



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 08:51 am BST

PDB ID : 4V55
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin and ribosome recycling factor (RRF).
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-17
Resolution : 4.00 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

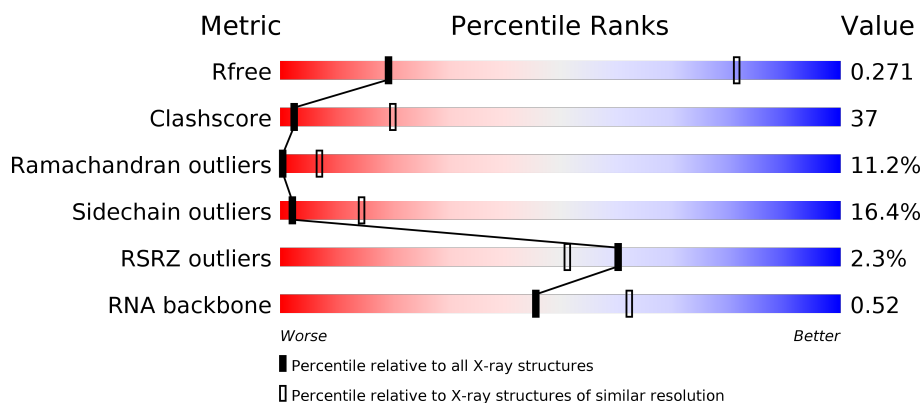
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1087 (4.30-3.70) |
| Clashscore | 141614 | 1148 (4.30-3.70) |
| Ramachandran outliers | 138981 | 1108 (4.30-3.70) |
| Sidechain outliers | 138945 | 1099 (4.30-3.70) |
| RSRZ outliers | 127900 | 1028 (4.34-3.66) |
| RNA backbone | 3102 | 1048 (5.00-3.00) |

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 | 1542 | <div> <div>24%</div> <div>62%</div> <div>12%</div> <div>..</div> </div> |
| 1 | CA | 1542 | <div> <div>22%</div> <div>65%</div> <div>12%</div> <div>..</div> </div> |
| 2 | AC | 232 | <div> <div>29%</div> <div>48%</div> <div>11%</div> <div>11%</div> </div> |
| 2 | CC | 232 | <div> <div>28%</div> <div>49%</div> <div>12%</div> <div>11%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AD | 205 | |
| 3 | CD | 205 | |
| 4 | AE | 166 | |
| 4 | CE | 166 | |
| 5 | AF | 135 | |
| 5 | CF | 135 | |
| 6 | AG | 178 | |
| 6 | CG | 178 | |
| 7 | AH | 129 | |
| 7 | CH | 129 | |
| 8 | AI | 129 | |
| 8 | CI | 129 | |
| 9 | AJ | 103 | |
| 9 | CJ | 103 | |
| 10 | AK | 128 | |
| 10 | CK | 128 | |
| 11 | AL | 123 | |
| 11 | CL | 123 | |
| 12 | AM | 117 | |
| 12 | CM | 117 | |
| 13 | AN | 100 | |
| 13 | CN | 100 | |
| 14 | AO | 89 | |
| 14 | CO | 89 | |
| 15 | AP | 82 | |

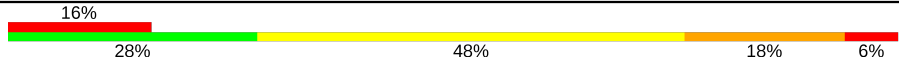
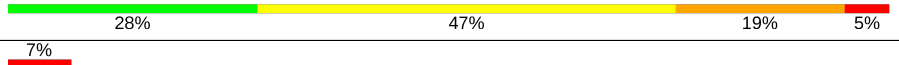
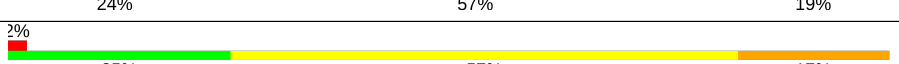
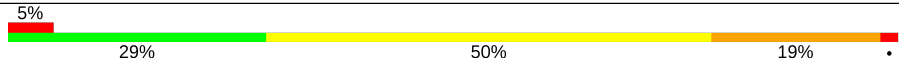
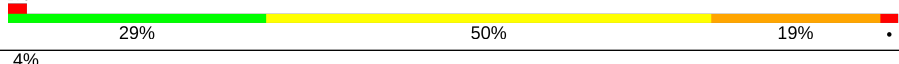

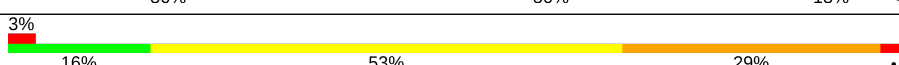
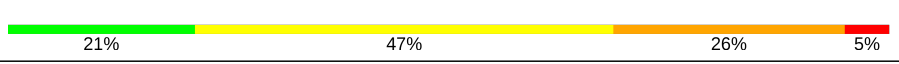
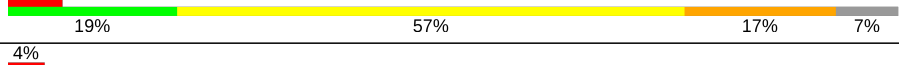
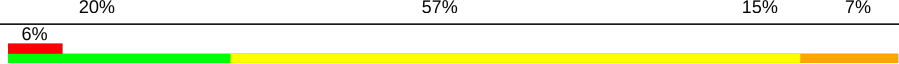
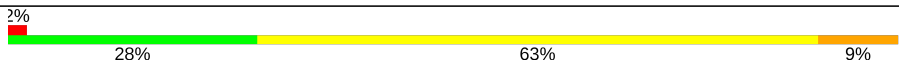

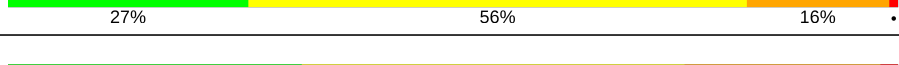
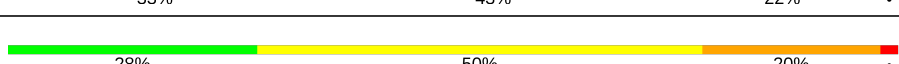
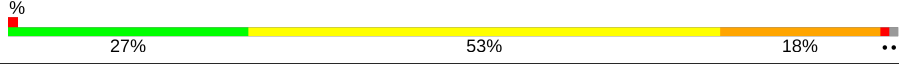
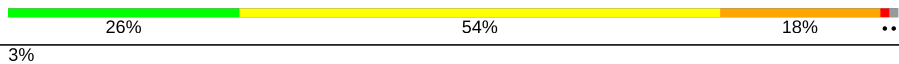
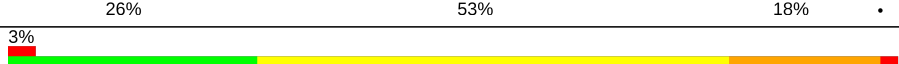
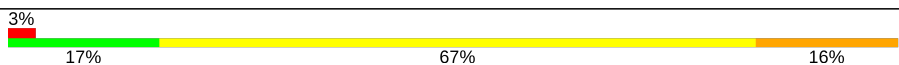
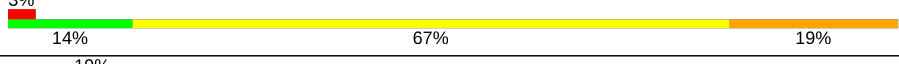




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | CP | 82 | |
| 16 | AQ | 83 | |
| 16 | CQ | 83 | |
| 17 | AR | 74 | |
| 17 | CR | 74 | |
| 18 | AS | 91 | |
| 18 | CS | 91 | |
| 19 | AT | 86 | |
| 19 | CT | 86 | |
| 20 | AB | 240 | |
| 20 | CB | 240 | |
| 21 | AU | 70 | |
| 21 | CU | 70 | |
| 22 | BA | 120 | |
| 22 | DA | 120 | |
| 23 | BB | 2904 | |
| 23 | DB | 2904 | |
| 24 | BI | 141 | |
| 24 | DI | 141 | |
| 25 | BC | 272 | |
| 25 | DC | 272 | |
| 26 | BD | 209 | |
| 26 | DD | 209 | |
| 27 | BK | 123 | |
| 27 | DK | 123 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | BP | 114 |  |
| 28 | DP | 114 |  |
| 29 | BE | 201 |  |
| 29 | DE | 201 |  |
| 30 | BY | 58 |  |
| 30 | DY | 58 |  |
| 31 | B0 | 56 |  |
| 31 | D0 | 56 |  |
| 32 | B4 | 38 |  |
| 32 | D4 | 38 |  |
| 33 | B1 | 54 |  |
| 33 | D1 | 54 |  |
| 34 | B3 | 64 |  |
| 34 | D3 | 64 |  |
| 35 | BV | 94 |  |
| 35 | DV | 94 |  |
| 36 | B2 | 46 |  |
| 36 | D2 | 46 |  |
| 37 | BL | 144 |  |
| 37 | DL | 144 |  |
| 38 | BM | 136 |  |
| 38 | DM | 136 |  |
| 39 | BX | 63 |  |
| 39 | DX | 63 | |
| 40 | BH | 149 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | DH | 149 | |
| 41 | BJ | 142 | |
| 41 | DJ | 142 | |
| 42 | BN | 127 | |
| 42 | DN | 127 | |
| 43 | BO | 117 | |
| 43 | DO | 117 | |
| 44 | BQ | 117 | |
| 44 | DQ | 117 | |
| 45 | BS | 110 | |
| 45 | DS | 110 | |
| 46 | BU | 103 | |
| 46 | DU | 103 | |
| 47 | BF | 178 | |
| 47 | DF | 178 | |
| 48 | BG | 176 | |
| 48 | DG | 176 | |
| 49 | BR | 103 | |
| 49 | DR | 103 | |
| 50 | BT | 100 | |
| 50 | DT | 100 | |
| 51 | BZ | 78 | |
| 51 | DZ | 78 | |
| 52 | BW | 84 | |
| 52 | DW | 84 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | B6 | 185 | |
| 53 | D6 | 185 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | AA | 1625 | - | - | - | X |
| 54 | MG | AA | 1637 | - | - | - | X |
| 54 | MG | AA | 1647 | - | - | - | X |
| 54 | MG | AA | 1656 | - | - | - | X |
| 54 | MG | AA | 1657 | - | - | - | X |
| 54 | MG | AA | 1659 | - | - | - | X |
| 54 | MG | BB | 3033 | - | - | - | X |

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287083 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 | 1530 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32831 | 14642 | 6024 | 10635 | 1530 | | | |
| 1 | CA | 1530 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32831 | 14642 | 6024 | 10635 | 1530 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | | |
| 2 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |
| 3 | CD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | AE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |
| 4 | CE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |
| 5 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AG | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1174 | 730 | 226 | 214 | 4 | | | |
| 6 | CG | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1196 | 745 | 230 | 217 | 4 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |
| 7 | CH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 8 | CI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 634 | 206 | 178 | 3 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | AJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |
| 9 | CJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |

- Molecule 10 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | CK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |
| 11 | CL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | | |
| 12 | CM | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 541 | 177 | 155 | 3 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |
| 13 | CN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | AO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |
| 14 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 15 | CP | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 400 | 126 | 111 | 1 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | | |
| 16 | CQ | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 657 | 417 | 122 | 115 | 3 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17 | AR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |
| 17 | CR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | AS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 637 | 408 | 120 | 107 | 2 | | | |
| 18 | CS | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 644 | 413 | 121 | 108 | 2 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |
| 19 | CT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 20 | AB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |
| 20 | CB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21 | AU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |
| 21 | CU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |

- Molecule 22 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 22 | BA | 117 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2507 | 1116 | 459 | 815 | 117 | | | |
| 22 | DA | 117 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2507 | 1116 | 459 | 815 | 117 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 23 | BB | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60995 | 27210 | 11229 | 19715 | 2841 | | | |
| 23 | DB | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60995 | 27210 | 11229 | 19715 | 2841 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | BI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 24 | DI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 25 | BC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |
| 25 | DC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | BD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | DD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | BK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |
| 27 | DK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |
| 28 | DP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 29 | DE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | BY | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |
| 30 | DY | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | B0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 31 | D0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32 | B4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 32 | D4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 33 | B1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |
| 33 | D1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 34 | B3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 34 | D3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 35 | DV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 36 | B2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 36 | D2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |
| 37 | DL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |
| 38 | DM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 39 | BX | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |
| 39 | DX | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |
| 40 | DH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |
| 41 | DJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | DN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 43 | BO | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |
| 43 | DO | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |

- Molecule 44 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 44 | BQ | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |
| 44 | DQ | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |

- Molecule 45 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |
| 45 | DS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 46 | BU | 102 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | | |
| 46 | DU | 102 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | | |

- Molecule 47 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | BF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |
| 47 | DF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | BG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 48 | DG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | BR | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |
| 49 | DR | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | BT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |
| 50 | DT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51 | BZ | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 51 | DZ | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | BW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |
| 52 | DW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |

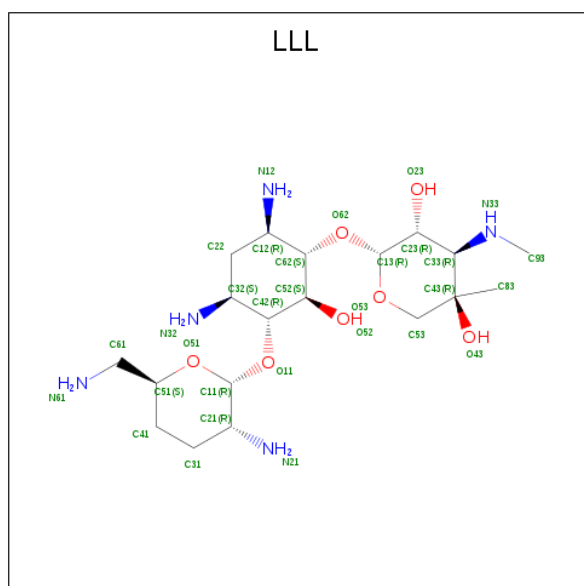
- Molecule 53 is a protein called 50S ribosomal protein RRF.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53 | B6 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1478 | 924 | 270 | 282 | 2 | | | |
| 53 | D6 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1478 | 924 | 270 | 282 | 2 | | | |

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54 | DB | 111 | Total | Mg | 0 | 0 |
| | | | 111 | 111 | | |
| 54 | BB | 110 | Total | Mg | 0 | 0 |
| | | | 110 | 110 | | |
| 54 | AA | 60 | Total | Mg | 0 | 0 |
| | | | 60 | 60 | | |
| 54 | CA | 61 | Total | Mg | 0 | 0 |
| | | | 61 | 61 | | |
| 54 | CE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 55 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 55 | AA | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 55 | BB | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 55 | CA | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 55 | DB | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 57 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57 | AA | 287 | Total | O | 0 | 0 |
| | | | 287 | 287 | | |
| 57 | AE | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | AK | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | AL | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | AN | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 57 | AT | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | BB | 492 | Total | O | 0 | 0 |
| | | | 492 | 492 | | |
| 57 | BC | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 57 | BD | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | BE | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | BL | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | BT | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

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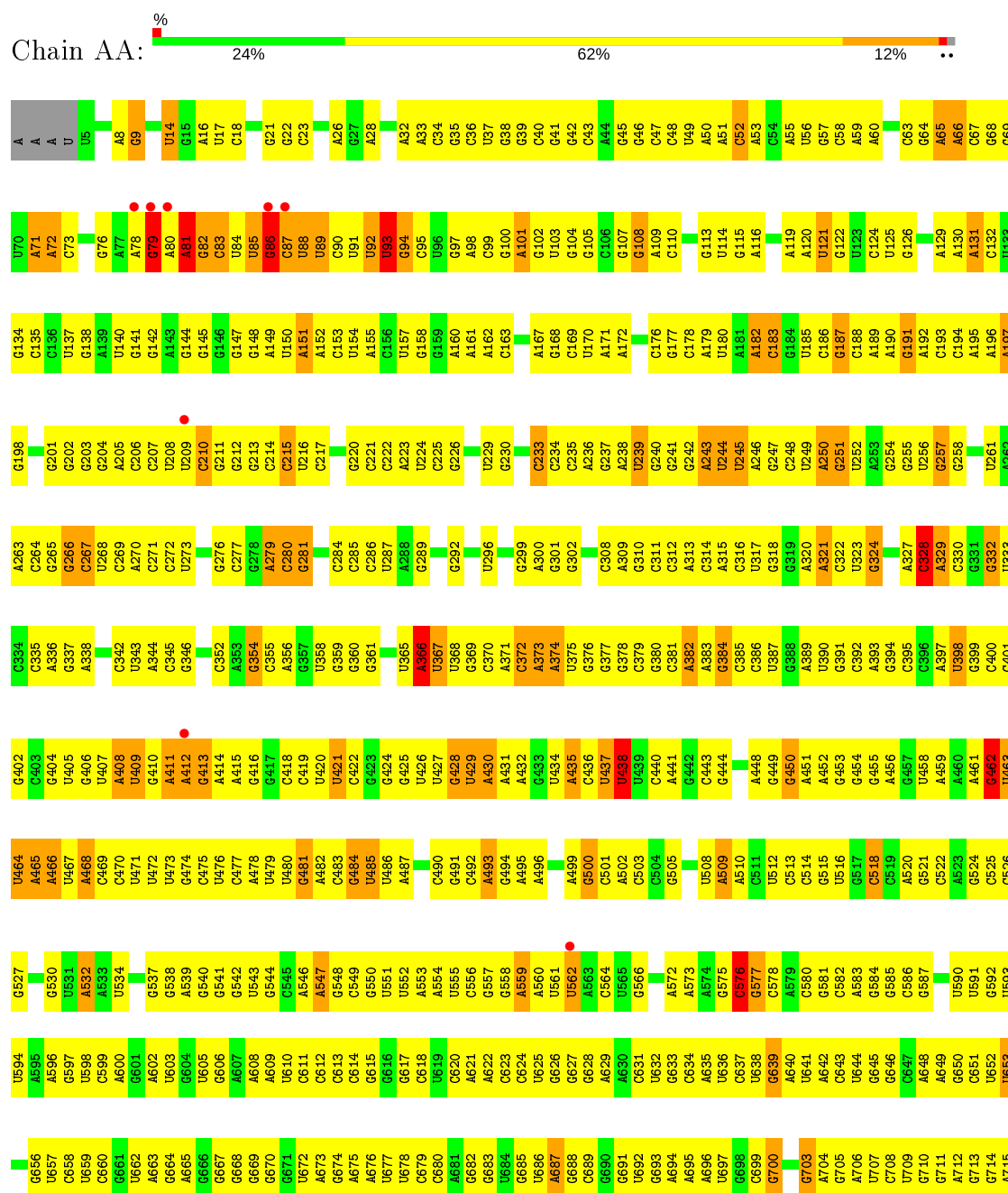
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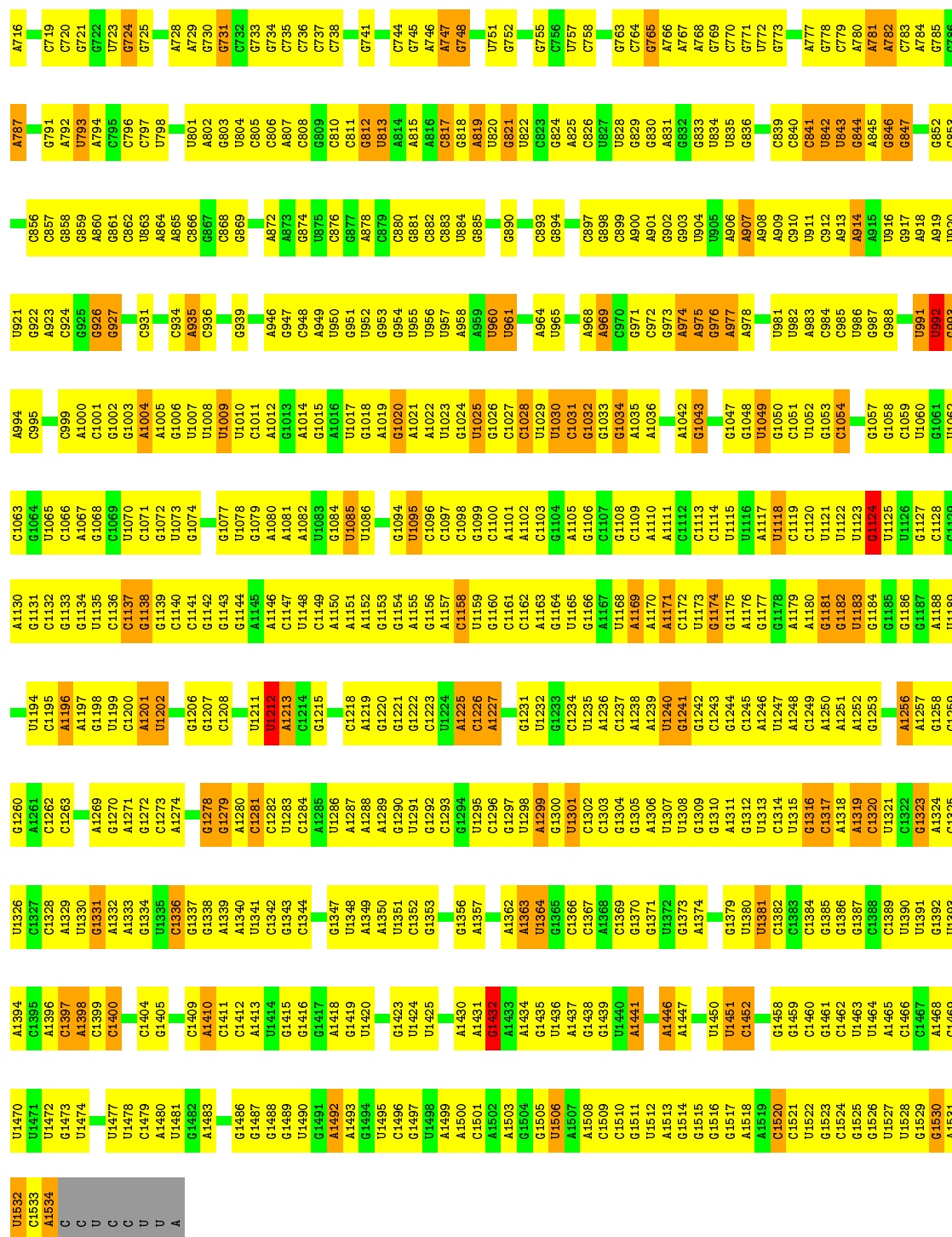
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 57 | CA | 296 | Total 296 | O 296 | 0 | 0 |
| 57 | CE | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | CK | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | CL | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | CN | 4 | Total 4 | O 4 | 0 | 0 |
| 57 | CT | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | DB | 500 | Total 500 | O 500 | 0 | 0 |
| 57 | DC | 6 | Total 6 | O 6 | 0 | 0 |
| 57 | DE | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | DL | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | DR | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | DT | 1 | Total 1 | O 1 | 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.

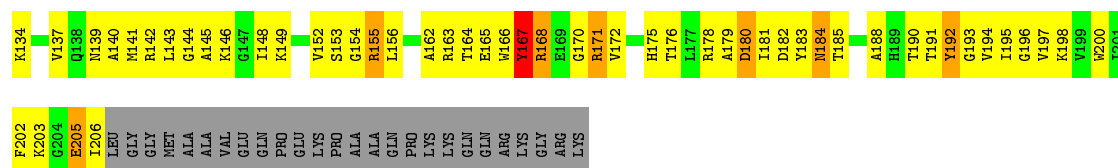
• Molecule 1: 16S rRNA



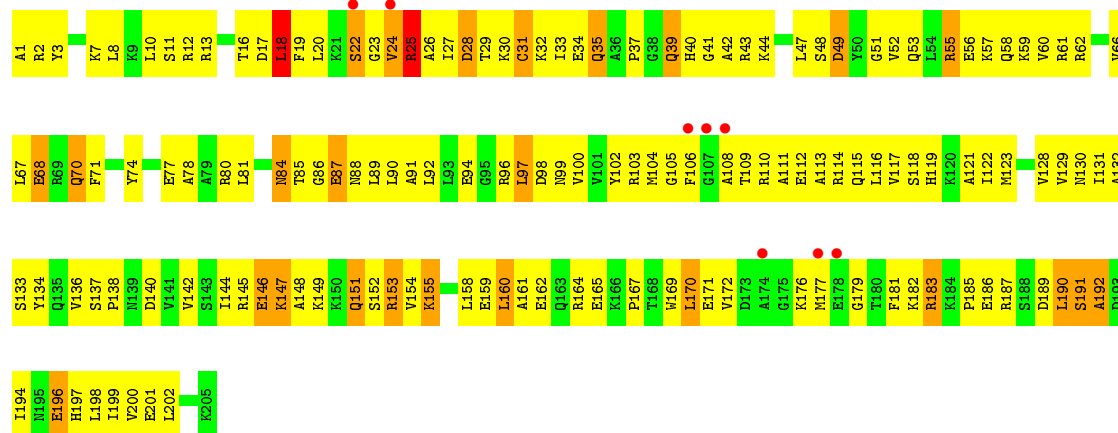




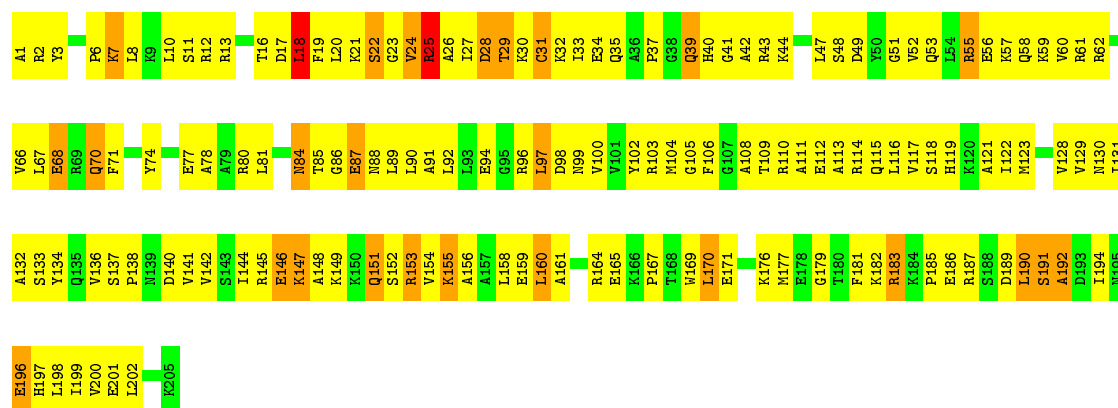




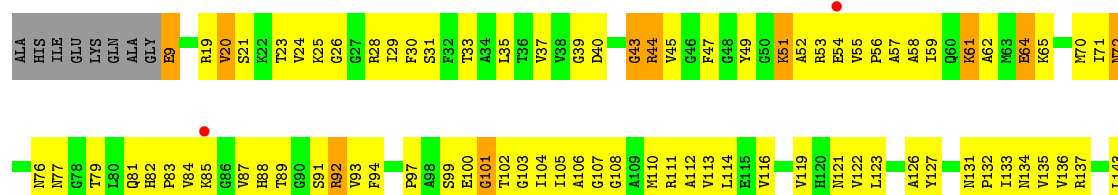
• Molecule 3: 30S ribosomal protein S4

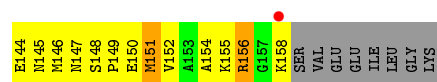


• Molecule 3: 30S ribosomal protein S4

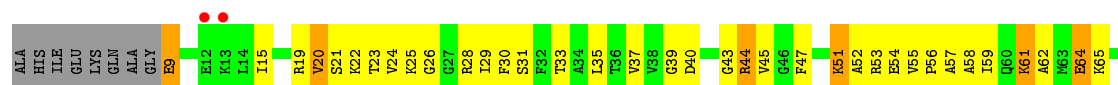


• Molecule 4: 30S ribosomal protein S5

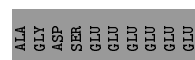
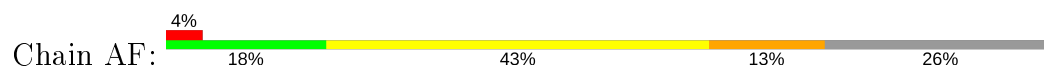




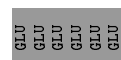
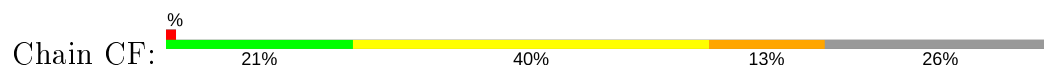
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6



