# WORLDWIDE wwPDB PROTEIN DATA BANK

# wwPDB EM Validation Summary Report (i)

Nov 10, 2024 – 07:33 am GMT

|  |  |  |
|---|---|---|
| PDB ID | : | 8RXH |
| EMDB ID | : | EMD-19576 |
| Title | : | CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME WITH A/P/E-site tRNA AND mRNA : PARENTAL STRAIN |
| Authors | : | Rajan, K.S.; Yonath, A. |
| Deposited on | : | 2024-02-07 |
| Resolution | : | 2.93 Å(reported) |

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# 1   Overall quality at a glance   ⓘ

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

The reported resolution of this entry is 2.93 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 | Percentile Ranks | Value |
|--------|------------------|-------|
| Ramachandran outliers | | 0.0% |
| Sidechain outliers | | 6.6% |
| RNA backbone | | 0.49 |

*Worse*          *Better*

█ Percentile relative to all structures

▯ Percentile relative to all EM structures
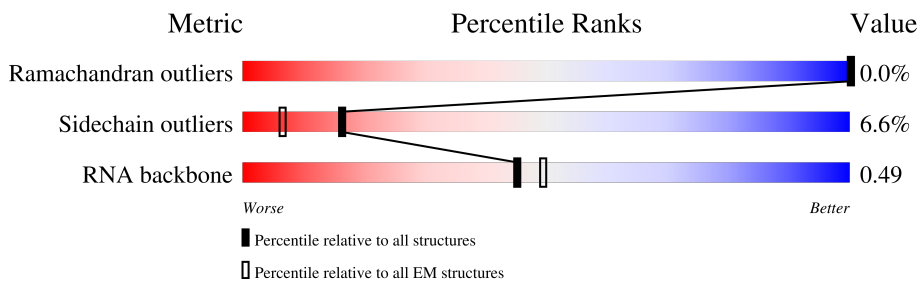
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|--------|--------------------------|--------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | L1 | 1782 | 66%   27%   6% |
| 2 | L2 | 1526 | 52%   22%   24% |
| 3 | L3 | 216 | 61%   23%   15% |
| 4 | L4 | 184 | 72%   28% |
| 5 | L5 | 135 | 5%   63%   26%   11% |
| 6 | L6 | 73 | 52%   45% |
| 7 | L7 | 171 | 65%   30% |
| 8 | L8 | 124 | 79%   18% |

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W O R L D W I D E
**wwPDB**
PROTEIN DATA BANK
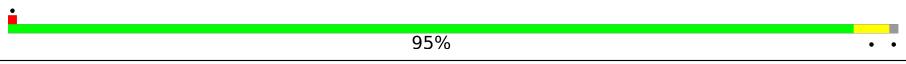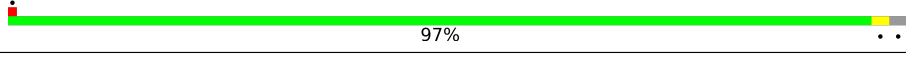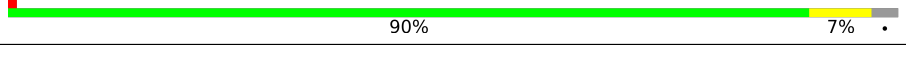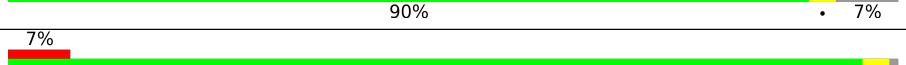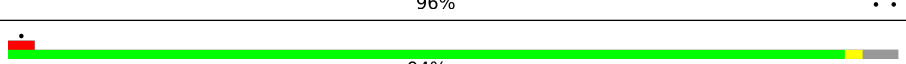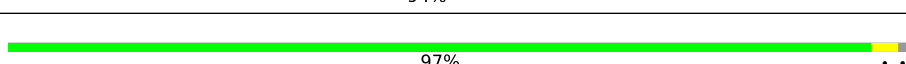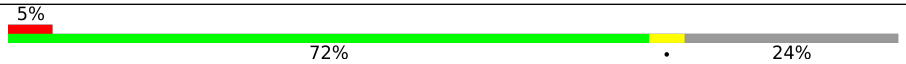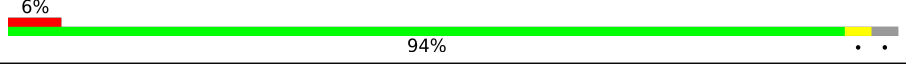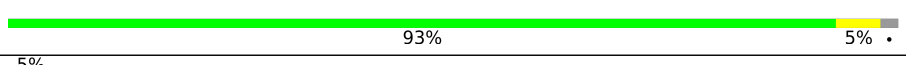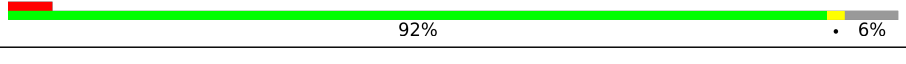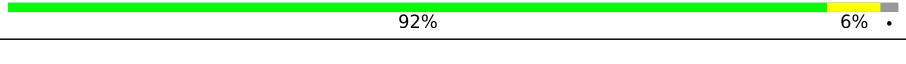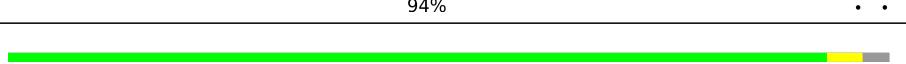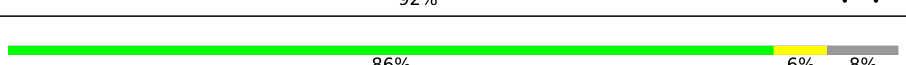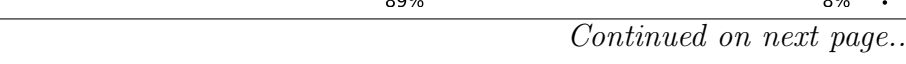
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9 | LA | 260 | 95% — 5% |
| 10 | LB | 419 | 94% |
| 11 | LC | 373 | 93% — 5% |
| 12 | LD | 188 | 5% — 87% — 6% — 7% |
| 13 | LE | 190 | 92% — 6% |
| 14 | LF | 195 | 72% — 24% |
| 15 | LG | 264 | 7% — 88% — 9% |
| 16 | LH | 222 | 95% — 5% |
| 17 | LI | 220 | 94% |
| 18 | LJ | 139 | 95% |
| 19 | LK | 175 | 6% — 92% — 5% |
| 20 | LL | 145 | 94% |
| 21 | LM | 204 | 92% — 6% |
| 22 | LN | 213 | 86% — 10% |
| 23 | LO | 305 | 8% — 94% |
| 24 | LP | 198 | 96% |
| 25 | LQ | 254 | 9% — 75% — 21% |
| 26 | LR | 179 | 95% |
| 27 | LS | 159 | 94% — 5% |
| 28 | LT | 166 | 89% — 8% |
| 29 | LU | 129 | 16% — 90% — 5% — 5% |
| 30 | LV | 145 | 80% — 18% |
| 31 | LW | 143 | 82% — 15% |
| 32 | LX | 124 | 17% — 66% — 31% |
| 33 | LY | 134 | 95% |
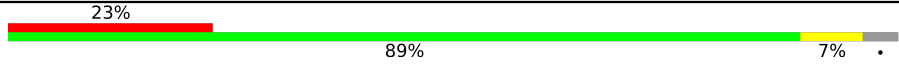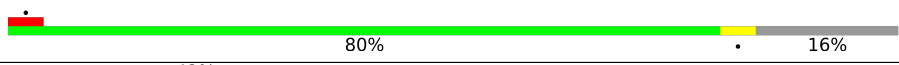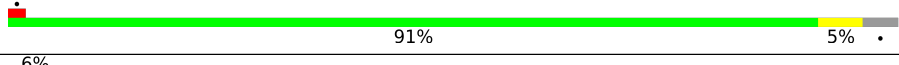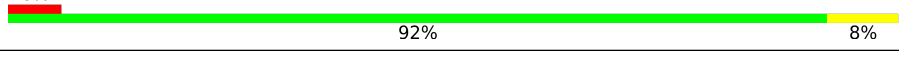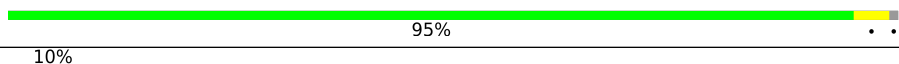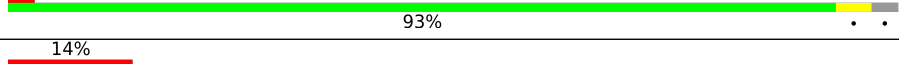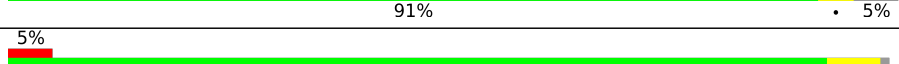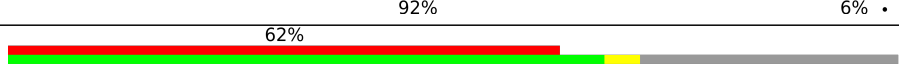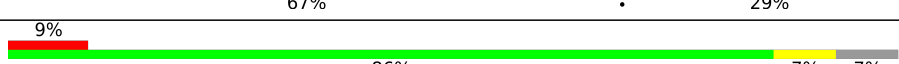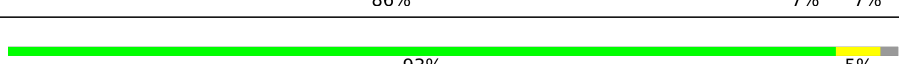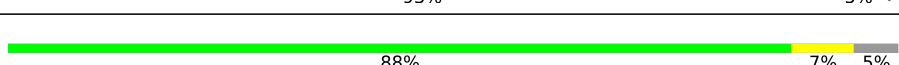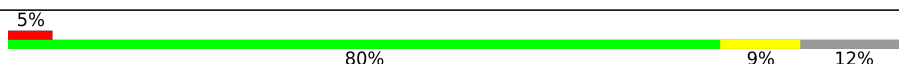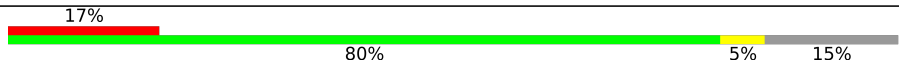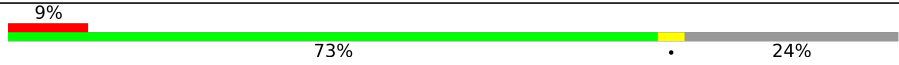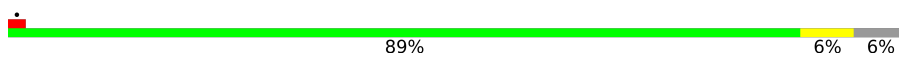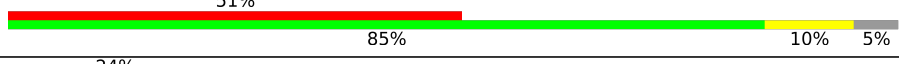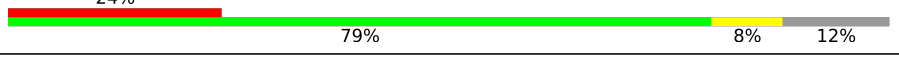
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 34 | LZ | 147 | 95% |
| 35 | La | 127 | 97% |
| 36 | Lb | 70 | 90%   7% |
| 37 | Lc | 252 | 88%   9% |
| 38 | Ld | 104 | 5%   90%   7% |
| 39 | Le | 188 | 7%   96% |
| 40 | Lf | 133 | 94% |
| 41 | Lg | 144 | 97% |
| 42 | Lh | 168 | 5%   72%   24% |
| 43 | Li | 105 | 6%   94% |
| 44 | Lj | 83 | 93%   5% |
| 45 | Lk | 83 | 5%   92%   6% |
| 46 | Ll | 51 | 92%   6% |
| 47 | Lm | 128 | 38%   59% |
| 48 | Ln | 34 | 94% |
| 49 | Lo | 92 | 92% |
| 50 | Lp | 106 | 86%   6%   8% |
| 51 | S1 | 2204 | 11%   61%   22%   16% |
| 52 | S2 | 76 | 80%   62%   38% |
| 53 | S3 | 77 | 21%   71%   25% |
| 54 | S4 | 76 | 63%   46%   51% |
| 55 | S5 | 13 | 8%   46%   46%   8% |
| 56 | SA | 264 | 5%   88%   5%   8% |
| 57 | SB | 246 | 83%   14% |
| 58 | SC | 219 | 10%   89%   8% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 59 | SD | 190 | 23% … 89% … 7% … |
| 60 | SE | 273 | 27% … 88% … 8% … 5% |
| 61 | SF | 265 | … 80% … 16% |
| 62 | SG | 249 | 42% … 80% … 12% … 8% |
| 63 | SH | 190 | … 91% … 5% … |
| 64 | SI | 200 | 6% … 92% … 8% |
| 65 | SJ | 130 | 95% … |
| 66 | SK | 220 | 10% … 80% … 7% … 13% |
| 67 | SL | 149 | … 93% … |
| 68 | SM | 116 | 14% … 80% … 7% … 13% |
| 69 | SN | 168 | 11% … 54% … 5% … 40% |
| 70 | SO | 144 | … 91% … 5% |
| 71 | SP | 143 | 5% … 92% … 6% … |
| 72 | SQ | 141 | 62% … 67% … 29% |
| 73 | SR | 153 | 9% … 86% … 7% … 7% |
| 74 | SS | 57 | 93% … 5% … |
| 75 | ST | 151 | 88% … 7% … 5% |
| 76 | SU | 173 | 5% … 80% … 9% … 12% |
| 77 | SV | 143 | 17% … 80% … 5% … 15% |
| 78 | SW | 152 | 9% … 73% … 24% |
| 79 | SX | 161 | … 89% … 6% … 6% |
| 80 | SY | 164 | … 51% … 46% |
| 81 | SZ | 137 | 51% … 85% … 10% … 5% |
| 82 | Sa | 120 | 24% … 79% … 8% … 12% |
| 83 | Sb | 112 | … 87% … 6% … 7% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 84 | Sc | 86 | 91%   8% |
| 85 | Sd | 87 | 10%   70%   6%   24% |
| 86 | Se | 66 | 26%   86%   6%   8% |
| 87 | Sf | 152 | 38%   45%   7%   47% |
| 88 | Sg | 312 | 33%   90%   7% |
| 89 | Sh | 235 | 40%   36%   5%   59% |

