



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 3, 2024 – 05:35 am GMT

PDB ID : 4V5F
Title : The structure of the ribosome with elongation factor G trapped in the post-translocational state
Authors : Gao, Y.-G.; Selmer, M.; Dunham, C.M.; Weixlbaumer, A.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-09-01
Resolution : 3.60 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

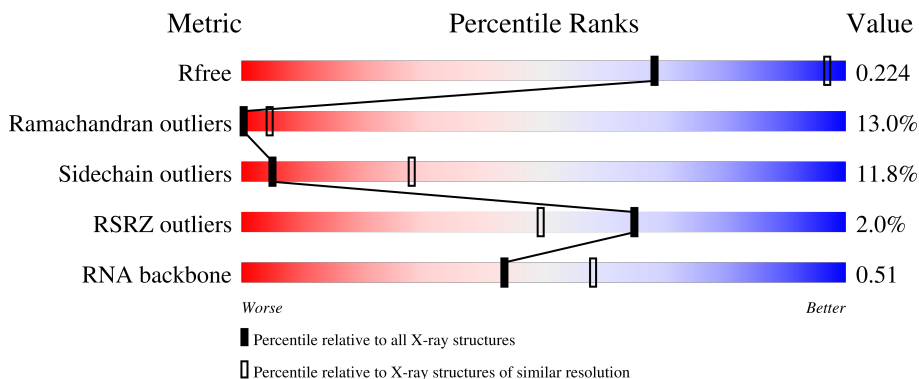
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.














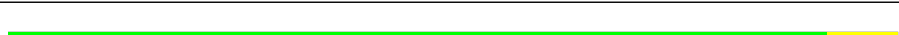

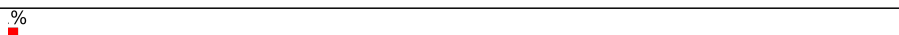
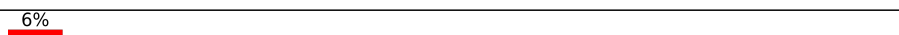
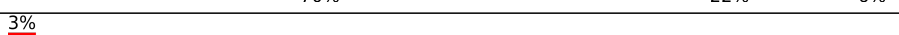

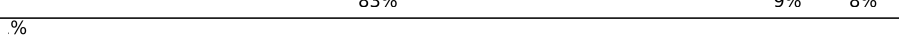







| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1257 (3.70-3.50) |
| Ramachandran outliers | 138981 | 1307 (3.70-3.50) |
| Sidechain outliers | 138945 | 1307 (3.70-3.50) |
| RSRZ outliers | 127900 | 1161 (3.70-3.50) |
| RNA backbone | 3102 | 1017 (4.20-3.00) |

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 of 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 | 1522 | 78% 19% .. |
| 1 | CA | 1522 | 78% 19% .. |
| 2 | AB | 256 | 70% 20% . 8% |
| 2 | CB | 256 | 70% 19% . 8% |









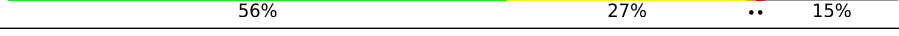

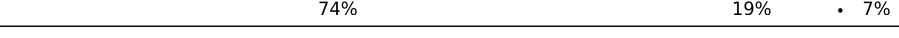
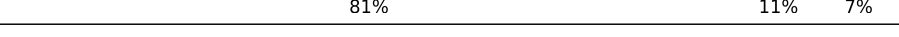

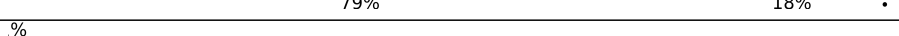


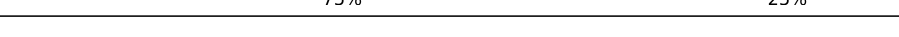

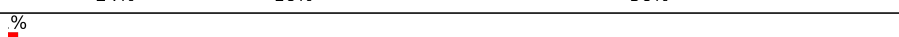






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | AC | 239 |  72% 13% 13% |
| 3 | CC | 239 |  72% 14% 13% |
| 4 | AD | 209 |  80% 19% |
| 4 | CD | 209 |  80% 19% |
| 5 | AE | 162 |  % 78% 15% 7% |
| 5 | CE | 162 |  % 79% 14% 7% |
| 6 | AF | 101 |  87% 12% |
| 6 | CF | 101 |  87% 12% |
| 7 | AG | 156 |  % 87% 12% |
| 7 | CG | 156 |  % 87% 13% |
| 8 | AH | 138 |  91% 9% |
| 8 | CH | 138 |  92% 8% |
| 9 | AI | 128 |  % 83% 16% .. |
| 9 | CI | 128 |  % 84% 14% .. |
| 10 | AJ | 105 |  6% 70% 22% 6% |
| 10 | CJ | 105 |  3% 70% 22% 6% |
| 11 | AK | 129 |  2% 83% 9% 8% |
| 11 | CK | 129 |  % 83% 9% 8% |
| 12 | AL | 132 |  76% 17% 5% |
| 12 | CL | 132 |  2% 74% 18% 5% |
| 13 | AM | 126 |  5% 79% 18% .. |
| 13 | CM | 126 |  6% 79% 17% .. |
| 14 | AN | 61 |  2% 87% 7% 5% |
| 14 | CN | 61 |  85% 8% 5% |
| 15 | AO | 89 |  81% 18% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | CO | 89 |  80% 19% . |
| 16 | AP | 88 |  83% 11% . 5% |
| 16 | CP | 88 |  83% 11% . 5% |
| 17 | AQ | 105 |  84% 11% 5% |
| 17 | CQ | 105 |  85% 10% 5% |
| 18 | AR | 88 |  72% 8% 20% |
| 18 | CR | 88 |  72% 8% 20% |
| 19 | AS | 93 |  55% 28% .. 15% |
| 19 | CS | 93 |  56% 27% .. 15% |
| 20 | AT | 106 |  74% 19% . 7% |
| 20 | CT | 106 |  74% 19% . 7% |
| 21 | AU | 27 |  81% 11% 7% |
| 21 | CU | 27 |  78% 15% 7% |
| 22 | AV | 77 |  79% 18% . |
| 22 | AW | 77 |  68% 32% |
| 22 | CV | 77 |  82% 17% . |
| 22 | CW | 77 |  75% 25% |
| 23 | AX | 25 |  20% 20% . 56% |
| 23 | CX | 25 |  24% 16% . 56% |
| 24 | AY | 691 |  74% 21% .. |
| 24 | CY | 691 |  77% 19% .. |
| 25 | B0 | 85 |  85% 13% .. |
| 25 | D0 | 85 |  85% 13% .. |
| 26 | B1 | 98 |  70% 24% .. |
| 26 | D1 | 98 |  77% 18% .. |

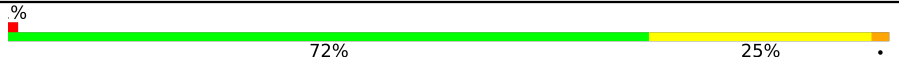

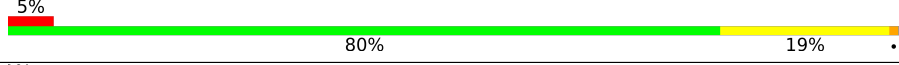

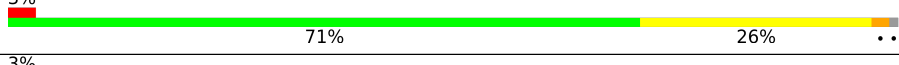
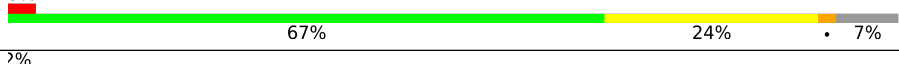
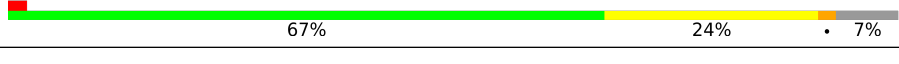
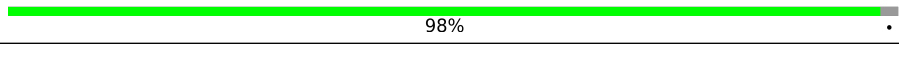
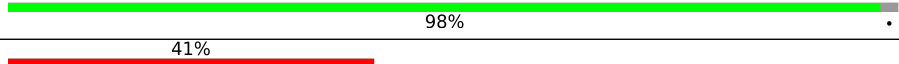








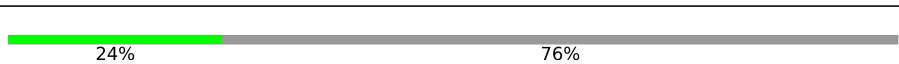
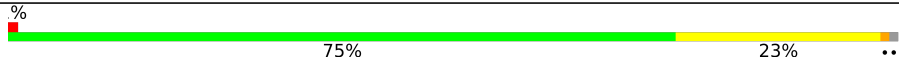


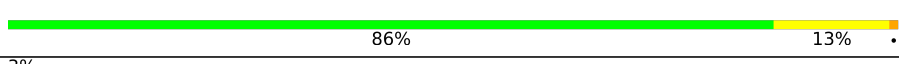
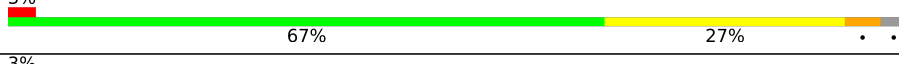


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------------|
| 27 | B2 | 72 | 3% 68% 29% .. |
| 27 | D2 | 72 | 3% 75% 24% . |
| 28 | B3 | 60 | 2% 87% 12% . |
| 28 | D3 | 60 | 3% 87% 12% . |
| 29 | B4 | 71 | 4% 49% 24% 7% . 18% |
| 29 | D4 | 71 | 10% 48% 25% 7% . 18% |
| 30 | B5 | 60 | 5% 75% 18% 5% . |
| 30 | D5 | 60 | 7% 73% 20% 5% . |
| 31 | B6 | 54 | 4% 52% 35% . . 7% |
| 31 | D6 | 54 | 2% 54% 31% 6% . 7% |
| 32 | B7 | 49 | 4% 88% 12% |
| 32 | D7 | 49 | 88% 12% |
| 33 | B8 | 65 | 2% 74% 17% 8% . |
| 33 | D8 | 65 | 2% 72% 18% 8% . |
| 34 | B9 | 37 | 78% 19% |
| 34 | D9 | 37 | 3% 76% 19% 5% |
| 35 | BA | 2915 | % 76% 22% . |
| 35 | DA | 2915 | % 76% 22% . |
| 36 | BB | 122 | 76% 20% .. |
| 36 | DB | 122 | 76% 21% . |
| 37 | BC | 229 | 2% 90% 10% |
| 37 | DC | 229 | 5% 89% 10% |
| 38 | BD | 276 | 75% 22% . |
| 38 | DD | 276 | 75% 22% . |
| 39 | BE | 206 | 2% 72% 25% . |





















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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 39 | DE | 206 |  72% 25% |
| 40 | BF | 210 |  80% 18% 5% |
| 40 | DF | 210 |  80% 19% 5% |
| 41 | BG | 182 |  74% 24% 2% |
| 41 | DG | 182 |  71% 26% 3% |
| 42 | BH | 180 |  67% 24% 3% 7% |
| 42 | DH | 180 |  67% 24% 2% 7% |
| 43 | BJ | 173 |  98% |
| 43 | DJ | 173 |  98% |
| 44 | BK | 147 |  41% 77% 18% 5% |
| 44 | DK | 147 |  33% 78% 18% 5% |
| 45 | BL | 125 |  82% 18% |
| 45 | BM | 125 |  25% 75% |
| 45 | Bl | 125 |  25% 75% |
| 45 | Bm | 125 |  24% 76% |
| 45 | DL | 125 |  82% 18% |
| 45 | DM | 125 |  25% 75% |
| 45 | DI | 125 |  25% 75% |
| 45 | Dm | 125 |  24% 76% |
| 46 | BN | 140 |  75% 23% 0% 2% |
| 46 | DN | 140 |  74% 24% 0% 2% |
| 47 | BO | 122 |  86% 13% 0% 1% |
| 47 | DO | 122 |  86% 13% 0% 1% |
| 48 | BP | 150 |  3% 67% 27% 3% |
| 48 | DP | 150 |  3% 66% 27% 4% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 49 | BQ | 141 |  85% 13% |
| 49 | DQ | 141 |  87% 12% |
| 50 | BR | 118 |  79% 19% |
| 50 | DR | 118 |  77% 21% |
| 51 | BS | 112 |  62% 25% 12% |
| 51 | DS | 112 |  62% 25% 12% |
| 52 | BT | 146 |  62% 29% 5% |
| 52 | DT | 146 |  61% 31% 5% |
| 53 | BU | 118 |  81% 18% |
| 53 | DU | 118 |  81% 19% |
| 54 | BV | 101 |  73% 25% |
| 54 | DV | 101 |  73% 25% |
| 55 | BW | 113 |  86% 13% |
| 55 | DW | 113 |  87% 12% |
| 56 | BX | 96 |  78% 18% |
| 56 | DX | 96 |  78% 18% |
| 57 | BY | 110 |  64% 32% |
| 57 | DY | 110 |  65% 31% |
| 58 | BZ | 206 |  65% 20% 5% 10% |
| 58 | DZ | 206 |  67% 21% 10% |

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 311552 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 ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------|------------|-----------|------------|-----------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | AA | 1504 | Total 32329 | C 14390 | N 5992 | O 10444 | P 1503 | 0 | 0 | 0 |
| 1 | CA | 1504 | Total 32329 | C 14390 | N 5992 | O 10444 | P 1503 | 0 | 0 | 0 |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | AB | 235 | Total 1901 | C 1213 | N 342 | O 341 | S 5 | 0 | 0 | 1 |
| 2 | CB | 235 | Total 1901 | C 1213 | N 342 | O 341 | S 5 | 0 | 0 | 1 |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | AC | 207 | Total 1613 | C 1016 | N 315 | O 281 | S 1 | 0 | 0 | 1 |
| 3 | CC | 207 | Total 1613 | C 1016 | N 315 | O 281 | S 1 | 0 | 0 | 1 |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | AD | 208 | Total 1703 | C 1066 | N 339 | O 291 | S 7 | 0 | 0 | 0 |
| 4 | CD | 208 | Total 1703 | C 1066 | N 339 | O 291 | S 7 | 0 | 0 | 0 |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 201 | 4 | | | |
| 5 | CE | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 201 | 4 | | | |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |
| 6 | CF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |
| 7 | CG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |
| 8 | CH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | AI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |
| 9 | CI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AJ | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 795 | 499 | 157 | 138 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | CJ | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 795 | 499 | 157 | 138 | 1 | | | |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |
| 11 | CK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 971 | 611 | 196 | 163 | 1 | | | |
| 12 | CL | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 971 | 611 | 196 | 163 | 1 | | | |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 988 | 611 | 206 | 169 | 2 | | | |
| 13 | CM | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 988 | 611 | 206 | 169 | 2 | | | |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14 | AN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 14 | CN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |
| 15 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 117 | 1 | | | |
| 16 | CP | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 117 | 1 | | | |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 100 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 824 | 528 | 152 | 142 | 2 | | | |
| 17 | CQ | 100 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 824 | 528 | 152 | 142 | 2 | | | |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | AR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |
| 18 | CR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 79 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 630 | 403 | 115 | 110 | 2 | | | |
| 19 | CS | 79 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 630 | 403 | 115 | 110 | 2 | | | |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |
| 20 | CT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AU | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |
| 21 | CU | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |

- Molecule 22 is a RNA chain called E-SITE TRNA FMET OR P-SITE TRNA FMET (UN-MODIFIED BASES EXCEPT FOR THYMINE 54).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | AV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1640 | 732 | 297 | 535 | 76 | | | |
| 22 | AW | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1640 | 732 | 297 | 535 | 76 | | | |
| 22 | CV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1640 | 732 | 297 | 535 | 76 | | | |
| 22 | CW | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1640 | 732 | 297 | 535 | 76 | | | |

- Molecule 23 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 23 | AX | 11 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 230 | 105 | 41 | 74 | 10 | | | |
| 23 | CX | 11 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 230 | 105 | 41 | 74 | 10 | | | |

- Molecule 24 is a protein called ELONGATION FACTOR G.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 24 | AY | 667 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 5215 | 3316 | 893 | 988 | 18 | | | |
| 24 | CY | 667 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 5215 | 3316 | 893 | 988 | 18 | | | |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|---|
| 25 | B0 | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 410 | 140 | 111 | 1 | | | |
| 25 | D0 | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 410 | 140 | 111 | 1 | | | |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | B1 | 94 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 732 | 460 | 146 | 125 | 1 | | | |
| 26 | D1 | 94 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 732 | 460 | 146 | 125 | 1 | | | |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | B2 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 598 | 370 | 121 | 106 | 1 | | | |
| 27 | D2 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 598 | 370 | 121 | 106 | 1 | | | |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | B3 | 60 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 468 | 298 | 91 | 78 | 1 | | | |
| 28 | D3 | 60 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 468 | 298 | 91 | 78 | 1 | | | |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | B4 | 58 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 451 | 285 | 78 | 83 | 5 | | | |
| 29 | D4 | 58 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 451 | 285 | 78 | 83 | 5 | | | |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 30 | D5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | B6 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 433 | 270 | 88 | 71 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | D6 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 433 | 270 | 88 | 71 | 4 | | | |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32 | B7 | 49 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 419 | 257 | 105 | 55 | 2 | | | |
| 32 | D7 | 49 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 419 | 257 | 105 | 55 | 2 | | | |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 508 | 326 | 102 | 78 | 2 | | | |
| 33 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 508 | 326 | 102 | 78 | 2 | | | |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 34 | B9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 34 | D9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 35 | BA | 2901 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62474 | 27806 | 11681 | 20087 | 2900 | | | |
| 35 | DA | 2901 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62474 | 27806 | 11681 | 20087 | 2900 | | | |

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 36 | BB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |
| 36 | DB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 37 | BC | 228 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1742 | 1101 | 319 | 319 | 3 | | | |
| 37 | DC | 228 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1742 | 1101 | 319 | 319 | 3 | | | |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 38 | BD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2145 | 1353 | 428 | 361 | 3 | | | |
| 38 | DD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2145 | 1353 | 428 | 361 | 3 | | | |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 39 | BE | 205 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1564 | 988 | 300 | 270 | 6 | | | |
| 39 | DE | 205 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1564 | 988 | 300 | 270 | 6 | | | |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 40 | BF | 208 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1624 | 1035 | 304 | 282 | 3 | | | |
| 40 | DF | 208 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1624 | 1035 | 304 | 282 | 3 | | | |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 41 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 41 | DG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BH | 167 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1269 | 803 | 238 | 227 | 1 | | | |
| 42 | DH | 167 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1269 | 803 | 238 | 227 | 1 | | | |

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BJ | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 851 | 510 | 170 | 171 | | | | |
| 43 | DJ | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 851 | 510 | 170 | 171 | | | | |

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BK | 140 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1026 | 653 | 182 | 186 | 5 | | | |
| 44 | DK | 140 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1026 | 653 | 182 | 186 | 5 | | | |