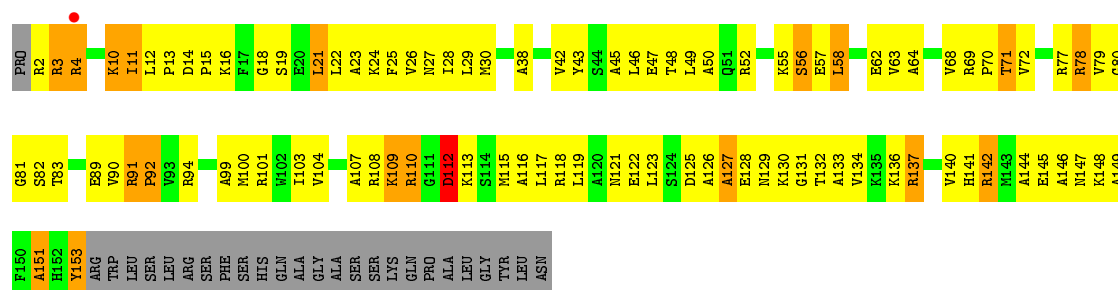
• Molecule 5: 30S ribosomal protein S6



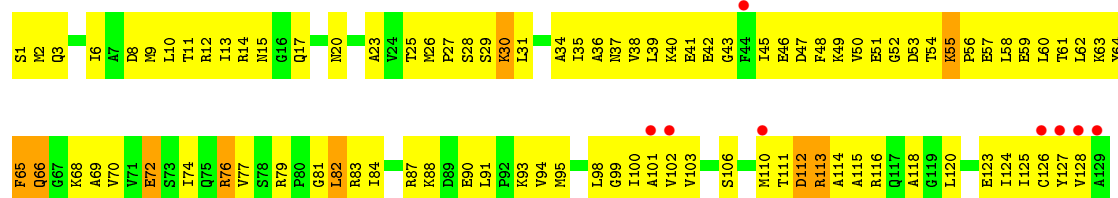
• Molecule 6: 30S ribosomal protein S7



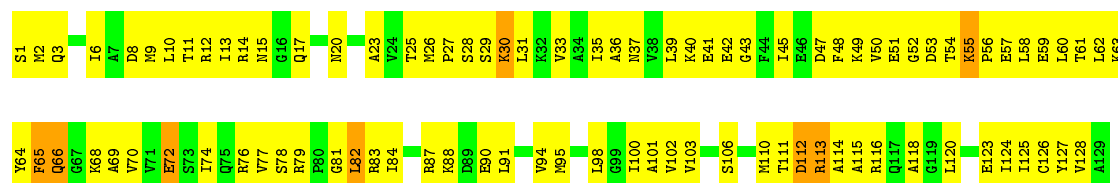
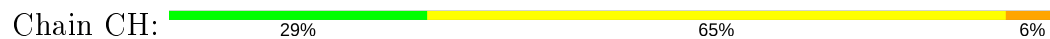
- Molecule 6: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S8

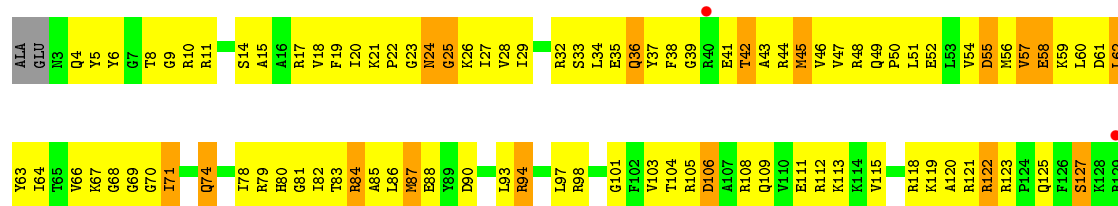


- Molecule 7: 30S ribosomal protein S8

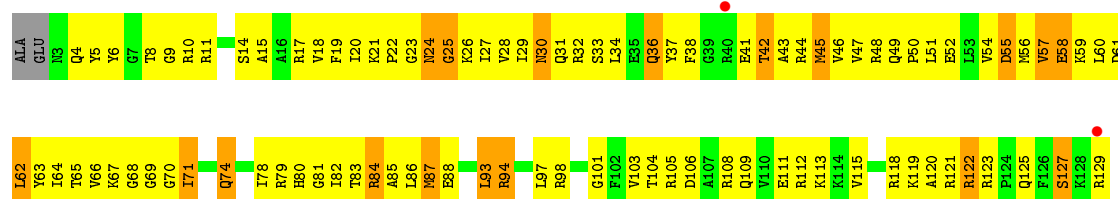


- Molecule 8: 30S ribosomal protein S9

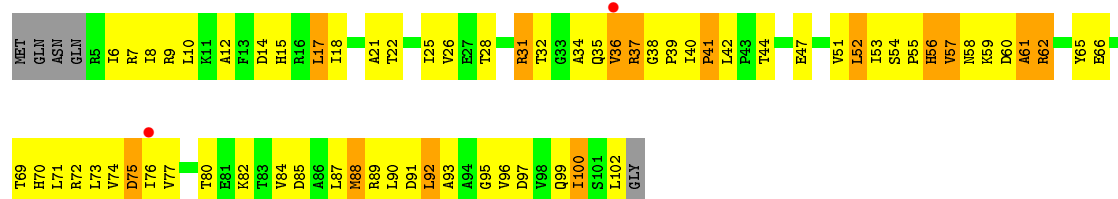




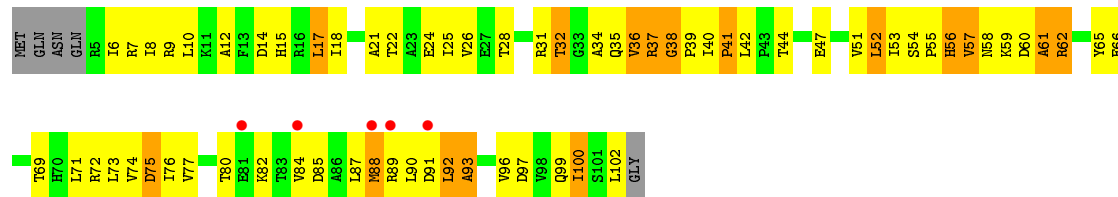
• Molecule 8: 30S ribosomal protein S9



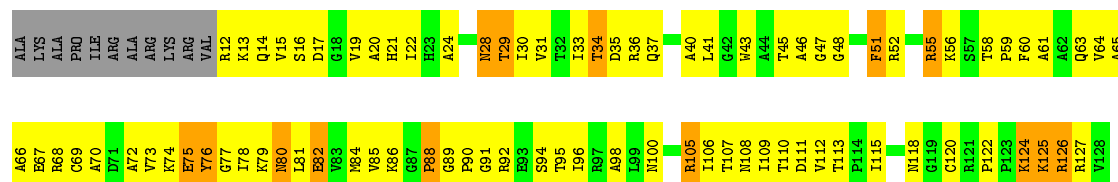
• Molecule 9: 30S ribosomal protein S10



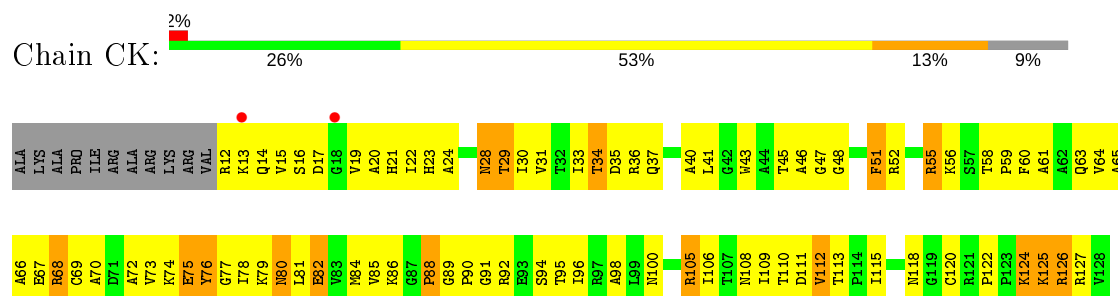
• Molecule 9: 30S ribosomal protein S10



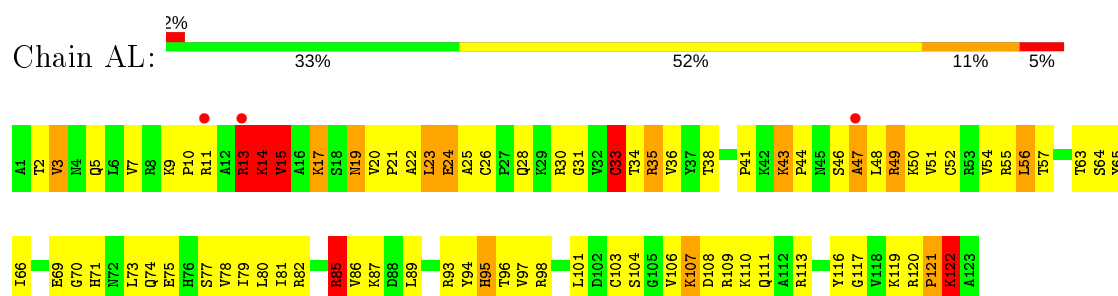
• Molecule 10: 30S ribosomal protein S11



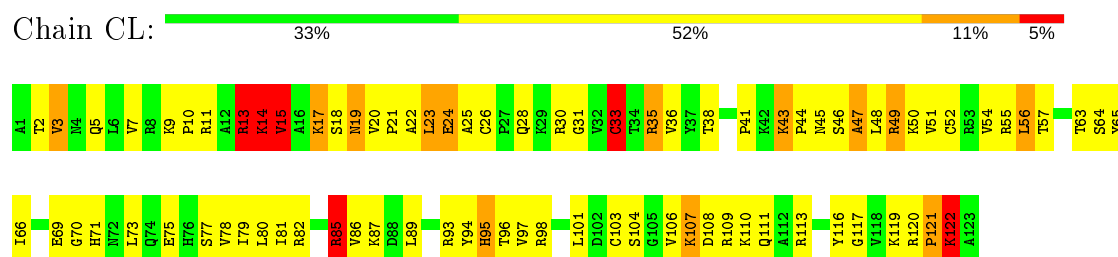
- Molecule 10: 30S ribosomal protein S11



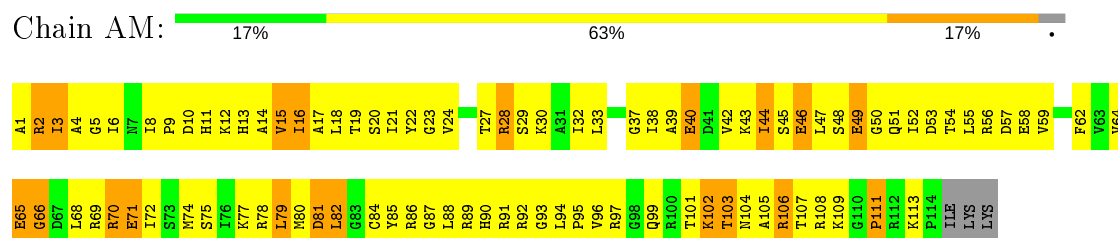
- Molecule 11: 30S ribosomal protein S12



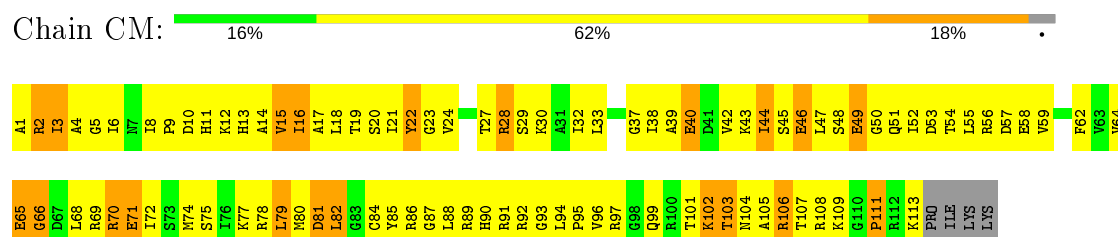
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

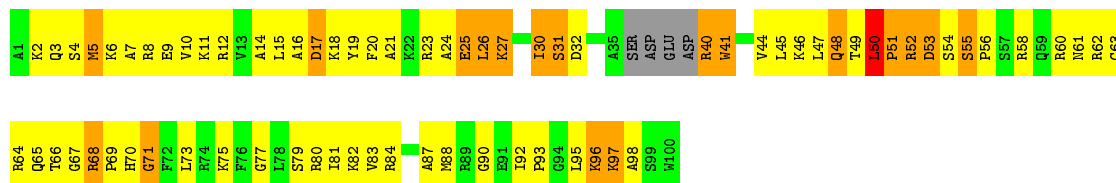


- Molecule 12: 30S ribosomal protein S13



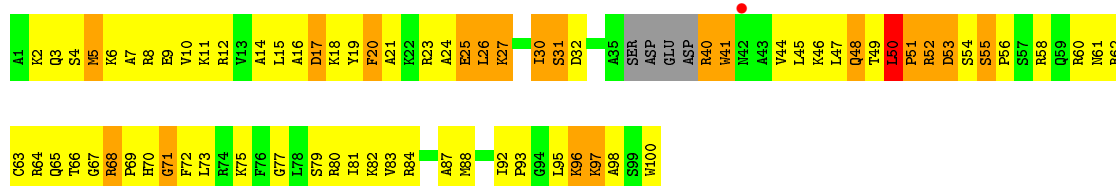
- Molecule 13: 30S ribosomal protein S14

Chain AN:  23% 54% 18% . .



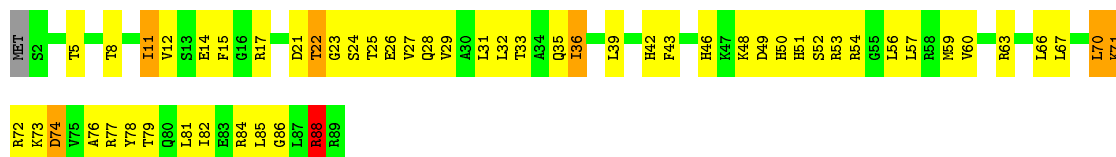
- Molecule 13: 30S ribosomal protein S14

Chain CN:  22% 54% 19% . .



- Molecule 14: 30S ribosomal protein S15

Chain AO:  38% 53% 7% . .



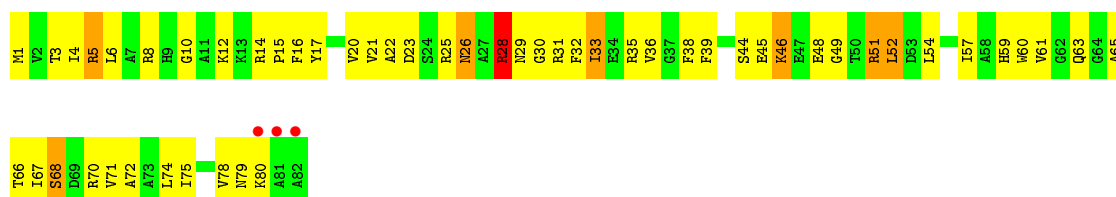
- Molecule 14: 30S ribosomal protein S15

Chain CO:  38% 53% 7% . .

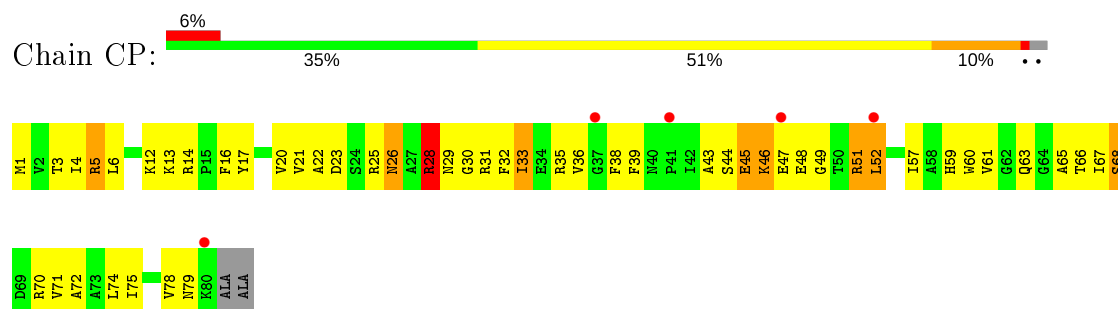


- Molecule 15: 30S ribosomal protein S16

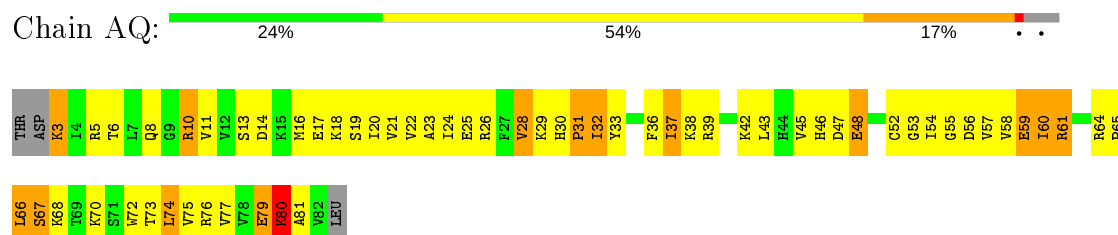
Chain AP:  4% 35% 55% 9% .



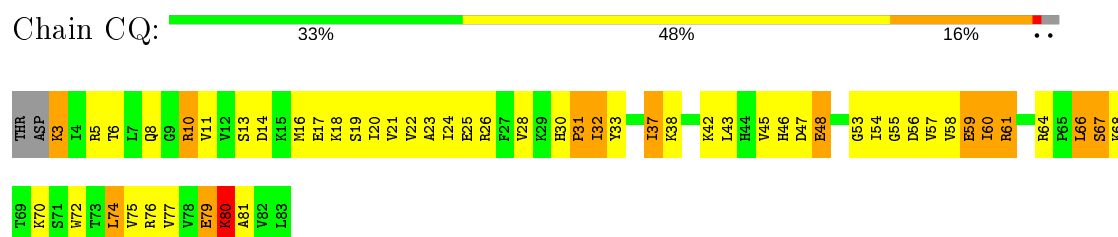
- Molecule 15: 30S ribosomal protein S16



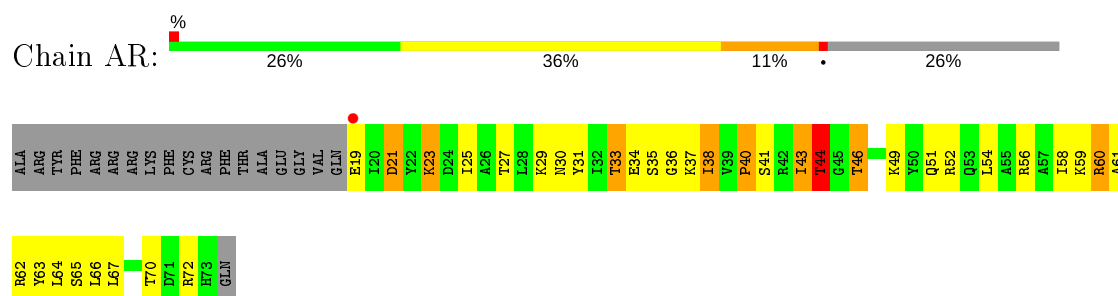
- Molecule 16: 30S ribosomal protein S17



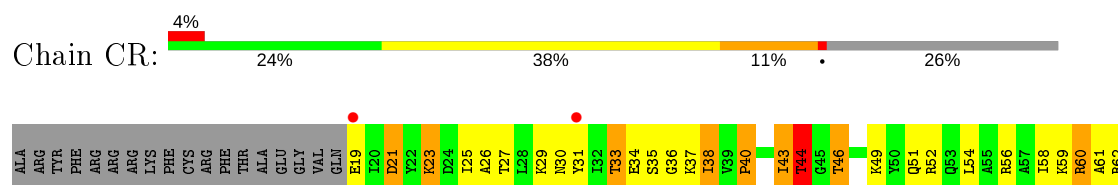
- Molecule 16: 30S ribosomal protein S17

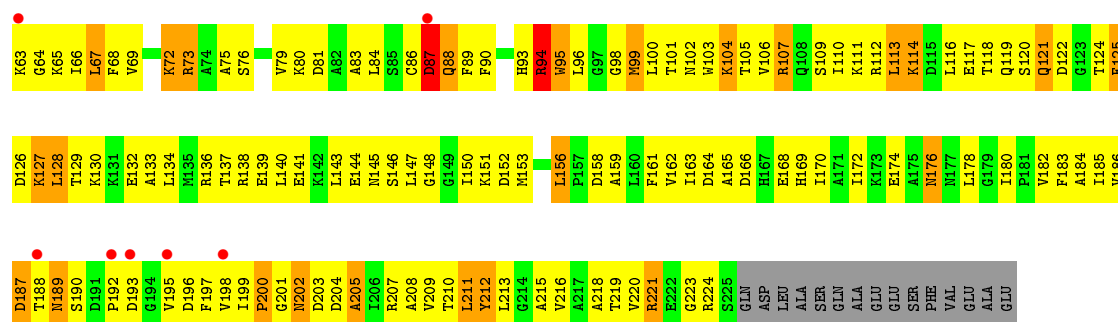


- Molecule 17: 30S ribosomal protein S18

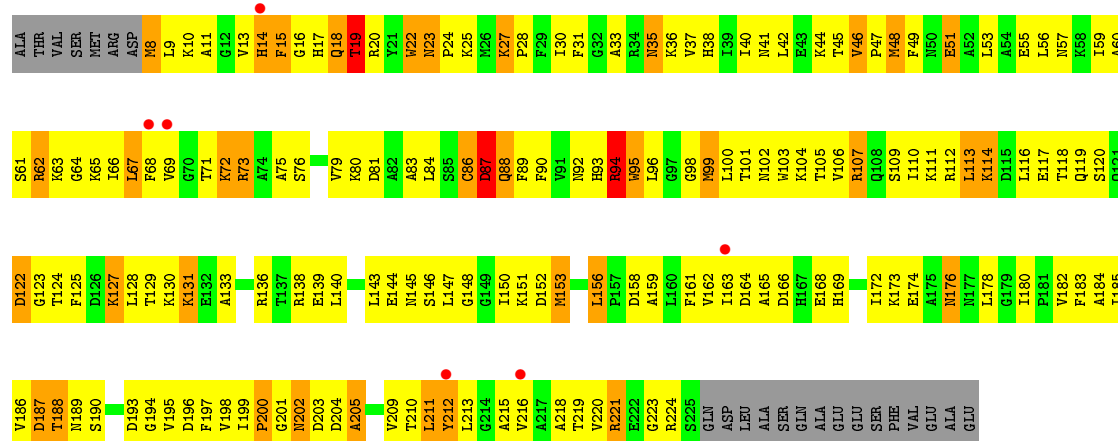


- Molecule 17: 30S ribosomal protein S18

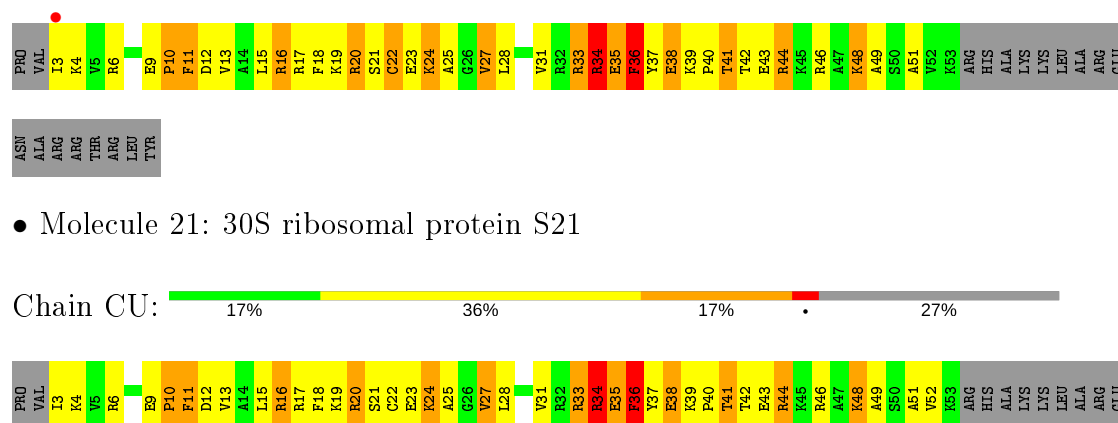
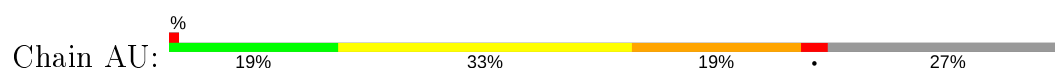




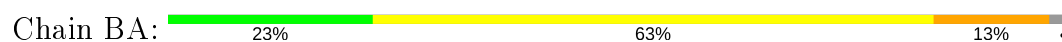
• Molecule 20: 30S ribosomal protein S2

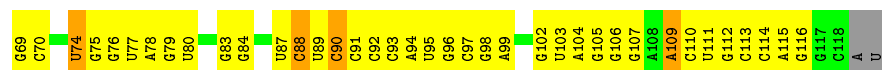
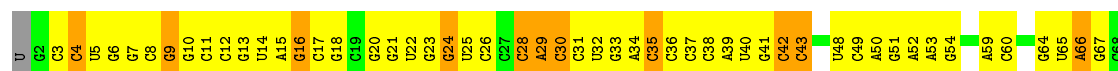


• Molecule 21: 30S ribosomal protein S21

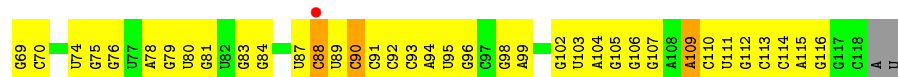


• Molecule 22: 5S rRNA

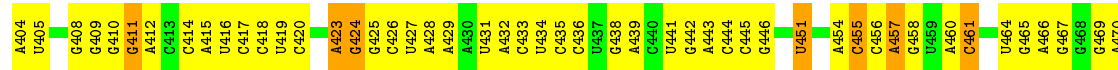
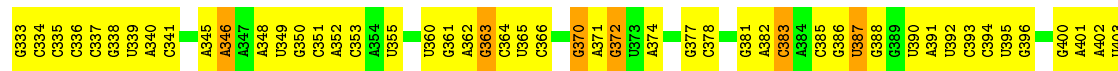
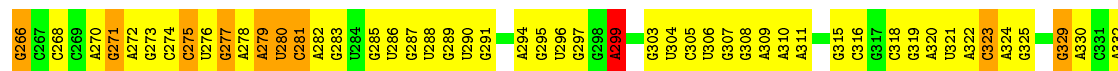
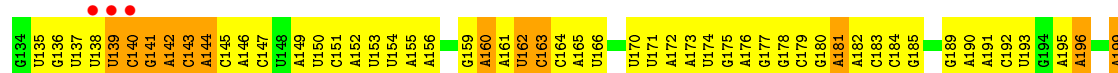
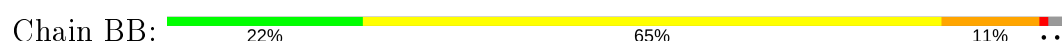