# 2   Entry composition  ⓘ

There are 95 unique types of molecules in this entry. The entry contains 216694 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called LSUa_rRNA_chain_1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | L1 | 1677 | 35987 | 16086 | 6578 | 11645 | 1678 | 1 | 0 |

- Molecule 2 is a RNA chain called LSUb_rRNA_chain_2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | L2 | 1155 | 24715 | 11065 | 4453 | 8042 | 1155 | 0 | 0 |

- Molecule 3 is a RNA chain called SR1_chain_3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | L3 | 183 | 3877 | 1735 | 669 | 1290 | 183 | 0 | 0 |

- Molecule 4 is a RNA chain called SR2_chain_4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | L4 | 184 | 3937 | 1756 | 712 | 1285 | 184 | 0 | 0 |

- Molecule 5 is a RNA chain called SR4_chain_5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | L5 | 120 | 2555 | 1140 | 455 | 840 | 120 | 0 | 0 |

- Molecule 6 is a RNA chain called SR6_chain_6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 6 | L6 | 71 | 1506 | 675 | 271 | 489 | 71 | 0 | 0 |

- Molecule 7 is a RNA chain called 5.8S_rRNA_chain_7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | L7 | 166 | Total 3533 | C 1583 | N 626 | O 1159 | P 165 | 0 | 0 |

- Molecule 8 is a RNA chain called 5S_rRNA_chain_8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | L8 | 120 | Total 2551 | C 1141 | N 454 | O 836 | P 120 | 0 | 0 |

- Molecule 9 is a protein called Putative 60S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | LA | 258 | Total 1962 | C 1223 | N 400 | O 329 | S 10 | 0 | 0 |

- Molecule 10 is a protein called Putative ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | LB | 404 | Total 3216 | C 2024 | N 638 | O 541 | S 13 | 0 | 0 |

- Molecule 11 is a protein called Putative ribosomal protein L1a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | LC | 366 | Total 2820 | C 1761 | N 561 | O 483 | S 15 | 0 | 0 |

- Molecule 12 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | LD | 175 | Total 1387 | C 875 | N 261 | O 243 | S 8 | 0 | 0 |

- Molecule 13 is a protein called Putative 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | LE | 186 | Total 1477 | C 936 | N 273 | O 262 | S 6 | 0 | 0 |

- Molecule 14 is a protein called Putative 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 14 | LF | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1151 | 731 | 216 | 202 | 2 | | |

- Molecule 15 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 15 | LG | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1905 | 1199 | 376 | 323 | 7 | | |

- Molecule 16 is a protein called Putative 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 16 | LH | 221 | Total | C | N | O | S | 0 | 0 |
| | | | 1767 | 1123 | 353 | 284 | 7 | | |

- Molecule 17 is a protein called Putative 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 17 | LI | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1695 | 1056 | 342 | 289 | 8 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| LI | 203 | ARG | ASN | conflict | UNP E9AEA8 |

- Molecule 18 is a protein called Putative 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 18 | LJ | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1012 | 638 | 191 | 177 | 6 | | |

- Molecule 19 is a protein called Putative 40S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 19 | LK | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1336 | 833 | 264 | 231 | 8 | | |

- Molecule 20 is a protein called Putative 60S ribosomal protein L27A/L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | LL | 144 | Total 1124 | C 707 | N 226 | O 185 | S 6 | 0 | 0 |

- Molecule 21 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | LM | 203 | Total 1711 | C 1079 | N 362 | O 262 | S 8 | 0 | 0 |

- Molecule 22 is a protein called Putative 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | LN | 205 | Total 1665 | C 1050 | N 329 | O 271 | S 15 | 0 | 0 |

- Molecule 23 is a protein called Putative 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | LO | 298 | Total 2329 | C 1480 | N 437 | O 406 | S 6 | 0 | 0 |

- Molecule 24 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | LP | 197 | Total 1539 | C 968 | N 307 | O 258 | S 6 | 0 | 0 |

- Molecule 25 is a protein called Putative 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | LQ | 201 | Total 1682 | C 1035 | N 367 | O 274 | S 6 | 0 | 0 |

- Molecule 26 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | LR | 178 | Total 1455 | C 925 | N 279 | O 246 | S 5 | 0 | 0 |

- Molecule 27 is a protein called Putative 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | LS | 158 | Total | C | N | O | S | 0 | 0 |
| | | | 1261 | 803 | 245 | 209 | 4 | | |

- Molecule 28 is a protein called Putative 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | LT | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1217 | 761 | 241 | 205 | 10 | | |

- Molecule 29 is a protein called Putative 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | LU | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 960 | 624 | 176 | 157 | 3 | | |

- Molecule 30 is a protein called Putative 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | LV | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 953 | 604 | 181 | 166 | 2 | | |

- Molecule 31 is a protein called Putative 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | LW | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 967 | 603 | 200 | 160 | 4 | | |

- Molecule 32 is a protein called Putative ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | LX | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 461 | 140 | 109 | 4 | | |

- Molecule 33 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | LY | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1067 | 684 | 215 | 165 | 3 | | |

- Molecule 34 is a protein called Putative 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 34 | LZ | 145 | Total 1117 | C 685 | N 238 | O 189 | S 5 | 0 | 0 |

- Molecule 35 is a protein called Putative 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 35 | La | 125 | Total 1043 | C 650 | N 217 | O 172 | S 4 | 0 | 0 |

- Molecule 36 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---------|-------|
| 36 | Lb | 68 | Total 546 | C 335 | N 125 | O 86 | 0 | 0 |

- Molecule 37 is a protein called Putative 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 37 | Lc | 229 | Total 1862 | C 1185 | N 358 | O 308 | S 11 | 0 | 0 |

- Molecule 38 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 38 | Ld | 97 | Total 744 | C 464 | N 136 | O 139 | S 5 | 0 | 0 |

- Molecule 39 is a protein called Putative 60S ribosomal subunit protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 39 | Le | 186 | Total 1469 | C 922 | N 296 | O 247 | S 4 | 0 | 0 |

- Molecule 40 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 40 | Lf | 128 | Total 1046 | C 658 | N 210 | O 174 | S 4 | 0 | 0 |

- Molecule 41 is a protein called Putative ribosomal protein l35a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 41 | Lg | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1149 | 714 | 240 | 190 | 5 | | |

- Molecule 42 is a protein called Putative 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 42 | Lh | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1029 | 633 | 224 | 166 | 6 | | |

- Molecule 43 is a protein called Putative 60S Ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 43 | Li | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 807 | 508 | 163 | 133 | 3 | | |

- Molecule 44 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 44 | Lj | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 672 | 409 | 154 | 103 | 6 | | |

- Molecule 45 is a protein called Putative ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 45 | Lk | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 608 | 383 | 119 | 103 | 3 | | |

- Molecule 46 is a protein called Putative 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 46 | Ll | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 450 | 291 | 95 | 63 | 1 | | |

- Molecule 47 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 47 | Lm | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 417 | 263 | 85 | 64 | 5 | | |

- Molecule 48 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | Ln | 33 | Total 296 | C 181 | N 76 | O 37 | S 2 | 0 | 0 |

- Molecule 49 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | Lo | 89 | Total 693 | C 431 | N 143 | O 113 | S 6 | 0 | 0 |

- Molecule 50 is a protein called Putative 60S ribosomal protein L44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | Lp | 97 | Total 784 | C 496 | N 158 | O 125 | S 5 | 0 | 0 |

- Molecule 51 is a RNA chain called SSU_rRNA_chain_S1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | S1 | 1844 | Total 39438 | C 17643 | N 7112 | O 12839 | P 1844 | 0 | 0 |

- Molecule 52 is a RNA chain called A-site_tRNA_chain_S2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | S2 | 76 | Total 1626 | C 729 | N 290 | O 531 | P 75 | S 1 | 0 | 0 |

- Molecule 53 is a RNA chain called P-site_tRNA_chain_S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | S3 | 75 | Total 1602 | C 714 | N 292 | O 521 | P 75 | 0 | 0 |

- Molecule 54 is a RNA chain called E-site_tRNA_chain_S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | S4 | 74 | Total 1574 | C 703 | N 280 | O 518 | P 73 | 0 | 0 |

- Molecule 55 is a RNA chain called mRNA_chain_S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 55 | S5 | 12 | Total | C | N | O | P | 0 | 0 |
| | | | 251 | 113 | 43 | 83 | 12 | | |

- Molecule 56 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 56 | SA | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1943 | 1213 | 375 | 344 | 11 | | |

- Molecule 57 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 57 | SB | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1661 | 1055 | 303 | 292 | 11 | | |

- Molecule 58 is a protein called Putative 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 58 | SC | 212 | Total | C | N | O | S | 1 | 0 |
| | | | 1646 | 1040 | 302 | 291 | 13 | | |

- Molecule 59 is a protein called Putative 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 59 | SD | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1508 | 949 | 305 | 246 | 8 | | |

- Molecule 60 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 60 | SE | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2054 | 1301 | 393 | 351 | 9 | | |

- Molecule 61 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 61 | SF | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1708 | 1088 | 301 | 309 | 10 | | |

- Molecule 62 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 62 | SG | 229 | Total<br>1829 | C<br>1140 | N<br>375 | O<br>311 | S<br>3 | 0 | 0 |

- Molecule 63 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 63 | SH | 183 | Total<br>1447 | C<br>899 | N<br>279 | O<br>262 | S<br>7 | 0 | 0 |

- Molecule 64 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 64 | SI | 200 | Total<br>1649 | C<br>1050 | N<br>320 | O<br>271 | S<br>8 | 0 | 0 |

- Molecule 65 is a protein called Putative 40S ribosomal protein S15A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 65 | SJ | 129 | Total<br>1021 | C<br>646 | N<br>188 | O<br>179 | S<br>8 | 0 | 0 |

- Molecule 66 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 66 | SK | 192 | Total<br>1550 | C<br>967 | N<br>320 | O<br>261 | S<br>2 | 0 | 0 |

- Molecule 67 is a protein called Putative 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 67 | SL | 144 | Total<br>1140 | C<br>731 | N<br>210 | O<br>196 | S<br>3 | 0 | 0 |

- Molecule 68 is a protein called Putative ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 68 | SM | 101 | Total<br>792 | C<br>496 | N<br>144 | O<br>150 | S<br>2 | 0 | 0 |

- Molecule 69 is a protein called Putative 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | SN | 100 | Total 818 | C 525 | N 143 | O 143 | S 7 | 0 | 0 |

- Molecule 70 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | SO | 137 | Total 1024 | C 633 | N 200 | O 183 | S 8 | 0 | 0 |

- Molecule 71 is a protein called Putative 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | SP | 141 | Total 1100 | C 694 | N 217 | O 186 | S 3 | 0 | 0 |

- Molecule 72 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | SQ | 100 | Total 670 | C 411 | N 121 | O 133 | S 5 | 0 | 0 |

- Molecule 73 is a protein called Putative 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | SR | 142 | Total 1138 | C 715 | N 226 | O 192 | S 5 | 0 | 0 |

- Molecule 74 is a protein called Putative ribosomal protein S29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | SS | 56 | Total 452 | C 279 | N 94 | O 73 | S 6 | 0 | 0 |

- Molecule 75 is a protein called Putative 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | ST | 143 | Total 1167 | C 736 | N 231 | O 191 | S 9 | 0 | 0 |

- Molecule 76 is a protein called Ribosomal protein S17 family protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76 | SU | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1257 | 795 | 251 | 206 | 5 | | |

