | 75 | OMG | O6-C6-C5 | -2.51 | 119.94 | 126.60 |
| 70 | L5 | 4220 | 6MZ | C4-C5-N7 | -2.51 | 107.56 | 110.62 |
| 74 | S2 | 918 | PSU | O2-C2-N1 | -2.50 | 120.03 | 122.79 |
| 70 | L5 | 4196 | OMG | O6-C6-C5 | -2.50 | 119.96 | 126.60 |
| 74 | S2 | 109 | PSU | C6-N1-C2 | -2.50 | 120.12 | 122.68 |
| 67 | Pt | 47 | G7M | N9-C8-N7 | -2.50 | 106.02 | 112.21 |
| 74 | S2 | 918 | PSU | C6-N1-C2 | -2.50 | 120.12 | 122.68 |
| 70 | L5 | 2843 | PSU | O2-C2-N1 | -2.50 | 120.04 | 122.79 |
| 70 | L5 | 4220 | 6MZ | C4-N9-C1' | -2.50 | 120.64 | 126.59 |
| 74 | S2 | 1842 | 4AC | C6-C5-C4 | 2.50 | 120.02 | 116.96 |
| 70 | L5 | 4442 | PSU | O2-C2-N1 | -2.50 | 120.04 | 122.79 |
| 70 | L5 | 3884 | PSU | C6-N1-C2 | -2.49 | 120.14 | 122.68 |
| 74 | S2 | 1678 | A2M | C4-C5-N7 | -2.49 | 107.59 | 110.62 |
| 70 | L5 | 4530 | UR3 | C6-N1-C2 | -2.49 | 119.56 | 121.79 |
| 70 | L5 | 4552 | PSU | O2-C2-N1 | -2.49 | 120.05 | 122.79 |
| 70 | L5 | 4499 | OMG | O6-C6-C5 | -2.48 | 120.02 | 126.60 |
| 74 | S2 | 93 | PSU | O2-C2-N1 | -2.48 | 120.06 | 122.79 |
| 74 | S2 | 509 | OMG | O6-C6-C5 | -2.48 | 120.02 | 126.60 |
| 70 | L5 | 4293 | PSU | O2-C2-N1 | -2.48 | 120.06 | 122.79 |
| 70 | L5 | 2508 | PSU | C6-N1-C2 | -2.47 | 120.15 | 122.68 |
| 70 | L5 | 2364 | OMG | O6-C6-C5 | -2.47 | 120.04 | 126.60 |
| 70 | L5 | 3782 | 5MC | CM5-C5-C6 | -2.47 | 119.55 | 122.85 |
| 70 | L5 | 4471 | PSU | C6-N1-C2 | -2.47 | 120.16 | 122.68 |
| 70 | L5 | 3627 | OMG | O6-C6-C5 | -2.47 | 120.06 | 126.60 |
| 70 | L5 | 4576 | PSU | O2-C2-N1 | -2.46 | 120.08 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 74 | S2 | 1004 | PSU | C6-N1-C2 | -2.46 | 120.17 | 122.68 |
| 70 | L5 | 3715 | PSU | O2-C2-N1 | -2.46 | 120.08 | 122.79 |
| 70 | L5 | 4673 | PSU | O2-C2-N1 | -2.46 | 120.08 | 122.79 |
| 70 | L5 | 3844 | PSU | O2-C2-N1 | -2.46 | 120.08 | 122.79 |
| 74 | S2 | 815 | PSU | C6-N1-C2 | -2.46 | 120.17 | 122.68 |
| 70 | L5 | 1536 | PSU | O2-C2-N1 | -2.46 | 120.08 | 122.79 |
| 74 | S2 | 867 | OMG | O6-C6-C5 | -2.46 | 120.08 | 126.60 |
| 70 | L5 | 4361 | PSU | O2-C2-N1 | -2.46 | 120.09 | 122.79 |
| 74 | S2 | 1243 | PSU | C6-N1-C2 | -2.45 | 120.17 | 122.68 |
| 70 | L5 | 3744 | OMG | O6-C6-C5 | -2.45 | 120.09 | 126.60 |
| 70 | L5 | 4673 | PSU | C6-N1-C2 | -2.45 | 120.17 | 122.68 |
| 74 | S2 | 1490 | OMG | O6-C6-C5 | -2.45 | 120.10 | 126.60 |
| 74 | S2 | 109 | PSU | O2-C2-N1 | -2.45 | 120.09 | 122.79 |
| 67 | Pt | 33 | OMC | O2-C2-N3 | -2.45 | 118.35 | 122.33 |
| 70 | L5 | 4392 | OMG | O6-C6-C5 | -2.45 | 120.11 | 126.60 |
| 70 | L5 | 4228 | OMG | O6-C6-C5 | -2.44 | 120.11 | 126.60 |
| 69 | L8 | 55 | PSU | O2-C2-N1 | -2.44 | 120.10 | 122.79 |
| 70 | L5 | 3853 | PSU | C6-N1-C2 | -2.44 | 120.19 | 122.68 |
| 70 | L5 | 4500 | PSU | C6-N1-C2 | -2.44 | 120.19 | 122.68 |
| 74 | S2 | 918 | PSU | O4'-C1'-C2' | 2.44 | 108.59 | 105.14 |
| 70 | L5 | 4521 | PSU | O2-C2-N1 | -2.44 | 120.10 | 122.79 |
| 74 | S2 | 1238 | PSU | C6-N1-C2 | -2.44 | 120.19 | 122.68 |
| 74 | S2 | 801 | PSU | O2-C2-N1 | -2.44 | 120.11 | 122.79 |
| 74 | S2 | 509 | OMG | N9-C8-N7 | -2.44 | 108.80 | 113.39 |
| 70 | L5 | 4637 | OMG | O6-C6-C5 | -2.44 | 120.13 | 126.60 |
| 70 | L5 | 3764 | PSU | C6-N1-C2 | -2.43 | 120.20 | 122.68 |
| 70 | L5 | 2351 | OMC | C1'-N1-C2 | 2.42 | 123.83 | 118.42 |
| 70 | L5 | 1322 | 1MA | N9-C8-N7 | -2.42 | 108.84 | 113.39 |
| 70 | L5 | 4972 | PSU | C6-N1-C2 | -2.41 | 120.21 | 122.68 |
| 70 | L5 | 3899 | OMG | O6-C6-C5 | -2.41 | 120.20 | 126.60 |
| 74 | S2 | 1232 | PSU | O2-C2-N1 | -2.41 | 120.14 | 122.79 |
| 74 | S2 | 218 | PSU | O2-C2-N1 | -2.41 | 120.14 | 122.79 |
| 70 | L5 | 4299 | PSU | C6-N1-C2 | -2.41 | 120.22 | 122.68 |
| 70 | L5 | 4493 | PSU | O2-C2-N1 | -2.41 | 120.14 | 122.79 |
| 70 | L5 | 4296 | PSU | O2-C2-N1 | -2.40 | 120.15 | 122.79 |
| 70 | L5 | 4532 | PSU | C6-N1-C2 | -2.40 | 120.23 | 122.68 |
| 70 | L5 | 5001 | PSU | O2-C2-N1 | -2.40 | 120.15 | 122.79 |
| 74 | S2 | 863 | PSU | C6-N1-C2 | -2.40 | 120.23 | 122.68 |
| 74 | S2 | 1643 | PSU | C6-N1-C2 | -2.40 | 120.23 | 122.68 |
| 70 | L5 | 1522 | OMG | O6-C6-C5 | -2.39 | 120.25 | 126.60 |
| 70 | L5 | 4531 | PSU | C6-C5-C4 | 2.39 | 119.87 | 118.20 |
| 70 | L5 | 1782 | PSU | O2-C2-N1 | -2.39 | 120.16 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 70 | L5 | 3734 | PSU | O2-C2-N1 | -2.39 | 120.16 | 122.79 |
| 74 | S2 | 34 | PSU | C6-N1-C2 | -2.39 | 120.24 | 122.68 |
| 70 | L5 | 4423 | PSU | C6-N1-C2 | -2.39 | 120.24 | 122.68 |
| 70 | L5 | 4689 | PSU | C6-N1-C2 | -2.39 | 120.24 | 122.68 |
| 70 | L5 | 3715 | PSU | C6-N1-C2 | -2.38 | 120.25 | 122.68 |
| 74 | S2 | 1337 | 4AC | C6-C5-C4 | 2.38 | 119.87 | 116.96 |
| 74 | S2 | 866 | PSU | C6-N1-C2 | -2.38 | 120.25 | 122.68 |
| 70 | L5 | 3770 | PSU | C6-N1-C2 | -2.37 | 120.25 | 122.68 |
| 70 | L5 | 5001 | PSU | C6-N1-C2 | -2.37 | 120.26 | 122.68 |
| 70 | L5 | 1582 | PSU | C6-N1-C2 | -2.37 | 120.26 | 122.68 |
| 70 | L5 | 1871 | A2M | C4-N9-C8 | 2.37 | 108.30 | 105.73 |
| 70 | L5 | 3729 | PSU | C6-N1-C2 | -2.36 | 120.27 | 122.68 |
| 70 | L5 | 4576 | PSU | C6-N1-C2 | -2.36 | 120.27 | 122.68 |
| 74 | S2 | 406 | PSU | C6-N1-C2 | -2.35 | 120.28 | 122.68 |
| 70 | L5 | 4293 | PSU | C6-N1-C2 | -2.34 | 120.29 | 122.68 |
| 74 | S2 | 1232 | PSU | C6-N1-C2 | -2.34 | 120.29 | 122.68 |
| 70 | L5 | 3637 | PSU | C6-N1-C2 | -2.34 | 120.29 | 122.68 |
| 70 | L5 | 4579 | PSU | C6-N1-C2 | -2.34 | 120.29 | 122.68 |
| 70 | L5 | 2815 | A2M | C6-C5-C4 | 2.33 | 120.31 | 117.18 |
| 70 | L5 | 3920 | PSU | C6-N1-C2 | -2.33 | 120.31 | 122.68 |
| 70 | L5 | 1860 | PSU | O2-C2-N1 | -2.33 | 120.23 | 122.79 |
| 74 | S2 | 1850 | MA6 | C4-N9-C8 | 2.32 | 108.25 | 105.73 |
| 70 | L5 | 1744 | PSU | C6-N1-C2 | -2.32 | 120.31 | 122.68 |
| 70 | L5 | 4431 | PSU | O2-C2-N1 | -2.32 | 120.24 | 122.79 |