• Molecule 22: 5S rRNA

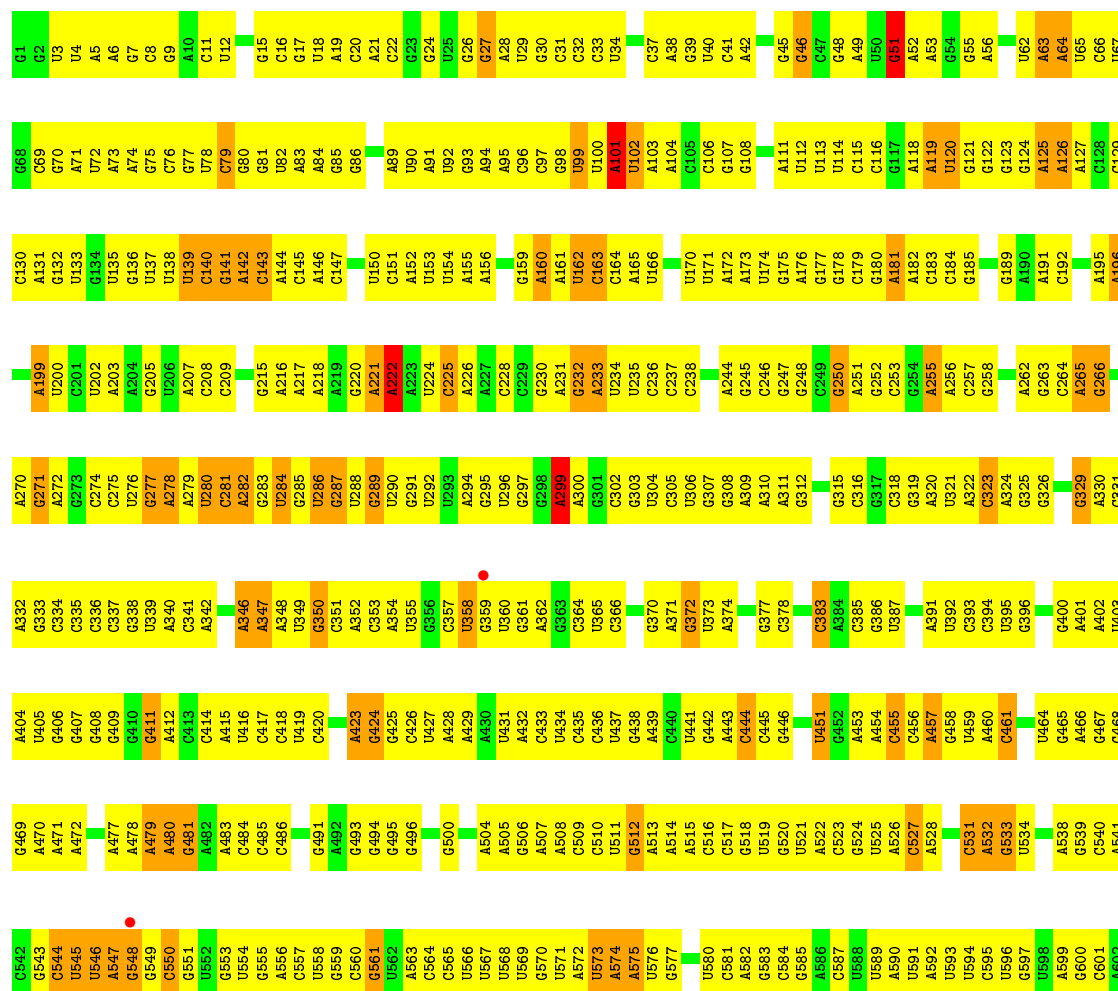


• Molecule 23: 23S rRNA



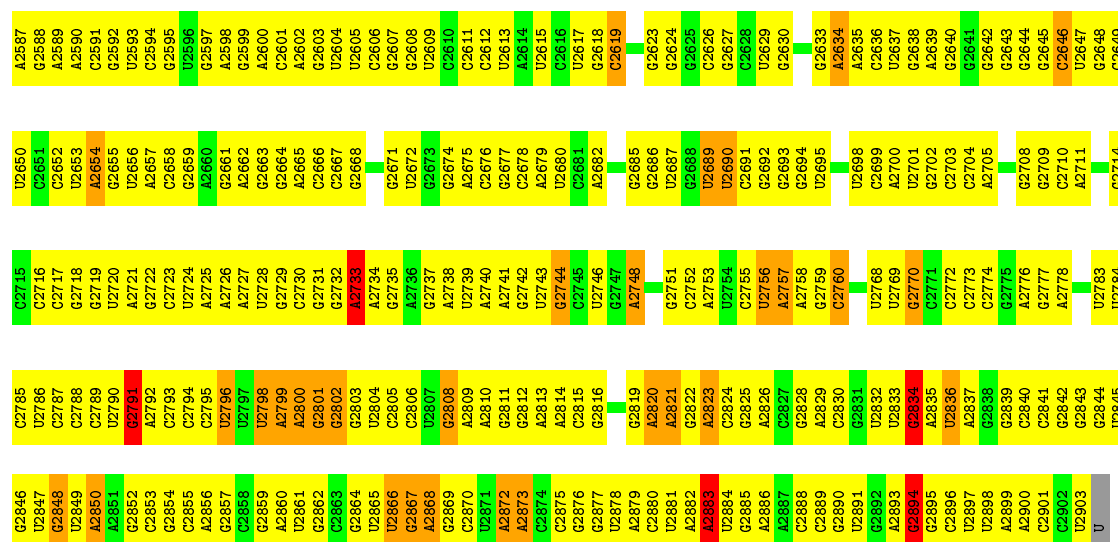
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| A1528 | U1467 | U1466 | C1403 | G1337 | C1269 | G1202 | G1137 | A1070 | A996 | C935 | G864 | A804 | G733 | A609 |
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| U1534 | A1470 | A1470 | G1408 | G1341 | U1273 | G1206 | C1140 | C1076 | G1002 | G939 | U870 | G808 | C737 | G612 |
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| U1539 | C1472 | C1472 | U1411 | C1345 | A1276 | C1208 | A1142 | U1078 | A1010 | G941 | U872 | U810 | C740 | U615 |
| G1540 | U1474 | U1474 | U1412 | A1346 | G1276 | U1209 | A1143 | U1078 | A1010 | G942 | C873 | U811 | U741 | A616 |
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| A1544 | U1478 | U1478 | G1418 | C1350 | G1280 | A1214 | A1147 | U1082 | C1013 | A945 | A877 | C815 | G745 | G620 |
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| C1547 | U1481 | U1481 | A1420 | A1353 | G1283 | U1217 | C1150 | A1085 | G1016 | C948 | A880 | C818 | U748 | C623 |
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| | | | | | | | | | | | | |
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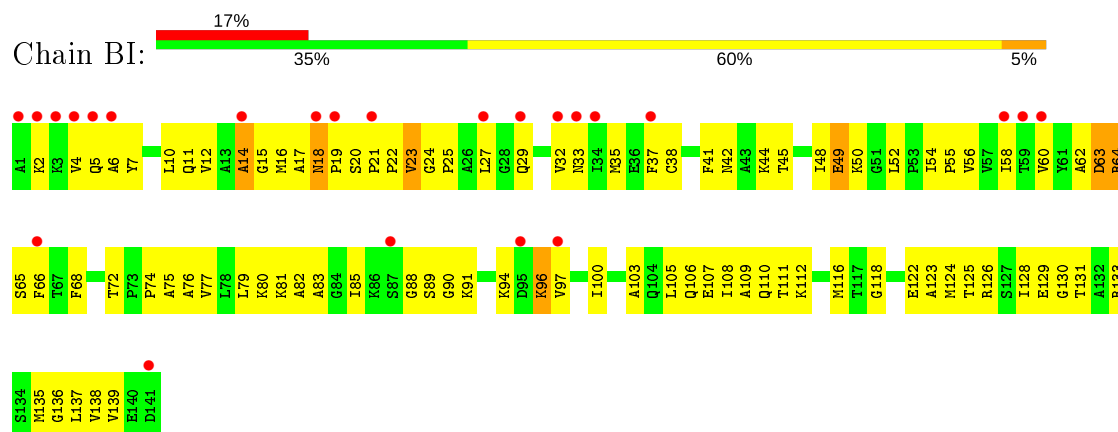


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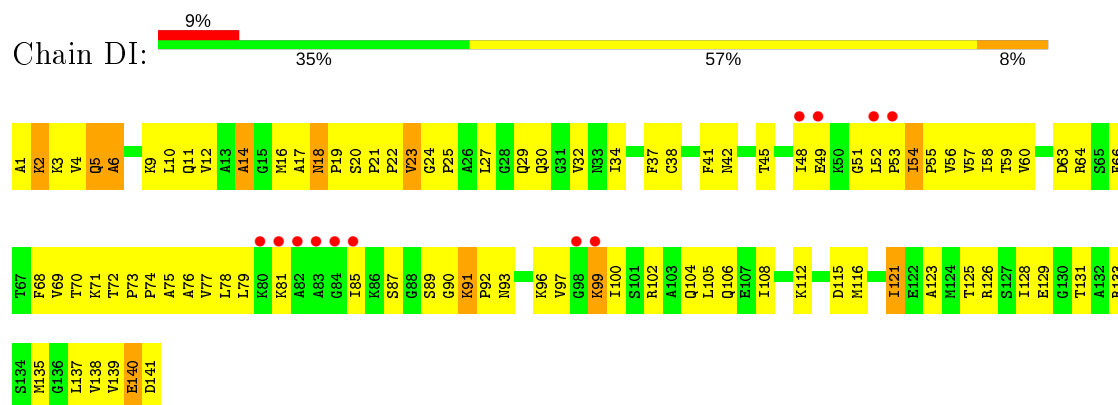
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PDB
PROTEIN DATA BANK



• Molecule 24: 50S ribosomal protein L11

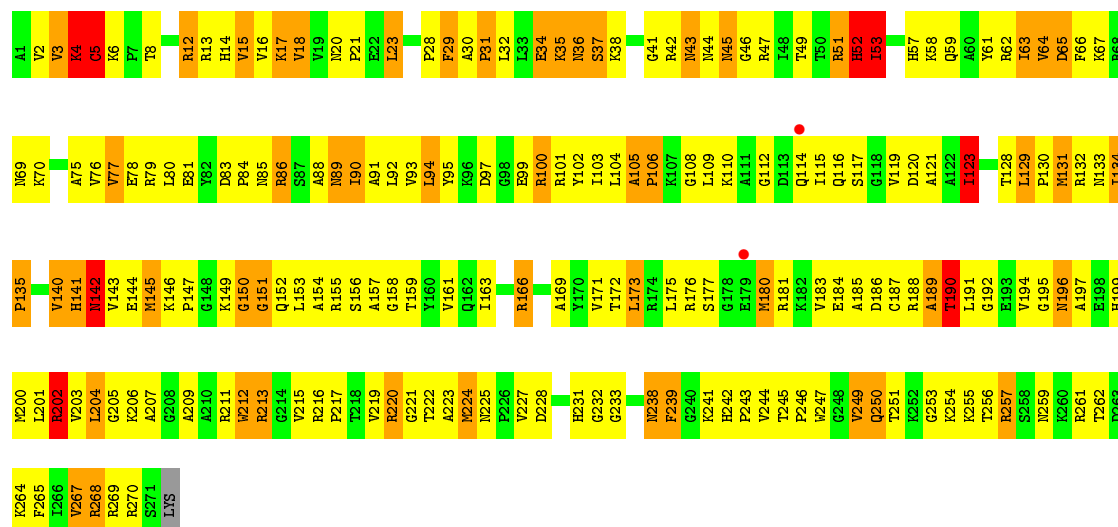


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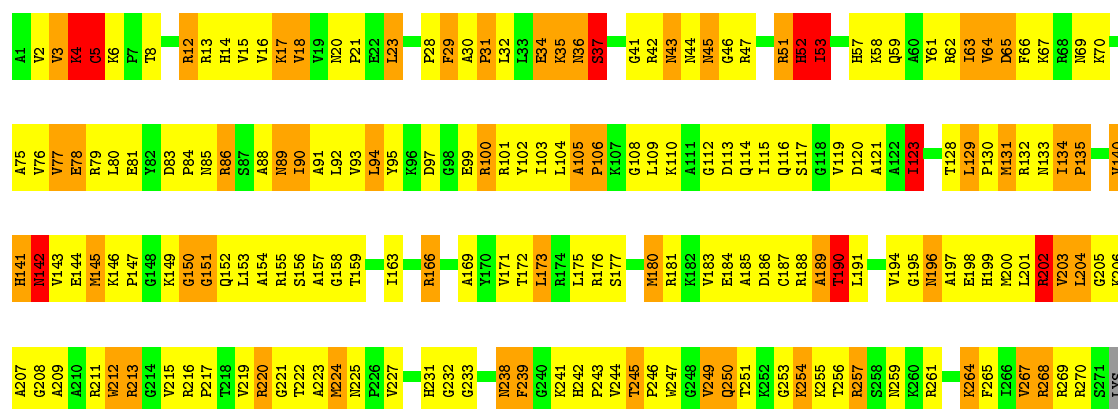
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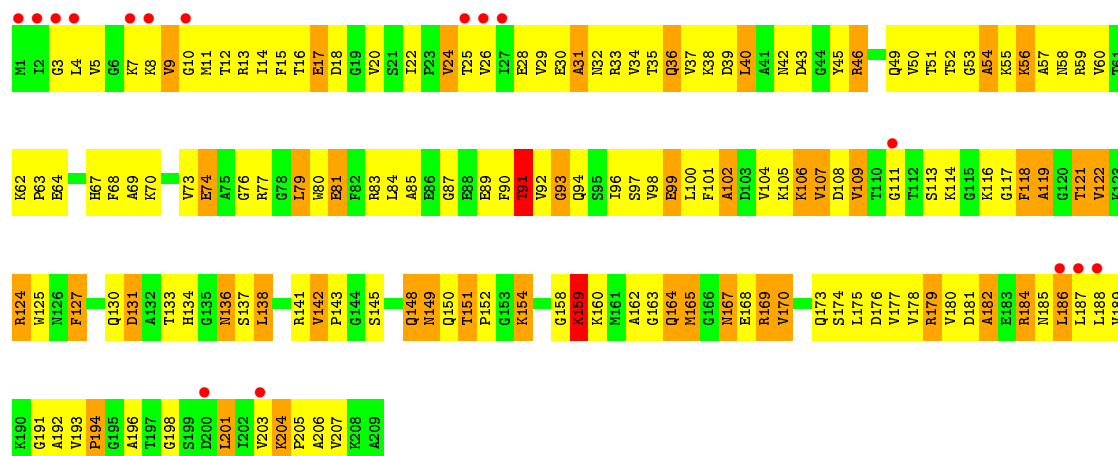
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Chain DC: 29% 47% 20%

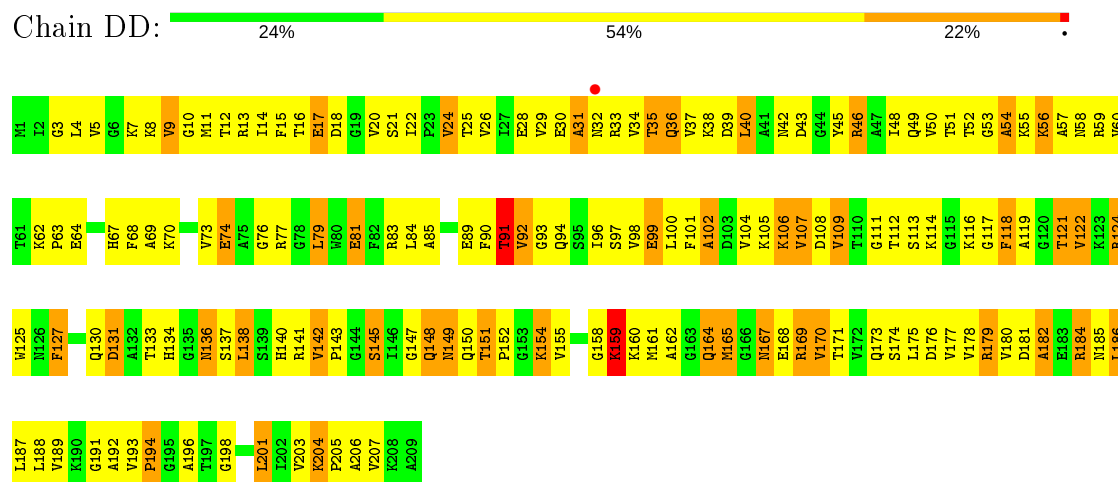


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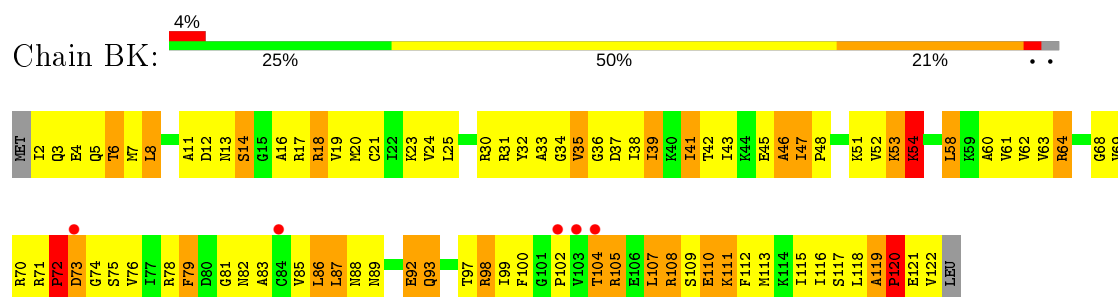
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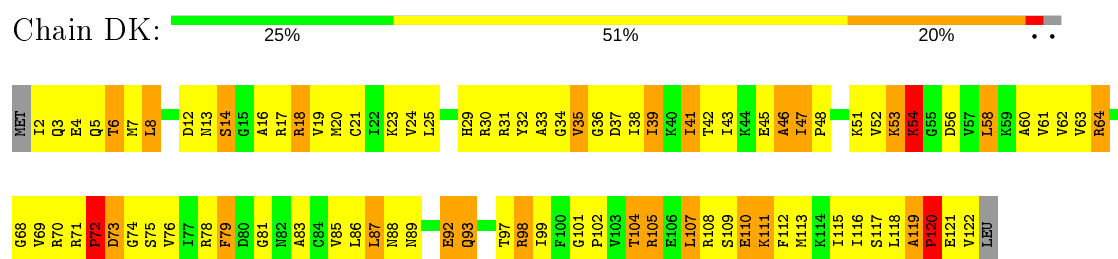
- Molecule 26: 50S ribosomal protein L3



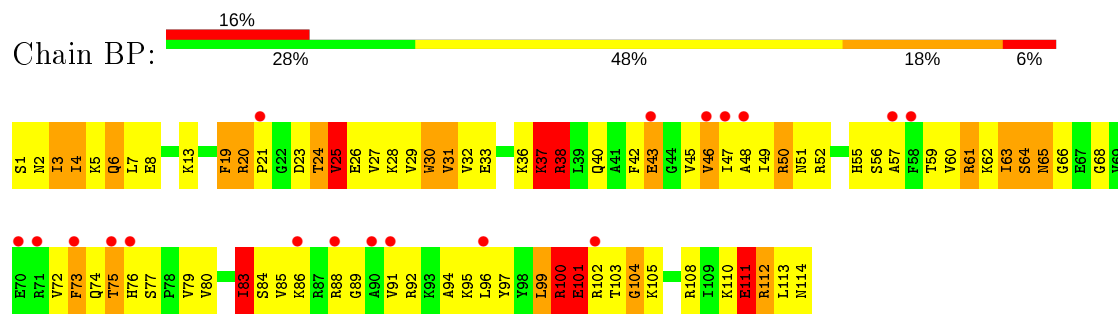
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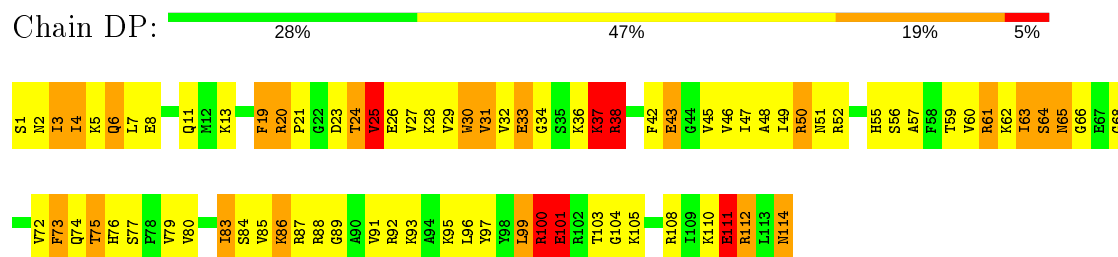
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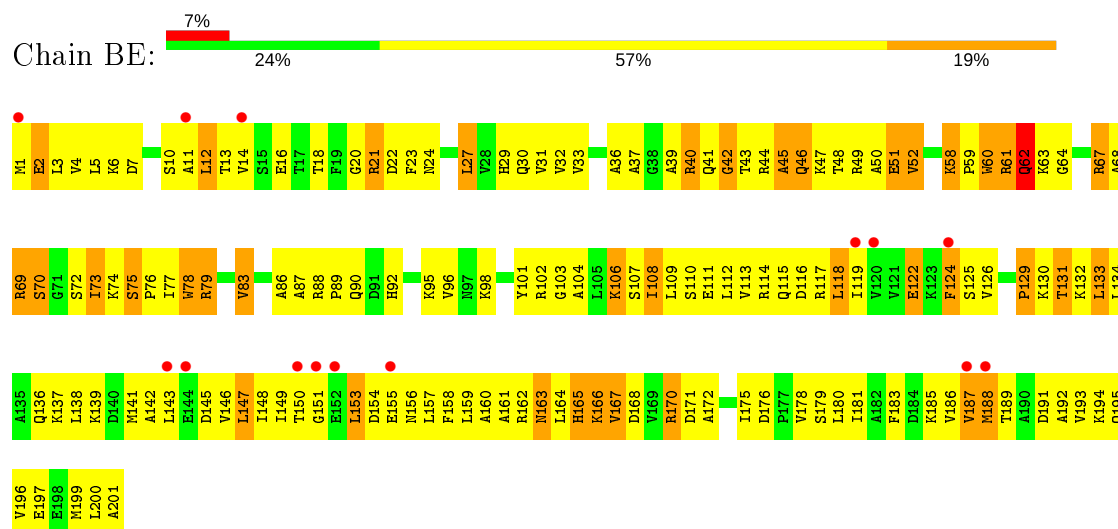
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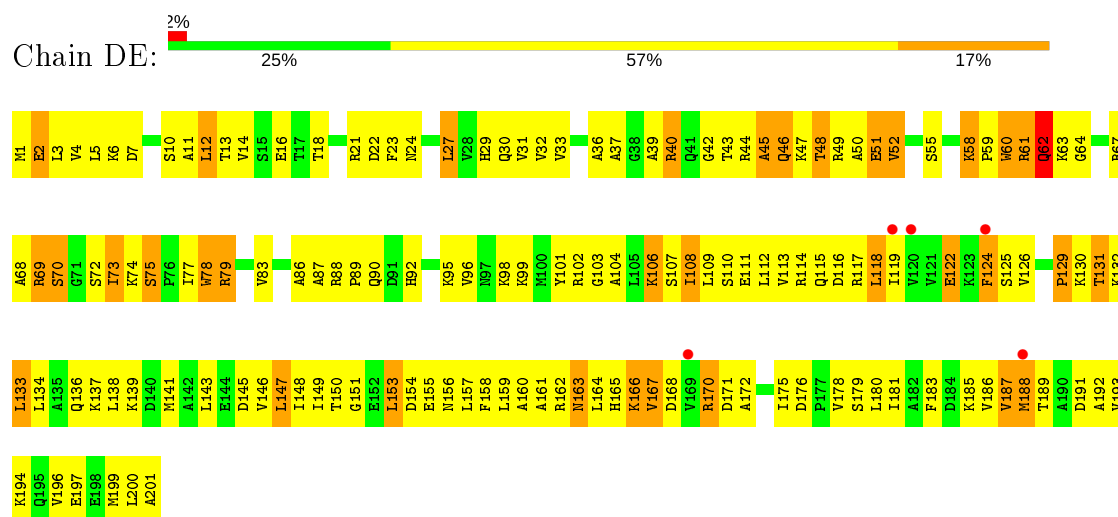
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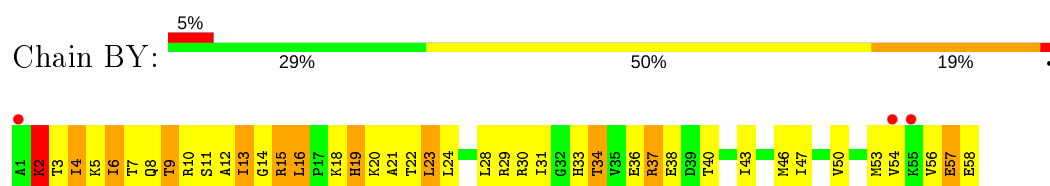
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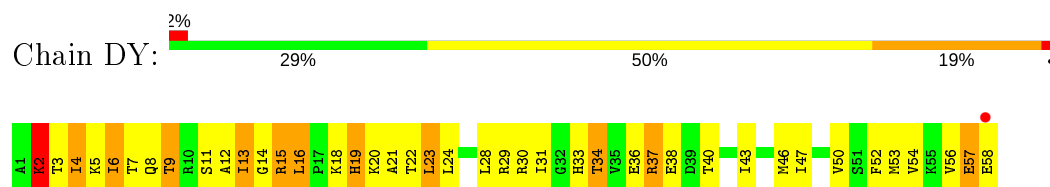
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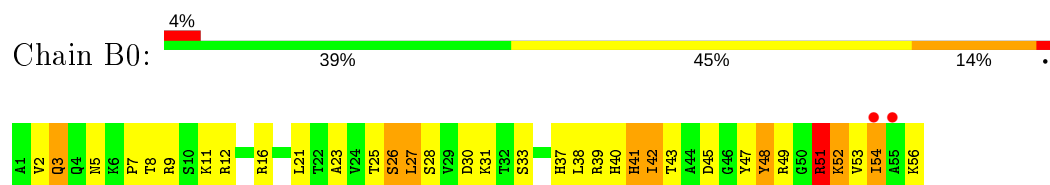
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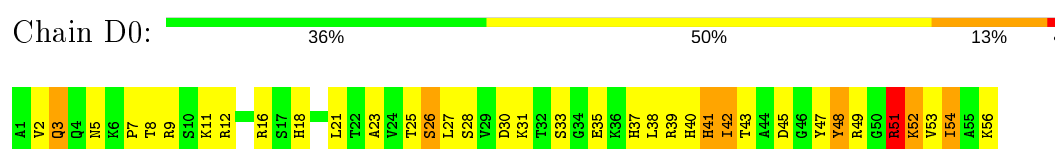
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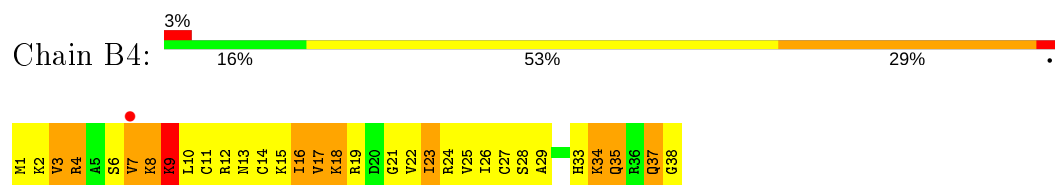
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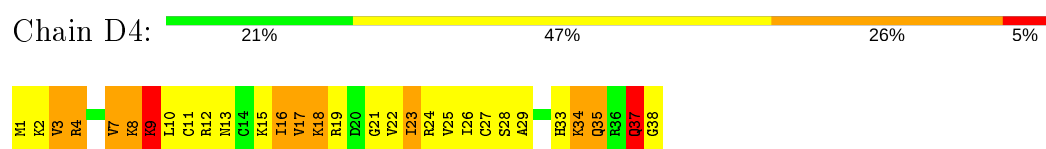
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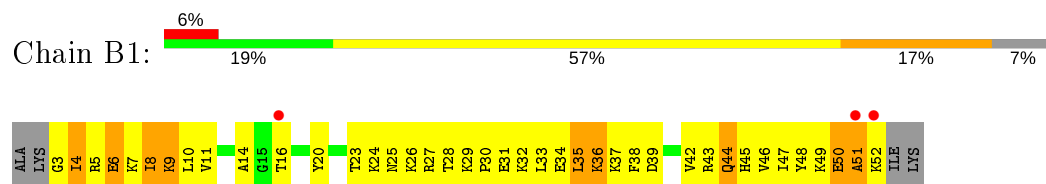
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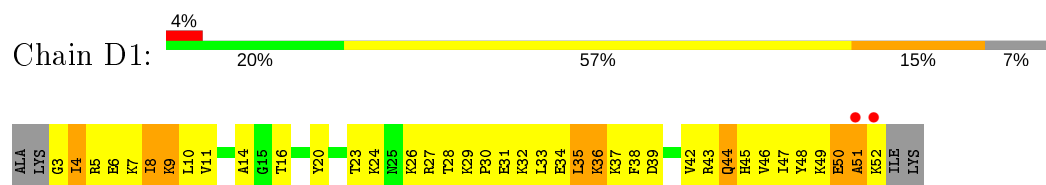
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- Molecule 33: 50S ribosomal protein L33



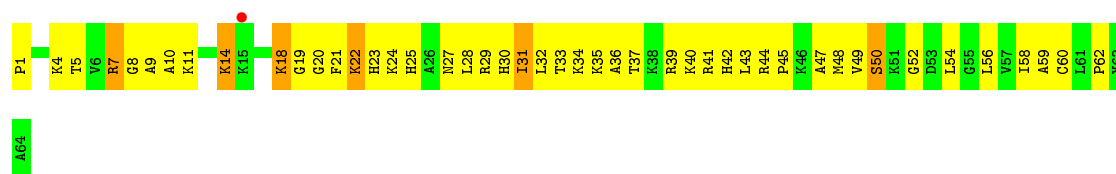
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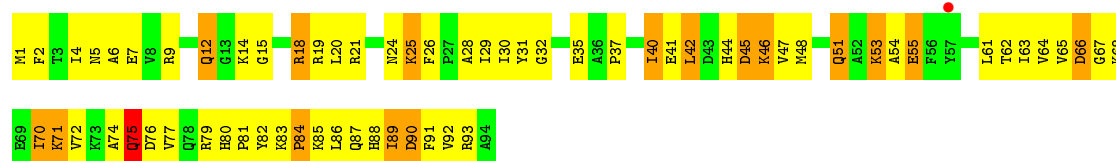
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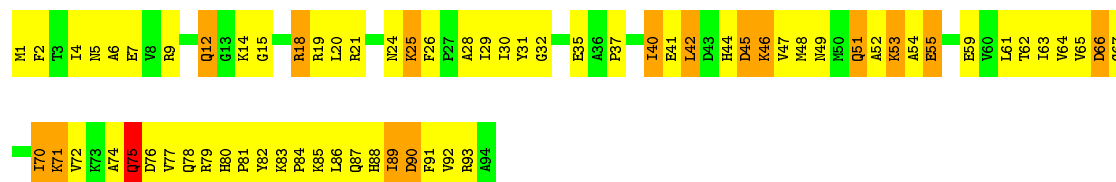
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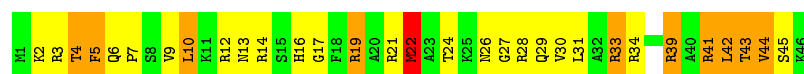
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- Molecule 35: 50S ribosomal protein L25

