



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 11:58 am BST

PDB ID : 5J8A
Title : Structure of the E coli 70S ribosome with the U1052G mutation in 16S rRNA bound to tigecycline
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-07
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

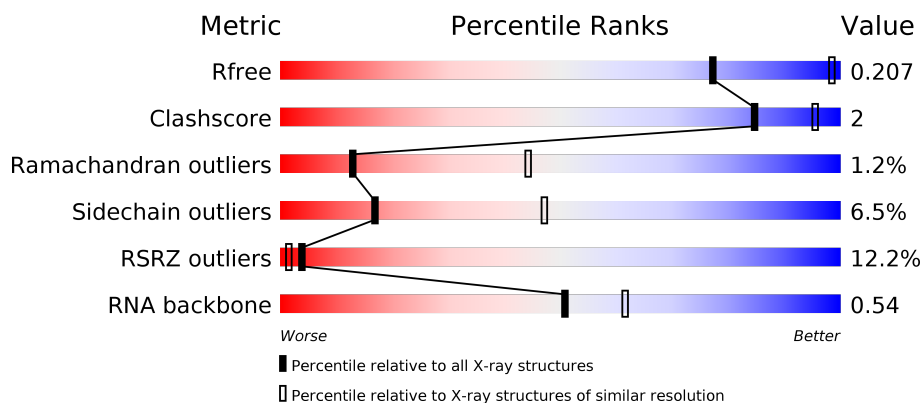
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1094 (3.10-3.10) |
| Clashscore | 141614 | 1184 (3.10-3.10) |
| Ramachandran outliers | 138981 | 1141 (3.10-3.10) |
| Sidechain outliers | 138945 | 1141 (3.10-3.10) |
| RSRZ outliers | 127900 | 1067 (3.10-3.10) |
| RNA backbone | 3102 | 1116 (3.40-2.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | AA | 1534 | <div> <div>3%</div> <div>76%</div> <div>21%</div> <div>.</div> </div> |
| 1 | BA | 1534 | <div> <div>13%</div> <div>75%</div> <div>23%</div> <div>.</div> </div> |
| 2 | AB | 224 | <div> <div>15%</div> <div>88%</div> <div>12%</div> <div>.</div> </div> |
| 2 | BB | 224 | <div> <div>14%</div> <div>88%</div> <div>11%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AC | 206 | |
| 3 | BC | 206 | |
| 4 | AD | 205 | |
| 4 | BD | 205 | |
| 5 | AE | 155 | |
| 5 | BE | 155 | |
| 6 | AF | 106 | |
| 6 | BF | 106 | |
| 7 | AG | 151 | |
| 7 | BG | 151 | |
| 8 | AH | 129 | |
| 8 | BH | 129 | |
| 9 | AI | 127 | |
| 9 | BI | 127 | |
| 10 | AJ | 99 | |
| 10 | BJ | 99 | |
| 11 | AK | 117 | |
| 11 | BK | 117 | |
| 12 | AL | 123 | |
| 12 | BL | 123 | |
| 13 | AM | 114 | |
| 13 | BM | 114 | |
| 14 | AN | 100 | |
| 14 | BN | 100 | |
| 15 | AO | 88 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 15 | BO | 88 | <div> <div>5%</div> <div>91%</div> <div>7%</div> <div>..</div> </div> |
| 16 | AP | 82 | <div> <div>9%</div> <div>85%</div> <div>15%</div> </div> |
| 16 | BP | 82 | <div> <div>13%</div> <div>80%</div> <div>18%</div> <div>.</div> </div> |
| 17 | AQ | 80 | <div> <div>%</div> <div>80%</div> <div>19%</div> <div>.</div> </div> |
| 17 | BQ | 80 | <div> <div>15%</div> <div>64%</div> <div>31%</div> <div>..</div> </div> |
| 18 | AR | 55 | <div> <div>7%</div> <div>87%</div> <div>13%</div> </div> |
| 18 | BR | 55 | <div> <div>5%</div> <div>89%</div> <div>11%</div> </div> |
| 19 | AS | 79 | <div> <div>8%</div> <div>81%</div> <div>18%</div> <div>.</div> </div> |
| 19 | BS | 79 | <div> <div>71%</div> <div>84%</div> <div>13%</div> <div>..</div> </div> |
| 20 | AT | 86 | <div> <div>%</div> <div>93%</div> <div>6%</div> <div>.</div> </div> |
| 20 | BT | 86 | <div> <div>16%</div> <div>78%</div> <div>17%</div> <div>..</div> </div> |
| 21 | AU | 56 | <div> <div>7%</div> <div>86%</div> <div>14%</div> </div> |
| 21 | BU | 56 | <div> <div>7%</div> <div>88%</div> <div>13%</div> </div> |
| 22 | C1 | 56 | <div> <div>30%</div> <div>82%</div> <div>14%</div> <div>.</div> </div> |
| 22 | D1 | 56 | <div> <div>82%</div> <div>18%</div> </div> |
| 23 | C2 | 51 | <div> <div>61%</div> <div>65%</div> <div>31%</div> <div>..</div> </div> |
| 23 | D2 | 51 | <div> <div>73%</div> <div>25%</div> <div>.</div> </div> |
| 24 | C3 | 46 | <div> <div>41%</div> <div>85%</div> <div>15%</div> </div> |
| 24 | D3 | 46 | <div> <div>2%</div> <div>93%</div> <div>7%</div> </div> |
| 25 | C4 | 64 | <div> <div>13%</div> <div>92%</div> <div>8%</div> </div> |
| 25 | D4 | 64 | <div> <div>94%</div> <div>5%</div> <div>.</div> </div> |
| 26 | C5 | 38 | <div> <div>26%</div> <div>71%</div> <div>29%</div> </div> |
| 26 | D5 | 38 | <div> <div>87%</div> <div>13%</div> </div> |
| 27 | C0 | 58 | <div> <div>33%</div> <div>78%</div> <div>19%</div> <div>.</div> </div> |
| 27 | D0 | 58 | <div> <div>93%</div> <div>7%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | CB | 120 | |
| 28 | DB | 120 | |
| 29 | CC | 272 | |
| 29 | DC | 272 | |
| 30 | CD | 209 | |
| 31 | CA | 2904 | |
| 32 | DD | 209 | |
| 33 | CE | 201 | |
| 33 | DE | 201 | |
| 34 | CF | 178 | |
| 34 | DF | 178 | |
| 35 | CG | 176 | |
| 35 | DG | 176 | |
| 36 | CH | 149 | |
| 36 | DH | 149 | |
| 37 | CJ | 135 | |
| 37 | DJ | 135 | |
| 38 | CK | 142 | |
| 38 | DK | 142 | |
| 39 | CL | 123 | |
| 39 | DL | 123 | |
| 40 | CM | 144 | |
| 40 | DM | 144 | |
| 41 | CN | 136 | |
| 41 | DN | 136 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 42 | CO | 125 | |
| 42 | DO | 125 | |
| 43 | CP | 117 | |
| 43 | DP | 117 | |
| 44 | CQ | 114 | |
| 44 | DQ | 114 | |
| 45 | CR | 117 | |
| 45 | DR | 117 | |
| 46 | CS | 103 | |
| 46 | DS | 103 | |
| 47 | CT | 110 | |
| 47 | DT | 110 | |
| 48 | CU | 93 | |
| 48 | DU | 93 | |
| 49 | CV | 103 | |
| 49 | DV | 103 | |
| 50 | CW | 94 | |
| 50 | DW | 94 | |
| 51 | CX | 83 | |
| 51 | DX | 83 | |
| 52 | CY | 77 | |
| 52 | DY | 77 | |
| 53 | CZ | 62 | |
| 53 | DZ | 62 | |
| 54 | DI | 135 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 55 | DA | 2904 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | AA | 1603 | - | - | - | X |
| 56 | MG | AA | 1612 | - | - | - | X |
| 56 | MG | AA | 1613 | - | - | - | X |
| 56 | MG | AA | 1615 | - | - | - | X |
| 56 | MG | AA | 1616 | - | - | - | X |
| 56 | MG | AA | 1618 | - | - | - | X |
| 56 | MG | AA | 1622 | - | - | - | X |
| 56 | MG | AA | 1626 | - | - | - | X |
| 56 | MG | AA | 1628 | - | - | - | X |
| 56 | MG | BA | 1612 | - | - | - | X |
| 56 | MG | BA | 1623 | - | - | - | X |
| 56 | MG | BA | 1624 | - | - | - | X |
| 56 | MG | BA | 1639 | - | - | - | X |
| 56 | MG | BA | 1647 | - | - | - | X |
| 56 | MG | CA | 3003 | - | - | - | X |
| 56 | MG | CA | 3047 | - | - | - | X |
| 56 | MG | CA | 3075 | - | - | - | X |
| 56 | MG | CA | 3077 | - | - | - | X |
| 56 | MG | CA | 3114 | - | - | - | X |
| 56 | MG | CA | 3122 | - | - | - | X |
| 56 | MG | CA | 3123 | - | - | - | X |
| 56 | MG | CA | 3132 | - | - | - | X |
| 56 | MG | CA | 3136 | - | - | - | X |
| 56 | MG | CA | 3139 | - | - | - | X |
| 56 | MG | CA | 3154 | - | - | - | X |
| 56 | MG | CA | 3156 | - | - | - | X |
| 56 | MG | DA | 3122 | - | - | - | X |
| 56 | MG | DA | 3129 | - | - | - | X |
| 56 | MG | DA | 3166 | - | - | - | X |
| 56 | MG | DA | 3167 | - | - | - | X |
| 56 | MG | DA | 3176 | - | - | - | X |
| 56 | MG | DA | 3179 | - | - | - | X |
| 56 | MG | DA | 3180 | - | - | - | X |
| 56 | MG | DA | 3181 | - | - | - | X |
| 56 | MG | DB | 206 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | DB | 207 | - | - | - | X |
| 58 | MPD | DA | 3204 | - | - | - | X |
| 58 | MPD | DE | 301 | - | - | - | X |
| 59 | PUT | AA | 1672 | - | - | - | X |
| 59 | PUT | AA | 1674 | - | - | - | X |
| 59 | PUT | AA | 1675 | - | - | - | X |
| 59 | PUT | DA | 3195 | - | - | - | X |
| 62 | PEG | D3 | 102 | - | - | - | X |
| 62 | PEG | DA | 3199 | - | - | - | X |
| 62 | PEG | DA | 3200 | - | - | - | X |
| 62 | PEG | DP | 201 | - | - | - | X |
| 62 | PEG | DQ | 201 | - | - | - | X |
| 64 | PGE | D1 | 102 | - | - | - | X |
| 69 | TRS | DA | 3220 | - | - | - | X |

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 295207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1534 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32933 | 14695 | 6044 | 10660 | 1534 | | | |
| 1 | BA | 1533 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32911 | 14685 | 6039 | 10654 | 1533 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|--------------|
| AA | 1052 | G | U | engineered mutation | GB 675819282 |
| BA | 1052 | G | U | engineered mutation | GB 675819282 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 224 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1753 | 1109 | 315 | 321 | 8 | | | |
| 2 | BB | 224 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1753 | 1109 | 315 | 321 | 8 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1625 | 1028 | 305 | 289 | 3 | | | |
| 3 | BC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1625 | 1028 | 305 | 289 | 3 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | AD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | BD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 711 | 216 | 211 | 6 | | | |
| 5 | BE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 862 | 545 | 156 | 154 | 7 | | | |
| 6 | BF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | | |
| 7 | BG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |
| 8 | BH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | AI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 9 | BI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 796 | 498 | 152 | 145 | 1 | | | |
| 10 | BJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 787 | 493 | 150 | 143 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |
| 11 | BK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 957 | 591 | 196 | 165 | 5 | | | |
| 12 | BL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 957 | 591 | 196 | 165 | 5 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | | |
| 13 | BM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | AN | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 805 | 499 | 164 | 139 | 3 | | | |
| 14 | BN | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 805 | 499 | 164 | 139 | 3 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |
| 15 | BO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 16 | BP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | | |
| 17 | BQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18 | AR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 456 | 288 | 86 | 82 | | | |
| 18 | BR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 456 | 288 | 86 | 82 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | | |
| 19 | BS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 86 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 670 | 414 | 138 | 115 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | BT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21 | AU | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 465 | 290 | 96 | 78 | 1 | | | |
| 21 | BU | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 465 | 290 | 96 | 78 | 1 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 22 | C1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 22 | D1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 23 | C2 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |
| 23 | D2 | 51 | Total | C | N | O | 0 | 0 | 0 |
| | | | 414 | 266 | 76 | 72 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 24 | C3 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 24 | D3 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 25 | C4 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 25 | D4 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | C5 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 26 | D5 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | C0 | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |
| 27 | D0 | 58 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 463 | 290 | 90 | 81 | 2 | | | |

- Molecule 28 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 28 | CB | 118 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | | |
| 28 | DB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2569 | 1144 | 468 | 837 | 120 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | CC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |
| 29 | DC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | CD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

- Molecule 31 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 31 | CA | 2898 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62229 | 27768 | 11448 | 20115 | 2898 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | DD | 209 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 1576 | 986 | 290 | 296 | 4 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | CE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 33 | DE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1551 | 974 | 283 | 289 | 5 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | CF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | | |
| 34 | DF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | CG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 35 | DG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | CH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 699 | 197 | 213 | 1 | | | |
| 36 | DH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 699 | 197 | 213 | 1 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | CJ | 134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 619 | 169 | 185 | 6 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | DJ | 134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 619 | 169 | 185 | 6 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | CK | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |
| 38 | DK | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | CL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | | |
| 39 | DL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 946 | 593 | 181 | 166 | 6 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | CM | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | | |
| 40 | DM | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | CN | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1075 | 686 | 205 | 178 | 6 | | | |
| 41 | DN | 136 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 1092 | 696 | 211 | 179 | 6 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| CN | 81 | 4D4 | ARG | conflict | UNP P0ADY7 |
| DN | 81 | 4D4 | ARG | conflict | UNP P0ADY7 |

- Molecule 42 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | CO | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |
| 42 | DO | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 993 | 613 | 202 | 173 | 5 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | CP | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |
| 43 | DP | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 557 | 179 | 163 | 1 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | CQ | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |
| 44 | DQ | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | CR | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |
| 45 | DR | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |

- Molecule 46 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | CS | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |
| 46 | DS | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | CT | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | DT | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | CU | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 739 | 466 | 139 | 132 | 2 | | | |
| 48 | DU | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | CV | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | | |
| 49 | DV | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | | |

- Molecule 50 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | CW | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 50 | DW | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51 | CX | 75 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 569 | 353 | 113 | 102 | 1 | | | |
| 51 | DX | 76 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 591 | 365 | 121 | 104 | 1 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | CY | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 52 | DY | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | CZ | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 501 | 308 | 98 | 94 | 1 | | | |
| 53 | DZ | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 501 | 308 | 98 | 94 | 1 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54 | DI | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1023 | 649 | 179 | 192 | 3 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| DI | 85 | VAL | SER | conflict | UNP P0A7J3 |
| DI | 86 | THR | MET | conflict | UNP P0A7J3 |

- Molecule 55 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 55 | DA | 2897 | Total | C | N | O | P | 0 | 11 | 0 |
| | | | 62423 | 27855 | 11485 | 20176 | 2907 | | | |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

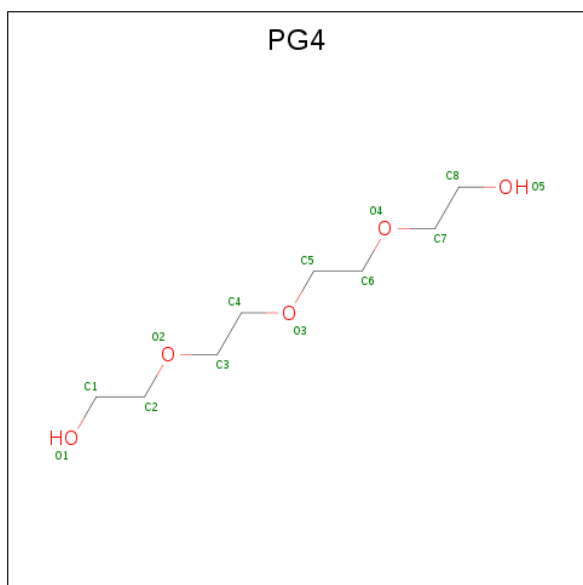
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | BA | 45 | Total | Mg | 0 | 0 |
| | | | 45 | 45 | | |
| 56 | CA | 156 | Total | Mg | 0 | 0 |
| | | | 156 | 156 | | |
| 56 | CB | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | DM | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DR | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | AA | 72 | Total | Mg | 0 | 0 |
| | | | 72 | 72 | | |
| 56 | DA | 184 | Total | Mg | 0 | 0 |
| | | | 184 | 184 | | |

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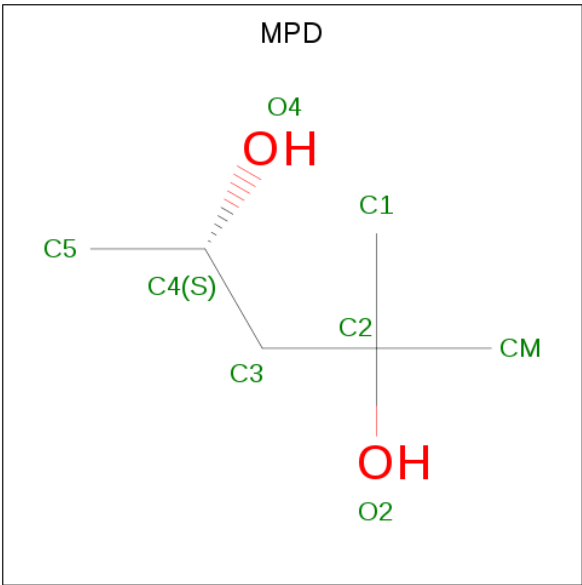
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56 | DB | 9 | Total | Mg | 0 | 0 |
| | | | 9 | 9 | | |
| 56 | DD | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



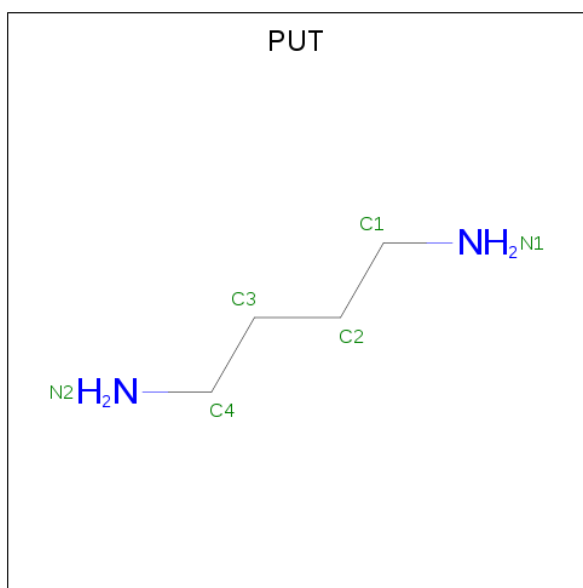
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 57 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | BA | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DQ | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DR | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DS | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 58 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DE | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DE | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DK | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DN | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DS | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DT | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DT | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 59 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



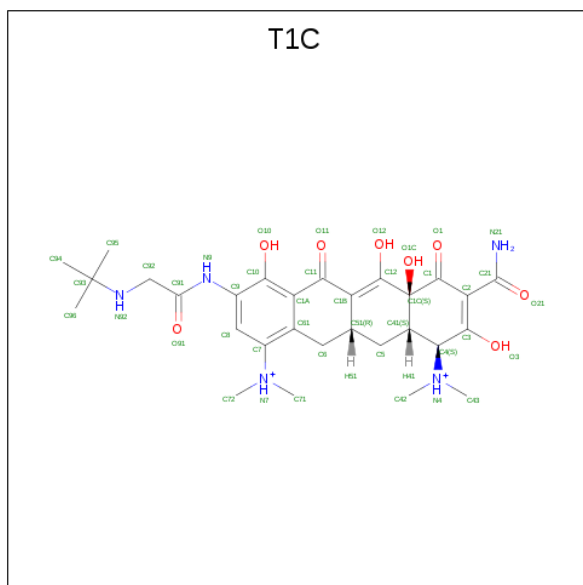
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 59 | AA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | AA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | AA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | AA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |

- Molecule 60 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



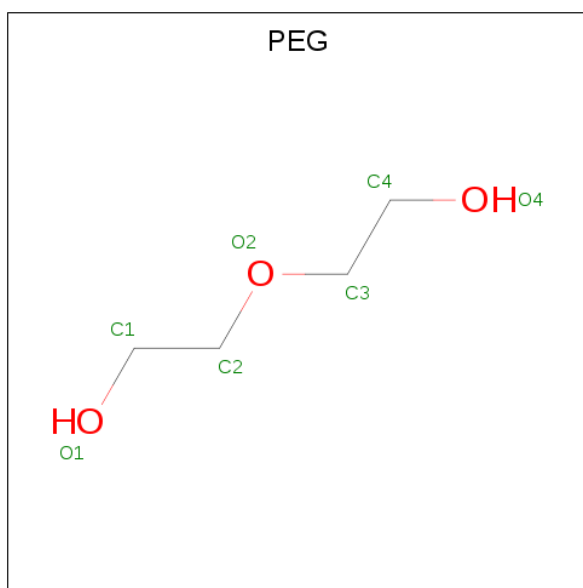
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 60 | AA | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 29 | 5 | 8 | | |
| 60 | BA | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 29 | 5 | 8 | | |

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 61 | C5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | AB | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | D5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

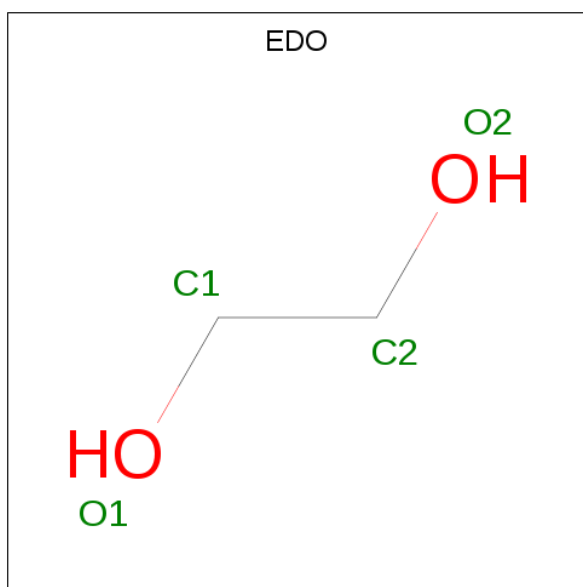
- Molecule 62 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:

C₄H₁₀O₃).



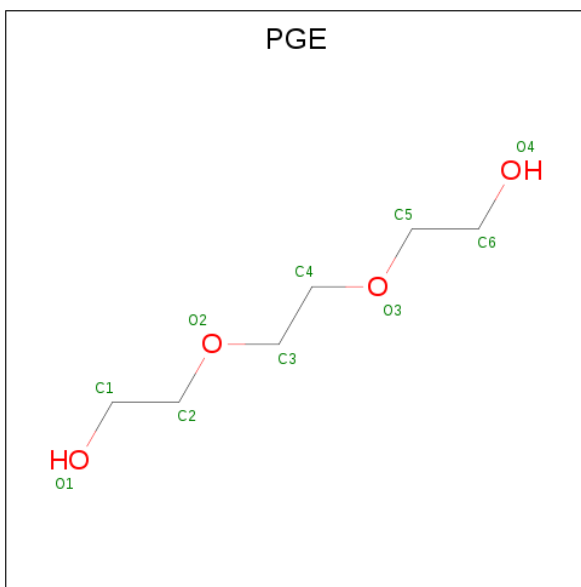
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 62 | AL | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | D1 | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | D3 | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | DL | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | DP | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | DQ | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 62 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |

- Molecule 63 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



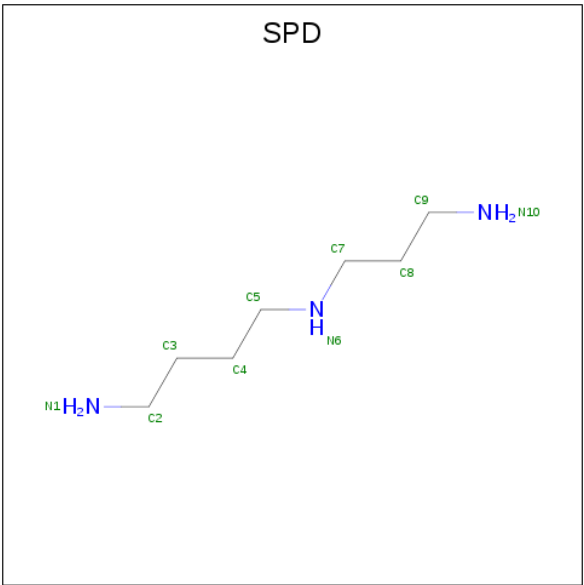
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 63 | D1 | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DB | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DB | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DB | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DB | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 63 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

- Molecule 64 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



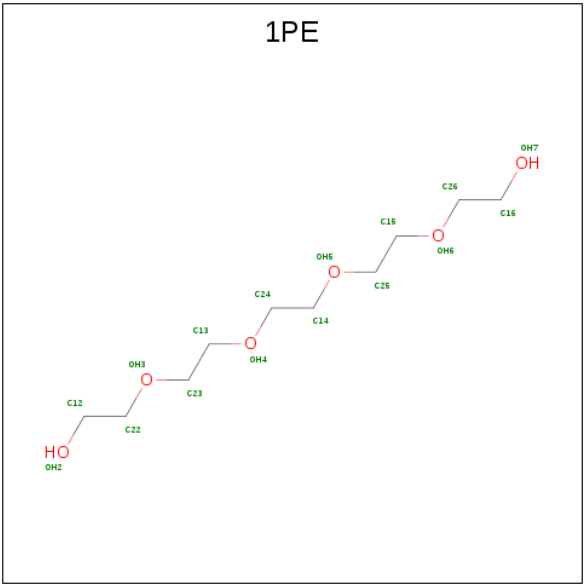
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 64 | D1 | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | D3 | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DS | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DU | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |

- Molecule 65 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



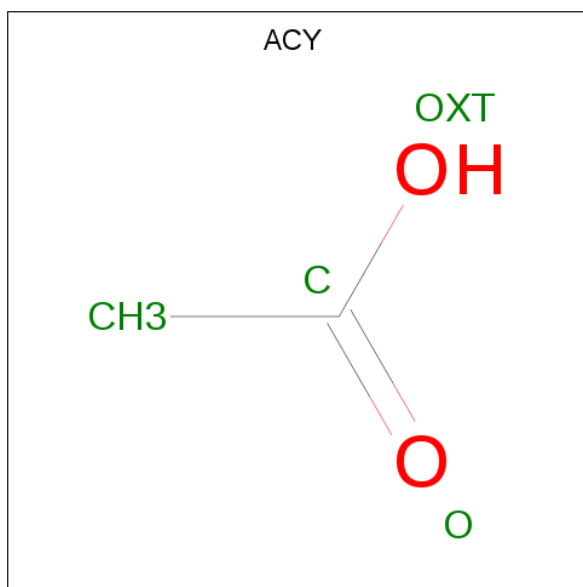
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 65 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 65 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 65 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 65 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |

- Molecule 66 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



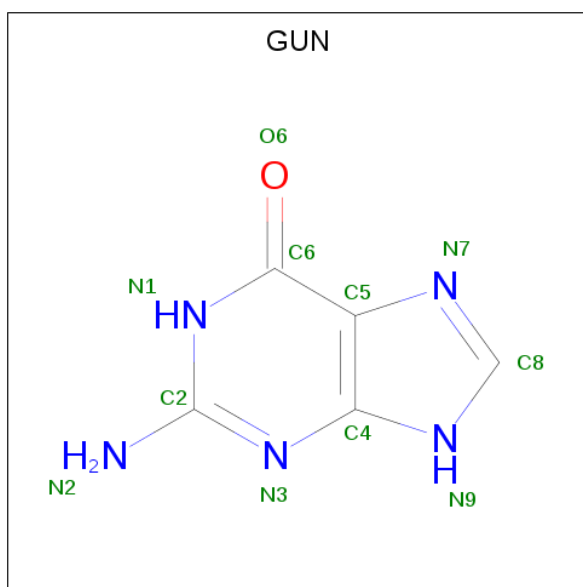
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 66 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 16 | 10 | 6 | | |
| 66 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 16 | 10 | 6 | | |

- Molecule 67 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



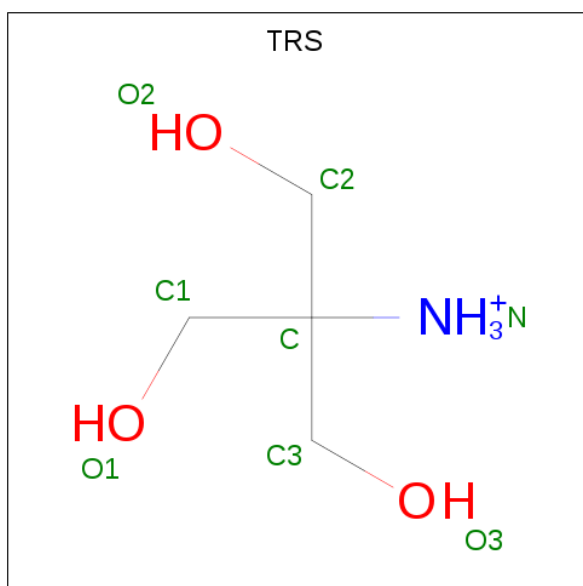
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 67 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 67 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 67 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

- Molecule 68 is GUANINE (three-letter code: GUN) (formula: C₅H₅N₅O).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 68 | DA | 1 | Total | C | N | O | 0 | 0 |
| | | | 11 | 5 | 5 | 1 | | |

- Molecule 69 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 69 | DA | 1 | Total | C | N | O | 0 | 0 |
| | | | 8 | 4 | 1 | 3 | | |

- Molecule 70 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 70 | AA | 500 | Total 500 | O 500 | 0 | 0 |
| 70 | AC | 5 | Total 5 | O 5 | 0 | 0 |
| 70 | AD | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | AE | 4 | Total 4 | O 4 | 0 | 0 |
| 70 | AF | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | AG | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | AH | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | AJ | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | AK | 6 | Total 6 | O 6 | 0 | 0 |
| 70 | AL | 10 | Total 10 | O 10 | 0 | 0 |
| 70 | AM | 4 | Total 4 | O 4 | 0 | 0 |
| 70 | AN | 7 | Total 7 | O 7 | 0 | 0 |
| 70 | AO | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | AP | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | AR | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | AT | 3 | Total 3 | O 3 | 0 | 0 |
| 70 | AU | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | C3 | 3 | Total 3 | O 3 | 0 | 0 |
| 70 | C4 | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | BA | 288 | Total 288 | O 288 | 0 | 0 |
| 70 | BD | 12 | Total 12 | O 12 | 0 | 0 |
| 70 | BE | 1 | Total 1 | O 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 70 | BF | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | BK | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | BL | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | BN | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | BO | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | BP | 3 | Total 3 | O 3 | 0 | 0 |
| 70 | BT | 4 | Total 4 | O 4 | 0 | 0 |
| 70 | BU | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | D1 | 45 | Total 45 | O 45 | 0 | 0 |
| 70 | D2 | 7 | Total 7 | O 7 | 0 | 0 |
| 70 | D3 | 23 | Total 23 | O 23 | 0 | 0 |
| 70 | D4 | 39 | Total 39 | O 39 | 0 | 0 |
| 70 | D5 | 12 | Total 12 | O 12 | 0 | 0 |
| 70 | D0 | 21 | Total 21 | O 21 | 0 | 0 |
| 70 | CB | 13 | Total 13 | O 13 | 0 | 0 |
| 70 | CC | 12 | Total 12 | O 12 | 0 | 0 |
| 70 | CD | 6 | Total 6 | O 6 | 0 | 0 |
| 70 | CA | 692 | Total 692 | O 692 | 0 | 0 |
| 70 | DC | 104 | Total 104 | O 104 | 0 | 0 |
| 70 | DD | 92 | Total 92 | O 92 | 0 | 0 |
| 70 | CE | 4 | Total 4 | O 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 70 | CL | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | CM | 4 | Total 4 | O 4 | 0 | 0 |
| 70 | CO | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | CU | 3 | Total 3 | O 3 | 0 | 0 |
| 70 | CV | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | CW | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | CY | 1 | Total 1 | O 1 | 0 | 0 |
| 70 | DE | 60 | Total 60 | O 60 | 0 | 0 |
| 70 | DF | 15 | Total 15 | O 15 | 0 | 0 |
| 70 | DG | 6 | Total 6 | O 6 | 0 | 0 |
| 70 | DH | 2 | Total 2 | O 2 | 0 | 0 |
| 70 | DK | 64 | Total 64 | O 64 | 0 | 0 |
| 70 | DL | 51 | Total 51 | O 51 | 0 | 0 |
| 70 | DM | 64 | Total 64 | O 64 | 0 | 0 |
| 70 | DN | 73 | Total 73 | O 73 | 0 | 0 |
| 70 | DO | 46 | Total 46 | O 46 | 0 | 0 |
| 70 | DP | 40 | Total 40 | O 40 | 0 | 0 |
| 70 | DQ | 32 | Total 32 | O 32 | 0 | 0 |
| 70 | DR | 63 | Total 63 | O 63 | 0 | 0 |
| 70 | DS | 44 | Total 44 | O 44 | 0 | 0 |
| 70 | DT | 69 | Total 69 | O 69 | 0 | 0 |

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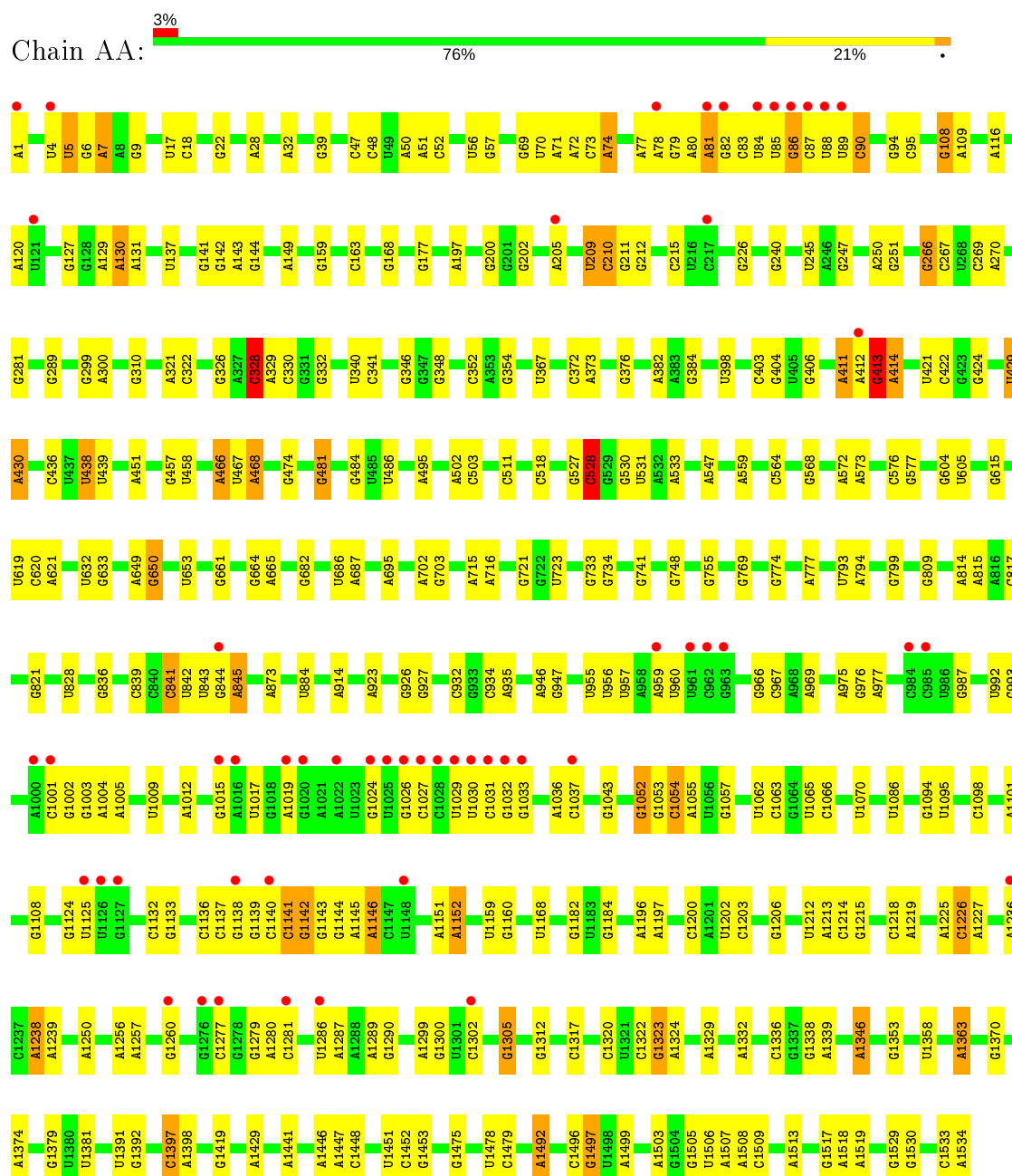
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 70 | DU | 21 | Total 21 | O 21 | 0 | 0 |
| 70 | DV | 20 | Total 20 | O 20 | 0 | 0 |
| 70 | DW | 31 | Total 31 | O 31 | 0 | 0 |
| 70 | DX | 26 | Total 26 | O 26 | 0 | 0 |
| 70 | DY | 11 | Total 11 | O 11 | 0 | 0 |
| 70 | DZ | 7 | Total 7 | O 7 | 0 | 0 |
| 70 | DB | 213 | Total 213 | O 213 | 0 | 0 |
| 70 | DA | 4829 | Total 4829 | O 4829 | 0 | 0 |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: 16S rRNA




Chain BA:

13% 75% 23%

Nodes (A to U93) are arranged in a grid, with each node represented by a colored square and a label. The nodes are connected by lines, forming a complex network. The colors of the nodes vary, with some nodes having a red dot.


- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A2 | | K10 | T17 | K22 | R26 | A27 | I28 | F38 | L48 | R56 | F107 | H120 | K121 | I132 | V143 | S144 | I145 | K151 | K177 | M178 | E179 | D194 | E197 | I200 | K206 |
|----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

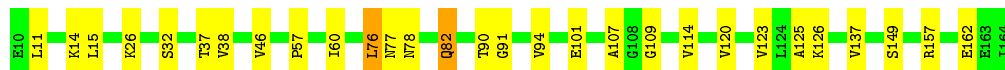
- Molecule 4: 30S ribosomal protein S4

Chain BD:  87% 13%




- Molecule 5: 30S ribosomal protein S5

Chain AE:  81% 17% .




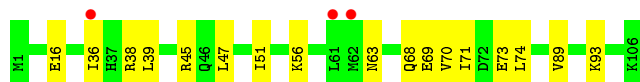
- Molecule 5: 30S ribosomal protein S5

Chain BE:  % 71% 20% 5% . .




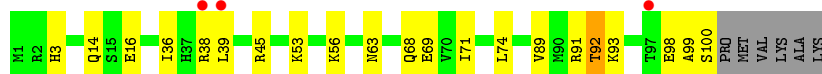
- Molecule 6: 30S ribosomal protein S6

Chain AF:  3% 84% 16%




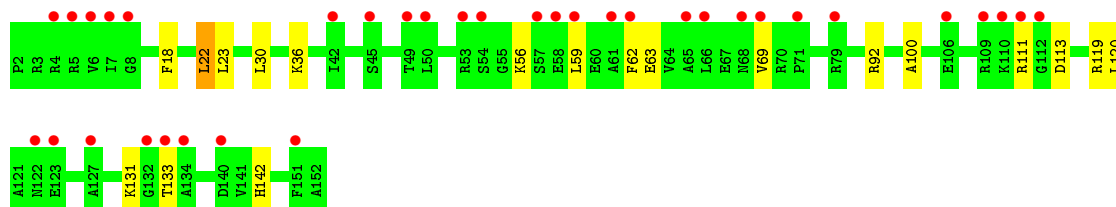
- Molecule 6: 30S ribosomal protein S6

Chain BF:  3% 75% 19% 6%



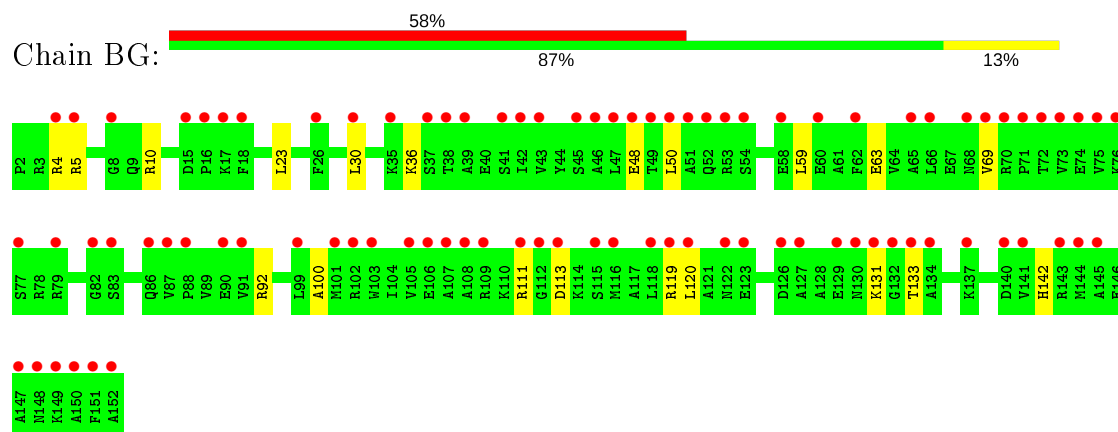
- Molecule 7: 30S ribosomal protein S7

Chain AG:  23% 87% 12% .



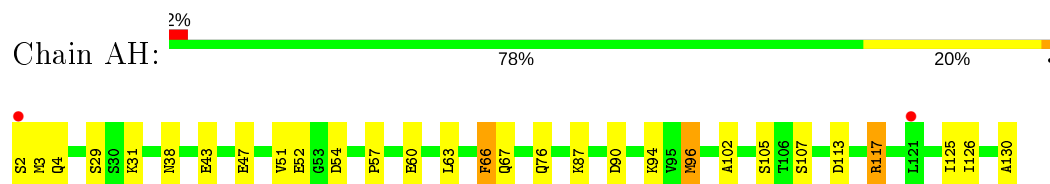
- Molecule 7: 30S ribosomal protein S7

Chain BG:



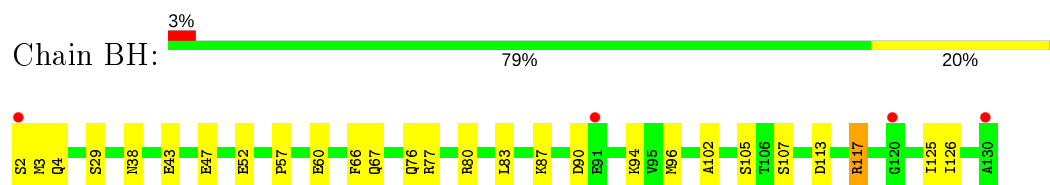
- Molecule 8: 30S ribosomal protein S8

Chain AH:



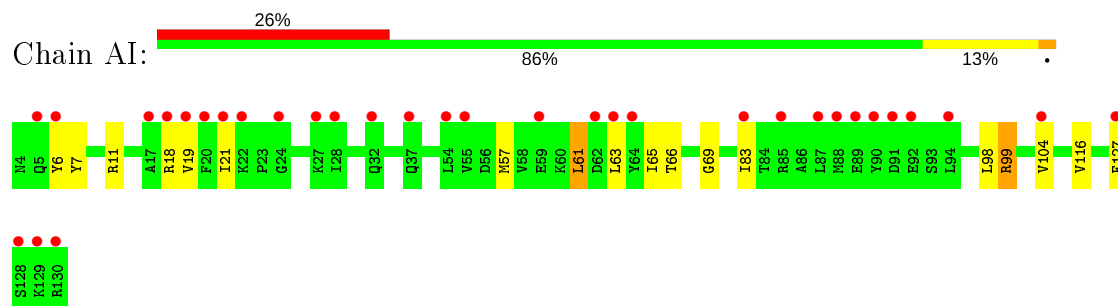
- Molecule 8: 30S ribosomal protein S8

Chain BH:



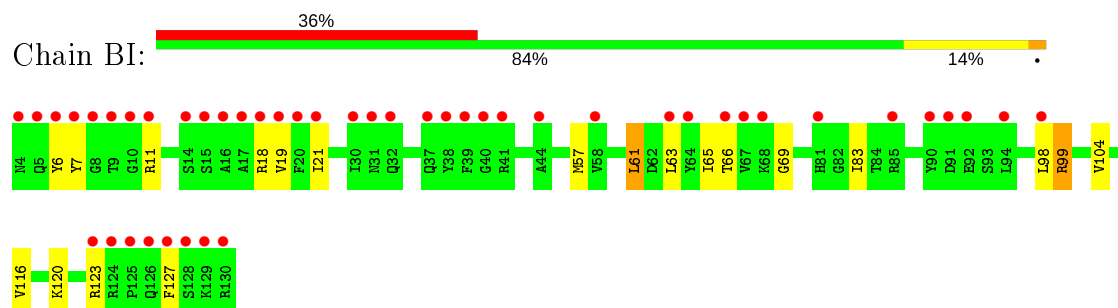
- Molecule 9: 30S ribosomal protein S9

Chain AI:

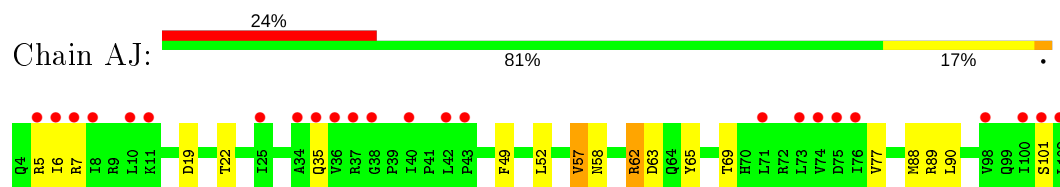


- Molecule 9: 30S ribosomal protein S9

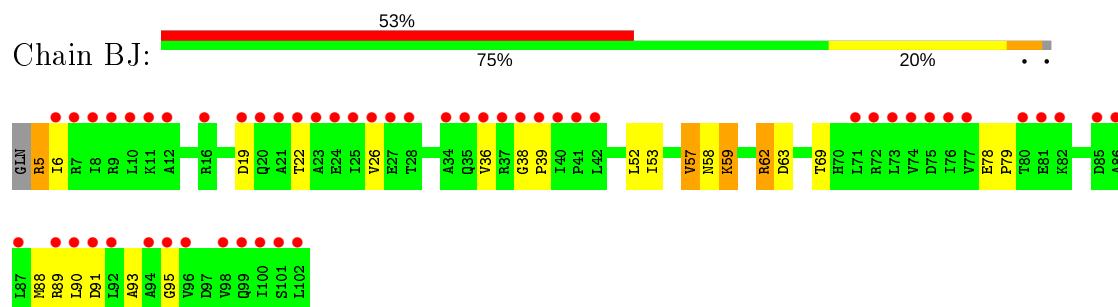
Chain BI:



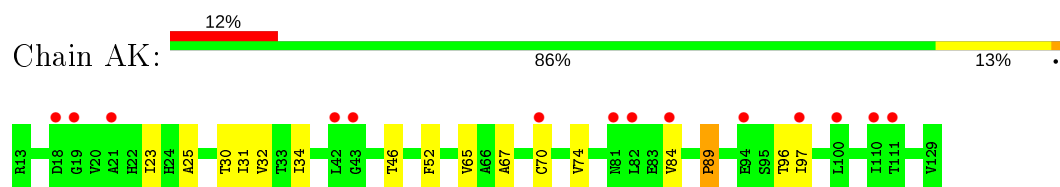
- Molecule 10: 30S ribosomal protein S10



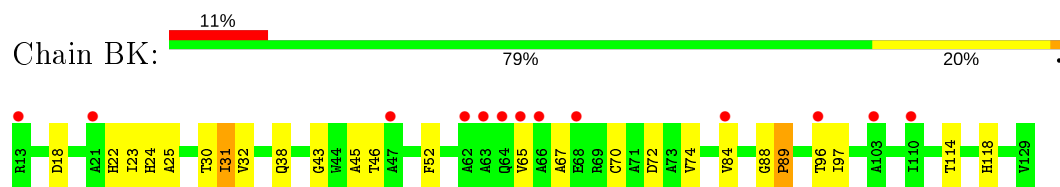
- Molecule 10: 30S ribosomal protein S10



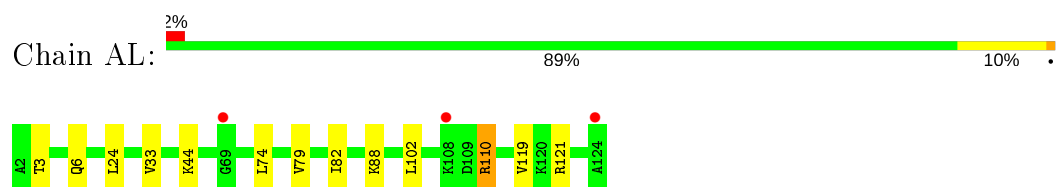
- Molecule 11: 30S ribosomal protein S11



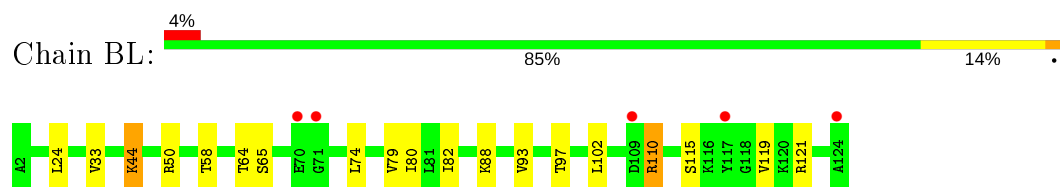
- Molecule 11: 30S ribosomal protein S11



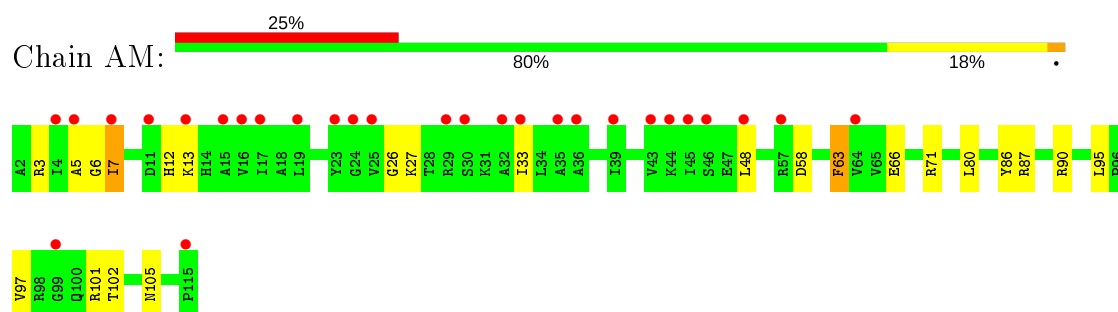
- Molecule 12: 30S ribosomal protein S12



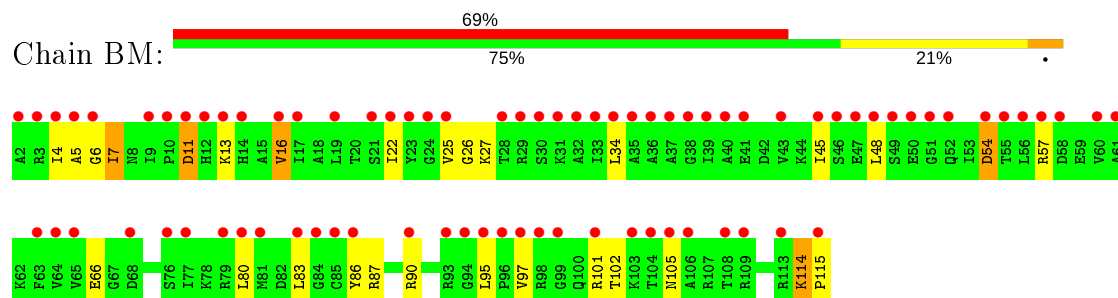
- Molecule 12: 30S ribosomal protein S12



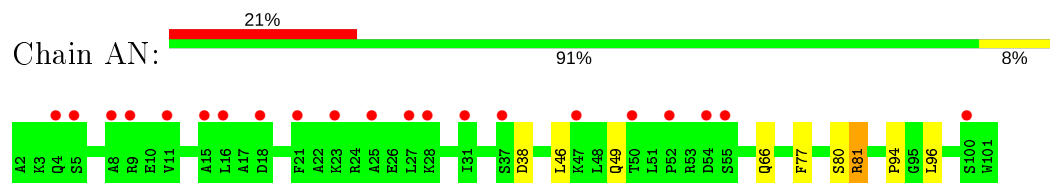
- Molecule 13: 30S ribosomal protein S13



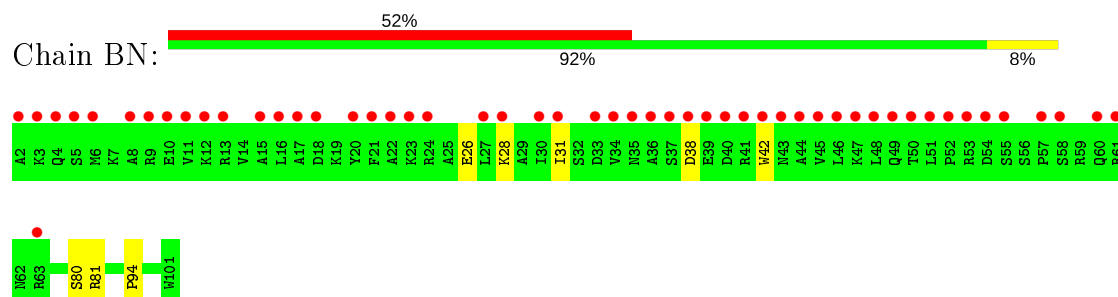
- Molecule 13: 30S ribosomal protein S13



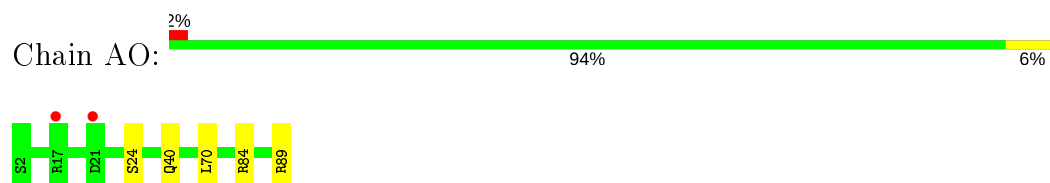
- Molecule 14: 30S ribosomal protein S14



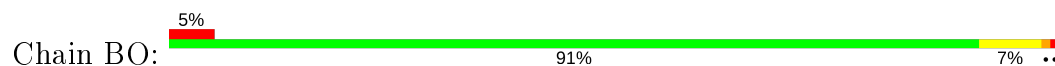
- Molecule 14: 30S ribosomal protein S14

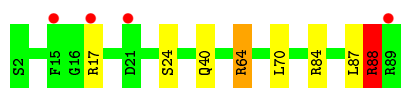


- Molecule 15: 30S ribosomal protein S15

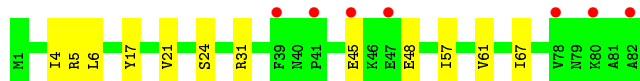
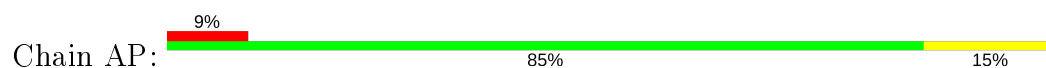


- Molecule 15: 30S ribosomal protein S15

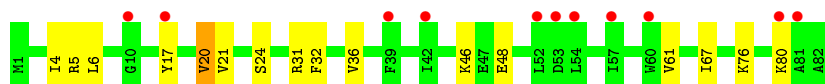
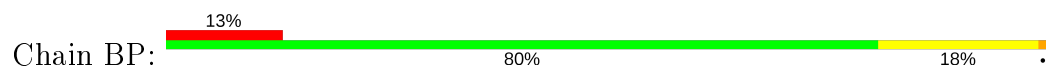




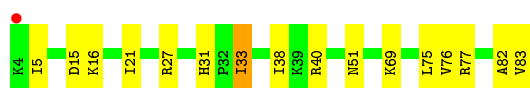
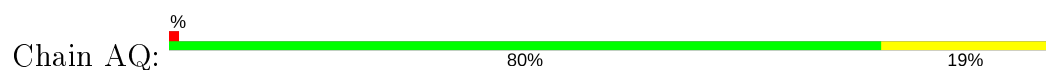
- Molecule 16: 30S ribosomal protein S16



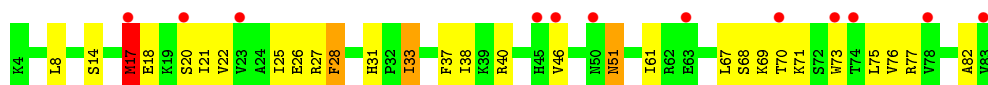
- Molecule 16: 30S ribosomal protein S16



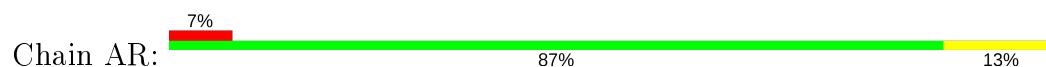
- Molecule 17: 30S ribosomal protein S17



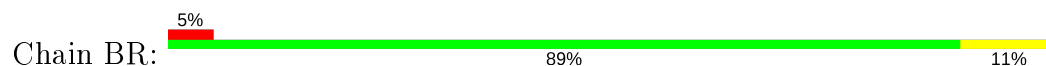
- Molecule 17: 30S ribosomal protein S17



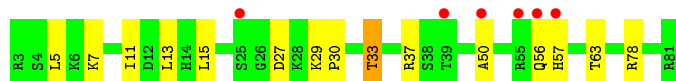
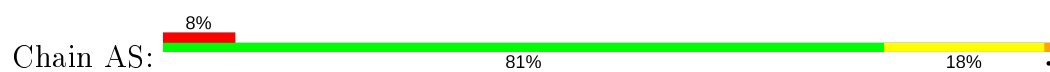
- Molecule 18: 30S ribosomal protein S18



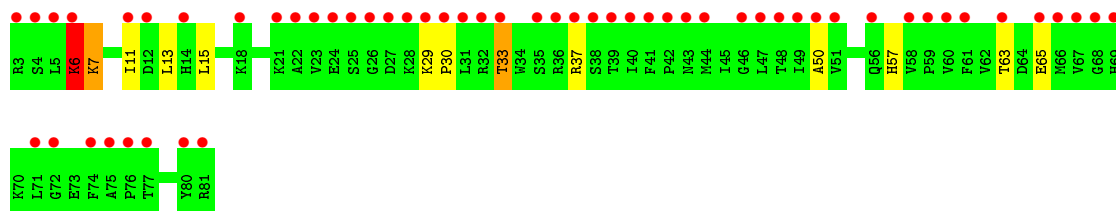
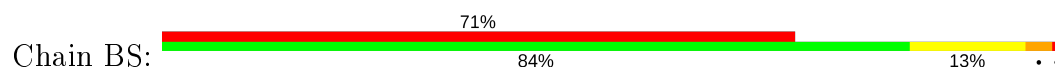
- Molecule 18: 30S ribosomal protein S18



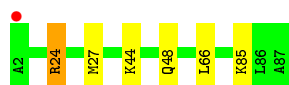
- Molecule 19: 30S ribosomal protein S19



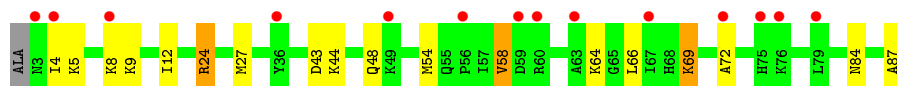
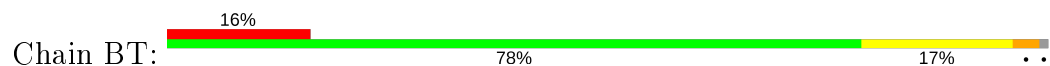
- Molecule 19: 30S ribosomal protein S19



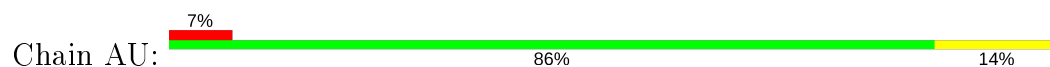
- Molecule 20: 30S ribosomal protein S20



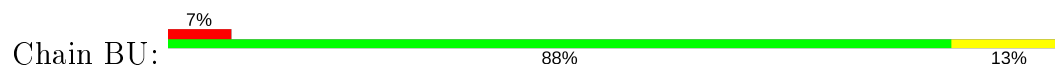
- Molecule 20: 30S ribosomal protein S20



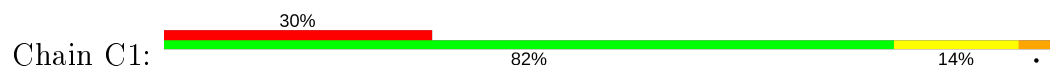
- Molecule 21: 30S ribosomal protein S21

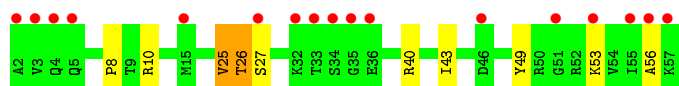


- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 50S ribosomal protein L32





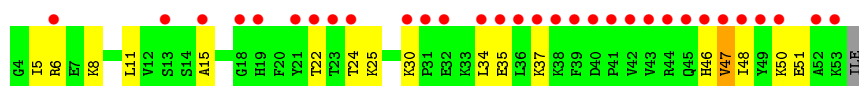
- Molecule 22: 50S ribosomal protein L32

Chain D1: 82% 18%



- Molecule 23: 50S ribosomal protein L33

Chain C2: 61% 65% 31% ..



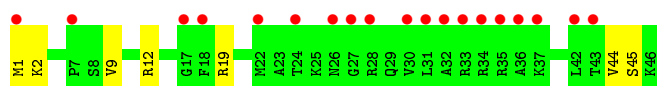
- Molecule 23: 50S ribosomal protein L33

Chain D2: 73% 25% .



- Molecule 24: 50S ribosomal protein L34

Chain C3: 41% 85% 15%



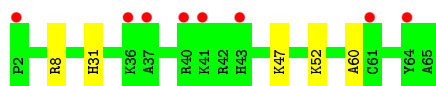
- Molecule 24: 50S ribosomal protein L34

Chain D3: 2% 93% 7%



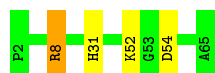
- Molecule 25: 50S ribosomal protein L35

Chain C4: 13% 92% 8%




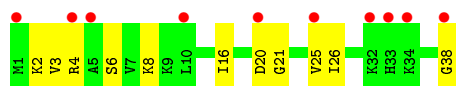
- Molecule 25: 50S ribosomal protein L35

Chain D4:  94% 5% .




- Molecule 26: 50S ribosomal protein L36

Chain C5:  26% 71% 29%




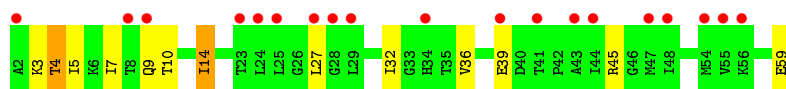
- Molecule 26: 50S ribosomal protein L36

Chain D5:  87% 13%



- Molecule 27: 50S ribosomal protein L30

Chain C0:  33% 78% 19% .




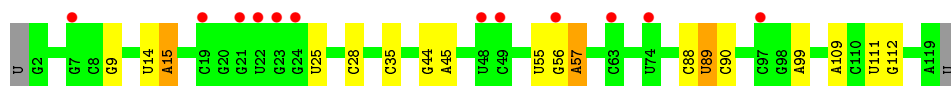
- Molecule 27: 50S ribosomal protein L30

Chain D0:  93% 7%



- Molecule 28: 5S rRNA

Chain CB:  10% 83% 13% . .

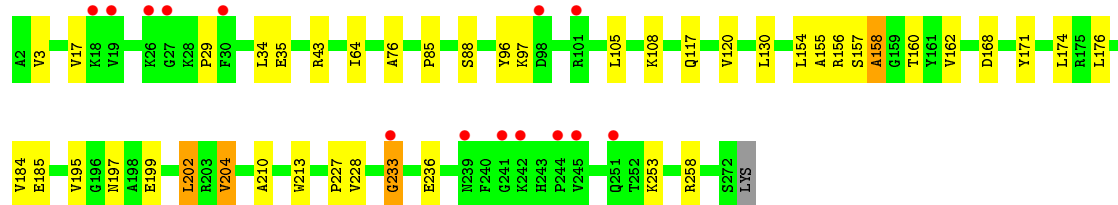
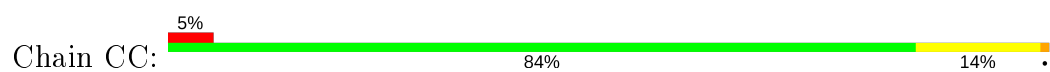


- Molecule 28: 5S rRNA

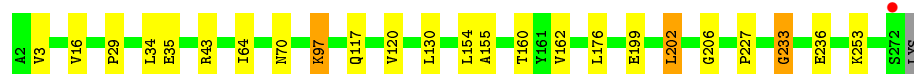
Chain DB:  91% 8% .