| 70 | L5 | 3851 | PSU | O2-C2-N1 | -2.31 | 120.24 | 122.79 |
| 70 | L5 | 2401 | A2M | C6-C5-C4 | 2.31 | 120.29 | 117.18 |
| 74 | S2 | 1692 | PSU | O2-C2-N1 | -2.31 | 120.25 | 122.79 |
| 74 | S2 | 1445 | PSU | C6-N1-C2 | -2.31 | 120.32 | 122.68 |
| 70 | L5 | 4431 | PSU | C6-N1-C2 | -2.31 | 120.32 | 122.68 |
| 74 | S2 | 801 | PSU | C6-N1-C2 | -2.30 | 120.33 | 122.68 |
| 70 | L5 | 1792 | PSU | O2-C2-N1 | -2.30 | 120.26 | 122.79 |
| 70 | L5 | 3695 | PSU | C6-N1-C2 | -2.30 | 120.33 | 122.68 |
| 74 | S2 | 576 | A2M | C6-C5-C4 | 2.30 | 120.27 | 117.18 |
| 70 | L5 | 3758 | PSU | C6-N1-C2 | -2.30 | 120.33 | 122.68 |
| 70 | L5 | 2837 | OMU | O2-C2-N1 | -2.29 | 119.74 | 122.79 |
| 70 | L5 | 4353 | PSU | O2-C2-N1 | -2.29 | 120.27 | 122.79 |
| 74 | S2 | 668 | A2M | C3'-C2'-C1' | 2.29 | 107.20 | 102.89 |
| 74 | S2 | 1056 | PSU | O2-C2-N1 | -2.29 | 120.27 | 122.79 |
| 74 | S2 | 1337 | 4AC | C5-C4-N3 | -2.28 | 118.92 | 122.59 |
| 70 | L5 | 1862 | PSU | C6-N1-C2 | -2.28 | 120.35 | 122.68 |
| 74 | S2 | 651 | PSU | C6-N1-C2 | -2.28 | 120.36 | 122.68 |
| 74 | S2 | 1031 | A2M | C6-C5-C4 | 2.28 | 120.24 | 117.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 70 | L5 | 4442 | PSU | C6-N1-C2 | -2.28 | 120.36 | 122.68 |
| 74 | S2 | 814 | PSU | O2-C2-N1 | -2.27 | 120.29 | 122.79 |
| 70 | L5 | 1779 | PSU | C6-N1-C2 | -2.27 | 120.36 | 122.68 |
| 74 | S2 | 573 | PSU | O2-C2-N1 | -2.27 | 120.29 | 122.79 |
| 74 | S2 | 1248 | B8N | O4'-C1'-C2' | 2.27 | 108.34 | 105.14 |
| 70 | L5 | 3920 | PSU | O2-C2-N1 | -2.27 | 120.30 | 122.79 |
| 74 | S2 | 296 | PSU | C6-N1-C2 | -2.27 | 120.37 | 122.68 |
| 74 | S2 | 105 | PSU | C6-N1-C2 | -2.27 | 120.37 | 122.68 |
| 70 | L5 | 3695 | PSU | O2-C2-N1 | -2.26 | 120.30 | 122.79 |
| 74 | S2 | 1625 | PSU | C6-N1-C2 | -2.26 | 120.37 | 122.68 |
| 70 | L5 | 4552 | PSU | C6-N1-C2 | -2.26 | 120.37 | 122.68 |
| 70 | L5 | 5010 | PSU | C6-N1-C2 | -2.26 | 120.37 | 122.68 |
| 70 | L5 | 4523 | A2M | C6-C5-C4 | 2.26 | 120.22 | 117.18 |
| 74 | S2 | 1832 | 6MZ | C4-N9-C8 | 2.26 | 108.18 | 105.73 |
| 74 | S2 | 590 | A2M | C6-C5-C4 | 2.25 | 120.21 | 117.18 |
| 70 | L5 | 3760 | A2M | C4-N9-C8 | 2.25 | 108.16 | 105.73 |
| 74 | S2 | 1174 | PSU | C6-N1-C2 | -2.25 | 120.39 | 122.68 |
| 74 | S2 | 681 | PSU | O2-C2-N1 | -2.24 | 120.32 | 122.79 |
| 70 | L5 | 3825 | A2M | C6-C5-C4 | 2.24 | 120.20 | 117.18 |
| 74 | S2 | 668 | A2M | C4-C5-N7 | -2.24 | 107.89 | 110.62 |
| 74 | S2 | 814 | PSU | C6-N1-C2 | -2.24 | 120.40 | 122.68 |
| 70 | L5 | 1524 | A2M | C4-C5-N7 | -2.24 | 107.90 | 110.62 |
| 70 | L5 | 4590 | A2M | C4-C5-N7 | -2.24 | 107.90 | 110.62 |
| 70 | L5 | 4220 | 6MZ | C4-N9-C8 | 2.23 | 108.15 | 105.73 |
| 67 | Pt | 56 | PSU | C6-N1-C2 | -2.23 | 120.40 | 122.68 |
| 69 | L8 | 69 | PSU | C6-N1-C2 | -2.23 | 120.41 | 122.68 |
| 70 | L5 | 1522 | OMG | C8-N7-C5 | 2.22 | 108.27 | 104.24 |
| 74 | S2 | 686 | PSU | C6-N1-C2 | -2.22 | 120.41 | 122.68 |
| 65 | La | 39 | V5N | O-C-CA | -2.22 | 118.96 | 124.78 |
| 74 | S2 | 815 | PSU | O2-C2-N1 | -2.22 | 120.35 | 122.79 |
| 70 | L5 | 3760 | A2M | C6-C5-C4 | 2.22 | 120.17 | 117.18 |
| 70 | L5 | 4442 | PSU | O4'-C1'-C2' | 2.22 | 108.27 | 105.14 |
| 74 | S2 | 627 | OMU | O2-C2-N1 | -2.21 | 119.84 | 122.79 |
| 70 | L5 | 3785 | A2M | C4-N9-C8 | 2.21 | 108.12 | 105.73 |
| 70 | L5 | 3627 | OMG | C8-N7-C5 | 2.21 | 108.24 | 104.24 |
| 74 | S2 | 1248 | B8N | C31-N3-C2 | 2.21 | 120.98 | 117.67 |
| 70 | L5 | 1683 | PSU | C6-N1-C2 | -2.21 | 120.43 | 122.68 |
| 70 | L5 | 4296 | PSU | C6-N1-C2 | -2.21 | 120.43 | 122.68 |
| 70 | L5 | 4493 | PSU | C6-N1-C2 | -2.21 | 120.43 | 122.68 |
| 70 | L5 | 4457 | PSU | C6-N1-C2 | -2.20 | 120.43 | 122.68 |
| 74 | S2 | 572 | PSU | C6-N1-C2 | -2.20 | 120.43 | 122.68 |
| 74 | S2 | 1244 | PSU | C6-N1-C2 | -2.20 | 120.43 | 122.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 70 | L5 | 1781 | PSU | C6-N1-C2 | -2.20 | 120.44 | 122.68 |
| 74 | S2 | 1177 | PSU | C6-N1-C2 | -2.20 | 120.44 | 122.68 |
| 74 | S2 | 1347 | PSU | C6-N1-C2 | -2.20 | 120.44 | 122.68 |
| 70 | L5 | 4312 | PSU | C6-N1-C2 | -2.20 | 120.44 | 122.68 |
| 70 | L5 | 2843 | PSU | C6-N1-C2 | -2.20 | 120.44 | 122.68 |
| 74 | S2 | 36 | PSU | C6-N1-C2 | -2.20 | 120.44 | 122.68 |
| 70 | L5 | 1781 | PSU | O2-C2-N1 | -2.19 | 120.38 | 122.79 |
| 74 | S2 | 1832 | 6MZ | C5-C4-N9 | 2.19 | 108.33 | 105.78 |
| 67 | Pt | 33 | OMC | C1'-N1-C2 | 2.19 | 123.31 | 118.42 |
| 70 | L5 | 2876 | OMG | C8-N7-C5 | 2.19 | 108.21 | 104.24 |
| 74 | S2 | 1678 | A2M | C6-C5-C4 | 2.19 | 120.13 | 117.18 |
| 74 | S2 | 1367 | PSU | C6-N1-C2 | -2.18 | 120.45 | 122.68 |
| 70 | L5 | 3899 | OMG | C8-N7-C5 | 2.18 | 108.19 | 104.24 |
| 74 | S2 | 609 | PSU | C6-N1-C2 | -2.18 | 120.45 | 122.68 |
| 74 | S2 | 668 | A2M | C4-N9-C8 | 2.18 | 108.09 | 105.73 |
| 74 | S2 | 867 | OMG | C8-N7-C5 | 2.18 | 108.18 | 104.24 |
| 70 | L5 | 1322 | 1MA | C2'-C1'-N9 | 2.17 | 119.38 | 113.22 |
| 70 | L5 | 1536 | PSU | C6-N1-C2 | -2.17 | 120.46 | 122.68 |
| 70 | L5 | 3851 | PSU | C6-N1-C2 | -2.17 | 120.46 | 122.68 |
| 70 | L5 | 4569 | PSU | C6-N1-C2 | -2.17 | 120.46 | 122.68 |
| 74 | S2 | 681 | PSU | C6-N1-C2 | -2.17 | 120.47 | 122.68 |
| 70 | L5 | 4403 | PSU | C6-N1-C2 | -2.17 | 120.47 | 122.68 |
| 74 | S2 | 1842 | 4AC | O2-C2-N3 | -2.16 | 118.81 | 122.33 |
| 70 | L5 | 4637 | OMG | C8-N7-C5 | 2.16 | 108.15 | 104.24 |
| 70 | L5 | 4521 | PSU | C6-N1-C2 | -2.16 | 120.48 | 122.68 |
| 74 | S2 | 1842 | 4AC | C5-C4-N3 | -2.16 | 119.12 | 122.59 |
| 70 | L5 | 1322 | 1MA | C5-C4-N9 | 2.16 | 109.54 | 105.63 |
| 70 | L5 | 3825 | A2M | C4-C5-N7 | -2.15 | 107.99 | 110.62 |
| 74 | S2 | 1851 | MA6 | C4-C5-N7 | -2.15 | 108.00 | 110.62 |
| 70 | L5 | 3768 | PSU | C6-N1-C2 | -2.15 | 120.48 | 122.68 |
| 70 | L5 | 398 | A2M | C4-C5-N7 | -2.15 | 108.00 | 110.62 |