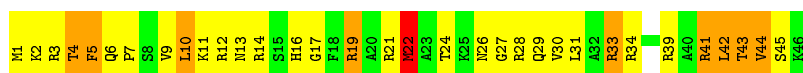


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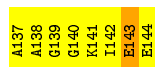


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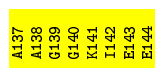
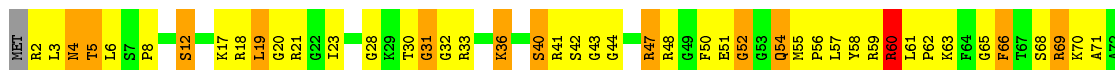




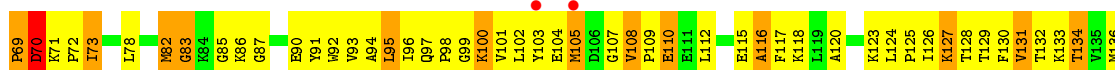
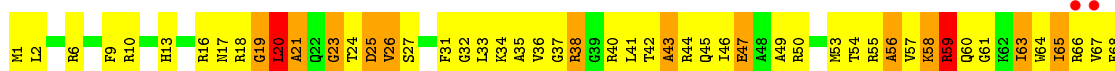
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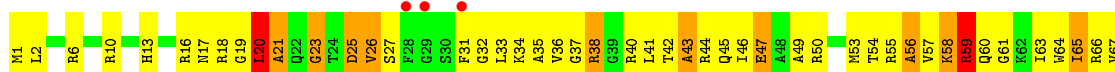
• Molecule 37: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L16



M136

- Molecule 39: 50S ribosomal protein L29



K1 K2 K3 K4 K5 K6 K7 K8 K9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 Q31 S34 Q35 Q36 Q37 Q38 Q39 Q40 Q41 Q42 Q43 Q44 Q45 Q46 Q47 Q48 Q49 Q50 Q51 Q52 Q53 Q54 Q55 Q56 Q57 Q58 Q59 Q60 Q61

G62 A63

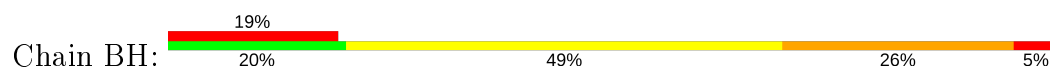
- Molecule 39: 50S ribosomal protein L29



K1 K2 K3 K4 K5 K6 K7 K8 K9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 Q31 S34 Q35 Q36 Q37 Q38 Q39 Q40 Q41 Q42 Q43 Q44 Q45 Q46 Q47 Q48 Q49 Q50 Q51 Q52 Q53 Q54 Q55 Q56 Q57 Q58 Q59 Q60 Q61

G62 A63

- Molecule 40: 50S ribosomal protein L9



K1 K2 K3 K4 K5 K6 K7 K8 K9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 Q31 S34 Q35 Q36 Q37 Q38 Q39 Q40 Q41 Q42 Q43 Q44 Q45 Q46 Q47 Q48 Q49 Q50 Q51 Q52 Q53 Q54 Q55 Q56 Q57 Q58 Q59 Q60 Q61 A64

A65 A66 A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A78 A79 A80 A81 A82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105 A106 A107 A108 A109 A110 A111 A112 A113 A114 A115 A116 A117 A118 A119 A120 A121 A122 A123 A124 A125 A126 A127 A128

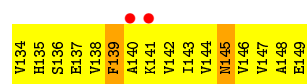
E129 V130 S131 F132 Q133 V134 H135 S136 E137 F138 V139 F140 A141 K142 K143 V144 I145 N146 V147 A148 E149

- Molecule 40: 50S ribosomal protein L9

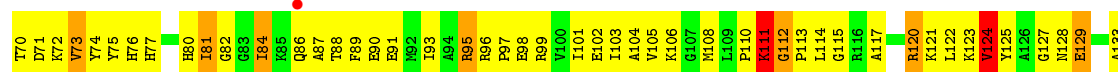
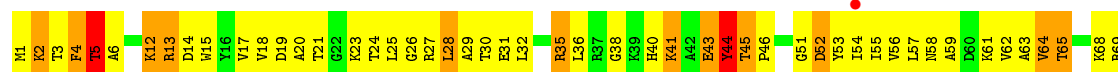


K1 K2 K3 K4 K5 K6 K7 K8 K9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 Q31 S34 Q35 Q36 Q37 Q38 Q39 Q40 Q41 Q42 Q43 Q44 Q45 Q46 Q47 Q48 Q49 Q50 Q51 Q52 Q53 Q54 Q55 Q56 Q57 Q58 Q59 Q60 Q61 A64

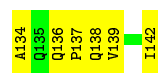
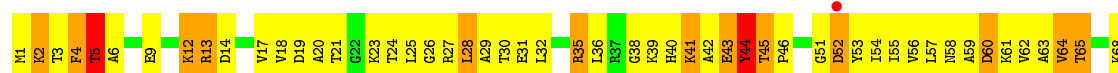
A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A78 A79 A80 A81 A82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105 A106 A107 A108 A109 A110 A111 A112 A113 A114 A115 A116 A117 A118 A119 A120 A121 A122 A123 A124 A125 A126 A127 A128 A129 A130 A131 A132 A133



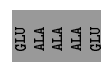
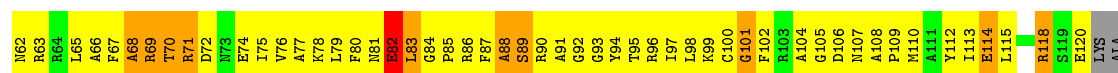
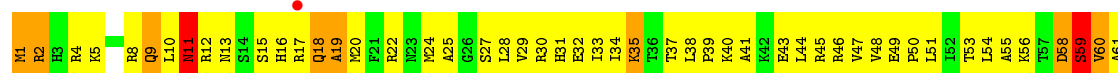
• Molecule 41: 50S ribosomal protein L13



• Molecule 41: 50S ribosomal protein L13

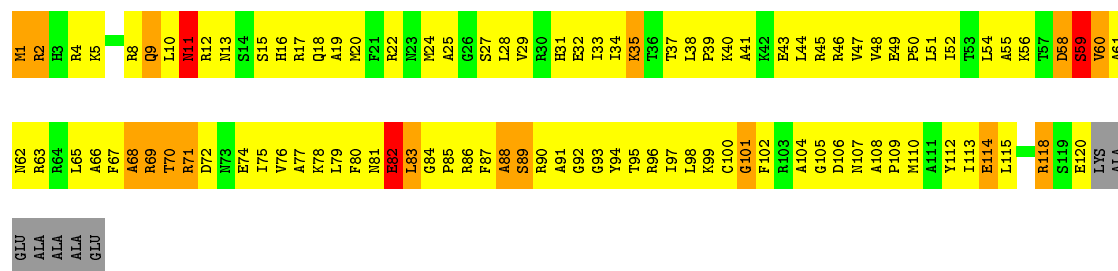


• Molecule 42: 50S ribosomal protein L17

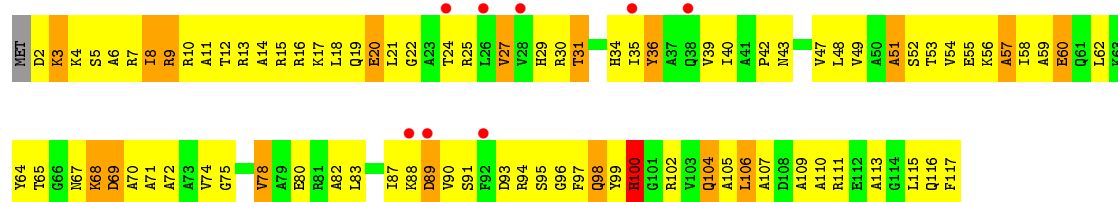


• Molecule 42: 50S ribosomal protein L17

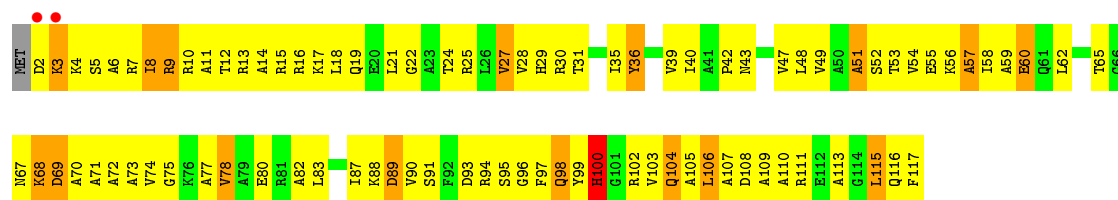




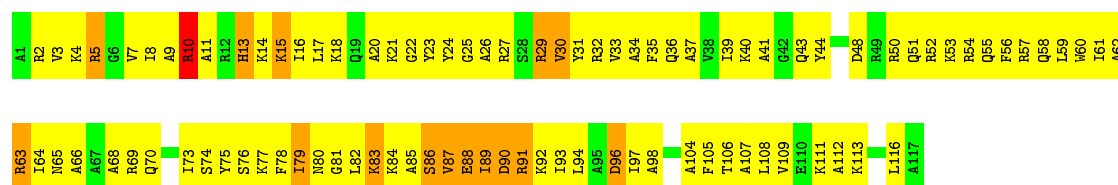
• Molecule 43: 50S ribosomal protein L18



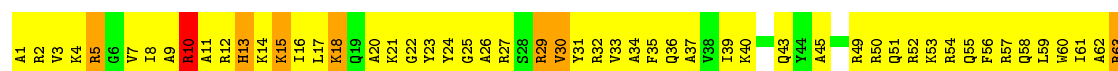
• Molecule 43: 50S ribosomal protein L18

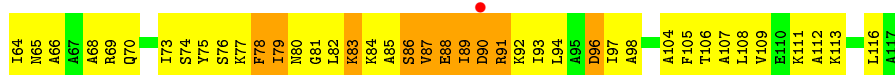


• Molecule 44: 50S ribosomal protein L20

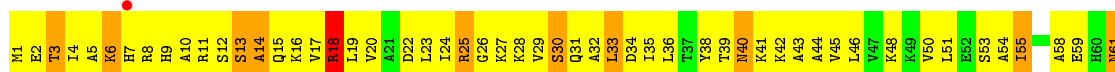


• Molecule 44: 50S ribosomal protein L20

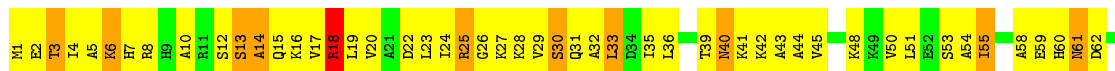




- Molecule 45: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L22



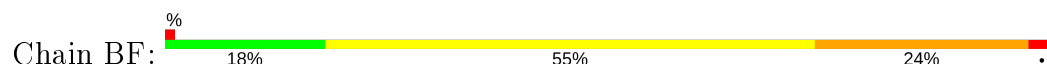
- Molecule 46: 50S ribosomal protein L24

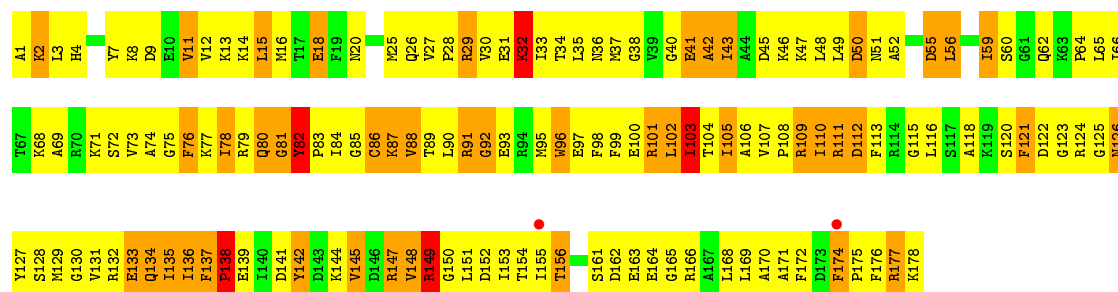


- Molecule 46: 50S ribosomal protein L24

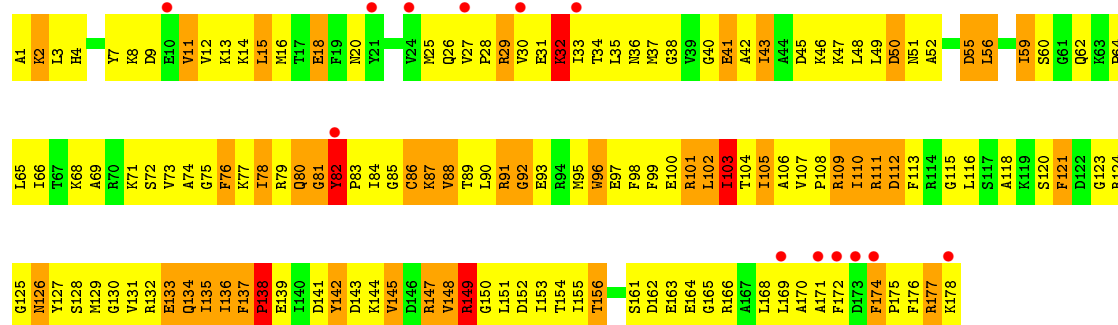


- Molecule 47: 50S ribosomal protein L5

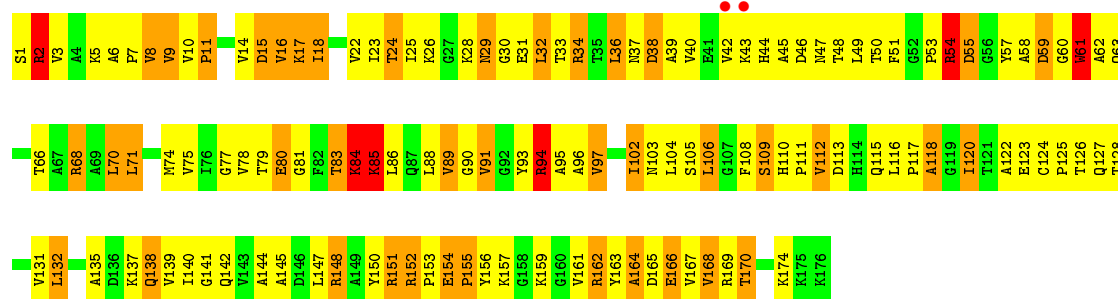




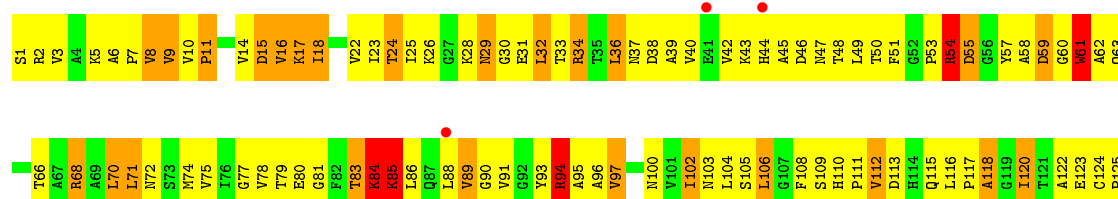
• Molecule 47: 50S ribosomal protein L5

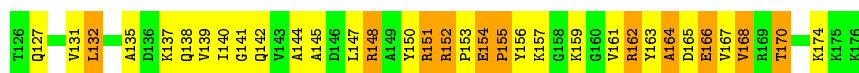


• Molecule 48: 50S ribosomal protein L6

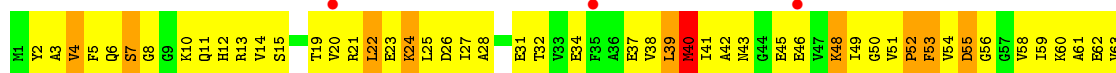


• Molecule 48: 50S ribosomal protein L6

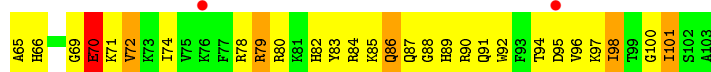




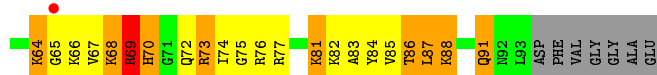
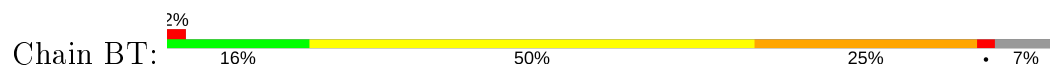
- Molecule 49: 50S ribosomal protein L21



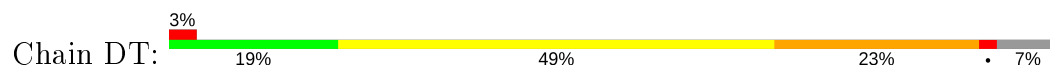
- Molecule 49: 50S ribosomal protein L21



- Molecule 50: 50S ribosomal protein L23

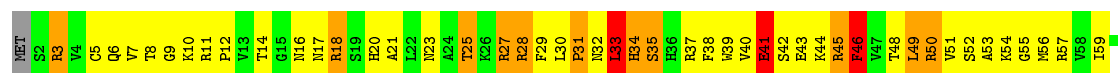


- Molecule 50: 50S ribosomal protein L23

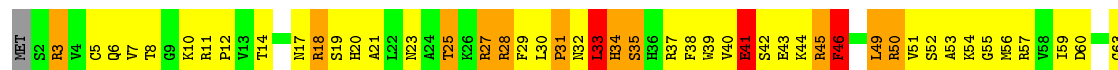


- Molecule 51: 50S ribosomal protein L28





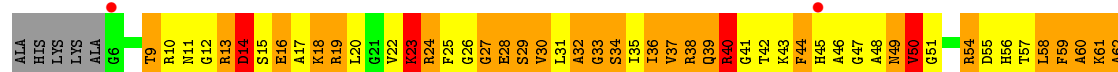
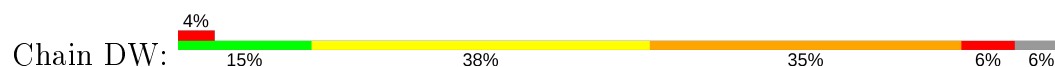
- Molecule 51: 50S ribosomal protein L28



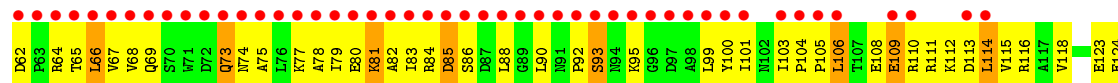
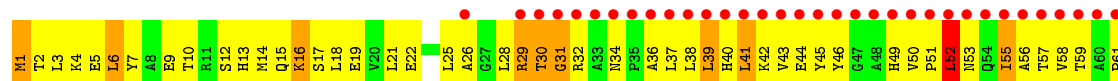
- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27

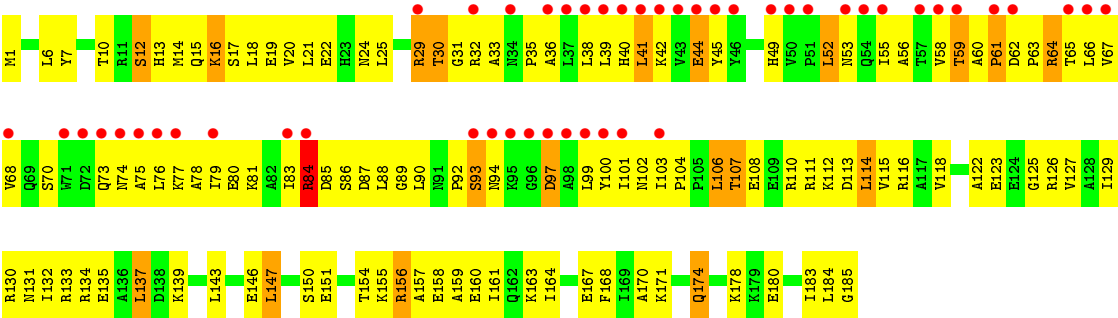


- Molecule 53: 50S ribosomal protein RRF





● Molecule 53: 50S ribosomal protein RRF



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.54Å 378.89Å 736.90Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 4.00 138.07 – 4.15 | Depositor EDS |
| % Data completeness (in resolution range) | 87.4 (40.00-4.00) 87.4 (138.07-4.15) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.14 (at 4.15Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.261 , 0.305 0.232 , 0.271 | Depositor DCC |
| R_{free} test set | 18876 reflections (4.93%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 133.1 | Xtriage |
| Anisotropy | 0.323 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.22 , 74.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 287083 | wwPDB-VP |
| Average B, all atoms (Å ²) | 72.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: ZN, MG, LLL

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 | 0.29 | 3/36762 (0.0%) | 0.78 | 21/57350 (0.0%) |
| 1 | CA | 0.29 | 4/36762 (0.0%) | 0.78 | 22/57350 (0.0%) |
| 2 | AC | 0.23 | 0/1651 | 0.44 | 0/2225 |
| 2 | CC | 0.23 | 0/1651 | 0.44 | 0/2225 |
| 3 | AD | 0.23 | 0/1665 | 0.44 | 0/2227 |
| 3 | CD | 0.23 | 0/1665 | 0.44 | 0/2227 |
| 4 | AE | 0.23 | 0/1118 | 0.46 | 0/1504 |
| 4 | CE | 0.23 | 0/1118 | 0.46 | 0/1504 |
| 5 | AF | 0.24 | 0/835 | 0.45 | 0/1128 |
| 5 | CF | 0.24 | 0/835 | 0.45 | 0/1128 |
| 6 | AG | 0.23 | 0/1187 | 0.46 | 0/1591 |
| 6 | CG | 0.23 | 0/1211 | 0.46 | 0/1624 |
| 7 | AH | 0.23 | 0/989 | 0.44 | 0/1326 |
| 7 | CH | 0.23 | 0/989 | 0.44 | 0/1326 |
| 8 | AI | 0.24 | 0/1034 | 0.46 | 0/1375 |
| 8 | CI | 0.24 | 0/1033 | 0.46 | 0/1375 |
| 9 | AJ | 0.22 | 0/796 | 0.48 | 0/1077 |
| 9 | CJ | 0.22 | 0/796 | 0.48 | 0/1077 |
| 10 | AK | 0.24 | 0/893 | 0.46 | 0/1205 |
| 10 | CK | 0.24 | 0/893 | 0.46 | 0/1205 |
| 11 | AL | 0.22 | 0/969 | 0.50 | 0/1300 |
| 11 | CL | 0.22 | 0/969 | 0.50 | 0/1300 |
| 12 | AM | 0.21 | 0/892 | 0.46 | 0/1193 |
| 12 | CM | 0.21 | 0/884 | 0.46 | 0/1181 |
| 13 | AN | 0.24 | 0/785 | 0.45 | 0/1043 |
| 13 | CN | 0.24 | 0/785 | 0.45 | 0/1043 |
| 14 | AO | 0.23 | 0/722 | 0.47 | 0/964 |
| 14 | CO | 0.23 | 0/722 | 0.47 | 0/964 |
| 15 | AP | 0.25 | 0/659 | 0.46 | 0/884 |
| 15 | CP | 0.25 | 0/648 | 0.47 | 0/870 |
| 16 | AQ | 0.24 | 0/657 | 0.47 | 0/881 |
| 16 | CQ | 0.24 | 0/666 | 0.47 | 0/892 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AR | 0.23 | 0/462 | 0.46 | 0/621 |
| 17 | CR | 0.23 | 0/462 | 0.46 | 0/621 |
| 18 | AS | 0.25 | 0/652 | 0.47 | 0/877 |
| 18 | CS | 0.25 | 0/660 | 0.48 | 0/888 |
| 19 | AT | 0.23 | 0/671 | 0.39 | 0/888 |
| 19 | CT | 0.23 | 0/671 | 0.39 | 0/888 |
| 20 | AB | 0.25 | 0/1735 | 0.45 | 0/2338 |
| 20 | CB | 0.25 | 0/1735 | 0.45 | 0/2338 |
| 21 | AU | 0.26 | 0/430 | 0.48 | 0/570 |
| 21 | CU | 0.26 | 0/430 | 0.48 | 0/570 |
| 22 | BA | 0.28 | 0/2803 | 0.76 | 1/4371 (0.0%) |
| 22 | DA | 0.28 | 0/2803 | 0.76 | 0/4371 |
| 23 | BB | 0.28 | 6/68314 (0.0%) | 0.78 | 48/106569 (0.0%) |
| 23 | DB | 0.30 | 6/68314 (0.0%) | 0.79 | 48/106569 (0.0%) |
| 24 | BI | 0.24 | 0/1046 | 0.47 | 0/1410 |
| 24 | DI | 0.25 | 0/1046 | 0.48 | 0/1410 |
| 25 | BC | 0.22 | 0/2121 | 0.48 | 0/2852 |
| 25 | DC | 0.22 | 0/2121 | 0.48 | 0/2852 |
| 26 | BD | 0.24 | 0/1586 | 0.49 | 0/2134 |
| 26 | DD | 0.24 | 0/1586 | 0.49 | 0/2134 |
| 27 | BK | 0.24 | 0/939 | 0.55 | 0/1258 |
| 27 | DK | 0.24 | 0/939 | 0.55 | 0/1258 |
| 28 | BP | 0.24 | 0/929 | 0.51 | 0/1242 |
| 28 | DP | 0.24 | 0/929 | 0.51 | 0/1242 |
| 29 | BE | 0.24 | 0/1571 | 0.51 | 0/2113 |
| 29 | DE | 0.24 | 0/1571 | 0.51 | 0/2113 |
| 30 | BY | 0.23 | 0/453 | 0.49 | 0/605 |
| 30 | DY | 0.23 | 0/453 | 0.49 | 0/605 |
| 31 | B0 | 0.22 | 0/450 | 0.55 | 0/599 |
| 31 | D0 | 0.23 | 0/450 | 0.55 | 0/599 |
| 32 | B4 | 0.23 | 0/303 | 0.47 | 0/397 |
| 32 | D4 | 0.23 | 0/303 | 0.47 | 0/397 |
| 33 | B1 | 0.27 | 0/416 | 0.49 | 0/554 |
| 33 | D1 | 0.27 | 0/416 | 0.49 | 0/554 |
| 34 | B3 | 0.24 | 0/513 | 0.48 | 0/676 |
| 34 | D3 | 0.24 | 0/513 | 0.48 | 0/676 |
| 35 | BV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 35 | DV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 36 | B2 | 0.25 | 0/380 | 0.48 | 0/498 |
| 36 | D2 | 0.25 | 0/380 | 0.48 | 0/498 |
| 37 | BL | 0.23 | 0/1054 | 0.48 | 0/1403 |
| 37 | DL | 0.23 | 0/1054 | 0.48 | 0/1403 |
| 38 | BM | 0.25 | 0/1093 | 0.48 | 0/1460 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DM | 0.25 | 0/1093 | 0.48 | 0/1460 |
| 39 | BX | 0.24 | 0/510 | 0.53 | 0/677 |
| 39 | DX | 0.24 | 0/510 | 0.53 | 0/677 |
| 40 | BH | 0.25 | 0/1122 | 0.48 | 0/1515 |
| 40 | DH | 0.25 | 0/1122 | 0.48 | 0/1515 |
| 41 | BJ | 0.24 | 0/1152 | 0.48 | 0/1551 |
| 41 | DJ | 0.23 | 0/1152 | 0.48 | 0/1551 |
| 42 | BN | 0.24 | 0/973 | 0.51 | 0/1301 |
| 42 | DN | 0.24 | 0/973 | 0.51 | 0/1301 |
| 43 | BO | 0.23 | 0/902 | 0.49 | 0/1209 |
| 43 | DO | 0.23 | 0/902 | 0.49 | 0/1209 |
| 44 | BQ | 0.25 | 0/960 | 0.49 | 0/1278 |
| 44 | DQ | 0.26 | 0/960 | 0.49 | 0/1278 |
| 45 | BS | 0.22 | 0/864 | 0.52 | 0/1156 |
| 45 | DS | 0.22 | 0/864 | 0.52 | 0/1156 |
| 46 | BU | 0.25 | 0/787 | 0.47 | 0/1051 |
| 46 | DU | 0.25 | 0/787 | 0.47 | 0/1051 |
| 47 | BF | 0.26 | 0/1444 | 0.52 | 0/1937 |
| 47 | DF | 0.26 | 0/1444 | 0.52 | 0/1937 |
| 48 | BG | 0.23 | 0/1343 | 0.47 | 0/1816 |
| 48 | DG | 0.23 | 0/1343 | 0.47 | 0/1816 |
| 49 | BR | 0.25 | 0/829 | 0.50 | 0/1107 |
| 49 | DR | 0.25 | 0/829 | 0.50 | 0/1107 |
| 50 | BT | 0.23 | 0/744 | 0.55 | 0/994 |
| 50 | DT | 0.22 | 0/744 | 0.55 | 0/994 |
| 51 | BZ | 0.25 | 0/635 | 0.51 | 0/848 |
| 51 | DZ | 0.25 | 0/635 | 0.52 | 0/848 |
| 52 | BW | 0.28 | 0/603 | 0.51 | 0/797 |
| 52 | DW | 0.28 | 0/603 | 0.51 | 0/797 |
| 53 | B6 | 0.23 | 0/1497 | 0.52 | 1/2017 (0.0%) |
| 53 | D6 | 0.30 | 0/1497 | 0.58 | 1/2017 (0.0%) |
| All | All | 0.28 | 19/309353 (0.0%) | 0.71 | 142/462003 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AA | 0 | 16 |
| 1 | CA | 0 | 17 |
| 23 | BB | 0 | 35 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 23 | DB | 0 | 47 |
| All | All | 0 | 115 |

The worst 5 of 19 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23 | BB | 1086 | A | C5-C6 | -16.56 | 1.26 | 1.41 |
| 23 | DB | 1086 | A | C5-C6 | -16.53 | 1.26 | 1.41 |
| 23 | DB | 1088 | A | C6-N1 | -10.57 | 1.28 | 1.35 |
| 23 | BB | 1088 | A | C6-N1 | -10.52 | 1.28 | 1.35 |
| 1 | CA | 1213 | A | P-OP1 | -9.61 | 1.32 | 1.49 |

The worst 5 of 142 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | CA | 1213 | A | O5'-P-OP1 | -31.90 | 72.42 | 110.70 |
| 1 | AA | 1213 | A | O5'-P-OP2 | -30.12 | 74.56 | 110.70 |
| 23 | DB | 2204 | G | O5'-P-OP1 | -29.74 | 75.02 | 110.70 |
| 23 | BB | 2204 | G | O5'-P-OP2 | -28.90 | 76.02 | 110.70 |
| 23 | BB | 2791 | G | O5'-P-OP1 | -28.07 | 77.02 | 110.70 |

There are no chirality outliers.