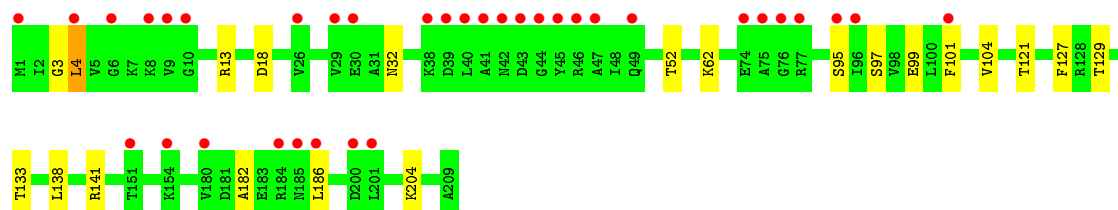
- Molecule 29: 50S ribosomal protein L2



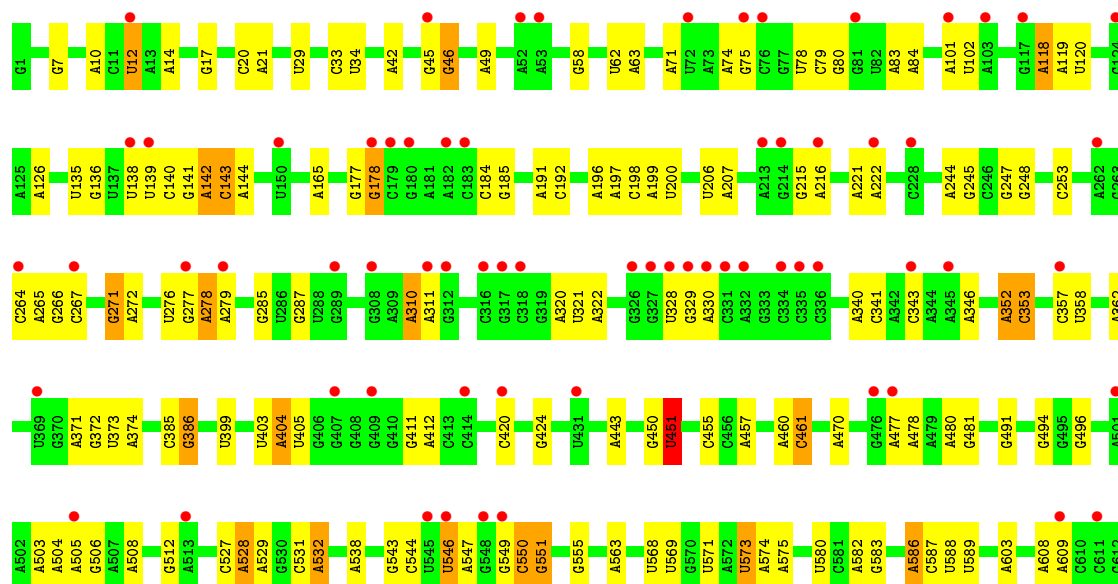
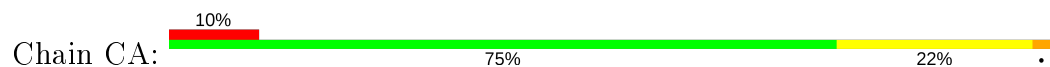
- Molecule 29: 50S ribosomal protein L2

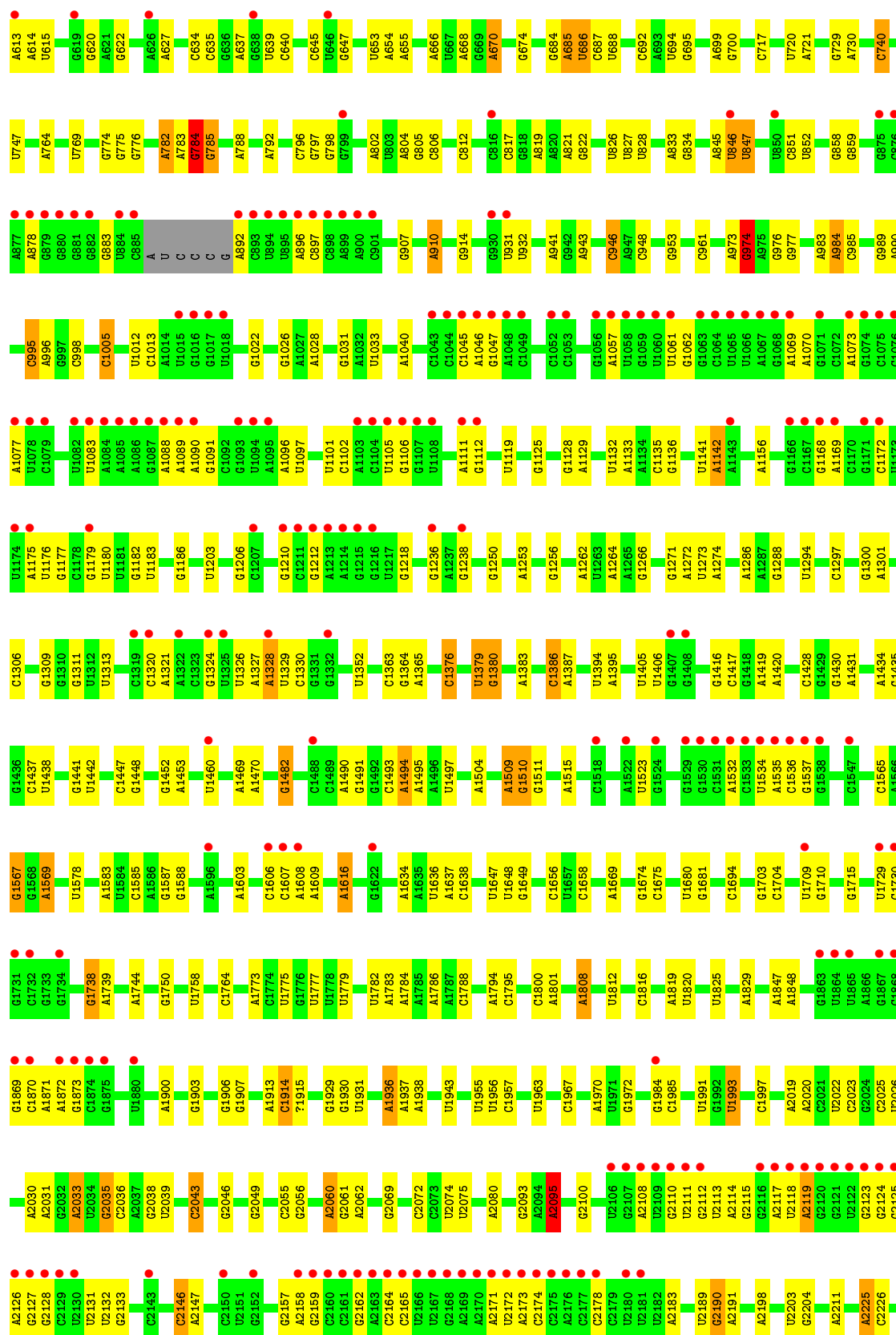


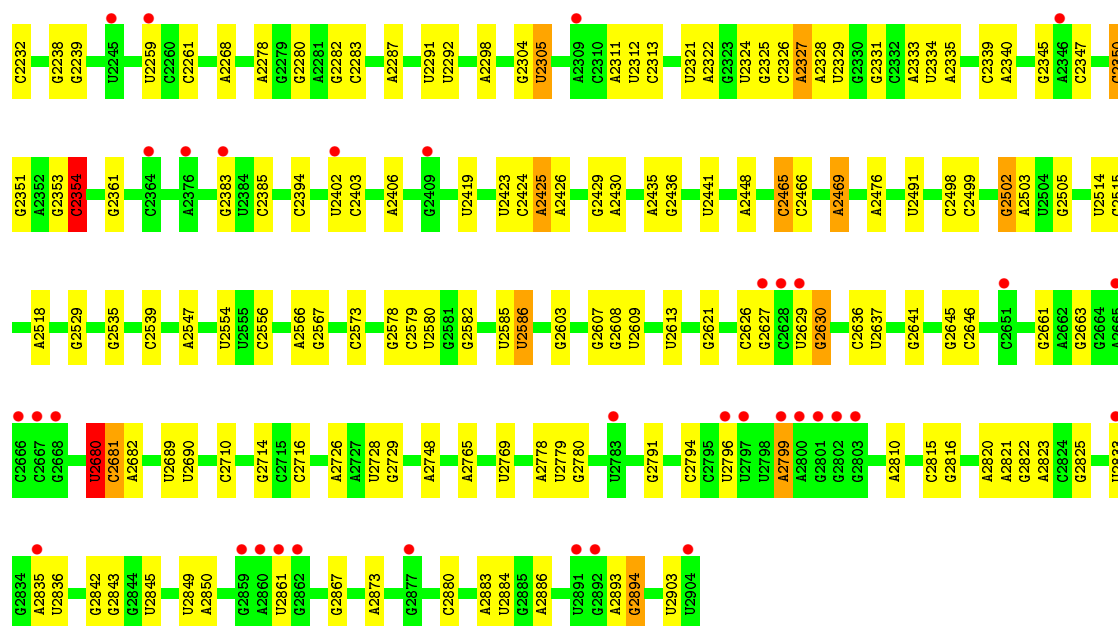
- Molecule 30: 50S ribosomal protein L3



- Molecule 31: 23S rRNA







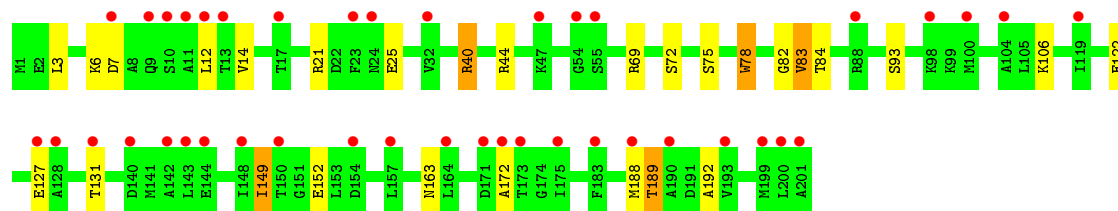
• Molecule 32: 50S ribosomal protein L3

Chain DD: 91% 9%



• Molecule 33: 50S ribosomal protein L4

Chain CE: 20% 86% 11%



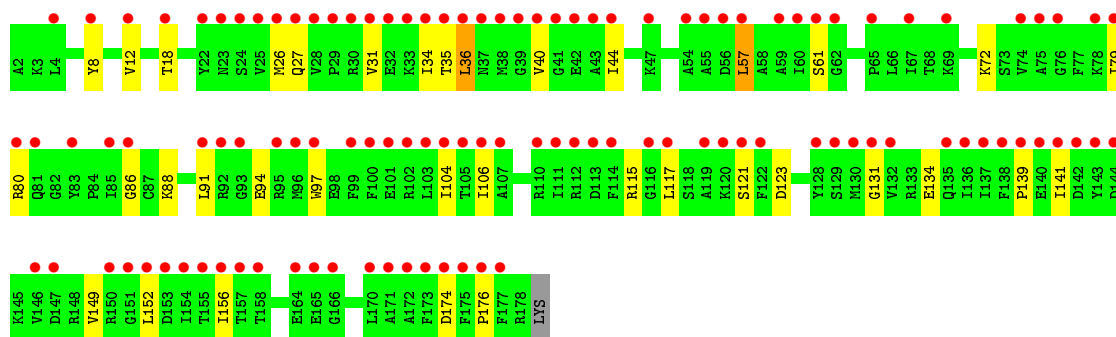
• Molecule 33: 50S ribosomal protein L4

Chain DE: 91% 8%

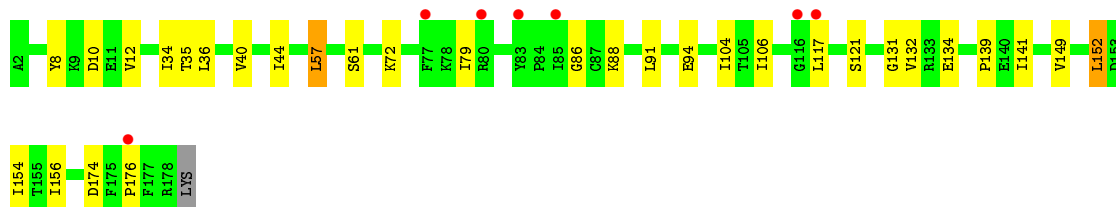
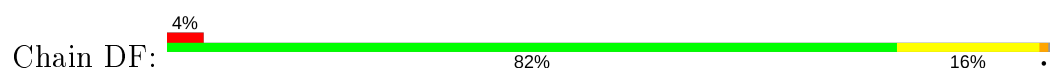


• Molecule 34: 50S ribosomal protein L5

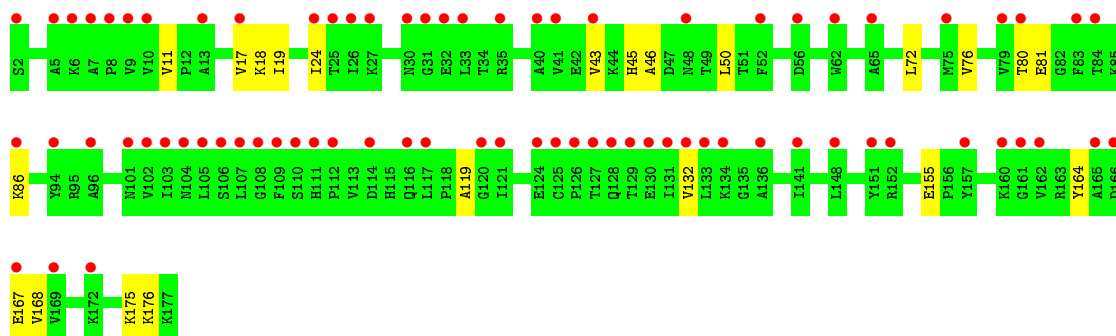
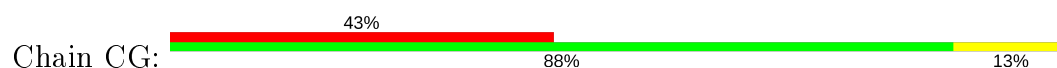
Chain CF: 63% 79% 19%



- Molecule 34: 50S ribosomal protein L5



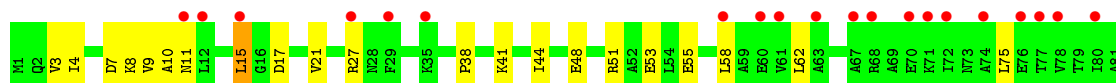
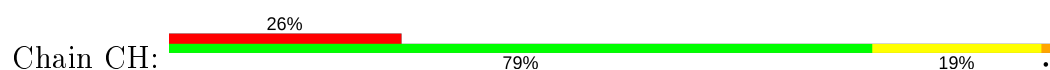
- Molecule 35: 50S ribosomal protein L6

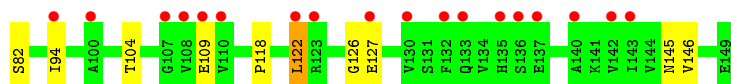


- Molecule 35: 50S ribosomal protein L6

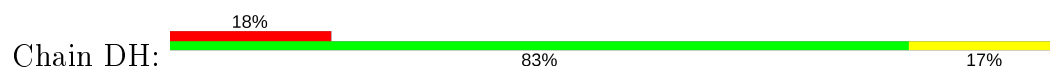


- Molecule 36: 50S ribosomal protein L9

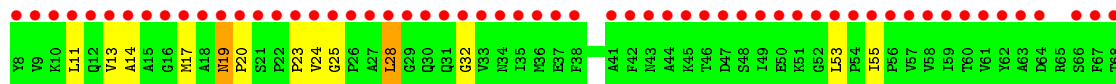
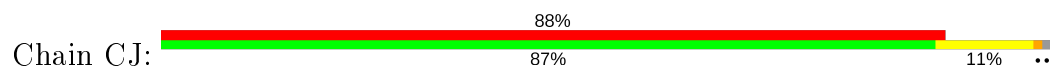




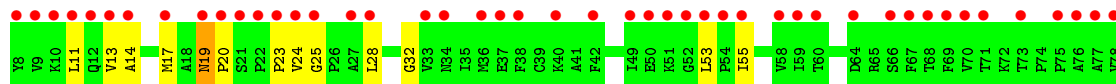
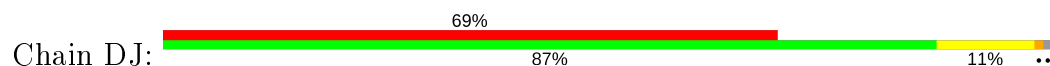
- Molecule 36: 50S ribosomal protein L9



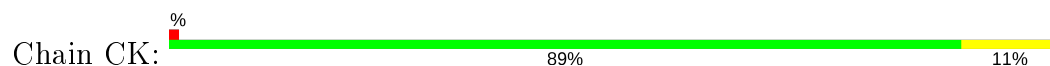
- Molecule 37: 50S ribosomal protein L11



- Molecule 37: 50S ribosomal protein L11



- Molecule 38: 50S ribosomal protein L13

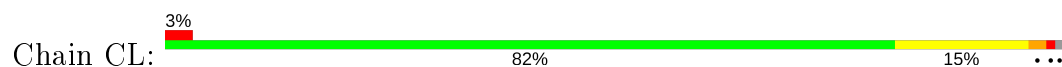


- Molecule 38: 50S ribosomal protein L13

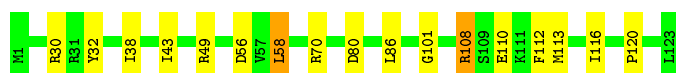




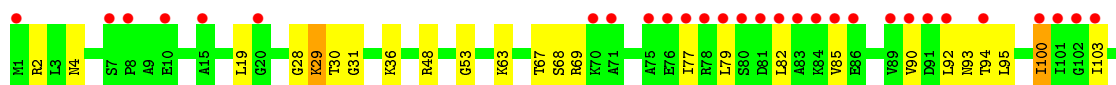
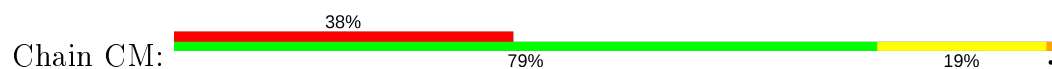
- Molecule 39: 50S ribosomal protein L14



- Molecule 39: 50S ribosomal protein L14



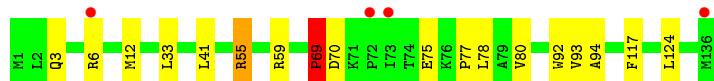
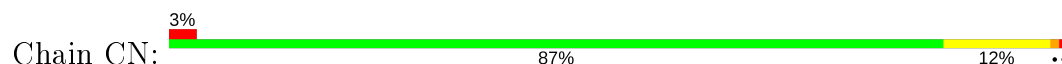
- Molecule 40: 50S ribosomal protein L15



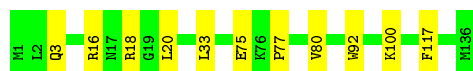
- Molecule 40: 50S ribosomal protein L15



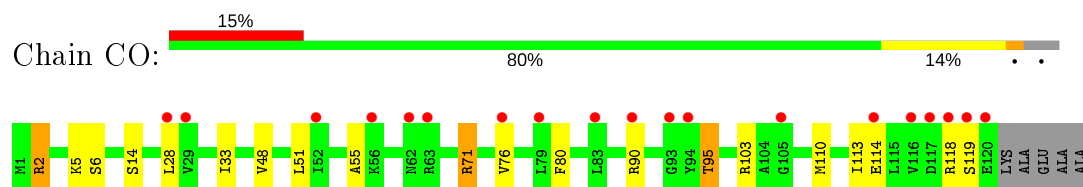
- Molecule 41: 50S ribosomal protein L16



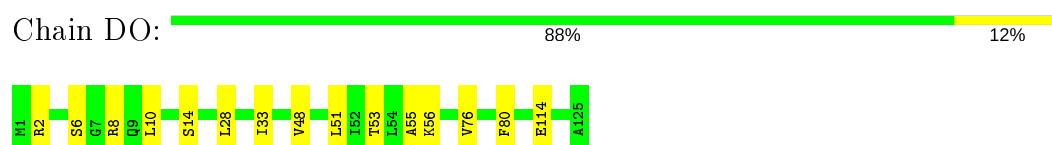
- Molecule 41: 50S ribosomal protein L16



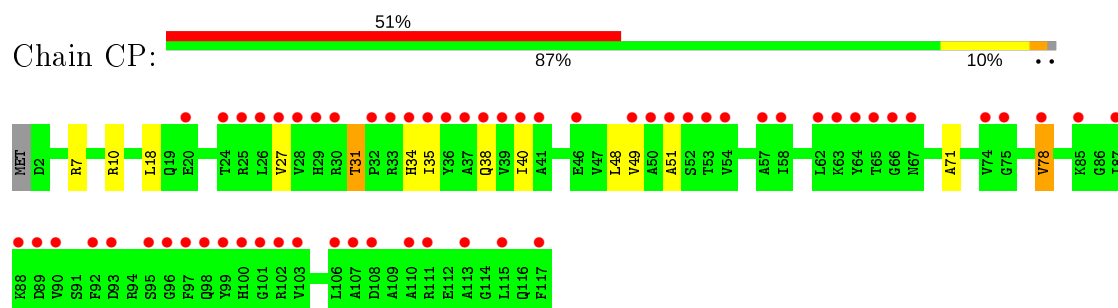
- Molecule 42: 50S ribosomal protein L17



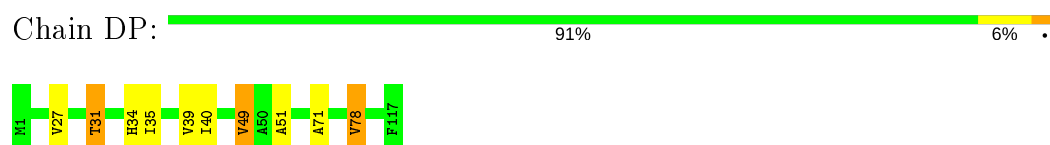
- Molecule 42: 50S ribosomal protein L17



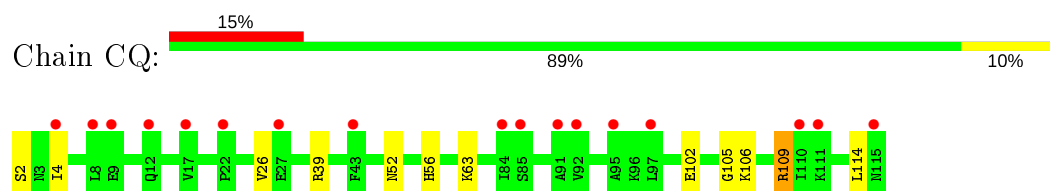
- Molecule 43: 50S ribosomal protein L18



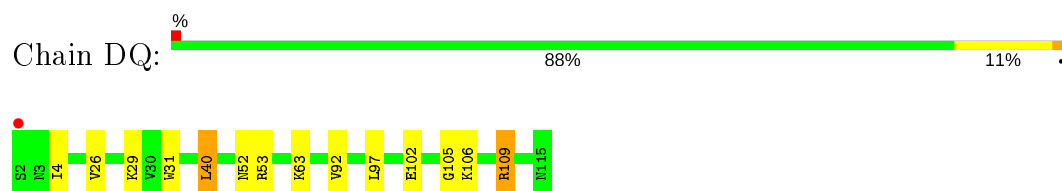
- Molecule 43: 50S ribosomal protein L18



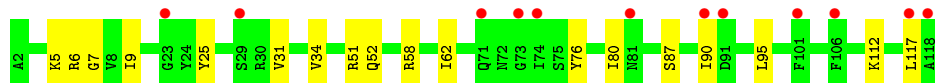
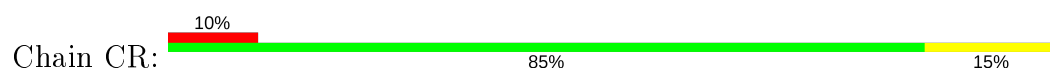
- Molecule 44: 50S ribosomal protein L19



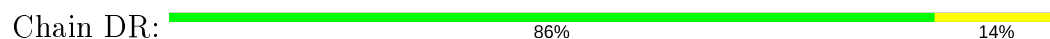
- Molecule 44: 50S ribosomal protein L19



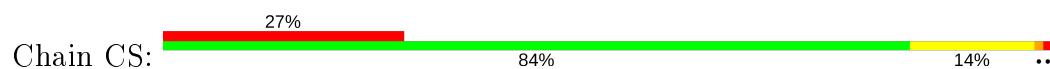
- Molecule 45: 50S ribosomal protein L20



- Molecule 45: 50S ribosomal protein L20



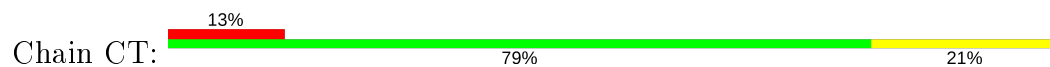
- Molecule 46: 50S ribosomal protein L21



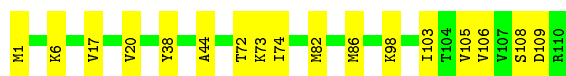
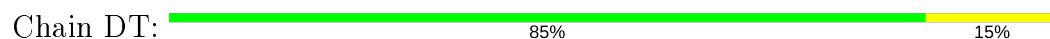
- Molecule 46: 50S ribosomal protein L21



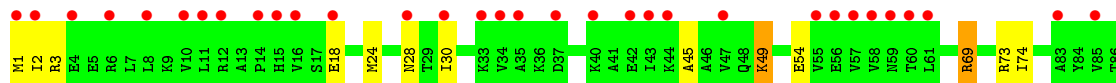
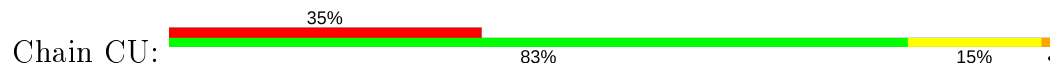
- Molecule 47: 50S ribosomal protein L22



- Molecule 47: 50S ribosomal protein L22

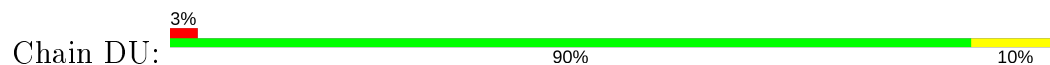


- Molecule 48: 50S ribosomal protein L23

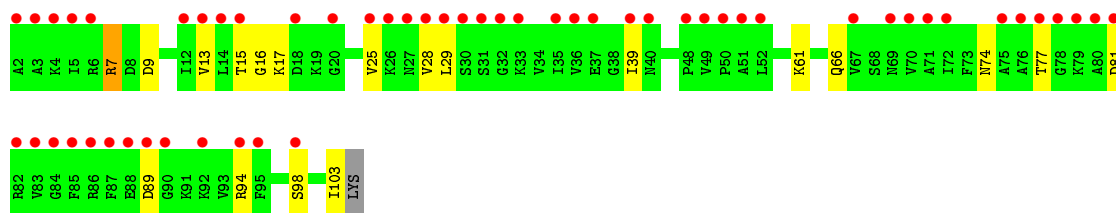
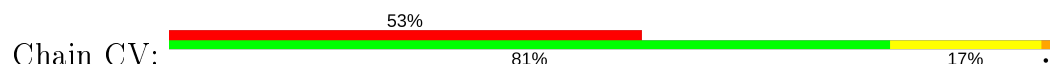




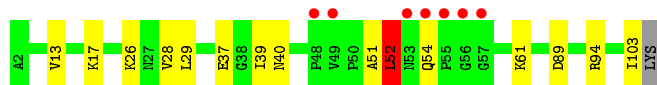
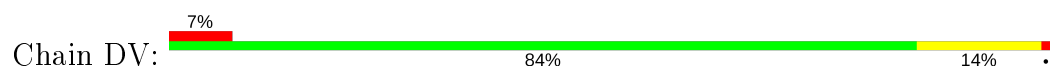
- Molecule 48: 50S ribosomal protein L23



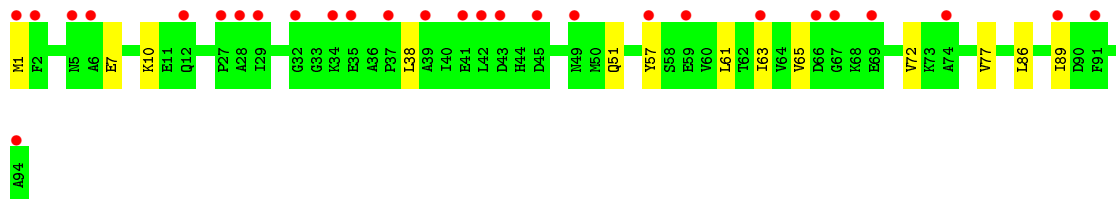
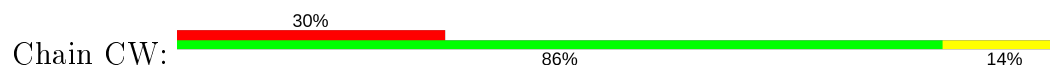
- Molecule 49: 50S ribosomal protein L24



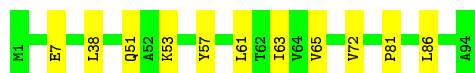
- Molecule 49: 50S ribosomal protein L24



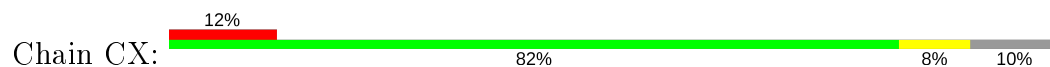
- Molecule 50: 50S ribosomal protein L25

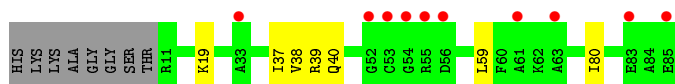


- Molecule 50: 50S ribosomal protein L25

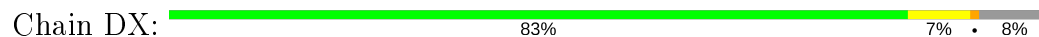


- Molecule 51: 50S ribosomal protein L27

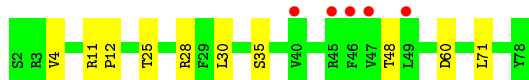
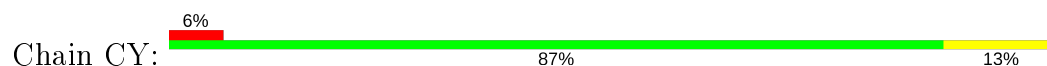




- Molecule 51: 50S ribosomal protein L27



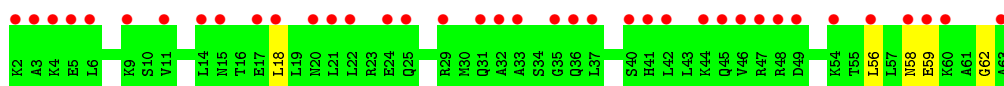
- Molecule 52: 50S ribosomal protein L28



- Molecule 52: 50S ribosomal protein L28



- Molecule 53: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L29

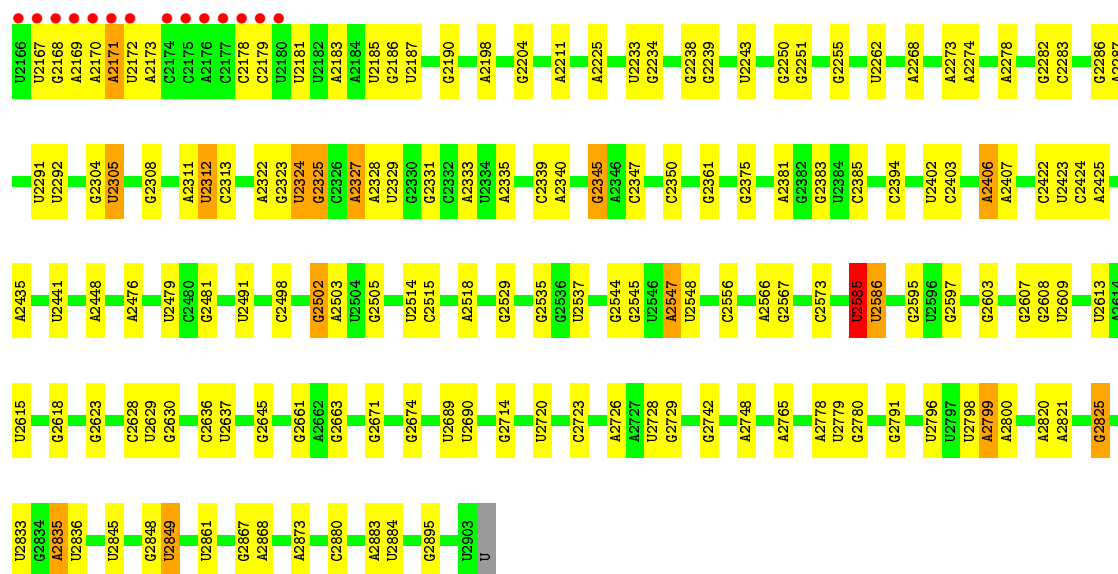


- Molecule 54: 50S ribosomal protein L10



Chain DA: 