- Molecule 77 is a protein called Putative 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77 | SV | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 992 | 619 | 193 | 175 | 5 | | |

- Molecule 78 is a protein called Putative 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78 | SW | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 928 | 591 | 176 | 157 | 4 | | |

- Molecule 79 is a protein called 40S ribosomal protein S19-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79 | SX | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1206 | 766 | 237 | 199 | 4 | | |

- Molecule 80 is a protein called Putative 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80 | SY | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 663 | 409 | 121 | 129 | 4 | | |

- Molecule 81 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81 | SZ | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1051 | 675 | 204 | 169 | 3 | | |

- Molecule 82 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82 | Sa | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 798 | 502 | 147 | 145 | 4 | | |

- Molecule 83 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 83 | Sb | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 825 | 511 | 177 | 130 | 7 | | |

- Molecule 84 is a protein called Putative 40S ribosomal protein S27-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 84 | Sc | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 674 | 416 | 131 | 119 | 8 | | |

- Molecule 85 is a protein called Putative 40S ribosomal protein S33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 85 | Sd | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 496 | 301 | 100 | 91 | 4 | | |

- Molecule 86 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 86 | Se | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 487 | 307 | 102 | 77 | 1 | | |

- Molecule 87 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 87 | Sf | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 659 | 413 | 130 | 110 | 6 | | |

- Molecule 88 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 88 | Sg | 303 | Total | C | N | O | S | 0 | 0 |
| | | | 2354 | 1475 | 420 | 446 | 13 | | |

- Molecule 89 is a protein called Putative RNA binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 89 | Sh | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 768 | 486 | 146 | 133 | 3 | | |

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|:---:|:---:|:---:|:---:|:---:|:---:|
| 90 | L1 | 116 | Total<br>116 | Mg<br>116 | 0 |
| 90 | L2 | 74 | Total<br>74 | Mg<br>74 | 0 |
| 90 | L3 | 4 | Total<br>4 | Mg<br>4 | 0 |
| 90 | L4 | 4 | Total<br>4 | Mg<br>4 | 0 |
| 90 | L5 | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | L6 | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | L7 | 9 | Total<br>9 | Mg<br>9 | 0 |
| 90 | L8 | 5 | Total<br>5 | Mg<br>5 | 0 |
| 90 | LA | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | LB | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | LJ | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | LS | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | LT | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | Lf | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | Lh | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | Lj | 1 | Total<br>1 | Mg<br>1 | 0 |
| 90 | S1 | 64 | Total<br>64 | Mg<br>64 | 0 |
| 90 | S5 | 2 | Total<br>2 | Mg<br>2 | 0 |
| 90 | SX | 1 | Total<br>1 | Mg<br>1 | 0 |

- Molecule 91 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | AltConf |
|:---:|:---:|:---:|:---:|:---:|:---:|
| 91 | L1 | 29 | Total<br>29 | Na<br>29 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 91 | L2 | 21 | Total 21 | Na 21 | 0 |
| 91 | L4 | 4 | Total 4 | Na 4 | 0 |
| 91 | L5 | 3 | Total 3 | Na 3 | 0 |
| 91 | L8 | 1 | Total 1 | Na 1 | 0 |
| 91 | LA | 2 | Total 2 | Na 2 | 0 |
| 91 | LE | 1 | Total 1 | Na 1 | 0 |
| 91 | LH | 1 | Total 1 | Na 1 | 0 |
| 91 | LM | 2 | Total 2 | Na 2 | 0 |
| 91 | LN | 2 | Total 2 | Na 2 | 0 |
| 91 | LR | 1 | Total 1 | Na 1 | 0 |
| 91 | Lf | 1 | Total 1 | Na 1 | 0 |
| 91 | S1 | 16 | Total 16 | Na 16 | 0 |
| 91 | SH | 1 | Total 1 | Na 1 | 0 |
| 91 | SP | 1 | Total 1 | Na 1 | 0 |

- Molecule 92 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 92 | L1 | 55 | Total 55 | K 55 | 0 |
| 92 | L2 | 33 | Total 33 | K 33 | 0 |
| 92 | L3 | 2 | Total 2 | K 2 | 0 |
| 92 | L4 | 6 | Total 6 | K 6 | 0 |
| 92 | L5 | 2 | Total 2 | K 2 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 92 | L7 | 5 | Total 5 | K 5 | 0 |
| 92 | L8 | 1 | Total 1 | K 1 | 0 |
| 92 | LB | 2 | Total 2 | K 2 | 0 |
| 92 | LC | 2 | Total 2 | K 2 | 0 |
| 92 | LZ | 1 | Total 1 | K 1 | 0 |
| 92 | Lh | 1 | Total 1 | K 1 | 0 |
| 92 | S1 | 30 | Total 30 | K 30 | 0 |
| 92 | SS | 1 | Total 1 | K 1 | 0 |
| 92 | ST | 1 | Total 1 | K 1 | 0 |
| 92 | Sb | 1 | Total 1 | K 1 | 0 |

- Molecule 93 is (2S)-2-[2-[4-[[(2R,3S,4S)-3-acetyloxy-4-oxidanyl-pyrrolidin-2-yl]methyl]phenoxy]ethanoylamino]-6-azanyl-hexanoic acid (three-letter code: A1H4F) (formula: $C_{21}H_{31}N_3O_7$).
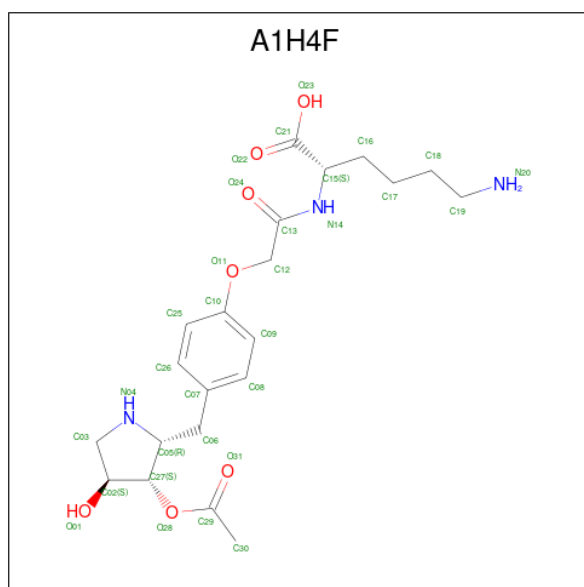
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 93 | L2 | 1 | Total 31 | C 21 | N 3 | O 7 | 0 |

- Molecule 94 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 94 | Lp | 1 | Total 1 | Zn 1 | 0 |

- Molecule 95 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 95 | L1 | 152 | Total 152 | O 152 | 0 |
| 95 | L2 | 119 | Total 119 | O 119 | 0 |
| 95 | L3 | 10 | Total 10 | O 10 | 0 |
| 95 | L4 | 11 | Total 11 | O 11 | 0 |
| 95 | L5 | 3 | Total 3 | O 3 | 0 |
| 95 | L7 | 11 | Total 11 | O 11 | 0 |
| 95 | L8 | 1 | Total 1 | O 1 | 0 |
| 95 | LA | 7 | Total 7 | O 7 | 0 |
| 95 | LB | 5 | Total 5 | O 5 | 0 |
| 95 | LC | 4 | Total 4 | O 4 | 0 |
| 95 | LG | 1 | Total 1 | O 1 | 0 |
| 95 | LH | 2 | Total 2 | O 2 | 0 |
| 95 | LI | 2 | Total 2 | O 2 | 0 |
| 95 | LL | 5 | Total 5 | O 5 | 0 |
| 95 | LM | 7 | Total 7 | O 7 | 0 |
| 95 | LP | 2 | Total 2 | O 2 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 95 | LQ | 2 | Total 2 | O 2 | 0 |
| 95 | LS | 2 | Total 2 | O 2 | 0 |
| 95 | LT | 2 | Total 2 | O 2 | 0 |
| 95 | LV | 1 | Total 1 | O 1 | 0 |
| 95 | LW | 1 | Total 1 | O 1 | 0 |
| 95 | La | 2 | Total 2 | O 2 | 0 |
| 95 | Lb | 2 | Total 2 | O 2 | 0 |
| 95 | Le | 1 | Total 1 | O 1 | 0 |
| 95 | Lf | 2 | Total 2 | O 2 | 0 |
| 95 | Lh | 1 | Total 1 | O 1 | 0 |
| 95 | Lj | 4 | Total 4 | O 4 | 0 |
| 95 | Lo | 1 | Total 1 | O 1 | 0 |
| 95 | Lp | 2 | Total 2 | O 2 | 0 |
| 95 | S1 | 47 | Total 47 | O 47 | 0 |
| 95 | SA | 1 | Total 1 | O 1 | 0 |

# 3   Residue-property plots ⓘ

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

• Molecule 1: LSUa_rRNA_chain_1
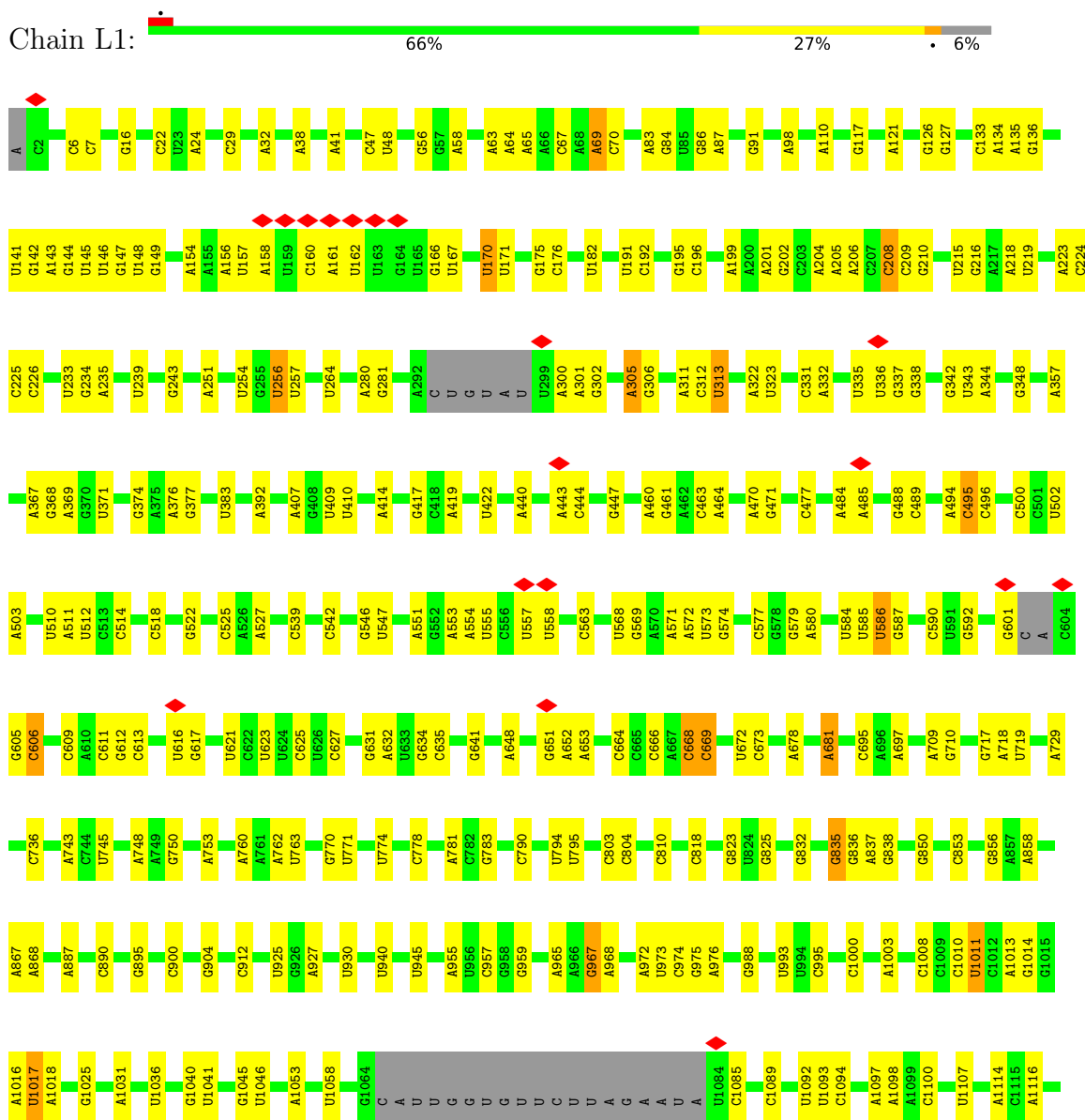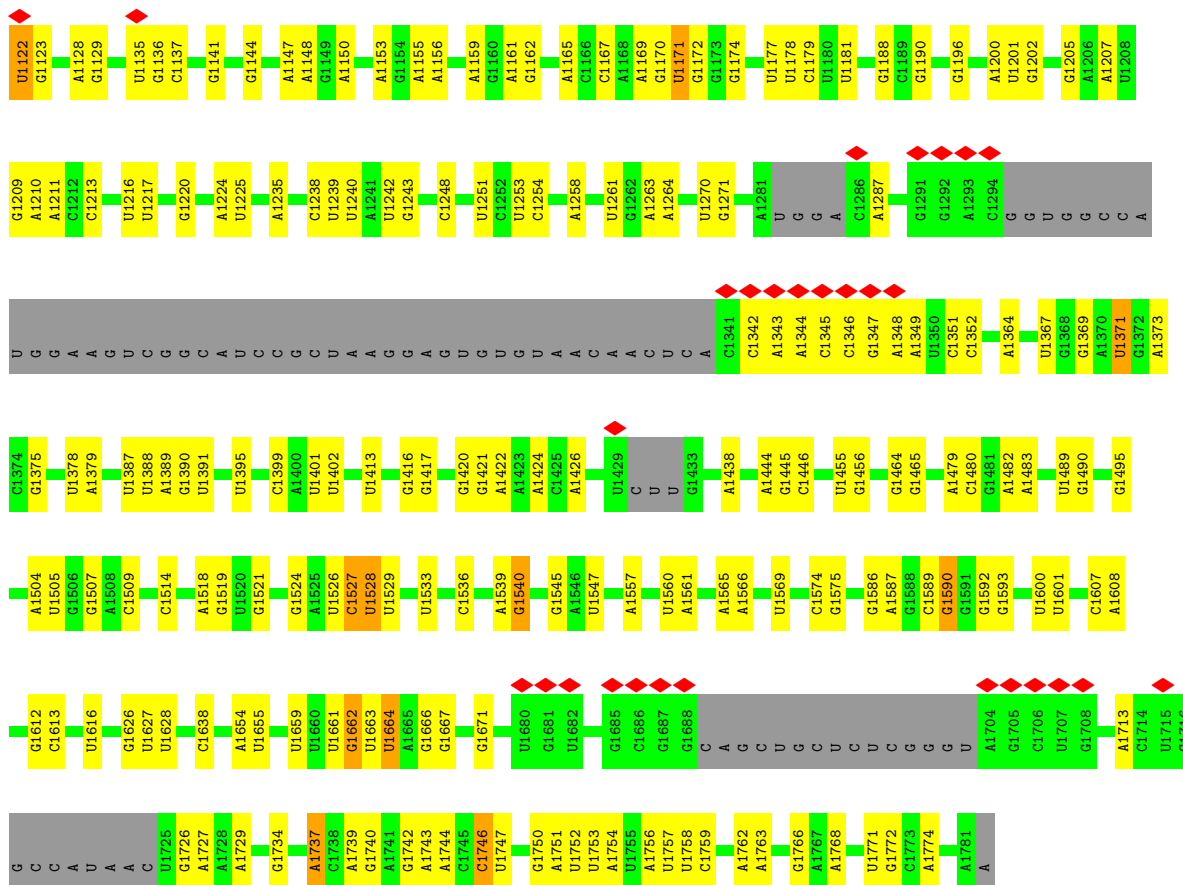
• Molecule 2: LSUb_rRNA_chain_2