5 of 115 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 187 | G | Sidechain |
| 1 | AA | 281 | G | Sidechain |
| 1 | AA | 324 | G | Sidechain |
| 1 | AA | 437 | U | Sidechain |
| 1 | AA | 86 | G | 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 | 32831 | 0 | 16521 | 1290 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | CA | 32831 | 0 | 16521 | 1350 | 0 |
| 2 | AC | 1624 | 0 | 1699 | 140 | 0 |
| 2 | CC | 1624 | 0 | 1699 | 146 | 0 |
| 3 | AD | 1643 | 0 | 1710 | 174 | 0 |
| 3 | CD | 1643 | 0 | 1710 | 170 | 0 |
| 4 | AE | 1105 | 0 | 1148 | 95 | 0 |
| 4 | CE | 1105 | 0 | 1148 | 96 | 0 |
| 5 | AF | 817 | 0 | 808 | 96 | 0 |
| 5 | CF | 817 | 0 | 808 | 94 | 0 |
| 6 | AG | 1174 | 0 | 1230 | 112 | 0 |
| 6 | CG | 1196 | 0 | 1246 | 106 | 0 |
| 7 | AH | 979 | 0 | 1034 | 95 | 0 |
| 7 | CH | 979 | 0 | 1034 | 96 | 0 |
| 8 | AI | 1022 | 0 | 1070 | 149 | 0 |
| 8 | CI | 1021 | 0 | 1070 | 149 | 0 |
| 9 | AJ | 786 | 0 | 828 | 77 | 0 |
| 9 | CJ | 786 | 0 | 828 | 80 | 0 |
| 10 | AK | 877 | 0 | 887 | 111 | 0 |
| 10 | CK | 877 | 0 | 887 | 114 | 0 |
| 11 | AL | 955 | 0 | 1019 | 92 | 0 |
| 11 | CL | 955 | 0 | 1019 | 91 | 0 |
| 12 | AM | 883 | 0 | 944 | 119 | 0 |
| 12 | CM | 876 | 0 | 937 | 120 | 0 |
| 13 | AN | 774 | 0 | 827 | 121 | 0 |
| 13 | CN | 774 | 0 | 827 | 131 | 0 |
| 14 | AO | 714 | 0 | 734 | 60 | 0 |
| 14 | CO | 714 | 0 | 734 | 54 | 0 |
| 15 | AP | 649 | 0 | 666 | 56 | 0 |
| 15 | CP | 638 | 0 | 656 | 57 | 0 |
| 16 | AQ | 648 | 0 | 691 | 71 | 0 |
| 16 | CQ | 657 | 0 | 702 | 67 | 0 |
| 17 | AR | 455 | 0 | 478 | 51 | 0 |
| 17 | CR | 455 | 0 | 478 | 56 | 0 |
| 18 | AS | 637 | 0 | 665 | 85 | 0 |
| 18 | CS | 644 | 0 | 675 | 87 | 0 |
| 19 | AT | 665 | 0 | 714 | 68 | 0 |
| 19 | CT | 665 | 0 | 714 | 70 | 0 |
| 20 | AB | 1704 | 0 | 1732 | 220 | 0 |
| 20 | CB | 1704 | 0 | 1732 | 211 | 0 |
| 21 | AU | 425 | 0 | 449 | 79 | 0 |
| 21 | CU | 425 | 0 | 449 | 89 | 0 |
| 22 | BA | 2507 | 0 | 1270 | 106 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22 | DA | 2507 | 0 | 1270 | 108 | 0 |
| 23 | BB | 60995 | 0 | 30678 | 2536 | 0 |
| 23 | DB | 60995 | 0 | 30678 | 2543 | 0 |
| 24 | BI | 1032 | 0 | 1088 | 119 | 0 |
| 24 | DI | 1032 | 0 | 1088 | 181 | 0 |
| 25 | BC | 2082 | 0 | 2157 | 239 | 0 |
| 25 | DC | 2082 | 0 | 2157 | 241 | 0 |
| 26 | BD | 1565 | 0 | 1616 | 206 | 0 |
| 26 | DD | 1565 | 0 | 1616 | 216 | 0 |
| 27 | BK | 930 | 0 | 1000 | 122 | 0 |
| 27 | DK | 930 | 0 | 1000 | 122 | 0 |
| 28 | BP | 917 | 0 | 965 | 102 | 0 |
| 28 | DP | 917 | 0 | 965 | 108 | 0 |
| 29 | BE | 1552 | 0 | 1619 | 194 | 0 |
| 29 | DE | 1552 | 0 | 1619 | 181 | 0 |
| 30 | BY | 449 | 0 | 491 | 49 | 0 |
| 30 | DY | 449 | 0 | 491 | 55 | 0 |
| 31 | B0 | 444 | 0 | 461 | 49 | 0 |
| 31 | D0 | 444 | 0 | 461 | 47 | 0 |
| 32 | B4 | 302 | 0 | 340 | 38 | 0 |
| 32 | D4 | 302 | 0 | 340 | 44 | 0 |
| 33 | B1 | 409 | 0 | 440 | 58 | 0 |
| 33 | D1 | 409 | 0 | 440 | 54 | 0 |
| 34 | B3 | 504 | 0 | 574 | 51 | 0 |
| 34 | D3 | 504 | 0 | 574 | 48 | 0 |
| 35 | BV | 753 | 0 | 780 | 97 | 0 |
| 35 | DV | 753 | 0 | 780 | 102 | 0 |
| 36 | B2 | 377 | 0 | 418 | 38 | 0 |
| 36 | D2 | 377 | 0 | 418 | 38 | 0 |
| 37 | BL | 1045 | 0 | 1117 | 148 | 0 |
| 37 | DL | 1045 | 0 | 1117 | 153 | 0 |
| 38 | BM | 1074 | 0 | 1157 | 129 | 0 |
| 38 | DM | 1074 | 0 | 1157 | 121 | 0 |
| 39 | BX | 509 | 0 | 543 | 55 | 0 |
| 39 | DX | 509 | 0 | 543 | 60 | 0 |
| 40 | BH | 1111 | 0 | 1148 | 186 | 0 |
| 40 | DH | 1111 | 0 | 1148 | 158 | 0 |
| 41 | BJ | 1129 | 0 | 1162 | 136 | 0 |
| 41 | DJ | 1129 | 0 | 1162 | 137 | 0 |
| 42 | BN | 960 | 0 | 1000 | 130 | 0 |
| 42 | DN | 960 | 0 | 1000 | 129 | 0 |
| 43 | BO | 892 | 0 | 923 | 94 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43 | DO | 892 | 0 | 923 | 96 | 0 |
| 44 | BQ | 947 | 0 | 1022 | 171 | 0 |
| 44 | DQ | 947 | 0 | 1022 | 178 | 0 |
| 45 | BS | 857 | 0 | 922 | 101 | 0 |
| 45 | DS | 857 | 0 | 922 | 101 | 0 |
| 46 | BU | 779 | 0 | 834 | 114 | 0 |
| 46 | DU | 779 | 0 | 834 | 109 | 0 |
| 47 | BF | 1420 | 0 | 1460 | 223 | 0 |
| 47 | DF | 1420 | 0 | 1460 | 216 | 0 |
| 48 | BG | 1323 | 0 | 1374 | 218 | 0 |
| 48 | DG | 1323 | 0 | 1374 | 195 | 0 |
| 49 | BR | 816 | 0 | 839 | 113 | 0 |
| 49 | DR | 816 | 0 | 839 | 128 | 0 |
| 50 | BT | 738 | 0 | 807 | 125 | 0 |
| 50 | DT | 738 | 0 | 807 | 121 | 0 |
| 51 | BZ | 625 | 0 | 652 | 82 | 0 |
| 51 | DZ | 625 | 0 | 652 | 82 | 0 |
| 52 | BW | 596 | 0 | 610 | 120 | 0 |
| 52 | DW | 596 | 0 | 610 | 126 | 0 |
| 53 | B6 | 1478 | 0 | 1526 | 192 | 0 |
| 53 | D6 | 1478 | 0 | 1526 | 150 | 0 |
| 54 | AA | 60 | 0 | 0 | 0 | 0 |
| 54 | BB | 110 | 0 | 0 | 0 | 0 |
| 54 | CA | 61 | 0 | 0 | 0 | 0 |
| 54 | CE | 1 | 0 | 0 | 0 | 0 |
| 54 | DB | 111 | 0 | 0 | 0 | 0 |
| 55 | AA | 31 | 0 | 39 | 0 | 0 |
| 55 | BB | 31 | 0 | 39 | 2 | 0 |
| 55 | CA | 31 | 0 | 39 | 3 | 0 |
| 55 | DB | 31 | 0 | 39 | 0 | 0 |
| 56 | B4 | 1 | 0 | 0 | 0 | 0 |
| 56 | D4 | 1 | 0 | 0 | 0 | 0 |
| 57 | AA | 287 | 0 | 0 | 1 | 0 |
| 57 | AE | 3 | 0 | 0 | 0 | 0 |
| 57 | AK | 1 | 0 | 0 | 0 | 0 |
| 57 | AL | 3 | 0 | 0 | 0 | 0 |
| 57 | AN | 4 | 0 | 0 | 0 | 0 |
| 57 | AT | 2 | 0 | 0 | 0 | 0 |
| 57 | BB | 492 | 0 | 0 | 8 | 0 |
| 57 | BC | 6 | 0 | 0 | 0 | 0 |
| 57 | BD | 1 | 0 | 0 | 0 | 0 |
| 57 | BE | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57 | BL | 3 | 0 | 0 | 0 | 0 |
| 57 | BT | 1 | 0 | 0 | 0 | 0 |
| 57 | CA | 296 | 0 | 0 | 2 | 0 |
| 57 | CE | 3 | 0 | 0 | 0 | 0 |
| 57 | CK | 1 | 0 | 0 | 0 | 0 |
| 57 | CL | 3 | 0 | 0 | 0 | 0 |
| 57 | CN | 4 | 0 | 0 | 0 | 0 |
| 57 | CT | 2 | 0 | 0 | 0 | 0 |
| 57 | DB | 500 | 0 | 0 | 7 | 0 |
| 57 | DC | 6 | 0 | 0 | 0 | 0 |
| 57 | DE | 2 | 0 | 0 | 0 | 0 |
| 57 | DL | 2 | 0 | 0 | 0 | 0 |
| 57 | DR | 1 | 0 | 0 | 0 | 0 |
| 57 | DT | 1 | 0 | 0 | 0 | 0 |
| All | All | 287083 | 0 | 193870 | 17818 | 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 37.

The worst 5 of 17818 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) |
|------------------|-------------------|--------------------------|-------------------|
| 23:DB:1099:G:H8 | 24:DI:3:LYS:N | 1.36 | 1.20 |
| 40:BH:31:VAL:HB | 40:BH:32:PRO:HD2 | 1.23 | 1.17 |
| 21:CU:36:PHE:HB3 | 21:CU:40:PRO:HD3 | 1.28 | 1.14 |
| 21:AU:36:PHE:HB3 | 21:AU:40:PRO:HD3 | 1.29 | 1.11 |
| 25:DC:144:GLU:HA | 25:DC:151:GLY:HA2 | 1.33 | 1.11 |

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 | AC | 204/232 (88%) | 151 (74%) | 38 (19%) | 15 (7%) | 1 | 15 |
| 2 | CC | 204/232 (88%) | 152 (74%) | 37 (18%) | 15 (7%) | 1 | 15 |
| 3 | AD | 203/205 (99%) | 151 (74%) | 39 (19%) | 13 (6%) | 1 | 18 |
| 3 | CD | 203/205 (99%) | 148 (73%) | 42 (21%) | 13 (6%) | 1 | 18 |
| 4 | AE | 148/166 (89%) | 117 (79%) | 25 (17%) | 6 (4%) | 3 | 25 |
| 4 | CE | 148/166 (89%) | 117 (79%) | 25 (17%) | 6 (4%) | 3 | 25 |
| 5 | AF | 98/135 (73%) | 64 (65%) | 25 (26%) | 9 (9%) | 1 | 11 |
| 5 | CF | 98/135 (73%) | 65 (66%) | 24 (24%) | 9 (9%) | 1 | 11 |
| 6 | AG | 148/178 (83%) | 106 (72%) | 33 (22%) | 9 (6%) | 1 | 19 |
| 6 | CG | 150/178 (84%) | 112 (75%) | 29 (19%) | 9 (6%) | 1 | 19 |
| 7 | AH | 127/129 (98%) | 98 (77%) | 23 (18%) | 6 (5%) | 2 | 23 |
| 7 | CH | 127/129 (98%) | 96 (76%) | 25 (20%) | 6 (5%) | 2 | 23 |
| 8 | AI | 125/129 (97%) | 99 (79%) | 17 (14%) | 9 (7%) | 1 | 16 |
| 8 | CI | 125/129 (97%) | 98 (78%) | 18 (14%) | 9 (7%) | 1 | 16 |
| 9 | AJ | 96/103 (93%) | 70 (73%) | 13 (14%) | 13 (14%) | 0 | 4 |
| 9 | CJ | 96/103 (93%) | 71 (74%) | 12 (12%) | 13 (14%) | 0 | 4 |
| 10 | AK | 115/128 (90%) | 87 (76%) | 22 (19%) | 6 (5%) | 2 | 21 |
| 10 | CK | 115/128 (90%) | 87 (76%) | 22 (19%) | 6 (5%) | 2 | 21 |
| 11 | AL | 121/123 (98%) | 73 (60%) | 33 (27%) | 15 (12%) | 0 | 5 |
| 11 | CL | 121/123 (98%) | 75 (62%) | 31 (26%) | 15 (12%) | 0 | 5 |
| 12 | AM | 112/117 (96%) | 79 (70%) | 24 (21%) | 9 (8%) | 1 | 14 |
| 12 | CM | 111/117 (95%) | 76 (68%) | 25 (22%) | 10 (9%) | 1 | 12 |
| 13 | AN | 92/100 (92%) | 59 (64%) | 26 (28%) | 7 (8%) | 1 | 14 |
| 13 | CN | 92/100 (92%) | 60 (65%) | 24 (26%) | 8 (9%) | 1 | 12 |
| 14 | AO | 86/89 (97%) | 59 (69%) | 22 (26%) | 5 (6%) | 1 | 19 |
| 14 | CO | 86/89 (97%) | 60 (70%) | 22 (26%) | 4 (5%) | 2 | 23 |
| 15 | AP | 80/82 (98%) | 59 (74%) | 16 (20%) | 5 (6%) | 1 | 18 |
| 15 | CP | 78/82 (95%) | 56 (72%) | 16 (20%) | 6 (8%) | 1 | 14 |
| 16 | AQ | 78/83 (94%) | 58 (74%) | 15 (19%) | 5 (6%) | 1 | 18 |
| 16 | CQ | 79/83 (95%) | 59 (75%) | 15 (19%) | 5 (6%) | 1 | 18 |
| 17 | AR | 53/74 (72%) | 41 (77%) | 9 (17%) | 3 (6%) | 1 | 19 |
| 17 | CR | 53/74 (72%) | 41 (77%) | 9 (17%) | 3 (6%) | 1 | 19 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 18 | AS | 77/91 (85%) | 60 (78%) | 12 (16%) | 5 (6%) | 1 | 18 |
| 18 | CS | 78/91 (86%) | 61 (78%) | 11 (14%) | 6 (8%) | 1 | 14 |
| 19 | AT | 83/86 (96%) | 63 (76%) | 15 (18%) | 5 (6%) | 1 | 19 |
| 19 | CT | 83/86 (96%) | 62 (75%) | 16 (19%) | 5 (6%) | 1 | 19 |
| 20 | AB | 216/240 (90%) | 142 (66%) | 57 (26%) | 17 (8%) | 1 | 14 |
| 20 | CB | 216/240 (90%) | 134 (62%) | 65 (30%) | 17 (8%) | 1 | 14 |
| 21 | AU | 49/70 (70%) | 28 (57%) | 11 (22%) | 10 (20%) | 0 | 2 |
| 21 | CU | 49/70 (70%) | 28 (57%) | 12 (24%) | 9 (18%) | 0 | 2 |
| 24 | BI | 139/141 (99%) | 120 (86%) | 14 (10%) | 5 (4%) | 3 | 28 |
| 24 | DI | 139/141 (99%) | 114 (82%) | 20 (14%) | 5 (4%) | 3 | 28 |
| 25 | BC | 269/272 (99%) | 155 (58%) | 66 (24%) | 48 (18%) | 0 | 2 |
| 25 | DC | 269/272 (99%) | 155 (58%) | 65 (24%) | 49 (18%) | 0 | 2 |
| 26 | BD | 207/209 (99%) | 122 (59%) | 54 (26%) | 31 (15%) | 0 | 3 |
| 26 | DD | 207/209 (99%) | 124 (60%) | 51 (25%) | 32 (16%) | 0 | 3 |
| 27 | BK | 119/123 (97%) | 78 (66%) | 24 (20%) | 17 (14%) | 0 | 3 |
| 27 | DK | 119/123 (97%) | 78 (66%) | 24 (20%) | 17 (14%) | 0 | 3 |
| 28 | BP | 112/114 (98%) | 61 (54%) | 32 (29%) | 19 (17%) | 0 | 3 |
| 28 | DP | 112/114 (98%) | 61 (54%) | 34 (30%) | 17 (15%) | 0 | 3 |
| 29 | BE | 199/201 (99%) | 125 (63%) | 50 (25%) | 24 (12%) | 0 | 5 |
| 29 | DE | 199/201 (99%) | 125 (63%) | 51 (26%) | 23 (12%) | 0 | 6 |
| 30 | BY | 56/58 (97%) | 39 (70%) | 12 (21%) | 5 (9%) | 1 | 12 |
| 30 | DY | 56/58 (97%) | 39 (70%) | 12 (21%) | 5 (9%) | 1 | 12 |
| 31 | B0 | 54/56 (96%) | 39 (72%) | 8 (15%) | 7 (13%) | 0 | 4 |
| 31 | D0 | 54/56 (96%) | 39 (72%) | 8 (15%) | 7 (13%) | 0 | 4 |
| 32 | B4 | 36/38 (95%) | 16 (44%) | 10 (28%) | 10 (28%) | 0 | 0 |
| 32 | D4 | 36/38 (95%) | 16 (44%) | 10 (28%) | 10 (28%) | 0 | 0 |
| 33 | B1 | 48/54 (89%) | 37 (77%) | 7 (15%) | 4 (8%) | 1 | 13 |
| 33 | D1 | 48/54 (89%) | 36 (75%) | 8 (17%) | 4 (8%) | 1 | 13 |
| 34 | B3 | 62/64 (97%) | 35 (56%) | 21 (34%) | 6 (10%) | 0 | 10 |
| 34 | D3 | 62/64 (97%) | 34 (55%) | 22 (36%) | 6 (10%) | 0 | 10 |
| 35 | BV | 92/94 (98%) | 64 (70%) | 22 (24%) | 6 (6%) | 1 | 18 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 35 | DV | 92/94 (98%) | 62 (67%) | 24 (26%) | 6 (6%) | 1 | 18 |
| 36 | B2 | 44/46 (96%) | 30 (68%) | 10 (23%) | 4 (9%) | 1 | 12 |
| 36 | D2 | 44/46 (96%) | 30 (68%) | 10 (23%) | 4 (9%) | 1 | 12 |
| 37 | BL | 141/144 (98%) | 89 (63%) | 31 (22%) | 21 (15%) | 0 | 3 |
| 37 | DL | 141/144 (98%) | 89 (63%) | 32 (23%) | 20 (14%) | 0 | 3 |
| 38 | BM | 134/136 (98%) | 84 (63%) | 29 (22%) | 21 (16%) | 0 | 3 |
| 38 | DM | 134/136 (98%) | 83 (62%) | 31 (23%) | 20 (15%) | 0 | 3 |
| 39 | BX | 61/63 (97%) | 36 (59%) | 17 (28%) | 8 (13%) | 0 | 4 |
| 39 | DX | 61/63 (97%) | 36 (59%) | 17 (28%) | 8 (13%) | 0 | 4 |
| 40 | BH | 147/149 (99%) | 76 (52%) | 46 (31%) | 25 (17%) | 0 | 3 |
| 40 | DH | 147/149 (99%) | 91 (62%) | 33 (22%) | 23 (16%) | 0 | 3 |
| 41 | BJ | 140/142 (99%) | 85 (61%) | 37 (26%) | 18 (13%) | 0 | 4 |
| 41 | DJ | 140/142 (99%) | 85 (61%) | 36 (26%) | 19 (14%) | 0 | 4 |
| 42 | BN | 118/127 (93%) | 76 (64%) | 29 (25%) | 13 (11%) | 0 | 7 |
| 42 | DN | 118/127 (93%) | 77 (65%) | 28 (24%) | 13 (11%) | 0 | 7 |
| 43 | BO | 114/117 (97%) | 74 (65%) | 29 (25%) | 11 (10%) | 0 | 10 |
| 43 | DO | 114/117 (97%) | 75 (66%) | 27 (24%) | 12 (10%) | 0 | 8 |
| 44 | BQ | 115/117 (98%) | 75 (65%) | 31 (27%) | 9 (8%) | 1 | 14 |
| 44 | DQ | 115/117 (98%) | 75 (65%) | 29 (25%) | 11 (10%) | 0 | 10 |
| 45 | BS | 108/110 (98%) | 68 (63%) | 29 (27%) | 11 (10%) | 0 | 9 |
| 45 | DS | 108/110 (98%) | 66 (61%) | 31 (29%) | 11 (10%) | 0 | 9 |
| 46 | BU | 100/103 (97%) | 58 (58%) | 23 (23%) | 19 (19%) | 0 | 2 |
| 46 | DU | 100/103 (97%) | 59 (59%) | 22 (22%) | 19 (19%) | 0 | 2 |
| 47 | BF | 176/178 (99%) | 103 (58%) | 44 (25%) | 29 (16%) | 0 | 3 |
| 47 | DF | 176/178 (99%) | 105 (60%) | 42 (24%) | 29 (16%) | 0 | 3 |
| 48 | BG | 174/176 (99%) | 99 (57%) | 42 (24%) | 33 (19%) | 0 | 2 |
| 48 | DG | 174/176 (99%) | 101 (58%) | 41 (24%) | 32 (18%) | 0 | 2 |
| 49 | BR | 101/103 (98%) | 72 (71%) | 20 (20%) | 9 (9%) | 1 | 12 |
| 49 | DR | 101/103 (98%) | 74 (73%) | 18 (18%) | 9 (9%) | 1 | 12 |
| 50 | BT | 91/100 (91%) | 48 (53%) | 23 (25%) | 20 (22%) | 0 | 1 |
| 50 | DT | 91/100 (91%) | 46 (50%) | 27 (30%) | 18 (20%) | 0 | 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 51 | BZ | 75/78 (96%) | 50 (67%) | 13 (17%) | 12 (16%) | 0 | 3 |
| 51 | DZ | 75/78 (96%) | 50 (67%) | 13 (17%) | 12 (16%) | 0 | 3 |
| 52 | BW | 77/84 (92%) | 28 (36%) | 23 (30%) | 26 (34%) | 0 | 0 |
| 52 | DW | 77/84 (92%) | 28 (36%) | 24 (31%) | 25 (32%) | 0 | 0 |
| 53 | B6 | 183/185 (99%) | 162 (88%) | 16 (9%) | 5 (3%) | 5 | 34 |
| 53 | D6 | 183/185 (99%) | 152 (83%) | 24 (13%) | 7 (4%) | 3 | 27 |
| All | All | 11607/12284 (94%) | 7731 (67%) | 2581 (22%) | 1295 (11%) | 0 | 7 |

5 of 1295 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AC | 14 | VAL |
| 2 | AC | 54 | ILE |
| 2 | AC | 205 | GLU |
| 3 | AD | 24 | VAL |
| 3 | AD | 25 | ARG |