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 211.72Å 435.19Å 622.83Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 48.53 – 3.10 48.53 – 3.10 | Depositor EDS |
| % Data completeness (in resolution range) | 99.7 (48.53-3.10) 99.7 (48.53-3.10) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.40 (at 3.12Å) | Xtriage |
| Refinement program | BUSTER-TNT 2.11.6 | Depositor |
| R, R_{free} | 0.171 , 0.192 0.185 , 0.207 | Depositor DCC |
| R_{free} test set | 4087 reflections (0.40%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 65.0 | Xtriage |
| Anisotropy | 0.428 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 91.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 295207 | wwPDB-VP |
| Average B, all atoms (Å ²) | 112.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, GUN, 1PE, 2MA, 2MG, ACY, PEG, 1MG, 3TD, PGE, D2T, UR3, 7MG, 4D4, 5MU, ZN, 5MC, MPD, PG4, 6MZ, TRS, OMC, MG, OMG, T1C, H2U, SPD, EDO, MEQ, OMU, PUT, 4OC, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | AA | 0.95 | 7/36597 (0.0%) | 0.85 | 6/57088 (0.0%) |
| 1 | BA | 0.96 | 5/36572 (0.0%) | 0.85 | 6/57049 (0.0%) |
| 2 | AB | 0.43 | 0/1784 | 0.62 | 0/2403 |
| 2 | BB | 0.42 | 0/1784 | 0.63 | 0/2403 |
| 3 | AC | 0.45 | 0/1652 | 0.65 | 0/2225 |
| 3 | BC | 0.44 | 0/1652 | 0.65 | 0/2225 |
| 4 | AD | 0.41 | 0/1665 | 0.65 | 0/2227 |
| 4 | BD | 0.41 | 0/1665 | 0.66 | 0/2227 |
| 5 | AE | 0.44 | 0/1157 | 0.74 | 0/1557 |
| 5 | BE | 0.47 | 0/1118 | 0.77 | 0/1504 |
| 6 | AF | 0.42 | 0/881 | 0.66 | 0/1189 |
| 6 | BF | 0.44 | 0/835 | 0.74 | 0/1128 |
| 7 | AG | 0.44 | 0/1196 | 0.61 | 0/1602 |
| 7 | BG | 0.44 | 0/1196 | 0.62 | 0/1602 |
| 8 | AH | 0.40 | 0/989 | 0.66 | 0/1326 |
| 8 | BH | 0.40 | 0/989 | 0.66 | 0/1326 |
| 9 | AI | 0.42 | 0/1034 | 0.64 | 0/1375 |
| 9 | BI | 0.42 | 0/1034 | 0.64 | 0/1375 |
| 10 | AJ | 0.41 | 0/806 | 0.64 | 0/1089 |
| 10 | BJ | 0.46 | 0/797 | 0.69 | 0/1077 |
| 11 | AK | 0.43 | 0/893 | 0.61 | 0/1205 |
| 11 | BK | 0.41 | 0/893 | 0.65 | 0/1205 |
| 12 | AL | 0.42 | 0/960 | 0.69 | 0/1286 |
| 12 | BL | 0.42 | 0/960 | 0.70 | 0/1286 |
| 13 | AM | 0.47 | 0/893 | 0.70 | 0/1193 |
| 13 | BM | 0.48 | 0/893 | 0.70 | 0/1193 |
| 14 | AN | 0.44 | 0/817 | 0.63 | 0/1088 |
| 14 | BN | 0.42 | 0/817 | 0.62 | 0/1088 |
| 15 | AO | 0.43 | 0/722 | 0.59 | 0/964 |
| 15 | BO | 0.42 | 0/722 | 0.59 | 0/964 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | AP | 0.43 | 0/659 | 0.68 | 0/884 |
| 16 | BP | 0.46 | 0/659 | 0.74 | 0/884 |
| 17 | AQ | 0.44 | 0/658 | 0.70 | 0/881 |
| 17 | BQ | 0.48 | 0/658 | 0.74 | 0/881 |
| 18 | AR | 0.46 | 0/463 | 0.63 | 0/621 |
| 18 | BR | 0.46 | 0/463 | 0.62 | 0/621 |
| 19 | AS | 0.46 | 0/653 | 0.59 | 0/877 |
| 19 | BS | 0.46 | 0/653 | 0.60 | 0/877 |
| 20 | AT | 0.45 | 0/676 | 0.64 | 0/895 |
| 20 | BT | 0.49 | 0/671 | 0.67 | 0/888 |
| 21 | AU | 0.40 | 0/472 | 0.60 | 0/627 |
| 21 | BU | 0.37 | 0/472 | 0.61 | 0/627 |
| 22 | C1 | 0.48 | 0/450 | 0.66 | 0/599 |
| 22 | D1 | 0.51 | 0/450 | 0.72 | 0/599 |
| 23 | C2 | 0.44 | 0/416 | 0.68 | 0/554 |
| 23 | D2 | 0.45 | 0/421 | 0.66 | 0/561 |
| 24 | C3 | 0.40 | 0/380 | 0.67 | 0/498 |
| 24 | D3 | 0.50 | 0/380 | 0.70 | 0/498 |
| 25 | C4 | 0.41 | 0/513 | 0.62 | 0/676 |
| 25 | D4 | 0.47 | 0/513 | 0.65 | 0/676 |
| 26 | C5 | 0.41 | 0/303 | 0.76 | 0/397 |
| 26 | D5 | 0.46 | 0/303 | 0.72 | 0/397 |
| 27 | C0 | 0.47 | 0/453 | 0.79 | 0/605 |
| 27 | D0 | 0.53 | 0/467 | 0.78 | 0/623 |
| 28 | CB | 0.92 | 0/2828 | 0.87 | 2/4410 (0.0%) |
| 28 | DB | 0.94 | 0/2872 | 0.86 | 0/4478 |
| 29 | CC | 0.41 | 0/2121 | 0.70 | 0/2852 |
| 29 | DC | 0.43 | 0/2121 | 0.70 | 0/2852 |
| 30 | CD | 0.40 | 0/1586 | 0.65 | 0/2134 |
| 31 | CA | 0.97 | 29/69165 (0.0%) | 0.86 | 10/107896 (0.0%) |
| 32 | DD | 0.44 | 0/1576 | 0.65 | 0/2119 |
| 33 | CE | 0.42 | 0/1571 | 0.68 | 0/2113 |
| 33 | DE | 0.44 | 0/1570 | 0.66 | 0/2113 |
| 34 | CF | 0.40 | 0/1434 | 0.65 | 0/1926 |
| 34 | DF | 0.43 | 0/1434 | 0.67 | 0/1926 |
| 35 | CG | 0.39 | 0/1343 | 0.64 | 0/1816 |
| 35 | DG | 0.41 | 0/1343 | 0.62 | 0/1816 |
| 36 | CH | 0.45 | 0/1121 | 0.67 | 0/1515 |
| 36 | DH | 0.45 | 0/1121 | 0.66 | 0/1515 |
| 37 | CJ | 0.48 | 0/993 | 0.62 | 0/1341 |
| 37 | DJ | 0.48 | 0/993 | 0.62 | 0/1341 |
| 38 | CK | 0.39 | 0/1152 | 0.65 | 0/1551 |
| 38 | DK | 0.47 | 0/1152 | 0.66 | 0/1551 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | CL | 0.43 | 0/947 | 0.69 | 0/1268 |
| 39 | DL | 0.46 | 0/955 | 0.68 | 0/1279 |
| 40 | CM | 0.42 | 0/1062 | 0.71 | 2/1413 (0.1%) |
| 40 | DM | 0.42 | 0/1062 | 0.67 | 0/1413 |
| 41 | CN | 0.42 | 0/1081 | 0.71 | 1/1443 (0.1%) |
| 41 | DN | 0.47 | 0/1092 | 0.71 | 0/1457 |
| 42 | CO | 0.41 | 0/973 | 0.67 | 0/1301 |
| 42 | DO | 0.48 | 0/1006 | 0.72 | 0/1345 |
| 43 | CP | 0.41 | 0/902 | 0.68 | 0/1209 |
| 43 | DP | 0.44 | 0/910 | 0.68 | 0/1219 |
| 44 | CQ | 0.38 | 0/929 | 0.68 | 0/1242 |
| 44 | DQ | 0.43 | 0/929 | 0.66 | 0/1242 |
| 45 | CR | 0.43 | 0/960 | 0.64 | 0/1278 |
| 45 | DR | 0.49 | 0/960 | 0.65 | 0/1278 |
| 46 | CS | 0.39 | 0/829 | 0.71 | 0/1107 |
| 46 | DS | 0.43 | 0/829 | 0.75 | 0/1107 |
| 47 | CT | 0.38 | 0/864 | 0.70 | 0/1156 |
| 47 | DT | 0.45 | 0/864 | 0.70 | 0/1156 |
| 48 | CU | 0.41 | 0/745 | 0.67 | 0/994 |
| 48 | DU | 0.43 | 0/744 | 0.68 | 0/994 |
| 49 | CV | 0.42 | 0/787 | 0.72 | 0/1051 |
| 49 | DV | 0.42 | 0/787 | 0.71 | 0/1051 |
| 50 | CW | 0.38 | 0/766 | 0.62 | 0/1025 |
| 50 | DW | 0.44 | 0/766 | 0.65 | 0/1025 |
| 51 | CX | 0.36 | 0/576 | 0.59 | 0/762 |
| 51 | DX | 0.43 | 0/598 | 0.63 | 0/790 |
| 52 | CY | 0.40 | 0/635 | 0.70 | 0/848 |
| 52 | DY | 0.44 | 0/635 | 0.69 | 0/848 |
| 53 | CZ | 0.40 | 0/502 | 0.60 | 0/667 |
| 53 | DZ | 0.42 | 0/502 | 0.59 | 0/667 |
| 54 | DI | 0.49 | 0/1037 | 0.73 | 1/1402 (0.1%) |
| 55 | DA | 1.02 | 20/69364 (0.0%) | 0.88 | 10/108207 (0.0%) |
| All | All | 0.86 | 61/309273 (0.0%) | 0.81 | 38/462224 (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 |
|-----|-------|---------------------|---------------------|
| 41 | CN | 0 | 1 |
| 55 | DA | 0 | 25 |
| All | All | 0 | 26 |

The worst 5 of 61 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 31 | CA | 2095 | A | O5'-C5' | -9.11 | 1.28 | 1.42 |
| 31 | CA | 2425 | A | C3'-O3' | 8.77 | 1.54 | 1.42 |
| 55 | DA | 12 | U | C1'-N1 | 8.01 | 1.60 | 1.48 |
| 31 | CA | 1936 | A | N9-C4 | -7.92 | 1.33 | 1.37 |
| 55 | DA | 2097 | A | O5'-C5' | -7.38 | 1.31 | 1.42 |

The worst 5 of 38 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28 | CB | 15 | A | O4'-C1'-N9 | 9.58 | 115.86 | 108.20 |
| 55 | DA | 1936 | A | O4'-C1'-N9 | 7.65 | 114.32 | 108.20 |
| 1 | AA | 1 | A | OP1-P-OP2 | -7.18 | 108.83 | 119.60 |
| 54 | DI | 132 | TYR | C-N-CA | 7.11 | 139.46 | 121.70 |
| 1 | AA | 413 | G | C1'-O4'-C4' | -7.07 | 104.24 | 109.90 |

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 41 | CN | 69 | PRO | Mainchain |
| 55 | DA | 15 | G | Sidechain |
| 55 | DA | 177 | G | Sidechain |
| 55 | DA | 221 | A | Sidechain |
| 55 | DA | 249 | C | Sidechain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32933 | 0 | 16593 | 81 | 0 |
| 1 | BA | 32911 | 0 | 16582 | 95 | 0 |
| 2 | AB | 1753 | 0 | 1780 | 7 | 0 |
| 2 | BB | 1753 | 0 | 1780 | 8 | 0 |
| 3 | AC | 1625 | 0 | 1696 | 12 | 0 |
| 3 | BC | 1625 | 0 | 1696 | 13 | 0 |
| 4 | AD | 1643 | 0 | 1707 | 11 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | BD | 1643 | 0 | 1707 | 16 | 0 |
| 5 | AE | 1144 | 0 | 1185 | 10 | 0 |
| 5 | BE | 1105 | 0 | 1148 | 19 | 0 |
| 6 | AF | 862 | 0 | 864 | 6 | 0 |
| 6 | BF | 817 | 0 | 808 | 7 | 0 |
| 7 | AG | 1182 | 0 | 1238 | 5 | 0 |
| 7 | BG | 1182 | 0 | 1238 | 3 | 0 |
| 8 | AH | 979 | 0 | 1031 | 11 | 0 |
| 8 | BH | 979 | 0 | 1031 | 8 | 0 |
| 9 | AI | 1022 | 0 | 1070 | 10 | 0 |
| 9 | BI | 1022 | 0 | 1070 | 11 | 0 |
| 10 | AJ | 796 | 0 | 836 | 10 | 0 |
| 10 | BJ | 787 | 0 | 828 | 8 | 0 |
| 11 | AK | 877 | 0 | 887 | 11 | 0 |
| 11 | BK | 877 | 0 | 887 | 13 | 0 |
| 12 | AL | 957 | 0 | 1017 | 6 | 0 |
| 12 | BL | 957 | 0 | 1017 | 8 | 0 |
| 13 | AM | 884 | 0 | 941 | 10 | 0 |
| 13 | BM | 884 | 0 | 941 | 15 | 0 |
| 14 | AN | 805 | 0 | 844 | 6 | 0 |
| 14 | BN | 805 | 0 | 844 | 5 | 0 |
| 15 | AO | 714 | 0 | 734 | 0 | 0 |
| 15 | BO | 714 | 0 | 734 | 1 | 0 |
| 16 | AP | 649 | 0 | 666 | 6 | 0 |
| 16 | BP | 649 | 0 | 666 | 6 | 0 |
| 17 | AQ | 649 | 0 | 691 | 4 | 0 |
| 17 | BQ | 649 | 0 | 691 | 11 | 0 |
| 18 | AR | 456 | 0 | 478 | 2 | 0 |
| 18 | BR | 456 | 0 | 478 | 3 | 0 |
| 19 | AS | 638 | 0 | 665 | 4 | 0 |
| 19 | BS | 638 | 0 | 665 | 6 | 0 |
| 20 | AT | 670 | 0 | 719 | 1 | 0 |
| 20 | BT | 665 | 0 | 714 | 6 | 0 |
| 21 | AU | 465 | 0 | 491 | 3 | 0 |
| 21 | BU | 465 | 0 | 491 | 3 | 0 |
| 22 | C1 | 444 | 0 | 458 | 4 | 0 |
| 22 | D1 | 444 | 0 | 458 | 10 | 0 |
| 23 | C2 | 409 | 0 | 440 | 7 | 0 |
| 23 | D2 | 414 | 0 | 442 | 5 | 0 |
| 24 | C3 | 377 | 0 | 418 | 4 | 0 |
| 24 | D3 | 377 | 0 | 418 | 2 | 0 |
| 25 | C4 | 504 | 0 | 572 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25 | D4 | 504 | 0 | 572 | 2 | 0 |
| 26 | C5 | 302 | 0 | 340 | 9 | 0 |
| 26 | D5 | 302 | 0 | 340 | 3 | 0 |
| 27 | C0 | 449 | 0 | 488 | 3 | 0 |
| 27 | D0 | 463 | 0 | 504 | 0 | 0 |
| 28 | CB | 2529 | 0 | 1281 | 7 | 0 |
| 28 | DB | 2569 | 0 | 1301 | 2 | 0 |
| 29 | CC | 2082 | 0 | 2154 | 20 | 0 |
| 29 | DC | 2082 | 0 | 2154 | 10 | 0 |
| 30 | CD | 1565 | 0 | 1616 | 12 | 0 |
| 31 | CA | 62229 | 0 | 31319 | 205 | 0 |
| 32 | DD | 1576 | 0 | 1627 | 11 | 0 |
| 33 | CE | 1552 | 0 | 1619 | 13 | 0 |
| 33 | DE | 1551 | 0 | 1619 | 10 | 0 |
| 34 | CF | 1410 | 0 | 1444 | 18 | 0 |
| 34 | DF | 1410 | 0 | 1444 | 13 | 0 |
| 35 | CG | 1323 | 0 | 1371 | 7 | 0 |
| 35 | DG | 1323 | 0 | 1371 | 6 | 0 |
| 36 | CH | 1110 | 0 | 1148 | 10 | 0 |
| 36 | DH | 1110 | 0 | 1148 | 7 | 0 |
| 37 | CJ | 979 | 0 | 1028 | 7 | 0 |
| 37 | DJ | 979 | 0 | 1028 | 5 | 0 |
| 38 | CK | 1129 | 0 | 1162 | 6 | 0 |
| 38 | DK | 1129 | 0 | 1162 | 6 | 0 |
| 39 | CL | 938 | 0 | 1012 | 8 | 0 |
| 39 | DL | 946 | 0 | 1023 | 7 | 0 |
| 40 | CM | 1053 | 0 | 1129 | 15 | 0 |
| 40 | DM | 1053 | 0 | 1129 | 7 | 0 |
| 41 | CN | 1075 | 0 | 1154 | 8 | 0 |
| 41 | DN | 1092 | 0 | 1177 | 8 | 0 |
| 42 | CO | 960 | 0 | 1000 | 7 | 0 |
| 42 | DO | 993 | 0 | 1034 | 6 | 0 |
| 43 | CP | 892 | 0 | 923 | 6 | 0 |
| 43 | DP | 900 | 0 | 935 | 6 | 0 |
| 44 | CQ | 917 | 0 | 962 | 4 | 0 |
| 44 | DQ | 917 | 0 | 962 | 7 | 0 |
| 45 | CR | 947 | 0 | 1019 | 11 | 0 |
| 45 | DR | 947 | 0 | 1019 | 13 | 0 |
| 46 | CS | 816 | 0 | 839 | 8 | 0 |
| 46 | DS | 816 | 0 | 839 | 4 | 0 |
| 47 | CT | 857 | 0 | 922 | 12 | 0 |
| 47 | DT | 857 | 0 | 922 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48 | CU | 739 | 0 | 807 | 6 | 0 |
| 48 | DU | 738 | 0 | 807 | 4 | 0 |
| 49 | CV | 779 | 0 | 831 | 6 | 0 |
| 49 | DV | 779 | 0 | 831 | 6 | 0 |
| 50 | CW | 753 | 0 | 780 | 7 | 0 |
| 50 | DW | 753 | 0 | 780 | 7 | 0 |
| 51 | CX | 569 | 0 | 581 | 4 | 0 |
| 51 | DX | 591 | 0 | 606 | 4 | 0 |
| 52 | CY | 625 | 0 | 652 | 4 | 0 |
| 52 | DY | 625 | 0 | 652 | 3 | 0 |
| 53 | CZ | 501 | 0 | 531 | 1 | 0 |
| 53 | DZ | 501 | 0 | 531 | 2 | 0 |
| 54 | DI | 1023 | 0 | 1052 | 20 | 0 |
| 55 | DA | 62423 | 0 | 31412 | 164 | 0 |
| 56 | AA | 72 | 0 | 0 | 0 | 0 |
| 56 | BA | 45 | 0 | 0 | 0 | 0 |
| 56 | CA | 156 | 0 | 0 | 0 | 0 |
| 56 | CB | 3 | 0 | 0 | 0 | 0 |
| 56 | DA | 184 | 0 | 0 | 0 | 0 |
| 56 | DB | 9 | 0 | 0 | 0 | 0 |
| 56 | DD | 1 | 0 | 0 | 0 | 0 |
| 56 | DM | 1 | 0 | 0 | 0 | 0 |
| 56 | DR | 1 | 0 | 0 | 0 | 0 |
| 57 | AA | 13 | 0 | 18 | 1 | 0 |
| 57 | BA | 13 | 0 | 18 | 1 | 0 |
| 57 | DA | 26 | 0 | 36 | 0 | 0 |
| 57 | DQ | 13 | 0 | 18 | 0 | 0 |
| 57 | DR | 13 | 0 | 18 | 4 | 0 |
| 57 | DS | 13 | 0 | 18 | 1 | 0 |
| 58 | AA | 16 | 0 | 28 | 0 | 0 |
| 58 | DA | 40 | 0 | 70 | 2 | 0 |
| 58 | DE | 16 | 0 | 28 | 0 | 0 |
| 58 | DK | 8 | 0 | 14 | 0 | 0 |
| 58 | DN | 8 | 0 | 14 | 1 | 0 |
| 58 | DS | 8 | 0 | 14 | 0 | 0 |
| 58 | DT | 16 | 0 | 28 | 0 | 0 |
| 59 | AA | 24 | 0 | 48 | 0 | 0 |
| 59 | DA | 72 | 0 | 144 | 3 | 0 |
| 60 | AA | 42 | 0 | 39 | 2 | 0 |
| 60 | BA | 42 | 0 | 38 | 0 | 0 |
| 61 | AB | 1 | 0 | 0 | 0 | 0 |
| 61 | C5 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61 | D5 | 1 | 0 | 0 | 0 | 0 |
| 62 | AL | 7 | 0 | 10 | 0 | 0 |
| 62 | D1 | 7 | 0 | 10 | 1 | 0 |
| 62 | D3 | 7 | 0 | 10 | 0 | 0 |
| 62 | DA | 35 | 0 | 50 | 0 | 0 |
| 62 | DL | 7 | 0 | 10 | 0 | 0 |
| 62 | DP | 7 | 0 | 10 | 0 | 0 |
| 62 | DQ | 7 | 0 | 10 | 0 | 0 |
| 63 | D1 | 4 | 0 | 6 | 0 | 0 |
| 63 | DA | 28 | 0 | 42 | 1 | 0 |
| 63 | DB | 16 | 0 | 24 | 0 | 0 |
| 64 | D1 | 10 | 0 | 14 | 2 | 0 |
| 64 | D3 | 10 | 0 | 14 | 0 | 0 |
| 64 | DA | 50 | 0 | 70 | 5 | 0 |
| 64 | DS | 10 | 0 | 14 | 1 | 0 |
| 64 | DU | 10 | 0 | 14 | 1 | 0 |
| 65 | DA | 40 | 0 | 76 | 2 | 0 |
| 66 | DA | 32 | 0 | 44 | 3 | 0 |
| 67 | DA | 12 | 0 | 9 | 0 | 0 |
| 68 | DA | 11 | 0 | 5 | 0 | 0 |
| 69 | DA | 8 | 0 | 12 | 1 | 0 |
| 70 | AA | 500 | 0 | 0 | 0 | 0 |
| 70 | AC | 5 | 0 | 0 | 0 | 0 |
| 70 | AD | 2 | 0 | 0 | 0 | 0 |
| 70 | AE | 4 | 0 | 0 | 0 | 0 |
| 70 | AF | 1 | 0 | 0 | 0 | 0 |
| 70 | AG | 1 | 0 | 0 | 0 | 0 |
| 70 | AH | 1 | 0 | 0 | 0 | 0 |
| 70 | AJ | 2 | 0 | 0 | 0 | 0 |
| 70 | AK | 6 | 0 | 0 | 0 | 0 |
| 70 | AL | 10 | 0 | 0 | 0 | 0 |
| 70 | AM | 4 | 0 | 0 | 1 | 0 |
| 70 | AN | 7 | 0 | 0 | 1 | 0 |
| 70 | AO | 2 | 0 | 0 | 0 | 0 |
| 70 | AP | 2 | 0 | 0 | 0 | 0 |
| 70 | AR | 1 | 0 | 0 | 0 | 0 |
| 70 | AT | 3 | 0 | 0 | 0 | 0 |
| 70 | AU | 2 | 0 | 0 | 0 | 0 |
| 70 | BA | 288 | 0 | 0 | 1 | 0 |
| 70 | BD | 12 | 0 | 0 | 0 | 0 |
| 70 | BE | 1 | 0 | 0 | 0 | 0 |
| 70 | BF | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 70 | BK | 2 | 0 | 0 | 0 | 0 |
| 70 | BL | 2 | 0 | 0 | 0 | 0 |
| 70 | BN | 2 | 0 | 0 | 0 | 0 |
| 70 | BO | 1 | 0 | 0 | 0 | 0 |
| 70 | BP | 3 | 0 | 0 | 0 | 0 |
| 70 | BT | 4 | 0 | 0 | 0 | 0 |
| 70 | BU | 1 | 0 | 0 | 0 | 0 |
| 70 | C3 | 3 | 0 | 0 | 0 | 0 |
| 70 | C4 | 1 | 0 | 0 | 0 | 0 |
| 70 | CA | 692 | 0 | 0 | 2 | 0 |
| 70 | CB | 13 | 0 | 0 | 0 | 0 |
| 70 | CC | 12 | 0 | 0 | 0 | 0 |
| 70 | CD | 6 | 0 | 0 | 0 | 0 |
| 70 | CE | 4 | 0 | 0 | 0 | 0 |
| 70 | CL | 1 | 0 | 0 | 0 | 0 |
| 70 | CM | 4 | 0 | 0 | 0 | 0 |
| 70 | CO | 1 | 0 | 0 | 0 | 0 |
| 70 | CU | 3 | 0 | 0 | 0 | 0 |
| 70 | CV | 1 | 0 | 0 | 0 | 0 |
| 70 | CW | 1 | 0 | 0 | 0 | 0 |
| 70 | CY | 1 | 0 | 0 | 0 | 0 |
| 70 | D0 | 21 | 0 | 0 | 0 | 0 |
| 70 | D1 | 45 | 0 | 0 | 0 | 0 |
| 70 | D2 | 7 | 0 | 0 | 0 | 0 |
| 70 | D3 | 23 | 0 | 0 | 0 | 0 |
| 70 | D4 | 39 | 0 | 0 | 0 | 0 |
| 70 | D5 | 12 | 0 | 0 | 0 | 0 |
| 70 | DA | 4829 | 0 | 0 | 13 | 0 |
| 70 | DB | 213 | 0 | 0 | 0 | 0 |
| 70 | DC | 104 | 0 | 0 | 0 | 0 |
| 70 | DD | 92 | 0 | 0 | 2 | 0 |
| 70 | DE | 60 | 0 | 0 | 2 | 0 |
| 70 | DF | 15 | 0 | 0 | 0 | 0 |
| 70 | DG | 6 | 0 | 0 | 0 | 0 |
| 70 | DH | 2 | 0 | 0 | 0 | 0 |
| 70 | DK | 64 | 0 | 0 | 2 | 0 |
| 70 | DL | 51 | 0 | 0 | 0 | 0 |
| 70 | DM | 64 | 0 | 0 | 0 | 0 |
| 70 | DN | 73 | 0 | 0 | 0 | 0 |
| 70 | DO | 46 | 0 | 0 | 0 | 0 |
| 70 | DP | 40 | 0 | 0 | 0 | 0 |
| 70 | DQ | 32 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 70 | DR | 63 | 0 | 0 | 1 | 0 |
| 70 | DS | 44 | 0 | 0 | 0 | 0 |
| 70 | DT | 69 | 0 | 0 | 1 | 0 |
| 70 | DU | 21 | 0 | 0 | 0 | 0 |
| 70 | DV | 20 | 0 | 0 | 0 | 0 |
| 70 | DW | 31 | 0 | 0 | 0 | 0 |
| 70 | DX | 26 | 0 | 0 | 0 | 0 |
| 70 | DY | 11 | 0 | 0 | 0 | 0 |
| 70 | DZ | 7 | 0 | 0 | 1 | 0 |
| All | All | 295207 | 0 | 194493 | 1128 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 1128 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:CS:14:VAL:HG21 | 46:CS:98:ILE:HG13 | 1.26 | 1.10 |
| 31:CA:1936:A:H2 | 31:CA:1943:U:H3 | 1.01 | 0.98 |
| 2:BB:20:THR:HA | 2:BB:39:HIS:CE1 | 1.98 | 0.97 |
| 1:BA:1052:G:H22 | 1:BA:1206:G:H1 | 0.98 | 0.94 |
| 55:DA:2796:U:H3 | 55:DA:2799:A:H61 | 1.20 | 0.88 |

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 X-ray entries followed by that with respect to entries of similar resolution.

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 | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 2 | AB | 222/224 (99%) | 207 (93%) | 11 (5%) | 4 (2%) | 8 | 34 |
| 2 | BB | 222/224 (99%) | 207 (93%) | 11 (5%) | 4 (2%) | 8 | 34 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | AC | 204/206 (99%) | 194 (95%) | 9 (4%) | 1 (0%) | 29 | 64 |
| 3 | BC | 204/206 (99%) | 195 (96%) | 7 (3%) | 2 (1%) | 15 | 49 |
| 4 | AD | 203/205 (99%) | 197 (97%) | 6 (3%) | 0 | 100 | 100 |
| 4 | BD | 203/205 (99%) | 197 (97%) | 6 (3%) | 0 | 100 | 100 |
| 5 | AE | 153/155 (99%) | 144 (94%) | 7 (5%) | 2 (1%) | 12 | 42 |
| 5 | BE | 148/155 (96%) | 131 (88%) | 14 (10%) | 3 (2%) | 7 | 31 |
| 6 | AF | 104/106 (98%) | 100 (96%) | 4 (4%) | 0 | 100 | 100 |
| 6 | BF | 98/106 (92%) | 91 (93%) | 5 (5%) | 2 (2%) | 7 | 31 |
| 7 | AG | 149/151 (99%) | 135 (91%) | 13 (9%) | 1 (1%) | 22 | 57 |
| 7 | BG | 149/151 (99%) | 137 (92%) | 12 (8%) | 0 | 100 | 100 |
| 8 | AH | 127/129 (98%) | 119 (94%) | 7 (6%) | 1 (1%) | 19 | 54 |
| 8 | BH | 127/129 (98%) | 118 (93%) | 7 (6%) | 2 (2%) | 9 | 37 |
| 9 | AI | 125/127 (98%) | 110 (88%) | 15 (12%) | 0 | 100 | 100 |
| 9 | BI | 125/127 (98%) | 110 (88%) | 15 (12%) | 0 | 100 | 100 |
| 10 | AJ | 97/99 (98%) | 89 (92%) | 7 (7%) | 1 (1%) | 15 | 49 |
| 10 | BJ | 96/99 (97%) | 77 (80%) | 13 (14%) | 6 (6%) | 1 | 8 |
| 11 | AK | 115/117 (98%) | 105 (91%) | 9 (8%) | 1 (1%) | 17 | 52 |
| 11 | BK | 115/117 (98%) | 104 (90%) | 10 (9%) | 1 (1%) | 17 | 52 |
| 12 | AL | 120/123 (98%) | 115 (96%) | 5 (4%) | 0 | 100 | 100 |
| 12 | BL | 120/123 (98%) | 111 (92%) | 8 (7%) | 1 (1%) | 19 | 54 |
| 13 | AM | 112/114 (98%) | 102 (91%) | 7 (6%) | 3 (3%) | 5 | 25 |
| 13 | BM | 112/114 (98%) | 101 (90%) | 6 (5%) | 5 (4%) | 2 | 15 |
| 14 | AN | 98/100 (98%) | 87 (89%) | 9 (9%) | 2 (2%) | 7 | 31 |
| 14 | BN | 98/100 (98%) | 87 (89%) | 10 (10%) | 1 (1%) | 15 | 49 |
| 15 | AO | 86/88 (98%) | 84 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | BO | 86/88 (98%) | 83 (96%) | 2 (2%) | 1 (1%) | 13 | 44 |
| 16 | AP | 80/82 (98%) | 73 (91%) | 5 (6%) | 2 (2%) | 5 | 27 |
| 16 | BP | 80/82 (98%) | 68 (85%) | 10 (12%) | 2 (2%) | 5 | 27 |
| 17 | AQ | 78/80 (98%) | 71 (91%) | 6 (8%) | 1 (1%) | 12 | 42 |
| 17 | BQ | 78/80 (98%) | 67 (86%) | 7 (9%) | 4 (5%) | 2 | 13 |
| 18 | AR | 53/55 (96%) | 50 (94%) | 3 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 18 | BR | 53/55 (96%) | 50 (94%) | 3 (6%) | 0 | 100 | 100 |
| 19 | AS | 77/79 (98%) | 67 (87%) | 10 (13%) | 0 | 100 | 100 |
| 19 | BS | 77/79 (98%) | 66 (86%) | 10 (13%) | 1 (1%) | 12 | 42 |
| 20 | AT | 84/86 (98%) | 82 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | BT | 83/86 (96%) | 79 (95%) | 3 (4%) | 1 (1%) | 13 | 44 |
| 21 | AU | 54/56 (96%) | 51 (94%) | 3 (6%) | 0 | 100 | 100 |
| 21 | BU | 54/56 (96%) | 51 (94%) | 3 (6%) | 0 | 100 | 100 |
| 22 | C1 | 54/56 (96%) | 47 (87%) | 4 (7%) | 3 (6%) | 2 | 11 |
| 22 | D1 | 54/56 (96%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 23 | C2 | 48/51 (94%) | 43 (90%) | 3 (6%) | 2 (4%) | 3 | 16 |
| 23 | D2 | 49/51 (96%) | 47 (96%) | 2 (4%) | 0 | 100 | 100 |
| 24 | C3 | 44/46 (96%) | 42 (96%) | 1 (2%) | 1 (2%) | 6 | 28 |
| 24 | D3 | 44/46 (96%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | C4 | 62/64 (97%) | 58 (94%) | 4 (6%) | 0 | 100 | 100 |
| 25 | D4 | 62/64 (97%) | 58 (94%) | 4 (6%) | 0 | 100 | 100 |
| 26 | C5 | 36/38 (95%) | 34 (94%) | 1 (3%) | 1 (3%) | 5 | 25 |
| 26 | D5 | 36/38 (95%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 27 | C0 | 56/58 (97%) | 51 (91%) | 3 (5%) | 2 (4%) | 3 | 20 |
| 27 | D0 | 57/58 (98%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 29 | CC | 269/272 (99%) | 249 (93%) | 15 (6%) | 5 (2%) | 8 | 33 |
| 29 | DC | 269/272 (99%) | 251 (93%) | 16 (6%) | 2 (1%) | 22 | 57 |
| 30 | CD | 207/209 (99%) | 199 (96%) | 8 (4%) | 0 | 100 | 100 |
| 32 | DD | 206/209 (99%) | 199 (97%) | 7 (3%) | 0 | 100 | 100 |
| 33 | CE | 199/201 (99%) | 189 (95%) | 7 (4%) | 3 (2%) | 10 | 39 |
| 33 | DE | 199/201 (99%) | 191 (96%) | 7 (4%) | 1 (0%) | 29 | 64 |
| 34 | CF | 175/178 (98%) | 166 (95%) | 9 (5%) | 0 | 100 | 100 |
| 34 | DF | 175/178 (98%) | 166 (95%) | 9 (5%) | 0 | 100 | 100 |
| 35 | CG | 174/176 (99%) | 162 (93%) | 7 (4%) | 5 (3%) | 4 | 24 |
| 35 | DG | 174/176 (99%) | 165 (95%) | 7 (4%) | 2 (1%) | 14 | 46 |
| 36 | CH | 147/149 (99%) | 130 (88%) | 11 (8%) | 6 (4%) | 3 | 16 |
| 36 | DH | 147/149 (99%) | 133 (90%) | 11 (8%) | 3 (2%) | 7 | 31 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 37 | CJ | 132/135 (98%) | 125 (95%) | 3 (2%) | 4 (3%) | 4 | 23 |
| 37 | DJ | 132/135 (98%) | 125 (95%) | 3 (2%) | 4 (3%) | 4 | 23 |
| 38 | CK | 140/142 (99%) | 135 (96%) | 2 (1%) | 3 (2%) | 7 | 30 |
| 38 | DK | 140/142 (99%) | 136 (97%) | 2 (1%) | 2 (1%) | 11 | 40 |
| 39 | CL | 120/123 (98%) | 114 (95%) | 4 (3%) | 2 (2%) | 9 | 36 |
| 39 | DL | 121/123 (98%) | 116 (96%) | 4 (3%) | 1 (1%) | 19 | 54 |
| 40 | CM | 142/144 (99%) | 132 (93%) | 7 (5%) | 3 (2%) | 7 | 30 |
| 40 | DM | 142/144 (99%) | 136 (96%) | 5 (4%) | 1 (1%) | 22 | 57 |
| 41 | CN | 133/136 (98%) | 125 (94%) | 7 (5%) | 1 (1%) | 19 | 54 |
| 41 | DN | 134/136 (98%) | 130 (97%) | 4 (3%) | 0 | 100 | 100 |
| 42 | CO | 118/125 (94%) | 110 (93%) | 6 (5%) | 2 (2%) | 9 | 36 |
| 42 | DO | 123/125 (98%) | 116 (94%) | 7 (6%) | 0 | 100 | 100 |
| 43 | CP | 114/117 (97%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 43 | DP | 115/117 (98%) | 114 (99%) | 1 (1%) | 0 | 100 | 100 |
| 44 | CQ | 112/114 (98%) | 107 (96%) | 4 (4%) | 1 (1%) | 17 | 52 |
| 44 | DQ | 112/114 (98%) | 107 (96%) | 4 (4%) | 1 (1%) | 17 | 52 |
| 45 | CR | 115/117 (98%) | 110 (96%) | 4 (4%) | 1 (1%) | 17 | 52 |
| 45 | DR | 115/117 (98%) | 110 (96%) | 4 (4%) | 1 (1%) | 17 | 52 |
| 46 | CS | 101/103 (98%) | 91 (90%) | 7 (7%) | 3 (3%) | 4 | 23 |
| 46 | DS | 101/103 (98%) | 94 (93%) | 6 (6%) | 1 (1%) | 15 | 49 |
| 47 | CT | 108/110 (98%) | 99 (92%) | 9 (8%) | 0 | 100 | 100 |
| 47 | DT | 108/110 (98%) | 103 (95%) | 5 (5%) | 0 | 100 | 100 |
| 48 | CU | 91/93 (98%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 48 | DU | 91/93 (98%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 49 | CV | 100/103 (97%) | 90 (90%) | 6 (6%) | 4 (4%) | 3 | 17 |
| 49 | DV | 100/103 (97%) | 96 (96%) | 2 (2%) | 2 (2%) | 7 | 31 |
| 50 | CW | 92/94 (98%) | 89 (97%) | 3 (3%) | 0 | 100 | 100 |
| 50 | DW | 92/94 (98%) | 87 (95%) | 5 (5%) | 0 | 100 | 100 |
| 51 | CX | 73/83 (88%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 51 | DX | 75/83 (90%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 52 | CY | 75/77 (97%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 52 | DY | 75/77 (97%) | 73 (97%) | 2 (3%) | 0 | 100 | 100 |
| 53 | CZ | 60/62 (97%) | 58 (97%) | 1 (2%) | 1 (2%) | 9 | 36 |
| 53 | DZ | 60/62 (97%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | DI | 133/135 (98%) | 112 (84%) | 15 (11%) | 6 (4%) | 2 | 15 |
| All | All | 11407/11651 (98%) | 10682 (94%) | 590 (5%) | 135 (1%) | 13 | 44 |