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BL | 102 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 506 | 303 | 102 | 101 | | | | |
| 45 | BM | 31 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 151 | 90 | 31 | 30 | | | | |
| 45 | Bl | 31 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 151 | 90 | 31 | 30 | | | | |
| 45 | Bm | 30 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 146 | 87 | 30 | 29 | | | | |
| 45 | DL | 102 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 506 | 303 | 102 | 101 | | | | |
| 45 | DM | 31 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 151 | 90 | 31 | 30 | | | | |
| 45 | Dl | 31 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 151 | 90 | 31 | 30 | | | | |
| 45 | Dm | 30 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 146 | 87 | 30 | 29 | | | | |

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BN | 139 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1105 | 712 | 207 | 182 | 4 | | | |
| 46 | DN | 139 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1105 | 712 | 207 | 182 | 4 | | | |

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | BO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 47 | DO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | BP | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |
| 48 | DP | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | BQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 49 | DQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 50 | BR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |
| 50 | DR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 51 | BS | 99 | Total | C | N | O | 0 | 0 | 1 |
| | | | 771 | 486 | 155 | 130 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 51 | DS | 99 | 771 | 486 | 155 | 130 | 0 | 0 | 1 |

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 52 | BT | 138 | 1142 | 710 | 235 | 196 | 1 | 0 | 0 | 1 |
| 52 | DT | 138 | 1142 | 710 | 235 | 196 | 1 | 0 | 0 | 1 |

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 53 | BU | 117 | 958 | 604 | 202 | 151 | 1 | 0 | 0 | 0 |
| 53 | DU | 117 | 958 | 604 | 202 | 151 | 1 | 0 | 0 | 0 |

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 54 | BV | 101 | 779 | 501 | 142 | 135 | 1 | 0 | 0 | 0 |
| 54 | DV | 101 | 779 | 501 | 142 | 135 | 1 | 0 | 0 | 0 |

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 55 | BW | 113 | 896 | 563 | 176 | 155 | 2 | 0 | 0 | 0 |
| 55 | DW | 113 | 896 | 563 | 176 | 155 | 2 | 0 | 0 | 0 |

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 56 | BX | 93 | 726 | 471 | 132 | 123 | 0 | 0 | 1 |
| 56 | DX | 93 | 726 | 471 | 132 | 123 | 0 | 0 | 1 |

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 57 | BY | 107 | Total 811 | C 520 | N 155 | O 131 | S 5 | 0 | 0 | 1 |
| 57 | DY | 107 | Total 811 | C 520 | N 155 | O 131 | S 5 | 0 | 0 | 1 |

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 58 | BZ | 185 | Total 1468 | C 936 | N 262 | O 268 | S 2 | 0 | 0 | 1 |
| 58 | DZ | 185 | Total 1468 | C 936 | N 262 | O 268 | S 2 | 0 | 0 | 1 |

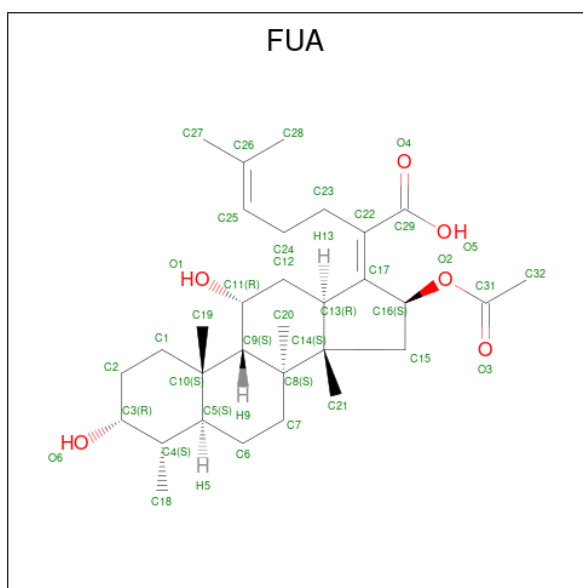
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59 | AD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | AN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | B4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | B9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | CD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | CN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | D4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

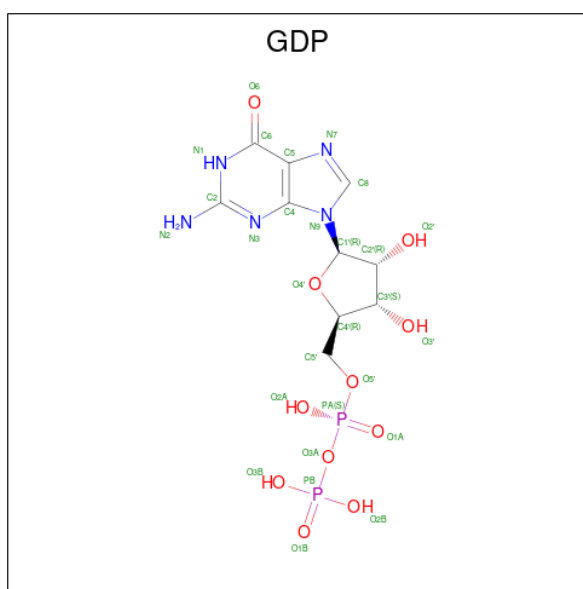
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 60 | AY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | CY | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).

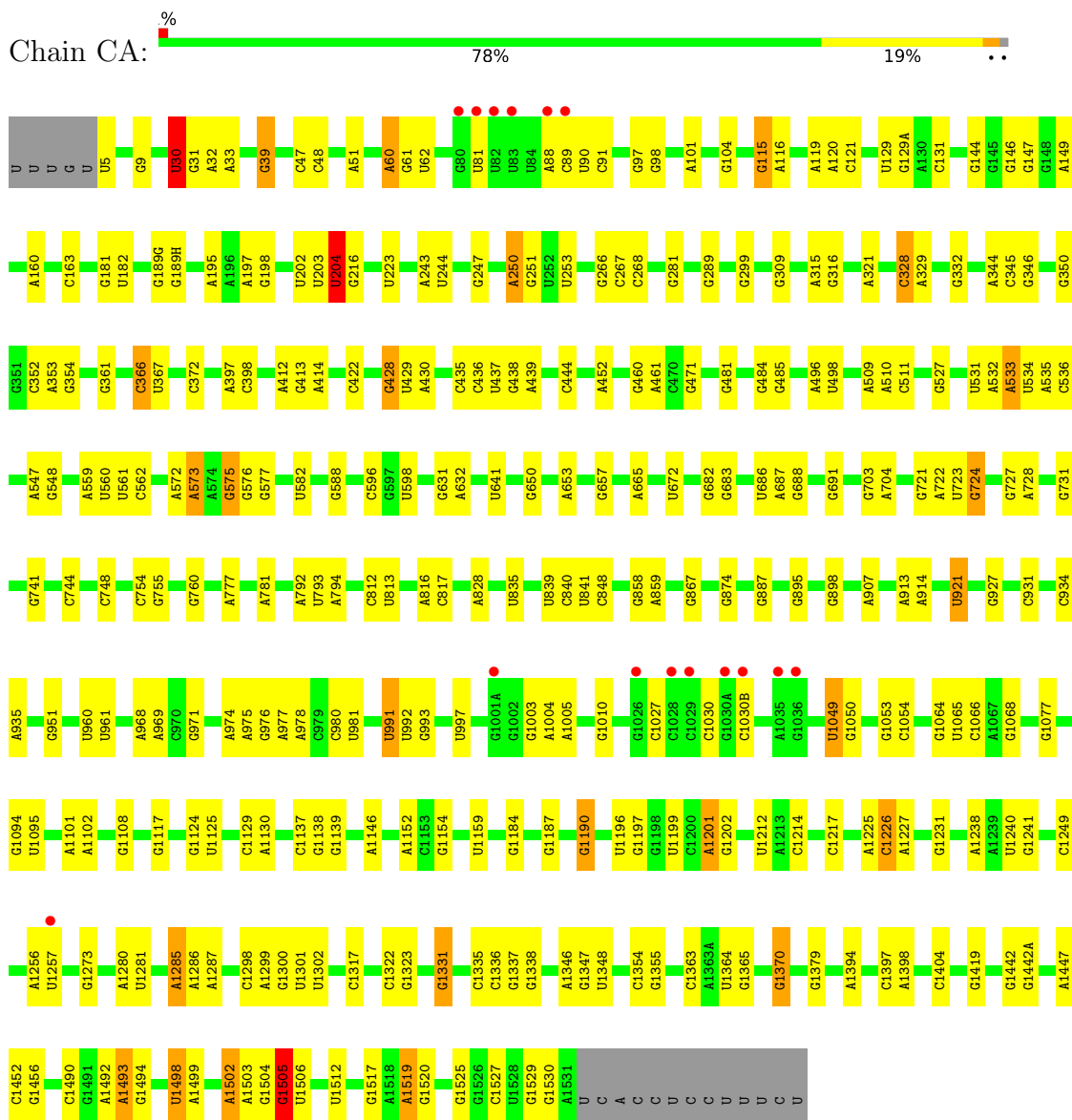


| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 61 | AY | 1 | Total C O 37 31 6 | 0 | 0 |
| 61 | CY | 1 | Total C O 37 31 6 | 0 | 0 |

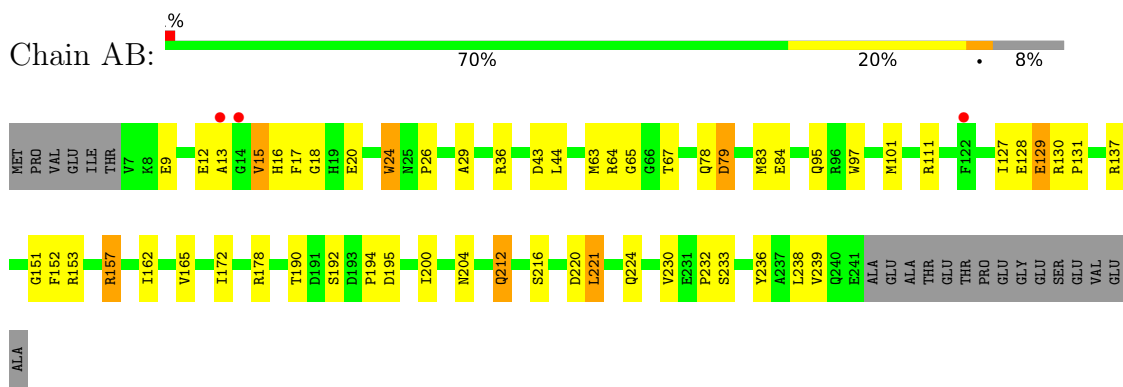
- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| | | | Total | C | N | O | P | | |
| 62 | AY | 1 | 28 | 10 | 5 | 11 | 2 | 0 | 0 |
| 62 | CY | 1 | 28 | 10 | 5 | 11 | 2 | 0 | 0 |

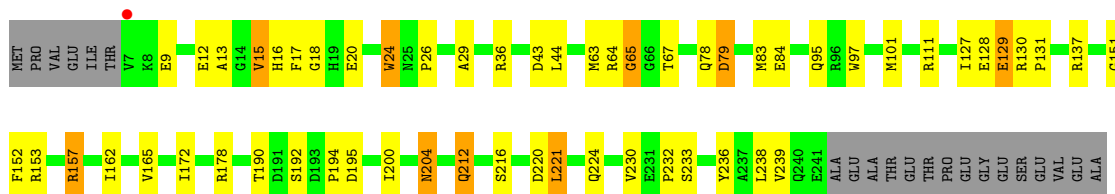


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

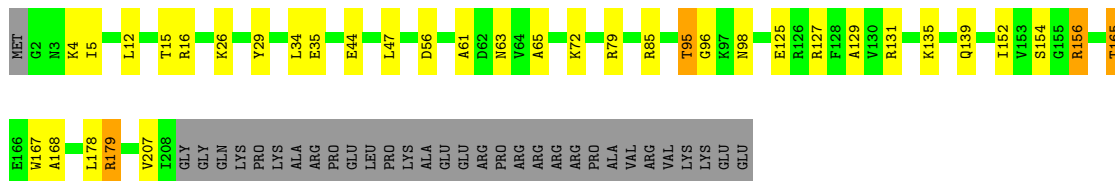


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

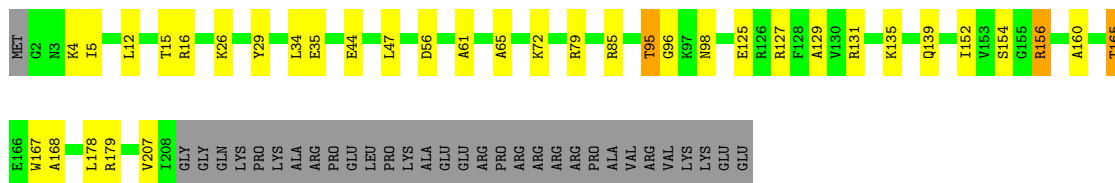




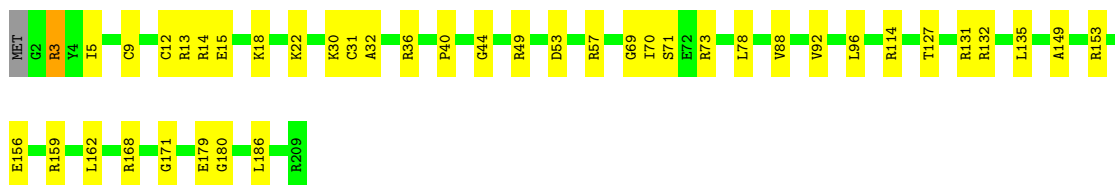
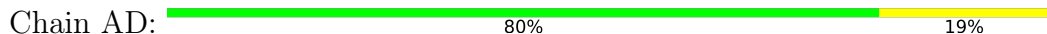
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



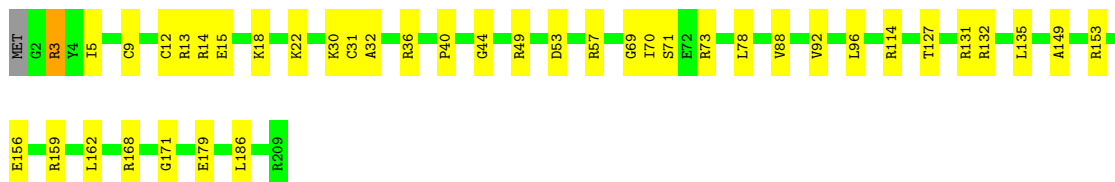
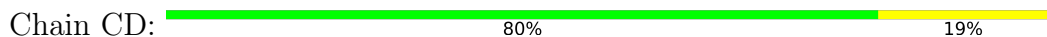
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



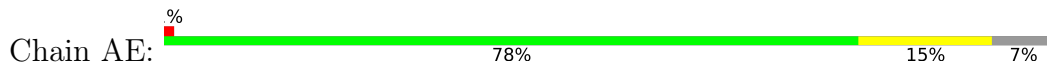
- Molecule 4: 30S RIBOSOMAL PROTEIN S4



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

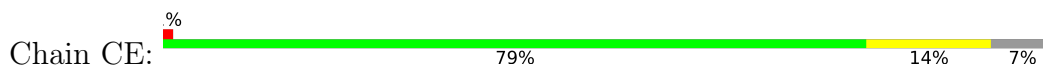


- Molecule 5: 30S RIBOSOMAL PROTEIN S5

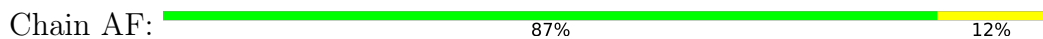




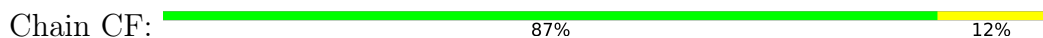
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



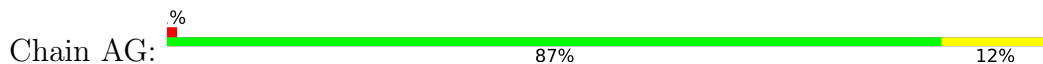
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



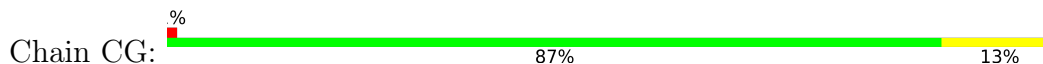
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



- Molecule 7: 30S RIBOSOMAL PROTEIN S7



- Molecule 7: 30S RIBOSOMAL PROTEIN S7



- Molecule 8: 30S RIBOSOMAL PROTEIN S8

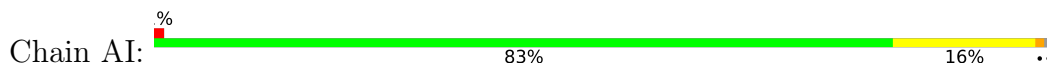


- Molecule 8: 30S RIBOSOMAL PROTEIN S8

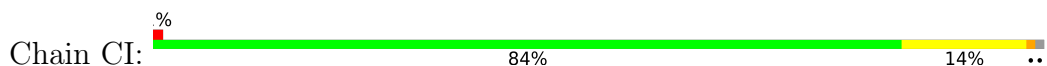




- Molecule 9: 30S RIBOSOMAL PROTEIN S9



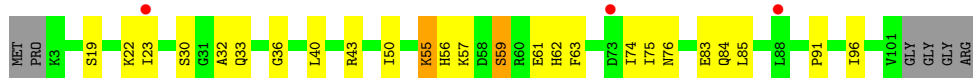
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



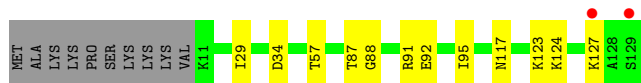
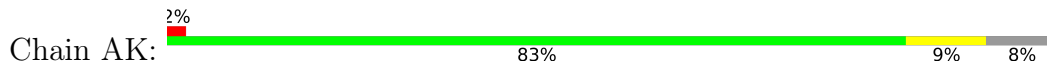
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



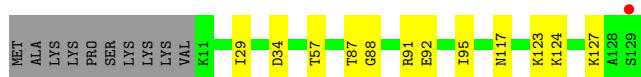
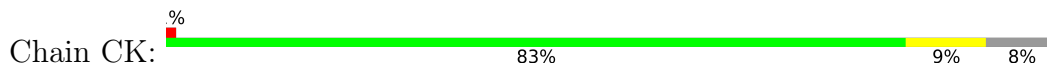
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



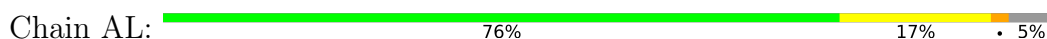
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

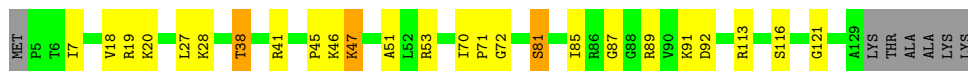


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

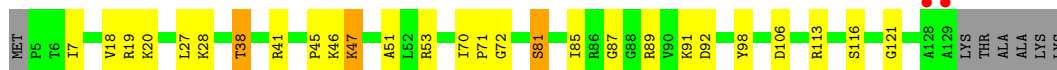
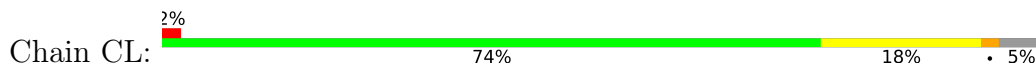