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 | AC | 170/189 (90%) | 144 (85%) | 26 (15%) | 2 | 16 |
| 2 | CC | 170/189 (90%) | 143 (84%) | 27 (16%) | 2 | 16 |
| 3 | AD | 172/172 (100%) | 146 (85%) | 26 (15%) | 3 | 17 |
| 3 | CD | 172/172 (100%) | 147 (86%) | 25 (14%) | 3 | 18 |
| 4 | AE | 113/125 (90%) | 95 (84%) | 18 (16%) | 2 | 16 |
| 4 | CE | 113/125 (90%) | 96 (85%) | 17 (15%) | 3 | 17 |
| 5 | AF | 87/116 (75%) | 76 (87%) | 11 (13%) | 4 | 22 |
| 5 | CF | 87/116 (75%) | 76 (87%) | 11 (13%) | 4 | 22 |
| 6 | AG | 123/146 (84%) | 105 (85%) | 18 (15%) | 3 | 18 |
| 6 | CG | 125/146 (86%) | 106 (85%) | 19 (15%) | 3 | 16 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 7 | AH | 104/104 (100%) | 96 (92%) | 8 (8%) | 13 | 40 |
| 7 | CH | 104/104 (100%) | 97 (93%) | 7 (7%) | 16 | 44 |
| 8 | AI | 105/106 (99%) | 91 (87%) | 14 (13%) | 4 | 21 |
| 8 | CI | 105/106 (99%) | 89 (85%) | 16 (15%) | 3 | 16 |
| 9 | AJ | 86/90 (96%) | 76 (88%) | 10 (12%) | 5 | 24 |
| 9 | CJ | 86/90 (96%) | 76 (88%) | 10 (12%) | 5 | 24 |
| 10 | AK | 90/98 (92%) | 77 (86%) | 13 (14%) | 3 | 18 |
| 10 | CK | 90/98 (92%) | 75 (83%) | 15 (17%) | 2 | 14 |
| 11 | AL | 103/103 (100%) | 86 (84%) | 17 (16%) | 2 | 14 |
| 11 | CL | 103/103 (100%) | 85 (82%) | 18 (18%) | 2 | 12 |
| 12 | AM | 92/95 (97%) | 77 (84%) | 15 (16%) | 2 | 15 |
| 12 | CM | 91/95 (96%) | 76 (84%) | 15 (16%) | 2 | 14 |
| 13 | AN | 79/83 (95%) | 62 (78%) | 17 (22%) | 1 | 6 |
| 13 | CN | 79/83 (95%) | 62 (78%) | 17 (22%) | 1 | 6 |
| 14 | AO | 76/77 (99%) | 69 (91%) | 7 (9%) | 9 | 32 |
| 14 | CO | 76/77 (99%) | 69 (91%) | 7 (9%) | 9 | 32 |
| 15 | AP | 65/65 (100%) | 59 (91%) | 6 (9%) | 9 | 32 |
| 15 | CP | 65/65 (100%) | 59 (91%) | 6 (9%) | 9 | 32 |
| 16 | AQ | 74/77 (96%) | 61 (82%) | 13 (18%) | 2 | 12 |
| 16 | CQ | 75/77 (97%) | 63 (84%) | 12 (16%) | 2 | 15 |
| 17 | AR | 48/64 (75%) | 40 (83%) | 8 (17%) | 2 | 14 |
| 17 | CR | 48/64 (75%) | 39 (81%) | 9 (19%) | 1 | 10 |
| 18 | AS | 70/78 (90%) | 56 (80%) | 14 (20%) | 1 | 8 |
| 18 | CS | 71/78 (91%) | 57 (80%) | 14 (20%) | 1 | 8 |
| 19 | AT | 65/65 (100%) | 55 (85%) | 10 (15%) | 2 | 16 |
| 19 | CT | 65/65 (100%) | 55 (85%) | 10 (15%) | 2 | 16 |
| 20 | AB | 180/198 (91%) | 148 (82%) | 32 (18%) | 2 | 12 |
| 20 | CB | 180/198 (91%) | 150 (83%) | 30 (17%) | 2 | 14 |
| 21 | AU | 44/60 (73%) | 32 (73%) | 12 (27%) | 0 | 3 |
| 21 | CU | 44/60 (73%) | 32 (73%) | 12 (27%) | 0 | 3 |
| 24 | BI | 109/109 (100%) | 107 (98%) | 2 (2%) | 59 | 77 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 24 | DI | 109/109 (100%) | 103 (94%) | 6 (6%) | 21 | 50 |
| 25 | BC | 216/217 (100%) | 179 (83%) | 37 (17%) | 2 | 13 |
| 25 | DC | 216/217 (100%) | 176 (82%) | 40 (18%) | 1 | 10 |
| 26 | BD | 164/164 (100%) | 135 (82%) | 29 (18%) | 2 | 12 |
| 26 | DD | 164/164 (100%) | 134 (82%) | 30 (18%) | 1 | 11 |
| 27 | BK | 102/104 (98%) | 80 (78%) | 22 (22%) | 1 | 6 |
| 27 | DK | 102/104 (98%) | 81 (79%) | 21 (21%) | 1 | 7 |
| 28 | BP | 99/99 (100%) | 80 (81%) | 19 (19%) | 1 | 9 |
| 28 | DP | 99/99 (100%) | 80 (81%) | 19 (19%) | 1 | 9 |
| 29 | BE | 165/165 (100%) | 143 (87%) | 22 (13%) | 4 | 21 |
| 29 | DE | 165/165 (100%) | 142 (86%) | 23 (14%) | 3 | 20 |
| 30 | BY | 48/48 (100%) | 38 (79%) | 10 (21%) | 1 | 6 |
| 30 | DY | 48/48 (100%) | 38 (79%) | 10 (21%) | 1 | 6 |
| 31 | B0 | 47/47 (100%) | 38 (81%) | 9 (19%) | 1 | 9 |
| 31 | D0 | 47/47 (100%) | 38 (81%) | 9 (19%) | 1 | 9 |
| 32 | B4 | 34/34 (100%) | 28 (82%) | 6 (18%) | 2 | 12 |
| 32 | D4 | 34/34 (100%) | 29 (85%) | 5 (15%) | 3 | 18 |
| 33 | B1 | 45/48 (94%) | 40 (89%) | 5 (11%) | 6 | 26 |
| 33 | D1 | 45/48 (94%) | 41 (91%) | 4 (9%) | 9 | 34 |
| 34 | B3 | 51/51 (100%) | 45 (88%) | 6 (12%) | 5 | 24 |
| 34 | D3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 8 | 29 |
| 35 | BV | 78/78 (100%) | 64 (82%) | 14 (18%) | 2 | 11 |
| 35 | DV | 78/78 (100%) | 64 (82%) | 14 (18%) | 2 | 11 |
| 36 | B2 | 38/38 (100%) | 28 (74%) | 10 (26%) | 0 | 3 |
| 36 | D2 | 38/38 (100%) | 28 (74%) | 10 (26%) | 0 | 3 |
| 37 | BL | 102/103 (99%) | 91 (89%) | 11 (11%) | 6 | 27 |
| 37 | DL | 102/103 (99%) | 91 (89%) | 11 (11%) | 6 | 27 |
| 38 | BM | 109/109 (100%) | 87 (80%) | 22 (20%) | 1 | 7 |
| 38 | DM | 109/109 (100%) | 87 (80%) | 22 (20%) | 1 | 7 |
| 39 | BX | 55/55 (100%) | 46 (84%) | 9 (16%) | 2 | 14 |
| 39 | DX | 55/55 (100%) | 46 (84%) | 9 (16%) | 2 | 14 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 40 | BH | 114/114 (100%) | 79 (69%) | 35 (31%) | 0 | 2 |
| 40 | DH | 114/114 (100%) | 89 (78%) | 25 (22%) | 1 | 6 |
| 41 | BJ | 116/116 (100%) | 100 (86%) | 16 (14%) | 3 | 20 |
| 41 | DJ | 116/116 (100%) | 100 (86%) | 16 (14%) | 3 | 20 |
| 42 | BN | 100/103 (97%) | 84 (84%) | 16 (16%) | 2 | 15 |
| 42 | DN | 100/103 (97%) | 84 (84%) | 16 (16%) | 2 | 15 |
| 43 | BO | 86/87 (99%) | 71 (83%) | 15 (17%) | 2 | 12 |
| 43 | DO | 86/87 (99%) | 72 (84%) | 14 (16%) | 2 | 15 |
| 44 | BQ | 89/89 (100%) | 79 (89%) | 10 (11%) | 6 | 25 |
| 44 | DQ | 89/89 (100%) | 79 (89%) | 10 (11%) | 6 | 25 |
| 45 | BS | 93/93 (100%) | 77 (83%) | 16 (17%) | 2 | 13 |
| 45 | DS | 93/93 (100%) | 77 (83%) | 16 (17%) | 2 | 13 |
| 46 | BU | 83/84 (99%) | 65 (78%) | 18 (22%) | 1 | 6 |
| 46 | DU | 83/84 (99%) | 65 (78%) | 18 (22%) | 1 | 6 |
| 47 | BF | 149/149 (100%) | 117 (78%) | 32 (22%) | 1 | 6 |
| 47 | DF | 149/149 (100%) | 117 (78%) | 32 (22%) | 1 | 6 |
| 48 | BG | 137/137 (100%) | 110 (80%) | 27 (20%) | 1 | 8 |
| 48 | DG | 137/137 (100%) | 112 (82%) | 25 (18%) | 1 | 11 |
| 49 | BR | 84/84 (100%) | 71 (84%) | 13 (16%) | 2 | 16 |
| 49 | DR | 84/84 (100%) | 70 (83%) | 14 (17%) | 2 | 14 |
| 50 | BT | 80/84 (95%) | 64 (80%) | 16 (20%) | 1 | 8 |
| 50 | DT | 80/84 (95%) | 64 (80%) | 16 (20%) | 1 | 8 |
| 51 | BZ | 67/68 (98%) | 53 (79%) | 14 (21%) | 1 | 6 |
| 51 | DZ | 67/68 (98%) | 56 (84%) | 11 (16%) | 2 | 14 |
| 52 | BW | 59/62 (95%) | 42 (71%) | 17 (29%) | 0 | 2 |
| 52 | DW | 59/62 (95%) | 42 (71%) | 17 (29%) | 0 | 2 |
| 53 | B6 | 157/157 (100%) | 137 (87%) | 20 (13%) | 4 | 22 |
| 53 | D6 | 157/157 (100%) | 134 (85%) | 23 (15%) | 3 | 18 |
| All | All | 9647/10014 (96%) | 8066 (84%) | 1581 (16%) | 2 | 14 |

5 of 1581 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | BR | 39 | LEU |
| 6 | CG | 110 | ARG |
| 47 | DF | 103 | ILE |
| 50 | BT | 68 | LYS |
| 2 | CC | 61 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 320 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | BG | 37 | ASN |
| 7 | CH | 3 | GLN |
| 46 | DU | 65 | GLN |
| 49 | BR | 86 | GLN |
| 2 | CC | 2 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1529/1542 (99%) | 244 (15%) | 21 (1%) |
| 1 | CA | 1529/1542 (99%) | 235 (15%) | 19 (1%) |
| 22 | BA | 116/120 (96%) | 17 (14%) | 0 |
| 22 | DA | 116/120 (96%) | 16 (13%) | 0 |
| 23 | BB | 2837/2904 (97%) | 457 (16%) | 17 (0%) |
| 23 | DB | 2837/2904 (97%) | 435 (15%) | 22 (0%) |
| All | All | 8964/9132 (98%) | 1404 (15%) | 79 (0%) |

5 of 1404 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 9 | G |
| 1 | AA | 14 | U |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |

5 of 79 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 2425 | A |
| 1 | CA | 372 | C |
| 23 | DB | 2336 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 2756 | U |
| 1 | CA | 243 | A |

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 55 | LLL | BB | 3111 | - | 29,33,33 | 2.33 | 11 (37%) | 34,49,49 | 1.20 | 4 (11%) |
| 55 | LLL | DB | 3112 | - | 29,33,33 | 2.38 | 12 (41%) | 34,49,49 | 1.23 | 5 (14%) |
| 55 | LLL | AA | 1661 | - | 29,33,33 | 2.37 | 11 (37%) | 34,49,49 | 1.26 | 4 (11%) |
| 55 | LLL | CA | 1662 | - | 29,33,33 | 2.37 | 11 (37%) | 34,49,49 | 1.26 | 4 (11%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 55 | LLL | BB | 3111 | - | - | 1/11/65/65 | 0/3/3/3 |
| 55 | LLL | DB | 3112 | - | - | 1/11/65/65 | 0/3/3/3 |
| 55 | LLL | AA | 1661 | - | - | 1/11/65/65 | 0/3/3/3 |
| 55 | LLL | CA | 1662 | - | - | 1/11/65/65 | 0/3/3/3 |

The worst 5 of 45 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 55 | CA | 1662 | LLL | O53-C53 | 6.36 | 1.52 | 1.43 |
| 55 | AA | 1661 | LLL | O53-C53 | 6.34 | 1.52 | 1.43 |
| 55 | DB | 3112 | LLL | O53-C53 | 6.32 | 1.52 | 1.43 |
| 55 | BB | 3111 | LLL | O53-C53 | 6.27 | 1.52 | 1.43 |
| 55 | CA | 1662 | LLL | O53-C13 | 4.57 | 1.51 | 1.41 |

The worst 5 of 17 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 55 | CA | 1662 | LLL | C53-O53-C13 | 3.78 | 117.62 | 111.53 |
| 55 | DB | 3112 | LLL | C53-O53-C13 | 3.76 | 117.59 | 111.53 |
| 55 | AA | 1661 | LLL | C53-O53-C13 | 3.68 | 117.45 | 111.53 |
| 55 | BB | 3111 | LLL | C53-O53-C13 | 3.68 | 117.45 | 111.53 |
| 55 | AA | 1661 | LLL | C13-O62-C62 | 2.64 | 124.50 | 117.96 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 55 | DB | 3112 | LLL | C23-C33-N33-C93 |
| 55 | AA | 1661 | LLL | C23-C33-N33-C93 |
| 55 | BB | 3111 | LLL | C23-C33-N33-C93 |
| 55 | CA | 1662 | LLL | C23-C33-N33-C93 |

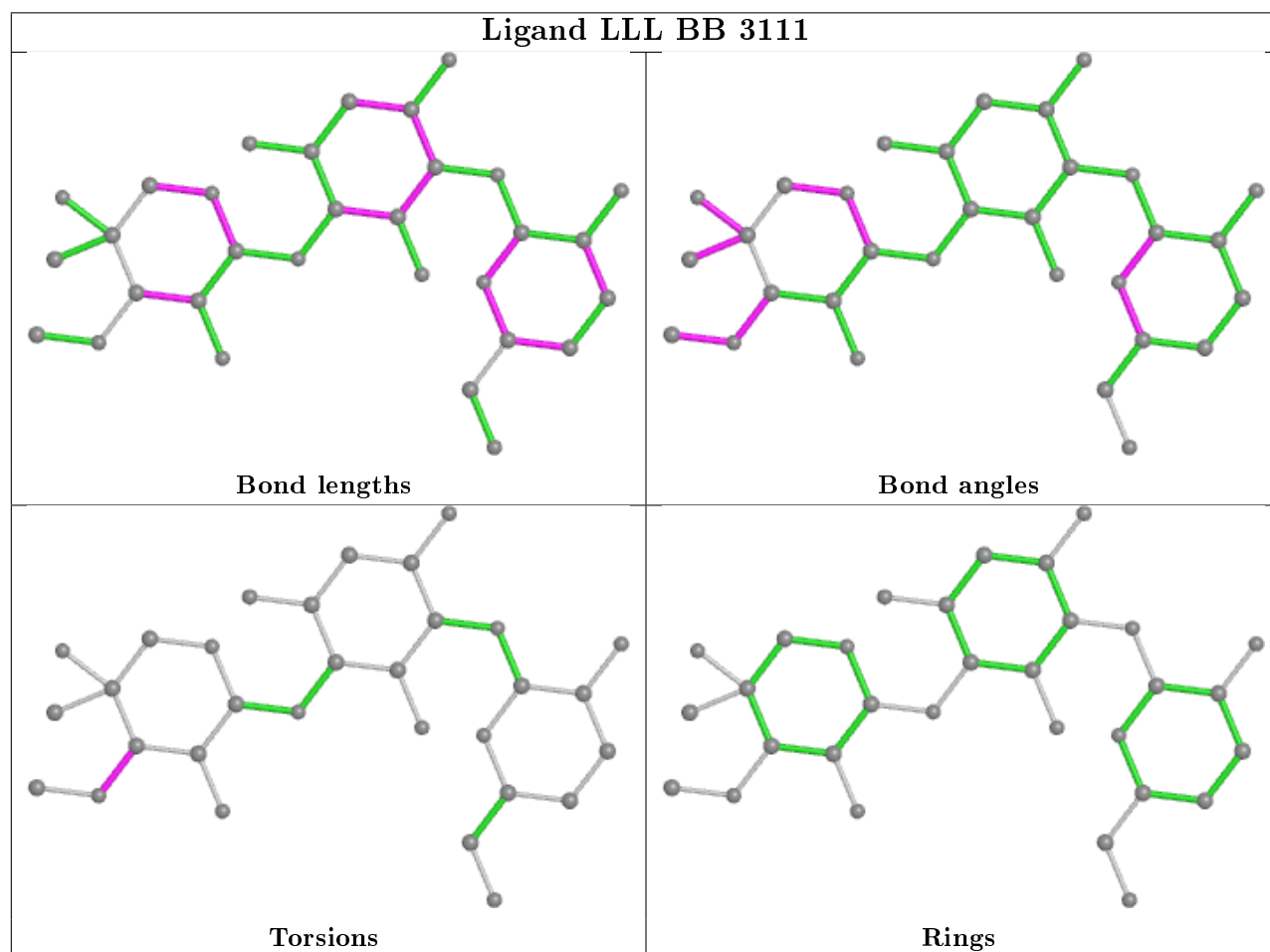
There are no ring outliers.

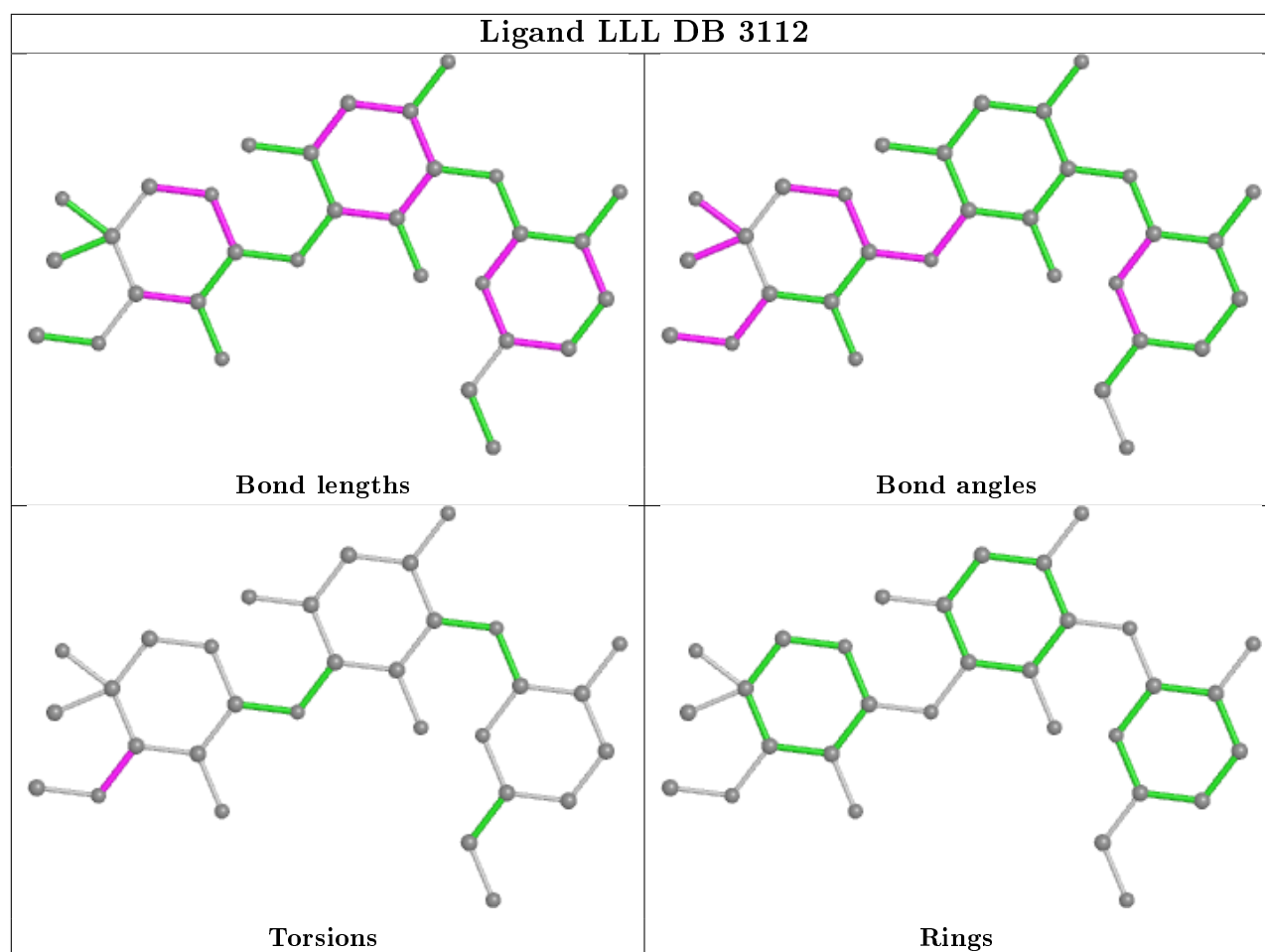
2 monomers are involved in 5 short contacts:

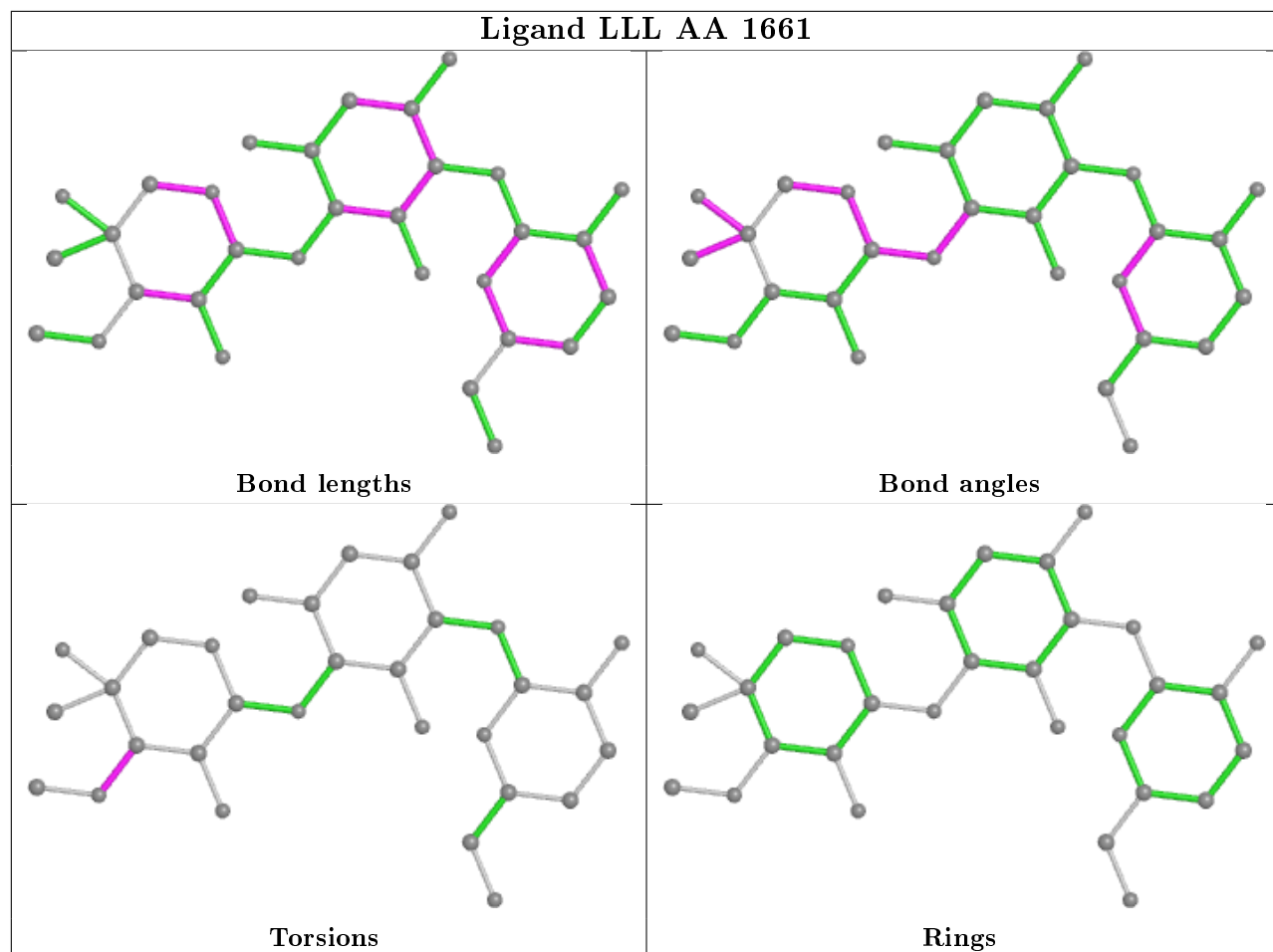
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 55 | BB | 3111 | LLL | 2 | 0 |
| 55 | CA | 1662 | LLL | 3 | 0 |