5 of 135 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 126 | PHE |
| 3 | AC | 156 | ARG |
| 13 | AM | 5 | ALA |
| 17 | AQ | 82 | ALA |
| 22 | C1 | 25 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | AB | 186/186 (100%) | 172 (92%) | 14 (8%) | 13 | 42 |
| 2 | BB | 186/186 (100%) | 171 (92%) | 15 (8%) | 11 | 39 |
| 3 | AC | 170/170 (100%) | 159 (94%) | 11 (6%) | 17 | 47 |
| 3 | BC | 170/170 (100%) | 157 (92%) | 13 (8%) | 13 | 41 |
| 4 | AD | 172/172 (100%) | 165 (96%) | 7 (4%) | 30 | 64 |
| 4 | BD | 172/172 (100%) | 165 (96%) | 7 (4%) | 30 | 64 |
| 5 | AE | 118/118 (100%) | 105 (89%) | 13 (11%) | 6 | 25 |
| 5 | BE | 113/118 (96%) | 92 (81%) | 21 (19%) | 1 | 7 |
| 6 | AF | 92/92 (100%) | 84 (91%) | 8 (9%) | 10 | 36 |
| 6 | BF | 87/92 (95%) | 76 (87%) | 11 (13%) | 4 | 18 |
| 7 | AG | 124/124 (100%) | 112 (90%) | 12 (10%) | 8 | 30 |
| 7 | BG | 124/124 (100%) | 109 (88%) | 15 (12%) | 5 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 8 | AH | 104/104 (100%) | 90 (86%) | 14 (14%) | 4 | 16 |
| 8 | BH | 104/104 (100%) | 91 (88%) | 13 (12%) | 4 | 18 |
| 9 | AI | 105/105 (100%) | 100 (95%) | 5 (5%) | 25 | 58 |
| 9 | BI | 105/105 (100%) | 100 (95%) | 5 (5%) | 25 | 58 |
| 10 | AJ | 87/87 (100%) | 80 (92%) | 7 (8%) | 12 | 40 |
| 10 | BJ | 86/87 (99%) | 76 (88%) | 10 (12%) | 5 | 22 |
| 11 | AK | 90/90 (100%) | 90 (100%) | 0 | 100 | 100 |
| 11 | BK | 90/90 (100%) | 84 (93%) | 6 (7%) | 16 | 46 |
| 12 | AL | 102/102 (100%) | 96 (94%) | 6 (6%) | 19 | 50 |
| 12 | BL | 102/102 (100%) | 95 (93%) | 7 (7%) | 15 | 45 |
| 13 | AM | 92/92 (100%) | 83 (90%) | 9 (10%) | 8 | 29 |
| 13 | BM | 92/92 (100%) | 85 (92%) | 7 (8%) | 13 | 41 |
| 14 | AN | 83/83 (100%) | 82 (99%) | 1 (1%) | 71 | 88 |
| 14 | BN | 83/83 (100%) | 81 (98%) | 2 (2%) | 49 | 76 |
| 15 | AO | 76/76 (100%) | 71 (93%) | 5 (7%) | 16 | 47 |
| 15 | BO | 76/76 (100%) | 68 (90%) | 8 (10%) | 7 | 26 |
| 16 | AP | 65/65 (100%) | 64 (98%) | 1 (2%) | 65 | 85 |
| 16 | BP | 65/65 (100%) | 60 (92%) | 5 (8%) | 13 | 41 |
| 17 | AQ | 74/74 (100%) | 65 (88%) | 9 (12%) | 5 | 19 |
| 17 | BQ | 74/74 (100%) | 63 (85%) | 11 (15%) | 3 | 13 |
| 18 | AR | 48/48 (100%) | 45 (94%) | 3 (6%) | 18 | 48 |
| 18 | BR | 48/48 (100%) | 47 (98%) | 1 (2%) | 53 | 79 |
| 19 | AS | 70/70 (100%) | 61 (87%) | 9 (13%) | 4 | 18 |
| 19 | BS | 70/70 (100%) | 63 (90%) | 7 (10%) | 7 | 28 |
| 20 | AT | 65/65 (100%) | 59 (91%) | 6 (9%) | 9 | 33 |
| 20 | BT | 65/65 (100%) | 56 (86%) | 9 (14%) | 3 | 16 |
| 21 | AU | 48/48 (100%) | 45 (94%) | 3 (6%) | 18 | 48 |
| 21 | BU | 48/48 (100%) | 46 (96%) | 2 (4%) | 30 | 62 |
| 22 | C1 | 47/47 (100%) | 45 (96%) | 2 (4%) | 29 | 62 |
| 22 | D1 | 47/47 (100%) | 46 (98%) | 1 (2%) | 53 | 79 |
| 23 | C2 | 45/46 (98%) | 42 (93%) | 3 (7%) | 16 | 46 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 23 | D2 | 45/46 (98%) | 40 (89%) | 5 (11%) | 6 | 24 |
| 24 | C3 | 38/38 (100%) | 37 (97%) | 1 (3%) | 46 | 74 |
| 24 | D3 | 38/38 (100%) | 37 (97%) | 1 (3%) | 46 | 74 |
| 25 | C4 | 51/51 (100%) | 48 (94%) | 3 (6%) | 19 | 50 |
| 25 | D4 | 51/51 (100%) | 48 (94%) | 3 (6%) | 19 | 50 |
| 26 | C5 | 34/34 (100%) | 32 (94%) | 2 (6%) | 19 | 50 |
| 26 | D5 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 27 | C0 | 48/48 (100%) | 40 (83%) | 8 (17%) | 2 | 9 |
| 27 | D0 | 49/48 (102%) | 45 (92%) | 4 (8%) | 11 | 38 |
| 29 | CC | 216/217 (100%) | 203 (94%) | 13 (6%) | 19 | 49 |
| 29 | DC | 216/217 (100%) | 208 (96%) | 8 (4%) | 34 | 66 |
| 30 | CD | 164/164 (100%) | 156 (95%) | 8 (5%) | 25 | 57 |
| 32 | DD | 163/163 (100%) | 157 (96%) | 6 (4%) | 34 | 66 |
| 33 | CE | 165/165 (100%) | 150 (91%) | 15 (9%) | 9 | 33 |
| 33 | DE | 165/165 (100%) | 160 (97%) | 5 (3%) | 41 | 71 |
| 34 | CF | 148/149 (99%) | 133 (90%) | 15 (10%) | 7 | 28 |
| 34 | DF | 148/149 (99%) | 137 (93%) | 11 (7%) | 13 | 42 |
| 35 | CG | 137/137 (100%) | 132 (96%) | 5 (4%) | 35 | 67 |
| 35 | DG | 137/137 (100%) | 133 (97%) | 4 (3%) | 42 | 72 |
| 36 | CH | 114/114 (100%) | 101 (89%) | 13 (11%) | 5 | 23 |
| 36 | DH | 114/114 (100%) | 104 (91%) | 10 (9%) | 10 | 36 |
| 37 | CJ | 104/105 (99%) | 99 (95%) | 5 (5%) | 25 | 58 |
| 37 | DJ | 104/105 (99%) | 99 (95%) | 5 (5%) | 25 | 58 |
| 38 | CK | 116/116 (100%) | 112 (97%) | 4 (3%) | 37 | 69 |
| 38 | DK | 116/116 (100%) | 114 (98%) | 2 (2%) | 60 | 83 |
| 39 | CL | 103/104 (99%) | 95 (92%) | 8 (8%) | 12 | 40 |
| 39 | DL | 104/104 (100%) | 97 (93%) | 7 (7%) | 16 | 46 |
| 40 | CM | 103/103 (100%) | 95 (92%) | 8 (8%) | 12 | 40 |
| 40 | DM | 103/103 (100%) | 98 (95%) | 5 (5%) | 25 | 57 |
| 41 | CN | 108/108 (100%) | 103 (95%) | 5 (5%) | 27 | 59 |
| 41 | DN | 109/108 (101%) | 107 (98%) | 2 (2%) | 59 | 82 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 42 | CO | 100/102 (98%) | 92 (92%) | 8 (8%) | 12 | 40 |
| 42 | DO | 102/102 (100%) | 98 (96%) | 4 (4%) | 32 | 65 |
| 43 | CP | 86/87 (99%) | 80 (93%) | 6 (7%) | 15 | 45 |
| 43 | DP | 87/87 (100%) | 84 (97%) | 3 (3%) | 37 | 69 |
| 44 | CQ | 99/99 (100%) | 92 (93%) | 7 (7%) | 14 | 44 |
| 44 | DQ | 99/99 (100%) | 94 (95%) | 5 (5%) | 24 | 56 |
| 45 | CR | 89/89 (100%) | 84 (94%) | 5 (6%) | 21 | 52 |
| 45 | DR | 89/89 (100%) | 86 (97%) | 3 (3%) | 37 | 69 |
| 46 | CS | 84/84 (100%) | 78 (93%) | 6 (7%) | 14 | 44 |
| 46 | DS | 84/84 (100%) | 83 (99%) | 1 (1%) | 71 | 88 |
| 47 | CT | 93/93 (100%) | 90 (97%) | 3 (3%) | 39 | 69 |
| 47 | DT | 93/93 (100%) | 90 (97%) | 3 (3%) | 39 | 69 |
| 48 | CU | 80/80 (100%) | 71 (89%) | 9 (11%) | 6 | 23 |
| 48 | DU | 80/80 (100%) | 78 (98%) | 2 (2%) | 47 | 75 |
| 49 | CV | 83/84 (99%) | 77 (93%) | 6 (7%) | 14 | 44 |
| 49 | DV | 83/84 (99%) | 79 (95%) | 4 (5%) | 25 | 58 |
| 50 | CW | 78/78 (100%) | 74 (95%) | 4 (5%) | 24 | 56 |
| 50 | DW | 78/78 (100%) | 75 (96%) | 3 (4%) | 33 | 66 |
| 51 | CX | 56/62 (90%) | 54 (96%) | 2 (4%) | 35 | 67 |
| 51 | DX | 58/62 (94%) | 54 (93%) | 4 (7%) | 15 | 45 |
| 52 | CY | 67/67 (100%) | 63 (94%) | 4 (6%) | 19 | 49 |
| 52 | DY | 67/67 (100%) | 65 (97%) | 2 (3%) | 41 | 71 |
| 53 | CZ | 54/54 (100%) | 52 (96%) | 2 (4%) | 34 | 66 |
| 53 | DZ | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |
| 54 | DI | 103/103 (100%) | 97 (94%) | 6 (6%) | 20 | 51 |
| All | All | 9461/9494 (100%) | 8844 (94%) | 617 (6%) | 17 | 47 |

5 of 617 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | BL | 44 | LYS |
| 25 | D4 | 31 | HIS |
| 40 | DM | 2 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | BM | 16 | VAL |
| 17 | BQ | 38 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | BE | 70 | ASN |
| 16 | BP | 9 | HIS |
| 35 | DG | 116 | GLN |
| 7 | BG | 97 | ASN |
| 7 | AG | 142 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1530/1534 (99%) | 263 (17%) | 31 (2%) |
| 1 | BA | 1529/1534 (99%) | 264 (17%) | 36 (2%) |
| 28 | CB | 117/120 (97%) | 12 (10%) | 0 |
| 28 | DB | 119/120 (99%) | 10 (8%) | 0 |
| 31 | CA | 2892/2904 (99%) | 466 (16%) | 78 (2%) |
| 55 | DA | 2880/2904 (99%) | 404 (14%) | 62 (2%) |
| All | All | 9067/9116 (99%) | 1419 (15%) | 207 (2%) |

5 of 1419 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 4 | U |
| 1 | AA | 5 | U |
| 1 | AA | 6 | G |
| 1 | AA | 9 | G |
| 1 | AA | 22 | G |

5 of 207 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | CA | 973 | A |
| 31 | CA | 1536 | C |
| 55 | DA | 2146 | C |
| 31 | CA | 1046 | A |
| 31 | CA | 1288 | G |

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

75 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$ |
| 31 | 6MZ | CA | 1618 | 31 | 18,25,26 | 0.89 | 0 | 16,36,39 | 0.93 | 1 (6%) |
| 1 | UR3 | BA | 1498 | 1 | 14,22,23 | 1.30 | 1 (7%) | 15,32,35 | 0.40 | 0 |
| 31 | OMC | CA | 2498 | 31,56 | 15,22,23 | 0.98 | 1 (6%) | 17,31,34 | 1.20 | 1 (5%) |
| 31 | PSU | CA | 2605 | 31 | 17,21,22 | 1.30 | 2 (11%) | 20,30,33 | 5.31 | 4 (20%) |
| 55 | 5MU | DA | 1939 | 55 | 15,22,23 | 1.32 | 2 (13%) | 16,32,35 | 3.69 | 2 (12%) |
| 12 | D2T | BL | 89 | 12 | 4,9,10 | 0.49 | 0 | 3,11,13 | 1.11 | 0 |
| 55 | OMC | DA | 2498 | 55,56 | 15,22,23 | 0.99 | 1 (6%) | 17,31,34 | 1.19 | 1 (5%) |
| 1 | 2MG | BA | 1207 | 1 | 19,26,27 | 1.18 | 2 (10%) | 21,38,41 | 2.39 | 4 (19%) |
| 1 | MA6 | BA | 1519 | 1 | 19,26,27 | 0.88 | 0 | 18,38,41 | 1.03 | 1 (5%) |
| 1 | 5MC | BA | 1407 | 1 | 15,22,23 | 0.97 | 1 (6%) | 19,32,35 | 1.21 | 2 (10%) |
| 41 | 4D4 | DN | 81[B] | - | 9,11,12 | 1.76 | 2 (22%) | 8,13,15 | 2.46 | 2 (25%) |
| 31 | 6MZ | CA | 2030 | 31 | 18,25,26 | 0.86 | 0 | 16,36,39 | 0.78 | 1 (6%) |
| 55 | 5MC | DA | 1962 | 55 | 15,22,23 | 0.99 | 1 (6%) | 19,32,35 | 1.16 | 2 (10%) |
| 31 | 2MG | CA | 1835 | 31 | 19,26,27 | 1.17 | 1 (5%) | 21,38,41 | 2.24 | 4 (19%) |
| 41 | 4D4 | DN | 81[A] | - | 9,11,12 | 1.68 | 2 (22%) | 8,13,15 | 2.40 | 3 (37%) |
| 55 | OMU | DA | 2552 | 55 | 14,22,23 | 1.20 | 1 (7%) | 14,31,34 | 1.08 | 1 (7%) |
| 1 | 7MG | BA | 527 | 1 | 22,26,27 | 1.66 | 3 (13%) | 28,39,42 | 2.56 | 8 (28%) |
| 12 | D2T | AL | 89 | 12 | 4,9,10 | 0.52 | 0 | 3,11,13 | 1.08 | 0 |
| 1 | PSU | AA | 516 | 1,56 | 17,21,22 | 1.28 | 2 (11%) | 20,30,33 | 5.30 | 4 (20%) |
| 31 | PSU | CA | 1917 | 31 | 17,21,22 | 1.19 | 2 (11%) | 20,30,33 | 5.35 | 4 (20%) |
| 31 | OMG | CA | 2251 | 31 | 18,26,27 | 1.23 | 2 (11%) | 20,38,41 | 2.52 | 5 (25%) |
| 31 | 7MG | CA | 2069 | 31 | 22,26,27 | 1.69 | 4 (18%) | 28,39,42 | 2.36 | 8 (28%) |
| 55 | OMG | DA | 2251 | 55 | 18,26,27 | 1.04 | 1 (5%) | 20,38,41 | 2.42 | 5 (25%) |
| 1 | 5MC | BA | 967 | 1 | 15,22,23 | 0.83 | 0 | 19,32,35 | 1.17 | 2 (10%) |
| 1 | 2MG | AA | 966 | 1 | 19,26,27 | 1.40 | 2 (10%) | 21,38,41 | 2.39 | 3 (14%) |
| 1 | MA6 | AA | 1518 | 1 | 19,26,27 | 0.84 | 0 | 18,38,41 | 1.25 | 1 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 31 | OMU | CA | 2552 | 31 | 14,22,23 | 1.30 | 2 (14%) | 14,31,34 | 1.10 | 1 (7%) |
| 55 | PSU | DA | 2604 | 55 | 17,21,22 | 1.54 | 3 (17%) | 20,30,33 | 5.35 | 4 (20%) |
| 55 | 2MG | DA | 1835 | 55 | 19,26,27 | 1.06 | 1 (5%) | 21,38,41 | 2.33 | 4 (19%) |
| 31 | 5MC | CA | 1962 | 31 | 15,22,23 | 0.85 | 1 (6%) | 19,32,35 | 1.14 | 2 (10%) |
| 31 | 2MA | CA | 2503 | 31 | 17,25,26 | 0.94 | 0 | 19,37,40 | 2.24 | 3 (15%) |
| 55 | 5MU | DA | 747 | 55 | 15,22,23 | 1.22 | 1 (6%) | 16,32,35 | 3.65 | 1 (6%) |
| 31 | PSU | CA | 1911 | 31 | 17,21,22 | 1.21 | 2 (11%) | 20,30,33 | 5.28 | 4 (20%) |
| 55 | 7MG | DA | 2069 | 55 | 22,26,27 | 1.64 | 3 (13%) | 28,39,42 | 2.37 | 6 (21%) |
| 1 | MA6 | BA | 1518 | 1 | 19,26,27 | 0.80 | 0 | 18,38,41 | 1.26 | 1 (5%) |
| 55 | H2U | DA | 2449 | 55 | 18,21,22 | 0.48 | 0 | 21,30,33 | 0.67 | 1 (4%) |
| 55 | PSU | DA | 955 | 55 | 17,21,22 | 1.46 | 3 (17%) | 20,30,33 | 5.30 | 4 (20%) |
| 31 | 2MG | CA | 2445 | 31 | 19,26,27 | 1.30 | 2 (10%) | 21,38,41 | 2.38 | 4 (19%) |
| 31 | PSU | CA | 746 | 31,56 | 17,21,22 | 1.40 | 4 (23%) | 20,30,33 | 5.32 | 5 (25%) |
| 55 | 1MG | DA | 745 | 55 | 18,26,27 | 1.25 | 2 (11%) | 19,39,42 | 1.17 | 2 (10%) |
| 31 | PSU | CA | 955 | 31 | 17,21,22 | 1.19 | 2 (11%) | 20,30,33 | 5.31 | 4 (20%) |
| 31 | 5MU | CA | 747 | 31 | 15,22,23 | 1.18 | 1 (6%) | 16,32,35 | 3.68 | 2 (12%) |
| 1 | 5MC | AA | 967 | 1 | 15,22,23 | 0.84 | 0 | 19,32,35 | 1.16 | 2 (10%) |
| 1 | 7MG | AA | 527 | 1 | 22,26,27 | 1.68 | 3 (13%) | 28,39,42 | 2.63 | 8 (28%) |
| 55 | PSU | DA | 2605 | 55 | 17,21,22 | 1.24 | 2 (11%) | 20,30,33 | 5.36 | 5 (25%) |
| 1 | 4OC | AA | 1402 | 1 | 16,23,24 | 0.81 | 1 (6%) | 17,32,35 | 0.85 | 1 (5%) |
| 1 | 2MG | BA | 1516 | 1 | 19,26,27 | 1.36 | 2 (10%) | 21,38,41 | 2.30 | 4 (19%) |
| 31 | 5MU | CA | 1939 | 31 | 15,22,23 | 1.22 | 1 (6%) | 16,32,35 | 3.69 | 2 (12%) |
| 32 | MEQ | DD | 150[B] | 32 | 8,9,10 | 1.10 | 1 (12%) | 5,10,12 | 0.73 | 0 |
| 32 | MEQ | DD | 150[A] | 32 | 8,9,10 | 0.38 | 0 | 5,10,12 | 0.54 | 0 |
| 55 | 2MA | DA | 2503 | 55,56 | 17,25,26 | 0.91 | 0 | 19,37,40 | 2.06 | 3 (15%) |
| 55 | PSU | DA | 2504 | 55 | 17,21,22 | 1.26 | 2 (11%) | 20,30,33 | 5.30 | 4 (20%) |
| 1 | 2MG | BA | 966 | 1 | 19,26,27 | 1.21 | 2 (10%) | 21,38,41 | 2.43 | 4 (19%) |
| 55 | PSU | DA | 2457 | 55 | 17,21,22 | 1.34 | 2 (11%) | 20,30,33 | 5.30 | 4 (20%) |
| 55 | 6MZ | DA | 1618 | 55 | 18,25,26 | 0.73 | 0 | 16,36,39 | 2.09 | 2 (12%) |
| 1 | 2MG | AA | 1516 | 1 | 19,26,27 | 1.30 | 2 (10%) | 21,38,41 | 2.28 | 4 (19%) |
| 55 | 3TD | DA | 1915 | 55 | 17,22,23 | 1.32 | 3 (17%) | 19,32,35 | 1.54 | 2 (10%) |
| 31 | PSU | CA | 2580 | 31 | 17,21,22 | 1.30 | 3 (17%) | 20,30,33 | 5.34 | 4 (20%) |
| 1 | UR3 | AA | 1498 | 1 | 14,22,23 | 1.00 | 1 (7%) | 15,32,35 | 0.40 | 0 |
| 55 | 6MZ | DA | 2030 | 55 | 18,25,26 | 1.06 | 2 (11%) | 16,36,39 | 0.99 | 2 (12%) |
| 1 | PSU | BA | 516 | 1 | 17,21,22 | 1.27 | 2 (11%) | 20,30,33 | 5.31 | 4 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 55 | PSU | DA | 1917 | 55 | 17,21,22 | 1.23 | 3 (17%) | 20,30,33 | 5.30 | 4 (20%) |
| 31 | 1MG | CA | 745 | 31 | 18,26,27 | 1.24 | 1 (5%) | 19,39,42 | 1.24 | 2 (10%) |
| 55 | PSU | DA | 2580 | 55 | 17,21,22 | 1.47 | 3 (17%) | 20,30,33 | 5.29 | 4 (20%) |
| 31 | PSU | CA | 2504 | 31 | 17,21,22 | 1.24 | 3 (17%) | 20,30,33 | 5.30 | 4 (20%) |
| 55 | 2MG | DA | 2445 | 55 | 19,26,27 | 1.30 | 3 (15%) | 21,38,41 | 2.42 | 4 (19%) |
| 1 | 2MG | AA | 1207 | 1 | 19,26,27 | 1.08 | 1 (5%) | 21,38,41 | 2.37 | 4 (19%) |
| 1 | 5MC | AA | 1407 | 1 | 15,22,23 | 0.90 | 0 | 19,32,35 | 1.25 | 2 (10%) |
| 1 | 4OC | BA | 1402 | 1 | 16,23,24 | 0.77 | 0 | 17,32,35 | 0.83 | 1 (5%) |
| 31 | 3TD | CA | 1915 | 31 | 17,22,23 | 1.29 | 3 (17%) | 19,32,35 | 1.51 | 2 (10%) |
| 55 | PSU | DA | 1911 | 55 | 17,21,22 | 1.21 | 2 (11%) | 20,30,33 | 5.28 | 4 (20%) |
| 55 | PSU | DA | 746 | 55,56 | 17,21,22 | 1.65 | 5 (29%) | 20,30,33 | 5.32 | 5 (25%) |
| 1 | MA6 | AA | 1519 | 1 | 19,26,27 | 0.86 | 0 | 18,38,41 | 1.03 | 1 (5%) |
| 31 | PSU | CA | 2457 | 31 | 17,21,22 | 1.46 | 4 (23%) | 20,30,33 | 5.29 | 4 (20%) |
| 41 | 4D4 | CN | 81 | 41 | 9,11,12 | 2.20 | 2 (22%) | 8,13,15 | 2.33 | 2 (25%) |

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 |
|-----|------|-------|-------|-------|---------|------------|---------|
| 31 | 6MZ | CA | 1618 | 31 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | UR3 | BA | 1498 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 31 | OMC | CA | 2498 | 31,56 | - | 0/7/27/28 | 0/2/2/2 |
| 31 | PSU | CA | 2605 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MU | DA | 1939 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 12 | D2T | BL | 89 | 12 | - | 1/3/12/14 | - |
| 55 | OMC | DA | 2498 | 55,56 | - | 0/7/27/28 | 0/2/2/2 |
| 1 | 2MG | BA | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | MA6 | BA | 1519 | 1 | - | 3/7/29/30 | 0/3/3/3 |
| 1 | 5MC | BA | 1407 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 41 | 4D4 | DN | 81[B] | - | - | 3/11/12/14 | - |
| 31 | 6MZ | CA | 2030 | 31 | - | 2/5/27/28 | 0/3/3/3 |
| 55 | 5MC | DA | 1962 | 55 | - | 2/5/25/26 | 0/2/2/2 |
| 31 | 2MG | CA | 1835 | 31 | - | 1/5/27/28 | 0/3/3/3 |
| 41 | 4D4 | DN | 81[A] | - | - | 1/11/12/14 | - |
| 55 | OMU | DA | 2552 | 55 | - | 1/7/27/28 | 0/2/2/2 |
| 1 | 7MG | BA | 527 | 1 | - | 2/7/37/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|-------|---------|-----------|---------|
| 12 | D2T | AL | 89 | 12 | - | 1/3/12/14 | - |
| 1 | PSU | AA | 516 | 1,56 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | PSU | CA | 1917 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | OMG | CA | 2251 | 31 | - | 0/5/27/28 | 0/3/3/3 |
| 31 | 7MG | CA | 2069 | 31 | - | 1/7/37/38 | 0/3/3/3 |
| 55 | OMG | DA | 2251 | 55 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | 5MC | BA | 967 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 2MG | AA | 966 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | MA6 | AA | 1518 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 31 | OMU | CA | 2552 | 31 | - | 1/7/27/28 | 0/2/2/2 |
| 55 | PSU | DA | 2604 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 2MG | DA | 1835 | 55 | - | 2/5/27/28 | 0/3/3/3 |
| 31 | 5MC | CA | 1962 | 31 | - | 2/5/25/26 | 0/2/2/2 |
| 31 | 2MA | CA | 2503 | 31 | - | 2/3/25/26 | 0/3/3/3 |
| 55 | 5MU | DA | 747 | 55 | - | 1/5/25/26 | 0/2/2/2 |
| 31 | PSU | CA | 1911 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 7MG | DA | 2069 | 55 | - | 2/7/37/38 | 0/3/3/3 |
| 1 | MA6 | BA | 1518 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 55 | H2U | DA | 2449 | 55 | - | 0/7/38/39 | 0/2/2/2 |
| 55 | PSU | DA | 955 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | 2MG | CA | 2445 | 31 | - | 0/5/27/28 | 0/3/3/3 |
| 31 | PSU | CA | 746 | 31,56 | - | 3/7/25/26 | 0/2/2/2 |
| 55 | 1MG | DA | 745 | 55 | - | 0/3/25/26 | 0/3/3/3 |
| 31 | PSU | CA | 955 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | 5MU | CA | 747 | 31 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MC | AA | 967 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 7MG | AA | 527 | 1 | - | 2/7/37/38 | 0/3/3/3 |
| 55 | PSU | DA | 2605 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | AA | 1402 | 1 | - | 0/9/29/30 | 0/2/2/2 |
| 1 | 2MG | BA | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 31 | 5MU | CA | 1939 | 31 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | MEQ | DD | 150[B] | 32 | - | 4/8/9/11 | - |
| 32 | MEQ | DD | 150[A] | 32 | - | 4/8/9/11 | - |
| 55 | 2MA | DA | 2503 | 55,56 | - | 2/3/25/26 | 0/3/3/3 |
| 55 | PSU | DA | 2504 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | BA | 966 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 55 | PSU | DA | 2457 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 6MZ | DA | 1618 | 55 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 2MG | AA | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 55 | 3TD | DA | 1915 | 55 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|------------|---------|
| 31 | PSU | CA | 2580 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | UR3 | AA | 1498 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 55 | 6MZ | DA | 2030 | 55 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | PSU | BA | 516 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | PSU | DA | 1917 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | 1MG | CA | 745 | 31 | - | 0/3/25/26 | 0/3/3/3 |
| 55 | PSU | DA | 2580 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | PSU | CA | 2504 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 2MG | DA | 2445 | 55 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | 2MG | AA | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | AA | 1407 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 4OC | BA | 1402 | 1 | - | 0/9/29/30 | 0/2/2/2 |
| 31 | 3TD | CA | 1915 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | PSU | DA | 1911 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | PSU | DA | 746 | 55,56 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | MA6 | AA | 1519 | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 31 | PSU | CA | 2457 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 41 | 4D4 | CN | 81 | 41 | - | 1/11/12/14 | - |

The worst 5 of 119 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 41 | CN | 81 | 4D4 | CZ-NE | 6.09 | 1.45 | 1.33 |
| 1 | AA | 527 | 7MG | C8-N9 | -5.35 | 1.33 | 1.45 |
| 55 | DA | 2069 | 7MG | C8-N9 | -5.32 | 1.33 | 1.45 |
| 1 | BA | 527 | 7MG | C8-N9 | -5.31 | 1.33 | 1.45 |
| 31 | CA | 2069 | 7MG | C8-N9 | -5.22 | 1.33 | 1.45 |

The worst 5 of 215 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 31 | CA | 1917 | PSU | N1-C2-N3 | -17.20 | 114.76 | 128.43 |
| 55 | DA | 2604 | PSU | N1-C2-N3 | -17.20 | 114.76 | 128.43 |
| 31 | CA | 746 | PSU | N1-C2-N3 | -17.18 | 114.77 | 128.43 |
| 55 | DA | 2605 | PSU | N1-C2-N3 | -17.16 | 114.78 | 128.43 |
| 31 | CA | 2580 | PSU | N1-C2-N3 | -17.16 | 114.79 | 128.43 |

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-------|------|-----------------|
| 12 | BL | 89 | D2T | CG-CB-SB-CB1 |
| 41 | DN | 81[B] | 4D4 | CA-CB-CG-CD |
| 31 | CA | 2030 | 6MZ | O4'-C4'-C5'-O5' |
| 55 | DA | 1962 | 5MC | O4'-C1'-N1-C6 |
| 55 | DA | 1962 | 5MC | C2'-C1'-N1-C6 |

There are no ring outliers.