• Molecule 3: SR1_chain_3



Chain L3:

- Molecule 4: SR2_chain_4

Chain L4:



- Molecule 5: SR4_chain_5

Chain L5:



- Molecule 6: SR6_chain_6

Chain L6:



- Molecule 7: 5.8S_rRNA_chain_7

Chain L7:



- Molecule 8: 5S_rRNA_chain_8

Chain L8:



- Molecule 9: Putative 60S ribosomal protein L2

Chain LA:

MET G2 R30 K46 M76 D122 L148 K155 K156 S157 S185 R190 V202 R242 R245 P258 E259 GLU
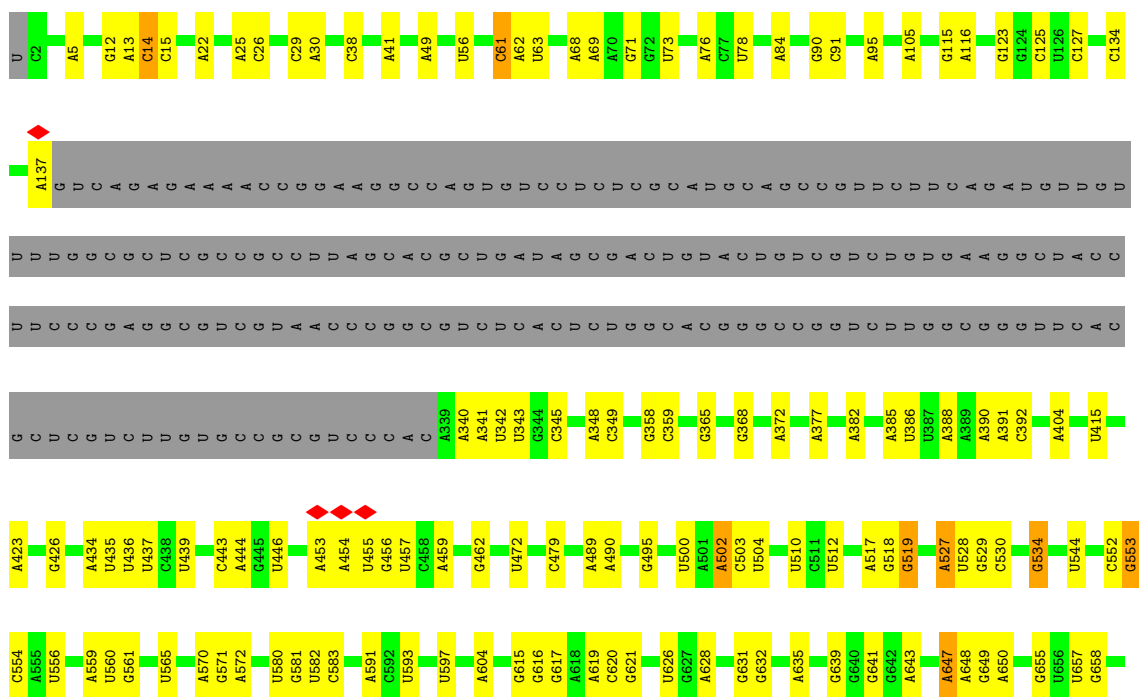
• Molecule 10: Putative ribosomal protein L3

Chain LB: 94%

MET S2 K40 D59 K66 L79 V87 L171 K206 L307 R339 K360 R376 K392 E398 E399 R400 L401 R402 K403 E404 R405 ALA ALA ARG ALA VAL GLU ARG LYS ALA LYS ALA ALA LYS LYS
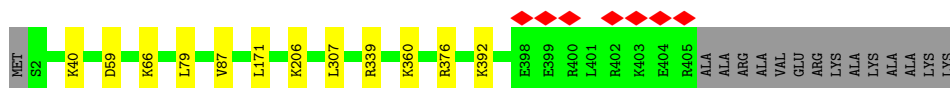
• Molecule 11: Putative ribosomal protein L1a

Chain LC: 93% 5%

MET SER ALA R4 S13 S14 D15 R55 L56 R70 T83 M94 F107 F121 R204 N213 K214 S253 D259 T276 T285 R312 R326 T337 R353 K369 SER ALA LYS GLN

• Molecule 12: 60S ribosomal protein L11

Chain LD: 5% 87% 6% 7%

MET VAL ALA GLU S5 K6 A7 A8 D30 R31 Q41 T46 S50 R57 R62 C71 E80 E83 S95 I116 K117 M127 S153 F174 K177 K178 K179 LYS LYS MET ILE ARG ARG ARG ARG ARG
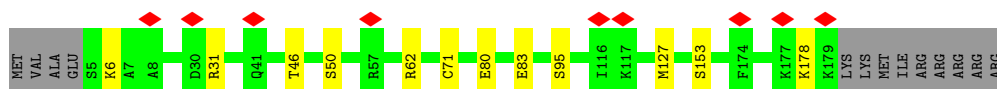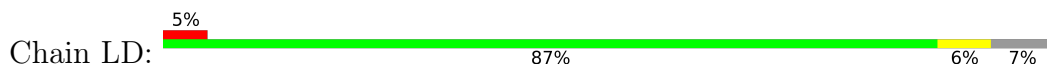
• Molecule 13: Putative 60S ribosomal protein L9

Chain LE: 92% 6%

MET V2 S6 L7 E14 G15 V16 V56 T81 R92 K130 S137 R155 I171 D176 T182 E187 GLY MET GLU
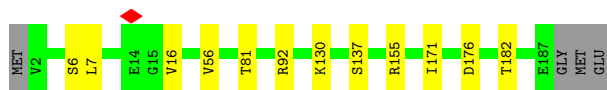
• Molecule 14: Putative 60S ribosomal protein L6

Chain LF: 72% 24%

MET ALA ALA THR LYS SER ALA VAL SER ALA ALA LYS ARG LYS ALA ALA LYS K18 K22 K31 S66 K70 R77 S81 V84 P109 K110 A111 E112 K113 P114 THR LYS SER GLU GLY ASP PHE MET GLY ASP LYS GLN LYS LYS ALA LYS ALA GLU LYS ALA ALA LYS

LYS THR SER LYS ALA GLY LYS LYS T144 L145 R150 W195
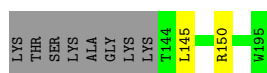
• Molecule 15: 60S ribosomal protein L7a

Chain LG: 7% 88% 9%

MET PRO GLY LYS GLU VAL LYS LYS VAL THR GLN PRO ALA LYS ALA ALA SER PRO TYR LYS LYS PRO ALA V24 A25 L66 S87 A114 E115 E116 K117 K118 K119 D120 P121 K122 K123 T124 V125 S126 T127 K128 M167 K175 D183 E209 N254 Q264
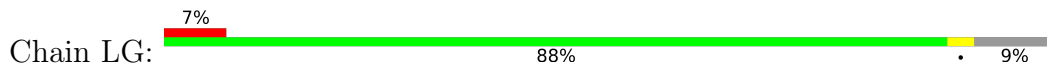
• Molecule 16: Putative 60S ribosomal protein L13a

Chain LH:
95%       5%

MET A2 R67 R77 T85 R108 T133 R136 R141 R149 S150 T155 S169 A222

• Molecule 17: Putative 60S ribosomal protein L13

Chain LI:
94%

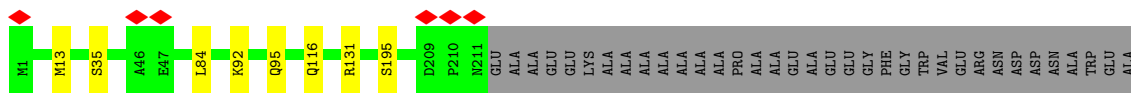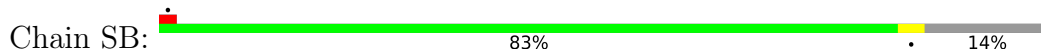MET P2 R39 K57 R60 V68 S81 K140 S170 E180 M184 E211 A212 A213 K214 E215 GLU LYS THR GLY LYS
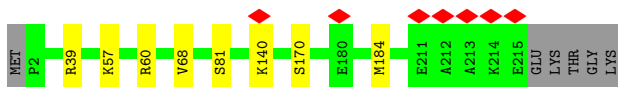
• Molecule 18: Putative 60S ribosomal protein L23

Chain LJ:
95%

MET GLY LYS ASP Q5 N35 K85 N100 V139
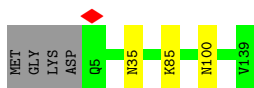
• Molecule 19: Putative 40S ribosomal protein L14

Chain LK:
6%
92%       5%

MET VAL K3 S4 K60 S64 R91 V115 D132 A133 K134 K149 K150 A151 A152 K153 S156 T157 E158 K166 A167 I168 A169 A170 R171 LYS ALA LYS LYS
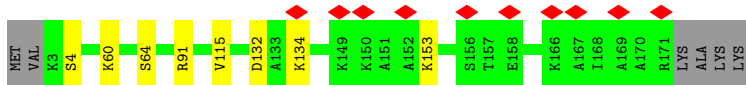
• Molecule 20: Putative 60S ribosomal protein L27A/L29

Chain LL:
94%

MET P2 C8 S30 H39 H40 H60 M68 E85 S104 V117 A145
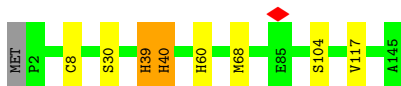
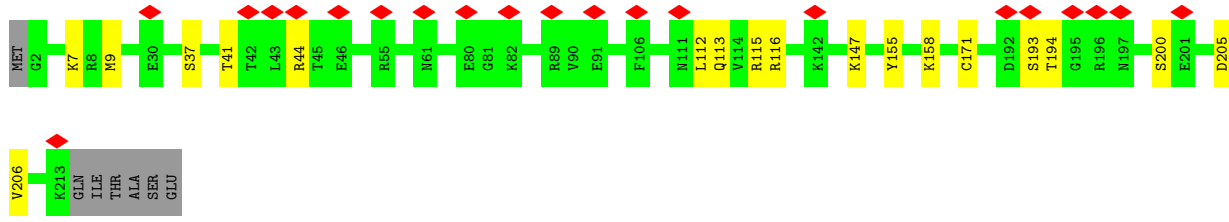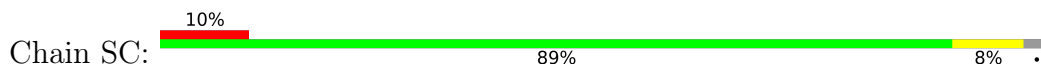• Molecule 21: Ribosomal protein L15