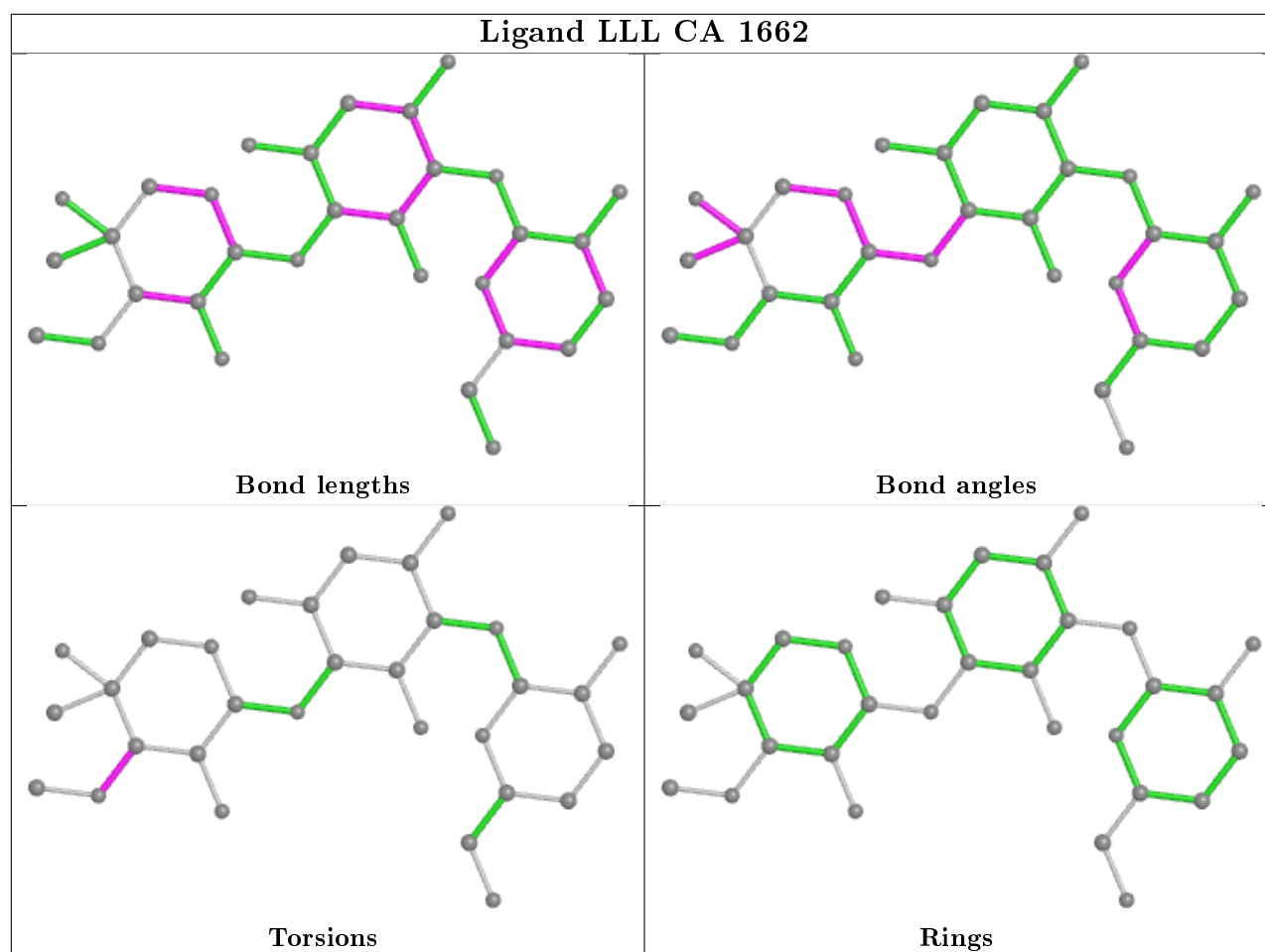
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 | 1530/1542 (99%) | -0.34 | 8 (0%) 91 85 | 13, 75, 157, 180 | 0 |
| 1 | CA | 1530/1542 (99%) | -0.40 | 1 (0%) 95 94 | 8, 52, 139, 180 | 0 |
| 2 | AC | 206/232 (88%) | -0.19 | 3 (1%) 73 64 | 5, 72, 147, 180 | 0 |
| 2 | CC | 206/232 (88%) | -0.10 | 1 (0%) 91 85 | 6, 72, 131, 180 | 0 |
| 3 | AD | 205/205 (100%) | 0.19 | 8 (3%) 39 31 | 20, 95, 159, 180 | 0 |
| 3 | CD | 205/205 (100%) | -0.17 | 0 100 100 | 5, 56, 145, 180 | 0 |
| 4 | AE | 150/166 (90%) | 0.16 | 3 (2%) 65 56 | 7, 69, 146, 180 | 0 |
| 4 | CE | 150/166 (90%) | 0.16 | 3 (2%) 65 56 | 5, 49, 112, 180 | 0 |
| 5 | AF | 100/135 (74%) | 0.24 | 6 (6%) 21 17 | 5, 69, 150, 177 | 0 |
| 5 | CF | 100/135 (74%) | -0.01 | 1 (1%) 82 74 | 5, 72, 143, 166 | 0 |
| 6 | AG | 150/178 (84%) | 0.01 | 4 (2%) 54 44 | 20, 97, 159, 175 | 0 |
| 6 | CG | 152/178 (85%) | -0.14 | 1 (0%) 87 82 | 29, 85, 147, 180 | 0 |
| 7 | AH | 129/129 (100%) | 0.26 | 8 (6%) 20 17 | 26, 80, 143, 177 | 0 |
| 7 | CH | 129/129 (100%) | 0.00 | 0 100 100 | 6, 49, 117, 174 | 0 |
| 8 | AI | 127/129 (98%) | 0.01 | 2 (1%) 72 62 | 18, 89, 171, 180 | 0 |
| 8 | CI | 127/129 (98%) | -0.05 | 2 (1%) 72 62 | 22, 92, 160, 180 | 0 |
| 9 | AJ | 98/103 (95%) | 0.21 | 2 (2%) 65 56 | 16, 92, 169, 180 | 0 |
| 9 | CJ | 98/103 (95%) | 0.30 | 5 (5%) 28 24 | 26, 87, 153, 180 | 0 |
| 10 | AK | 117/128 (91%) | -0.16 | 0 100 100 | 7, 59, 119, 180 | 0 |
| 10 | CK | 117/128 (91%) | -0.19 | 2 (1%) 70 60 | 5, 52, 120, 180 | 0 |
| 11 | AL | 123/123 (100%) | 0.10 | 3 (2%) 59 49 | 14, 78, 152, 180 | 0 |
| 11 | CL | 123/123 (100%) | -0.05 | 0 100 100 | 5, 46, 127, 170 | 0 |
| 12 | AM | 114/117 (97%) | -0.18 | 0 100 100 | 40, 114, 180, 180 | 0 |
| 12 | CM | 113/117 (96%) | -0.23 | 0 100 100 | 27, 100, 173, 180 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AN | 96/100 (96%) | -0.01 | 0 100 100 | 8, 86, 158, 180 | 0 |
| 13 | CN | 96/100 (96%) | 0.08 | 1 (1%) 82 74 | 14, 87, 147, 178 | 0 |
| 14 | AO | 88/89 (98%) | -0.35 | 0 100 100 | 5, 76, 128, 180 | 0 |
| 14 | CO | 88/89 (98%) | -0.20 | 0 100 100 | 10, 63, 132, 159 | 0 |
| 15 | AP | 82/82 (100%) | 0.67 | 3 (3%) 41 32 | 24, 94, 154, 180 | 0 |
| 15 | CP | 80/82 (97%) | 0.43 | 5 (6%) 20 16 | 5, 46, 128, 180 | 0 |
| 16 | AQ | 80/83 (96%) | 0.02 | 0 100 100 | 36, 96, 168, 180 | 0 |
| 16 | CQ | 81/83 (97%) | 0.02 | 0 100 100 | 5, 52, 135, 180 | 0 |
| 17 | AR | 55/74 (74%) | -0.05 | 1 (1%) 68 59 | 14, 70, 148, 180 | 0 |
| 17 | CR | 55/74 (74%) | 0.39 | 3 (5%) 25 21 | 12, 64, 136, 180 | 0 |
| 18 | AS | 79/91 (86%) | 0.40 | 6 (7%) 13 11 | 44, 120, 176, 180 | 0 |
| 18 | CS | 80/91 (87%) | -0.18 | 0 100 100 | 34, 107, 180, 180 | 0 |
| 19 | AT | 85/86 (98%) | -0.20 | 0 100 100 | 34, 101, 168, 180 | 0 |
| 19 | CT | 85/86 (98%) | -0.40 | 0 100 100 | 5, 62, 140, 180 | 0 |
| 20 | AB | 218/240 (90%) | 0.13 | 8 (3%) 41 32 | 18, 97, 160, 180 | 0 |
| 20 | CB | 218/240 (90%) | 0.11 | 6 (2%) 53 42 | 16, 93, 160, 180 | 0 |
| 21 | AU | 51/70 (72%) | 0.00 | 1 (1%) 65 56 | 27, 89, 171, 180 | 0 |
| 21 | CU | 51/70 (72%) | -0.11 | 0 100 100 | 23, 81, 137, 180 | 0 |
| 22 | BA | 117/120 (97%) | -0.42 | 0 100 100 | 49, 85, 136, 180 | 0 |
| 22 | DA | 117/120 (97%) | -0.35 | 2 (1%) 70 60 | 36, 88, 148, 180 | 0 |
| 23 | BB | 2841/2904 (97%) | -0.16 | 14 (0%) 91 85 | 6, 60, 150, 180 | 0 |
| 23 | DB | 2841/2904 (97%) | -0.20 | 8 (0%) 94 90 | 5, 46, 154, 180 | 0 |
| 24 | BI | 141/141 (100%) | 0.97 | 24 (17%) 1 2 | 72, 166, 180, 180 | 0 |
| 24 | DI | 141/141 (100%) | 0.58 | 12 (8%) 10 9 | 63, 162, 180, 180 | 0 |
| 25 | BC | 271/272 (99%) | 0.09 | 2 (0%) 87 82 | 5, 47, 107, 156 | 0 |
| 25 | DC | 271/272 (99%) | 0.03 | 0 100 100 | 5, 38, 99, 145 | 0 |
| 26 | BD | 209/209 (100%) | 0.38 | 16 (7%) 13 11 | 8, 72, 145, 180 | 0 |
| 26 | DD | 209/209 (100%) | 0.10 | 1 (0%) 91 85 | 5, 51, 131, 180 | 0 |
| 27 | BK | 121/123 (98%) | 0.62 | 5 (4%) 37 30 | 16, 62, 142, 180 | 0 |
| 27 | DK | 121/123 (98%) | 0.24 | 0 100 100 | 5, 42, 103, 180 | 0 |
| 28 | BP | 114/114 (100%) | 1.10 | 18 (15%) 2 2 | 28, 86, 155, 173 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | DP | 114/114 (100%) | -0.22 | 0 100 100 | 5, 52, 119, 161 | 0 |
| 29 | BE | 201/201 (100%) | 0.34 | 14 (6%) 16 13 | 5, 76, 143, 180 | 0 |
| 29 | DE | 201/201 (100%) | 0.08 | 5 (2%) 57 47 | 5, 66, 138, 180 | 0 |
| 30 | BY | 58/58 (100%) | 0.28 | 3 (5%) 27 24 | 22, 84, 137, 180 | 0 |
| 30 | DY | 58/58 (100%) | -0.05 | 1 (1%) 70 60 | 10, 66, 149, 158 | 0 |
| 31 | B0 | 56/56 (100%) | 0.16 | 2 (3%) 42 34 | 5, 81, 149, 180 | 0 |
| 31 | D0 | 56/56 (100%) | -0.25 | 0 100 100 | 9, 54, 119, 180 | 0 |
| 32 | B4 | 38/38 (100%) | 0.08 | 1 (2%) 56 46 | 5, 71, 153, 168 | 0 |
| 32 | D4 | 38/38 (100%) | -0.01 | 0 100 100 | 17, 62, 132, 171 | 0 |
| 33 | B1 | 50/54 (92%) | 0.40 | 3 (6%) 21 17 | 32, 87, 132, 174 | 0 |
| 33 | D1 | 50/54 (92%) | 0.17 | 2 (4%) 38 30 | 24, 73, 125, 155 | 0 |
| 34 | B3 | 64/64 (100%) | 0.59 | 4 (6%) 20 16 | 19, 64, 105, 133 | 0 |
| 34 | D3 | 64/64 (100%) | 0.14 | 1 (1%) 72 62 | 6, 49, 107, 180 | 0 |
| 35 | BV | 94/94 (100%) | -0.11 | 1 (1%) 80 72 | 37, 92, 143, 180 | 0 |
| 35 | DV | 94/94 (100%) | -0.09 | 0 100 100 | 27, 94, 160, 180 | 0 |
| 36 | B2 | 46/46 (100%) | 0.00 | 0 100 100 | 5, 50, 123, 143 | 0 |
| 36 | D2 | 46/46 (100%) | -0.12 | 0 100 100 | 7, 43, 103, 180 | 0 |
| 37 | BL | 143/144 (99%) | 0.25 | 1 (0%) 87 82 | 7, 72, 131, 180 | 0 |
| 37 | DL | 143/144 (99%) | 0.12 | 0 100 100 | 5, 61, 128, 162 | 0 |
| 38 | BM | 136/136 (100%) | 0.08 | 4 (2%) 51 41 | 16, 68, 144, 165 | 0 |
| 38 | DM | 136/136 (100%) | 0.22 | 4 (2%) 51 41 | 5, 63, 134, 171 | 0 |
| 39 | BX | 63/63 (100%) | 0.26 | 2 (3%) 47 37 | 24, 92, 169, 180 | 0 |
| 39 | DX | 63/63 (100%) | -0.09 | 2 (3%) 47 37 | 38, 94, 166, 180 | 0 |
| 40 | BH | 149/149 (100%) | 1.22 | 28 (18%) 1 1 | 13, 125, 180, 180 | 0 |
| 40 | DH | 149/149 (100%) | 0.38 | 6 (4%) 38 30 | 5, 109, 171, 180 | 0 |
| 41 | BJ | 142/142 (100%) | 0.03 | 2 (1%) 75 65 | 13, 77, 132, 166 | 0 |
| 41 | DJ | 142/142 (100%) | -0.13 | 1 (0%) 87 82 | 5, 65, 128, 180 | 0 |
| 42 | BN | 120/127 (94%) | 0.06 | 1 (0%) 86 79 | 5, 68, 136, 180 | 0 |
| 42 | DN | 120/127 (94%) | -0.38 | 0 100 100 | 5, 44, 116, 141 | 0 |
| 43 | BO | 116/117 (99%) | 0.39 | 8 (6%) 16 13 | 29, 94, 144, 180 | 0 |
| 43 | DO | 116/117 (99%) | -0.10 | 2 (1%) 70 60 | 5, 93, 156, 180 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | BQ | 117/117 (100%) | -0.37 | 0 100 100 | 5, 72, 134, 171 | 0 |
| 44 | DQ | 117/117 (100%) | 0.05 | 1 (0%) 84 77 | 5, 50, 131, 156 | 0 |
| 45 | BS | 110/110 (100%) | 0.44 | 2 (1%) 68 59 | 5, 67, 129, 180 | 0 |
| 45 | DS | 110/110 (100%) | 0.29 | 0 100 100 | 5, 50, 120, 157 | 0 |
| 46 | BU | 102/103 (99%) | 0.71 | 6 (5%) 22 18 | 13, 88, 148, 177 | 0 |
| 46 | DU | 102/103 (99%) | -0.00 | 1 (0%) 82 74 | 26, 93, 154, 180 | 0 |
| 47 | BF | 178/178 (100%) | 0.29 | 2 (1%) 80 72 | 39, 115, 174, 180 | 0 |
| 47 | DF | 178/178 (100%) | 0.60 | 13 (7%) 15 12 | 22, 106, 175, 180 | 0 |
| 48 | BG | 176/176 (100%) | 0.23 | 2 (1%) 80 72 | 8, 102, 172, 180 | 0 |
| 48 | DG | 176/176 (100%) | 0.03 | 3 (1%) 70 60 | 32, 104, 164, 180 | 0 |
| 49 | BR | 103/103 (100%) | 0.14 | 3 (2%) 51 41 | 18, 99, 151, 173 | 0 |
| 49 | DR | 103/103 (100%) | 0.29 | 4 (3%) 39 31 | 5, 85, 144, 180 | 0 |
| 50 | BT | 93/100 (93%) | 0.23 | 2 (2%) 62 52 | 13, 83, 160, 180 | 0 |
| 50 | DT | 93/100 (93%) | 0.31 | 3 (3%) 47 37 | 15, 79, 167, 180 | 0 |
| 51 | BZ | 77/78 (98%) | 0.29 | 3 (3%) 39 31 | 12, 57, 112, 152 | 0 |
| 51 | DZ | 77/78 (98%) | -0.13 | 1 (1%) 77 68 | 5, 56, 101, 131 | 0 |
| 52 | BW | 79/84 (94%) | 0.60 | 7 (8%) 9 8 | 19, 88, 139, 180 | 0 |
| 52 | DW | 79/84 (94%) | 0.03 | 3 (3%) 40 32 | 5, 79, 143, 180 | 0 |
| 53 | B6 | 185/185 (100%) | 2.72 | 83 (44%) 0 0 | 23, 123, 180, 180 | 0 |
| 53 | D6 | 185/185 (100%) | 1.06 | 49 (26%) 0 0 | 5, 104, 180, 180 | 0 |
| All | All | 20787/21416 (97%) | 0.00 | 485 (2%) 60 51 | 5, 69, 159, 180 | 0 |

The worst 5 of 485 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 53 | B6 | 96 | GLY | 15.3 |
| 53 | B6 | 97 | ASP | 15.0 |
| 53 | B6 | 98 | ALA | 13.2 |
| 53 | B6 | 88 | LEU | 10.7 |
| 53 | B6 | 94 | ASN | 10.0 |

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

There are no non-standard protein/DNA/RNA residues in this entry.