18 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 31 | CA | 2498 | OMC | 2 | 0 |
| 55 | DA | 2498 | OMC | 1 | 0 |
| 1 | BA | 1519 | MA6 | 1 | 0 |
| 31 | CA | 2030 | 6MZ | 1 | 0 |
| 55 | DA | 2251 | OMG | 1 | 0 |
| 1 | BA | 967 | 5MC | 1 | 0 |
| 1 | AA | 1518 | MA6 | 1 | 0 |
| 31 | CA | 2503 | 2MA | 1 | 0 |
| 1 | BA | 1518 | MA6 | 1 | 0 |
| 55 | DA | 745 | 1MG | 1 | 0 |
| 1 | AA | 967 | 5MC | 1 | 0 |
| 32 | DD | 150[B] | MEQ | 1 | 0 |
| 32 | DD | 150[A] | MEQ | 3 | 0 |
| 55 | DA | 2503 | 2MA | 1 | 0 |
| 31 | CA | 2580 | PSU | 1 | 0 |
| 55 | DA | 2030 | 6MZ | 1 | 0 |
| 31 | CA | 1915 | 3TD | 1 | 0 |
| 1 | AA | 1519 | MA6 | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 557 ligands modelled in this entry, 475 are monoatomic - leaving 82 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$ |
| 59 | PUT | DA | 3213 | - | 5,5,5 | 0.17 | 0 | 4,4,4 | 0.17 | 0 |
| 63 | EDO | D1 | 101 | - | 3,3,3 | 0.62 | 0 | 2,2,2 | 0.09 | 0 |
| 58 | MPD | DA | 3207 | - | 7,7,7 | 0.76 | 0 | 9,10,10 | 0.51 | 0 |
| 59 | PUT | AA | 1673 | - | 5,5,5 | 0.12 | 0 | 4,4,4 | 0.10 | 0 |
| 62 | PEG | DA | 3199 | - | 6,6,6 | 0.24 | 0 | 5,5,5 | 0.15 | 0 |
| 67 | ACY | DA | 3191 | - | 1,3,3 | 1.32 | 0 | 0,3,3 | 0.00 | - |
| 58 | MPD | DA | 3204 | - | 7,7,7 | 0.77 | 0 | 9,10,10 | 0.70 | 0 |
| 57 | PG4 | DR | 202 | - | 12,12,12 | 0.26 | 0 | 11,11,11 | 0.36 | 0 |
| 69 | TRS | DA | 3220 | - | 7,7,7 | 0.26 | 0 | 9,9,9 | 0.27 | 0 |
| 58 | MPD | DK | 201 | - | 7,7,7 | 0.66 | 0 | 9,10,10 | 0.30 | 0 |
| 59 | PUT | DA | 3184 | - | 5,5,5 | 0.16 | 0 | 4,4,4 | 0.12 | 0 |
| 64 | PGE | DA | 3225 | - | 9,9,9 | 0.12 | 0 | 8,8,8 | 0.17 | 0 |
| 58 | MPD | DS | 203 | - | 7,7,7 | 0.37 | 0 | 9,10,10 | 0.49 | 0 |
| 60 | T1C | AA | 1680 | 56 | 44,45,45 | 1.04 | 3 (6%) | 53,72,72 | 1.53 | 3 (5%) |
| 58 | MPD | DN | 201 | - | 7,7,7 | 0.87 | 0 | 9,10,10 | 0.54 | 0 |
| 62 | PEG | DP | 201 | - | 6,6,6 | 0.16 | 0 | 5,5,5 | 0.09 | 0 |
| 64 | PGE | DA | 3214 | - | 9,9,9 | 0.19 | 0 | 8,8,8 | 0.27 | 0 |
| 59 | PUT | DA | 3223 | - | 5,5,5 | 0.16 | 0 | 4,4,4 | 0.15 | 0 |
| 63 | EDO | DA | 3209 | - | 3,3,3 | 0.61 | 0 | 2,2,2 | 0.28 | 0 |
| 57 | PG4 | DA | 3193 | - | 12,12,12 | 0.30 | 0 | 11,11,11 | 0.25 | 0 |
| 64 | PGE | DA | 3186 | - | 9,9,9 | 0.24 | 0 | 8,8,8 | 0.29 | 0 |
| 62 | PEG | DA | 3226 | - | 6,6,6 | 0.24 | 0 | 5,5,5 | 0.13 | 0 |
| 57 | PG4 | BA | 1642 | - | 12,12,12 | 0.15 | 0 | 11,11,11 | 0.20 | 0 |
| 57 | PG4 | DA | 3216 | - | 12,12,12 | 0.11 | 0 | 11,11,11 | 0.17 | 0 |
| 62 | PEG | DA | 3218 | - | 6,6,6 | 0.16 | 0 | 5,5,5 | 0.09 | 0 |
| 59 | PUT | DA | 3188 | - | 5,5,5 | 0.21 | 0 | 4,4,4 | 0.13 | 0 |
| 59 | PUT | AA | 1674 | - | 5,5,5 | 0.16 | 0 | 4,4,4 | 0.10 | 0 |
| 58 | MPD | DE | 302 | - | 7,7,7 | 0.88 | 1 (14%) | 9,10,10 | 0.56 | 0 |
| 59 | PUT | DA | 3205 | - | 5,5,5 | 0.12 | 0 | 4,4,4 | 0.12 | 0 |
| 62 | PEG | D3 | 102 | - | 6,6,6 | 0.21 | 0 | 5,5,5 | 0.20 | 0 |
| 62 | PEG | DQ | 201 | - | 6,6,6 | 0.12 | 0 | 5,5,5 | 0.09 | 0 |
| 59 | PUT | AA | 1672 | - | 5,5,5 | 0.20 | 0 | 4,4,4 | 0.20 | 0 |
| 59 | PUT | AA | 1675 | - | 5,5,5 | 0.21 | 0 | 4,4,4 | 0.12 | 0 |
| 63 | EDO | DA | 3197 | - | 3,3,3 | 0.67 | 0 | 2,2,2 | 0.18 | 0 |
| 64 | PGE | D3 | 101 | - | 9,9,9 | 0.22 | 0 | 8,8,8 | 0.22 | 0 |
| 57 | PG4 | AA | 1670 | - | 12,12,12 | 0.31 | 0 | 11,11,11 | 0.28 | 0 |
| 58 | MPD | DE | 301 | - | 7,7,7 | 0.81 | 0 | 9,10,10 | 0.56 | 0 |
| 63 | EDO | DB | 212 | - | 3,3,3 | 0.58 | 0 | 2,2,2 | 0.30 | 0 |
| 58 | MPD | DA | 3190 | - | 7,7,7 | 0.37 | 0 | 9,10,10 | 0.48 | 0 |
| 62 | PEG | DA | 3200 | - | 6,6,6 | 0.34 | 0 | 5,5,5 | 0.22 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 58 | MPD | AA | 1676 | - | 7,7,7 | 0.60 | 0 | 9,10,10 | 0.54 | 0 |
| 62 | PEG | DA | 3227 | - | 6,6,6 | 0.21 | 0 | 5,5,5 | 0.14 | 0 |
| 57 | PG4 | DQ | 202 | - | 12,12,12 | 0.20 | 0 | 11,11,11 | 0.14 | 0 |
| 58 | MPD | DA | 3210 | - | 7,7,7 | 0.63 | 0 | 9,10,10 | 0.28 | 0 |
| 59 | PUT | DA | 3001 | - | 5,5,5 | 0.25 | 0 | 4,4,4 | 0.13 | 0 |
| 58 | MPD | DT | 202 | - | 7,7,7 | 0.70 | 0 | 9,10,10 | 0.39 | 0 |
| 58 | MPD | DT | 201 | - | 7,7,7 | 0.52 | 0 | 9,10,10 | 0.30 | 0 |
| 66 | 1PE | DA | 3185 | - | 15,15,15 | 0.19 | 0 | 14,14,14 | 0.21 | 0 |
| 59 | PUT | DA | 3212 | - | 5,5,5 | 0.18 | 0 | 4,4,4 | 0.04 | 0 |
| 63 | EDO | DB | 213 | - | 3,3,3 | 0.74 | 0 | 2,2,2 | 0.03 | 0 |
| 58 | MPD | DA | 3192 | - | 7,7,7 | 0.52 | 0 | 9,10,10 | 0.54 | 0 |
| 62 | PEG | DL | 201 | - | 6,6,6 | 0.07 | 0 | 5,5,5 | 0.10 | 0 |
| 65 | SPD | DA | 3187 | - | 9,9,9 | 0.21 | 0 | 8,8,8 | 0.17 | 0 |
| 63 | EDO | DB | 201 | - | 3,3,3 | 0.68 | 0 | 2,2,2 | 0.13 | 0 |
| 63 | EDO | DA | 3215 | - | 3,3,3 | 0.69 | 0 | 2,2,2 | 0.18 | 0 |
| 65 | SPD | DA | 3183 | - | 9,9,9 | 0.11 | 0 | 8,8,8 | 0.10 | 0 |
| 64 | PGE | DA | 3203 | - | 9,9,9 | 0.21 | 0 | 8,8,8 | 0.20 | 0 |
| 67 | ACY | DA | 3201 | - | 1,3,3 | 2.22 | 1 (100%) | 0,3,3 | 0.00 | - |
| 62 | PEG | AL | 201 | - | 6,6,6 | 0.23 | 0 | 5,5,5 | 0.13 | 0 |
| 59 | PUT | DA | 3219 | - | 5,5,5 | 0.17 | 0 | 4,4,4 | 0.20 | 0 |
| 63 | EDO | DB | 211 | - | 3,3,3 | 0.71 | 0 | 2,2,2 | 0.13 | 0 |
| 58 | MPD | AA | 1671 | - | 7,7,7 | 0.67 | 0 | 9,10,10 | 0.49 | 0 |
| 59 | PUT | DA | 3221 | - | 5,5,5 | 0.17 | 0 | 4,4,4 | 0.10 | 0 |
| 60 | T1C | BA | 1643 | 56 | 44,45,45 | 1.02 | 3 (6%) | 53,72,72 | 1.52 | 3 (5%) |
| 64 | PGE | DU | 101 | - | 9,9,9 | 0.23 | 0 | 8,8,8 | 0.12 | 0 |
| 67 | ACY | DA | 3196 | - | 1,3,3 | 2.73 | 1 (100%) | 0,3,3 | 0.00 | - |
| 62 | PEG | D1 | 103 | - | 6,6,6 | 0.30 | 0 | 5,5,5 | 0.16 | 0 |
| 65 | SPD | DA | 3224 | - | 9,9,9 | 0.20 | 0 | 8,8,8 | 0.38 | 0 |
| 68 | GUN | DA | 3211 | - | 9,12,12 | 1.74 | 2 (22%) | 8,17,17 | 3.85 | 4 (50%) |
| 64 | PGE | DS | 201 | - | 9,9,9 | 0.25 | 0 | 8,8,8 | 0.20 | 0 |
| 63 | EDO | DA | 3002 | - | 3,3,3 | 0.69 | 0 | 2,2,2 | 0.19 | 0 |
| 65 | SPD | DA | 3206 | - | 9,9,9 | 0.21 | 0 | 8,8,8 | 0.15 | 0 |
| 57 | PG4 | DS | 202 | - | 12,12,12 | 0.45 | 0 | 11,11,11 | 0.30 | 0 |
| 59 | PUT | DA | 3222 | - | 5,5,5 | 0.44 | 0 | 4,4,4 | 0.54 | 0 |
| 64 | PGE | D1 | 102 | - | 9,9,9 | 0.20 | 0 | 8,8,8 | 0.14 | 0 |
| 64 | PGE | DA | 3217 | - | 9,9,9 | 0.16 | 0 | 8,8,8 | 0.14 | 0 |
| 63 | EDO | DA | 3194 | - | 3,3,3 | 0.80 | 0 | 2,2,2 | 0.13 | 0 |
| 63 | EDO | DA | 3198 | - | 3,3,3 | 0.66 | 0 | 2,2,2 | 0.20 | 0 |
| 66 | 1PE | DA | 3202 | - | 15,15,15 | 0.32 | 0 | 14,14,14 | 0.34 | 0 |
| 63 | EDO | DA | 3208 | - | 3,3,3 | 0.68 | 0 | 2,2,2 | 0.16 | 0 |
| 59 | PUT | DA | 3195 | - | 5,5,5 | 0.31 | 0 | 4,4,4 | 0.32 | 0 |
| 59 | PUT | DA | 3189 | - | 5,5,5 | 0.30 | 0 | 4,4,4 | 0.18 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 59 | PUT | DA | 3213 | - | - | 0/3/3/3 | - |
| 63 | EDO | D1 | 101 | - | - | 0/1/1/1 | - |
| 58 | MPD | DA | 3207 | - | - | 3/5/5/5 | - |
| 59 | PUT | AA | 1673 | - | - | 0/3/3/3 | - |
| 62 | PEG | DA | 3199 | - | - | 2/4/4/4 | - |
| 63 | EDO | DA | 3194 | - | - | 0/1/1/1 | - |
| 58 | MPD | DA | 3204 | - | - | 2/5/5/5 | - |
| 57 | PG4 | DR | 202 | - | - | 5/10/10/10 | - |
| 69 | TRS | DA | 3220 | - | - | 0/9/9/9 | - |
| 58 | MPD | DK | 201 | - | - | 2/5/5/5 | - |
| 59 | PUT | DA | 3184 | - | - | 0/3/3/3 | - |
| 64 | PGE | DA | 3225 | - | - | 4/7/7/7 | - |
| 58 | MPD | DS | 203 | - | - | 0/5/5/5 | - |
| 60 | T1C | AA | 1680 | 56 | - | 6/22/80/80 | 0/4/4/4 |
| 58 | MPD | DN | 201 | - | - | 2/5/5/5 | - |
| 62 | PEG | DP | 201 | - | - | 2/4/4/4 | - |
| 64 | PGE | DA | 3214 | - | - | 2/7/7/7 | - |
| 59 | PUT | DA | 3223 | - | - | 1/3/3/3 | - |
| 63 | EDO | DA | 3209 | - | - | 0/1/1/1 | - |
| 57 | PG4 | DA | 3193 | - | - | 6/10/10/10 | - |
| 62 | PEG | DA | 3226 | - | - | 2/4/4/4 | - |
| 57 | PG4 | BA | 1642 | - | - | 0/10/10/10 | - |
| 57 | PG4 | DA | 3216 | - | - | 3/10/10/10 | - |
| 62 | PEG | DA | 3218 | - | - | 1/4/4/4 | - |
| 59 | PUT | DA | 3188 | - | - | 0/3/3/3 | - |
| 59 | PUT | AA | 1674 | - | - | 0/3/3/3 | - |
| 64 | PGE | DA | 3186 | - | - | 3/7/7/7 | - |
| 59 | PUT | DA | 3205 | - | - | 0/3/3/3 | - |
| 62 | PEG | D3 | 102 | - | - | 1/4/4/4 | - |
| 62 | PEG | DQ | 201 | - | - | 1/4/4/4 | - |
| 59 | PUT | AA | 1672 | - | - | 0/3/3/3 | - |
| 59 | PUT | AA | 1675 | - | - | 1/3/3/3 | - |
| 63 | EDO | DA | 3197 | - | - | 0/1/1/1 | - |
| 64 | PGE | D3 | 101 | - | - | 2/7/7/7 | - |
| 57 | PG4 | AA | 1670 | - | - | 3/10/10/10 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 58 | MPD | DE | 301 | - | - | 2/5/5/5 | - |
| 63 | EDO | DB | 212 | - | - | 1/1/1/1 | - |
| 58 | MPD | DA | 3190 | - | - | 2/5/5/5 | - |
| 62 | PEG | DA | 3200 | - | - | 2/4/4/4 | - |
| 58 | MPD | AA | 1676 | - | - | 2/5/5/5 | - |
| 62 | PEG | DA | 3227 | - | - | 0/4/4/4 | - |
| 57 | PG4 | DQ | 202 | - | - | 1/10/10/10 | - |
| 58 | MPD | DA | 3210 | - | - | 0/5/5/5 | - |
| 59 | PUT | DA | 3001 | - | - | 0/3/3/3 | - |
| 58 | MPD | DT | 201 | - | - | 2/5/5/5 | - |
| 66 | 1PE | DA | 3185 | - | - | 5/13/13/13 | - |
| 59 | PUT | DA | 3212 | - | - | 0/3/3/3 | - |
| 63 | EDO | DB | 213 | - | - | 0/1/1/1 | - |
| 58 | MPD | DA | 3192 | - | - | 2/5/5/5 | - |
| 62 | PEG | DL | 201 | - | - | 2/4/4/4 | - |
| 65 | SPD | DA | 3187 | - | - | 2/7/7/7 | - |
| 63 | EDO | DB | 201 | - | - | 1/1/1/1 | - |
| 63 | EDO | DA | 3215 | - | - | 1/1/1/1 | - |
| 65 | SPD | DA | 3183 | - | - | 1/7/7/7 | - |
| 64 | PGE | DA | 3203 | - | - | 5/7/7/7 | - |
| 58 | MPD | DT | 202 | - | - | 1/5/5/5 | - |
| 62 | PEG | AL | 201 | - | - | 2/4/4/4 | - |
| 59 | PUT | DA | 3219 | - | - | 0/3/3/3 | - |
| 68 | GUN | DA | 3211 | - | - | - | 0/2/2/2 |
| 63 | EDO | DB | 211 | - | - | 0/1/1/1 | - |
| 59 | PUT | DA | 3221 | - | - | 0/3/3/3 | - |
| 60 | T1C | BA | 1643 | 56 | - | 11/22/80/80 | 0/4/4/4 |
| 64 | PGE | DU | 101 | - | - | 3/7/7/7 | - |
| 62 | PEG | D1 | 103 | - | - | 0/4/4/4 | - |
| 65 | SPD | DA | 3224 | - | - | 3/7/7/7 | - |
| 58 | MPD | AA | 1671 | - | - | 0/5/5/5 | - |
| 64 | PGE | DS | 201 | - | - | 3/7/7/7 | - |
| 63 | EDO | DA | 3002 | - | - | 0/1/1/1 | - |
| 65 | SPD | DA | 3206 | - | - | 3/7/7/7 | - |
| 57 | PG4 | DS | 202 | - | - | 5/10/10/10 | - |
| 59 | PUT | DA | 3222 | - | - | 0/3/3/3 | - |
| 64 | PGE | D1 | 102 | - | - | 3/7/7/7 | - |
| 64 | PGE | DA | 3217 | - | - | 4/7/7/7 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 63 | EDO | DA | 3198 | - | - | 1/1/1/1 | - |
| 58 | MPD | DE | 302 | - | - | 3/5/5/5 | - |
| 66 | 1PE | DA | 3202 | - | - | 4/13/13/13 | - |
| 63 | EDO | DA | 3208 | - | - | 0/1/1/1 | - |
| 59 | PUT | DA | 3195 | - | - | 1/3/3/3 | - |
| 59 | PUT | DA | 3189 | - | - | 0/3/3/3 | - |

The worst 5 of 11 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 68 | DA | 3211 | GUN | C6-C5 | 3.40 | 1.47 | 1.41 |
| 68 | DA | 3211 | GUN | C6-N1 | 3.33 | 1.38 | 1.33 |
| 60 | BA | 1643 | T1C | C4-C3 | 3.16 | 1.58 | 1.51 |
| 60 | AA | 1680 | T1C | C4-C3 | 2.86 | 1.57 | 1.51 |
| 60 | AA | 1680 | T1C | C7-C61 | 2.76 | 1.43 | 1.40 |

The worst 5 of 10 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 68 | DA | 3211 | GUN | C5-C6-N1 | -7.96 | 112.55 | 123.43 |
| 60 | BA | 1643 | T1C | C92-N92-C93 | 7.94 | 125.80 | 115.84 |
| 60 | AA | 1680 | T1C | C92-N92-C93 | 7.70 | 125.49 | 115.84 |
| 68 | DA | 3211 | GUN | C6-N1-C2 | 5.66 | 124.93 | 115.93 |
| 60 | AA | 1680 | T1C | C8-C9-C10 | -5.12 | 115.41 | 120.49 |

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 58 | DA | 3192 | MPD | C2-C3-C4-O4 |
| 60 | AA | 1680 | T1C | C95-C93-N92-C92 |
| 60 | AA | 1680 | T1C | C96-C93-N92-C92 |
| 60 | AA | 1680 | T1C | C91-C92-N92-C93 |
| 60 | BA | 1643 | T1C | C1-C2-C21-O21 |

There are no ring outliers.

24 monomers are involved in 32 short contacts:

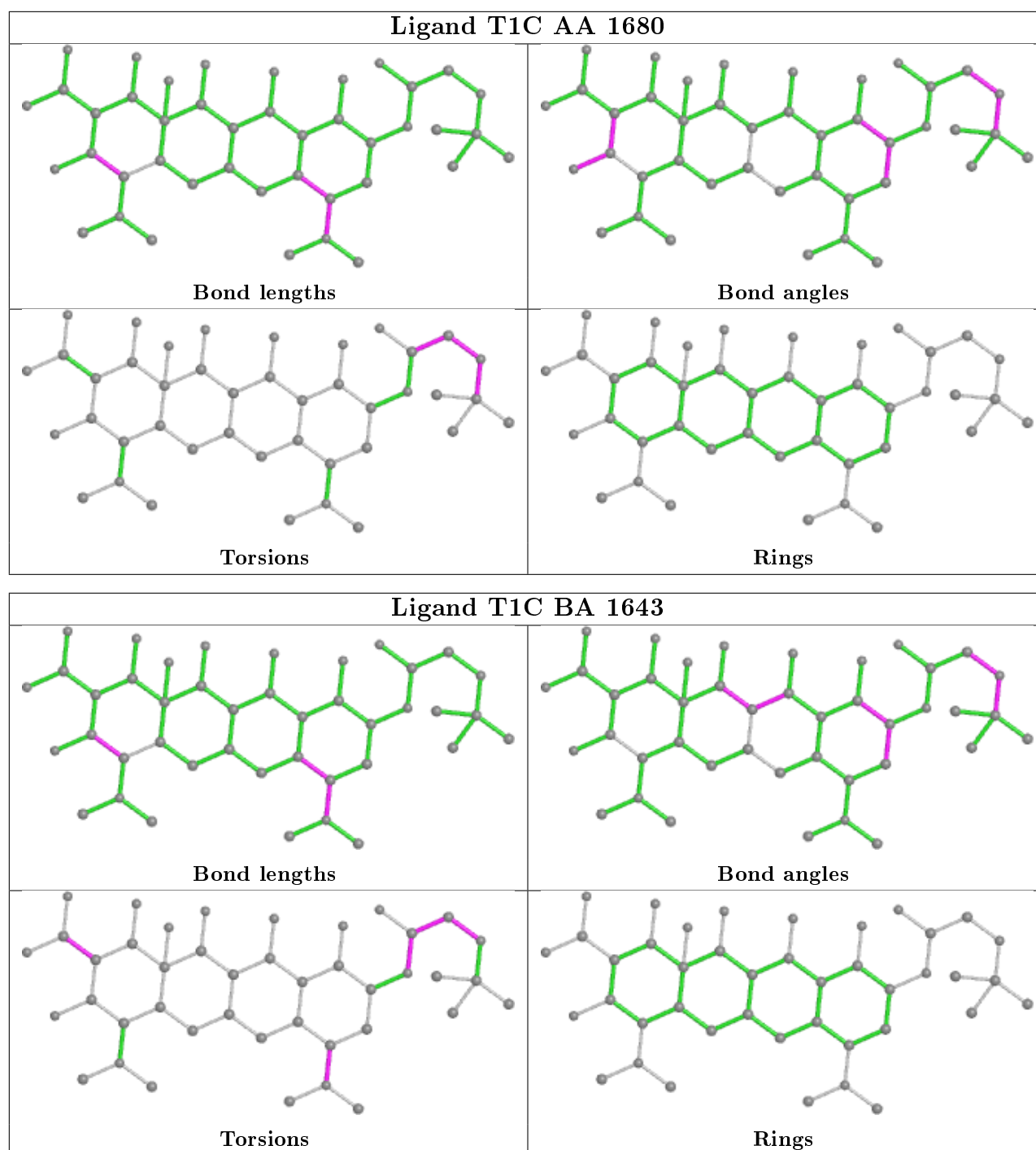
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58 | DA | 3204 | MPD | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57 | DR | 202 | PG4 | 4 | 0 |
| 69 | DA | 3220 | TRS | 1 | 0 |
| 64 | DA | 3225 | PGE | 2 | 0 |
| 60 | AA | 1680 | T1C | 2 | 0 |
| 58 | DN | 201 | MPD | 1 | 0 |
| 64 | DA | 3214 | PGE | 1 | 0 |
| 59 | DA | 3223 | PUT | 1 | 0 |
| 63 | DA | 3209 | EDO | 1 | 0 |
| 57 | BA | 1642 | PG4 | 1 | 0 |
| 57 | AA | 1670 | PG4 | 1 | 0 |
| 66 | DA | 3185 | 1PE | 1 | 0 |
| 58 | DA | 3192 | MPD | 1 | 0 |
| 64 | DA | 3203 | PGE | 1 | 0 |
| 59 | DA | 3219 | PUT | 1 | 0 |
| 64 | DU | 101 | PGE | 1 | 0 |
| 62 | D1 | 103 | PEG | 1 | 0 |
| 65 | DA | 3224 | SPD | 2 | 0 |
| 64 | DS | 201 | PGE | 1 | 0 |
| 57 | DS | 202 | PG4 | 1 | 0 |
| 64 | D1 | 102 | PGE | 2 | 0 |
| 64 | DA | 3217 | PGE | 1 | 0 |
| 66 | DA | 3202 | 1PE | 2 | 0 |
| 59 | DA | 3195 | PUT | 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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1523/1534 (99%) | 0.12 | 53 (3%) 44 23 | 43, 96, 240, 296 | 0 |
| 1 | BA | 1522/1534 (99%) | 0.59 | 195 (12%) 3 1 | 59, 109, 268, 280 | 0 |
| 2 | AB | 224/224 (100%) | 0.69 | 33 (14%) 2 1 | 72, 125, 197, 249 | 0 |
| 2 | BB | 224/224 (100%) | 0.65 | 31 (13%) 2 1 | 101, 143, 205, 240 | 0 |
| 3 | AC | 206/206 (100%) | 0.13 | 8 (3%) 39 20 | 78, 108, 137, 154 | 0 |
| 3 | BC | 206/206 (100%) | 1.33 | 55 (26%) 0 0 | 103, 151, 181, 204 | 0 |
| 4 | AD | 205/205 (100%) | -0.19 | 0 100 100 | 71, 104, 137, 164 | 0 |
| 4 | BD | 205/205 (100%) | -0.34 | 0 100 100 | 51, 77, 108, 132 | 0 |
| 5 | AE | 155/155 (100%) | 0.02 | 0 100 100 | 59, 84, 116, 155 | 0 |
| 5 | BE | 150/155 (96%) | 0.14 | 1 (0%) 87 75 | 68, 94, 135, 207 | 0 |
| 6 | AF | 106/106 (100%) | 0.17 | 3 (2%) 53 30 | 78, 107, 128, 148 | 0 |
| 6 | BF | 100/106 (94%) | 0.32 | 3 (3%) 50 27 | 88, 124, 147, 160 | 0 |
| 7 | AG | 151/151 (100%) | 0.93 | 35 (23%) 0 0 | 108, 141, 166, 178 | 0 |
| 7 | BG | 151/151 (100%) | 3.03 | 88 (58%) 0 0 | 145, 205, 222, 231 | 0 |
| 8 | AH | 129/129 (100%) | 0.03 | 2 (1%) 72 51 | 67, 89, 116, 132 | 0 |
| 8 | BH | 129/129 (100%) | 0.10 | 4 (3%) 49 26 | 90, 113, 141, 157 | 0 |
| 9 | AI | 127/127 (100%) | 1.25 | 33 (25%) 0 0 | 86, 142, 167, 175 | 0 |
| 9 | BI | 127/127 (100%) | 1.95 | 46 (36%) 0 0 | 141, 172, 209, 221 | 0 |
| 10 | AJ | 99/99 (100%) | 1.14 | 24 (24%) 0 0 | 91, 129, 150, 161 | 0 |
| 10 | BJ | 98/99 (98%) | 2.76 | 52 (53%) 0 0 | 144, 175, 196, 202 | 0 |
| 11 | AK | 117/117 (100%) | 0.75 | 14 (11%) 4 2 | 59, 117, 141, 150 | 0 |
| 11 | BK | 117/117 (100%) | 0.63 | 13 (11%) 5 2 | 69, 115, 149, 175 | 0 |
| 12 | AL | 122/123 (99%) | 0.02 | 3 (2%) 57 34 | 50, 70, 99, 133 | 0 |
| 12 | BL | 122/123 (99%) | 0.33 | 5 (4%) 37 18 | 71, 86, 117, 143 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13 | AM | 114/114 (100%) | 1.30 | 28 (24%) 0 0 | 116, 139, 175, 182 | 0 |
| 13 | BM | 114/114 (100%) | 3.30 | 79 (69%) 0 0 | 202, 239, 249, 254 | 0 |
| 14 | AN | 100/100 (100%) | 1.03 | 21 (21%) 1 0 | 84, 124, 192, 203 | 0 |
| 14 | BN | 100/100 (100%) | 2.33 | 52 (52%) 0 0 | 134, 185, 229, 236 | 0 |
| 15 | AO | 88/88 (100%) | 0.17 | 2 (2%) 60 39 | 68, 92, 115, 136 | 0 |
| 15 | BO | 88/88 (100%) | 0.44 | 4 (4%) 33 16 | 79, 113, 132, 152 | 0 |
| 16 | AP | 82/82 (100%) | 0.54 | 7 (8%) 10 4 | 62, 86, 128, 142 | 0 |
| 16 | BP | 82/82 (100%) | 0.76 | 11 (13%) 3 1 | 77, 94, 149, 159 | 0 |
| 17 | AQ | 80/80 (100%) | 0.00 | 1 (1%) 77 59 | 64, 88, 118, 134 | 0 |
| 17 | BQ | 80/80 (100%) | 0.77 | 12 (15%) 2 1 | 83, 120, 149, 157 | 0 |
| 18 | AR | 55/55 (100%) | 0.36 | 4 (7%) 15 6 | 74, 101, 142, 166 | 0 |
| 18 | BR | 55/55 (100%) | 0.52 | 3 (5%) 25 11 | 75, 97, 134, 166 | 0 |
| 19 | AS | 79/79 (100%) | 0.76 | 6 (7%) 13 5 | 123, 139, 159, 165 | 0 |
| 19 | BS | 79/79 (100%) | 3.47 | 56 (70%) 0 0 | 217, 233, 247, 254 | 0 |
| 20 | AT | 86/86 (100%) | 0.22 | 1 (1%) 79 61 | 68, 86, 116, 133 | 0 |
| 20 | BT | 85/86 (98%) | 0.89 | 14 (16%) 1 1 | 90, 119, 151, 161 | 0 |
| 21 | AU | 56/56 (100%) | 0.50 | 4 (7%) 16 6 | 81, 118, 163, 176 | 0 |
| 21 | BU | 56/56 (100%) | 0.30 | 4 (7%) 16 6 | 75, 110, 147, 155 | 0 |
| 22 | C1 | 56/56 (100%) | 1.53 | 17 (30%) 0 0 | 93, 147, 170, 185 | 0 |
| 22 | D1 | 56/56 (100%) | -0.40 | 0 100 100 | 21, 47, 73, 112 | 0 |
| 23 | C2 | 50/51 (98%) | 2.71 | 31 (62%) 0 0 | 145, 160, 172, 198 | 0 |
| 23 | D2 | 51/51 (100%) | 0.03 | 0 100 100 | 56, 69, 100, 116 | 0 |
| 24 | C3 | 46/46 (100%) | 1.85 | 19 (41%) 0 0 | 102, 130, 139, 152 | 0 |
| 24 | D3 | 46/46 (100%) | -0.10 | 1 (2%) 62 41 | 30, 40, 58, 116 | 0 |
| 25 | C4 | 64/64 (100%) | 1.00 | 8 (12%) 3 1 | 108, 134, 150, 161 | 0 |
| 25 | D4 | 64/64 (100%) | -0.33 | 0 100 100 | 32, 41, 57, 75 | 0 |
| 26 | C5 | 38/38 (100%) | 1.54 | 10 (26%) 0 0 | 115, 134, 145, 151 | 0 |
| 26 | D5 | 38/38 (100%) | -0.10 | 0 100 100 | 43, 55, 72, 99 | 0 |
| 27 | C0 | 58/58 (100%) | 1.69 | 19 (32%) 0 0 | 109, 132, 151, 162 | 0 |
| 27 | D0 | 58/58 (100%) | -0.39 | 0 100 100 | 29, 39, 64, 83 | 0 |
| 28 | CB | 118/120 (98%) | 0.63 | 12 (10%) 6 2 | 110, 181, 234, 243 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28 | DB | 120/120 (100%) | -0.14 | 0 100 100 | 34, 63, 99, 131 | 0 |
| 29 | CC | 271/272 (99%) | 0.32 | 14 (5%) 27 12 | 73, 100, 126, 136 | 0 |
| 29 | DC | 271/272 (99%) | -0.32 | 1 (0%) 92 84 | 26, 57, 84, 99 | 0 |
| 30 | CD | 209/209 (100%) | 0.91 | 35 (16%) 1 1 | 79, 116, 143, 158 | 0 |
| 31 | CA | 2876/2904 (99%) | 0.70 | 304 (10%) 6 2 | 64, 133, 248, 291 | 0 |
| 32 | DD | 208/209 (99%) | -0.40 | 0 100 100 | 20, 41, 71, 100 | 0 |
| 33 | CE | 201/201 (100%) | 1.05 | 41 (20%) 1 0 | 90, 160, 190, 200 | 0 |
| 33 | DE | 201/201 (100%) | -0.25 | 1 (0%) 91 81 | 25, 62, 104, 136 | 0 |
| 34 | CF | 177/178 (99%) | 2.86 | 112 (63%) 0 0 | 201, 219, 227, 235 | 0 |
| 34 | DF | 177/178 (99%) | 0.15 | 7 (3%) 38 19 | 54, 89, 132, 150 | 0 |
| 35 | CG | 176/176 (100%) | 2.02 | 76 (43%) 0 0 | 140, 167, 194, 206 | 0 |
| 35 | DG | 176/176 (100%) | -0.11 | 1 (0%) 89 78 | 44, 75, 103, 136 | 0 |
| 36 | CH | 149/149 (100%) | 1.24 | 38 (25%) 0 0 | 89, 149, 175, 187 | 0 |
| 36 | DH | 149/149 (100%) | 0.90 | 27 (18%) 1 0 | 71, 150, 190, 207 | 0 |
| 37 | CJ | 134/135 (99%) | 5.86 | 119 (88%) 0 0 | 241, 258, 269, 276 | 0 |
| 37 | DJ | 134/135 (99%) | 3.91 | 93 (69%) 0 0 | 210, 234, 245, 252 | 0 |
| 38 | CK | 142/142 (100%) | 0.31 | 1 (0%) 87 75 | 84, 109, 134, 142 | 0 |
| 38 | DK | 142/142 (100%) | -0.45 | 0 100 100 | 23, 37, 67, 88 | 0 |
| 39 | CL | 122/123 (99%) | 0.23 | 4 (3%) 46 24 | 76, 99, 141, 159 | 0 |
| 39 | DL | 123/123 (100%) | -0.42 | 0 100 100 | 28, 44, 71, 110 | 0 |
| 40 | CM | 144/144 (100%) | 1.98 | 55 (38%) 0 0 | 94, 152, 193, 222 | 0 |
| 40 | DM | 144/144 (100%) | -0.32 | 1 (0%) 87 75 | 18, 56, 88, 121 | 0 |
| 41 | CN | 135/136 (99%) | 0.29 | 4 (2%) 50 27 | 76, 111, 139, 174 | 0 |
| 41 | DN | 135/136 (99%) | -0.54 | 0 100 100 | 26, 43, 73, 95 | 0 |
| 42 | CO | 120/125 (96%) | 1.00 | 19 (15%) 2 1 | 93, 124, 143, 189 | 0 |
| 42 | DO | 125/125 (100%) | -0.38 | 0 100 100 | 27, 40, 76, 125 | 0 |
| 43 | CP | 116/117 (99%) | 2.38 | 60 (51%) 0 0 | 142, 164, 181, 187 | 0 |
| 43 | DP | 117/117 (100%) | -0.16 | 0 100 100 | 42, 61, 90, 99 | 0 |
| 44 | CQ | 114/114 (100%) | 0.83 | 17 (14%) 2 1 | 96, 114, 138, 154 | 0 |
| 44 | DQ | 114/114 (100%) | -0.32 | 1 (0%) 84 69 | 28, 52, 86, 125 | 0 |
| 45 | CR | 117/117 (100%) | 0.73 | 12 (10%) 6 2 | 82, 109, 134, 148 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|--|-----------------------|--------|
| 45 | DR | 117/117 (100%) | -0.30 | 0 100 100 | 19, 34, 52, 82 | 0 |
| 46 | CS | 103/103 (100%) | 1.66 | 28 (27%) 0 0 | 101, 124, 166, 174 | 0 |
| 46 | DS | 103/103 (100%) | -0.36 | 0 100 100 | 22, 45, 74, 101 | 0 |
| 47 | CT | 110/110 (100%) | 0.71 | 14 (12%) 3 1 | 99, 126, 157, 172 | 0 |
| 47 | DT | 110/110 (100%) | -0.45 | 0 100 100 | 26, 37, 67, 120 | 0 |
| 48 | CU | 93/93 (100%) | 1.83 | 33 (35%) 0 0 | 124, 154, 178, 190 | 0 |
| 48 | DU | 93/93 (100%) | 0.18 | 3 (3%) 47 25 | 41, 63, 120, 139 | 0 |
| 49 | CV | 102/103 (99%) | 2.69 | 55 (53%) 0 0 | 132, 164, 197, 206 | 0 |
| 49 | DV | 102/103 (99%) | -0.04 | 7 (6%) 16 7 | 49, 67, 116, 143 | 0 |
| 50 | CW | 94/94 (100%) | 1.35 | 28 (29%) 0 0 | 122, 144, 158, 167 | 0 |
| 50 | DW | 94/94 (100%) | -0.43 | 0 100 100 | 38, 58, 88, 96 | 0 |
| 51 | CX | 75/83 (90%) | 0.74 | 10 (13%) 3 1 | 95, 126, 138, 176 | 0 |
| 51 | DX | 76/83 (91%) | -0.49 | 0 100 100 | 29, 43, 72, 108 | 0 |
| 52 | CY | 77/77 (100%) | 0.35 | 5 (6%) 18 8 | 87, 116, 146, 163 | 0 |
| 52 | DY | 77/77 (100%) | -0.19 | 0 100 100 | 34, 58, 96, 112 | 0 |
| 53 | CZ | 62/62 (100%) | 2.52 | 38 (61%) 0 0 | 139, 171, 185, 191 | 0 |
| 53 | DZ | 62/62 (100%) | 0.32 | 2 (3%) 47 25 | 51, 81, 123, 140 | 0 |
| 54 | DI | 135/135 (100%) | 1.33 | 33 (24%) 0 0 | 82, 161, 211, 226 | 1 (0%) |
| 55 | DA | 2873/2904 (98%) | 0.09 | 101 (3%) 44 23 | 22, 47, 217, 299 | 0 |
| All | All | 20634/20767 (99%) | 0.59 | 2527 (12%) 4 1 | 18, 106, 237, 299 | 1 (0%) |