- Molecule 12: 30S RIBOSOMAL PROTEIN S12

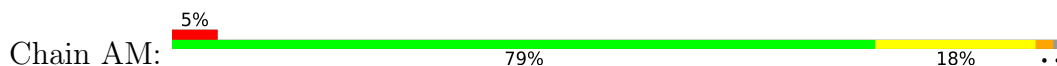




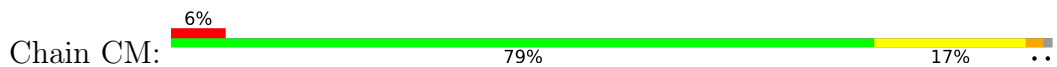
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



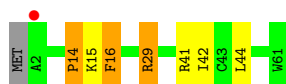
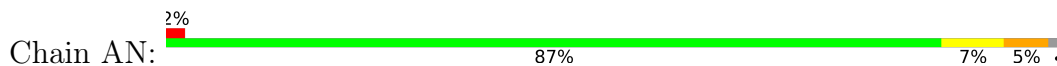
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



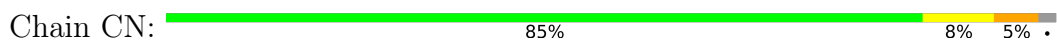
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



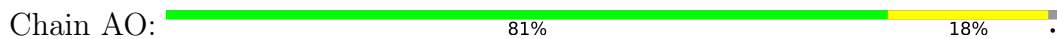
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



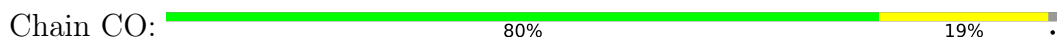
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

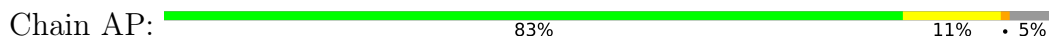


- Molecule 15: 30S RIBOSOMAL PROTEIN S15

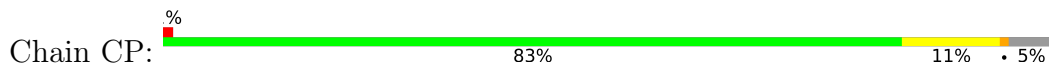




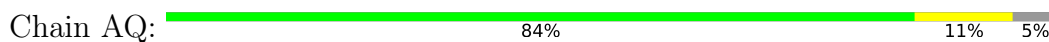
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



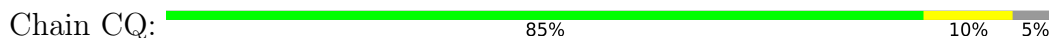
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



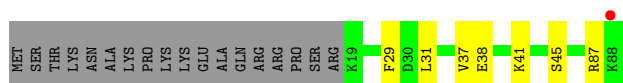
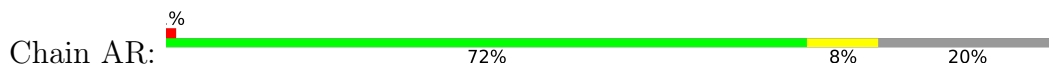
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



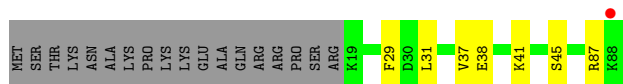
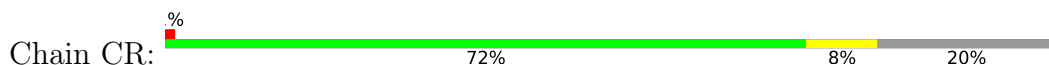
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



- Molecule 18: 30S RIBOSOMAL PROTEIN S18



- Molecule 18: 30S RIBOSOMAL PROTEIN S18



- Molecule 19: 30S RIBOSOMAL PROTEIN S19





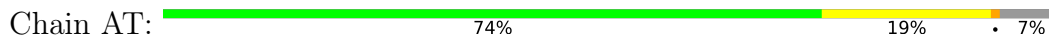
LYS

• Molecule 19: 30S RIBOSOMAL PROTEIN S19



LYS
LYS
LYS

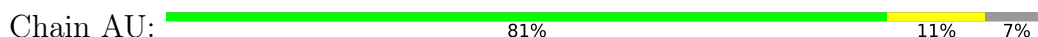
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



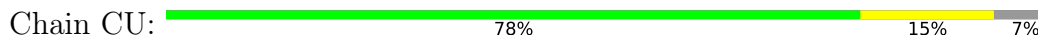
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



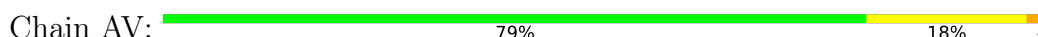
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

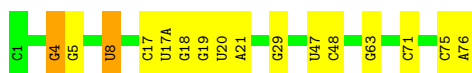


• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

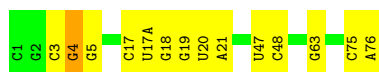
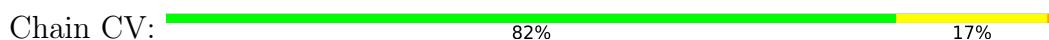




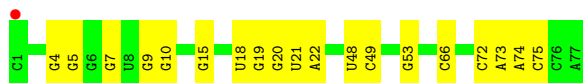
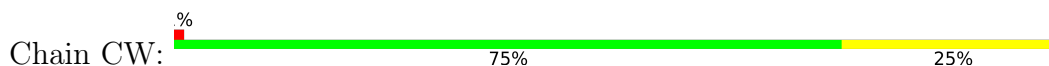
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



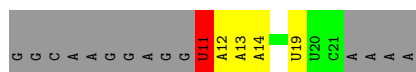
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



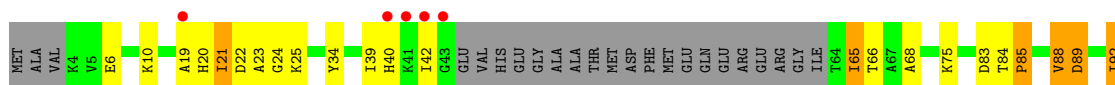
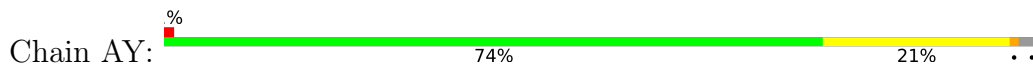
- Molecule 23: MRNA

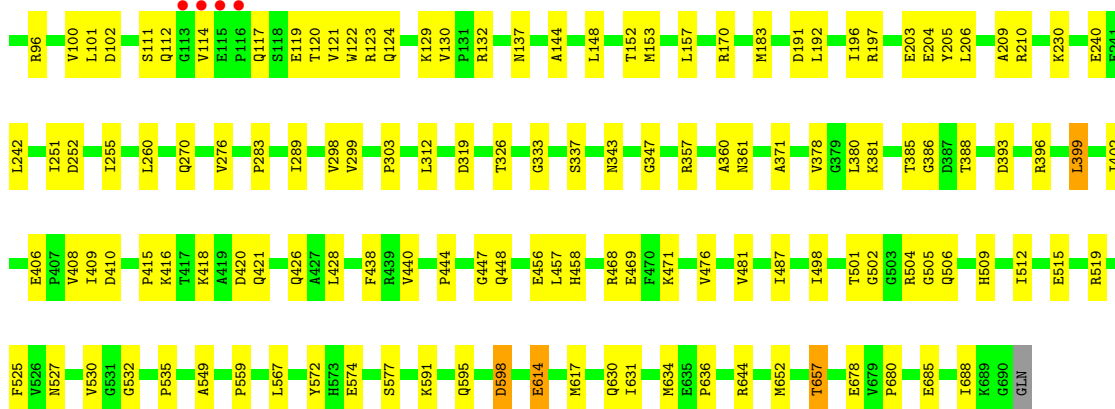


- Molecule 23: MRNA

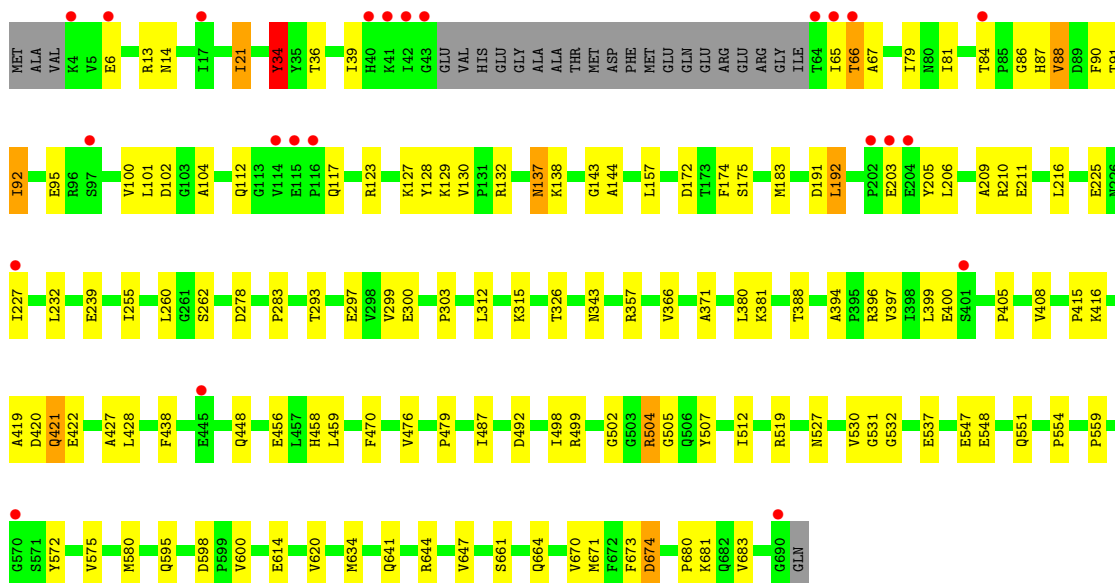
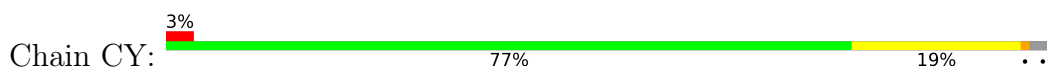


- Molecule 24: ELONGATION FACTOR G

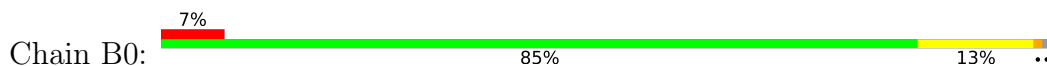




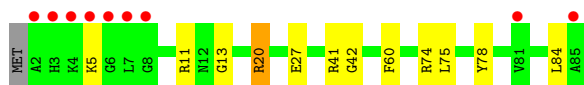
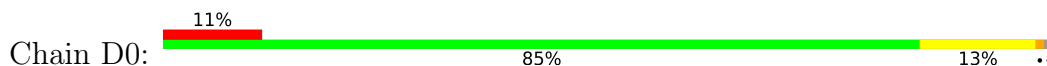
- Molecule 24: ELONGATION FACTOR G



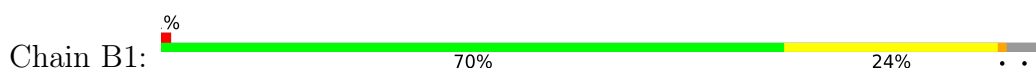
- Molecule 25: 50S RIBOSOMAL PROTEIN L27



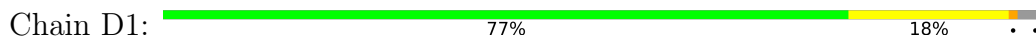
- Molecule 25: 50S RIBOSOMAL PROTEIN L27



- Molecule 26: 50S RIBOSOMAL PROTEIN L28



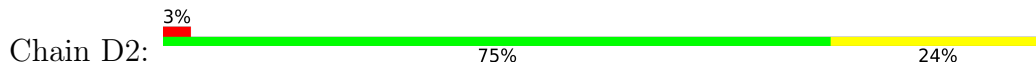
- Molecule 26: 50S RIBOSOMAL PROTEIN L28



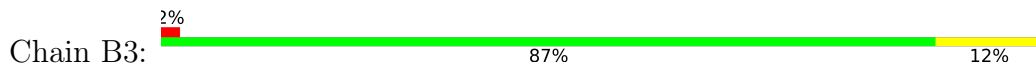
- Molecule 27: 50S RIBOSOMAL PROTEIN L29



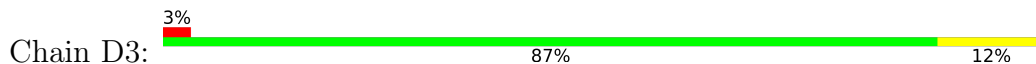
- Molecule 27: 50S RIBOSOMAL PROTEIN L29



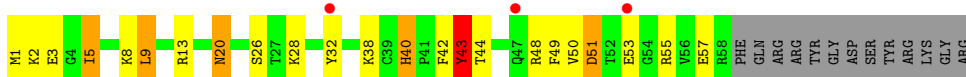
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



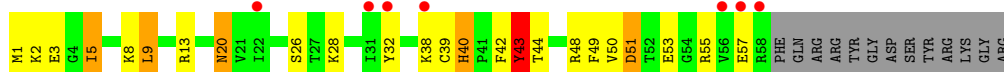
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



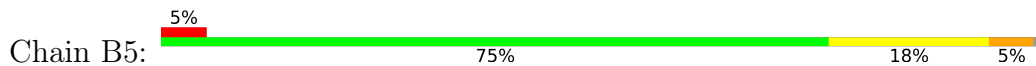
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



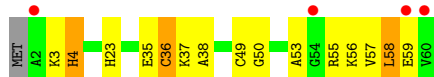
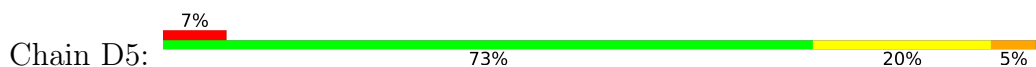
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



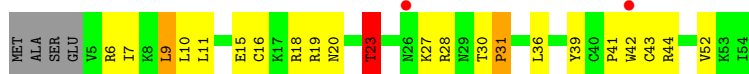
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



- Molecule 30: 50S RIBOSOMAL PROTEIN L32



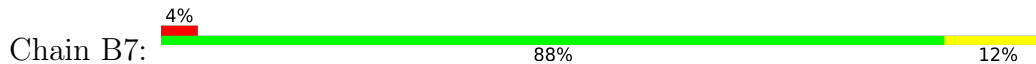
- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 31: 50S RIBOSOMAL PROTEIN L33



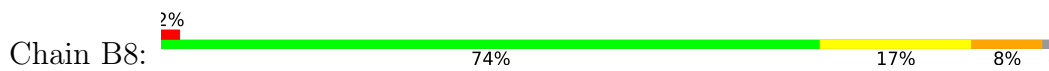
- Molecule 32: 50S RIBOSOMAL PROTEIN L34



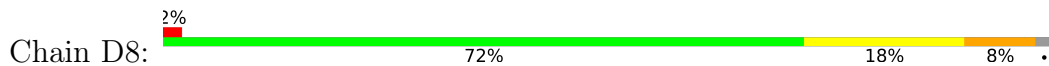
- Molecule 32: 50S RIBOSOMAL PROTEIN L34



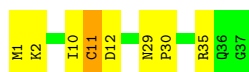
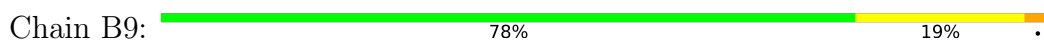
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



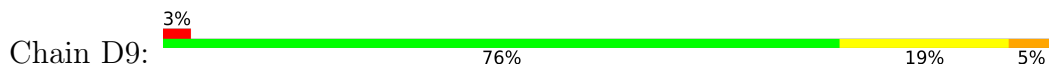
● Molecule 33: 50S RIBOSOMAL PROTEIN L35



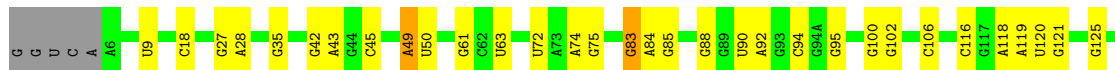
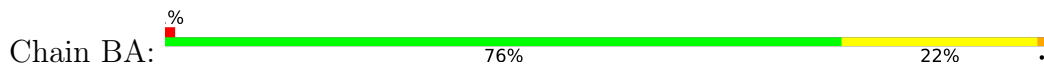
● Molecule 34: 50S RIBOSOMAL PROTEIN L36