Chain LM:
92%       6%

MET G2 E46 V61 R71 T80 K96 N117 D124 V155 R159 S182 K183 S187 Y188 R189 R193 R194 R204

• Molecule 22: Putative 60S ribosomal protein L10

Chain LN:

86%          10%

MET A2 R3 D28 P29 K30 I31 R32 D35 R40 V43 D44 V48 S54 R55 E63 N81 L103 S104 CYS ALA GLY ALA ASP ARG L111 Q112 M115 K156 R162 M167 K189 K205 M208 R209 N210 V211 M212 ALA

• Molecule 23: Putative 60S ribosomal protein L5

8%

Chain LO:

94%

MET PRO F3 V4 K5 R15 H31 P84 D137 D138 E139 G140 D141 D142 E143 E144 R185 E220 S223 N224 P225 D226 E227 K228 C229 K239 E246 K266 K267 A268 K269 LYS GLU GLY V273 A274 R302 L303 GLY LYS

• Molecule 24: 60S ribosomal protein L18

Chain LP:

96%

MET G2 S21 S41 S81 Y144 R157 S162 S189 R196 H197 V198

• Molecule 25: Putative 60S ribosomal protein L19

9%

Chain LQ:

75%          21%

MET V2 K5 S13 S40 M66 V78 M89 R117 N134 Q154 E157 Q158 L159 K162 R165 D166 R174 E177 R185 E186 R187 A188 R189 R190 D191 D192 A193 A194 A195 A196 A197 Q198 K199 K200 K201 A202 ASP ALA ALA LYS LYS SER ALA ALA

PRO ALA ALA LYS SER ALA ALA PRO ALA ALA LYS ALA ALA PRO ALA THR LYS ALA ALA ALA PRO ALA THR LYS GLY ALA ALA PRO VAL LYS LYS SER LYS LYS

• Molecule 26: 60S ribosomal protein L18a

Chain LR:

95%

MET V2 E19 S41 K50 L61 V65 N75 D98 R156 A179

• Molecule 27: Putative 60S ribosomal protein L21

Chain LS:

94%          5%

MET V2 S46 K55 T61 T68 K78 R83 T84 K98 A124 R148 Y159

• Molecule 28: Putative 60S ribosomal protein L17

Chain LT:

89%          8%

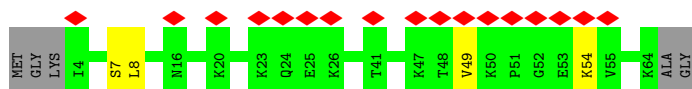MET T2 N37 C57 E75 R126 R127 R128 K153 LYS GLU ARG VAL PRO ALA PRO LYS SER ALA PRO LYS LYS

• Molecule 29: Putative 60S ribosomal protein L22

16%

Chain LU:
90%                    5%   5%

MET V2 R5 R15 Q16 K17 Q18 L19 A20 K23 C30 A35 D36 G37 I38 F39 S40 E41 D42 V43 L44 G45 N46 K63 L64 S65 D66 R69 D74 N75 T78 W106 I107 R108 N123 ILE GLN ASP GLN GLU GLU
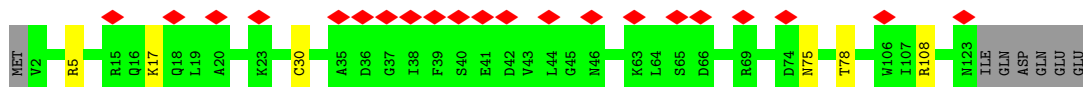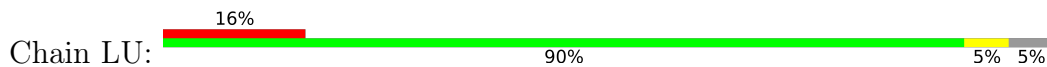
• Molecule 30: Putative 60S ribosomal protein L23a

Chain LV:
80%                    .   18%

MET PRO PRO ALA GLN LYS THR ALA LYS ALA ALA PRO LYS ASP ALA LYS ALA THR LYS VAL VAL LYS VAL THR THR R27 H39 S50 K77 V145
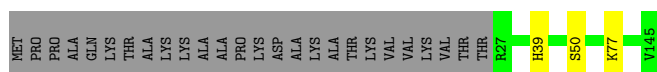
• Molecule 31: Putative 60S ribosomal protein L26

Chain LW:
82%                    .   15%

MET A2 R37 Y71 K81 R112 S122 SER LYS SER ASP LYS GLY LYS GLY LYS ILE SER ALA ALA ASP LYS ALA MET GLN GLN MET ASP
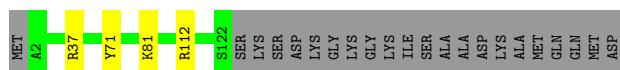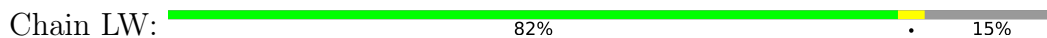
• Molecule 32: Putative ribosomal protein L24

17%

Chain LX:
66%                    .   31%

M1 R2 Y59 R64 LYS THR THR THR ASP ARG VAL ASN ARG ARG ALA ALA ALA ARG ALA VAL R81 V82 Q83 R84 A85 I86 V87 G88 A89 D90 L91 S92 Y93 I94 Q95 E96 V97 R98 A99 A100 R101 LYS GLU ASP ARG SER ALA LYS ALA LYS ALA VAL ARG ALA GLU VAL ALA GLU

ARG LYS ALA ALA LYS LYS

• Molecule 33: 60S ribosomal protein L27

Chain LY:
95%

MET T2 K9 K47 K59 M89 S103 K104 F134

• Molecule 34: Putative 60S ribosomal protein L28

Chain LZ:
95%

MET S2 Q14 R17 C62 T81 S93 S138 A144 K145 R146 ASN

• Molecule 35: Putative 60S ribosomal protein L35

Chain La:

97%

MET S2 K78 T92 R110 K126 ILE
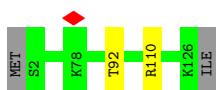
• Molecule 36: 60S ribosomal protein L29

Chain Lb:

90% 7%

MET A2 H10 S14 K33 R34 K53 A68 K69 ASN
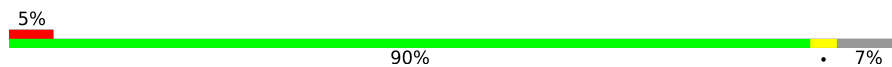
• Molecule 37: Putative 60S ribosomal protein L7

Chain Lc:

88% 9%

MET ALA THR HIS SER VAL TYR GLY ASN ALA SER ASP MET PRO ALA VAL PRO ALA PRO GLU SER ALA ILE K24 L72 N123 E141 M157 D175 I188 Y237 D241 I252

• Molecule 38: 60S ribosomal protein L30

Chain Ld:

5%
90% 7%

MET ALA LYS LYS THR K6 S7 K8 V9 D10 V26 L27 C90 D101 I102 ALA ALA

• Molecule 39: Putative 60S ribosomal subunit protein L31

Chain Le:

7%
96%

MET T2 R3 E14 A18 D21 A22 R23 K24 K25 A26 A27 E28 S29 R30 M45 D46 E47 E48 K49 R50 K51 H54 E159 I170 E187 GLN

• Molecule 40: 60S ribosomal protein L32

Chain Lf:

94%

MET V2 R17 R37 D82 N124 A125 K126 K129 ILE ALA ASN GLN

• Molecule 41: Putative ribosomal protein l35a

Chain Lg:

97%

MET T2 T21 R26 C76 S142 Q143 I144

• Molecule 42: Putative 60S ribosomal protein L34

5%

Chain Lh:      72%      24%

MET S2 C3 Q7 R17 K52 K105 H111 M114 H118 A122 N123 K124 K125 K126 S127 K128 GLN SER LYS LYS GLU ALA ILE ALA LYS LYS ILE SER THR LYS THR VAL SER LYS LYS LYS VAL PRO ALA LYS LYS ALA THR THR ARG GLN PRO VAL GLY SER

LYS LEU VAL LYS LYS

• Molecule 43: Putative 60S Ribosomal protein L36

6%

Chain Li:      94%

M1 S2 T5 S91 H99 A100 T101 K102 LYS HIS HIS

• Molecule 44: Ribosomal protein L37

Chain Lj:      93%      5%

MET T2 R24 R33 R63 R72 K82 ALA

• Molecule 45: Putative ribosomal protein L38

5%

Chain Lk:      92%      6%

MET P2 K26 D49 R58 S59 I60 H61 A79 GLY SER LYS GLN

• Molecule 46: Putative 60S ribosomal protein L39

Chain Ll:      92%      6%

MET G2 K5 R28 W37 Y51

• Molecule 47: Ubiquitin-60S ribosomal protein L40

Chain Lm:      38%      59%

MET GLN ILE PHE VAL LYS THR LEU THR GLY LYS THR ILE ALA LEU GLU VAL GLU PRO SER ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP LYS GLU GLY ILE PRO PRO ASP GLN GLN ARG LEU ILE PHE ALA GLY LYS GLN LEU GLU GLU GLY ARG THR LEU SER ASP TYR ASN

ILE GLN LYS GLU SER THR LEU HIS LEU VAL LEU ARG LEU ARG GLY GLY V77 C99 V105 H117 R128

- Molecule 48: 60S ribosomal protein L41

Chain Ln:

94%

MET G2 R8 K34

- Molecule 49: 60S ribosomal protein L37a

Chain Lo:

92%

MET A2 F41 C42 F47 R80 A90 LYS ILE

- Molecule 50: Putative 60S ribosomal protein L44

Chain Lp:

86%    6%    8%

MET V2 V26 K61 L72 K78 S79 K98 THR GLY ASN LYS ASP PRO THR TRP

- Molecule 51: SSU_rRNA_chain_S1

Chain S1:

11%

61%    22%    16%

G1 A2 U3 U8 U12 C17 C18 A26 U27 A28 U29 U33 G34 C38 G42 U45 U46 A47 U60 C61 A65 U66 C67 A68 A73 U U U G77 C95 A98 A102 A103 G110 U111 A112 A113 U114 G117 A122 A123 A124

U127 C128 U129 C132 G133 G134 U U U C138 C139 G140 C141 A142 A143 A144 A145 U146 U147 G148 G149 A152 U155 G158 C164 C167 G170 C171 A174 U175 A176 A182 C188 G189 G190 U191 U192 G193 U194 U195 C196 U197 C198 C199 A200 C201 U C C A

G A C G G U G G G C A A C C A U C G U C G226 U227 G228 A229 G230 A231 C232 G233 C234 C235 C236 A237 A249 C250 A251 G252 U253 A254 A255 A256 A257 C258 C259 A260 A261 U262 G263 C264 C265 U266 U267 C A C U G G273 C274 A275

G276 U277 A278 A279 C280 A281 C282 C283 C284 A285 G286 C287 A288 G289 G294 A295 C296 U297 C298 U302 C308 G309 U310 G313 A316 G321 C322 U323 U324 G325 U326 U327 C328 C329 C332 U336 G340 A341 A356 U357 C358 A359 G360 G364 A377 G381 A382

A388 G396 C404 G433 A434 G435 A443 A444 U445 A446 G447 C454 U455 C460 G465 G466 C467 U468 G469 G475 C476 U477 A478 A479 A480 U481 U482 U483 G484 C487 A488 A497 A500 A501 A502 C503 G507 A508 C511 A512 A516 A523 U524 A525

G528 U529 U530 C531 U532 C A C G U C C C A U U U G G A U546 U547 G548 U549 C550 A551 U552 U553 U554 C555 U565 C574 A580 A581 U582 A583 U584 C585 G586 A587 A590 A591 C592 A593 G600 G606 U607 C608 U609 U612 G613 C614 C615 A616

• Molecule 52: A-site_tRNA_chain_S2

Chain S2:



• Molecule 53: P-site_tRNA_chain_S3

Chain S3:



• Molecule 54: E-site_tRNA_chain_S4
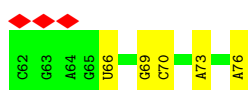
Chain S4:



• Molecule 55: mRNA_chain_S5

Chain S5:



• Molecule 56: 40S ribosomal protein S3a

Chain SA:

MET A2 G13 K14 R15 G16 LYS R18 G19 K20 A21 GLN E22 R26 D31 R55 S76 A77 G78 E79 E80 K85 D110 N150 N155 Q182 V194 L195 S196 N204 L207 K224 R246 GLU VAL GLU GLU ALA VAL GLU ALA ALA PRO ALA ALA