| 70 | L5 | 2363 | A2M | C4-C5-N7 | -2.15 | 108.00 | 110.62 |
| 74 | S2 | 1678 | A2M | C4-N9-C8 | 2.15 | 108.06 | 105.73 |
| 70 | L5 | 4403 | PSU | O4'-C1'-C2' | 2.15 | 108.17 | 105.14 |
| 70 | L5 | 3867 | A2M | C4-C5-N7 | -2.14 | 108.01 | 110.62 |
| 74 | S2 | 93 | PSU | C6-N1-C2 | -2.14 | 120.49 | 122.68 |
| 70 | L5 | 3853 | PSU | O2-C2-N1 | -2.14 | 120.44 | 122.79 |
| 70 | L5 | 2632 | PSU | C6-N1-C2 | -2.13 | 120.50 | 122.68 |
| 70 | L5 | 1316 | OMG | C8-N7-C5 | 2.13 | 108.10 | 104.24 |
| 70 | L5 | 1524 | A2M | C4'-O4'-C1' | -2.13 | 104.78 | 109.47 |
| 70 | L5 | 3639 | PSU | C6-N1-C2 | -2.13 | 120.51 | 122.68 |
| 74 | S2 | 99 | A2M | C6-C5-C4 | 2.13 | 120.04 | 117.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 69 | L8 | 55 | PSU | C6-N1-C2 | -2.13 | 120.51 | 122.68 |
| 74 | S2 | 218 | PSU | C6-N1-C2 | -2.13 | 120.51 | 122.68 |
| 70 | L5 | 1677 | PSU | C6-N1-C2 | -2.12 | 120.51 | 122.68 |
| 70 | L5 | 4228 | OMG | C8-N7-C5 | 2.12 | 108.08 | 104.24 |
| 74 | S2 | 572 | PSU | O4'-C1'-C2' | 2.12 | 108.13 | 105.14 |
| 70 | L5 | 3830 | A2M | C4-N9-C8 | 2.12 | 108.02 | 105.73 |
| 74 | S2 | 512 | A2M | C6-C5-C4 | 2.12 | 120.03 | 117.18 |
| 74 | S2 | 99 | A2M | C4-C5-N7 | -2.12 | 108.04 | 110.62 |
| 70 | L5 | 2351 | OMC | O2-C2-N1 | 2.11 | 123.26 | 118.89 |
| 70 | L5 | 4500 | PSU | C6-C5-C4 | 2.11 | 119.68 | 118.20 |
| 70 | L5 | 1792 | PSU | C6-N1-C2 | -2.11 | 120.52 | 122.68 |
| 74 | S2 | 1056 | PSU | C6-N1-C2 | -2.11 | 120.52 | 122.68 |
| 70 | L5 | 2839 | PSU | C6-N1-C2 | -2.11 | 120.53 | 122.68 |
| 74 | S2 | 1692 | PSU | C6-N1-C2 | -2.11 | 120.53 | 122.68 |
| 70 | L5 | 4353 | PSU | C6-N1-C2 | -2.10 | 120.53 | 122.68 |
| 70 | L5 | 3695 | PSU | O4'-C1'-C2' | 2.10 | 108.11 | 105.14 |
| 70 | L5 | 1860 | PSU | C6-N1-C2 | -2.10 | 120.53 | 122.68 |
| 70 | L5 | 4392 | OMG | C8-N7-C5 | 2.10 | 108.04 | 104.24 |
| 74 | S2 | 484 | A2M | C6-C5-C4 | 2.10 | 120.01 | 117.18 |
| 69 | L8 | 75 | OMG | C8-N7-C5 | 2.10 | 108.04 | 104.24 |
| 70 | L5 | 3718 | A2M | C6-C5-C4 | 2.10 | 120.00 | 117.18 |
| 74 | S2 | 1031 | A2M | C4-C5-N7 | -2.10 | 108.06 | 110.62 |
| 74 | S2 | 1639 | G7M | N9-C8-N7 | -2.10 | 107.02 | 112.21 |
| 74 | S2 | 218 | PSU | O4'-C1'-C2' | 2.09 | 108.10 | 105.14 |
| 74 | S2 | 512 | A2M | C4-C5-N7 | -2.09 | 108.07 | 110.62 |
| 70 | L5 | 3785 | A2M | C4-C5-N7 | -2.09 | 108.07 | 110.62 |
| 74 | S2 | 1136 | PSU | C6-N1-C2 | -2.09 | 120.55 | 122.68 |
| 70 | L5 | 4361 | PSU | C6-N1-C2 | -2.09 | 120.55 | 122.68 |
| 74 | S2 | 119 | PSU | O2-C2-N1 | -2.08 | 120.50 | 122.79 |
| 70 | L5 | 1625 | OMG | C8-N7-C5 | 2.08 | 108.01 | 104.24 |
| 70 | L5 | 4196 | OMG | C8-N7-C5 | 2.08 | 108.01 | 104.24 |
| 70 | L5 | 3925 | OMU | O2-C2-N1 | -2.08 | 120.02 | 122.79 |
| 70 | L5 | 1582 | PSU | O2-C2-N1 | -2.08 | 120.50 | 122.79 |
| 74 | S2 | 27 | A2M | C6-C5-C4 | 2.08 | 119.97 | 117.18 |
| 70 | L5 | 398 | A2M | C4-N9-C8 | 2.08 | 107.98 | 105.73 |
| 74 | S2 | 590 | A2M | C4-C5-N7 | -2.08 | 108.09 | 110.62 |
| 70 | L5 | 4623 | OMG | C8-N7-C5 | 2.07 | 107.99 | 104.24 |
| 70 | L5 | 2363 | A2M | C4-N9-C8 | 2.07 | 107.97 | 105.73 |
| 70 | L5 | 1534 | A2M | C4-C5-N7 | -2.07 | 108.10 | 110.62 |
| 70 | L5 | 2815 | A2M | C4-C5-N7 | -2.07 | 108.10 | 110.62 |
| 74 | S2 | 822 | PSU | O4'-C1'-C2' | 2.07 | 108.06 | 105.14 |
| 74 | S2 | 1445 | PSU | C6-C5-C4 | 2.07 | 119.64 | 118.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 70 | L5 | 398 | A2M | C6-C5-C4 | 2.07 | 119.96 | 117.18 |
| 74 | S2 | 468 | A2M | C6-C5-C4 | 2.07 | 119.96 | 117.18 |
| 70 | L5 | 4618 | OMG | C8-N7-C5 | 2.06 | 107.98 | 104.24 |
| 70 | L5 | 3760 | A2M | C4-C5-N7 | -2.06 | 108.11 | 110.62 |
| 70 | L5 | 2364 | OMG | C8-N7-C5 | 2.06 | 107.97 | 104.24 |
| 74 | S2 | 436 | OMG | C8-N7-C5 | 2.06 | 107.97 | 104.24 |
| 70 | L5 | 3744 | OMG | C8-N7-C5 | 2.06 | 107.97 | 104.24 |
| 70 | L5 | 4456 | OMC | O2-C2-N3 | -2.06 | 118.98 | 122.33 |
| 74 | S2 | 468 | A2M | C4-N9-C8 | 2.06 | 107.96 | 105.73 |
| 74 | S2 | 1328 | OMG | C8-N7-C5 | 2.06 | 107.96 | 104.24 |
| 70 | L5 | 3830 | A2M | C4-C5-N7 | -2.05 | 108.12 | 110.62 |
| 69 | L8 | 69 | PSU | O4'-C1'-C2' | 2.05 | 108.04 | 105.14 |
| 74 | S2 | 1031 | A2M | C4-N9-C8 | 2.05 | 107.95 | 105.73 |
| 70 | L5 | 3844 | PSU | C6-N1-C2 | -2.05 | 120.59 | 122.68 |
| 70 | L5 | 4499 | OMG | C8-N7-C5 | 2.05 | 107.95 | 104.24 |
| 70 | L5 | 3867 | A2M | C6-C5-C4 | 2.05 | 119.94 | 117.18 |
| 64 | LA | 216 | V5N | O-C-CA | -2.04 | 119.42 | 124.78 |
| 70 | L5 | 3825 | A2M | C4-N9-C8 | 2.04 | 107.94 | 105.73 |
| 74 | S2 | 1383 | A2M | C6-C5-C4 | 2.04 | 119.92 | 117.18 |
| 74 | S2 | 27 | A2M | C4-C5-N7 | -2.04 | 108.14 | 110.62 |
| 70 | L5 | 3734 | PSU | C6-N1-C2 | -2.04 | 120.60 | 122.68 |
| 74 | S2 | 1248 | B8N | O36-C34-C33 | 2.04 | 120.32 | 113.38 |
| 70 | L5 | 400 | A2M | C4-C5-N7 | -2.03 | 108.14 | 110.62 |
| 70 | L5 | 2401 | A2M | C4-C5-N7 | -2.03 | 108.14 | 110.62 |
| 70 | L5 | 1524 | A2M | C6-C5-C4 | 2.03 | 119.91 | 117.18 |
| 70 | L5 | 4571 | A2M | C4-N9-C8 | 2.03 | 107.93 | 105.73 |
| 70 | L5 | 3637 | PSU | O2-C2-N1 | -2.03 | 120.56 | 122.79 |
| 70 | L5 | 3830 | A2M | C6-C5-C4 | 2.03 | 119.91 | 117.18 |
| 70 | L5 | 4531 | PSU | C6-N1-C2 | -2.03 | 120.61 | 122.68 |
| 74 | S2 | 116 | OMU | O2-C2-N1 | -2.02 | 120.11 | 122.79 |
| 70 | L5 | 4571 | A2M | C6-C5-C4 | 2.02 | 119.89 | 117.18 |
| 67 | Pt | 8 | 4SU | O2-C2-N1 | -2.01 | 120.11 | 122.79 |
| 70 | L5 | 1871 | A2M | C4-C5-N7 | -2.01 | 108.17 | 110.62 |
| 74 | S2 | 683 | OMG | C8-N7-C5 | 2.01 | 107.87 | 104.24 |
| 74 | S2 | 590 | A2M | C4'-O4'-C1' | -2.01 | 105.05 | 109.47 |
| 70 | L5 | 4420 | PSU | O4'-C1'-C2' | 2.00 | 107.97 | 105.14 |
| 74 | S2 | 1490 | OMG | C8-N7-C5 | 2.00 | 107.87 | 104.24 |
| 74 | S2 | 644 | OMG | C8-N7-C5 | 2.00 | 107.86 | 104.24 |