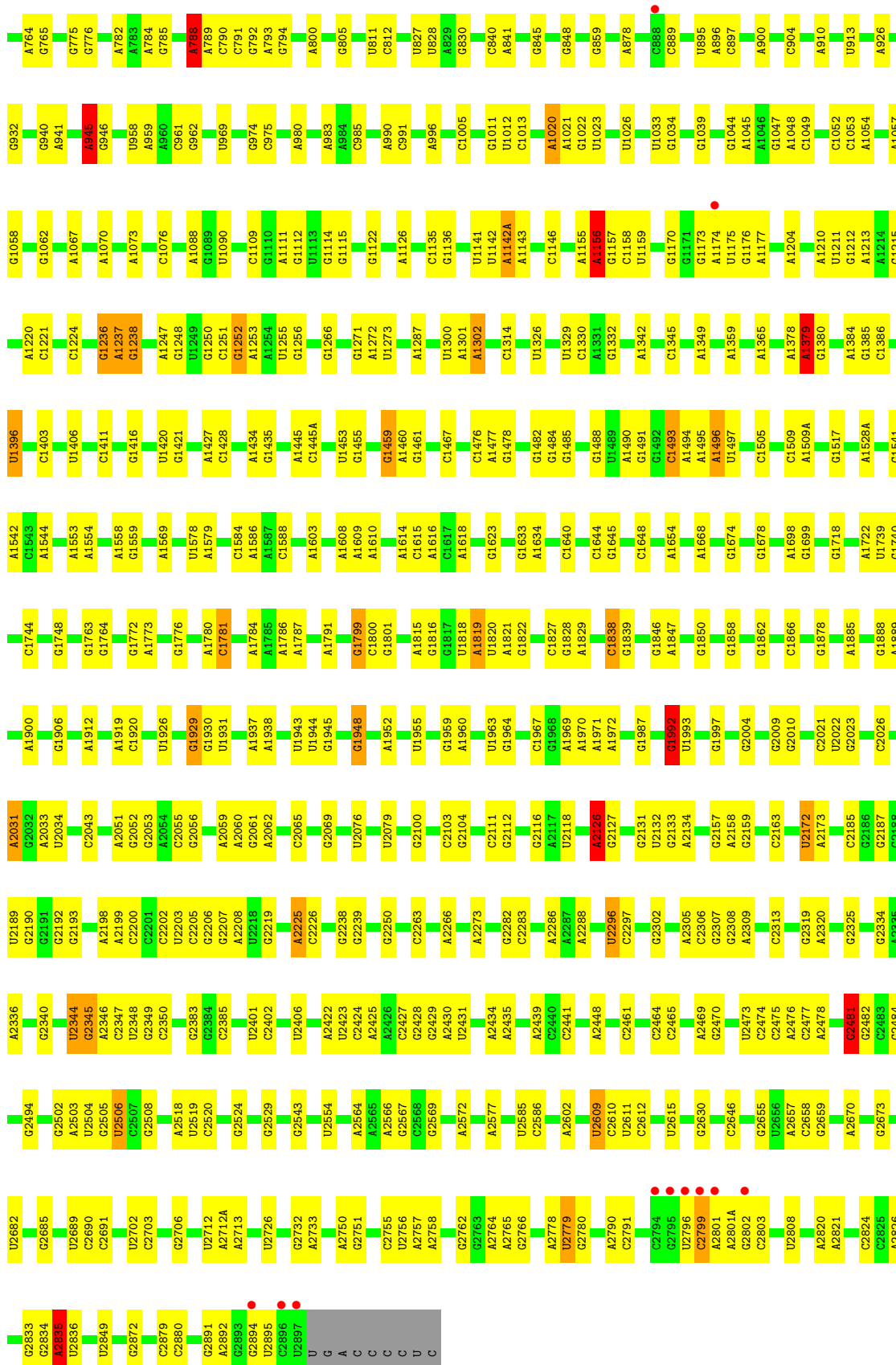


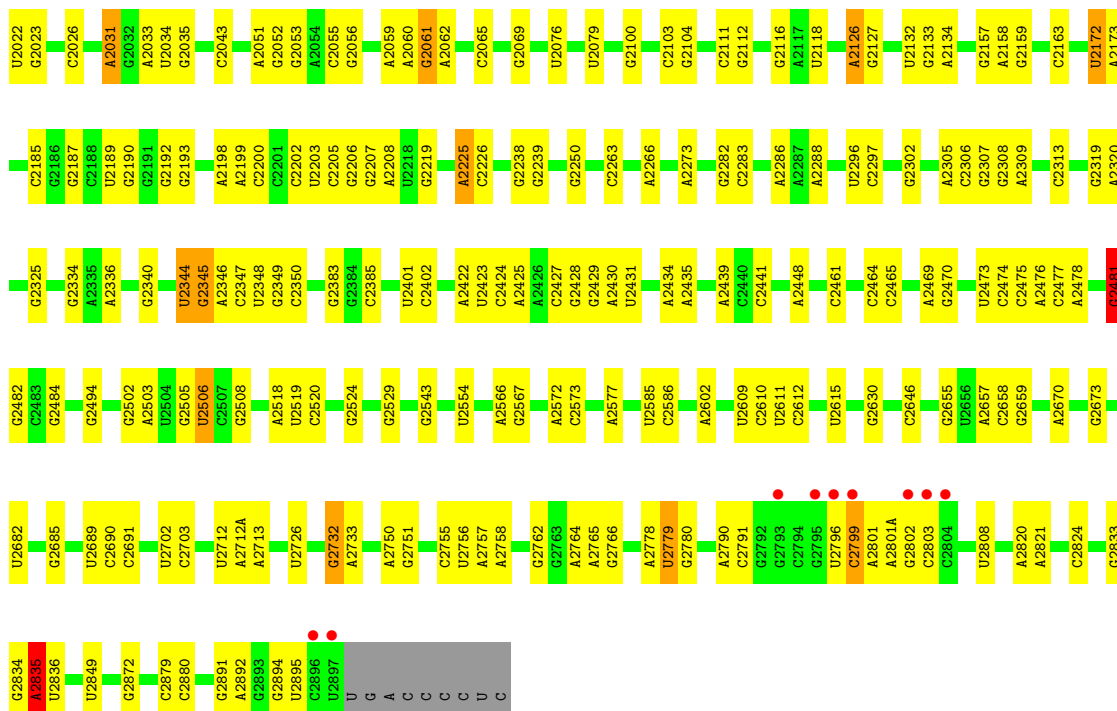
● Molecule 34: 50S RIBOSOMAL PROTEIN L36



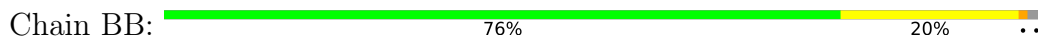
● Molecule 35: 23S RIBOSOMAL RNA



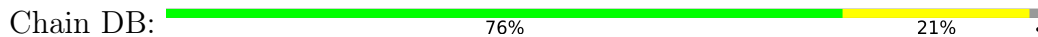




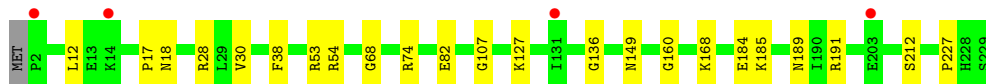
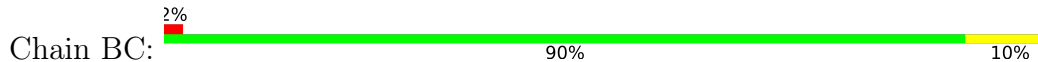
• Molecule 36: 5S RIBOSOMAL RNA



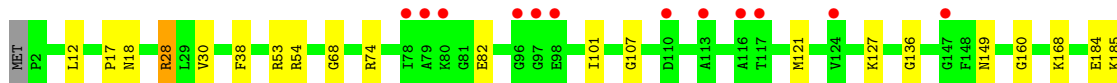
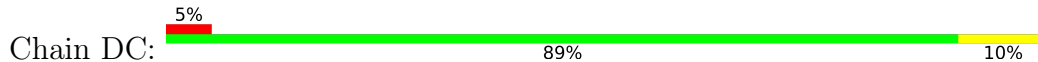
• Molecule 36: 5S RIBOSOMAL RNA



• Molecule 37: 50S RIBOSOMAL PROTEIN L1

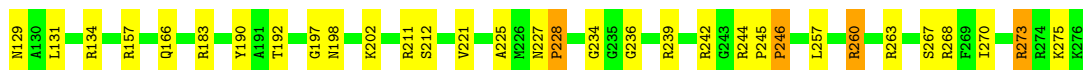
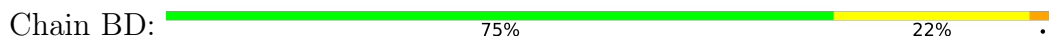


• Molecule 37: 50S RIBOSOMAL PROTEIN L1

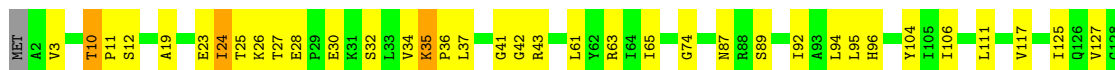
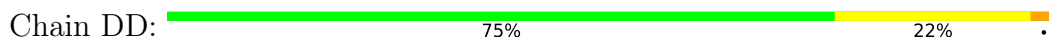




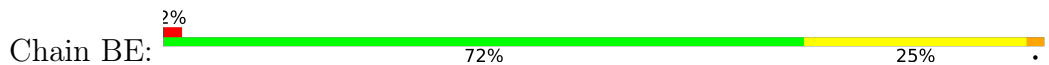
• Molecule 38: 50S RIBOSOMAL PROTEIN L2



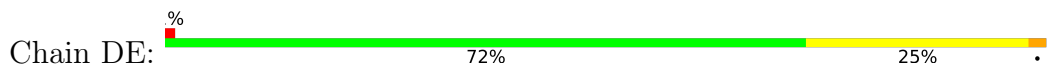
• Molecule 38: 50S RIBOSOMAL PROTEIN L2



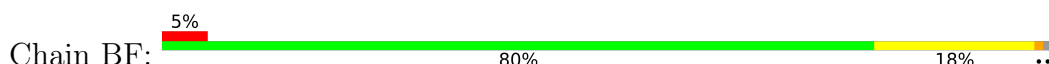
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

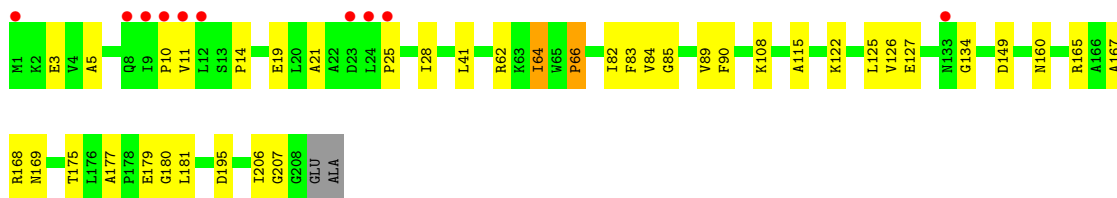


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

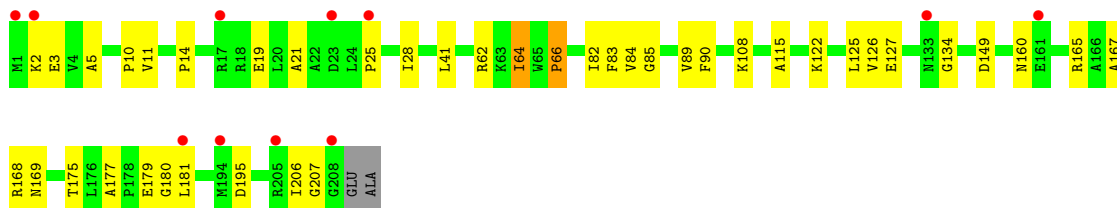
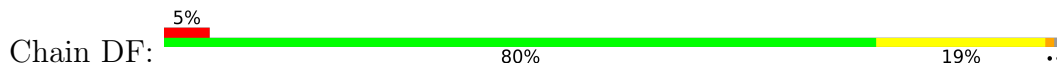


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

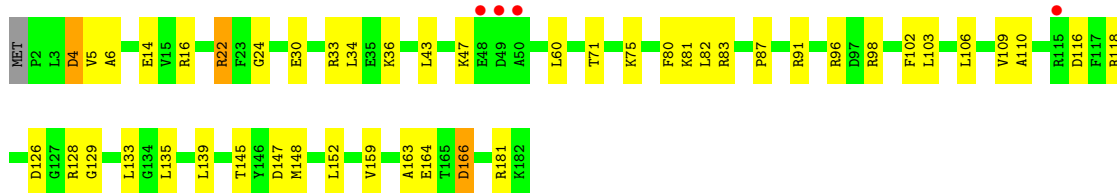
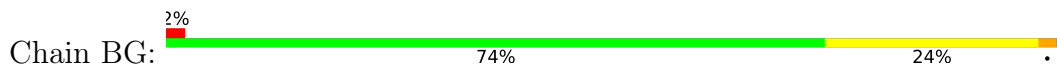




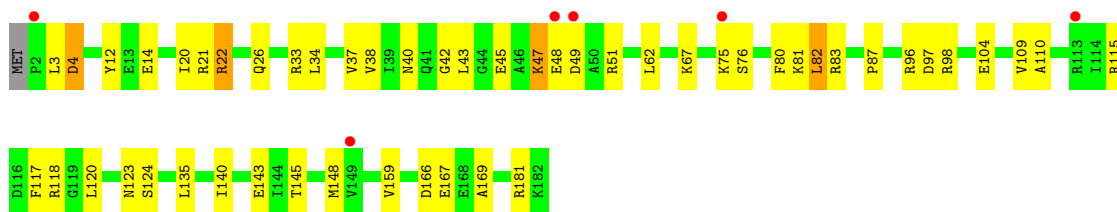
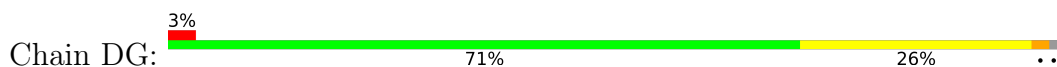
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



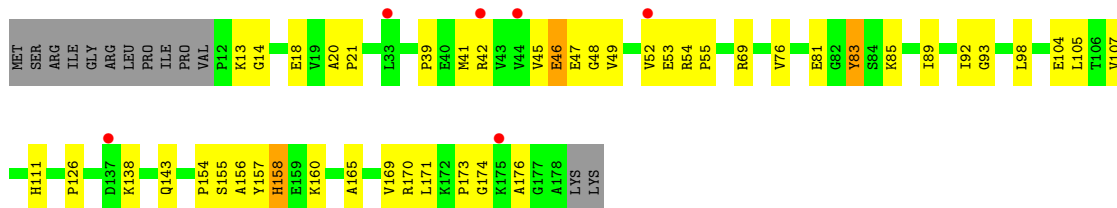
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



• Molecule 41: 50S RIBOSOMAL PROTEIN L5

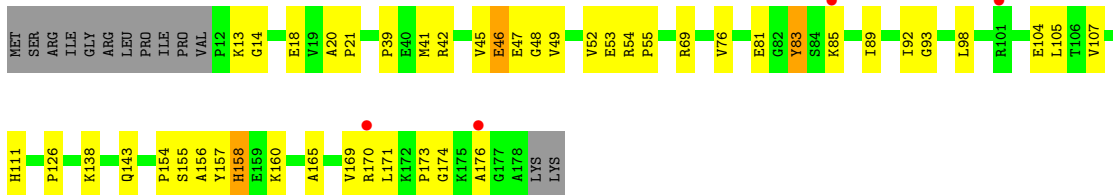


• Molecule 42: 50S RIBOSOMAL PROTEIN L6



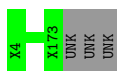
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH:  2% 67% 24% 7%



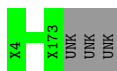
- Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain BJ:  98%




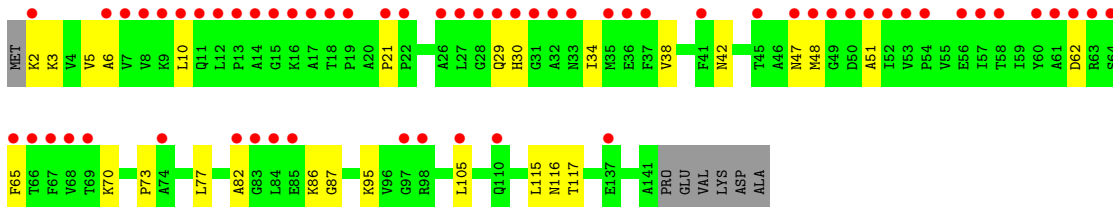
- Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain DJ:  98%




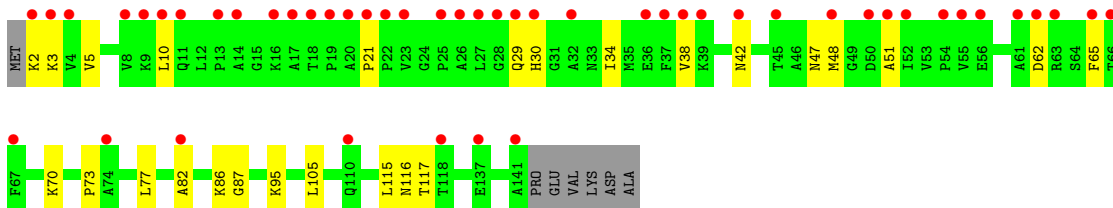
- Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain BK:  41% 77% 18% 5%




- Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain DK:  33% 78% 18% 5%

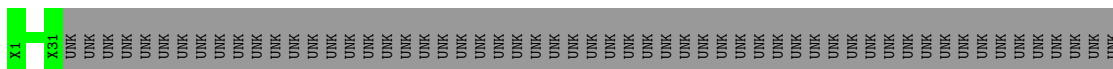


- Molecule 45: 50S RIBOSOMAL PROTEIN L12

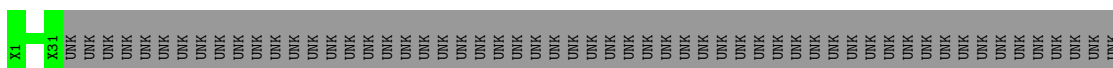
Chain BL:  82% 18%



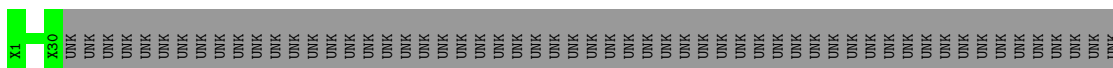
• Molecule 45: 50S RIBOSOMAL PROTEIN L12



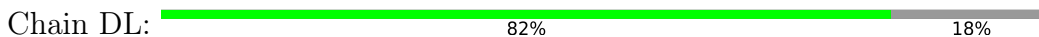
• Molecule 45: 50S RIBOSOMAL PROTEIN L12



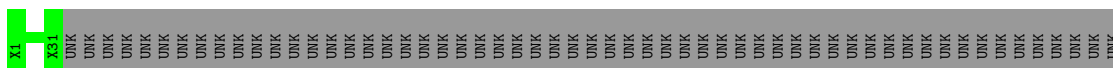
• Molecule 45: 50S RIBOSOMAL PROTEIN L12



• Molecule 45: 50S RIBOSOMAL PROTEIN L12



• Molecule 45: 50S RIBOSOMAL PROTEIN L12



• Molecule 45: 50S RIBOSOMAL PROTEIN L12

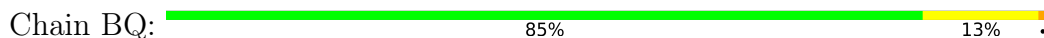




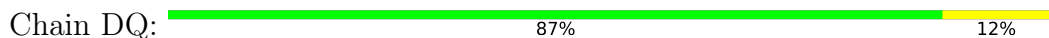
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



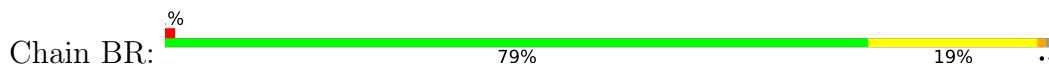
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



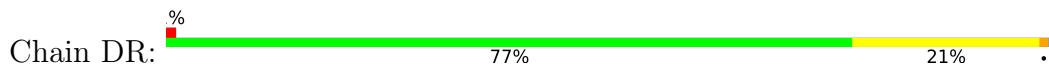
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



• Molecule 50: 50S RIBOSOMAL PROTEIN L17



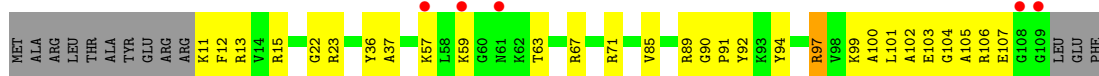
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



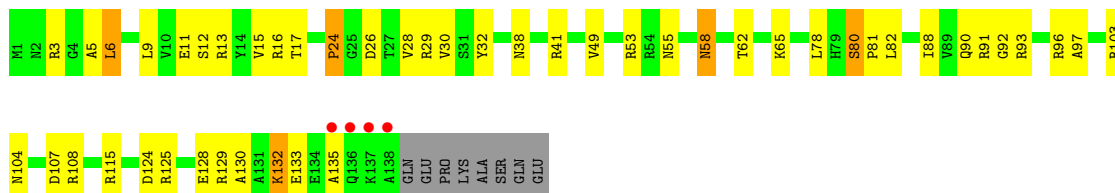
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