The worst 5 of 2527 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | DJ | 54 | PRO | 22.9 |
| 37 | CJ | 76 | ALA | 22.4 |
| 37 | CJ | 13 | VAL | 18.2 |
| 37 | CJ | 87 | LYS | 17.4 |
| 55 | DA | 2120 | G | 16.3 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-------|-------|------|------|-----------------------------|-------|
| 1 | 5MC | BA | 967 | 21/22 | 0.78 | 0.38 | 156,162,165,165 | 0 |
| 1 | 2MG | BA | 966 | 24/25 | 0.79 | 0.31 | 161,163,169,169 | 0 |
| 1 | 2MG | BA | 1207 | 24/25 | 0.85 | 0.27 | 169,172,175,177 | 0 |
| 31 | PSU | CA | 1917 | 20/21 | 0.89 | 0.20 | 106,115,121,121 | 0 |
| 31 | PSU | CA | 2504 | 20/21 | 0.90 | 0.24 | 87,89,95,96 | 0 |
| 31 | PSU | CA | 955 | 20/21 | 0.91 | 0.19 | 92,93,95,95 | 0 |
| 1 | 5MC | AA | 967 | 21/22 | 0.91 | 0.21 | 90,100,103,105 | 0 |
| 1 | 2MG | AA | 966 | 24/25 | 0.91 | 0.21 | 84,94,103,105 | 0 |
| 1 | PSU | BA | 516 | 20/21 | 0.91 | 0.18 | 93,98,101,102 | 0 |
| 1 | 2MG | AA | 1207 | 24/25 | 0.91 | 0.17 | 124,129,130,132 | 0 |
| 31 | 3TD | CA | 1915 | 21/22 | 0.91 | 0.23 | 132,137,140,141 | 0 |
| 31 | PSU | CA | 1911 | 20/21 | 0.92 | 0.18 | 112,123,126,126 | 0 |
| 31 | 2MA | CA | 2503 | 23/24 | 0.92 | 0.23 | 90,95,99,100 | 0 |
| 41 | 4D4 | CN | 81 | 12/13 | 0.92 | 0.32 | 85,88,108,110 | 0 |
| 31 | 5MU | CA | 747 | 21/22 | 0.93 | 0.20 | 95,101,103,106 | 0 |
| 31 | PSU | CA | 2457 | 20/21 | 0.93 | 0.20 | 83,88,93,96 | 0 |
| 31 | 7MG | CA | 2069 | 24/25 | 0.93 | 0.21 | 84,89,94,94 | 0 |
| 55 | PSU | DA | 1911 | 20/21 | 0.93 | 0.20 | 82,85,87,88 | 0 |
| 12 | D2T | BL | 89 | 10/11 | 0.94 | 0.26 | 77,82,93,93 | 0 |
| 31 | 2MG | CA | 2445 | 24/25 | 0.94 | 0.24 | 74,83,85,89 | 0 |
| 31 | 6MZ | CA | 2030 | 23/24 | 0.94 | 0.20 | 82,91,100,102 | 0 |
| 31 | OMU | CA | 2552 | 21/22 | 0.94 | 0.32 | 80,82,86,88 | 0 |
| 12 | D2T | AL | 89 | 10/11 | 0.94 | 0.22 | 61,65,85,86 | 0 |
| 55 | 3TD | DA | 1915 | 21/22 | 0.94 | 0.19 | 105,109,117,117 | 0 |
| 1 | 5MC | BA | 1407 | 21/22 | 0.94 | 0.17 | 81,92,94,95 | 0 |
| 31 | 6MZ | CA | 1618 | 23/24 | 0.95 | 0.29 | 112,116,119,120 | 0 |
| 1 | MA6 | BA | 1519 | 24/25 | 0.95 | 0.24 | 74,77,81,83 | 0 |
| 1 | 2MG | BA | 1516 | 24/25 | 0.95 | 0.17 | 67,75,78,81 | 0 |
| 31 | PSU | CA | 746 | 20/21 | 0.95 | 0.17 | 98,101,104,104 | 0 |
| 31 | OMG | CA | 2251 | 24/25 | 0.95 | 0.18 | 69,79,82,84 | 0 |
| 31 | 1MG | CA | 745 | 24/25 | 0.96 | 0.20 | 92,96,97,98 | 0 |
| 41 | 4D4 | DN | 81[A] | 12/13 | 0.96 | 0.22 | 32,40,49,51 | 9 |
| 1 | 7MG | BA | 527 | 24/25 | 0.96 | 0.18 | 76,81,88,89 | 0 |
| 41 | 4D4 | DN | 81[B] | 12/13 | 0.96 | 0.22 | 12,25,36,36 | 9 |
| 31 | OMC | CA | 2498 | 21/22 | 0.96 | 0.25 | 82,84,89,92 | 0 |
| 1 | 4OC | BA | 1402 | 22/23 | 0.96 | 0.17 | 79,83,83,84 | 0 |
| 31 | 2MG | CA | 1835 | 24/25 | 0.96 | 0.17 | 61,72,77,78 | 0 |
| 1 | MA6 | BA | 1518 | 24/25 | 0.96 | 0.18 | 67,73,76,77 | 0 |
| 31 | PSU | CA | 2580 | 20/21 | 0.96 | 0.18 | 86,88,93,94 | 0 |
| 55 | PSU | DA | 1917 | 20/21 | 0.96 | 0.18 | 79,84,93,93 | 0 |
| 1 | UR3 | AA | 1498 | 21/22 | 0.97 | 0.16 | 58,63,67,70 | 0 |
| 1 | PSU | AA | 516 | 20/21 | 0.97 | 0.14 | 81,85,86,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 1 | 2MG | AA | 1516 | 24/25 | 0.97 | 0.16 | 58,62,63,63 | 0 |
| 1 | 5MC | AA | 1407 | 21/22 | 0.97 | 0.15 | 55,57,60,62 | 0 |
| 31 | PSU | CA | 2605 | 20/21 | 0.97 | 0.15 | 73,75,78,80 | 0 |
| 1 | UR3 | BA | 1498 | 21/22 | 0.97 | 0.15 | 81,84,87,88 | 0 |
| 55 | 2MG | DA | 1835 | 24/25 | 0.97 | 0.20 | 41,47,52,52 | 0 |
| 31 | 5MC | CA | 1962 | 21/22 | 0.97 | 0.19 | 67,69,73,76 | 0 |
| 1 | 4OC | AA | 1402 | 22/23 | 0.97 | 0.17 | 53,61,66,66 | 0 |
| 31 | 5MU | CA | 1939 | 21/22 | 0.98 | 0.17 | 70,73,82,85 | 0 |
| 1 | 7MG | AA | 527 | 24/25 | 0.98 | 0.15 | 60,65,72,74 | 0 |
| 32 | MEQ | DD | 150[B] | 10/11 | 0.98 | 0.23 | 23,32,41,41 | 10 |
| 32 | MEQ | DD | 150[A] | 10/11 | 0.98 | 0.23 | 7,15,29,31 | 10 |
| 55 | PSU | DA | 2604 | 20/21 | 0.98 | 0.17 | 41,46,56,56 | 0 |
| 1 | MA6 | AA | 1519 | 24/25 | 0.98 | 0.17 | 53,56,61,64 | 0 |
| 55 | 5MC | DA | 1962 | 21/22 | 0.98 | 0.23 | 36,44,48,49 | 0 |
| 1 | MA6 | AA | 1518 | 24/25 | 0.98 | 0.17 | 51,55,58,61 | 0 |
| 55 | 5MU | DA | 1939 | 21/22 | 0.99 | 0.19 | 35,37,41,47 | 0 |
| 55 | PSU | DA | 2580 | 20/21 | 0.99 | 0.19 | 20,25,32,34 | 0 |
| 55 | 5MU | DA | 747 | 21/22 | 0.99 | 0.18 | 28,33,36,41 | 0 |
| 55 | PSU | DA | 2605 | 20/21 | 0.99 | 0.15 | 31,41,43,43 | 0 |
| 55 | 2MG | DA | 2445 | 24/25 | 0.99 | 0.19 | 26,29,35,37 | 0 |
| 55 | 7MG | DA | 2069 | 24/25 | 0.99 | 0.18 | 32,37,41,43 | 0 |
| 55 | OMU | DA | 2552 | 21/22 | 0.99 | 0.20 | 31,34,39,46 | 0 |
| 55 | H2U | DA | 2449 | 20/21 | 0.99 | 0.19 | 25,29,31,32 | 0 |
| 55 | PSU | DA | 955 | 20/21 | 0.99 | 0.19 | 25,27,30,30 | 0 |
| 55 | 2MA | DA | 2503 | 23/24 | 0.99 | 0.19 | 21,35,41,42 | 0 |
| 55 | PSU | DA | 2504 | 20/21 | 0.99 | 0.20 | 37,40,44,44 | 0 |
| 55 | OMG | DA | 2251 | 24/25 | 0.99 | 0.18 | 27,32,37,42 | 0 |
| 55 | PSU | DA | 2457 | 20/21 | 0.99 | 0.18 | 27,31,37,37 | 0 |
| 55 | PSU | DA | 746 | 20/21 | 0.99 | 0.17 | 21,28,31,35 | 0 |
| 55 | 6MZ | DA | 1618 | 23/24 | 0.99 | 0.18 | 26,33,36,36 | 0 |
| 55 | OMC | DA | 2498 | 21/22 | 0.99 | 0.19 | 21,26,29,30 | 0 |
| 55 | 1MG | DA | 745 | 24/25 | 0.99 | 0.18 | 25,29,37,41 | 0 |
| 55 | 6MZ | DA | 2030 | 23/24 | 1.00 | 0.19 | 22,25,29,34 | 0 |