There are no chirality outliers.

All (132) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 3 | Lo | 53 | MLZ | N-CA-CB-CG |
| 3 | Lo | 53 | MLZ | C-CA-CB-CG |
| 63 | Lb | 5 | MLZ | N-CA-CB-CG |
| 63 | Lb | 5 | MLZ | C-CA-CB-CG |
| 64 | LA | 216 | V5N | O-C-CA-CB |
| 67 | Pt | 33 | OMC | C1'-C2'-O2'-CM2 |
| 69 | L8 | 75 | OMG | C1'-C2'-O2'-CM2 |
| 70 | L5 | 1625 | OMG | O4'-C4'-C5'-O5' |
| 70 | L5 | 1677 | PSU | C2'-C1'-C5-C6 |
| 70 | L5 | 3701 | OMC | C2'-C1'-N1-C2 |
| 70 | L5 | 3701 | OMC | C2'-C1'-N1-C6 |
| 70 | L5 | 3729 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 3762 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 3867 | A2M | C1'-C2'-O2'-CM' |
| 70 | L5 | 3925 | OMU | C1'-C2'-O2'-CM2 |
| 70 | L5 | 4196 | OMG | C1'-C2'-O2'-CM2 |
| 70 | L5 | 4420 | PSU | C2'-C1'-C5-C4 |
| 70 | L5 | 4420 | PSU | C2'-C1'-C5-C6 |
| 70 | L5 | 4420 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 4590 | A2M | C4'-C5'-O5'-P |
| 70 | L5 | 4620 | OMU | C1'-C2'-O2'-CM2 |
| 70 | L5 | 4623 | OMG | C1'-C2'-O2'-CM2 |
| 70 | L5 | 4636 | PSU | C2'-C1'-C5-C6 |
| 70 | L5 | 4637 | OMG | O4'-C4'-C5'-O5' |
| 74 | S2 | 116 | OMU | C1'-C2'-O2'-CM2 |
| 74 | S2 | 428 | OMU | C2'-C1'-N1-C2 |
| 74 | S2 | 428 | OMU | C2'-C1'-N1-C6 |
| 74 | S2 | 509 | OMG | C1'-C2'-O2'-CM2 |
| 74 | S2 | 576 | A2M | C3'-C4'-C5'-O5' |
| 74 | S2 | 644 | OMG | O4'-C4'-C5'-O5' |
| 74 | S2 | 867 | OMG | C1'-C2'-O2'-CM2 |
| 74 | S2 | 1243 | PSU | C3'-C4'-C5'-O5' |
| 74 | S2 | 1243 | PSU | O4'-C4'-C5'-O5' |
| 74 | S2 | 1248 | B8N | C31-C32-C33-C34 |
| 74 | S2 | 1248 | B8N | C31-C32-C33-N34 |
| 74 | S2 | 1328 | OMG | C1'-C2'-O2'-CM2 |
| 74 | S2 | 1804 | OMU | C1'-C2'-O2'-CM2 |
| 74 | S2 | 1832 | 6MZ | C5-C6-N6-C9 |
| 74 | S2 | 1832 | 6MZ | N1-C6-N6-C9 |
| 67 | Pt | 21 | H2U | O4'-C4'-C5'-O5' |
| 70 | L5 | 1625 | OMG | C3'-C4'-C5'-O5' |
| 70 | L5 | 3729 | PSU | C3'-C4'-C5'-O5' |
| 70 | L5 | 3760 | A2M | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 70 | L5 | 3760 | A2M | C3'-C4'-C5'-O5' |
| 70 | L5 | 3762 | PSU | C3'-C4'-C5'-O5' |
| 70 | L5 | 3844 | PSU | C3'-C4'-C5'-O5' |
| 70 | L5 | 3844 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 4420 | PSU | C3'-C4'-C5'-O5' |
| 74 | S2 | 512 | A2M | O4'-C4'-C5'-O5' |
| 74 | S2 | 590 | A2M | O4'-C4'-C5'-O5' |
| 74 | S2 | 590 | A2M | C3'-C4'-C5'-O5' |
| 74 | S2 | 644 | OMG | C3'-C4'-C5'-O5' |
| 74 | S2 | 668 | A2M | O4'-C4'-C5'-O5' |
| 74 | S2 | 668 | A2M | C3'-C4'-C5'-O5' |
| 74 | S2 | 822 | PSU | C3'-C4'-C5'-O5' |
| 74 | S2 | 822 | PSU | O4'-C4'-C5'-O5' |
| 3 | Lo | 53 | MLZ | CD-CE-NZ-CM |
| 67 | Pt | 21 | H2U | C3'-C4'-C5'-O5' |
| 70 | L5 | 1677 | PSU | C3'-C4'-C5'-O5' |
| 70 | L5 | 1677 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 4196 | OMG | O4'-C4'-C5'-O5' |
| 70 | L5 | 4196 | OMG | C3'-C4'-C5'-O5' |
| 70 | L5 | 4637 | OMG | C3'-C4'-C5'-O5' |
| 74 | S2 | 576 | A2M | O4'-C4'-C5'-O5' |
| 74 | S2 | 918 | PSU | O4'-C4'-C5'-O5' |
| 3 | Lo | 53 | MLZ | CG-CD-CE-NZ |
| 70 | L5 | 3764 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 4447 | 5MC | C2'-C1'-N1-C6 |
| 74 | S2 | 512 | A2M | C3'-C4'-C5'-O5' |
| 63 | Lb | 5 | MLZ | CE-CD-CG-CB |
| 70 | L5 | 4293 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 2508 | PSU | C3'-C4'-C5'-O5' |
| 70 | L5 | 3760 | A2M | C4'-C5'-O5'-P |
| 74 | S2 | 590 | A2M | C4'-C5'-O5'-P |
| 74 | S2 | 428 | OMU | O4'-C4'-C5'-O5' |
| 63 | Lb | 5 | MLZ | CG-CD-CE-NZ |
| 70 | L5 | 400 | A2M | C1'-C2'-O2'-CM' |
| 70 | L5 | 4447 | 5MC | O4'-C1'-N1-C6 |
| 70 | L5 | 4447 | 5MC | C2'-C1'-N1-C2 |
| 70 | L5 | 4500 | PSU | C4'-C5'-O5'-P |
| 74 | S2 | 644 | OMG | C4'-C5'-O5'-P |
| 74 | S2 | 1490 | OMG | C4'-C5'-O5'-P |
| 70 | L5 | 398 | A2M | O4'-C4'-C5'-O5' |
| 74 | S2 | 627 | OMU | O4'-C4'-C5'-O5' |
| 74 | S2 | 428 | OMU | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 70 | L5 | 1534 | A2M | C4'-C5'-O5'-P |
| 70 | L5 | 2508 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 4590 | A2M | C3'-C4'-C5'-O5' |
| 74 | S2 | 119 | PSU | O4'-C4'-C5'-O5' |
| 74 | S2 | 1703 | OMC | O4'-C4'-C5'-O5' |
| 70 | L5 | 4447 | 5MC | O4'-C1'-N1-C2 |
| 67 | Pt | 21 | H2U | C4'-C5'-O5'-P |
| 70 | L5 | 3701 | OMC | O4'-C1'-N1-C6 |
| 74 | S2 | 428 | OMU | O4'-C1'-N1-C6 |
| 69 | L8 | 69 | PSU | C3'-C4'-C5'-O5' |
| 74 | S2 | 918 | PSU | C3'-C4'-C5'-O5' |
| 70 | L5 | 2876 | OMG | C3'-C2'-O2'-CM2 |
| 70 | L5 | 3785 | A2M | C3'-C2'-O2'-CM' |
| 70 | L5 | 3764 | PSU | C3'-C4'-C5'-O5' |
| 70 | L5 | 3844 | PSU | C4'-C5'-O5'-P |
| 70 | L5 | 4636 | PSU | O4'-C4'-C5'-O5' |
| 70 | L5 | 4521 | PSU | O4'-C1'-C5-C4 |
| 70 | L5 | 3869 | OMC | C3'-C2'-O2'-CM2 |
| 70 | L5 | 3701 | OMC | O4'-C1'-N1-C2 |
| 74 | S2 | 428 | OMU | O4'-C1'-N1-C2 |
| 70 | L5 | 2351 | OMC | C2'-C1'-N1-C6 |
| 70 | L5 | 1524 | A2M | O4'-C1'-N9-C8 |
| 74 | S2 | 1248 | B8N | N34-C33-C34-O35 |
| 70 | L5 | 2422 | OMC | C3'-C4'-C5'-O5' |
| 70 | L5 | 4293 | PSU | C3'-C4'-C5'-O5' |
| 63 | Lb | 5 | MLZ | CD-CE-NZ-CM |
| 70 | L5 | 2351 | OMC | C2'-C1'-N1-C2 |
| 70 | L5 | 4442 | PSU | O4'-C4'-C5'-O5' |
| 74 | S2 | 99 | A2M | O4'-C4'-C5'-O5' |
| 74 | S2 | 462 | OMC | C1'-C2'-O2'-CM2 |
| 67 | Pt | 33 | OMC | C2'-C1'-N1-C2 |
| 70 | L5 | 1534 | A2M | O4'-C4'-C5'-O5' |
| 70 | L5 | 2422 | OMC | O4'-C4'-C5'-O5' |
| 70 | L5 | 4499 | OMG | O4'-C4'-C5'-O5' |
| 70 | L5 | 4499 | OMG | C3'-C4'-C5'-O5' |
| 70 | L5 | 1677 | PSU | O4'-C1'-C5-C6 |
| 70 | L5 | 4636 | PSU | O4'-C1'-C5-C6 |
| 67 | Pt | 47 | G7M | C4'-C5'-O5'-P |
| 74 | S2 | 1248 | B8N | N34-C33-C34-O36 |
| 70 | L5 | 2351 | OMC | O4'-C4'-C5'-O5' |
| 70 | L5 | 3758 | PSU | C3'-C4'-C5'-O5' |
| 70 | L5 | 4361 | PSU | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 74 | S2 | 668 | A2M | C2'-C1'-N9-C8 |
| 67 | Pt | 21 | H2U | C2'-C1'-N1-C2 |
| 74 | S2 | 1851 | MA6 | C4'-C5'-O5'-P |
| 70 | L5 | 4636 | PSU | C4'-C5'-O5'-P |
| 74 | S2 | 1643 | PSU | O4'-C4'-C5'-O5' |