GLU LYS ALA ALA GLU

• Molecule 57: 40S ribosomal protein SA

Chain SB:　　83%　　14%

M1 M13 S35 A46 E47 L84 K92 Q95 Q116 R131 S195 D209 P210 N211 GLU ALA ALA GLU GLU LYS ALA ALA ALA ALA ALA PRO ALA ALA GLU ALA GLU GLU GLY PHE GLY TRP VAL GLU ARG ASN ASP ASP ASN ALA TRP GLU ALA

• Molecule 58: Putative 40S ribosomal protein S3

Chain SC:　　10%　　89%　　8%

MET G2 K7 R8 M9 E30 S37 T41 T42 L43 R44 T45 E46 R55 N61 E80 G81 K82 R89 V90 E91 F106 N111 L112 Q113 V114 R115 R116 K142 K147 Y155 K158 C171 D192 S193 T194 G195 R196 N197 S200 E201 D205

V206 K213 GLN ILE THR ALA SER GLU

• Molecule 59: Putative 40S ribosomal protein S9

Chain SD:　　23%　　89%　　7%

M1 N6 R15 E21 K28 K38 T47 L48 S49 L57 T60 N64 R67 R78 D86 E87 E88 K89 D90 K91 L92 D93 D102 R106 F113 K114 A115 G116 L117 A118 K119 A124 L127 K137 V149 S150 S151 E152 R153 H154

A158 D159 G164 N165 T168 V171 K172 R173 V174 R175 K176 K177 A178 A179 K180 R181 H182 A183 GLY GLY GLY ASP ASP ASP GLU

• Molecule 60: 40S ribosomal protein S4

Chain SE:　　27%　　88%　　8%　　5%

MET A2 Y10 K13 L17 S18 K19 L20 T21 R27 L35 V43 L49 A52 L53 N54 A55 G65 D70 G77 A81 E88 I89 P90 G93 D94 V102 F106 A107 L111 S112 E113 A114 E115 A116 Q117 I118 K119 L120 L126 Y127 T128

A129 T130 G141 I144 D148 P149 H150 N160 V161 K162 E163 K164 K165 D168 L169 I170 K171 N172 R173 Q174 T181 A184 V193 K194 V195 E196 A201 D209 A210 A213 E214 K227 D228 L229 N230 N231 L232 Q233 V234 T235 V236 P237 K238 Q239 Q240 G241 L242 R243

M244 N245 V246 I247 Q248 E251 E252 R253 L254 I255 A256 A257 E258 A259 R260 K261 ASN ALA PRO ALA ARG GLY ALA ARG ALA ARG ALA LYS

• Molecule 61: 40S ribosomal protein S2

Chain SF:

• Molecule 62: 40S ribosomal protein S6

Chain SG:

• Molecule 63: 40S ribosomal protein S5

Chain SH:

• Molecule 64: 40S ribosomal protein S7

Chain SI:

• Molecule 65: Putative 40S ribosomal protein S15A

Chain SJ:

• Molecule 66: 40S ribosomal protein S8

**Chain SK:**

10%

80%    7%    13%

MET G2 I3 V4 R22 R31 R47 L58 N64 V81 A107 R111 D120 L121 D122 A123 ASP LYS LYS THR LYS ALA ALA VAL ALA GLU LYS LYS GLY ARG LYS SER ALA HIS ALA ALA D147 K148 Y149 D150 V151 N152 K153 A154 S155 P156 K157 L158

Q159 R160 T163 R164 R165 R166 R167 N168 H169 R170 V171 A176 E181 G182 R183 Q209 E216 LYS LYS LYS

• Molecule 67: Putative 40S ribosomal protein S16

**Chain SL:**

93%

MET PRO ALA ASP LYS S6 Y7 A8 T28 Q32 D48 T49 S63 Q80 K108 R149

• Molecule 68: Putative ribosomal protein S20

**Chain SM:**

14%

80%    7%    13%

MET ASP TYR PRO LYS LYS ASN GLN ALA ALA PRO ALA GLU GLY Q15 T22 K27 A28 V29 S34 R41 D42 E43 K44 V45 T46 D87 E93 Q94 V95 K96 K97 T102 M103 S110 I111 T112 I113 L114 D115 ARG

• Molecule 69: Putative 40S ribosomal protein S10

**Chain SN:**

11%

54%    5%    40%

M1 S2 T3 S9 R10 D11 R15 F16 F17 K27 D28 T36 L37 G38 G39 N40 T41 V44 V49 D77 A81 Y82 M83 L89 A90 P91 S92 A93 M94 K99 P100 SER VAL ASN PHE GLU LYS VAL THR GLU GLY ARG GLY ARG GLY ARG GLY ARG GLY

GLY ARG GLY ARG GLY GLU GLY ARG GLY ARG GLY ARG GLY GLU GLY ARG GLY ARG GLY ARG GLY ARG GLY PHE GLY GLY GLU ARG MET ASN TYR ARG ALA ALA ALA THR SER ASP GLY GLU ALA ALA PRO ALA PRO ALA ALA GLU

• Molecule 70: 40S ribosomal protein S14

**Chain SO:**

91%    5%

MET SER LYS LYS GLN GLU VAL K8 A9 K16 G17 D18 R59 M68 R77 K89 R97 L144

• Molecule 71: Putative 40S ribosomal protein S23

**Chain SP:**

5%

92%    6%

MET T2 R21 R36 I55 G56 V57 R71 N77 V85 E95 D98 F105 N127 Q136 E139 K140 P141 R142 ASN

• Molecule 72: 40S ribosomal protein S12

**Chain SQ:**

62%
67%
29%

MET ALA GLU GLU THR VAL ARG VAL GLU VAL PRO ALA VAL GLU GLU ASN VAL VAL VAL ASP VAL ALA PRO GLU SER LEU E27 D28 A29 V30 R31 I32 V33 I34 Q35 K36 S37 L38 E39 A40 N41 G42 L43 V44 R45 G46 L47 S48 E49 V50 A51 R52 T53 L54 D55 C56 K57 T58 A59 H60

M61 L64 A65 D66 D67 C68 E69 D70 E71 E72 Y73 K74 K75 L76 V77 T78 A79 L80 A81 K82 Q83 G84 N85 I86 D87 L88 I89 N90 V91 E92 E93 R94 E95 K96 L97 A98 Q99 W100 A101 G102 L103 V104 R105 R106 D107 VAL A109 G110 E111 V112 T113 K114 T115 L116 K117 C118 S119 S120

R124 D125 F126 G127 GLU ARG THR LYS ALA LEU ASP TYR LEU LEU SER GLN LEU HIS

• Molecule 73: Putative 40S ribosomal protein S18

**Chain SR:**

9%
86%
7%
7%

MET S2 L3 T4 H12 N18 R32 L44 R56 E63 E66 A73 K79 R87 Q88 K92 K95 S100 M103 V104 D105 K117 T137 S140 G141 R142 H143 GLY LYS THR VAL GLY VAL SER ARG GLY LYS

• Molecule 74: Putative ribosomal protein S29

**Chain SS:**

93%
5%

MET G2 S9 M15 L56 R57

• Molecule 75: Putative 40S ribosomal protein S13

**Chain ST:**

88%
7%
5%

M1 V2 T21 S30 M36 K100 R104 T107 D108 R109 R114 R127 S143 SER THR ALA SER ALA MET VAL ALA

• Molecule 76: Ribosomal protein S17 family protein

**Chain SU:**

5%
80%
9%
12%

MET PRO VAL ALA PRO Q6 H9 A10 H11 H19 E20 K21 R25 M33 H34 R35 P36 S37 R38 K43 N65 R82 V89 T93 R97 K117 E137 N153 V158 SER LYS SER SER ALA ASP LYS MET GLY LYS LYS PHE ALA LYS ASN

• Molecule 77: Putative 40S ribosomal protein S17

**Chain SV:**

17%
80%
5%
15%

MET G2 R5 T6 K7 T8 D37 E42 R67 L71 K72 L73 Q74 E75 E76 E77 R78 E79 R80 R81 M82 D83 H84 A85 P86 A87 T88 Q96 S97 G98 V99 S100 V101 D102 R118 K121 R122 A123 ASP ALA ALA VAL THR LYS VAL LYS ALA ALA PRO ARG ARG ARG

GLN GLN LYS SER LYS

• Molecule 78: Putative 40S ribosomal protein S15

9%

Chain SW:

73% 24%

MET ALA SER ASN ILE THR ALA GLU ARG TYR GLU GLN LEU LYS LYS GLU ARG THR PHE HIS K21 F22 E28 I29 D30 S36 E37 E38 E39 K71 K72 H73 V74 K75 V76 G77 E78 H107 H135 GLY ARG PRO GLY VAL GLY ALA THR HIS SER SER ARG PHE ILE PRO ILE

LYS

• Molecule 79: 40S ribosomal protein S19-like protein

Chain SX:

89% 6% 6%

MET THR ALA PRO ARG N6 K7 I8 H9 R10 K13 D21 R33 R80 S100 R101 Q131 K142 G157 GLN SER LYS ALA

• Molecule 80: Putative 40S ribosomal protein S21

Chain SY:

51% 46%

MET ALA T3 D15 S40 T55 Y62 R80 K89 P90 LYS ARG ALA SER LYS SER SER LYS PRO ALA ALA LYS GLY ALA ALA GLY ALA ALA GLN LYS GLY ALA ARG PRO ALA GLN LYS GLY ALA ARG PRO PRO ALA GLN LYS GLY ALA ARG PRO

PRO ALA GLN LYS GLY ALA ARG PRO PRO ALA GLN LYS GLY ALA ARG PRO PRO ALA GLN LYS GLY ALA ALA PRO ALA ARG LYS ASN ARG ALA

• Molecule 81: 40S ribosomal protein S24

51%

Chain SZ:

85% 10% 5%

MET V2 F3 Q4 K5 K6 K7 A8 E9 V10 C11 I12 R13 T14 S15 Q16 F17 K18 V19 N20 K21 L22 L23 N24 F28 E31 V32 N33 H34 P35 H36 T43 Q44 L45 I46 R47 K48 K49 L50 A51 T52 L53 Y54 K55 V56 P57 D58 A59 S60 Q61 G66 F67 K68 T69 G73

T76 L81 D84 D85 L86 A87 R91 R100 M101 G102 F103 G104 K105 A106 R107 L108 P109 A110 R111 K112 E116 R117 R120 N121 K122 K123 L124 R125 G126 K127 A128 K129 G130 K131 GLN VAL ALA LYS LYS LYS

• Molecule 82: 40S ribosomal protein S25

24%

Chain Sa:

79% 8% 12%

MET P2 P3 K4 A5 G6 Q7 T8 K9 K10 A11 E14 N17 A20 K21 K22 T23 T24 K25 K26 K29 G30 Q31 S32 R33 E34 D43 K44 F45 D48 R51 S52 E53 K58 K87 C94 T98 V105 Q106 ALA ALA PRO ALA GLU ALA ALA ALA ALA

ALA PRO ALA ALA GLU

• Molecule 83: 40S ribosomal protein S26

Chain Sb:

87%                                                          6%    7%

M1 T2 T32 V42 S59 N65 C78 T87 V88 V104 PRO PHE ARG PRO ALA GLY LYS LYS

• Molecule 84: Putative 40S ribosomal protein S27-1

Chain Sc:

91%                                                          8%

MET G2 F3 L8 D35 V36 S37 R42 K58 K63 R82 D85 H86

• Molecule 85: Putative 40S ribosomal protein S33

10%

Chain Sd:

70%                                 6%              24%

MET ALA ASP SER LYS LYS ASP ASN LYS LYS THR GLU GLU VAL VAL THR GLN GLY THR ASP Q20 A21 Q22 K28 E49 A50 G51 S52 P53 D54 R57 L73 S74 R83 R84 L85 ARG

• Molecule 86: 40S ribosomal protein S30

26%

Chain Se:

86%                                                          6%    8%

MET GLY LYS I4 S7 L8 N16 K20 K23 Q24 E25 K26 T41 K47 T48 V49 K50 P51 G52 E53 K54 V55 K64 ALA GLY

• Molecule 87: Ubiquitin-60S ribosomal protein L40

38%

Chain Sf:

45%                  7%                         47%

MET GLN ILE PHE ILE LYS ASP ALA ALA GLY ARG SER VAL ALA VAL ARG VAL SER ALA GLU ASP THR VAL GLY PHE LEU LYS ALA GLN ALA ASN VAL THR GLN GLY ASN LEU PHE PHE ALA GLY MET CYS LEU ALA GLU GLU GLU THR LEU ALA ALA TYR GLY LEU SER LYS GLU SER THR

VAL ASP VAL VAL ILE PRO VAL GLU G69 G70 K71 G72 K73 K74 K75 K76 K77 R78 I79 F80 T81 P86 T87 H88 R89 H90 K91 L92 E93 K94 M95 R96 A97 L98 K99 Y100 F101 K102 V103 T104 E105 N106 D107 D108 G109 S110 Y111 K112 V113 E114 R115 T116 R117 Q118 D119 C120 P121 H122 P123