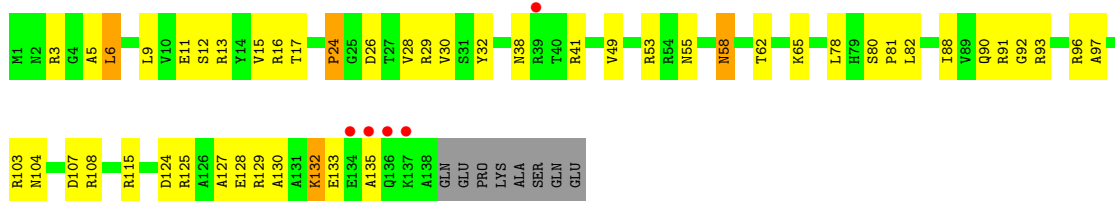
- Molecule 51: 50S RIBOSOMAL PROTEIN L18



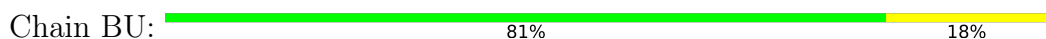
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



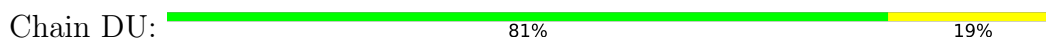
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



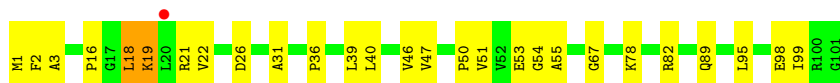
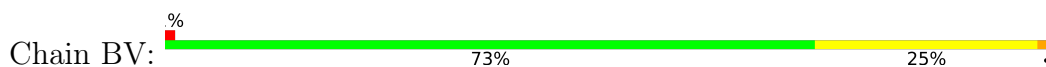
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



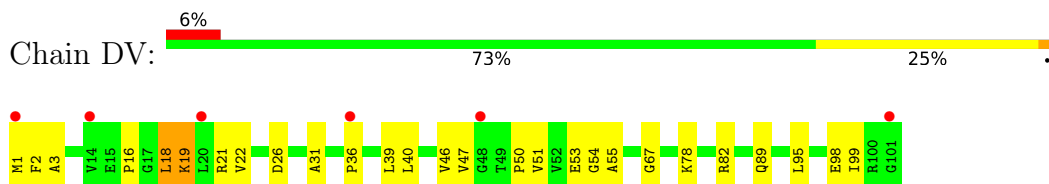
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



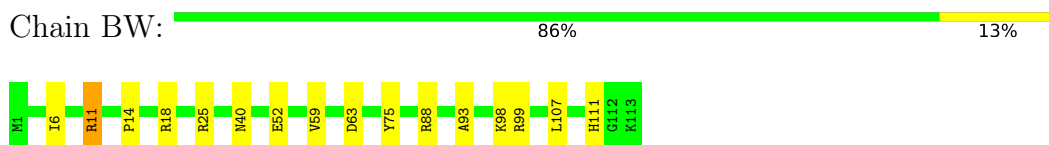
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



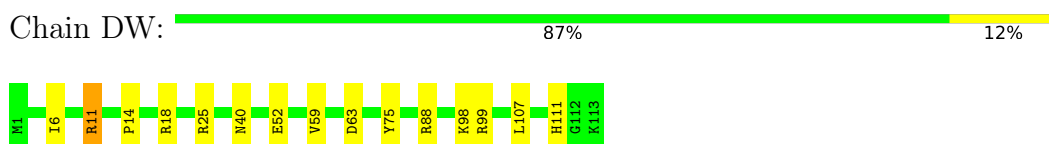
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



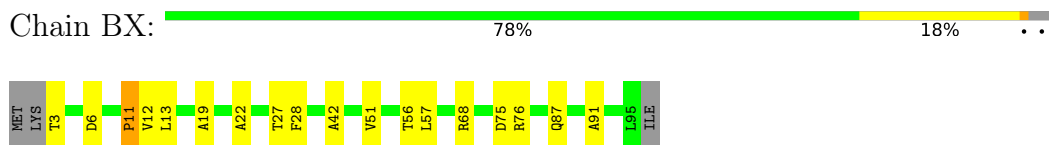
● Molecule 55: 50S RIBOSOMAL PROTEIN L22



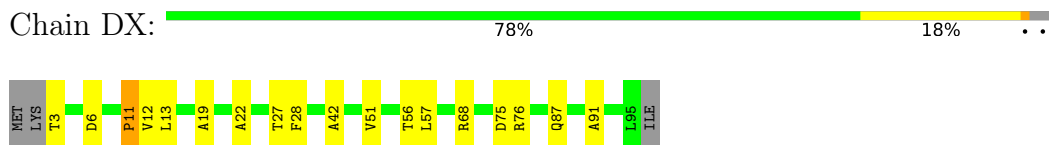
● Molecule 55: 50S RIBOSOMAL PROTEIN L22



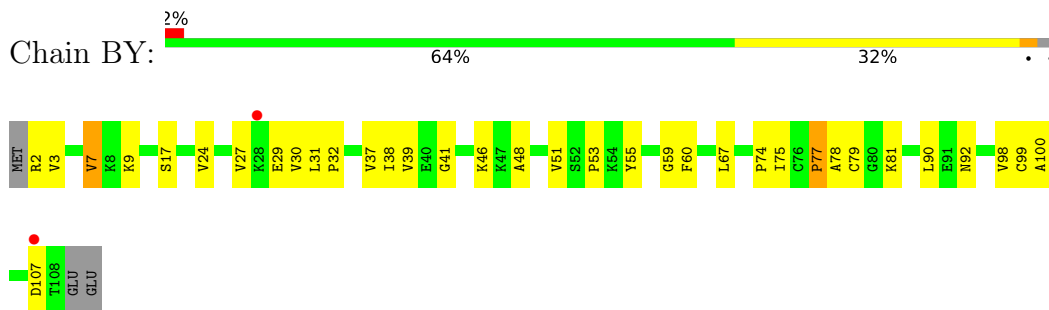
● Molecule 56: 50S RIBOSOMAL PROTEIN L23



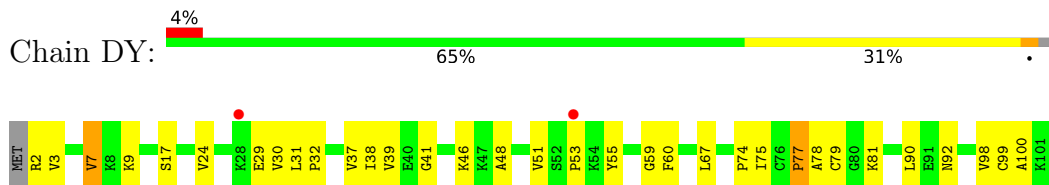
● Molecule 56: 50S RIBOSOMAL PROTEIN L23

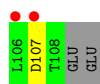


● Molecule 57: 50S RIBOSOMAL PROTEIN L24



● Molecule 57: 50S RIBOSOMAL PROTEIN L24





- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ: 65% 20% 5% 10%



- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ: 67% 21% 10%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 291.84Å 270.36Å 402.36Å 90.00° 91.73° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.60 49.57 – 3.40 | Depositor EDS |
| % Data completeness (in resolution range) | 96.0 (50.00-3.60) 95.0 (49.57-3.40) | Depositor EDS |
| R_{merge} | 0.37 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.57 (at 3.40Å) | Xtrriage |
| Refinement program | CNS 1.2 | Depositor |
| R, R_{free} | 0.227 , 0.260 0.225 , 0.224 | Depositor DCC |
| R_{free} test set | 40387 reflections (4.98%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 78.6 | Xtrriage |
| Anisotropy | 0.084 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 34.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$ | Xtrriage |
| Estimated twinning fraction | 0.048 for h,-k,-l | Xtrriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 311552 | wwPDB-VP |
| Average B, all atoms (Å ²) | 86.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP, FUA, ZN, MG

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 | 0.61 | 1/36190 (0.0%) | 0.76 | 26/56486 (0.0%) |
| 1 | CA | 0.60 | 2/36190 (0.0%) | 0.76 | 20/56486 (0.0%) |
| 2 | AB | 0.46 | 0/1936 | 0.70 | 0/2611 |
| 2 | CB | 0.44 | 0/1936 | 0.70 | 0/2611 |
| 3 | AC | 0.52 | 0/1637 | 0.69 | 0/2207 |
| 3 | CC | 0.46 | 0/1637 | 0.69 | 0/2207 |
| 4 | AD | 0.42 | 0/1733 | 0.66 | 0/2318 |
| 4 | CD | 0.41 | 0/1733 | 0.66 | 0/2318 |
| 5 | AE | 0.59 | 0/1163 | 0.72 | 0/1566 |
| 5 | CE | 0.55 | 0/1163 | 0.71 | 0/1566 |
| 6 | AF | 0.44 | 0/856 | 0.67 | 0/1154 |
| 6 | CF | 0.40 | 0/856 | 0.66 | 0/1154 |
| 7 | AG | 0.45 | 0/1276 | 0.65 | 0/1709 |
| 7 | CG | 0.45 | 0/1276 | 0.65 | 0/1709 |
| 8 | AH | 0.51 | 0/1136 | 0.74 | 0/1527 |
| 8 | CH | 0.46 | 0/1136 | 0.74 | 0/1527 |
| 9 | AI | 0.44 | 0/1027 | 0.68 | 0/1373 |
| 9 | CI | 0.41 | 0/1027 | 0.67 | 0/1373 |
| 10 | AJ | 0.47 | 0/808 | 0.72 | 0/1087 |
| 10 | CJ | 0.42 | 0/808 | 0.71 | 0/1087 |
| 11 | AK | 0.50 | 0/900 | 0.70 | 0/1213 |
| 11 | CK | 0.47 | 0/900 | 0.70 | 0/1213 |
| 12 | AL | 0.52 | 0/987 | 0.75 | 0/1322 |
| 12 | CL | 0.48 | 0/987 | 0.74 | 0/1322 |
| 13 | AM | 0.41 | 0/999 | 0.69 | 0/1338 |
| 13 | CM | 0.39 | 0/999 | 0.69 | 0/1338 |
| 14 | AN | 0.49 | 0/501 | 0.69 | 0/664 |
| 14 | CN | 0.47 | 0/501 | 0.69 | 0/664 |
| 15 | AO | 0.45 | 0/745 | 0.67 | 0/992 |
| 15 | CO | 0.43 | 0/745 | 0.66 | 0/992 |
| 16 | AP | 0.45 | 0/717 | 0.68 | 0/965 |
| 16 | CP | 0.43 | 0/717 | 0.68 | 0/965 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.51 | 0/837 | 0.69 | 0/1119 |
| 17 | CQ | 0.49 | 0/837 | 0.69 | 0/1119 |
| 18 | AR | 0.47 | 0/579 | 0.72 | 0/768 |
| 18 | CR | 0.45 | 0/579 | 0.73 | 0/768 |
| 19 | AS | 0.46 | 0/643 | 0.68 | 1/867 (0.1%) |
| 19 | CS | 0.44 | 0/643 | 0.67 | 1/867 (0.1%) |
| 20 | AT | 0.40 | 0/765 | 0.66 | 0/1007 |
| 20 | CT | 0.39 | 0/765 | 0.66 | 0/1007 |
| 21 | AU | 0.52 | 0/213 | 0.65 | 0/279 |
| 21 | CU | 0.50 | 0/213 | 0.65 | 0/279 |
| 22 | AV | 0.57 | 0/1810 | 0.73 | 0/2821 |
| 22 | AW | 0.41 | 0/1810 | 0.72 | 0/2821 |
| 22 | CV | 0.54 | 0/1810 | 0.70 | 0/2821 |
| 22 | CW | 0.38 | 0/1810 | 0.69 | 0/2821 |
| 23 | AX | 0.82 | 0/257 | 0.86 | 0/398 |
| 23 | CX | 0.79 | 0/257 | 0.84 | 1/398 (0.3%) |
| 24 | AY | 0.40 | 0/5313 | 0.69 | 0/7195 |
| 24 | CY | 0.42 | 0/5313 | 0.69 | 1/7195 (0.0%) |
| 25 | B0 | 0.43 | 0/671 | 0.66 | 0/892 |
| 25 | D0 | 0.42 | 0/671 | 0.67 | 0/892 |
| 26 | B1 | 0.48 | 0/739 | 0.78 | 0/983 |
| 26 | D1 | 0.45 | 0/739 | 0.69 | 0/983 |
| 27 | B2 | 0.36 | 0/600 | 0.66 | 0/793 |
| 27 | D2 | 0.37 | 0/600 | 0.62 | 0/793 |
| 28 | B3 | 0.43 | 0/473 | 0.63 | 0/636 |
| 28 | D3 | 0.43 | 0/473 | 0.64 | 0/636 |
| 29 | B4 | 0.68 | 0/461 | 0.92 | 2/623 (0.3%) |
| 29 | D4 | 0.74 | 0/461 | 0.93 | 2/623 (0.3%) |
| 30 | B5 | 0.43 | 0/473 | 0.75 | 0/639 |
| 30 | D5 | 0.44 | 0/473 | 0.74 | 0/639 |
| 31 | B6 | 0.64 | 0/440 | 0.96 | 1/586 (0.2%) |
| 31 | D6 | 0.64 | 0/440 | 0.96 | 1/586 (0.2%) |
| 32 | B7 | 0.45 | 0/427 | 0.71 | 0/563 |
| 32 | D7 | 0.45 | 0/427 | 0.71 | 0/563 |
| 33 | B8 | 0.54 | 0/516 | 0.83 | 0/681 |
| 33 | D8 | 0.54 | 0/516 | 0.83 | 0/681 |
| 34 | B9 | 0.47 | 0/310 | 0.69 | 0/407 |
| 34 | D9 | 0.46 | 0/310 | 0.70 | 0/407 |
| 35 | BA | 0.56 | 3/69972 (0.0%) | 0.75 | 35/109237 (0.0%) |
| 35 | DA | 0.55 | 4/69972 (0.0%) | 0.75 | 36/109237 (0.0%) |
| 36 | BB | 0.44 | 0/2853 | 0.72 | 1/4451 (0.0%) |
| 36 | DB | 0.44 | 0/2853 | 0.72 | 0/4451 |
| 37 | BC | 0.35 | 0/1774 | 0.61 | 0/2391 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 37 | DC | 0.34 | 0/1774 | 0.61 | 0/2391 |
| 38 | BD | 0.54 | 0/2195 | 0.83 | 0/2955 |
| 38 | DD | 0.53 | 0/2195 | 0.82 | 0/2955 |
| 39 | BE | 0.48 | 0/1597 | 0.74 | 0/2155 |
| 39 | DE | 0.46 | 0/1597 | 0.74 | 0/2155 |
| 40 | BF | 0.39 | 0/1659 | 0.66 | 0/2246 |
| 40 | DF | 0.38 | 0/1659 | 0.66 | 0/2246 |
| 41 | BG | 0.42 | 0/1498 | 0.78 | 1/2013 (0.0%) |
| 41 | DG | 0.43 | 0/1498 | 0.74 | 0/2013 |
| 42 | BH | 0.36 | 0/1293 | 0.71 | 0/1746 |
| 42 | DH | 0.35 | 0/1293 | 0.69 | 0/1746 |
| 44 | BK | 0.35 | 0/1045 | 0.60 | 0/1418 |
| 44 | DK | 0.36 | 0/1045 | 0.60 | 0/1418 |
| 46 | BN | 0.40 | 0/1132 | 0.73 | 1/1527 (0.1%) |
| 46 | DN | 0.39 | 0/1132 | 0.73 | 1/1527 (0.1%) |
| 47 | BO | 0.49 | 0/943 | 0.72 | 0/1269 |
| 47 | DO | 0.47 | 0/943 | 0.72 | 0/1269 |
| 48 | BP | 0.44 | 0/1131 | 0.93 | 4/1504 (0.3%) |
| 48 | DP | 0.44 | 0/1131 | 0.91 | 4/1504 (0.3%) |
| 49 | BQ | 0.49 | 0/1143 | 0.69 | 0/1527 |
| 49 | DQ | 0.48 | 0/1143 | 0.70 | 0/1527 |
| 50 | BR | 0.39 | 0/974 | 0.68 | 0/1302 |
| 50 | DR | 0.38 | 0/974 | 0.68 | 1/1302 (0.1%) |
| 51 | BS | 0.41 | 0/779 | 0.69 | 0/1038 |
| 51 | DS | 0.40 | 0/779 | 0.70 | 0/1038 |
| 52 | BT | 0.47 | 0/1156 | 0.79 | 2/1544 (0.1%) |
| 52 | DT | 0.49 | 0/1156 | 0.79 | 1/1544 (0.1%) |
| 53 | BU | 0.43 | 0/975 | 0.68 | 0/1297 |
| 53 | DU | 0.44 | 0/975 | 0.69 | 0/1297 |
| 54 | BV | 0.39 | 0/790 | 0.70 | 0/1057 |
| 54 | DV | 0.39 | 0/790 | 0.70 | 0/1057 |
| 55 | BW | 0.37 | 0/907 | 0.65 | 0/1216 |
| 55 | DW | 0.39 | 0/907 | 0.65 | 0/1216 |
| 56 | BX | 0.42 | 0/740 | 0.66 | 0/995 |
| 56 | DX | 0.42 | 0/740 | 0.66 | 0/995 |
| 57 | BY | 0.41 | 0/824 | 0.67 | 0/1100 |
| 57 | DY | 0.42 | 0/824 | 0.68 | 0/1100 |
| 58 | BZ | 0.48 | 0/1500 | 0.74 | 0/2037 |
| 58 | DZ | 0.46 | 0/1500 | 0.73 | 0/2037 |
| All | All | 0.53 | 10/333656 (0.0%) | 0.74 | 143/497270 (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 | 48 |
| 1 | CA | 0 | 43 |
| 22 | AV | 0 | 3 |
| 22 | CV | 0 | 1 |
| 23 | AX | 0 | 2 |
| 23 | CX | 0 | 1 |
| 35 | BA | 2 | 69 |
| 35 | DA | 2 | 58 |
| 36 | BB | 0 | 1 |
| 36 | DB | 0 | 1 |
| 37 | BC | 0 | 1 |
| 37 | DC | 0 | 1 |
| 44 | BK | 0 | 1 |
| 44 | DK | 0 | 1 |
| 46 | DN | 0 | 1 |
| All | All | 4 | 232 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 35 | BA | 2506 | U | N1-C2 | 7.05 | 1.44 | 1.38 |
| 35 | DA | 2506 | U | N1-C2 | 6.48 | 1.44 | 1.38 |
| 35 | BA | 272(I) | U | C1'-N1 | 5.69 | 1.57 | 1.48 |
| 1 | AA | 1417 | G | C6-O6 | 5.55 | 1.29 | 1.24 |
| 35 | DA | 272(I) | U | C1'-N1 | 5.49 | 1.56 | 1.48 |

The worst 5 of 143 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35 | BA | 1992 | G | C2'-C3'-O3' | 10.77 | 133.19 | 109.50 |
| 35 | DA | 1992 | G | C2'-C3'-O3' | 10.61 | 132.85 | 109.50 |
| 1 | CA | 575 | G | C2'-C3'-O3' | 9.68 | 130.80 | 109.50 |
| 1 | AA | 575 | G | C2'-C3'-O3' | 9.65 | 130.72 | 109.50 |
| 35 | BA | 945 | A | N9-C1'-C2' | 9.34 | 126.14 | 114.00 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 35 | BA | 1799 | G | C3' |
| 35 | BA | 1992 | G | C3' |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 35 | DA | 1799 | G | C3' |
| 35 | DA | 1992 | G | C3' |