There are no ring outliers.

48 monomers are involved in 54 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 74 | S2 | 509 | OMG | 2 | 0 |
| 70 | L5 | 1871 | A2M | 1 | 0 |
| 70 | L5 | 2424 | OMG | 1 | 0 |
| 67 | Pt | 21 | H2U | 1 | 0 |
| 74 | S2 | 1232 | PSU | 1 | 0 |
| 74 | S2 | 1804 | OMU | 1 | 0 |
| 70 | L5 | 400 | A2M | 1 | 0 |
| 70 | L5 | 3830 | A2M | 1 | 0 |
| 70 | L5 | 2363 | A2M | 1 | 0 |
| 70 | L5 | 1683 | PSU | 1 | 0 |
| 70 | L5 | 4521 | PSU | 1 | 0 |
| 70 | L5 | 4523 | A2M | 1 | 0 |
| 70 | L5 | 4618 | OMG | 1 | 0 |
| 74 | S2 | 484 | A2M | 1 | 0 |
| 70 | L5 | 1340 | OMC | 1 | 0 |
| 70 | L5 | 4579 | PSU | 1 | 0 |
| 74 | S2 | 573 | PSU | 1 | 0 |
| 74 | S2 | 867 | OMG | 1 | 0 |
| 67 | Pt | 33 | OMC | 1 | 0 |
| 74 | S2 | 1031 | A2M | 1 | 0 |
| 74 | S2 | 512 | A2M | 1 | 0 |
| 74 | S2 | 576 | A2M | 1 | 0 |
| 70 | L5 | 1326 | A2M | 1 | 0 |
| 70 | L5 | 4196 | OMG | 1 | 0 |
| 74 | S2 | 627 | OMU | 1 | 0 |
| 70 | L5 | 4220 | 6MZ | 1 | 0 |
| 74 | S2 | 116 | OMU | 2 | 0 |
| 74 | S2 | 1490 | OMG | 1 | 0 |
| 70 | L5 | 3770 | PSU | 2 | 0 |
| 70 | L5 | 4552 | PSU | 1 | 0 |
| 70 | L5 | 4623 | OMG | 1 | 0 |
| 70 | L5 | 4456 | OMC | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 74 | S2 | 1639 | G7M | 1 | 0 |
| 69 | L8 | 75 | OMG | 2 | 0 |
| 74 | S2 | 436 | OMG | 1 | 0 |
| 70 | L5 | 1625 | OMG | 1 | 0 |
| 70 | L5 | 3718 | A2M | 2 | 0 |
| 70 | L5 | 2351 | OMC | 1 | 0 |
| 74 | S2 | 1391 | OMC | 1 | 0 |
| 70 | L5 | 3867 | A2M | 1 | 0 |
| 70 | L5 | 4637 | OMG | 1 | 0 |
| 70 | L5 | 2837 | OMU | 1 | 0 |
| 74 | S2 | 1703 | OMC | 1 | 0 |
| 70 | L5 | 3925 | OMU | 1 | 0 |
| 70 | L5 | 4620 | OMU | 2 | 0 |
| 70 | L5 | 1322 | 1MA | 1 | 0 |
| 74 | S2 | 1244 | PSU | 2 | 0 |
| 70 | L5 | 2815 | A2M | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 266 ligands modelled in this entry, 262 are monoatomic - leaving 4 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 | $\# Z > 2$ |
| 85 | SPD | L5 | 5103 | 70 | 9,9,9 | 0.28 | 0 | 8,8,8 | 0.23 | 0 |
| 85 | SPD | L5 | 5102 | - | 9,9,9 | 0.28 | 0 | 8,8,8 | 0.22 | 0 |
| 85 | SPD | L5 | 5101 | - | 9,9,9 | 0.28 | 0 | 8,8,8 | 0.19 | 0 |
| 86 | HYG | S2 | 1901 | - | 35,39,39 | 3.13 | 12 (34%) | 43,60,60 | 1.88 | 8 (18%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 85 | SPD | L5 | 5103 | 70 | - | 4/7/7/7 | - |
| 85 | SPD | L5 | 5102 | - | - | 4/7/7/7 | - |
| 85 | SPD | L5 | 5101 | - | - | 2/7/7/7 | - |
| 86 | HYG | S2 | 1901 | - | - | 2/12/87/87 | 0/4/4/4 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 86 | S2 | 1901 | HYG | O29-C12 | 11.00 | 1.61 | 1.43 |
| 86 | S2 | 1901 | HYG | O22-C17 | 6.65 | 1.54 | 1.43 |
| 86 | S2 | 1901 | HYG | O14-C13 | 6.47 | 1.58 | 1.41 |
| 86 | S2 | 1901 | HYG | O28-C23 | 6.07 | 1.47 | 1.40 |
| 86 | S2 | 1901 | HYG | C16-C15 | 4.31 | 1.62 | 1.53 |
| 86 | S2 | 1901 | HYG | C17-C12 | -4.06 | 1.44 | 1.53 |
| 86 | S2 | 1901 | HYG | O28-C27 | 3.73 | 1.49 | 1.44 |
| 86 | S2 | 1901 | HYG | C25-C24 | -3.26 | 1.47 | 1.53 |
| 86 | S2 | 1901 | HYG | O18-C13 | -2.64 | 1.34 | 1.41 |
| 86 | S2 | 1901 | HYG | O30-C24 | 2.39 | 1.47 | 1.42 |
| 86 | S2 | 1901 | HYG | C26-C25 | -2.17 | 1.46 | 1.52 |
| 86 | S2 | 1901 | HYG | O31-C25 | 2.07 | 1.47 | 1.43 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 86 | S2 | 1901 | HYG | O28-C27-C26 | 6.61 | 117.91 | 108.52 |
| 86 | S2 | 1901 | HYG | O29-C12-C13 | 4.84 | 123.57 | 110.86 |
| 86 | S2 | 1901 | HYG | O22-C17-C16 | 4.08 | 121.16 | 111.22 |
| 86 | S2 | 1901 | HYG | C23-O28-C27 | 3.91 | 119.44 | 112.00 |
| 86 | S2 | 1901 | HYG | O22-C17-C12 | 2.75 | 107.97 | 103.58 |
| 86 | S2 | 1901 | HYG | O14-C15-C16 | 2.72 | 114.63 | 109.69 |
| 86 | S2 | 1901 | HYG | C13-O18-C6 | -2.48 | 111.81 | 117.96 |
| 86 | S2 | 1901 | HYG | C19-C15-C16 | -2.24 | 107.76 | 113.00 |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 85 | L5 | 5103 | SPD | C3-C4-C5-N6 |
| 85 | L5 | 5102 | SPD | C3-C4-C5-N6 |

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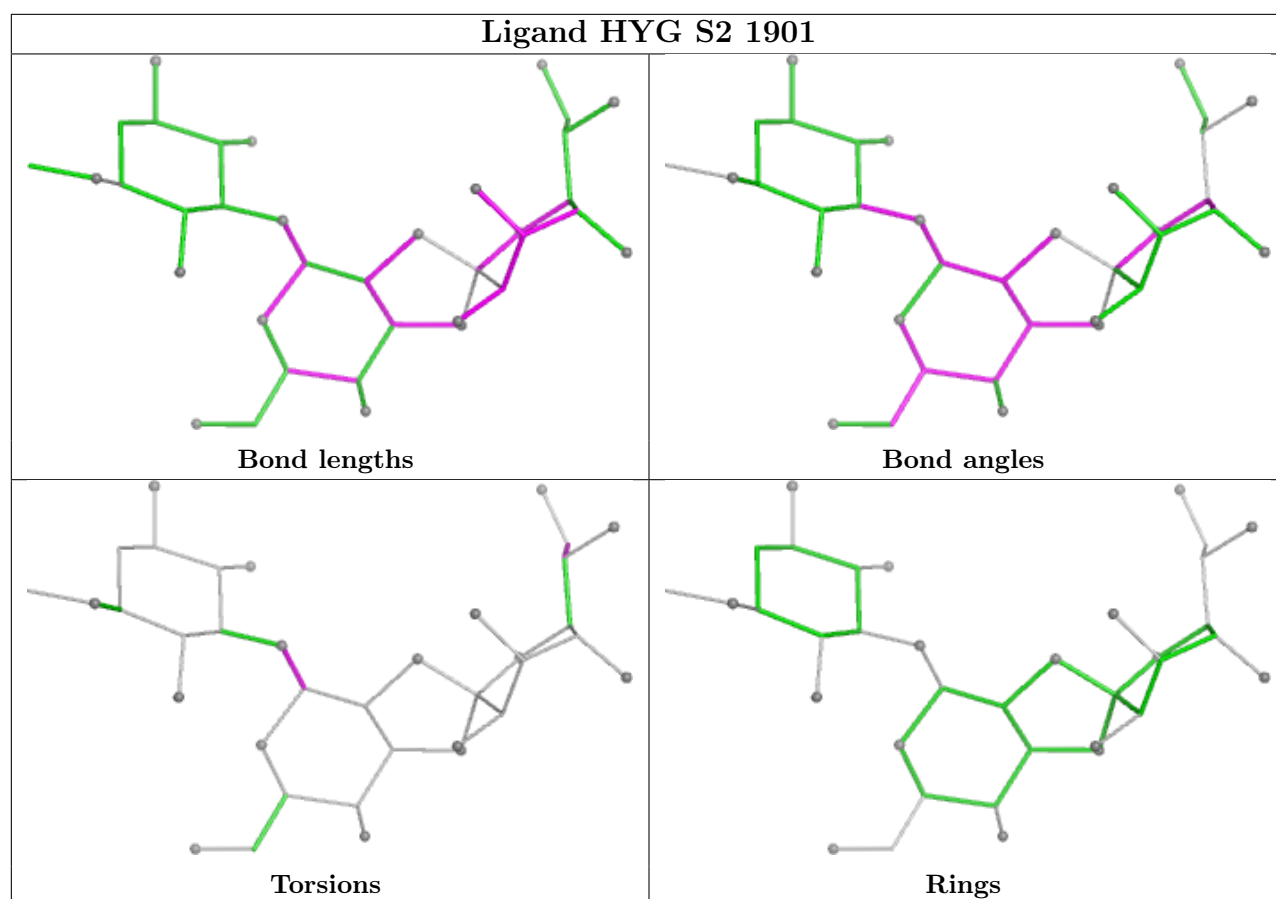
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 86 | S2 | 1901 | HYG | O14-C13-O18-C6 |
| 85 | L5 | 5103 | SPD | C7-C8-C9-N10 |
| 85 | L5 | 5103 | SPD | N6-C7-C8-C9 |
| 85 | L5 | 5101 | SPD | C8-C7-N6-C5 |
| 86 | S2 | 1901 | HYG | N36-C33-C34-O35 |
| 85 | L5 | 5101 | SPD | C7-C8-C9-N10 |
| 85 | L5 | 5102 | SPD | C7-C8-C9-N10 |
| 85 | L5 | 5102 | SPD | C2-C3-C4-C5 |
| 85 | L5 | 5102 | SPD | C4-C5-N6-C7 |
| 85 | L5 | 5103 | SPD | C2-C3-C4-C5 |

There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 85 | L5 | 5102 | SPD | 3 | 0 |
| 85 | L5 | 5101 | SPD | 1 | 0 |

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

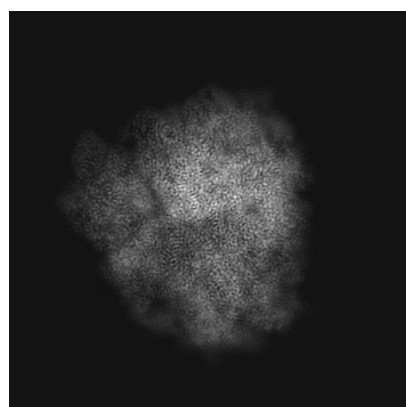
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54266. These allow visual inspection of the internal detail of the map and identification of artifacts.