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 56 | MG | AA | 1628 | 1/1 | -0.13 | 0.61 | 159,159,159,159 | 0 |
| 56 | MG | CA | 3154 | 1/1 | 0.03 | 0.72 | 147,147,147,147 | 0 |
| 56 | MG | BA | 1639 | 1/1 | 0.19 | 0.63 | 94,94,94,94 | 0 |
| 56 | MG | BA | 1625 | 1/1 | 0.38 | 0.16 | 256,256,256,256 | 0 |
| 56 | MG | CA | 3122 | 1/1 | 0.39 | 1.73 | 126,126,126,126 | 0 |
| 56 | MG | CA | 3123 | 1/1 | 0.40 | 0.90 | 113,113,113,113 | 0 |
| 56 | MG | DA | 3168 | 1/1 | 0.43 | 0.19 | 141,141,141,141 | 0 |
| 56 | MG | CA | 3139 | 1/1 | 0.44 | 0.47 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3167 | 1/1 | 0.46 | 0.55 | 102,102,102,102 | 0 |
| 56 | MG | CA | 3075 | 1/1 | 0.46 | 1.38 | 230,230,230,230 | 0 |
| 59 | PUT | AA | 1674 | 6/6 | 0.51 | 0.87 | 133,134,135,135 | 0 |
| 56 | MG | CA | 3077 | 1/1 | 0.52 | 0.44 | 249,249,249,249 | 0 |
| 56 | MG | DA | 3129 | 1/1 | 0.55 | 0.67 | 102,102,102,102 | 0 |
| 56 | MG | AA | 1603 | 1/1 | 0.55 | 0.52 | 83,83,83,83 | 0 |
| 56 | MG | CA | 3060 | 1/1 | 0.55 | 0.28 | 234,234,234,234 | 0 |
| 56 | MG | AA | 1615 | 1/1 | 0.56 | 0.84 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1622 | 1/1 | 0.56 | 0.89 | 100,100,100,100 | 0 |
| 56 | MG | DA | 3136 | 1/1 | 0.57 | 0.33 | 77,77,77,77 | 0 |
| 56 | MG | BA | 1647 | 1/1 | 0.58 | 0.60 | 91,91,91,91 | 0 |
| 56 | MG | CA | 3140 | 1/1 | 0.59 | 0.29 | 84,84,84,84 | 0 |
| 56 | MG | CA | 3028 | 1/1 | 0.59 | 0.37 | 278,278,278,278 | 0 |
| 56 | MG | CA | 3132 | 1/1 | 0.60 | 0.59 | 105,105,105,105 | 0 |
| 56 | MG | AA | 1618 | 1/1 | 0.61 | 0.50 | 92,92,92,92 | 0 |
| 56 | MG | CA | 3124 | 1/1 | 0.62 | 0.20 | 118,118,118,118 | 0 |
| 56 | MG | CB | 201 | 1/1 | 0.62 | 0.07 | 168,168,168,168 | 0 |
| 56 | MG | CA | 3156 | 1/1 | 0.64 | 0.51 | 232,232,232,232 | 0 |
| 62 | PEG | D3 | 102 | 7/7 | 0.64 | 1.36 | 114,119,124,125 | 0 |
| 56 | MG | CA | 3136 | 1/1 | 0.64 | 0.52 | 84,84,84,84 | 0 |
| 56 | MG | CA | 3047 | 1/1 | 0.64 | 0.45 | 229,229,229,229 | 0 |
| 56 | MG | CA | 3114 | 1/1 | 0.66 | 0.48 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1626 | 1/1 | 0.66 | 1.61 | 99,99,99,99 | 0 |
| 56 | MG | DA | 3163 | 1/1 | 0.66 | 0.38 | 91,91,91,91 | 0 |
| 59 | PUT | AA | 1672 | 6/6 | 0.67 | 0.69 | 99,100,102,103 | 0 |
| 56 | MG | CA | 3131 | 1/1 | 0.67 | 0.34 | 78,78,78,78 | 0 |
| 62 | PEG | DQ | 201 | 7/7 | 0.68 | 0.97 | 124,127,128,129 | 0 |
| 56 | MG | BA | 1612 | 1/1 | 0.68 | 0.46 | 182,182,182,182 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1614 | 1/1 | 0.68 | 0.13 | 85,85,85,85 | 0 |
| 56 | MG | DA | 3128 | 1/1 | 0.69 | 0.17 | 72,72,72,72 | 0 |
| 62 | PEG | DP | 201 | 7/7 | 0.69 | 0.79 | 126,127,131,132 | 0 |
| 56 | MG | CA | 3094 | 1/1 | 0.69 | 0.15 | 105,105,105,105 | 0 |
| 56 | MG | DA | 3151 | 1/1 | 0.70 | 0.25 | 82,82,82,82 | 0 |
| 56 | MG | CA | 3006 | 1/1 | 0.70 | 0.08 | 155,155,155,155 | 0 |
| 63 | EDO | DB | 212 | 4/4 | 0.72 | 0.39 | 115,115,116,116 | 0 |
| 65 | SPD | DA | 3206 | 10/10 | 0.73 | 0.36 | 87,102,109,110 | 0 |
| 56 | MG | CA | 3130 | 1/1 | 0.73 | 0.35 | 89,89,89,89 | 0 |
| 56 | MG | BA | 1624 | 1/1 | 0.73 | 0.82 | 262,262,262,262 | 0 |
| 59 | PUT | DA | 3195 | 6/6 | 0.73 | 0.63 | 87,91,91,92 | 0 |
| 56 | MG | CA | 3002 | 1/1 | 0.73 | 0.23 | 265,265,265,265 | 0 |
| 56 | MG | DA | 3176 | 1/1 | 0.73 | 0.42 | 98,98,98,98 | 0 |
| 56 | MG | DA | 3122 | 1/1 | 0.73 | 0.87 | 100,100,100,100 | 0 |
| 69 | TRS | DA | 3220 | 8/8 | 0.73 | 0.56 | 125,128,134,134 | 0 |
| 58 | MPD | DE | 301 | 8/8 | 0.73 | 1.08 | 139,140,142,142 | 0 |
| 56 | MG | BA | 1623 | 1/1 | 0.73 | 0.59 | 248,248,248,248 | 0 |
| 56 | MG | CA | 3129 | 1/1 | 0.73 | 0.18 | 104,104,104,104 | 0 |
| 56 | MG | DA | 3179 | 1/1 | 0.74 | 0.51 | 104,104,104,104 | 0 |
| 56 | MG | DB | 206 | 1/1 | 0.74 | 1.11 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3181 | 1/1 | 0.74 | 0.58 | 83,83,83,83 | 0 |
| 62 | PEG | DA | 3200 | 7/7 | 0.75 | 0.50 | 83,85,95,96 | 0 |
| 59 | PUT | AA | 1675 | 6/6 | 0.75 | 0.48 | 106,109,109,109 | 0 |
| 56 | MG | CA | 3141 | 1/1 | 0.76 | 0.31 | 80,80,80,80 | 0 |
| 56 | MG | CA | 3034 | 1/1 | 0.76 | 0.19 | 246,246,246,246 | 0 |
| 56 | MG | CA | 3135 | 1/1 | 0.76 | 0.38 | 101,101,101,101 | 0 |
| 62 | PEG | DA | 3218 | 7/7 | 0.76 | 0.36 | 123,129,133,134 | 0 |
| 56 | MG | BA | 1641 | 1/1 | 0.77 | 0.20 | 120,120,120,120 | 0 |
| 56 | MG | DA | 3180 | 1/1 | 0.77 | 2.06 | 106,106,106,106 | 0 |
| 62 | PEG | DA | 3199 | 7/7 | 0.77 | 0.48 | 80,89,93,95 | 0 |
| 56 | MG | DA | 3165 | 1/1 | 0.77 | 0.30 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1613 | 1/1 | 0.77 | 1.07 | 65,65,65,65 | 0 |
| 56 | MG | CA | 3111 | 1/1 | 0.77 | 0.25 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3166 | 1/1 | 0.77 | 1.04 | 81,81,81,81 | 0 |
| 56 | MG | CA | 3055 | 1/1 | 0.77 | 0.14 | 169,169,169,169 | 0 |
| 56 | MG | AA | 1612 | 1/1 | 0.78 | 0.43 | 77,77,77,77 | 0 |
| 59 | PUT | DA | 3219 | 6/6 | 0.78 | 0.37 | 70,75,78,79 | 0 |
| 58 | MPD | DT | 202 | 8/8 | 0.78 | 0.38 | 128,128,130,130 | 0 |
| 64 | PGE | D1 | 102 | 10/10 | 0.78 | 0.50 | 122,127,128,128 | 0 |
| 56 | MG | CA | 3003 | 1/1 | 0.78 | 1.90 | 278,278,278,278 | 0 |
| 56 | MG | CA | 3115 | 1/1 | 0.78 | 0.35 | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3127 | 1/1 | 0.78 | 0.14 | 73,73,73,73 | 0 |
| 56 | MG | DB | 207 | 1/1 | 0.78 | 0.56 | 92,92,92,92 | 0 |
| 56 | MG | CA | 3007 | 1/1 | 0.79 | 0.32 | 214,214,214,214 | 0 |
| 56 | MG | DA | 3142 | 1/1 | 0.79 | 0.31 | 62,62,62,62 | 0 |
| 56 | MG | BA | 1603 | 1/1 | 0.79 | 0.20 | 263,263,263,263 | 0 |
| 56 | MG | CA | 3031 | 1/1 | 0.79 | 0.08 | 64,64,64,64 | 0 |
| 56 | MG | BA | 1606 | 1/1 | 0.79 | 0.19 | 227,227,227,227 | 0 |
| 63 | EDO | DA | 3209 | 4/4 | 0.80 | 0.28 | 135,136,137,138 | 0 |
| 56 | MG | CA | 3125 | 1/1 | 0.80 | 0.33 | 89,89,89,89 | 0 |
| 58 | MPD | DA | 3204 | 8/8 | 0.80 | 0.61 | 112,114,117,117 | 0 |
| 64 | PGE | DS | 201 | 10/10 | 0.80 | 0.37 | 77,89,91,92 | 0 |
| 56 | MG | AA | 1616 | 1/1 | 0.80 | 0.97 | 85,85,85,85 | 0 |
| 63 | EDO | DB | 211 | 4/4 | 0.80 | 0.39 | 88,90,92,92 | 0 |
| 57 | PG4 | DR | 202 | 13/13 | 0.80 | 0.35 | 109,117,120,121 | 0 |
| 56 | MG | CA | 3080 | 1/1 | 0.81 | 0.17 | 151,151,151,151 | 0 |
| 56 | MG | CA | 3145 | 1/1 | 0.81 | 0.79 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3171 | 1/1 | 0.81 | 0.69 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3172 | 1/1 | 0.81 | 0.34 | 103,103,103,103 | 0 |
| 58 | MPD | DK | 201 | 8/8 | 0.81 | 0.29 | 120,121,123,124 | 0 |
| 56 | MG | DA | 3143 | 1/1 | 0.81 | 0.59 | 114,114,114,114 | 0 |
| 61 | ZN | C5 | 101 | 1/1 | 0.81 | 0.06 | 149,149,149,149 | 0 |
| 56 | MG | DA | 3137 | 1/1 | 0.81 | 0.68 | 37,37,37,37 | 1 |
| 56 | MG | AA | 1617 | 1/1 | 0.81 | 0.32 | 96,96,96,96 | 0 |
| 56 | MG | DA | 3152 | 1/1 | 0.81 | 0.42 | 66,66,66,66 | 0 |
| 56 | MG | CA | 3038 | 1/1 | 0.82 | 0.28 | 263,263,263,263 | 0 |
| 56 | MG | AA | 1624 | 1/1 | 0.82 | 0.44 | 95,95,95,95 | 0 |
| 56 | MG | CA | 3128 | 1/1 | 0.82 | 0.28 | 75,75,75,75 | 0 |
| 60 | T1C | BA | 1643 | 42/42 | 0.82 | 0.23 | 170,174,179,179 | 0 |
| 56 | MG | DA | 3123 | 1/1 | 0.82 | 0.19 | 62,62,62,62 | 0 |
| 67 | ACY | DA | 3196 | 4/4 | 0.82 | 0.30 | 84,85,87,87 | 0 |
| 62 | PEG | D1 | 103 | 7/7 | 0.82 | 0.38 | 85,90,91,91 | 0 |
| 56 | MG | AA | 1627 | 1/1 | 0.82 | 0.54 | 91,91,91,91 | 0 |
| 56 | MG | DA | 3147 | 1/1 | 0.82 | 0.24 | 65,65,65,65 | 0 |
| 59 | PUT | AA | 1673 | 6/6 | 0.82 | 0.64 | 100,102,103,104 | 0 |
| 56 | MG | AA | 1606 | 1/1 | 0.82 | 0.28 | 91,91,91,91 | 0 |
| 58 | MPD | DN | 201 | 8/8 | 0.83 | 0.36 | 106,111,116,117 | 0 |
| 59 | PUT | DA | 3221 | 6/6 | 0.83 | 0.48 | 138,140,141,141 | 0 |
| 59 | PUT | DA | 3222 | 6/6 | 0.83 | 0.34 | 48,52,57,58 | 0 |
| 56 | MG | DA | 3162 | 1/1 | 0.83 | 0.34 | 85,85,85,85 | 0 |
| 56 | MG | BA | 1640 | 1/1 | 0.83 | 0.42 | 124,124,124,124 | 0 |
| 56 | MG | CA | 3078 | 1/1 | 0.83 | 0.16 | 149,149,149,149 | 0 |
| 56 | MG | CA | 3005 | 1/1 | 0.83 | 0.60 | 237,237,237,237 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3160 | 1/1 | 0.83 | 0.61 | 74,74,74,74 | 0 |
| 56 | MG | CA | 3146 | 1/1 | 0.83 | 0.15 | 144,144,144,144 | 0 |
| 57 | PG4 | AA | 1670 | 13/13 | 0.83 | 0.25 | 78,87,97,97 | 0 |
| 56 | MG | CA | 3113 | 1/1 | 0.83 | 0.41 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3177 | 1/1 | 0.84 | 0.41 | 77,77,77,77 | 0 |
| 56 | MG | CA | 3149 | 1/1 | 0.84 | 0.31 | 67,67,67,67 | 0 |
| 56 | MG | CA | 3106 | 1/1 | 0.84 | 0.24 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3182 | 1/1 | 0.84 | 0.32 | 61,61,61,61 | 0 |
| 56 | MG | BA | 1644 | 1/1 | 0.84 | 0.13 | 133,133,133,133 | 0 |
| 56 | MG | CA | 3119 | 1/1 | 0.84 | 0.43 | 89,89,89,89 | 0 |
| 56 | MG | DA | 3153 | 1/1 | 0.84 | 0.45 | 52,52,52,52 | 0 |
| 62 | PEG | DA | 3227 | 7/7 | 0.84 | 0.38 | 97,99,103,104 | 0 |
| 56 | MG | CA | 3152 | 1/1 | 0.85 | 0.35 | 151,151,151,151 | 0 |
| 56 | MG | CA | 3070 | 1/1 | 0.85 | 0.09 | 91,91,91,91 | 0 |
| 56 | MG | BA | 1646 | 1/1 | 0.85 | 0.11 | 108,108,108,108 | 0 |
| 63 | EDO | DB | 201 | 4/4 | 0.85 | 0.31 | 94,97,98,99 | 0 |
| 56 | MG | CA | 3071 | 1/1 | 0.85 | 0.13 | 166,166,166,166 | 0 |
| 56 | MG | CA | 3116 | 1/1 | 0.85 | 0.34 | 95,95,95,95 | 0 |
| 57 | PG4 | DA | 3193 | 13/13 | 0.85 | 0.84 | 85,95,100,101 | 0 |
| 64 | PGE | D3 | 101 | 10/10 | 0.85 | 0.61 | 97,99,102,103 | 0 |
| 56 | MG | CA | 3063 | 1/1 | 0.85 | 0.17 | 125,125,125,125 | 0 |
| 56 | MG | BA | 1637 | 1/1 | 0.85 | 0.66 | 85,85,85,85 | 0 |
| 58 | MPD | DT | 201 | 8/8 | 0.85 | 0.34 | 102,108,109,109 | 0 |
| 56 | MG | DB | 208 | 1/1 | 0.85 | 0.71 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3140 | 1/1 | 0.86 | 0.27 | 54,54,54,54 | 0 |
| 63 | EDO | DA | 3002 | 4/4 | 0.86 | 0.71 | 93,94,95,95 | 0 |
| 62 | PEG | DL | 201 | 7/7 | 0.86 | 0.28 | 82,85,87,87 | 0 |
| 63 | EDO | DA | 3194 | 4/4 | 0.86 | 0.27 | 76,77,78,78 | 0 |
| 56 | MG | CA | 3105 | 1/1 | 0.86 | 0.31 | 262,262,262,262 | 0 |
| 56 | MG | AA | 1661 | 1/1 | 0.86 | 0.24 | 173,173,173,173 | 0 |
| 56 | MG | CA | 3142 | 1/1 | 0.86 | 0.42 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3131 | 1/1 | 0.86 | 0.21 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3022 | 1/1 | 0.86 | 0.83 | 195,195,195,195 | 0 |
| 56 | MG | DA | 3170 | 1/1 | 0.86 | 0.40 | 77,77,77,77 | 0 |
| 58 | MPD | DA | 3190 | 8/8 | 0.86 | 0.32 | 95,97,99,102 | 0 |
| 59 | PUT | DA | 3205 | 6/6 | 0.86 | 0.37 | 108,109,111,111 | 0 |
| 56 | MG | AA | 1621 | 1/1 | 0.86 | 0.51 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3133 | 1/1 | 0.86 | 0.41 | 91,91,91,91 | 0 |
| 56 | MG | DA | 3155 | 1/1 | 0.86 | 0.38 | 58,58,58,58 | 0 |
| 57 | PG4 | DA | 3216 | 13/13 | 0.86 | 0.32 | 99,104,109,110 | 0 |
| 56 | MG | CA | 3126 | 1/1 | 0.86 | 0.20 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3146 | 1/1 | 0.87 | 0.19 | 122,122,122,122 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CB | 203 | 1/1 | 0.87 | 0.08 | 145,145,145,145 | 0 |
| 59 | PUT | DA | 3189 | 6/6 | 0.87 | 0.43 | 45,54,56,56 | 0 |
| 56 | MG | CA | 3056 | 1/1 | 0.87 | 0.35 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1625 | 1/1 | 0.87 | 0.35 | 86,86,86,86 | 0 |
| 56 | MG | AA | 1609 | 1/1 | 0.87 | 0.33 | 89,89,89,89 | 0 |
| 56 | MG | CA | 3076 | 1/1 | 0.87 | 0.19 | 182,182,182,182 | 0 |
| 56 | MG | DA | 3141 | 1/1 | 0.88 | 0.32 | 86,86,86,86 | 0 |
| 56 | MG | CA | 3108 | 1/1 | 0.88 | 0.22 | 83,83,83,83 | 0 |
| 56 | MG | DR | 201 | 1/1 | 0.88 | 0.57 | 42,42,42,42 | 0 |
| 65 | SPD | DA | 3224 | 10/10 | 0.88 | 0.28 | 50,54,66,68 | 0 |
| 56 | MG | CA | 3001 | 1/1 | 0.88 | 0.18 | 296,296,296,296 | 0 |
| 57 | PG4 | DS | 202 | 13/13 | 0.88 | 0.34 | 43,51,72,73 | 0 |
| 59 | PUT | DA | 3213 | 6/6 | 0.88 | 0.32 | 105,107,110,110 | 0 |
| 56 | MG | CA | 3057 | 1/1 | 0.88 | 0.17 | 133,133,133,133 | 0 |
| 56 | MG | DA | 3132 | 1/1 | 0.88 | 0.31 | 70,70,70,70 | 0 |
| 58 | MPD | DE | 302 | 8/8 | 0.88 | 0.68 | 93,97,102,102 | 0 |
| 59 | PUT | DA | 3184 | 6/6 | 0.88 | 0.26 | 78,80,81,82 | 0 |
| 56 | MG | AA | 1601 | 1/1 | 0.88 | 0.68 | 67,67,67,67 | 0 |
| 58 | MPD | DA | 3192 | 8/8 | 0.89 | 0.49 | 95,100,104,105 | 0 |
| 56 | MG | CA | 3068 | 1/1 | 0.89 | 0.38 | 216,216,216,216 | 0 |
| 60 | T1C | AA | 1680 | 42/42 | 0.89 | 0.26 | 96,107,123,124 | 0 |
| 63 | EDO | DA | 3208 | 4/4 | 0.89 | 0.22 | 89,90,90,91 | 0 |
| 56 | MG | BA | 1609 | 1/1 | 0.89 | 0.12 | 166,166,166,166 | 0 |
| 56 | MG | CA | 3133 | 1/1 | 0.89 | 0.33 | 72,72,72,72 | 0 |
| 56 | MG | AA | 1605 | 1/1 | 0.89 | 0.64 | 89,89,89,89 | 0 |
| 56 | MG | BA | 1614 | 1/1 | 0.89 | 0.18 | 171,171,171,171 | 0 |
| 66 | 1PE | DA | 3202 | 16/16 | 0.89 | 0.29 | 61,64,72,73 | 0 |
| 56 | MG | CA | 3019 | 1/1 | 0.89 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | CA | 3151 | 1/1 | 0.89 | 0.42 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3110 | 1/1 | 0.89 | 0.34 | 295,295,295,295 | 0 |
| 57 | PG4 | DQ | 202 | 13/13 | 0.89 | 0.21 | 60,63,76,76 | 0 |
| 56 | MG | AA | 1642 | 1/1 | 0.89 | 0.25 | 158,158,158,158 | 0 |
| 56 | MG | AA | 1620 | 1/1 | 0.89 | 0.25 | 78,78,78,78 | 0 |
| 62 | PEG | DA | 3226 | 7/7 | 0.89 | 0.24 | 89,91,98,98 | 0 |
| 56 | MG | CA | 3064 | 1/1 | 0.89 | 0.36 | 249,249,249,249 | 0 |
| 56 | MG | CA | 3061 | 1/1 | 0.89 | 0.11 | 247,247,247,247 | 0 |
| 56 | MG | CA | 3059 | 1/1 | 0.89 | 0.10 | 86,86,86,86 | 0 |
| 56 | MG | DB | 209 | 1/1 | 0.90 | 0.37 | 66,66,66,66 | 0 |
| 64 | PGE | DA | 3214 | 10/10 | 0.90 | 0.38 | 72,73,77,78 | 0 |
| 56 | MG | AA | 1608 | 1/1 | 0.90 | 0.47 | 96,96,96,96 | 0 |
| 56 | MG | CA | 3110 | 1/1 | 0.90 | 0.19 | 93,93,93,93 | 0 |
| 56 | MG | CA | 3048 | 1/1 | 0.90 | 0.12 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3120 | 1/1 | 0.90 | 0.17 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3130 | 1/1 | 0.90 | 0.24 | 54,54,54,54 | 0 |
| 63 | EDO | D1 | 101 | 4/4 | 0.90 | 0.24 | 59,60,60,60 | 0 |
| 64 | PGE | DU | 101 | 10/10 | 0.90 | 0.55 | 89,97,104,105 | 0 |
| 56 | MG | AA | 1638 | 1/1 | 0.90 | 0.07 | 114,114,114,114 | 0 |
| 56 | MG | CA | 3112 | 1/1 | 0.90 | 0.24 | 75,75,75,75 | 0 |
| 56 | MG | CA | 3072 | 1/1 | 0.90 | 0.64 | 249,249,249,249 | 0 |
| 56 | MG | CA | 3009 | 1/1 | 0.90 | 0.19 | 243,243,243,243 | 0 |
| 56 | MG | CA | 3134 | 1/1 | 0.90 | 0.17 | 108,108,108,108 | 0 |
| 56 | MG | BA | 1645 | 1/1 | 0.90 | 0.15 | 102,102,102,102 | 0 |
| 59 | PUT | DA | 3212 | 6/6 | 0.90 | 0.23 | 81,84,85,85 | 0 |
| 56 | MG | DA | 3121 | 1/1 | 0.90 | 0.59 | 68,68,68,68 | 0 |
| 56 | MG | CA | 3008 | 1/1 | 0.91 | 0.10 | 136,136,136,136 | 0 |
| 56 | MG | BA | 1635 | 1/1 | 0.91 | 0.10 | 102,102,102,102 | 0 |
| 56 | MG | BA | 1638 | 1/1 | 0.91 | 0.58 | 78,78,78,78 | 0 |
| 56 | MG | DB | 210 | 1/1 | 0.91 | 0.46 | 97,97,97,97 | 0 |
| 57 | PG4 | BA | 1642 | 13/13 | 0.91 | 0.58 | 88,89,99,100 | 0 |
| 65 | SPD | DA | 3183 | 10/10 | 0.91 | 0.61 | 79,83,87,87 | 0 |
| 56 | MG | CA | 3093 | 1/1 | 0.91 | 0.11 | 88,88,88,88 | 0 |
| 56 | MG | DA | 3061 | 1/1 | 0.91 | 0.15 | 233,233,233,233 | 0 |
| 56 | MG | CA | 3012 | 1/1 | 0.91 | 0.17 | 95,95,95,95 | 0 |
| 68 | GUN | DA | 3211 | 11/11 | 0.91 | 0.29 | 98,100,101,102 | 0 |
| 56 | MG | CA | 3090 | 1/1 | 0.91 | 0.25 | 185,185,185,185 | 0 |
| 56 | MG | BA | 1608 | 1/1 | 0.91 | 0.11 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3178 | 1/1 | 0.91 | 0.45 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1654 | 1/1 | 0.91 | 0.39 | 262,262,262,262 | 0 |
| 56 | MG | CA | 3107 | 1/1 | 0.91 | 0.35 | 83,83,83,83 | 0 |
| 64 | PGE | DA | 3203 | 10/10 | 0.91 | 0.31 | 83,85,88,90 | 0 |
| 58 | MPD | AA | 1676 | 8/8 | 0.91 | 0.42 | 95,99,100,101 | 0 |
| 56 | MG | DA | 3145 | 1/1 | 0.91 | 0.25 | 79,79,79,79 | 0 |
| 56 | MG | CA | 3046 | 1/1 | 0.91 | 0.13 | 111,111,111,111 | 0 |
| 58 | MPD | DA | 3207 | 8/8 | 0.91 | 0.40 | 77,78,80,80 | 0 |
| 56 | MG | DA | 3174 | 1/1 | 0.91 | 0.24 | 74,74,74,74 | 0 |
| 56 | MG | CA | 3137 | 1/1 | 0.91 | 0.20 | 106,106,106,106 | 0 |
| 56 | MG | CA | 3036 | 1/1 | 0.91 | 0.17 | 193,193,193,193 | 0 |
| 56 | MG | CA | 3023 | 1/1 | 0.91 | 0.08 | 158,158,158,158 | 0 |
| 56 | MG | CA | 3053 | 1/1 | 0.91 | 0.16 | 65,65,65,65 | 0 |
| 56 | MG | CB | 202 | 1/1 | 0.91 | 0.10 | 116,116,116,116 | 0 |
| 66 | 1PE | DA | 3185 | 16/16 | 0.91 | 0.24 | 50,55,84,87 | 0 |
| 56 | MG | CA | 3109 | 1/1 | 0.91 | 0.25 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1659 | 1/1 | 0.91 | 0.10 | 115,115,115,115 | 0 |
| 56 | MG | AA | 1604 | 1/1 | 0.92 | 0.39 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3150 | 1/1 | 0.92 | 0.96 | 75,75,75,75 | 0 |
| 59 | PUT | DA | 3188 | 6/6 | 0.92 | 0.26 | 50,53,55,56 | 0 |
| 56 | MG | BA | 1619 | 1/1 | 0.92 | 0.19 | 96,96,96,96 | 0 |
| 56 | MG | CA | 3051 | 1/1 | 0.92 | 0.20 | 80,80,80,80 | 0 |
| 64 | PGE | DA | 3217 | 10/10 | 0.92 | 0.34 | 85,88,91,92 | 0 |
| 63 | EDO | DA | 3215 | 4/4 | 0.92 | 0.25 | 65,66,68,70 | 0 |
| 56 | MG | CA | 3029 | 1/1 | 0.92 | 0.20 | 143,143,143,143 | 0 |
| 56 | MG | CA | 3026 | 1/1 | 0.92 | 0.87 | 173,173,173,173 | 0 |
| 56 | MG | CA | 3101 | 1/1 | 0.92 | 0.15 | 151,151,151,151 | 0 |
| 56 | MG | DA | 3157 | 1/1 | 0.92 | 0.54 | 73,73,73,73 | 0 |
| 56 | MG | BA | 1617 | 1/1 | 0.92 | 0.12 | 131,131,131,131 | 0 |
| 56 | MG | CA | 3054 | 1/1 | 0.92 | 0.15 | 156,156,156,156 | 0 |
| 56 | MG | AA | 1623 | 1/1 | 0.92 | 0.37 | 69,69,69,69 | 0 |
| 56 | MG | CA | 3086 | 1/1 | 0.92 | 0.07 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1665 | 1/1 | 0.92 | 0.30 | 161,161,161,161 | 0 |
| 56 | MG | AA | 1658 | 1/1 | 0.92 | 0.08 | 98,98,98,98 | 0 |
| 56 | MG | AA | 1602 | 1/1 | 0.92 | 0.30 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3175 | 1/1 | 0.92 | 0.48 | 63,63,63,63 | 0 |
| 62 | PEG | AL | 201 | 7/7 | 0.93 | 0.34 | 83,85,94,95 | 0 |
| 56 | MG | BA | 1629 | 1/1 | 0.93 | 0.45 | 168,168,168,168 | 0 |
| 56 | MG | DA | 3011 | 1/1 | 0.93 | 0.18 | 115,115,115,115 | 0 |
| 56 | MG | CA | 3010 | 1/1 | 0.93 | 0.13 | 234,234,234,234 | 0 |
| 56 | MG | DA | 3120 | 1/1 | 0.93 | 0.21 | 70,70,70,70 | 0 |
| 56 | MG | BA | 1627 | 1/1 | 0.93 | 0.53 | 124,124,124,124 | 0 |
| 56 | MG | CA | 3155 | 1/1 | 0.93 | 0.17 | 156,156,156,156 | 0 |
| 56 | MG | DA | 3126 | 1/1 | 0.93 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | CA | 3079 | 1/1 | 0.93 | 0.07 | 115,115,115,115 | 0 |
| 56 | MG | CA | 3138 | 1/1 | 0.93 | 0.08 | 66,66,66,66 | 0 |
| 56 | MG | CA | 3083 | 1/1 | 0.93 | 0.16 | 204,204,204,204 | 0 |
| 56 | MG | CA | 3092 | 1/1 | 0.93 | 0.12 | 152,152,152,152 | 0 |
| 64 | PGE | DA | 3225 | 10/10 | 0.93 | 0.23 | 73,83,94,96 | 0 |
| 56 | MG | AA | 1678 | 1/1 | 0.93 | 0.17 | 78,78,78,78 | 0 |
| 56 | MG | CA | 3089 | 1/1 | 0.93 | 0.19 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1677 | 1/1 | 0.93 | 0.10 | 194,194,194,194 | 0 |
| 63 | EDO | DA | 3197 | 4/4 | 0.93 | 0.23 | 65,67,68,69 | 0 |
| 56 | MG | CA | 3018 | 1/1 | 0.93 | 0.08 | 85,85,85,85 | 0 |
| 56 | MG | CA | 3021 | 1/1 | 0.93 | 1.26 | 264,264,264,264 | 0 |
| 56 | MG | CA | 3014 | 1/1 | 0.93 | 0.18 | 216,216,216,216 | 0 |
| 56 | MG | BA | 1630 | 1/1 | 0.93 | 0.05 | 153,153,153,153 | 0 |
| 56 | MG | CA | 3082 | 1/1 | 0.93 | 0.24 | 114,114,114,114 | 0 |
| 56 | MG | BA | 1605 | 1/1 | 0.93 | 0.09 | 107,107,107,107 | 0 |
| 56 | MG | CA | 3148 | 1/1 | 0.93 | 0.48 | 51,51,51,51 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3032 | 1/1 | 0.93 | 0.17 | 241,241,241,241 | 0 |
| 56 | MG | CA | 3040 | 1/1 | 0.94 | 0.08 | 76,76,76,76 | 0 |
| 56 | MG | AA | 1619 | 1/1 | 0.94 | 0.23 | 92,92,92,92 | 0 |
| 56 | MG | DA | 3124 | 1/1 | 0.94 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1667 | 1/1 | 0.94 | 0.11 | 47,47,47,47 | 0 |
| 63 | EDO | DA | 3198 | 4/4 | 0.94 | 0.38 | 78,81,83,83 | 0 |
| 56 | MG | DA | 3036 | 1/1 | 0.94 | 0.22 | 24,24,24,24 | 0 |
| 56 | MG | AA | 1664 | 1/1 | 0.94 | 0.49 | 212,212,212,212 | 0 |
| 56 | MG | CA | 3050 | 1/1 | 0.94 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | CA | 3104 | 1/1 | 0.94 | 0.37 | 258,258,258,258 | 0 |
| 56 | MG | BA | 1604 | 1/1 | 0.94 | 0.17 | 153,153,153,153 | 0 |
| 56 | MG | CA | 3066 | 1/1 | 0.94 | 0.18 | 89,89,89,89 | 0 |
| 58 | MPD | AA | 1671 | 8/8 | 0.94 | 0.55 | 88,88,90,92 | 0 |
| 56 | MG | DA | 3156 | 1/1 | 0.94 | 0.23 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1663 | 1/1 | 0.94 | 0.10 | 90,90,90,90 | 0 |
| 56 | MG | CA | 3067 | 1/1 | 0.94 | 0.32 | 277,277,277,277 | 0 |
| 56 | MG | DA | 3138 | 1/1 | 0.94 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | BA | 1602 | 1/1 | 0.94 | 0.10 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1611 | 1/1 | 0.94 | 0.24 | 108,108,108,108 | 0 |
| 56 | MG | AA | 1656 | 1/1 | 0.94 | 0.19 | 196,196,196,196 | 0 |
| 56 | MG | CA | 3037 | 1/1 | 0.94 | 0.40 | 189,189,189,189 | 0 |
| 56 | MG | AA | 1610 | 1/1 | 0.94 | 0.24 | 90,90,90,90 | 0 |
| 56 | MG | AA | 1632 | 1/1 | 0.94 | 0.05 | 94,94,94,94 | 0 |
| 56 | MG | CA | 3020 | 1/1 | 0.94 | 0.10 | 86,86,86,86 | 0 |
| 58 | MPD | DA | 3210 | 8/8 | 0.94 | 0.29 | 87,89,90,91 | 0 |
| 56 | MG | CA | 3084 | 1/1 | 0.94 | 0.47 | 174,174,174,174 | 0 |
| 56 | MG | BA | 1633 | 1/1 | 0.94 | 0.11 | 229,229,229,229 | 0 |
| 56 | MG | CA | 3069 | 1/1 | 0.94 | 0.19 | 88,88,88,88 | 0 |
| 56 | MG | CA | 3143 | 1/1 | 0.94 | 0.18 | 70,70,70,70 | 0 |
| 56 | MG | BA | 1610 | 1/1 | 0.94 | 0.05 | 93,93,93,93 | 0 |
| 56 | MG | CA | 3004 | 1/1 | 0.94 | 0.07 | 159,159,159,159 | 0 |
| 56 | MG | AA | 1641 | 1/1 | 0.94 | 0.07 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1645 | 1/1 | 0.94 | 0.13 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3161 | 1/1 | 0.95 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | CA | 3065 | 1/1 | 0.95 | 0.19 | 109,109,109,109 | 0 |
| 56 | MG | CA | 3118 | 1/1 | 0.95 | 0.39 | 59,59,59,59 | 0 |
| 56 | MG | CA | 3117 | 1/1 | 0.95 | 0.35 | 67,67,67,67 | 0 |
| 63 | EDO | DB | 213 | 4/4 | 0.95 | 0.19 | 82,82,84,84 | 0 |
| 56 | MG | DA | 3169 | 1/1 | 0.95 | 0.20 | 69,69,69,69 | 0 |
| 56 | MG | CA | 3058 | 1/1 | 0.95 | 0.16 | 98,98,98,98 | 0 |
| 56 | MG | BA | 1616 | 1/1 | 0.95 | 0.10 | 122,122,122,122 | 0 |
| 56 | MG | CA | 3035 | 1/1 | 0.95 | 0.19 | 91,91,91,91 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3044 | 1/1 | 0.95 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3053 | 1/1 | 0.95 | 0.13 | 89,89,89,89 | 0 |
| 56 | MG | DA | 3043 | 1/1 | 0.95 | 0.07 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3116 | 1/1 | 0.95 | 0.14 | 72,72,72,72 | 0 |
| 56 | MG | CA | 3016 | 1/1 | 0.95 | 0.29 | 107,107,107,107 | 0 |
| 56 | MG | CA | 3088 | 1/1 | 0.95 | 0.08 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3099 | 1/1 | 0.95 | 0.28 | 160,160,160,160 | 0 |
| 56 | MG | AA | 1655 | 1/1 | 0.95 | 0.17 | 163,163,163,163 | 0 |
| 59 | PUT | DA | 3001 | 6/6 | 0.95 | 0.17 | 46,50,58,60 | 0 |
| 59 | PUT | DA | 3223 | 6/6 | 0.95 | 0.27 | 61,62,65,67 | 0 |
| 56 | MG | DA | 3064 | 1/1 | 0.95 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3154 | 1/1 | 0.95 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | AA | 1650 | 1/1 | 0.96 | 0.07 | 114,114,114,114 | 0 |
| 56 | MG | CA | 3030 | 1/1 | 0.96 | 0.07 | 78,78,78,78 | 0 |
| 56 | MG | CA | 3147 | 1/1 | 0.96 | 0.56 | 58,58,58,58 | 1 |
| 56 | MG | DA | 3135 | 1/1 | 0.96 | 0.20 | 72,72,72,72 | 0 |
| 56 | MG | CA | 3081 | 1/1 | 0.96 | 0.07 | 104,104,104,104 | 0 |
| 56 | MG | CA | 3039 | 1/1 | 0.96 | 0.20 | 175,175,175,175 | 0 |
| 56 | MG | CA | 3015 | 1/1 | 0.96 | 0.19 | 51,51,51,51 | 0 |
| 56 | MG | CA | 3144 | 1/1 | 0.96 | 0.06 | 49,49,49,49 | 0 |
| 64 | PGE | DA | 3186 | 10/10 | 0.96 | 0.18 | 39,48,55,57 | 0 |
| 56 | MG | CA | 3098 | 1/1 | 0.96 | 0.07 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1636 | 1/1 | 0.96 | 0.22 | 97,97,97,97 | 0 |
| 56 | MG | DA | 3042 | 1/1 | 0.96 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | BA | 1626 | 1/1 | 0.96 | 0.09 | 102,102,102,102 | 0 |
| 56 | MG | CA | 3033 | 1/1 | 0.96 | 0.09 | 110,110,110,110 | 0 |
| 56 | MG | CA | 3017 | 1/1 | 0.96 | 0.09 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1630 | 1/1 | 0.96 | 0.12 | 134,134,134,134 | 0 |
| 56 | MG | CA | 3062 | 1/1 | 0.96 | 0.12 | 175,175,175,175 | 0 |
| 56 | MG | AA | 1639 | 1/1 | 0.96 | 0.11 | 118,118,118,118 | 0 |
| 56 | MG | AA | 1657 | 1/1 | 0.96 | 0.38 | 136,136,136,136 | 0 |
| 56 | MG | DA | 3173 | 1/1 | 0.96 | 0.33 | 98,98,98,98 | 0 |
| 67 | ACY | DA | 3201 | 4/4 | 0.96 | 0.21 | 78,79,79,79 | 0 |
| 56 | MG | BA | 1634 | 1/1 | 0.96 | 0.06 | 99,99,99,99 | 0 |
| 56 | MG | BA | 1628 | 1/1 | 0.96 | 0.15 | 89,89,89,89 | 0 |
| 56 | MG | DA | 3073 | 1/1 | 0.97 | 0.05 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3119 | 1/1 | 0.97 | 0.40 | 57,57,57,57 | 0 |
| 56 | MG | AA | 1666 | 1/1 | 0.97 | 0.06 | 57,57,57,57 | 0 |
| 56 | MG | CA | 3091 | 1/1 | 0.97 | 0.08 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1669 | 1/1 | 0.97 | 0.27 | 134,134,134,134 | 0 |
| 56 | MG | AA | 1607 | 1/1 | 0.97 | 0.45 | 65,65,65,65 | 0 |
| 56 | MG | BA | 1622 | 1/1 | 0.97 | 0.07 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DB | 202 | 1/1 | 0.97 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3080 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | CA | 3013 | 1/1 | 0.97 | 0.10 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3027 | 1/1 | 0.97 | 0.11 | 94,94,94,94 | 0 |
| 56 | MG | AA | 1679 | 1/1 | 0.97 | 0.16 | 77,77,77,77 | 0 |
| 56 | MG | BA | 1636 | 1/1 | 0.97 | 0.43 | 72,72,72,72 | 0 |
| 67 | ACY | DA | 3191 | 4/4 | 0.97 | 0.20 | 68,70,70,71 | 0 |
| 56 | MG | CA | 3085 | 1/1 | 0.97 | 0.08 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3106 | 1/1 | 0.97 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | AA | 1629 | 1/1 | 0.97 | 0.18 | 93,93,93,93 | 0 |
| 56 | MG | CA | 3042 | 1/1 | 0.97 | 0.08 | 88,88,88,88 | 0 |
| 56 | MG | DA | 3048 | 1/1 | 0.97 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | CA | 3043 | 1/1 | 0.97 | 0.07 | 81,81,81,81 | 0 |
| 56 | MG | DA | 3144 | 1/1 | 0.97 | 0.12 | 72,72,72,72 | 0 |
| 56 | MG | AA | 1668 | 1/1 | 0.97 | 0.11 | 75,75,75,75 | 0 |
| 56 | MG | BA | 1607 | 1/1 | 0.97 | 0.35 | 207,207,207,207 | 0 |
| 56 | MG | DA | 3088 | 1/1 | 0.97 | 0.17 | 24,24,24,24 | 0 |
| 56 | MG | AA | 1649 | 1/1 | 0.97 | 0.07 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1634 | 1/1 | 0.97 | 0.12 | 130,130,130,130 | 0 |
| 56 | MG | CA | 3052 | 1/1 | 0.97 | 0.10 | 68,68,68,68 | 0 |
| 56 | MG | CA | 3097 | 1/1 | 0.97 | 0.09 | 90,90,90,90 | 0 |
| 56 | MG | CA | 3121 | 1/1 | 0.97 | 0.13 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3117 | 1/1 | 0.97 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3158 | 1/1 | 0.97 | 0.28 | 191,191,191,191 | 0 |
| 56 | MG | DA | 3066 | 1/1 | 0.97 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | CA | 3024 | 1/1 | 0.97 | 0.05 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3125 | 1/1 | 0.97 | 0.34 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3148 | 1/1 | 0.97 | 0.15 | 61,61,61,61 | 0 |
| 65 | SPD | DA | 3187 | 10/10 | 0.97 | 0.25 | 34,42,45,48 | 0 |
| 56 | MG | CA | 3074 | 1/1 | 0.97 | 0.24 | 131,131,131,131 | 0 |
| 56 | MG | AA | 1644 | 1/1 | 0.97 | 0.17 | 106,106,106,106 | 0 |
| 56 | MG | DA | 3134 | 1/1 | 0.97 | 0.07 | 96,96,96,96 | 0 |
| 56 | MG | DA | 3139 | 1/1 | 0.97 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | BA | 1621 | 1/1 | 0.97 | 0.21 | 33,33,33,33 | 0 |
| 56 | MG | CA | 3102 | 1/1 | 0.97 | 0.17 | 113,113,113,113 | 0 |
| 56 | MG | DA | 3127 | 1/1 | 0.97 | 0.92 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3164 | 1/1 | 0.97 | 0.53 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1640 | 1/1 | 0.97 | 0.11 | 73,73,73,73 | 0 |
| 56 | MG | BA | 1601 | 1/1 | 0.97 | 0.22 | 106,106,106,106 | 0 |
| 56 | MG | CA | 3087 | 1/1 | 0.97 | 0.13 | 77,77,77,77 | 0 |
| 56 | MG | CA | 3073 | 1/1 | 0.97 | 0.28 | 222,222,222,222 | 0 |
| 56 | MG | CA | 3049 | 1/1 | 0.98 | 0.11 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3153 | 1/1 | 0.98 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | BA | 1615 | 1/1 | 0.98 | 0.06 | 72,72,72,72 | 0 |
| 56 | MG | AA | 1633 | 1/1 | 0.98 | 0.14 | 123,123,123,123 | 0 |
| 56 | MG | DA | 3118 | 1/1 | 0.98 | 0.41 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3091 | 1/1 | 0.98 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | BA | 1631 | 1/1 | 0.98 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3008 | 1/1 | 0.98 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3069 | 1/1 | 0.98 | 0.10 | 79,79,79,79 | 0 |
| 56 | MG | AA | 1647 | 1/1 | 0.98 | 0.24 | 179,179,179,179 | 0 |
| 56 | MG | DA | 3006 | 1/1 | 0.98 | 0.07 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3097 | 1/1 | 0.98 | 0.13 | 128,128,128,128 | 0 |
| 61 | ZN | AB | 301 | 1/1 | 0.98 | 0.19 | 171,171,171,171 | 0 |
| 56 | MG | AA | 1660 | 1/1 | 0.98 | 0.15 | 284,284,284,284 | 0 |
| 56 | MG | CA | 3027 | 1/1 | 0.98 | 0.18 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3005 | 1/1 | 0.98 | 0.06 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3109 | 1/1 | 0.98 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | CA | 3103 | 1/1 | 0.98 | 0.15 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3071 | 1/1 | 0.98 | 0.23 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3025 | 1/1 | 0.98 | 0.10 | 108,108,108,108 | 0 |
| 56 | MG | DA | 3030 | 1/1 | 0.98 | 0.13 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3039 | 1/1 | 0.98 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3051 | 1/1 | 0.98 | 0.10 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3021 | 1/1 | 0.98 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | AA | 1653 | 1/1 | 0.98 | 0.05 | 50,50,50,50 | 0 |
| 56 | MG | CA | 3096 | 1/1 | 0.98 | 0.06 | 61,61,61,61 | 0 |
| 56 | MG | AA | 1637 | 1/1 | 0.98 | 0.05 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3031 | 1/1 | 0.98 | 0.20 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3079 | 1/1 | 0.98 | 0.11 | 119,119,119,119 | 0 |
| 56 | MG | DA | 3096 | 1/1 | 0.98 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3029 | 1/1 | 0.98 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3102 | 1/1 | 0.98 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3092 | 1/1 | 0.98 | 0.20 | 35,35,35,35 | 0 |
| 56 | MG | BA | 1632 | 1/1 | 0.98 | 0.12 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3093 | 1/1 | 0.98 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1631 | 1/1 | 0.98 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3003 | 1/1 | 0.98 | 0.11 | 85,85,85,85 | 0 |
| 56 | MG | DA | 3068 | 1/1 | 0.98 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | BA | 1613 | 1/1 | 0.98 | 0.16 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3087 | 1/1 | 0.98 | 0.08 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3078 | 1/1 | 0.98 | 0.22 | 96,96,96,96 | 0 |
| 56 | MG | DA | 3076 | 1/1 | 0.98 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3098 | 1/1 | 0.98 | 0.14 | 23,23,23,23 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 1618 | 1/1 | 0.98 | 0.11 | 129,129,129,129 | 0 |
| 56 | MG | DA | 3150 | 1/1 | 0.98 | 0.31 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3032 | 1/1 | 0.98 | 0.15 | 27,27,27,27 | 0 |
| 56 | MG | AA | 1643 | 1/1 | 0.98 | 0.11 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1662 | 1/1 | 0.98 | 0.15 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3065 | 1/1 | 0.98 | 0.14 | 45,45,45,45 | 0 |
| 58 | MPD | DS | 203 | 8/8 | 0.98 | 0.19 | 48,52,58,59 | 0 |
| 56 | MG | AA | 1648 | 1/1 | 0.98 | 0.07 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3077 | 1/1 | 0.98 | 0.05 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3099 | 1/1 | 0.99 | 0.15 | 31,31,31,31 | 0 |
| 56 | MG | DM | 201 | 1/1 | 0.99 | 0.05 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3082 | 1/1 | 0.99 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | DB | 204 | 1/1 | 0.99 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3017 | 1/1 | 0.99 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3038 | 1/1 | 0.99 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3070 | 1/1 | 0.99 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3113 | 1/1 | 0.99 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3054 | 1/1 | 0.99 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3004 | 1/1 | 0.99 | 0.13 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3015 | 1/1 | 0.99 | 0.17 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3075 | 1/1 | 0.99 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3114 | 1/1 | 0.99 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3049 | 1/1 | 0.99 | 0.16 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3095 | 1/1 | 0.99 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3067 | 1/1 | 0.99 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3014 | 1/1 | 0.99 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | CA | 3045 | 1/1 | 0.99 | 0.07 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3105 | 1/1 | 0.99 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | CA | 3100 | 1/1 | 0.99 | 0.22 | 92,92,92,92 | 0 |
| 56 | MG | AA | 1651 | 1/1 | 0.99 | 0.11 | 76,76,76,76 | 0 |
| 56 | MG | AA | 1646 | 1/1 | 0.99 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3104 | 1/1 | 0.99 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3229 | 1/1 | 0.99 | 0.06 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3231 | 1/1 | 0.99 | 0.28 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3055 | 1/1 | 0.99 | 0.20 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3081 | 1/1 | 0.99 | 0.06 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3063 | 1/1 | 0.99 | 0.12 | 72,72,72,72 | 0 |
| 56 | MG | DB | 205 | 1/1 | 0.99 | 0.18 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3012 | 1/1 | 0.99 | 0.18 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3009 | 1/1 | 0.99 | 0.12 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3019 | 1/1 | 0.99 | 0.07 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3022 | 1/1 | 0.99 | 0.18 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3101 | 1/1 | 0.99 | 0.11 | 42,42,42,42 | 0 |
| 56 | MG | CA | 3011 | 1/1 | 0.99 | 0.11 | 59,59,59,59 | 0 |
| 61 | ZN | D5 | 101 | 1/1 | 0.99 | 0.10 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3047 | 1/1 | 0.99 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3024 | 1/1 | 0.99 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3018 | 1/1 | 0.99 | 0.24 | 8,8,8,8 | 0 |
| 56 | MG | DA | 3026 | 1/1 | 0.99 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3149 | 1/1 | 0.99 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3041 | 1/1 | 0.99 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | BA | 1620 | 1/1 | 0.99 | 0.09 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3094 | 1/1 | 0.99 | 0.12 | 80,80,80,80 | 0 |
| 56 | MG | CA | 3025 | 1/1 | 0.99 | 0.07 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1652 | 1/1 | 0.99 | 0.23 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3085 | 1/1 | 0.99 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | DB | 203 | 1/1 | 0.99 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3086 | 1/1 | 0.99 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3028 | 1/1 | 0.99 | 0.17 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3058 | 1/1 | 0.99 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | BA | 1611 | 1/1 | 0.99 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3050 | 1/1 | 0.99 | 0.10 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3084 | 1/1 | 0.99 | 0.08 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3041 | 1/1 | 0.99 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3090 | 1/1 | 0.99 | 0.16 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3107 | 1/1 | 0.99 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3100 | 1/1 | 0.99 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3230 | 1/1 | 0.99 | 0.05 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3037 | 1/1 | 0.99 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3007 | 1/1 | 0.99 | 0.07 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1635 | 1/1 | 0.99 | 0.10 | 104,104,104,104 | 0 |
| 56 | MG | DA | 3115 | 1/1 | 0.99 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3035 | 1/1 | 0.99 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3046 | 1/1 | 0.99 | 0.08 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3059 | 1/1 | 0.99 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3052 | 1/1 | 0.99 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | DD | 301 | 1/1 | 0.99 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3045 | 1/1 | 0.99 | 0.17 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3056 | 1/1 | 0.99 | 0.11 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3089 | 1/1 | 0.99 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3040 | 1/1 | 0.99 | 0.23 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3083 | 1/1 | 0.99 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3016 | 1/1 | 1.00 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3159 | 1/1 | 1.00 | 0.13 | 72,72,72,72 | 0 |

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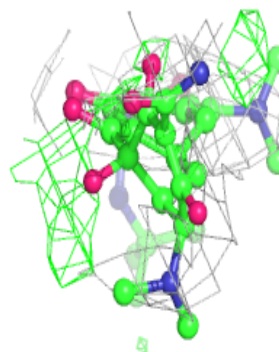
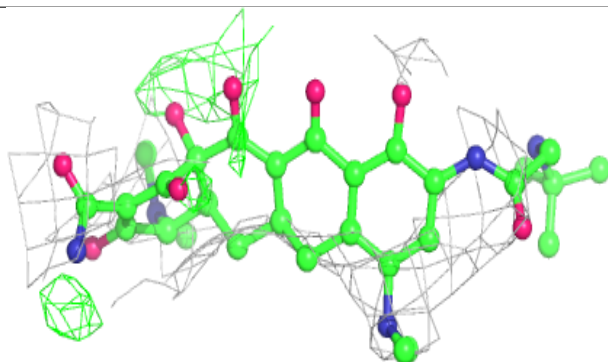
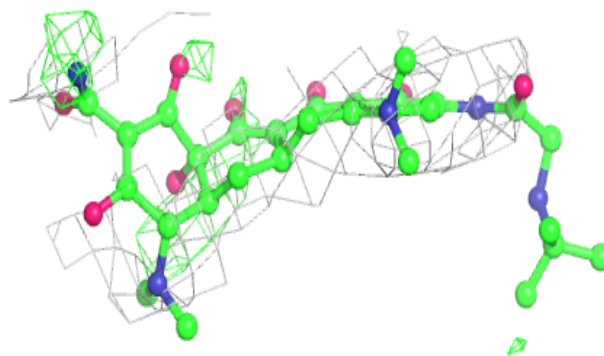
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3108 | 1/1 | 1.00 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3013 | 1/1 | 1.00 | 0.17 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3103 | 1/1 | 1.00 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3020 | 1/1 | 1.00 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3034 | 1/1 | 1.00 | 0.18 | 35,35,35,35 | 0 |
| 56 | MG | CA | 3095 | 1/1 | 1.00 | 0.06 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3057 | 1/1 | 1.00 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3111 | 1/1 | 1.00 | 0.17 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3074 | 1/1 | 1.00 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3112 | 1/1 | 1.00 | 0.08 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3072 | 1/1 | 1.00 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3228 | 1/1 | 1.00 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3010 | 1/1 | 1.00 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3033 | 1/1 | 1.00 | 0.12 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3062 | 1/1 | 1.00 | 0.09 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3060 | 1/1 | 1.00 | 0.16 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3044 | 1/1 | 1.00 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3023 | 1/1 | 1.00 | 0.16 | 29,29,29,29 | 0 |

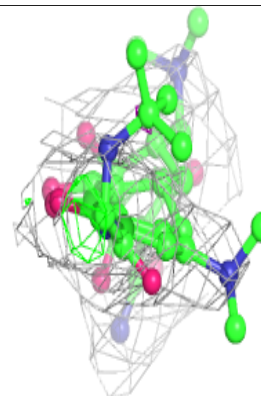
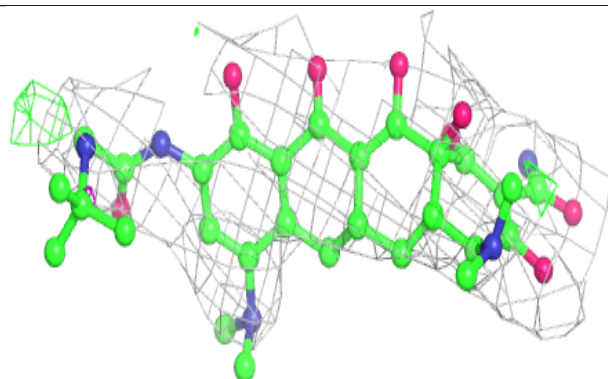
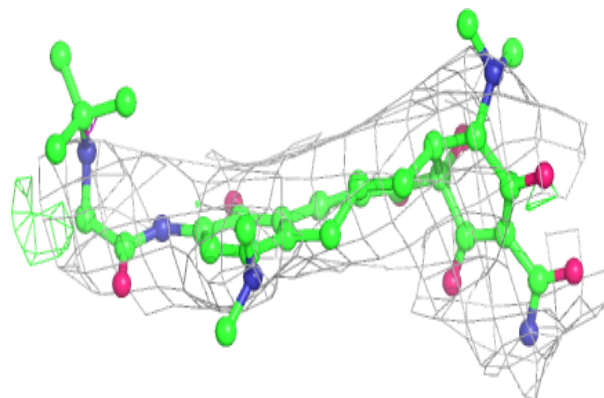
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around T1C BA 1643:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around T1C AA 1680:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.