5 of 232 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 108 | G | Sidechain |
| 1 | AA | 112 | G | Sidechain |
| 1 | AA | 30 | U | Sidechain |
| 1 | AA | 39 | G | Sidechain |
| 1 | AA | 5 | U | Sidechain |

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | AB | 233/256 (91%) | 139 (60%) | 53 (23%) | 41 (18%) | 0 | 2 |
| 2 | CB | 233/256 (91%) | 140 (60%) | 51 (22%) | 42 (18%) | 0 | 2 |
| 3 | AC | 205/239 (86%) | 133 (65%) | 50 (24%) | 22 (11%) | 0 | 7 |
| 3 | CC | 205/239 (86%) | 132 (64%) | 52 (25%) | 21 (10%) | 0 | 7 |
| 4 | AD | 206/209 (99%) | 134 (65%) | 50 (24%) | 22 (11%) | 0 | 7 |
| 4 | CD | 206/209 (99%) | 134 (65%) | 51 (25%) | 21 (10%) | 0 | 7 |
| 5 | AE | 149/162 (92%) | 119 (80%) | 21 (14%) | 9 (6%) | 1 | 17 |
| 5 | CE | 149/162 (92%) | 117 (78%) | 24 (16%) | 8 (5%) | 2 | 19 |
| 6 | AF | 99/101 (98%) | 75 (76%) | 17 (17%) | 7 (7%) | 1 | 14 |
| 6 | CF | 99/101 (98%) | 74 (75%) | 18 (18%) | 7 (7%) | 1 | 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|-----------|----------|-------------|----|
| 7 | AG | 153/156 (98%) | 109 (71%) | 34 (22%) | 10 (6%) | 1 | 16 |
| 7 | CG | 153/156 (98%) | 110 (72%) | 32 (21%) | 11 (7%) | 1 | 13 |
| 8 | AH | 136/138 (99%) | 103 (76%) | 30 (22%) | 3 (2%) | 6 | 39 |
| 8 | CH | 136/138 (99%) | 105 (77%) | 27 (20%) | 4 (3%) | 4 | 33 |
| 9 | AI | 121/128 (94%) | 81 (67%) | 26 (22%) | 14 (12%) | 0 | 6 |
| 9 | CI | 121/128 (94%) | 82 (68%) | 27 (22%) | 12 (10%) | 0 | 8 |
| 10 | AJ | 97/105 (92%) | 60 (62%) | 21 (22%) | 16 (16%) | 0 | 3 |
| 10 | CJ | 97/105 (92%) | 61 (63%) | 20 (21%) | 16 (16%) | 0 | 3 |
| 11 | AK | 117/129 (91%) | 91 (78%) | 20 (17%) | 6 (5%) | 2 | 20 |
| 11 | CK | 117/129 (91%) | 91 (78%) | 20 (17%) | 6 (5%) | 2 | 20 |
| 12 | AL | 123/132 (93%) | 82 (67%) | 23 (19%) | 18 (15%) | 0 | 3 |
| 12 | CL | 123/132 (93%) | 82 (67%) | 22 (18%) | 19 (15%) | 0 | 3 |
| 13 | AM | 123/126 (98%) | 77 (63%) | 25 (20%) | 21 (17%) | 0 | 2 |
| 13 | CM | 123/126 (98%) | 77 (63%) | 26 (21%) | 20 (16%) | 0 | 3 |
| 14 | AN | 58/61 (95%) | 47 (81%) | 7 (12%) | 4 (7%) | 1 | 14 |
| 14 | CN | 58/61 (95%) | 46 (79%) | 7 (12%) | 5 (9%) | 1 | 10 |
| 15 | AO | 86/89 (97%) | 55 (64%) | 23 (27%) | 8 (9%) | 0 | 9 |
| 15 | CO | 86/89 (97%) | 53 (62%) | 24 (28%) | 9 (10%) | 0 | 7 |
| 16 | AP | 82/88 (93%) | 60 (73%) | 15 (18%) | 7 (8%) | 1 | 10 |
| 16 | CP | 82/88 (93%) | 60 (73%) | 15 (18%) | 7 (8%) | 1 | 10 |
| 17 | AQ | 98/105 (93%) | 78 (80%) | 15 (15%) | 5 (5%) | 2 | 20 |
| 17 | CQ | 98/105 (93%) | 78 (80%) | 16 (16%) | 4 (4%) | 3 | 26 |
| 18 | AR | 68/88 (77%) | 52 (76%) | 11 (16%) | 5 (7%) | 1 | 13 |
| 18 | CR | 68/88 (77%) | 51 (75%) | 12 (18%) | 5 (7%) | 1 | 13 |
| 19 | AS | 77/93 (83%) | 43 (56%) | 14 (18%) | 20 (26%) | 0 | 0 |
| 19 | CS | 77/93 (83%) | 43 (56%) | 15 (20%) | 19 (25%) | 0 | 0 |
| 20 | AT | 97/106 (92%) | 52 (54%) | 30 (31%) | 15 (16%) | 0 | 3 |
| 20 | CT | 97/106 (92%) | 53 (55%) | 29 (30%) | 15 (16%) | 0 | 3 |
| 21 | AU | 23/27 (85%) | 14 (61%) | 6 (26%) | 3 (13%) | 0 | 5 |
| 21 | CU | 23/27 (85%) | 14 (61%) | 5 (22%) | 4 (17%) | 0 | 2 |
| 24 | AY | 663/691 (96%) | 435 (66%) | 137 (21%) | 91 (14%) | 0 | 4 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|-----------|----------|-------------|----|
| 24 | CY | 663/691 (96%) | 449 (68%) | 134 (20%) | 80 (12%) | 0 | 5 |
| 25 | B0 | 82/85 (96%) | 64 (78%) | 14 (17%) | 4 (5%) | 2 | 21 |
| 25 | D0 | 82/85 (96%) | 64 (78%) | 14 (17%) | 4 (5%) | 2 | 21 |
| 26 | B1 | 92/98 (94%) | 64 (70%) | 15 (16%) | 13 (14%) | 0 | 4 |
| 26 | D1 | 92/98 (94%) | 67 (73%) | 13 (14%) | 12 (13%) | 0 | 5 |
| 27 | B2 | 69/72 (96%) | 35 (51%) | 18 (26%) | 16 (23%) | 0 | 0 |
| 27 | D2 | 69/72 (96%) | 29 (42%) | 31 (45%) | 9 (13%) | 0 | 5 |
| 28 | B3 | 58/60 (97%) | 41 (71%) | 12 (21%) | 5 (9%) | 1 | 10 |
| 28 | D3 | 58/60 (97%) | 41 (71%) | 12 (21%) | 5 (9%) | 1 | 10 |
| 29 | B4 | 56/71 (79%) | 27 (48%) | 14 (25%) | 15 (27%) | 0 | 0 |
| 29 | D4 | 56/71 (79%) | 28 (50%) | 13 (23%) | 15 (27%) | 0 | 0 |
| 30 | B5 | 57/60 (95%) | 37 (65%) | 9 (16%) | 11 (19%) | 0 | 2 |
| 30 | D5 | 57/60 (95%) | 38 (67%) | 7 (12%) | 12 (21%) | 0 | 1 |
| 31 | B6 | 48/54 (89%) | 21 (44%) | 12 (25%) | 15 (31%) | 0 | 0 |
| 31 | D6 | 48/54 (89%) | 22 (46%) | 12 (25%) | 14 (29%) | 0 | 0 |
| 32 | B7 | 47/49 (96%) | 35 (74%) | 11 (23%) | 1 (2%) | 7 | 40 |
| 32 | D7 | 47/49 (96%) | 35 (74%) | 11 (23%) | 1 (2%) | 7 | 40 |
| 33 | B8 | 62/65 (95%) | 34 (55%) | 16 (26%) | 12 (19%) | 0 | 2 |
| 33 | D8 | 62/65 (95%) | 34 (55%) | 16 (26%) | 12 (19%) | 0 | 2 |
| 34 | B9 | 35/37 (95%) | 21 (60%) | 9 (26%) | 5 (14%) | 0 | 4 |
| 34 | D9 | 35/37 (95%) | 21 (60%) | 8 (23%) | 6 (17%) | 0 | 2 |
| 37 | BC | 226/229 (99%) | 163 (72%) | 51 (23%) | 12 (5%) | 2 | 19 |
| 37 | DC | 226/229 (99%) | 163 (72%) | 50 (22%) | 13 (6%) | 1 | 18 |
| 38 | BD | 273/276 (99%) | 189 (69%) | 50 (18%) | 34 (12%) | 0 | 5 |
| 38 | DD | 273/276 (99%) | 188 (69%) | 50 (18%) | 35 (13%) | 0 | 5 |
| 39 | BE | 203/206 (98%) | 122 (60%) | 45 (22%) | 36 (18%) | 0 | 2 |
| 39 | DE | 203/206 (98%) | 124 (61%) | 44 (22%) | 35 (17%) | 0 | 2 |
| 40 | BF | 206/210 (98%) | 132 (64%) | 44 (21%) | 30 (15%) | 0 | 3 |
| 40 | DF | 206/210 (98%) | 133 (65%) | 42 (20%) | 31 (15%) | 0 | 3 |
| 41 | BG | 177/182 (97%) | 110 (62%) | 43 (24%) | 24 (14%) | 0 | 4 |
| 41 | DG | 177/182 (97%) | 115 (65%) | 36 (20%) | 26 (15%) | 0 | 3 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 42 | BH | 165/180 (92%) | 86 (52%) | 40 (24%) | 39 (24%) | 0 | 0 |
| 42 | DH | 165/180 (92%) | 86 (52%) | 40 (24%) | 39 (24%) | 0 | 0 |
| 44 | BK | 138/147 (94%) | 92 (67%) | 35 (25%) | 11 (8%) | 1 | 11 |
| 44 | DK | 138/147 (94%) | 92 (67%) | 35 (25%) | 11 (8%) | 1 | 11 |
| 46 | BN | 137/140 (98%) | 88 (64%) | 28 (20%) | 21 (15%) | 0 | 3 |
| 46 | DN | 137/140 (98%) | 88 (64%) | 28 (20%) | 21 (15%) | 0 | 3 |
| 47 | BO | 120/122 (98%) | 91 (76%) | 19 (16%) | 10 (8%) | 1 | 10 |
| 47 | DO | 120/122 (98%) | 93 (78%) | 17 (14%) | 10 (8%) | 1 | 10 |
| 48 | BP | 144/150 (96%) | 72 (50%) | 45 (31%) | 27 (19%) | 0 | 2 |
| 48 | DP | 144/150 (96%) | 72 (50%) | 44 (31%) | 28 (19%) | 0 | 2 |
| 49 | BQ | 139/141 (99%) | 106 (76%) | 26 (19%) | 7 (5%) | 2 | 21 |
| 49 | DQ | 139/141 (99%) | 106 (76%) | 26 (19%) | 7 (5%) | 2 | 21 |
| 50 | BR | 115/118 (98%) | 81 (70%) | 20 (17%) | 14 (12%) | 0 | 5 |
| 50 | DR | 115/118 (98%) | 81 (70%) | 20 (17%) | 14 (12%) | 0 | 5 |
| 51 | BS | 97/112 (87%) | 41 (42%) | 35 (36%) | 21 (22%) | 0 | 1 |
| 51 | DS | 97/112 (87%) | 41 (42%) | 35 (36%) | 21 (22%) | 0 | 1 |
| 52 | BT | 136/146 (93%) | 76 (56%) | 32 (24%) | 28 (21%) | 0 | 1 |
| 52 | DT | 136/146 (93%) | 75 (55%) | 32 (24%) | 29 (21%) | 0 | 1 |
| 53 | BU | 115/118 (98%) | 66 (57%) | 37 (32%) | 12 (10%) | 0 | 7 |
| 53 | DU | 115/118 (98%) | 67 (58%) | 35 (30%) | 13 (11%) | 0 | 6 |
| 54 | BV | 99/101 (98%) | 69 (70%) | 12 (12%) | 18 (18%) | 0 | 2 |
| 54 | DV | 99/101 (98%) | 69 (70%) | 12 (12%) | 18 (18%) | 0 | 2 |
| 55 | BW | 111/113 (98%) | 80 (72%) | 21 (19%) | 10 (9%) | 1 | 9 |
| 55 | DW | 111/113 (98%) | 81 (73%) | 21 (19%) | 9 (8%) | 1 | 11 |
| 56 | BX | 91/96 (95%) | 56 (62%) | 26 (29%) | 9 (10%) | 0 | 8 |
| 56 | DX | 91/96 (95%) | 57 (63%) | 25 (28%) | 9 (10%) | 0 | 8 |
| 57 | BY | 105/110 (96%) | 42 (40%) | 36 (34%) | 27 (26%) | 0 | 0 |
| 57 | DY | 105/110 (96%) | 43 (41%) | 36 (34%) | 26 (25%) | 0 | 0 |
| 58 | BZ | 183/206 (89%) | 108 (59%) | 42 (23%) | 33 (18%) | 0 | 2 |
| 58 | DZ | 183/206 (89%) | 114 (62%) | 37 (20%) | 32 (18%) | 0 | 2 |
| All | All | 13200/13966 (94%) | 8607 (65%) | 2874 (22%) | 1719 (13%) | 0 | 5 |

5 of 1719 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 12 | GLU |
| 2 | AB | 13 | ALA |
| 2 | AB | 15 | VAL |
| 2 | AB | 20 | GLU |
| 2 | AB | 95 | GLN |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|----------------|-----------|----------|-------------|
| 2 | AB | 202/220 (92%) | 179 (89%) | 23 (11%) | 5 29 |
| 2 | CB | 202/220 (92%) | 179 (89%) | 23 (11%) | 5 29 |
| 3 | AC | 160/188 (85%) | 142 (89%) | 18 (11%) | 6 30 |
| 3 | CC | 160/188 (85%) | 142 (89%) | 18 (11%) | 6 30 |
| 4 | AD | 180/181 (99%) | 160 (89%) | 20 (11%) | 6 31 |
| 4 | CD | 180/181 (99%) | 160 (89%) | 20 (11%) | 6 31 |
| 5 | AE | 115/123 (94%) | 100 (87%) | 15 (13%) | 4 24 |
| 5 | CE | 115/123 (94%) | 100 (87%) | 15 (13%) | 4 24 |
| 6 | AF | 90/90 (100%) | 83 (92%) | 7 (8%) | 12 44 |
| 6 | CF | 90/90 (100%) | 83 (92%) | 7 (8%) | 12 44 |
| 7 | AG | 126/127 (99%) | 117 (93%) | 9 (7%) | 14 48 |
| 7 | CG | 126/127 (99%) | 117 (93%) | 9 (7%) | 14 48 |
| 8 | AH | 119/119 (100%) | 110 (92%) | 9 (8%) | 13 45 |
| 8 | CH | 119/119 (100%) | 112 (94%) | 7 (6%) | 19 55 |
| 9 | AI | 98/99 (99%) | 90 (92%) | 8 (8%) | 11 42 |
| 9 | CI | 98/99 (99%) | 90 (92%) | 8 (8%) | 11 42 |
| 10 | AJ | 88/92 (96%) | 77 (88%) | 11 (12%) | 4 25 |
| 10 | CJ | 88/92 (96%) | 77 (88%) | 11 (12%) | 4 25 |
| 11 | AK | 90/99 (91%) | 84 (93%) | 6 (7%) | 16 50 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 11 | CK | 90/99 (91%) | 84 (93%) | 6 (7%) | 16 | 50 |
| 12 | AL | 104/109 (95%) | 94 (90%) | 10 (10%) | 8 | 37 |
| 12 | CL | 104/109 (95%) | 93 (89%) | 11 (11%) | 6 | 32 |
| 13 | AM | 99/101 (98%) | 91 (92%) | 8 (8%) | 11 | 43 |
| 13 | CM | 99/101 (98%) | 91 (92%) | 8 (8%) | 11 | 43 |
| 14 | AN | 49/50 (98%) | 43 (88%) | 6 (12%) | 5 | 26 |
| 14 | CN | 49/50 (98%) | 43 (88%) | 6 (12%) | 5 | 26 |
| 15 | AO | 79/80 (99%) | 71 (90%) | 8 (10%) | 7 | 34 |
| 15 | CO | 79/80 (99%) | 71 (90%) | 8 (10%) | 7 | 34 |
| 16 | AP | 72/74 (97%) | 67 (93%) | 5 (7%) | 15 | 49 |
| 16 | CP | 72/74 (97%) | 67 (93%) | 5 (7%) | 15 | 49 |
| 17 | AQ | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 46 |
| 17 | CQ | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 46 |
| 18 | AR | 61/77 (79%) | 59 (97%) | 2 (3%) | 38 | 69 |
| 18 | CR | 61/77 (79%) | 59 (97%) | 2 (3%) | 38 | 69 |
| 19 | AS | 69/80 (86%) | 59 (86%) | 10 (14%) | 3 | 20 |
| 19 | CS | 69/80 (86%) | 59 (86%) | 10 (14%) | 3 | 20 |
| 20 | AT | 76/82 (93%) | 69 (91%) | 7 (9%) | 9 | 39 |
| 20 | CT | 76/82 (93%) | 69 (91%) | 7 (9%) | 9 | 39 |
| 21 | AU | 19/22 (86%) | 19 (100%) | 0 | 100 | 100 |
| 21 | CU | 19/22 (86%) | 19 (100%) | 0 | 100 | 100 |
| 24 | AY | 563/582 (97%) | 489 (87%) | 74 (13%) | 4 | 23 |
| 24 | CY | 563/582 (97%) | 495 (88%) | 68 (12%) | 5 | 26 |
| 25 | B0 | 66/67 (98%) | 57 (86%) | 9 (14%) | 3 | 22 |
| 25 | D0 | 66/67 (98%) | 57 (86%) | 9 (14%) | 3 | 22 |
| 26 | B1 | 78/83 (94%) | 65 (83%) | 13 (17%) | 2 | 14 |
| 26 | D1 | 78/83 (94%) | 70 (90%) | 8 (10%) | 7 | 34 |
| 27 | B2 | 66/67 (98%) | 59 (89%) | 7 (11%) | 6 | 32 |
| 27 | D2 | 66/67 (98%) | 58 (88%) | 8 (12%) | 5 | 26 |
| 28 | B3 | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 44 |
| 28 | D3 | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 44 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 29 | B4 | 51/63 (81%) | 38 (74%) | 13 (26%) | 0 | 4 |
| 29 | D4 | 51/63 (81%) | 37 (72%) | 14 (28%) | 0 | 3 |
| 30 | B5 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 28 |
| 30 | D5 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 28 |
| 31 | B6 | 49/52 (94%) | 39 (80%) | 10 (20%) | 1 | 8 |
| 31 | D6 | 49/52 (94%) | 38 (78%) | 11 (22%) | 1 | 6 |
| 32 | B7 | 41/42 (98%) | 36 (88%) | 5 (12%) | 5 | 26 |
| 32 | D7 | 41/42 (98%) | 36 (88%) | 5 (12%) | 5 | 26 |
| 33 | B8 | 53/55 (96%) | 44 (83%) | 9 (17%) | 2 | 14 |
| 33 | D8 | 53/55 (96%) | 43 (81%) | 10 (19%) | 1 | 9 |
| 34 | B9 | 34/34 (100%) | 30 (88%) | 4 (12%) | 5 | 28 |
| 34 | D9 | 34/34 (100%) | 29 (85%) | 5 (15%) | 3 | 20 |
| 37 | BC | 180/181 (99%) | 170 (94%) | 10 (6%) | 21 | 56 |
| 37 | DC | 180/181 (99%) | 169 (94%) | 11 (6%) | 18 | 53 |
| 38 | BD | 217/218 (100%) | 177 (82%) | 40 (18%) | 1 | 10 |
| 38 | DD | 217/218 (100%) | 178 (82%) | 39 (18%) | 1 | 11 |
| 39 | BE | 165/166 (99%) | 139 (84%) | 26 (16%) | 2 | 17 |
| 39 | DE | 165/166 (99%) | 140 (85%) | 25 (15%) | 3 | 19 |
| 40 | BF | 165/166 (99%) | 153 (93%) | 12 (7%) | 14 | 46 |
| 40 | DF | 165/166 (99%) | 153 (93%) | 12 (7%) | 14 | 46 |
| 41 | BG | 155/156 (99%) | 131 (84%) | 24 (16%) | 2 | 18 |
| 41 | DG | 155/156 (99%) | 126 (81%) | 29 (19%) | 1 | 10 |
| 42 | BH | 136/148 (92%) | 126 (93%) | 10 (7%) | 13 | 46 |
| 42 | DH | 136/148 (92%) | 126 (93%) | 10 (7%) | 13 | 46 |
| 44 | BK | 104/111 (94%) | 89 (86%) | 15 (14%) | 3 | 20 |
| 44 | DK | 104/111 (94%) | 90 (86%) | 14 (14%) | 4 | 23 |
| 46 | BN | 117/119 (98%) | 103 (88%) | 14 (12%) | 5 | 27 |
| 46 | DN | 117/119 (98%) | 102 (87%) | 15 (13%) | 4 | 24 |
| 47 | BO | 100/100 (100%) | 92 (92%) | 8 (8%) | 12 | 43 |
| 47 | DO | 100/100 (100%) | 92 (92%) | 8 (8%) | 12 | 43 |
| 48 | BP | 112/116 (97%) | 91 (81%) | 21 (19%) | 1 | 9 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|-------------|----|
| 48 | DP | 112/116 (97%) | 91 (81%) | 21 (19%) | 1 | 9 |
| 49 | BQ | 111/111 (100%) | 95 (86%) | 16 (14%) | 3 | 20 |
| 49 | DQ | 111/111 (100%) | 97 (87%) | 14 (13%) | 4 | 24 |
| 50 | BR | 100/101 (99%) | 89 (89%) | 11 (11%) | 6 | 31 |
| 50 | DR | 100/101 (99%) | 88 (88%) | 12 (12%) | 5 | 27 |
| 51 | BS | 77/88 (88%) | 68 (88%) | 9 (12%) | 5 | 29 |
| 51 | DS | 77/88 (88%) | 68 (88%) | 9 (12%) | 5 | 29 |
| 52 | BT | 120/127 (94%) | 97 (81%) | 23 (19%) | 1 | 9 |
| 52 | DT | 120/127 (94%) | 97 (81%) | 23 (19%) | 1 | 9 |
| 53 | BU | 92/94 (98%) | 83 (90%) | 9 (10%) | 8 | 36 |
| 53 | DU | 92/94 (98%) | 83 (90%) | 9 (10%) | 8 | 36 |
| 54 | BV | 82/82 (100%) | 71 (87%) | 11 (13%) | 4 | 23 |
| 54 | DV | 82/82 (100%) | 71 (87%) | 11 (13%) | 4 | 23 |
| 55 | BW | 91/92 (99%) | 84 (92%) | 7 (8%) | 13 | 45 |
| 55 | DW | 91/92 (99%) | 84 (92%) | 7 (8%) | 13 | 45 |
| 56 | BX | 74/78 (95%) | 64 (86%) | 10 (14%) | 4 | 23 |
| 56 | DX | 74/78 (95%) | 64 (86%) | 10 (14%) | 4 | 23 |
| 57 | BY | 87/91 (96%) | 75 (86%) | 12 (14%) | 3 | 22 |
| 57 | DY | 87/91 (96%) | 75 (86%) | 12 (14%) | 3 | 22 |
| 58 | BZ | 162/179 (90%) | 134 (83%) | 28 (17%) | 2 | 12 |
| 58 | DZ | 162/179 (90%) | 144 (89%) | 18 (11%) | 6 | 31 |
| All | All | 11080/11566 (96%) | 9776 (88%) | 1304 (12%) | 5 | 28 |