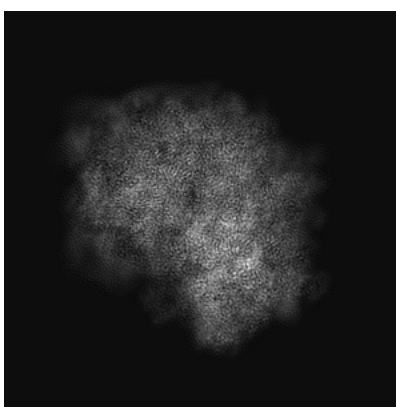
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

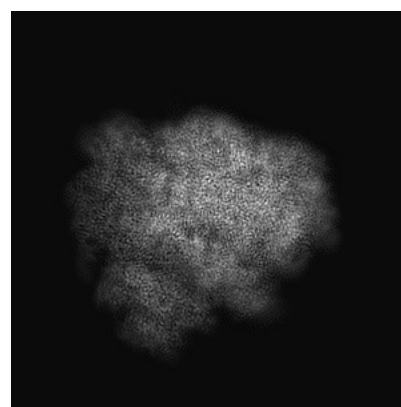
6.1.1 Primary map



X



Y

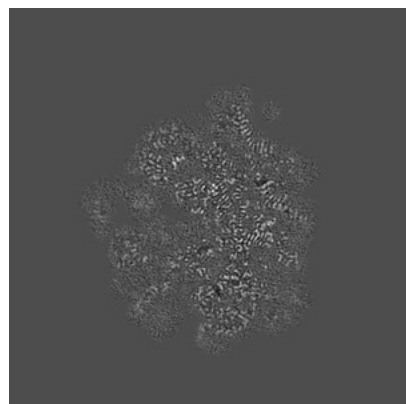


Z

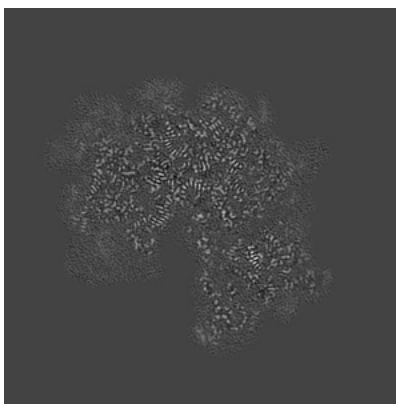
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

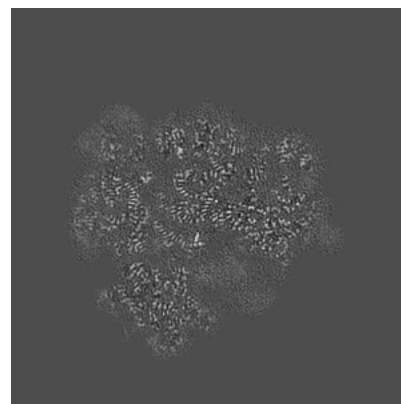
6.2.1 Primary map



X Index: 240



Y Index: 240

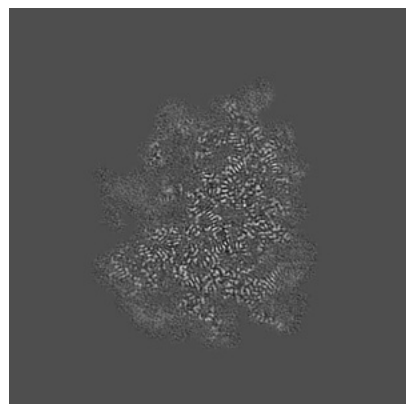


Z Index: 240

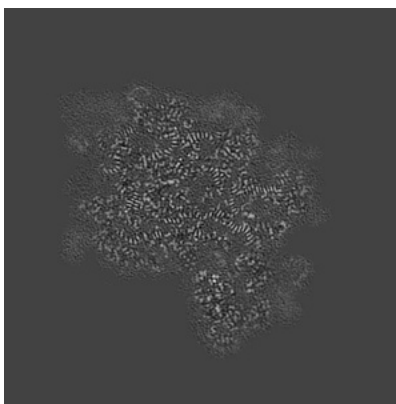
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

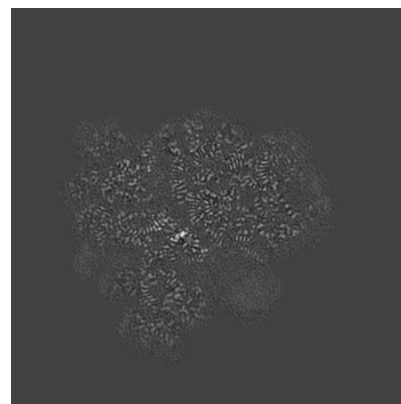
6.3.1 Primary map



X Index: 265



Y Index: 271

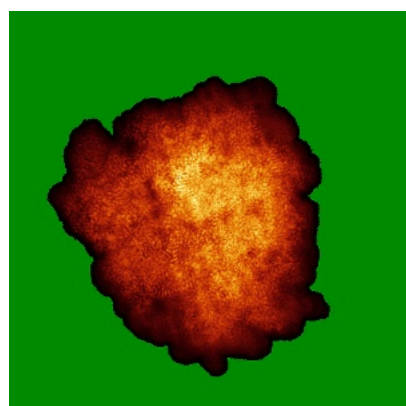


Z Index: 265

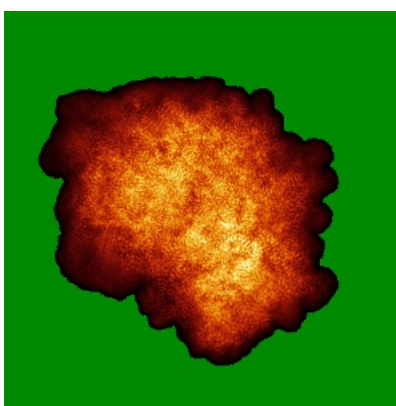
The images above show the largest variance slices of the map in three orthogonal directions.

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

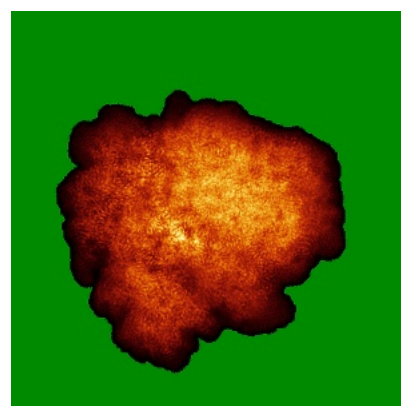
6.4.1 Primary map



X



Y

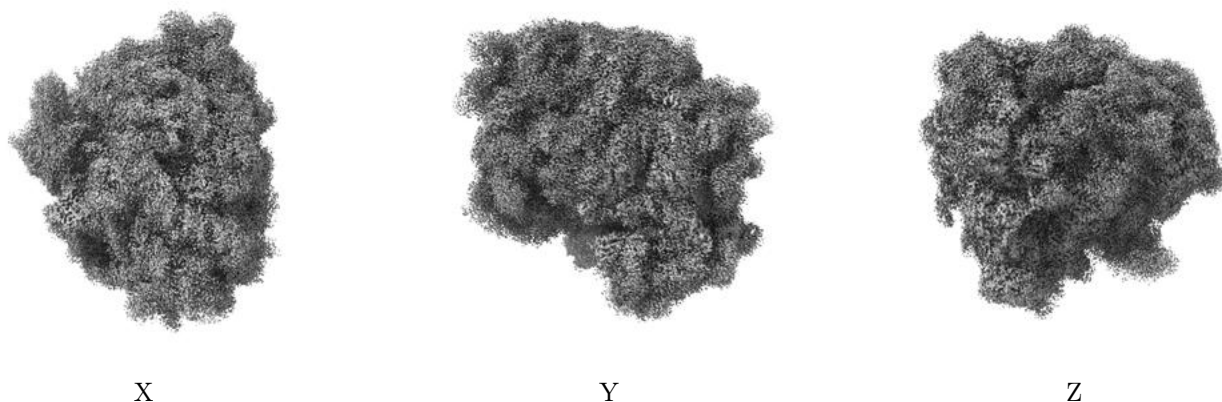


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

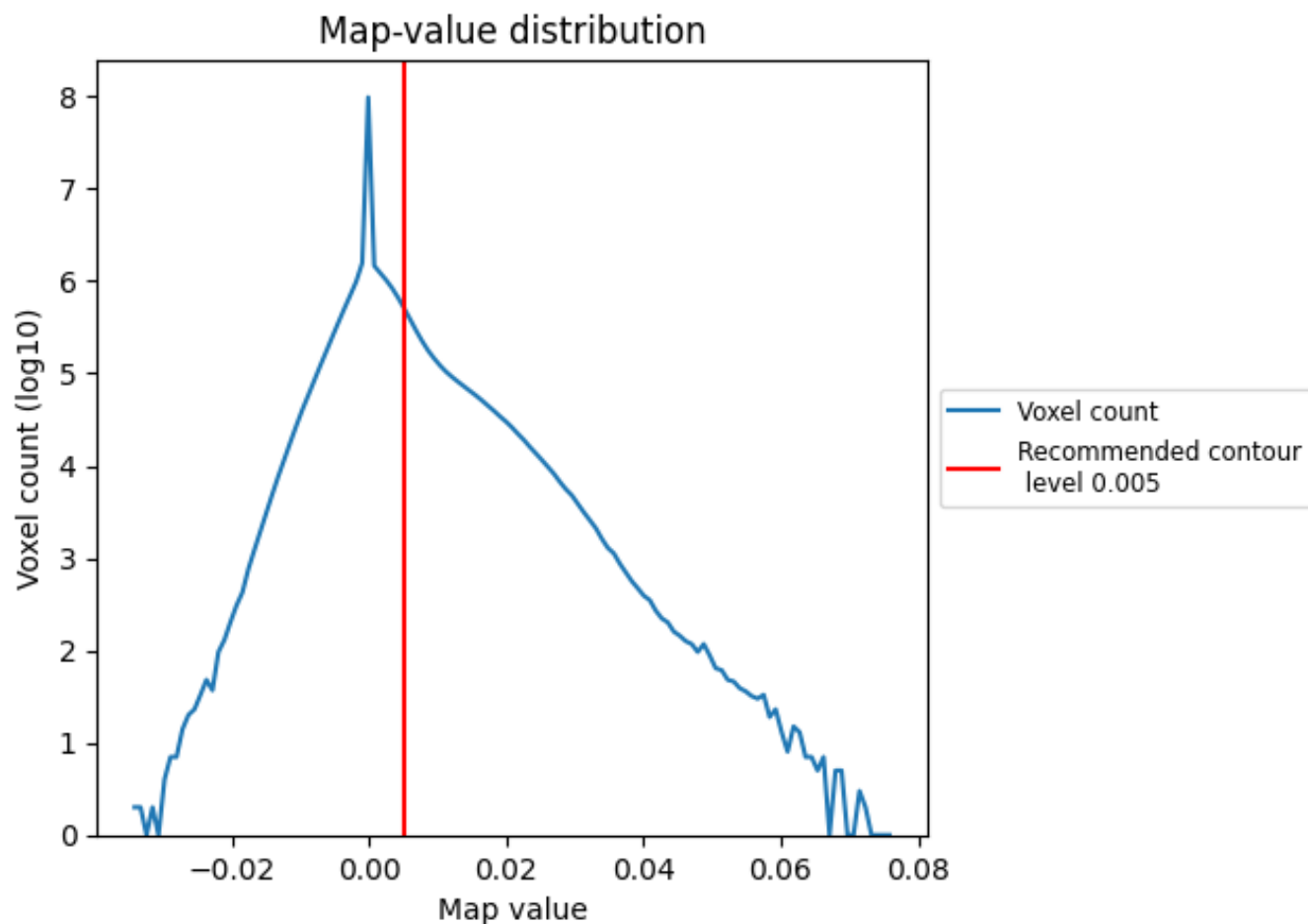
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