Q124 C125 G126 A127 G128 V129 Q133 H134 K135 D136 R137 Q138 Y139 C143 H144 L145 K148 ALA GLU SER LYS

• Molecule 88: Guanine nucleotide-binding protein subunit beta-like protein

33%

Chain Sg:

90%                                                          7%

M1 N2 W13 Q21 Q22 A23 G24 S25 Y26 P45 D46 R47 H48 S49 V50 D51 S52 D53 S69 S72 L73 A74 H75 A76 T77 D78 Y79 D86 F115 D118 D119 R120 L121 I122 D128 V133 W134 N135 V136 A137 G138 E139 C140 M141 H142 E143 F144 L145 R146 D147

G148 H149 E150 D151 F158 S159 P160 S161 LEU GLU HIS P165 I166 V167 V168 W179 N180 V181 N182 G183 G184 K185 C186 E187 R188 S194 T199 S203 P204 D205 G206 S207 L208 C209 D215 D222 L223 S224 T225 G226 E227 Q228 L229 F230 K231 I232 N233 V234 E235 P245 N246 R247

F248 R256 S257 L258 S259 V260 Y261 D262 L263 E264 S265 K266 A267 V268 I269 A270 E271 L272 T273 P274 ASP GLY ALA K278 P279 A289 D290 G291 N292 T293 L294 K299 R304 S307 I308 S309 ASP ALA GLU

• Molecule 89: Putative RNA binding protein

40%

Chain Sh:

36%　　　　　5%　　　　　59%

MET PRO ALA LYS ALA ALA LYS PRO VAL LYS PRO ALA ALA LYS ALA ALA PRO LYS PRO ALA ASN LYS ALA PRO ALA PRO LYS ALA ALA ALA LYS PRO VAL ALA LYS ALA ALA PRO LYS ALA ALA ALA PRO ALA ALA ARG PRO ALA SER GLY SER SER ASN GLY VAL TYR VAL LYS

ASN TRP GLY THR GLY SER VAL ALA ASP ALA ALA ASN VAL PHE SER ALA ALA GLY LYS LYS VAL VAL LYS VAL GLN LEU ARG ARG GLN ARG TYR ALA ILE VAL PHE PHE GLU GLU ASN SER ALA ALA VAL LYS LYS ALA ILE ASP LEU PHE ASN GLU LYS GLU VAL LEU LEU GLY LYS THR VAL LEU VAL

VAL PRO ALA LYS THR SER PRO LYS PRO ASP ALA HIS GLU N134 S135 S136 C137 V138 F139 V140 S141 P142 I143 F144 R145 P146 S147 T148 T149 K150 A151 Q152 V153 M154 E155 L156 F157 A158 G159 V160 K161 V162 Q163 R164 L165 R166 M167 Y168 R169 Q170 N171 F172 A173 Y174 A175 Y176 L177 D178 S179 P180

A181 A182 A183 K184 K185 F186 V187 E188 E189 K190 N191 G192 T193 E194 F195 R196 G197 H198 T199 L200 R201 V202 A203 L204 S205 A206 R207 S208 L209 E210 K211 L212 R213 A214 R215 Q216 E217 A218 A219 N220 V221 V222 I223 A224 A225 H226 R227 H228 Y229 LYS THR HIS GLU ARG GLN

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 419524 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 0.9340390798620625 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 1700 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.181 | Depositor |
| Minimum map value | -0.118 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.007 | Depositor |
| Recommended contour level | 0.015 | Depositor |
| Map size (Å) | 395.76, 395.76, 395.76 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.8245, 0.8245, 0.8245 | Depositor |

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, B8N, OMC, 5MC, MG, ZN, A1H4F, OMG, PSU, 7MG, OMU, MA6, NA, K, A2M

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 | L1 | 0.42 | 0/39236 | 0.91 | 56/61175 (0.1%) |
| 2 | L2 | 0.42 | 0/25973 | 0.92 | 49/40481 (0.1%) |
| 3 | L3 | 0.37 | 0/4302 | 0.91 | 11/6687 (0.2%) |
| 4 | L4 | 0.41 | 0/4376 | 0.90 | 9/6822 (0.1%) |
| 5 | L5 | 0.43 | 0/2852 | 0.99 | 4/4438 (0.1%) |
| 6 | L6 | 0.35 | 0/1683 | 0.90 | 1/2618 (0.0%) |
| 7 | L7 | 0.40 | 0/3782 | 1.01 | 13/5889 (0.2%) |
| 8 | L8 | 0.42 | 0/2851 | 0.91 | 3/4439 (0.1%) |
| 9 | LA | 0.30 | 0/2007 | 0.60 | 0/2696 |
| 10 | LB | 0.27 | 0/3283 | 0.55 | 0/4412 |
| 11 | LC | 0.26 | 0/2870 | 0.53 | 0/3861 |
| 12 | LD | 0.25 | 0/1410 | 0.51 | 0/1884 |
| 13 | LE | 0.26 | 0/1497 | 0.52 | 0/2017 |
| 14 | LF | 0.26 | 0/1173 | 0.52 | 0/1586 |
| 15 | LG | 0.25 | 0/1932 | 0.54 | 0/2599 |
| 16 | LH | 0.28 | 0/1803 | 0.54 | 0/2422 |
| 17 | LI | 0.27 | 0/1728 | 0.54 | 0/2313 |
| 18 | LJ | 0.28 | 0/1029 | 0.52 | 0/1388 |
| 19 | LK | 0.28 | 0/1355 | 0.52 | 0/1816 |
| 20 | LL | 0.30 | 0/1151 | 0.58 | 1/1538 (0.1%) |
| 21 | LM | 0.32 | 0/1751 | 0.59 | 0/2338 |
| 22 | LN | 0.27 | 0/1697 | 0.57 | 0/2269 |
| 23 | LO | 0.27 | 0/2370 | 0.51 | 1/3172 (0.0%) |
| 24 | LP | 0.33 | 0/1564 | 0.58 | 0/2092 |
| 25 | LQ | 0.24 | 0/1701 | 0.54 | 0/2250 |
| 26 | LR | 0.29 | 0/1489 | 0.52 | 0/2008 |
| 27 | LS | 0.31 | 0/1290 | 0.60 | 2/1736 (0.1%) |
| 28 | LT | 0.27 | 0/1241 | 0.52 | 0/1665 |
| 29 | LU | 0.25 | 0/976 | 0.50 | 0/1303 |
| 30 | LV | 0.26 | 0/968 | 0.51 | 0/1302 |
| 31 | LW | 0.25 | 0/981 | 0.56 | 0/1310 |
| 32 | LX | 0.27 | 0/735 | 0.55 | 0/989 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | LY | 0.27 | 0/1088 | 0.53 | 0/1455 |
| 34 | LZ | 0.26 | 0/1133 | 0.55 | 0/1516 |
| 35 | La | 0.24 | 0/1054 | 0.53 | 0/1399 |
| 36 | Lb | 0.30 | 0/557 | 0.55 | 0/743 |
| 37 | Lc | 0.27 | 0/1896 | 0.53 | 0/2540 |
| 38 | Ld | 0.26 | 0/754 | 0.47 | 0/1019 |
| 39 | Le | 0.25 | 0/1488 | 0.54 | 0/1979 |
| 40 | Lf | 0.33 | 0/1066 | 0.61 | 0/1424 |
| 41 | Lg | 0.30 | 0/1172 | 0.57 | 0/1573 |
| 42 | Lh | 0.26 | 0/1045 | 0.56 | 0/1390 |
| 43 | Li | 0.26 | 0/822 | 0.53 | 0/1099 |
| 44 | Lj | 0.31 | 0/686 | 0.65 | 0/915 |
| 45 | Lk | 0.26 | 0/617 | 0.52 | 0/828 |
| 46 | Ll | 0.26 | 0/463 | 0.54 | 0/617 |
| 47 | Lm | 0.26 | 0/423 | 0.57 | 0/563 |
| 48 | Ln | 0.26 | 0/300 | 0.70 | 0/390 |
| 49 | Lo | 0.28 | 0/705 | 0.60 | 0/940 |
| 50 | Lp | 0.29 | 0/797 | 0.49 | 0/1053 |
| 51 | S1 | 0.34 | 0/42995 | 0.86 | 33/66976 (0.0%) |
| 52 | S2 | 0.49 | 0/1783 | 0.95 | 0/2776 |
| 53 | S3 | 0.39 | 0/1790 | 0.88 | 1/2789 (0.0%) |
| 54 | S4 | 0.26 | 0/1757 | 0.88 | 1/2735 (0.0%) |
| 55 | S5 | 0.28 | 0/279 | 0.90 | 0/431 |
| 56 | SA | 0.25 | 0/1967 | 0.55 | 0/2641 |
| 57 | SB | 0.25 | 0/1695 | 0.50 | 0/2292 |
| 58 | SC | 0.27 | 0/1674 | 0.53 | 0/2240 |
| 59 | SD | 0.25 | 0/1536 | 0.58 | 0/2059 |
| 60 | SE | 0.25 | 0/2092 | 0.54 | 0/2819 |
| 61 | SF | 0.25 | 0/1744 | 0.50 | 1/2362 (0.0%) |
| 62 | SG | 0.25 | 0/1851 | 0.59 | 0/2474 |
| 63 | SH | 0.24 | 0/1469 | 0.51 | 0/1970 |
| 64 | SI | 0.25 | 0/1679 | 0.54 | 0/2255 |
| 65 | SJ | 0.26 | 0/1038 | 0.53 | 0/1391 |
| 66 | SK | 0.25 | 0/1573 | 0.58 | 0/2107 |
| 67 | SL | 0.28 | 0/1161 | 0.49 | 0/1559 |
| 68 | SM | 0.25 | 0/802 | 0.54 | 0/1088 |
| 69 | SN | 0.25 | 0/842 | 0.53 | 1/1141 (0.1%) |
| 70 | SO | 0.31 | 0/1039 | 0.59 | 0/1395 |
| 71 | SP | 0.25 | 0/1120 | 0.52 | 0/1500 |
| 72 | SQ | 0.26 | 0/671 | 0.58 | 0/911 |
| 73 | SR | 0.24 | 0/1158 | 0.53 | 0/1553 |
| 74 | SS | 0.25 | 0/458 | 0.55 | 0/607 |
| 75 | ST | 0.28 | 0/1190 | 0.55 | 0/1594 |

| Mol | Chain | Bond lengths | | Bond angles | |
| --- | --- | --- | --- | --- | --- |
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 76 | SU | 0.26 | 0/1286 | 0.54 | 0/1727 |
| 77 | SV | 0.24 | 0/1002 | 0.51 | 0/1334 |
| 78 | SW | 0.25 | 0/948 | 0.51 | 0/1275 |
| 79 | SX | 0.29 | 0/1237 | 0.51 | 0/1661 |
| 80 | SY | 0.24 | 0/673 | 0.50 | 0/913 |
| 81 | SZ | 0.25 | 0/1071 | 0.51 | 0/1425 |
| 82 | Sa | 0.25 | 0/807 | 0.51 | 0/1082 |
| 83 | Sb | 0.26 | 0/842 | 0.58 | 0/1127 |
| 84 | Sc | 0.28 | 0/688 | 0.54 | 0/921 |
| 85 | Sd | 0.23 | 0/498 | 0.58 | 0/668 |
| 86 | Se | 0.36 | 0/496 | 0.61 | 0/658 |
| 87 | Sf | 0.26 | 0/674 | 0.52 | 0/892 |
| 88 | Sg | 0.24 | 0/2412 | 0.51 | 0/3276 |
| 89 | Sh | 0.26 | 0/783 | 0.54 | 0/1053 |
| All | All | 0.35 | 0/227902 | 0.78 | 187/334635 (0.1%) |

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 |
| --- | --- | --- | --- |
| 16 | LH | 0 | 1 |
| 21 | LM | 0 | 4 |
| 24 | LP | 0 | 1 |
| 40 | Lf | 0 | 1 |
| 44 | Lj | 0 | 2 |
| 70 | SO | 0 | 1 |
| 79 | SX | 0 | 1 |
| All | All | 0 | 11 |

There are no bond length outliers.