5 of 1304 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | D1 | 45 | ASN |
| 46 | DN | 78 | TYR |
| 29 | D4 | 42 | PHE |
| 26 | D1 | 39 | LYS |
| 38 | DD | 260 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 348 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CT | 45 | GLN |
| 39 | DE | 143 | ASN |
| 24 | CY | 343 | ASN |
| 31 | D6 | 20 | ASN |
| 42 | DH | 147 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1503/1522 (98%) | 270 (17%) | 43 (2%) |
| 1 | CA | 1503/1522 (98%) | 266 (17%) | 43 (2%) |
| 22 | AV | 76/77 (98%) | 15 (19%) | 0 |
| 22 | AW | 76/77 (98%) | 25 (32%) | 1 (1%) |
| 22 | CV | 76/77 (98%) | 14 (18%) | 0 |
| 22 | CW | 76/77 (98%) | 19 (25%) | 1 (1%) |
| 23 | AX | 11/25 (44%) | 4 (36%) | 1 (9%) |
| 23 | CX | 11/25 (44%) | 4 (36%) | 1 (9%) |
| 35 | BA | 2900/2915 (99%) | 597 (20%) | 71 (2%) |
| 35 | DA | 2900/2915 (99%) | 594 (20%) | 71 (2%) |
| 36 | BB | 118/122 (96%) | 25 (21%) | 0 |
| 36 | DB | 118/122 (96%) | 25 (21%) | 0 |
| All | All | 9368/9476 (98%) | 1858 (19%) | 232 (2%) |

5 of 1858 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 9 | G |
| 1 | AA | 31 | G |
| 1 | AA | 32 | A |
| 1 | AA | 33 | A |
| 1 | AA | 39 | G |

5 of 232 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | BA | 2891 | G |
| 35 | DA | 2689 | U |
| 1 | CA | 992 | U |
| 35 | DA | 2481 | G |
| 35 | DA | 1819 | A |

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | 5MU | AV | 54 | 22 | 18,21,23 | 0.40 | 0 | 26,30,35 | 0.49 | 0 |
| 22 | 5MU | AW | 55 | 22 | 18,21,23 | 0.28 | 0 | 26,30,35 | 0.49 | 0 |
| 22 | 5MU | CW | 55 | 22 | 18,21,23 | 0.30 | 0 | 26,30,35 | 0.50 | 0 |
| 22 | 5MU | CV | 54 | 22 | 18,21,23 | 0.29 | 0 | 26,30,35 | 0.47 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 22 | 5MU | AV | 54 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | AW | 55 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | CW | 55 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | CV | 54 | 22 | - | 0/7/25/26 | 0/2/2/2 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 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 |
| 62 | GDP | AY | 703 | 60 | 24,30,30 | 1.29 | 2 (8%) | 30,47,47 | 1.57 | 6 (20%) |
| 61 | FUA | CY | 702 | - | 39,40,40 | 1.67 | 7 (17%) | 49,64,64 | 1.44 | 9 (18%) |
| 62 | GDP | CY | 703 | 60 | 24,30,30 | 1.30 | 2 (8%) | 30,47,47 | 1.69 | 6 (20%) |
| 61 | FUA | AY | 702 | - | 39,40,40 | 1.68 | 7 (17%) | 49,64,64 | 1.51 | 5 (10%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 62 | GDP | AY | 703 | 60 | - | 3/12/32/32 | 0/3/3/3 |
| 61 | FUA | CY | 702 | - | - | 9/15/92/92 | 0/4/4/4 |
| 62 | GDP | CY | 703 | 60 | - | 3/12/32/32 | 0/3/3/3 |
| 61 | FUA | AY | 702 | - | - | 6/15/92/92 | 0/4/4/4 |

The worst 5 of 18 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 61 | CY | 702 | FUA | C23-C22 | -4.50 | 1.39 | 1.51 |
| 61 | AY | 702 | FUA | C23-C22 | -4.38 | 1.39 | 1.51 |
| 61 | AY | 702 | FUA | C23-C24 | -4.27 | 1.39 | 1.53 |
| 61 | CY | 702 | FUA | C23-C24 | -4.26 | 1.39 | 1.53 |
| 61 | AY | 702 | FUA | C29-C22 | 4.19 | 1.53 | 1.47 |

The worst 5 of 26 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 61 | AY | 702 | FUA | C13-C12-C11 | -4.33 | 105.84 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 62 | CY | 703 | GDP | PA-O3A-PB | -4.29 | 118.11 | 132.83 |
| 61 | CY | 702 | FUA | C16-O2-C31 | -4.20 | 110.67 | 117.06 |
| 62 | AY | 703 | GDP | PA-O3A-PB | -3.92 | 119.36 | 132.83 |
| 61 | AY | 702 | FUA | C16-O2-C31 | -3.91 | 111.12 | 117.06 |

There are no chirality outliers.

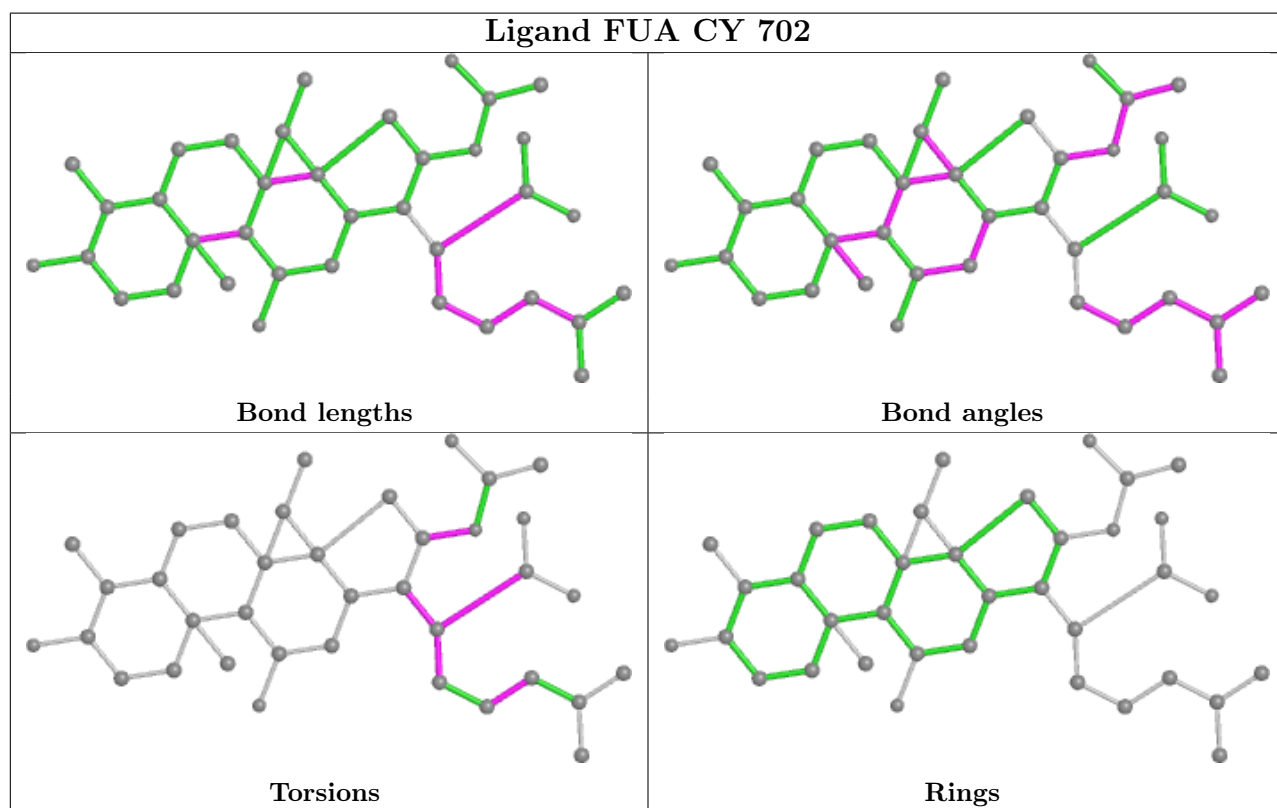
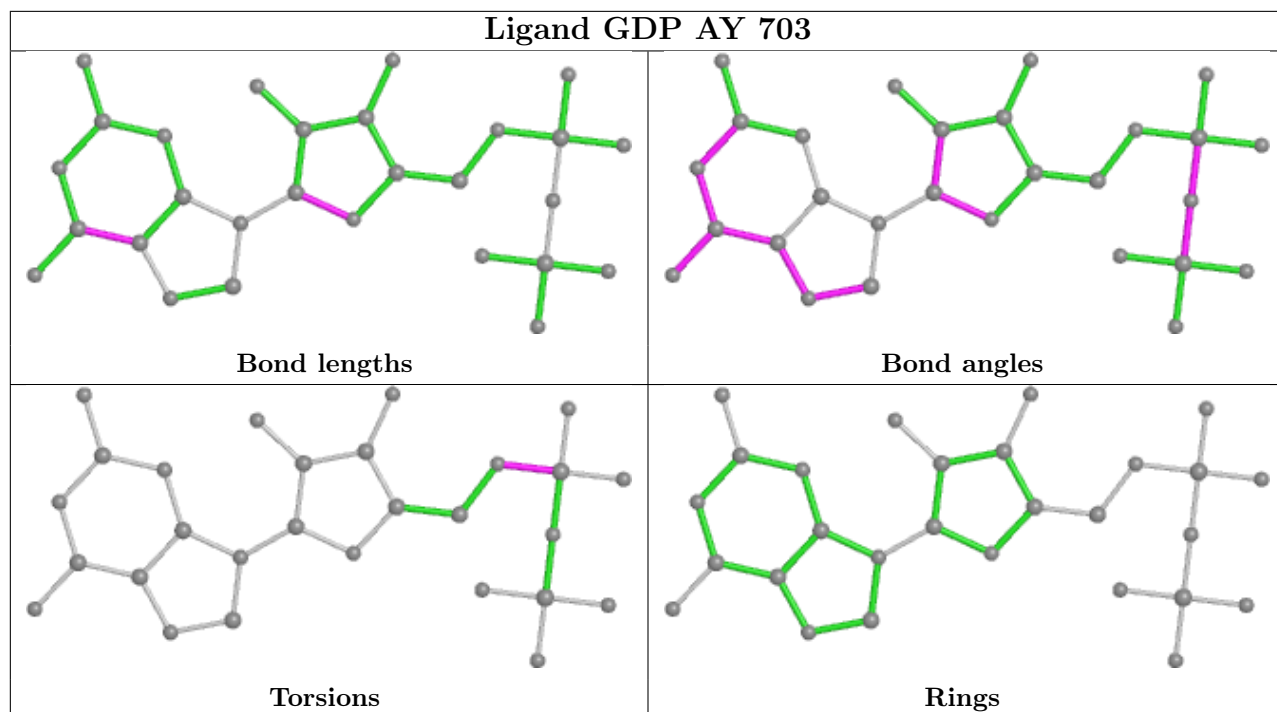
5 of 21 torsion outliers are listed below:

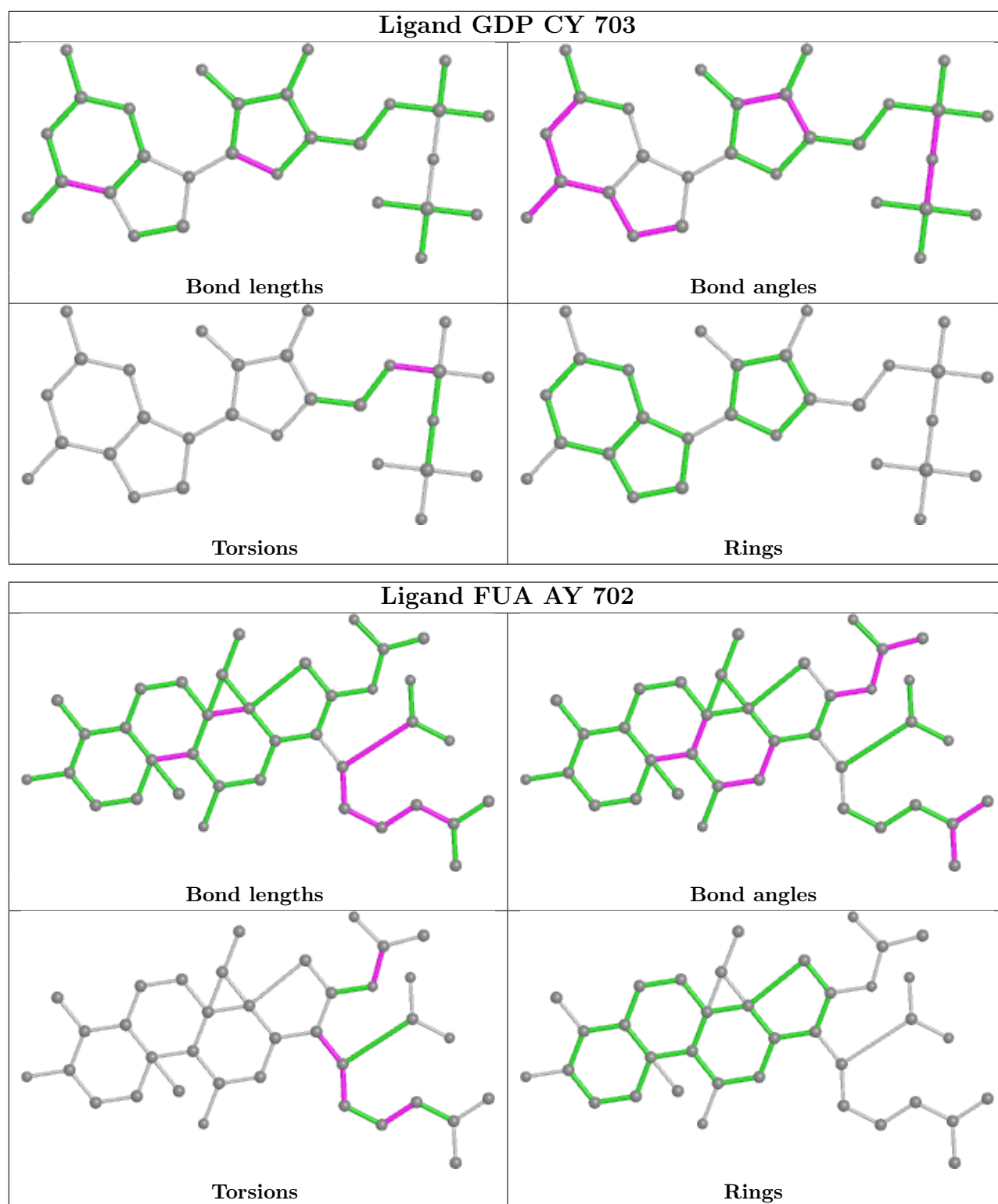
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 61 | AY | 702 | FUA | C13-C17-C22-C29 |
| 61 | AY | 702 | FUA | C17-C22-C23-C24 |
| 61 | AY | 702 | FUA | C29-C22-C23-C24 |
| 61 | CY | 702 | FUA | C13-C17-C22-C29 |
| 61 | CY | 702 | FUA | C17-C22-C23-C24 |