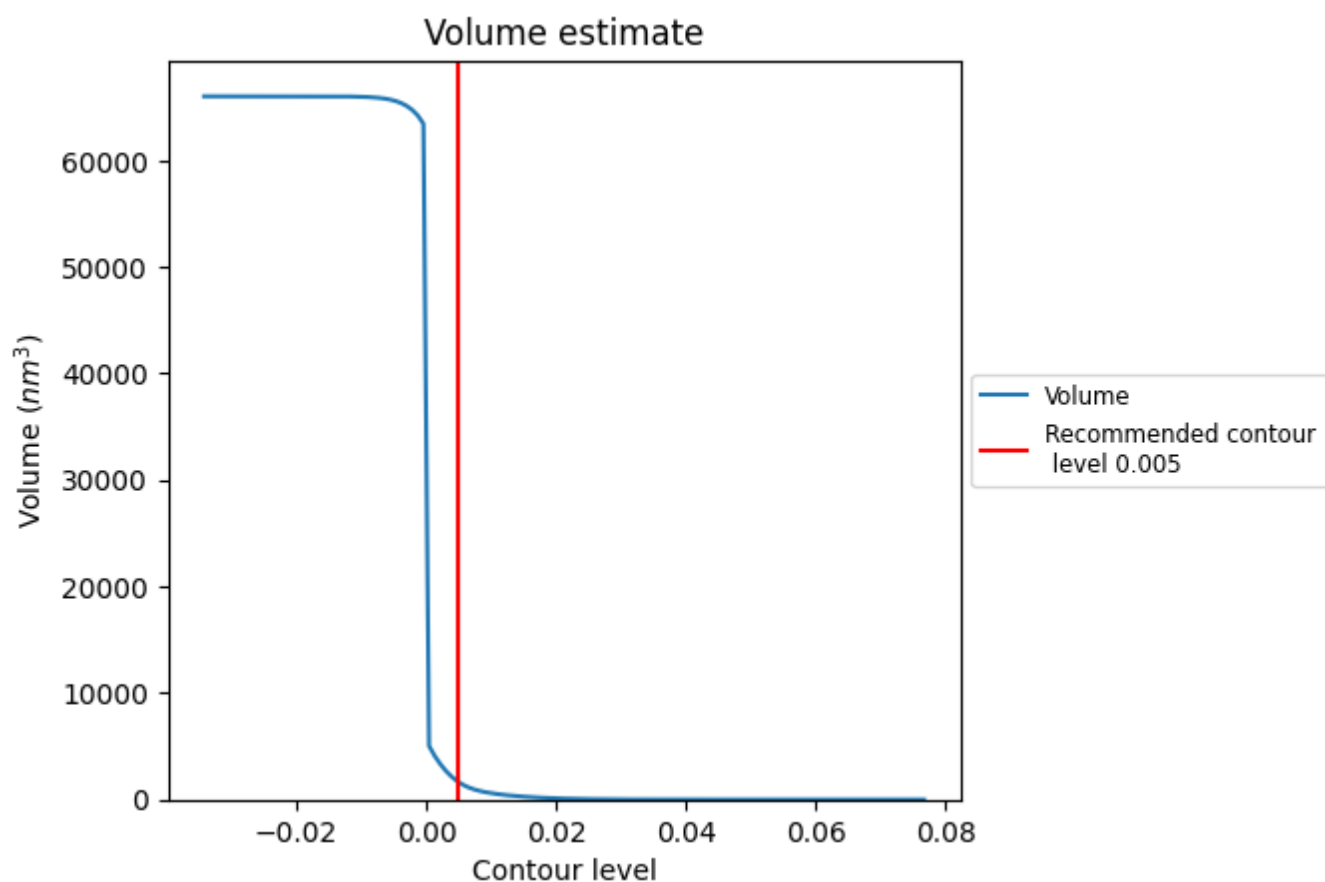
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

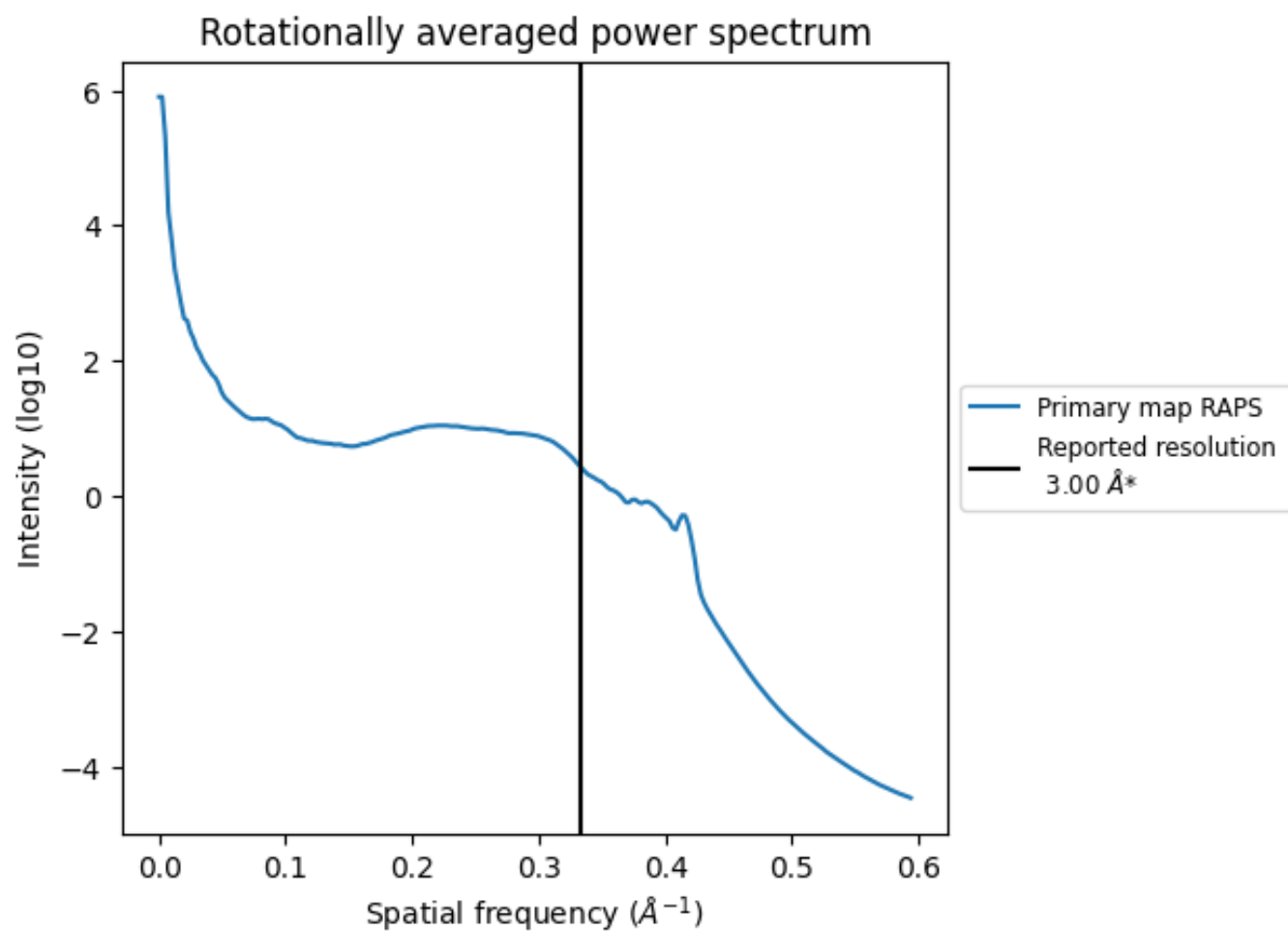
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1649 nm^3 ; this corresponds to an approximate mass of 1489 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 0.333 Å⁻¹

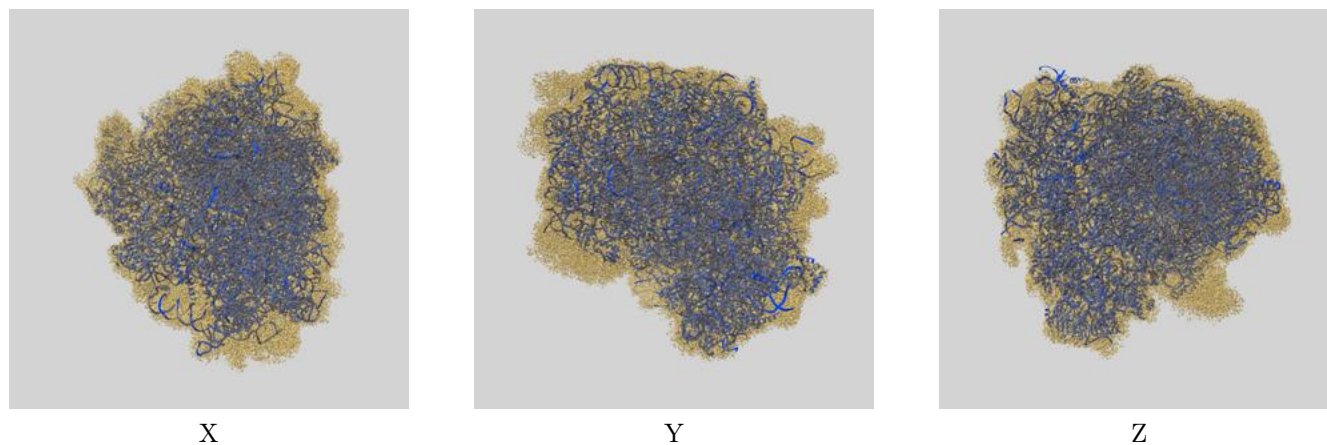
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