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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | AA | 1625 | 1/1 | 0.26 | 0.88 | 84,84,84,84 | 1 |
| 54 | MG | BB | 3033 | 1/1 | 0.48 | 0.65 | 141,141,141,141 | 0 |
| 54 | MG | AA | 1608 | 1/1 | 0.48 | 0.29 | 147,147,147,147 | 0 |
| 54 | MG | CA | 1627 | 1/1 | 0.52 | 0.33 | 69,69,69,69 | 1 |
| 54 | MG | AA | 1635 | 1/1 | 0.52 | 0.09 | 103,103,103,103 | 0 |
| 54 | MG | AA | 1622 | 1/1 | 0.53 | 0.39 | 163,163,163,163 | 0 |
| 54 | MG | AA | 1626 | 1/1 | 0.54 | 0.18 | 49,49,49,49 | 1 |
| 54 | MG | DB | 3060 | 1/1 | 0.55 | 0.10 | 104,104,104,104 | 0 |
| 54 | MG | AA | 1647 | 1/1 | 0.55 | 0.99 | 180,180,180,180 | 0 |
| 54 | MG | BB | 3042 | 1/1 | 0.56 | 0.12 | 135,135,135,135 | 0 |
| 54 | MG | AA | 1639 | 1/1 | 0.60 | 0.34 | 134,134,134,134 | 0 |
| 54 | MG | AA | 1632 | 1/1 | 0.65 | 0.26 | 62,62,62,62 | 0 |
| 54 | MG | AA | 1619 | 1/1 | 0.65 | 0.25 | 180,180,180,180 | 0 |
| 54 | MG | AA | 1637 | 1/1 | 0.66 | 2.40 | 151,151,151,151 | 0 |
| 54 | MG | DB | 3066 | 1/1 | 0.68 | 0.30 | 158,158,158,158 | 0 |
| 54 | MG | AA | 1650 | 1/1 | 0.69 | 0.14 | 122,122,122,122 | 0 |
| 54 | MG | AA | 1659 | 1/1 | 0.69 | 0.45 | 180,180,180,180 | 0 |
| 54 | MG | DB | 3059 | 1/1 | 0.69 | 0.23 | 166,166,166,166 | 0 |
| 54 | MG | BB | 3093 | 1/1 | 0.70 | 0.37 | 131,131,131,131 | 0 |
| 54 | MG | CA | 1619 | 1/1 | 0.70 | 0.19 | 70,70,70,70 | 0 |
| 54 | MG | AA | 1656 | 1/1 | 0.71 | 0.79 | 161,161,161,161 | 0 |
| 54 | MG | AA | 1614 | 1/1 | 0.71 | 0.11 | 113,113,113,113 | 0 |
| 54 | MG | CA | 1614 | 1/1 | 0.71 | 0.16 | 90,90,90,90 | 0 |
| 54 | MG | AA | 1602 | 1/1 | 0.73 | 0.18 | 147,147,147,147 | 0 |
| 54 | MG | AA | 1646 | 1/1 | 0.73 | 0.18 | 104,104,104,104 | 0 |
| 54 | MG | AA | 1657 | 1/1 | 0.76 | 0.42 | 124,124,124,124 | 0 |
| 54 | MG | CA | 1623 | 1/1 | 0.76 | 0.08 | 173,173,173,173 | 0 |
| 54 | MG | BB | 3080 | 1/1 | 0.79 | 0.20 | 77,77,77,77 | 0 |
| 54 | MG | AA | 1627 | 1/1 | 0.79 | 0.19 | 68,68,68,68 | 0 |
| 54 | MG | BB | 3079 | 1/1 | 0.79 | 0.20 | 63,63,63,63 | 0 |
| 54 | MG | BB | 3097 | 1/1 | 0.80 | 0.07 | 88,88,88,88 | 0 |
| 54 | MG | DB | 3057 | 1/1 | 0.80 | 0.10 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | CE | 201 | 1/1 | 0.80 | 0.22 | 113,113,113,113 | 0 |
| 54 | MG | AA | 1613 | 1/1 | 0.81 | 0.08 | 71,71,71,71 | 0 |
| 54 | MG | BB | 3013 | 1/1 | 0.81 | 0.18 | 92,92,92,92 | 0 |
| 54 | MG | CA | 1641 | 1/1 | 0.81 | 0.17 | 42,42,42,42 | 0 |
| 54 | MG | DB | 3034 | 1/1 | 0.81 | 0.20 | 69,69,69,69 | 0 |
| 54 | MG | BB | 3043 | 1/1 | 0.82 | 0.08 | 122,122,122,122 | 0 |
| 54 | MG | CA | 1658 | 1/1 | 0.83 | 0.34 | 53,53,53,53 | 0 |
| 54 | MG | CA | 1616 | 1/1 | 0.83 | 0.14 | 88,88,88,88 | 0 |
| 54 | MG | DB | 3058 | 1/1 | 0.83 | 0.85 | 162,162,162,162 | 0 |
| 54 | MG | CA | 1635 | 1/1 | 0.83 | 0.14 | 98,98,98,98 | 0 |
| 54 | MG | AA | 1623 | 1/1 | 0.83 | 0.65 | 73,73,73,73 | 1 |
| 54 | MG | BB | 3010 | 1/1 | 0.84 | 0.13 | 40,40,40,40 | 0 |
| 55 | LLL | DB | 3112 | 31/31 | 0.84 | 0.34 | 121,121,121,121 | 0 |
| 54 | MG | CA | 1643 | 1/1 | 0.84 | 0.07 | 32,32,32,32 | 0 |
| 54 | MG | AA | 1620 | 1/1 | 0.85 | 0.06 | 113,113,113,113 | 0 |
| 54 | MG | DB | 3100 | 1/1 | 0.85 | 0.21 | 46,46,46,46 | 0 |
| 54 | MG | DB | 3030 | 1/1 | 0.86 | 0.17 | 10,10,10,10 | 0 |
| 54 | MG | AA | 1651 | 1/1 | 0.86 | 0.09 | 112,112,112,112 | 0 |
| 54 | MG | AA | 1658 | 1/1 | 0.86 | 0.09 | 85,85,85,85 | 0 |
| 54 | MG | BB | 3019 | 1/1 | 0.86 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | CA | 1638 | 1/1 | 0.86 | 0.11 | 98,98,98,98 | 0 |
| 54 | MG | AA | 1606 | 1/1 | 0.87 | 0.08 | 47,47,47,47 | 0 |
| 55 | LLL | BB | 3111 | 31/31 | 0.87 | 0.26 | 107,107,107,107 | 0 |
| 54 | MG | DB | 3013 | 1/1 | 0.88 | 0.14 | 41,41,41,41 | 0 |
| 54 | MG | DB | 3026 | 1/1 | 0.88 | 0.18 | 54,54,54,54 | 0 |
| 54 | MG | BB | 3081 | 1/1 | 0.88 | 0.17 | 16,16,16,16 | 0 |
| 54 | MG | DB | 3055 | 1/1 | 0.88 | 0.13 | 41,41,41,41 | 0 |
| 54 | MG | BB | 3049 | 1/1 | 0.88 | 0.15 | 35,35,35,35 | 0 |
| 54 | MG | DB | 3029 | 1/1 | 0.88 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | CA | 1629 | 1/1 | 0.89 | 0.12 | 65,65,65,65 | 1 |
| 54 | MG | BB | 3092 | 1/1 | 0.89 | 0.08 | 45,45,45,45 | 0 |
| 54 | MG | BB | 3008 | 1/1 | 0.89 | 0.20 | 75,75,75,75 | 0 |
| 54 | MG | BB | 3053 | 1/1 | 0.89 | 0.07 | 79,79,79,79 | 0 |
| 54 | MG | AA | 1645 | 1/1 | 0.89 | 0.09 | 95,95,95,95 | 0 |
| 54 | MG | DB | 3015 | 1/1 | 0.89 | 0.10 | 24,24,24,24 | 0 |
| 54 | MG | DB | 3072 | 1/1 | 0.90 | 0.09 | 54,54,54,54 | 0 |
| 54 | MG | DB | 3033 | 1/1 | 0.90 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | BB | 3057 | 1/1 | 0.90 | 0.36 | 65,65,65,65 | 0 |
| 54 | MG | BB | 3072 | 1/1 | 0.90 | 0.14 | 79,79,79,79 | 0 |
| 54 | MG | BB | 3037 | 1/1 | 0.90 | 0.11 | 44,44,44,44 | 0 |
| 54 | MG | AA | 1601 | 1/1 | 0.91 | 0.12 | 41,41,41,41 | 0 |
| 54 | MG | CA | 1609 | 1/1 | 0.91 | 0.04 | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1646 | 1/1 | 0.91 | 0.08 | 99,99,99,99 | 0 |
| 54 | MG | BB | 3078 | 1/1 | 0.91 | 0.21 | 101,101,101,101 | 0 |
| 54 | MG | DB | 3074 | 1/1 | 0.91 | 0.09 | 17,17,17,17 | 0 |
| 54 | MG | CA | 1649 | 1/1 | 0.91 | 0.14 | 127,127,127,127 | 0 |
| 54 | MG | BB | 3061 | 1/1 | 0.91 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | AA | 1649 | 1/1 | 0.91 | 0.06 | 82,82,82,82 | 0 |
| 54 | MG | DB | 3052 | 1/1 | 0.91 | 0.24 | 113,113,113,113 | 0 |
| 54 | MG | CA | 1621 | 1/1 | 0.91 | 0.53 | 110,110,110,110 | 0 |
| 54 | MG | BB | 3088 | 1/1 | 0.92 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | CA | 1657 | 1/1 | 0.92 | 0.24 | 89,89,89,89 | 0 |
| 54 | MG | AA | 1641 | 1/1 | 0.92 | 0.04 | 69,69,69,69 | 0 |
| 54 | MG | AA | 1630 | 1/1 | 0.92 | 0.11 | 88,88,88,88 | 0 |
| 54 | MG | DB | 3006 | 1/1 | 0.92 | 0.14 | 15,15,15,15 | 0 |
| 54 | MG | DB | 3045 | 1/1 | 0.92 | 0.07 | 68,68,68,68 | 0 |
| 54 | MG | BB | 3003 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | CA | 1660 | 1/1 | 0.92 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | BB | 3108 | 1/1 | 0.92 | 0.22 | 44,44,44,44 | 0 |
| 54 | MG | CA | 1659 | 1/1 | 0.92 | 0.09 | 90,90,90,90 | 0 |
| 54 | MG | DB | 3064 | 1/1 | 0.92 | 0.10 | 19,19,19,19 | 0 |
| 54 | MG | AA | 1615 | 1/1 | 0.92 | 0.23 | 106,106,106,106 | 0 |
| 54 | MG | DB | 3053 | 1/1 | 0.92 | 0.09 | 80,80,80,80 | 0 |
| 54 | MG | BB | 3018 | 1/1 | 0.92 | 0.18 | 50,50,50,50 | 0 |
| 54 | MG | BB | 3035 | 1/1 | 0.93 | 0.13 | 82,82,82,82 | 0 |
| 54 | MG | CA | 1642 | 1/1 | 0.93 | 0.13 | 108,108,108,108 | 0 |
| 54 | MG | DB | 3080 | 1/1 | 0.93 | 0.08 | 5,5,5,5 | 0 |
| 54 | MG | DB | 3037 | 1/1 | 0.93 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | DB | 3003 | 1/1 | 0.93 | 0.16 | 33,33,33,33 | 0 |
| 54 | MG | CA | 1636 | 1/1 | 0.93 | 0.05 | 92,92,92,92 | 0 |
| 54 | MG | CA | 1606 | 1/1 | 0.93 | 0.13 | 138,138,138,138 | 0 |
| 54 | MG | DB | 3035 | 1/1 | 0.93 | 0.19 | 75,75,75,75 | 0 |
| 54 | MG | BB | 3004 | 1/1 | 0.93 | 0.19 | 73,73,73,73 | 0 |
| 54 | MG | CA | 1624 | 1/1 | 0.93 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | CA | 1620 | 1/1 | 0.93 | 0.14 | 37,37,37,37 | 0 |
| 54 | MG | CA | 1615 | 1/1 | 0.93 | 0.09 | 180,180,180,180 | 0 |
| 54 | MG | AA | 1624 | 1/1 | 0.93 | 0.10 | 77,77,77,77 | 0 |
| 54 | MG | BB | 3017 | 1/1 | 0.93 | 0.17 | 73,73,73,73 | 0 |
| 54 | MG | DB | 3020 | 1/1 | 0.94 | 0.20 | 13,13,13,13 | 0 |
| 54 | MG | DB | 3110 | 1/1 | 0.94 | 0.18 | 38,38,38,38 | 0 |
| 54 | MG | CA | 1654 | 1/1 | 0.94 | 0.10 | 59,59,59,59 | 0 |
| 55 | LLL | CA | 1662 | 31/31 | 0.94 | 0.22 | 14,14,14,14 | 0 |
| 54 | MG | DB | 3042 | 1/1 | 0.94 | 0.07 | 23,23,23,23 | 0 |
| 54 | MG | BB | 3065 | 1/1 | 0.94 | 0.06 | 5,5,5,5 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | DB | 3097 | 1/1 | 0.94 | 0.18 | 64,64,64,64 | 0 |
| 54 | MG | CA | 1652 | 1/1 | 0.94 | 0.17 | 65,65,65,65 | 0 |
| 54 | MG | AA | 1660 | 1/1 | 0.94 | 0.08 | 37,37,37,37 | 0 |
| 54 | MG | DB | 3022 | 1/1 | 0.94 | 0.08 | 71,71,71,71 | 0 |
| 54 | MG | AA | 1631 | 1/1 | 0.94 | 0.12 | 88,88,88,88 | 0 |
| 54 | MG | DB | 3106 | 1/1 | 0.94 | 0.18 | 64,64,64,64 | 0 |
| 54 | MG | BB | 3100 | 1/1 | 0.94 | 0.22 | 151,151,151,151 | 0 |
| 54 | MG | DB | 3061 | 1/1 | 0.94 | 0.09 | 69,69,69,69 | 0 |
| 56 | ZN | D4 | 101 | 1/1 | 0.94 | 0.07 | 45,45,45,45 | 0 |
| 54 | MG | DB | 3093 | 1/1 | 0.94 | 0.17 | 10,10,10,10 | 0 |
| 54 | MG | AA | 1644 | 1/1 | 0.94 | 0.13 | 98,98,98,98 | 0 |
| 54 | MG | CA | 1628 | 1/1 | 0.94 | 0.07 | 44,44,44,44 | 0 |
| 54 | MG | DB | 3016 | 1/1 | 0.95 | 0.07 | 25,25,25,25 | 0 |
| 54 | MG | DB | 3038 | 1/1 | 0.95 | 0.15 | 37,37,37,37 | 0 |
| 54 | MG | BB | 3038 | 1/1 | 0.95 | 0.23 | 152,152,152,152 | 0 |
| 54 | MG | AA | 1655 | 1/1 | 0.95 | 0.06 | 54,54,54,54 | 0 |
| 54 | MG | BB | 3095 | 1/1 | 0.95 | 0.11 | 81,81,81,81 | 0 |
| 54 | MG | DB | 3024 | 1/1 | 0.95 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | DB | 3083 | 1/1 | 0.95 | 0.17 | 83,83,83,83 | 0 |
| 54 | MG | AA | 1654 | 1/1 | 0.95 | 0.07 | 82,82,82,82 | 0 |
| 54 | MG | AA | 1636 | 1/1 | 0.95 | 0.06 | 93,93,93,93 | 0 |
| 54 | MG | DB | 3109 | 1/1 | 0.95 | 0.09 | 83,83,83,83 | 0 |
| 54 | MG | AA | 1648 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 54 | MG | BB | 3031 | 1/1 | 0.95 | 0.13 | 63,63,63,63 | 0 |
| 54 | MG | CA | 1625 | 1/1 | 0.95 | 0.18 | 6,6,6,6 | 0 |
| 54 | MG | AA | 1618 | 1/1 | 0.95 | 0.13 | 93,93,93,93 | 0 |
| 55 | LLL | AA | 1661 | 31/31 | 0.95 | 0.21 | 21,21,21,21 | 0 |
| 54 | MG | DB | 3036 | 1/1 | 0.95 | 0.08 | 20,20,20,20 | 0 |
| 56 | ZN | B4 | 101 | 1/1 | 0.95 | 0.09 | 64,64,64,64 | 0 |
| 54 | MG | BB | 3026 | 1/1 | 0.95 | 0.21 | 43,43,43,43 | 0 |
| 54 | MG | DB | 3081 | 1/1 | 0.95 | 0.11 | 19,19,19,19 | 0 |
| 54 | MG | BB | 3020 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 54 | MG | BB | 3110 | 1/1 | 0.95 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | DB | 3089 | 1/1 | 0.95 | 0.19 | 61,61,61,61 | 0 |
| 54 | MG | BB | 3024 | 1/1 | 0.95 | 0.06 | 44,44,44,44 | 0 |
| 54 | MG | BB | 3027 | 1/1 | 0.95 | 0.13 | 42,42,42,42 | 0 |
| 54 | MG | BB | 3050 | 1/1 | 0.95 | 0.10 | 33,33,33,33 | 0 |
| 54 | MG | BB | 3048 | 1/1 | 0.95 | 0.10 | 7,7,7,7 | 0 |
| 54 | MG | BB | 3001 | 1/1 | 0.95 | 0.07 | 29,29,29,29 | 0 |
| 54 | MG | CA | 1651 | 1/1 | 0.95 | 0.11 | 38,38,38,38 | 0 |
| 54 | MG | BB | 3067 | 1/1 | 0.95 | 0.13 | 24,24,24,24 | 0 |
| 54 | MG | BB | 3022 | 1/1 | 0.95 | 0.29 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | BB | 3099 | 1/1 | 0.95 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | DB | 3085 | 1/1 | 0.96 | 0.13 | 49,49,49,49 | 0 |
| 54 | MG | BB | 3077 | 1/1 | 0.96 | 0.07 | 83,83,83,83 | 0 |
| 54 | MG | DB | 3032 | 1/1 | 0.96 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | DB | 3017 | 1/1 | 0.96 | 0.10 | 5,5,5,5 | 0 |
| 54 | MG | DB | 3027 | 1/1 | 0.96 | 0.17 | 28,28,28,28 | 0 |
| 54 | MG | DB | 3063 | 1/1 | 0.96 | 0.06 | 19,19,19,19 | 0 |
| 54 | MG | DB | 3008 | 1/1 | 0.96 | 0.14 | 17,17,17,17 | 0 |
| 54 | MG | BB | 3034 | 1/1 | 0.96 | 0.24 | 59,59,59,59 | 0 |
| 54 | MG | BB | 3002 | 1/1 | 0.96 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | AA | 1603 | 1/1 | 0.96 | 0.10 | 14,14,14,14 | 0 |
| 54 | MG | DB | 3090 | 1/1 | 0.96 | 0.31 | 64,64,64,64 | 0 |
| 54 | MG | BB | 3036 | 1/1 | 0.96 | 0.13 | 62,62,62,62 | 0 |
| 54 | MG | BB | 3107 | 1/1 | 0.96 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | BB | 3054 | 1/1 | 0.96 | 0.14 | 46,46,46,46 | 0 |
| 54 | MG | CA | 1608 | 1/1 | 0.96 | 0.09 | 139,139,139,139 | 0 |
| 54 | MG | BB | 3071 | 1/1 | 0.96 | 0.09 | 89,89,89,89 | 0 |
| 54 | MG | CA | 1661 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | DB | 3092 | 1/1 | 0.96 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | BB | 3051 | 1/1 | 0.96 | 0.18 | 65,65,65,65 | 0 |
| 54 | MG | DB | 3104 | 1/1 | 0.96 | 0.19 | 71,71,71,71 | 0 |
| 54 | MG | CA | 1634 | 1/1 | 0.96 | 0.10 | 23,23,23,23 | 0 |
| 54 | MG | CA | 1626 | 1/1 | 0.96 | 0.23 | 41,41,41,41 | 1 |
| 54 | MG | BB | 3029 | 1/1 | 0.96 | 0.11 | 17,17,17,17 | 0 |
| 54 | MG | AA | 1612 | 1/1 | 0.96 | 0.12 | 88,88,88,88 | 0 |
| 54 | MG | DB | 3095 | 1/1 | 0.96 | 0.12 | 88,88,88,88 | 0 |
| 54 | MG | BB | 3103 | 1/1 | 0.96 | 0.09 | 20,20,20,20 | 0 |
| 54 | MG | CA | 1607 | 1/1 | 0.96 | 0.07 | 83,83,83,83 | 0 |
| 54 | MG | CA | 1610 | 1/1 | 0.96 | 0.07 | 75,75,75,75 | 0 |
| 54 | MG | AA | 1607 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 54 | MG | BB | 3086 | 1/1 | 0.96 | 0.17 | 18,18,18,18 | 0 |
| 54 | MG | DB | 3050 | 1/1 | 0.96 | 0.14 | 123,123,123,123 | 0 |
| 54 | MG | BB | 3014 | 1/1 | 0.96 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | CA | 1633 | 1/1 | 0.96 | 0.14 | 50,50,50,50 | 0 |
| 54 | MG | DB | 3068 | 1/1 | 0.96 | 0.17 | 22,22,22,22 | 0 |
| 54 | MG | BB | 3041 | 1/1 | 0.96 | 0.15 | 8,8,8,8 | 0 |
| 54 | MG | BB | 3009 | 1/1 | 0.96 | 0.14 | 96,96,96,96 | 0 |
| 54 | MG | BB | 3047 | 1/1 | 0.96 | 0.13 | 116,116,116,116 | 0 |
| 54 | MG | DB | 3054 | 1/1 | 0.96 | 0.06 | 29,29,29,29 | 0 |
| 54 | MG | DB | 3102 | 1/1 | 0.97 | 0.09 | 22,22,22,22 | 0 |
| 54 | MG | BB | 3028 | 1/1 | 0.97 | 0.15 | 61,61,61,61 | 0 |
| 54 | MG | DB | 3039 | 1/1 | 0.97 | 0.08 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | BB | 3039 | 1/1 | 0.97 | 0.07 | 5,5,5,5 | 0 |
| 54 | MG | CA | 1640 | 1/1 | 0.97 | 0.08 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3075 | 1/1 | 0.97 | 0.16 | 29,29,29,29 | 0 |
| 54 | MG | CA | 1656 | 1/1 | 0.97 | 0.05 | 11,11,11,11 | 0 |
| 54 | MG | AA | 1628 | 1/1 | 0.97 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | AA | 1633 | 1/1 | 0.97 | 0.03 | 48,48,48,48 | 0 |
| 54 | MG | CA | 1611 | 1/1 | 0.97 | 0.06 | 57,57,57,57 | 0 |
| 54 | MG | DB | 3108 | 1/1 | 0.97 | 0.10 | 5,5,5,5 | 0 |
| 54 | MG | AA | 1642 | 1/1 | 0.97 | 0.12 | 41,41,41,41 | 0 |
| 54 | MG | AA | 1643 | 1/1 | 0.97 | 0.03 | 29,29,29,29 | 0 |
| 54 | MG | CA | 1605 | 1/1 | 0.97 | 0.12 | 18,18,18,18 | 0 |
| 54 | MG | BB | 3052 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | BB | 3058 | 1/1 | 0.97 | 0.09 | 11,11,11,11 | 0 |
| 54 | MG | DB | 3011 | 1/1 | 0.97 | 0.27 | 33,33,33,33 | 0 |
| 54 | MG | AA | 1652 | 1/1 | 0.97 | 0.08 | 90,90,90,90 | 0 |
| 54 | MG | AA | 1605 | 1/1 | 0.97 | 0.09 | 47,47,47,47 | 0 |
| 54 | MG | AA | 1653 | 1/1 | 0.97 | 0.18 | 87,87,87,87 | 0 |
| 54 | MG | DB | 3111 | 1/1 | 0.97 | 0.18 | 32,32,32,32 | 0 |
| 54 | MG | AA | 1634 | 1/1 | 0.97 | 0.07 | 67,67,67,67 | 0 |
| 54 | MG | AA | 1621 | 1/1 | 0.97 | 0.17 | 26,26,26,26 | 0 |
| 54 | MG | CA | 1604 | 1/1 | 0.97 | 0.27 | 16,16,16,16 | 0 |
| 54 | MG | DB | 3001 | 1/1 | 0.97 | 0.09 | 6,6,6,6 | 0 |
| 54 | MG | DB | 3065 | 1/1 | 0.97 | 0.06 | 45,45,45,45 | 0 |
| 54 | MG | DB | 3105 | 1/1 | 0.97 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | AA | 1616 | 1/1 | 0.97 | 0.06 | 42,42,42,42 | 0 |
| 54 | MG | BB | 3005 | 1/1 | 0.97 | 0.19 | 20,20,20,20 | 0 |
| 54 | MG | DB | 3007 | 1/1 | 0.97 | 0.11 | 13,13,13,13 | 0 |
| 54 | MG | BB | 3032 | 1/1 | 0.97 | 0.21 | 49,49,49,49 | 0 |
| 54 | MG | DB | 3067 | 1/1 | 0.97 | 0.13 | 16,16,16,16 | 0 |
| 54 | MG | BB | 3044 | 1/1 | 0.97 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | DB | 3018 | 1/1 | 0.97 | 0.10 | 22,22,22,22 | 0 |
| 54 | MG | BB | 3074 | 1/1 | 0.97 | 0.14 | 13,13,13,13 | 0 |
| 54 | MG | BB | 3023 | 1/1 | 0.97 | 0.20 | 11,11,11,11 | 0 |
| 54 | MG | CA | 1648 | 1/1 | 0.97 | 0.19 | 14,14,14,14 | 0 |
| 54 | MG | DB | 3046 | 1/1 | 0.97 | 0.07 | 11,11,11,11 | 0 |
| 54 | MG | CA | 1630 | 1/1 | 0.97 | 0.28 | 52,52,52,52 | 0 |
| 54 | MG | DB | 3062 | 1/1 | 0.97 | 0.04 | 67,67,67,67 | 0 |
| 54 | MG | AA | 1617 | 1/1 | 0.97 | 0.12 | 100,100,100,100 | 0 |
| 54 | MG | CA | 1603 | 1/1 | 0.97 | 0.09 | 29,29,29,29 | 0 |
| 54 | MG | CA | 1647 | 1/1 | 0.97 | 0.07 | 65,65,65,65 | 0 |
| 54 | MG | BB | 3091 | 1/1 | 0.97 | 0.10 | 37,37,37,37 | 0 |
| 54 | MG | BB | 3021 | 1/1 | 0.97 | 0.10 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | BB | 3056 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 54 | MG | DB | 3023 | 1/1 | 0.97 | 0.10 | 17,17,17,17 | 0 |
| 54 | MG | DB | 3025 | 1/1 | 0.97 | 0.17 | 42,42,42,42 | 0 |
| 54 | MG | DB | 3073 | 1/1 | 0.98 | 0.21 | 67,67,67,67 | 0 |
| 54 | MG | DB | 3076 | 1/1 | 0.98 | 0.14 | 104,104,104,104 | 0 |
| 54 | MG | CA | 1653 | 1/1 | 0.98 | 0.04 | 51,51,51,51 | 0 |
| 54 | MG | DB | 3070 | 1/1 | 0.98 | 0.10 | 38,38,38,38 | 0 |
| 54 | MG | DB | 3044 | 1/1 | 0.98 | 0.07 | 21,21,21,21 | 0 |
| 54 | MG | BB | 3066 | 1/1 | 0.98 | 0.15 | 25,25,25,25 | 0 |
| 54 | MG | DB | 3075 | 1/1 | 0.98 | 0.12 | 35,35,35,35 | 0 |
| 54 | MG | BB | 3096 | 1/1 | 0.98 | 0.15 | 67,67,67,67 | 0 |
| 54 | MG | DB | 3002 | 1/1 | 0.98 | 0.08 | 6,6,6,6 | 0 |
| 54 | MG | BB | 3090 | 1/1 | 0.98 | 0.10 | 91,91,91,91 | 0 |
| 54 | MG | DB | 3019 | 1/1 | 0.98 | 0.06 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3098 | 1/1 | 0.98 | 0.16 | 16,16,16,16 | 0 |
| 54 | MG | BB | 3064 | 1/1 | 0.98 | 0.08 | 37,37,37,37 | 0 |
| 54 | MG | DB | 3049 | 1/1 | 0.98 | 0.07 | 9,9,9,9 | 0 |
| 54 | MG | CA | 1612 | 1/1 | 0.98 | 0.07 | 72,72,72,72 | 0 |
| 54 | MG | DB | 3084 | 1/1 | 0.98 | 0.14 | 16,16,16,16 | 0 |
| 54 | MG | DB | 3103 | 1/1 | 0.98 | 0.11 | 42,42,42,42 | 0 |
| 54 | MG | BB | 3012 | 1/1 | 0.98 | 0.09 | 53,53,53,53 | 0 |
| 54 | MG | DB | 3082 | 1/1 | 0.98 | 0.08 | 57,57,57,57 | 0 |
| 54 | MG | BB | 3007 | 1/1 | 0.98 | 0.07 | 53,53,53,53 | 0 |
| 54 | MG | DB | 3099 | 1/1 | 0.98 | 0.20 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3106 | 1/1 | 0.98 | 0.11 | 39,39,39,39 | 0 |
| 54 | MG | AA | 1611 | 1/1 | 0.98 | 0.09 | 77,77,77,77 | 0 |
| 54 | MG | CA | 1617 | 1/1 | 0.98 | 0.08 | 5,5,5,5 | 0 |
| 54 | MG | DB | 3010 | 1/1 | 0.98 | 0.09 | 16,16,16,16 | 0 |
| 54 | MG | DB | 3079 | 1/1 | 0.98 | 0.12 | 34,34,34,34 | 0 |
| 54 | MG | BB | 3070 | 1/1 | 0.98 | 0.19 | 59,59,59,59 | 0 |
| 54 | MG | DB | 3009 | 1/1 | 0.98 | 0.17 | 18,18,18,18 | 0 |
| 54 | MG | CA | 1632 | 1/1 | 0.98 | 0.08 | 18,18,18,18 | 0 |
| 54 | MG | CA | 1601 | 1/1 | 0.98 | 0.17 | 5,5,5,5 | 0 |
| 54 | MG | DB | 3086 | 1/1 | 0.98 | 0.20 | 52,52,52,52 | 0 |
| 54 | MG | DB | 3069 | 1/1 | 0.98 | 0.20 | 14,14,14,14 | 0 |
| 54 | MG | DB | 3088 | 1/1 | 0.98 | 0.16 | 46,46,46,46 | 0 |
| 54 | MG | DB | 3040 | 1/1 | 0.98 | 0.09 | 18,18,18,18 | 0 |
| 54 | MG | DB | 3041 | 1/1 | 0.98 | 0.08 | 34,34,34,34 | 0 |
| 54 | MG | BB | 3089 | 1/1 | 0.98 | 0.19 | 25,25,25,25 | 0 |
| 54 | MG | DB | 3051 | 1/1 | 0.98 | 0.20 | 32,32,32,32 | 0 |
| 54 | MG | DB | 3028 | 1/1 | 0.98 | 0.18 | 58,58,58,58 | 0 |
| 54 | MG | CA | 1637 | 1/1 | 0.98 | 0.07 | 92,92,92,92 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | BB | 3082 | 1/1 | 0.98 | 0.19 | 5,5,5,5 | 0 |
| 54 | MG | AA | 1604 | 1/1 | 0.98 | 0.09 | 19,19,19,19 | 0 |
| 54 | MG | BB | 3101 | 1/1 | 0.98 | 0.05 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3102 | 1/1 | 0.98 | 0.04 | 31,31,31,31 | 0 |
| 54 | MG | BB | 3055 | 1/1 | 0.98 | 0.19 | 53,53,53,53 | 0 |
| 54 | MG | BB | 3087 | 1/1 | 0.98 | 0.22 | 114,114,114,114 | 0 |
| 54 | MG | BB | 3063 | 1/1 | 0.98 | 0.14 | 28,28,28,28 | 0 |
| 54 | MG | DB | 3031 | 1/1 | 0.98 | 0.07 | 24,24,24,24 | 0 |
| 54 | MG | DB | 3107 | 1/1 | 0.98 | 0.07 | 11,11,11,11 | 0 |
| 54 | MG | DB | 3077 | 1/1 | 0.98 | 0.08 | 15,15,15,15 | 0 |
| 54 | MG | CA | 1639 | 1/1 | 0.98 | 0.07 | 7,7,7,7 | 0 |
| 54 | MG | DB | 3071 | 1/1 | 0.98 | 0.05 | 37,37,37,37 | 0 |
| 54 | MG | DB | 3012 | 1/1 | 0.98 | 0.09 | 12,12,12,12 | 0 |
| 54 | MG | BB | 3030 | 1/1 | 0.98 | 0.04 | 70,70,70,70 | 0 |
| 54 | MG | CA | 1622 | 1/1 | 0.98 | 0.10 | 18,18,18,18 | 0 |
| 54 | MG | DB | 3005 | 1/1 | 0.98 | 0.16 | 45,45,45,45 | 0 |
| 54 | MG | BB | 3094 | 1/1 | 0.98 | 0.13 | 47,47,47,47 | 0 |
| 54 | MG | BB | 3083 | 1/1 | 0.98 | 0.21 | 28,28,28,28 | 0 |
| 54 | MG | BB | 3109 | 1/1 | 0.98 | 0.07 | 59,59,59,59 | 0 |
| 54 | MG | CA | 1645 | 1/1 | 0.98 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | BB | 3046 | 1/1 | 0.98 | 0.08 | 64,64,64,64 | 0 |
| 54 | MG | CA | 1618 | 1/1 | 0.98 | 0.12 | 30,30,30,30 | 0 |
| 54 | MG | BB | 3084 | 1/1 | 0.98 | 0.20 | 77,77,77,77 | 0 |
| 54 | MG | DB | 3094 | 1/1 | 0.98 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | CA | 1631 | 1/1 | 0.98 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | CA | 1613 | 1/1 | 0.98 | 0.11 | 40,40,40,40 | 0 |
| 54 | MG | CA | 1644 | 1/1 | 0.98 | 0.07 | 68,68,68,68 | 0 |
| 54 | MG | AA | 1610 | 1/1 | 0.98 | 0.06 | 62,62,62,62 | 0 |
| 54 | MG | AA | 1638 | 1/1 | 0.98 | 0.07 | 20,20,20,20 | 0 |
| 54 | MG | BB | 3062 | 1/1 | 0.98 | 0.05 | 27,27,27,27 | 0 |
| 54 | MG | BB | 3069 | 1/1 | 0.98 | 0.14 | 10,10,10,10 | 0 |
| 54 | MG | DB | 3047 | 1/1 | 0.98 | 0.11 | 19,19,19,19 | 0 |
| 54 | MG | AA | 1640 | 1/1 | 0.98 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | AA | 1609 | 1/1 | 0.99 | 0.11 | 5,5,5,5 | 0 |
| 54 | MG | DB | 3043 | 1/1 | 0.99 | 0.08 | 32,32,32,32 | 0 |
| 54 | MG | BB | 3025 | 1/1 | 0.99 | 0.06 | 42,42,42,42 | 0 |
| 54 | MG | BB | 3059 | 1/1 | 0.99 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | BB | 3040 | 1/1 | 0.99 | 0.12 | 27,27,27,27 | 0 |
| 54 | MG | DB | 3004 | 1/1 | 0.99 | 0.13 | 69,69,69,69 | 0 |
| 54 | MG | DB | 3091 | 1/1 | 0.99 | 0.14 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3016 | 1/1 | 0.99 | 0.13 | 91,91,91,91 | 0 |
| 54 | MG | BB | 3085 | 1/1 | 0.99 | 0.11 | 43,43,43,43 | 0 |

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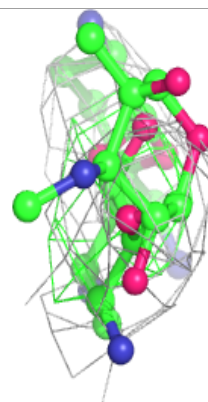
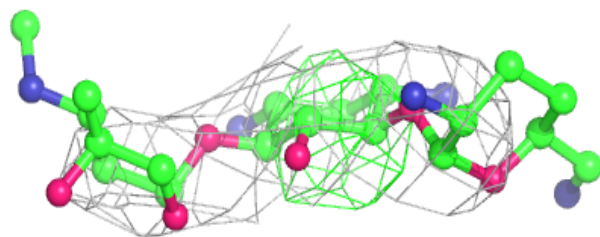
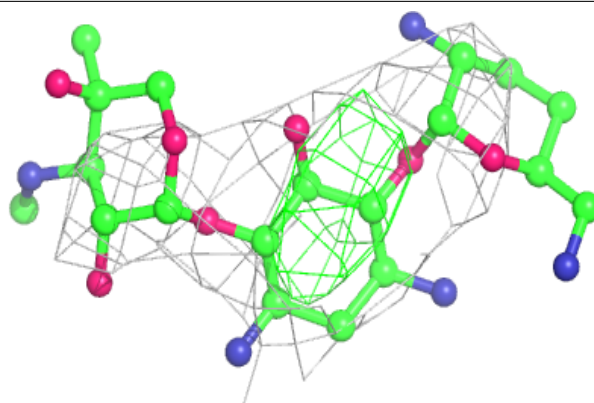
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | BB | 3015 | 1/1 | 0.99 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | BB | 3060 | 1/1 | 0.99 | 0.08 | 22,22,22,22 | 0 |
| 54 | MG | BB | 3076 | 1/1 | 0.99 | 0.06 | 20,20,20,20 | 0 |
| 54 | MG | BB | 3104 | 1/1 | 0.99 | 0.16 | 28,28,28,28 | 0 |
| 54 | MG | DB | 3096 | 1/1 | 0.99 | 0.16 | 20,20,20,20 | 0 |
| 54 | MG | BB | 3006 | 1/1 | 0.99 | 0.08 | 20,20,20,20 | 0 |
| 54 | MG | DB | 3014 | 1/1 | 0.99 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | CA | 1602 | 1/1 | 0.99 | 0.12 | 11,11,11,11 | 0 |
| 54 | MG | AA | 1629 | 1/1 | 0.99 | 0.05 | 26,26,26,26 | 0 |
| 54 | MG | DB | 3087 | 1/1 | 0.99 | 0.15 | 75,75,75,75 | 0 |
| 54 | MG | BB | 3073 | 1/1 | 0.99 | 0.23 | 38,38,38,38 | 0 |
| 54 | MG | DB | 3021 | 1/1 | 0.99 | 0.08 | 51,51,51,51 | 0 |
| 54 | MG | BB | 3105 | 1/1 | 0.99 | 0.05 | 60,60,60,60 | 0 |
| 54 | MG | CA | 1650 | 1/1 | 0.99 | 0.07 | 33,33,33,33 | 0 |
| 54 | MG | DB | 3056 | 1/1 | 0.99 | 0.12 | 12,12,12,12 | 0 |
| 54 | MG | DB | 3101 | 1/1 | 0.99 | 0.25 | 25,25,25,25 | 0 |
| 54 | MG | DB | 3098 | 1/1 | 0.99 | 0.17 | 28,28,28,28 | 0 |
| 54 | MG | DB | 3078 | 1/1 | 0.99 | 0.08 | 32,32,32,32 | 0 |
| 54 | MG | BB | 3045 | 1/1 | 0.99 | 0.04 | 38,38,38,38 | 0 |
| 54 | MG | CA | 1655 | 1/1 | 0.99 | 0.07 | 25,25,25,25 | 0 |
| 54 | MG | BB | 3011 | 1/1 | 0.99 | 0.21 | 29,29,29,29 | 0 |
| 54 | MG | DB | 3048 | 1/1 | 0.99 | 0.08 | 34,34,34,34 | 0 |
| 54 | MG | BB | 3068 | 1/1 | 1.00 | 0.05 | 61,61,61,61 | 0 |

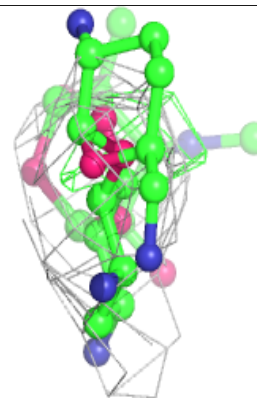
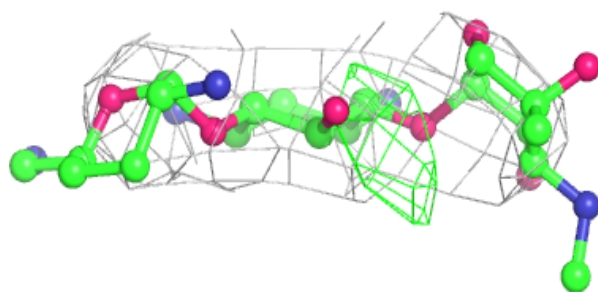
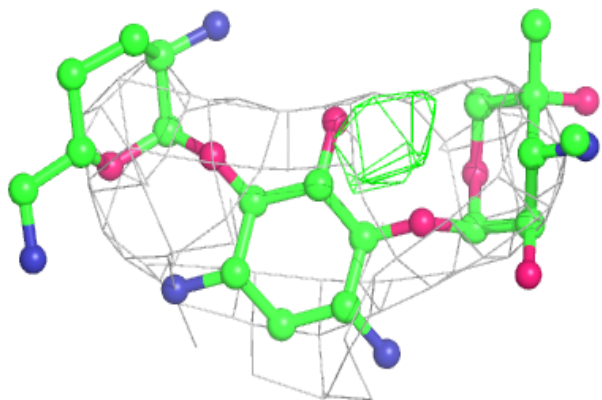
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LLL DB 3112:

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

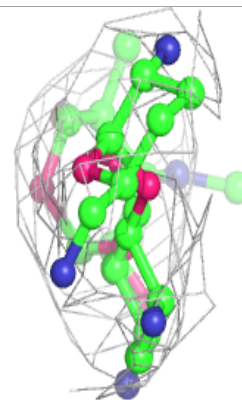
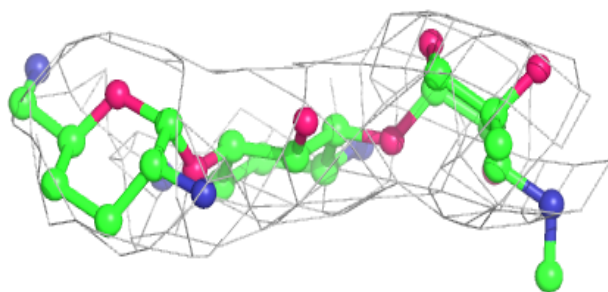
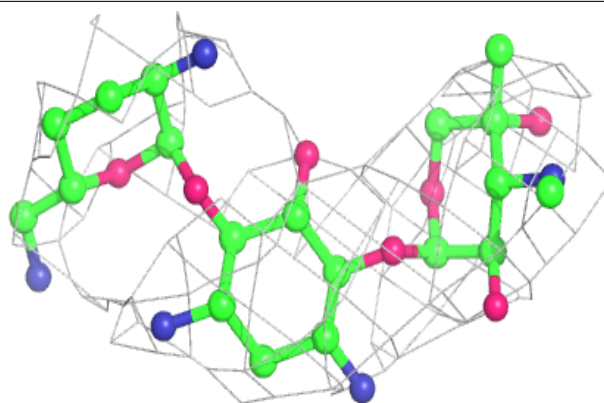
**Electron density around LLL BB 3111:**

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

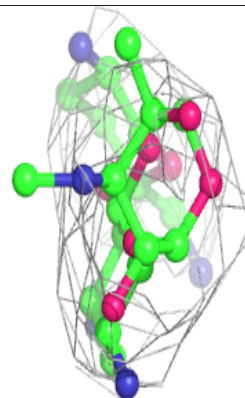
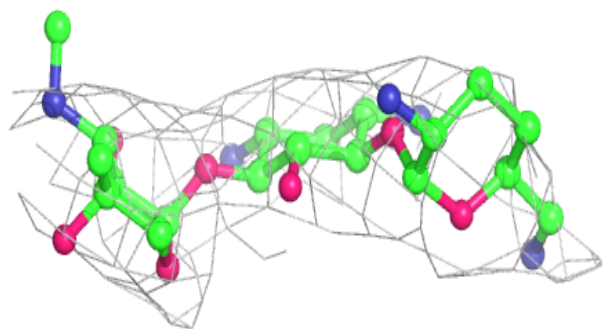
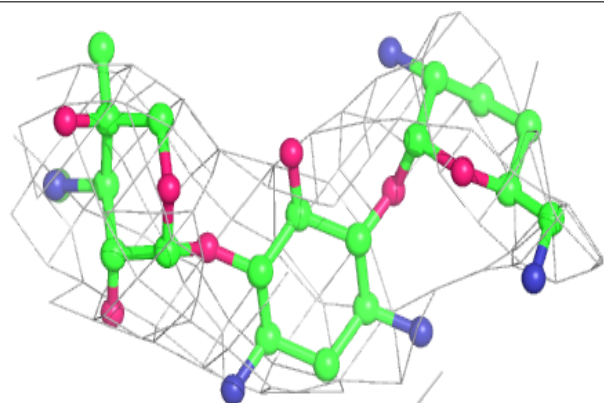


Electron density around LLL CA 1662:

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

**Electron density around LLL AA 1661:**

$2mF_o-DF_c$ (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.