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 9 | CI | 2 |
| 9 | AI | 2 |
| 45 | DL | 1 |
| 45 | BL | 1 |
| 41 | BG | 1 |
| 41 | DG | 1 |

The worst 5 of 8 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | DL | 30:UNK | C | 52:UNK | N | 38.40 |
| 1 | BL | 30:UNK | C | 52:UNK | N | 36.36 |
| 1 | BG | 112:PRO | C | 113:ARG | N | 3.27 |
| 1 | DG | 112:PRO | C | 113:ARG | N | 3.05 |
| 1 | CI | 53:VAL | C | 54:ASP | N | 2.98 |

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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 | 1504/1522 (98%) | -0.27 | 22 (1%) 73 60 | 23, 62, 148, 220 | 0 |
| 1 | CA | 1504/1522 (98%) | -0.51 | 15 (0%) 82 70 | 26, 65, 148, 220 | 0 |
| 2 | AB | 235/256 (91%) | -0.30 | 3 (1%) 77 63 | 40, 81, 147, 159 | 0 |
| 2 | CB | 235/256 (91%) | -0.32 | 1 (0%) 92 86 | 43, 82, 147, 158 | 0 |
| 3 | AC | 207/239 (86%) | -0.41 | 0 100 100 | 31, 72, 113, 118 | 0 |
| 3 | CC | 207/239 (86%) | -0.38 | 0 100 100 | 33, 75, 115, 121 | 0 |
| 4 | AD | 208/209 (99%) | -0.39 | 0 100 100 | 46, 79, 115, 124 | 0 |
| 4 | CD | 208/209 (99%) | -0.43 | 0 100 100 | 48, 80, 116, 125 | 0 |
| 5 | AE | 151/162 (93%) | -0.49 | 1 (0%) 87 78 | 25, 50, 90, 112 | 0 |
| 5 | CE | 151/162 (93%) | -0.46 | 1 (0%) 87 78 | 27, 52, 91, 112 | 0 |
| 6 | AF | 101/101 (100%) | -0.44 | 0 100 100 | 55, 85, 110, 118 | 0 |
| 6 | CF | 101/101 (100%) | -0.29 | 0 100 100 | 60, 87, 111, 118 | 0 |
| 7 | AG | 155/156 (99%) | -0.38 | 1 (0%) 89 81 | 51, 79, 109, 136 | 0 |
| 7 | CG | 155/156 (99%) | -0.39 | 2 (1%) 77 63 | 55, 81, 111, 136 | 0 |
| 8 | AH | 138/138 (100%) | -0.41 | 0 100 100 | 32, 54, 75, 82 | 0 |
| 8 | CH | 138/138 (100%) | -0.49 | 0 100 100 | 35, 56, 76, 83 | 0 |
| 9 | AI | 127/128 (99%) | -0.23 | 1 (0%) 86 75 | 50, 83, 114, 120 | 0 |
| 9 | CI | 127/128 (99%) | -0.36 | 1 (0%) 86 75 | 53, 86, 114, 120 | 0 |
| 10 | AJ | 99/105 (94%) | 0.08 | 6 (6%) 21 12 | 47, 100, 155, 159 | 0 |
| 10 | CJ | 99/105 (94%) | 0.18 | 3 (3%) 50 34 | 50, 102, 156, 159 | 0 |
| 11 | AK | 119/129 (92%) | -0.34 | 2 (1%) 70 55 | 42, 59, 100, 123 | 0 |
| 11 | CK | 119/129 (92%) | -0.28 | 1 (0%) 86 75 | 44, 60, 102, 124 | 0 |
| 12 | AL | 125/132 (94%) | -0.49 | 0 100 100 | 38, 57, 87, 127 | 0 |
| 12 | CL | 125/132 (94%) | -0.43 | 2 (1%) 72 57 | 39, 58, 88, 129 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 13 | AM | 125/126 (99%) | -0.15 | 6 (4%) 30 19 | 68, 111, 139, 171 | 0 |
| 13 | CM | 125/126 (99%) | -0.16 | 8 (6%) 19 11 | 70, 112, 139, 172 | 0 |
| 14 | AN | 60/61 (98%) | -0.41 | 1 (1%) 70 55 | 39, 59, 92, 97 | 0 |
| 14 | CN | 60/61 (98%) | -0.42 | 0 100 100 | 44, 61, 93, 98 | 0 |
| 15 | AO | 88/89 (98%) | -0.57 | 0 100 100 | 35, 61, 91, 100 | 0 |
| 15 | CO | 88/89 (98%) | -0.54 | 0 100 100 | 38, 61, 94, 100 | 0 |
| 16 | AP | 84/88 (95%) | -0.45 | 0 100 100 | 54, 73, 96, 131 | 0 |
| 16 | CP | 84/88 (95%) | -0.43 | 1 (1%) 79 66 | 57, 74, 98, 132 | 0 |
| 17 | AQ | 100/105 (95%) | -0.56 | 0 100 100 | 43, 64, 89, 98 | 0 |
| 17 | CQ | 100/105 (95%) | -0.50 | 0 100 100 | 46, 66, 90, 97 | 0 |
| 18 | AR | 70/88 (79%) | -0.42 | 1 (1%) 75 61 | 42, 69, 94, 108 | 0 |
| 18 | CR | 70/88 (79%) | -0.51 | 1 (1%) 75 61 | 45, 70, 95, 109 | 0 |
| 19 | AS | 79/93 (84%) | -0.02 | 2 (2%) 57 41 | 77, 106, 144, 149 | 0 |
| 19 | CS | 79/93 (84%) | 0.15 | 4 (5%) 28 17 | 78, 107, 144, 150 | 0 |
| 20 | AT | 99/106 (93%) | -0.37 | 0 100 100 | 63, 84, 126, 129 | 0 |
| 20 | CT | 99/106 (93%) | -0.37 | 0 100 100 | 64, 85, 127, 129 | 0 |
| 21 | AU | 25/27 (92%) | -0.24 | 0 100 100 | 63, 82, 118, 122 | 0 |
| 21 | CU | 25/27 (92%) | 0.12 | 0 100 100 | 66, 86, 120, 123 | 0 |
| 22 | AV | 76/77 (98%) | -0.48 | 0 100 100 | 32, 67, 110, 127 | 0 |
| 22 | AW | 76/77 (98%) | -0.43 | 1 (1%) 77 63 | 71, 168, 192, 201 | 0 |
| 22 | CV | 76/77 (98%) | -0.61 | 0 100 100 | 47, 84, 121, 151 | 0 |
| 22 | CW | 76/77 (98%) | -0.37 | 1 (1%) 77 63 | 78, 176, 200, 210 | 0 |
| 23 | AX | 11/25 (44%) | 0.09 | 0 100 100 | 28, 94, 149, 166 | 0 |
| 23 | CX | 11/25 (44%) | 0.01 | 0 100 100 | 45, 106, 156, 168 | 0 |
| 24 | AY | 667/691 (96%) | -0.17 | 9 (1%) 77 63 | 61, 99, 140, 150 | 0 |
| 24 | CY | 667/691 (96%) | 0.08 | 23 (3%) 45 30 | 73, 108, 148, 161 | 0 |
| 25 | B0 | 84/85 (98%) | 0.05 | 6 (7%) 16 9 | 67, 82, 140, 163 | 0 |
| 25 | D0 | 84/85 (98%) | 0.37 | 9 (10%) 6 3 | 69, 84, 141, 163 | 0 |
| 26 | B1 | 94/98 (95%) | -0.46 | 1 (1%) 80 68 | 41, 70, 118, 128 | 0 |
| 26 | D1 | 94/98 (95%) | -0.34 | 0 100 100 | 53, 80, 123, 131 | 0 |
| 27 | B2 | 71/72 (98%) | -0.30 | 2 (2%) 53 37 | 77, 116, 150, 161 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 27 | D2 | 71/72 (98%) | -0.15 | 2 (2%) 53 37 | 95, 119, 146, 163 | 0 |
| 28 | B3 | 60/60 (100%) | -0.08 | 1 (1%) 70 55 | 63, 88, 114, 135 | 0 |
| 28 | D3 | 60/60 (100%) | -0.02 | 2 (3%) 46 31 | 64, 89, 114, 134 | 0 |
| 29 | B4 | 58/71 (81%) | 0.07 | 3 (5%) 27 17 | 76, 135, 220, 222 | 0 |
| 29 | D4 | 58/71 (81%) | 0.27 | 7 (12%) 4 3 | 77, 137, 220, 222 | 0 |
| 30 | B5 | 59/60 (98%) | -0.08 | 3 (5%) 28 17 | 52, 80, 153, 172 | 0 |
| 30 | D5 | 59/60 (98%) | -0.03 | 4 (6%) 17 10 | 52, 80, 153, 172 | 0 |
| 31 | B6 | 50/54 (92%) | 0.00 | 2 (4%) 38 25 | 56, 89, 107, 117 | 0 |
| 31 | D6 | 50/54 (92%) | -0.26 | 1 (2%) 65 49 | 56, 90, 108, 117 | 0 |
| 32 | B7 | 49/49 (100%) | -0.34 | 2 (4%) 37 24 | 47, 64, 119, 132 | 0 |
| 32 | D7 | 49/49 (100%) | -0.39 | 0 100 100 | 47, 64, 120, 132 | 0 |
| 33 | B8 | 64/65 (98%) | -0.37 | 1 (1%) 72 57 | 63, 75, 105, 125 | 0 |
| 33 | D8 | 64/65 (98%) | -0.26 | 1 (1%) 72 57 | 65, 76, 105, 126 | 0 |
| 34 | B9 | 37/37 (100%) | -0.43 | 0 100 100 | 60, 71, 85, 89 | 0 |
| 34 | D9 | 37/37 (100%) | -0.30 | 1 (2%) 54 38 | 60, 73, 87, 91 | 0 |
| 35 | BA | 2901/2915 (99%) | -0.39 | 27 (0%) 84 73 | 30, 76, 162, 221 | 0 |
| 35 | DA | 2901/2915 (99%) | -0.52 | 32 (1%) 80 68 | 29, 77, 162, 221 | 0 |
| 36 | BB | 119/122 (97%) | -0.54 | 0 100 100 | 65, 106, 138, 183 | 0 |
| 36 | DB | 119/122 (97%) | -0.72 | 0 100 100 | 66, 108, 138, 183 | 0 |
| 37 | BC | 228/229 (99%) | -0.13 | 4 (1%) 68 53 | 42, 97, 147, 160 | 0 |
| 37 | DC | 228/229 (99%) | 0.09 | 12 (5%) 26 16 | 43, 98, 148, 162 | 0 |
| 38 | BD | 275/276 (99%) | -0.52 | 0 100 100 | 31, 52, 82, 101 | 0 |
| 38 | DD | 275/276 (99%) | -0.51 | 1 (0%) 92 86 | 32, 52, 82, 101 | 0 |
| 39 | BE | 205/206 (99%) | -0.33 | 4 (1%) 65 49 | 44, 77, 128, 135 | 0 |
| 39 | DE | 205/206 (99%) | -0.29 | 3 (1%) 73 60 | 44, 77, 128, 134 | 0 |
| 40 | BF | 208/210 (99%) | 0.01 | 10 (4%) 30 19 | 53, 110, 166, 177 | 0 |
| 40 | DF | 208/210 (99%) | -0.01 | 11 (5%) 26 16 | 53, 111, 166, 176 | 0 |
| 41 | BG | 181/182 (99%) | -0.27 | 4 (2%) 62 45 | 63, 95, 131, 143 | 0 |
| 41 | DG | 181/182 (99%) | -0.03 | 6 (3%) 46 31 | 86, 110, 137, 151 | 0 |
| 42 | BH | 167/180 (92%) | 0.06 | 6 (3%) 42 28 | 81, 117, 143, 159 | 0 |
| 42 | DH | 167/180 (92%) | 0.04 | 4 (2%) 59 42 | 81, 118, 143, 160 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 43 | BJ | 0/173 | - | - | - | - |
| 43 | DJ | 0/173 | - | - | - | - |
| 44 | BK | 140/147 (95%) | 1.96 | 61 (43%) 0 0 | 162, 180, 186, 188 | 0 |
| 44 | DK | 140/147 (95%) | 1.68 | 49 (35%) 0 0 | 162, 180, 186, 187 | 0 |
| 45 | BL | 0/125 | - | - | - | - |
| 45 | BM | 0/125 | - | - | - | - |
| 45 | Bl | 0/125 | - | - | - | - |
| 45 | Bm | 0/125 | - | - | - | - |
| 45 | DL | 0/125 | - | - | - | - |
| 45 | DM | 0/125 | - | - | - | - |
| 45 | Dl | 0/125 | - | - | - | - |
| 45 | Dm | 0/125 | - | - | - | - |
| 46 | BN | 139/140 (99%) | -0.30 | 2 (1%) 75 61 | 60, 91, 132, 137 | 0 |
| 46 | DN | 139/140 (99%) | -0.25 | 1 (0%) 87 78 | 61, 91, 132, 137 | 0 |
| 47 | BO | 122/122 (100%) | -0.45 | 0 100 100 | 35, 60, 73, 86 | 0 |
| 47 | DO | 122/122 (100%) | -0.43 | 0 100 100 | 36, 61, 73, 88 | 0 |
| 48 | BP | 146/150 (97%) | 0.02 | 4 (2%) 54 38 | 46, 111, 137, 157 | 0 |
| 48 | DP | 146/150 (97%) | 0.10 | 4 (2%) 54 38 | 50, 113, 137, 157 | 0 |
| 49 | BQ | 141/141 (100%) | -0.38 | 0 100 100 | 45, 65, 88, 119 | 0 |
| 49 | DQ | 141/141 (100%) | -0.41 | 0 100 100 | 45, 66, 89, 120 | 0 |
| 50 | BR | 117/118 (99%) | -0.37 | 1 (0%) 84 73 | 49, 81, 101, 128 | 0 |
| 50 | DR | 117/118 (99%) | -0.28 | 1 (0%) 84 73 | 53, 82, 101, 128 | 0 |
| 51 | BS | 99/112 (88%) | -0.19 | 2 (2%) 65 49 | 82, 116, 140, 144 | 0 |
| 51 | DS | 99/112 (88%) | 0.28 | 5 (5%) 28 17 | 83, 117, 141, 145 | 0 |
| 52 | BT | 138/146 (94%) | -0.13 | 4 (2%) 51 35 | 55, 83, 149, 176 | 0 |
| 52 | DT | 138/146 (94%) | -0.18 | 5 (3%) 42 28 | 57, 84, 149, 177 | 0 |
| 53 | BU | 117/118 (99%) | -0.36 | 0 100 100 | 62, 80, 114, 135 | 0 |
| 53 | DU | 117/118 (99%) | -0.36 | 0 100 100 | 62, 81, 115, 134 | 0 |
| 54 | BV | 101/101 (100%) | -0.02 | 1 (0%) 82 70 | 59, 116, 133, 141 | 0 |
| 54 | DV | 101/101 (100%) | 0.18 | 6 (5%) 22 13 | 61, 116, 134, 140 | 0 |
| 55 | BW | 113/113 (100%) | -0.28 | 0 100 100 | 61, 79, 119, 158 | 0 |
| 55 | DW | 113/113 (100%) | -0.16 | 0 100 100 | 63, 80, 120, 159 | 0 |
| 56 | BX | 93/96 (96%) | -0.18 | 0 100 100 | 76, 91, 110, 114 | 0 |
| 56 | DX | 93/96 (96%) | -0.22 | 0 100 100 | 76, 92, 111, 114 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 57 | BY | 107/110 (97%) | 0.08 | 2 (1%) 66 51 | 78, 127, 149, 155 | 0 |
| 57 | DY | 107/110 (97%) | 0.41 | 4 (3%) 41 27 | 78, 127, 149, 155 | 0 |
| 58 | BZ | 185/206 (89%) | -0.23 | 1 (0%) 91 83 | 47, 90, 135, 143 | 0 |
| 58 | DZ | 185/206 (89%) | -0.09 | 1 (0%) 91 83 | 68, 99, 138, 146 | 0 |
| All | All | 22794/24788 (91%) | -0.29 | 446 (1%) 65 49 | 23, 82, 154, 222 | 0 |

The worst 5 of 446 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 35 | BA | 654(K) | C | 14.8 |
| 1 | CA | 1036 | G | 13.4 |
| 52 | BT | 138 | ALA | 13.1 |
| 35 | DA | 654(D) | G | 13.0 |
| 35 | BA | 654(F) | C | 11.4 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 22 | 5MU | CW | 55 | 20/22 | 0.81 | 0.13 | 178,179,186,186 | 0 |
| 22 | 5MU | AW | 55 | 20/22 | 0.82 | 0.14 | 161,165,168,168 | 0 |
| 22 | 5MU | AV | 54 | 20/22 | 0.95 | 0.13 | 82,84,86,86 | 0 |
| 22 | 5MU | CV | 54 | 20/22 | 0.97 | 0.11 | 89,92,95,96 | 0 |

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 59 | ZN | D4 | 101 | 1/1 | 0.90 | 0.07 | 164,164,164,164 | 0 |
| 61 | FUA | AY | 702 | 37/37 | 0.90 | 0.43 | 98,102,110,111 | 0 |
| 61 | FUA | CY | 702 | 37/37 | 0.90 | 0.35 | 102,104,107,109 | 0 |
| 59 | ZN | B4 | 101 | 1/1 | 0.91 | 0.12 | 122,122,122,122 | 0 |
| 62 | GDP | CY | 703 | 28/28 | 0.95 | 0.15 | 81,87,94,95 | 0 |
| 62 | GDP | AY | 703 | 28/28 | 0.96 | 0.17 | 78,82,83,84 | 0 |
| 60 | MG | AY | 701 | 1/1 | 0.98 | 0.22 | 30,30,30,30 | 0 |
| 59 | ZN | CD | 301 | 1/1 | 0.99 | 0.28 | 49,49,49,49 | 0 |
| 60 | MG | CY | 701 | 1/1 | 0.99 | 0.12 | 39,39,39,39 | 0 |
| 59 | ZN | B9 | 101 | 1/1 | 0.99 | 0.15 | 62,62,62,62 | 0 |
| 59 | ZN | AN | 101 | 1/1 | 1.00 | 0.16 | 35,35,35,35 | 0 |
| 59 | ZN | D9 | 101 | 1/1 | 1.00 | 0.12 | 86,86,86,86 | 0 |
| 59 | ZN | AD | 301 | 1/1 | 1.00 | 0.28 | 32,32,32,32 | 0 |
| 59 | ZN | CN | 101 | 1/1 | 1.00 | 0.16 | 66,66,66,66 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.