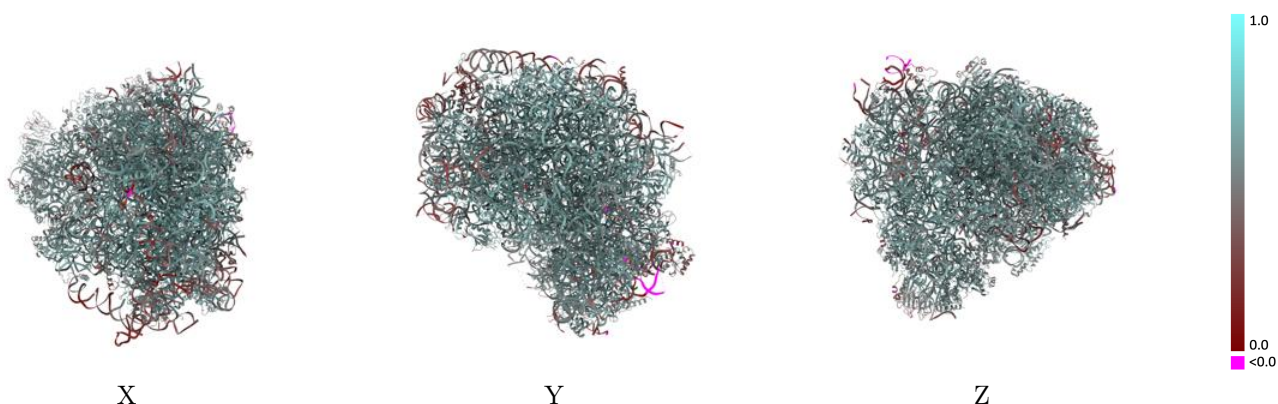
This section contains information regarding the fit between EMDB map EMD-54266 and PDB model 9RU8. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



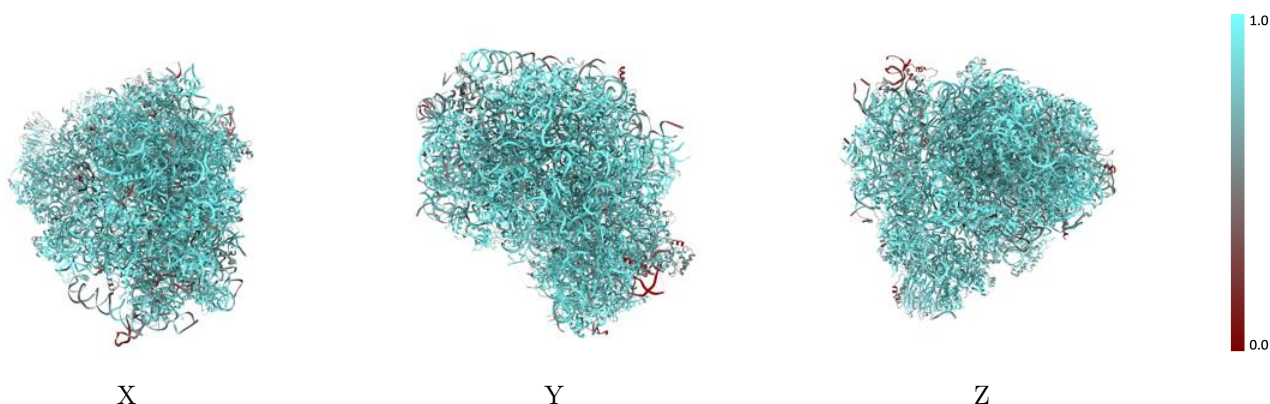
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



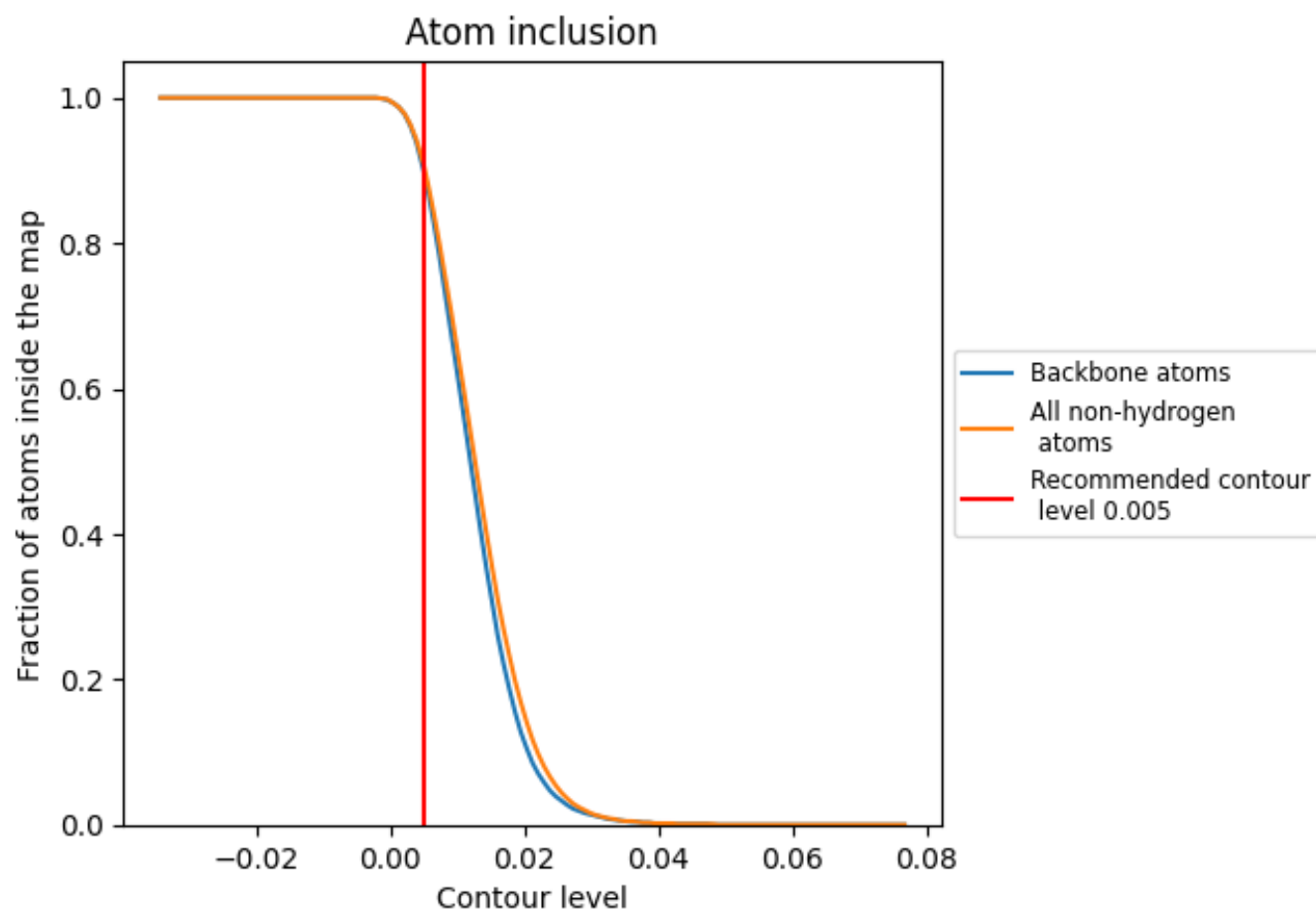
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9090 |  0.5780 |
| L5 |  0.9140 |  0.5720 |
| L7 |  0.9750 |  0.6100 |
| L8 |  0.9410 |  0.5860 |
| LA |  0.9690 |  0.6410 |
| LB |  0.9470 |  0.6230 |
| LC |  0.9460 |  0.6210 |
| LD |  0.8770 |  0.5690 |
| LE |  0.8870 |  0.5750 |
| LF |  0.9540 |  0.6310 |
| LG |  0.8670 |  0.5620 |
| LH |  0.9040 |  0.5880 |
| LI |  0.9310 |  0.6130 |
| LJ |  0.8270 |  0.5380 |
| LL |  0.9120 |  0.5950 |
| LM |  0.9200 |  0.6000 |
| LN |  0.9780 |  0.6450 |
| LO |  0.9600 |  0.6320 |
| LP |  0.9670 |  0.6320 |
| LQ |  0.9540 |  0.6300 |
| LR |  0.8940 |  0.5860 |
| LS |  0.9510 |  0.6290 |
| LT |  0.8990 |  0.5950 |
| LU |  0.7430 |  0.4810 |
| LV |  0.9320 |  0.6190 |
| LW |  0.9400 |  0.6140 |
| LX |  0.9000 |  0.5840 |
| LY |  0.9510 |  0.6130 |
| LZ |  0.9180 |  0.5850 |
| La |  0.9560 |  0.6310 |
| Lb |  0.8280 |  0.5510 |
| Lc |  0.9270 |  0.5910 |
| Ld |  0.9330 |  0.5980 |
| Le |  0.9540 |  0.6350 |
| Lf |  0.9650 |  0.6410 |









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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Lg |  0.9490 |  0.6180 |
| Lh |  0.9300 |  0.5980 |
| Li |  0.8900 |  0.5760 |
| Lj |  0.9640 |  0.6400 |
| Lk |  0.8590 |  0.5500 |
| Ll |  0.9450 |  0.6250 |
| Lm |  0.9470 |  0.6170 |
| Ln |  0.9200 |  0.6000 |
| Lo |  0.9170 |  0.6130 |
| Lp |  0.9560 |  0.6190 |
| Lr |  0.9470 |  0.6180 |
| Pt |  0.7240 |  0.4580 |
| S2 |  0.9220 |  0.5740 |
| S6 |  0.6020 |  0.3170 |
| SA |  0.9020 |  0.5890 |
| SB |  0.9210 |  0.5860 |
| SC |  0.8860 |  0.5890 |
| SD |  0.8630 |  0.5640 |
| SE |  0.9090 |  0.5910 |
| SF |  0.9030 |  0.5740 |
| SG |  0.7860 |  0.5220 |
| SH |  0.7330 |  0.4950 |
| SI |  0.8250 |  0.5530 |
| SJ |  0.9020 |  0.5850 |
| SK |  0.8710 |  0.5440 |
| SL |  0.9020 |  0.6060 |
| SN |  0.9250 |  0.5940 |
| SO |  0.9260 |  0.5980 |
| SP |  0.8690 |  0.5390 |
| SQ |  0.9140 |  0.5910 |
| SR |  0.7880 |  0.5280 |
| SS |  0.9210 |  0.5730 |
| ST |  0.9280 |  0.5890 |
| SU |  0.6930 |  0.5030 |
| SV |  0.8800 |  0.5800 |
| SW |  0.9510 |  0.6230 |
| SX |  0.9320 |  0.6060 |
| SY |  0.9000 |  0.5760 |
| SZ |  0.8630 |  0.5290 |
| Sa |  0.9390 |  0.5950 |
| Sb |  0.8410 |  0.5560 |
| Sc |  0.8740 |  0.5630 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Sd |  0.9590 |  0.6120 |
| Se |  0.8520 |  0.5610 |
| Sg |  0.7270 |  0.4590 |
| mR |  0.7960 |  0.4980 |