The worst 5 of 187 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 7 | L7 | 6 | G | O3'-P-O5' | -24.52 | 57.42 | 104.00 |
| 7 | L7 | 7 | U | O5'-P-OP1 | -18.18 | 88.89 | 110.70 |
| 7 | L7 | 6 | G | OP1-P-O3' | 14.95 | 138.08 | 105.20 |
| 1 | L1 | 563 | C | N1-C2-O2 | 8.73 | 124.14 | 118.90 |
| 1 | L1 | 563 | C | C2-N1-C1' | 8.11 | 127.72 | 118.80 |

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 16 | LH | 108 | ARG | Sidechain |
| 21 | LM | 189 | ARG | Sidechain |
| 21 | LM | 193 | ARG | Sidechain |
| 21 | LM | 194 | ARG | Sidechain |
| 21 | LM | 71 | ARG | Sidechain |

## 5.2   Too-close contacts ⓘ

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

## 5.3   Torsion angles ⓘ

### 5.3.1   Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|-----|-----|
| 9 | LA | 256/260 (98%) | 249 (97%) | 7 (3%) | 0 | 100 | 100 |
| 10 | LB | 402/419 (96%) | 390 (97%) | 12 (3%) | 0 | 100 | 100 |
| 11 | LC | 364/373 (98%) | 353 (97%) | 11 (3%) | 0 | 100 | 100 |
| 12 | LD | 173/188 (92%) | 170 (98%) | 3 (2%) | 0 | 100 | 100 |
| 13 | LE | 184/190 (97%) | 175 (95%) | 9 (5%) | 0 | 100 | 100 |
| 14 | LF | 145/195 (74%) | 138 (95%) | 7 (5%) | 0 | 100 | 100 |
| 15 | LG | 239/264 (90%) | 234 (98%) | 5 (2%) | 0 | 100 | 100 |
| 16 | LH | 219/222 (99%) | 216 (99%) | 3 (1%) | 0 | 100 | 100 |
| 17 | LI | 212/220 (96%) | 206 (97%) | 6 (3%) | 0 | 100 | 100 |
| 18 | LJ | 133/139 (96%) | 131 (98%) | 2 (2%) | 0 | 100 | 100 |
| 19 | LK | 167/175 (95%) | 161 (96%) | 6 (4%) | 0 | 100 | 100 |
| 20 | LL | 142/145 (98%) | 135 (95%) | 6 (4%) | 1 (1%) | 19 | 41 |
| 21 | LM | 201/204 (98%) | 199 (99%) | 2 (1%) | 0 | 100 | 100 |
| 22 | LN | 201/213 (94%) | 195 (97%) | 6 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|-----|-----|
| 23 | LO | 294/305 (96%) | 288 (98%) | 6 (2%) | 0 | 100 | 100 |
| 24 | LP | 195/198 (98%) | 190 (97%) | 4 (2%) | 1 (0%) | 25 | 50 |
| 25 | LQ | 199/254 (78%) | 198 (100%) | 1 (0%) | 0 | 100 | 100 |
| 26 | LR | 176/179 (98%) | 175 (99%) | 1 (1%) | 0 | 100 | 100 |
| 27 | LS | 156/159 (98%) | 149 (96%) | 7 (4%) | 0 | 100 | 100 |
| 28 | LT | 150/166 (90%) | 146 (97%) | 4 (3%) | 0 | 100 | 100 |
| 29 | LU | 120/129 (93%) | 117 (98%) | 3 (2%) | 0 | 100 | 100 |
| 30 | LV | 117/145 (81%) | 116 (99%) | 1 (1%) | 0 | 100 | 100 |
| 31 | LW | 119/143 (83%) | 117 (98%) | 2 (2%) | 0 | 100 | 100 |
| 32 | LX | 81/124 (65%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 33 | LY | 131/134 (98%) | 131 (100%) | 0 | 0 | 100 | 100 |
| 34 | LZ | 143/147 (97%) | 141 (99%) | 2 (1%) | 0 | 100 | 100 |
| 35 | La | 123/127 (97%) | 122 (99%) | 1 (1%) | 0 | 100 | 100 |
| 36 | Lb | 66/70 (94%) | 63 (96%) | 2 (3%) | 1 (2%) | 8 | 24 |
| 37 | Lc | 227/252 (90%) | 221 (97%) | 6 (3%) | 0 | 100 | 100 |
| 38 | Ld | 95/104 (91%) | 95 (100%) | 0 | 0 | 100 | 100 |
| 39 | Le | 184/188 (98%) | 183 (100%) | 1 (0%) | 0 | 100 | 100 |
| 40 | Lf | 126/133 (95%) | 122 (97%) | 4 (3%) | 0 | 100 | 100 |
| 41 | Lg | 141/144 (98%) | 141 (100%) | 0 | 0 | 100 | 100 |
| 42 | Lh | 125/168 (74%) | 122 (98%) | 3 (2%) | 0 | 100 | 100 |
| 43 | Li | 100/105 (95%) | 98 (98%) | 2 (2%) | 0 | 100 | 100 |
| 44 | Lj | 79/83 (95%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 45 | Lk | 76/83 (92%) | 75 (99%) | 1 (1%) | 0 | 100 | 100 |
| 46 | Ll | 48/51 (94%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 47 | Lm | 50/128 (39%) | 50 (100%) | 0 | 0 | 100 | 100 |
| 48 | Ln | 31/34 (91%) | 31 (100%) | 0 | 0 | 100 | 100 |
| 49 | Lo | 87/92 (95%) | 80 (92%) | 7 (8%) | 0 | 100 | 100 |
| 50 | Lp | 95/106 (90%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 56 | SA | 240/264 (91%) | 232 (97%) | 8 (3%) | 0 | 100 | 100 |
| 57 | SB | 209/246 (85%) | 202 (97%) | 7 (3%) | 0 | 100 | 100 |
| 58 | SC | 211/219 (96%) | 207 (98%) | 4 (2%) | 0 | 100 | 100 |

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|-------------|--|
| 59 | SD | 181/190 (95%) | 178 (98%) | 3 (2%) | 0 | 100 | 100 |
| 60 | SE | 258/273 (94%) | 253 (98%) | 5 (2%) | 0 | 100 | 100 |
| 61 | SF | 220/265 (83%) | 220 (100%) | 0 | 0 | 100 | 100 |
| 62 | SG | 225/249 (90%) | 218 (97%) | 7 (3%) | 0 | 100 | 100 |
| 63 | SH | 179/190 (94%) | 177 (99%) | 2 (1%) | 0 | 100 | 100 |
| 64 | SI | 198/200 (99%) | 195 (98%) | 3 (2%) | 0 | 100 | 100 |
| 65 | SJ | 127/130 (98%) | 125 (98%) | 2 (2%) | 0 | 100 | 100 |
| 66 | SK | 188/220 (86%) | 188 (100%) | 0 | 0 | 100 | 100 |
| 67 | SL | 142/149 (95%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 68 | SM | 99/116 (85%) | 99 (100%) | 0 | 0 | 100 | 100 |
| 69 | SN | 98/168 (58%) | 93 (95%) | 4 (4%) | 1 (1%) | 13 | 32 |
| 70 | SO | 135/144 (94%) | 131 (97%) | 4 (3%) | 0 | 100 | 100 |
| 71 | SP | 139/143 (97%) | 136 (98%) | 3 (2%) | 0 | 100 | 100 |
| 72 | SQ | 96/141 (68%) | 93 (97%) | 3 (3%) | 0 | 100 | 100 |
| 73 | SR | 140/153 (92%) | 138 (99%) | 2 (1%) | 0 | 100 | 100 |
| 74 | SS | 54/57 (95%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 75 | ST | 141/151 (93%) | 139 (99%) | 2 (1%) | 0 | 100 | 100 |
| 76 | SU | 151/173 (87%) | 144 (95%) | 7 (5%) | 0 | 100 | 100 |
| 77 | SV | 120/143 (84%) | 119 (99%) | 1 (1%) | 0 | 100 | 100 |
| 78 | SW | 113/152 (74%) | 113 (100%) | 0 | 0 | 100 | 100 |
| 79 | SX | 150/161 (93%) | 144 (96%) | 6 (4%) | 0 | 100 | 100 |
| 80 | SY | 86/164 (52%) | 86 (100%) | 0 | 0 | 100 | 100 |
| 81 | SZ | 128/137 (93%) | 122 (95%) | 6 (5%) | 0 | 100 | 100 |
| 82 | Sa | 103/120 (86%) | 94 (91%) | 9 (9%) | 0 | 100 | 100 |
| 83 | Sb | 102/112 (91%) | 101 (99%) | 1 (1%) | 0 | 100 | 100 |
| 84 | Sc | 83/86 (96%) | 82 (99%) | 1 (1%) | 0 | 100 | 100 |
| 85 | Sd | 64/87 (74%) | 61 (95%) | 3 (5%) | 0 | 100 | 100 |
| 86 | Se | 59/66 (89%) | 57 (97%) | 2 (3%) | 0 | 100 | 100 |
| 87 | Sf | 78/152 (51%) | 73 (94%) | 5 (6%) | 0 | 100 | 100 |
| 88 | Sg | 297/312 (95%) | 286 (96%) | 11 (4%) | 0 | 100 | 100 |
| 89 | Sh | 94/235 (40%) | 92 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|----------|----------|---------|----------|-------------|
| All | All | 11480/12926 (89%) | 11208 (98%) | 268 (2%) | 4 (0%) | 100   100 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 69 | SN | 40 | ASN |
| 36 | Lb | 10 | HIS |
| 20 | LL | 40 | HIS |
| 24 | LP | 189 | SER |

### 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|------|------|
| 9 | LA | 200/204 (98%) | 188 (94%) | 12 (6%) | 16 | 35 |
| 10 | LB | 337/351 (96%) | 325 (96%) | 12 (4%) | 30 | 54 |
| 11 | LC | 291/301 (97%) | 271 (93%) | 20 (7%) | 13 | 30 |
| 12 | LD | 147/162 (91%) | 135 (92%) | 12 (8%) | 9 | 23 |
| 13 | LE | 166/172 (96%) | 154 (93%) | 12 (7%) | 12 | 29 |
| 14 | LF | 122/153 (80%) | 114 (93%) | 8 (7%) | 14 | 31 |
| 15 | LG | 198/221 (90%) | 189 (96%) | 9 (4%) | 23 | 47 |
| 16 | LH | 182/188 (97%) | 172 (94%) | 10 (6%) | 18 | 39 |
| 17 | LI | 178/183 (97%) | 170 (96%) | 8 (4%) | 23 | 47 |
| 18 | LJ | 106/111 (96%) | 103 (97%) | 3 (3%) | 38 | 63 |
| 19 | LK | 138/145 (95%) | 130 (94%) | 8 (6%) | 17 | 37 |
| 20 | LL | 113/114 (99%) | 105 (93%) | 8 (7%) | 12 | 29 |
| 21 | LM | 178/180 (99%) | 164 (92%) | 14 (8%) | 10 | 24 |
| 22 | LN | 175/179 (98%) | 153 (87%) | 22 (13%) | 3 | 10 |
| 23 | LO | 232/242 (96%) | 222 (96%) | 10 (4%) | 25 | 49 |
| 24 | LP | 163/164 (99%) | 157 (96%) | 6 (4%) | 29 | 53 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 25 | LQ | 170/198 (86%) | 159 (94%) | 11 (6%) | 14 | 32 |
| 26 | LR | 157/159 (99%) | 149 (95%) | 8 (5%) | 20 | 42 |
| 27 | LS | 132/134 (98%) | 123 (93%) | 9 (7%) | 13 | 31 |
| 28 | LT | 127/143 (89%) | 122 (96%) | 5 (4%) | 27 | 52 |
| 29 | LU | 93/114 (82%) | 87 (94%) | 6 (6%) | 14 | 32 |
| 30 | LV | 102/124 (82%) | 99 (97%) | 3 (3%) | 37 | 62 |
| 31 | LW | 104/122 (85%) | 100 (96%) | 4 (4%) | 28 | 52 |
| 32 | LX | 74/104 (71%) | 71 (96%) | 3 (4%) | 26 | 50 |
| 33 | LY | 111/116 (96%) | 105 (95%) | 6 (5%) | 18 | 40 |
| 34 | LZ | 114/118 (97%) | 108 (95%) | 6 (5%) | 19 | 40 |
| 35 | La | 114/118 (97%) | 112 (98%) | 2 (2%) | 54 | 75 |
| 36 | Lb | 56/58 (97%) | 52 (93%) | 4 (7%) | 12 | 29 |
| 37 | Lc | 191/209 (91%) | 183 (96%) | 8 (4%) | 25 | 49 |
| 38 | Ld | 85/89 (96%) | 82 (96%) | 3 (4%) | 31 | 55 |
| 39 | Le | 154/158 (98%) | 149 (97%) | 5 (3%) | 34 | 59 |
| 40 | Lf | 111/115 (96%) | 109 (98%) | 2 (2%) | 54 | 75 |
| 41 | Lg | 120/121 (99%) | 116 (97%) | 4 (3%) | 33 | 57 |
| 42 | Lh | 107/146 (73%) | 101 (94%) | 6 (6%) | 17 | 39 |
| 43 | Li | 84/88 (96%) | 81 (96%) | 3 (4%) | 30 | 54 |
| 44 | Lj | 68/70 (97%) | 66 (97%) | 2 (3%) | 37 | 62 |
| 45 | Lk | 65/74 (88%) | 63 (97%) | 2 (3%) | 35 | 59 |
| 46 | Ll | 46/47 (98%) | 43 (94%) | 3 (6%) | 14 | 32 |
| 47 | Lm | 43/113 (38%) | 40 (93%) | 3 (7%) | 12 | 29 |
| 48 | Ln | 31/32 (97%) | 30 (97%) | 1 (3%) | 34 | 59 |
| 49 | Lo | 69/74 (93%) | 65 (94%) | 4 (6%) | 17 | 37 |
| 50 | Lp | 83/92 (90%) | 77 (93%) | 6 (7%) | 12 | 29 |
| 56 | SA | 206/222 (93%) | 193 (94%) | 13 (6%) | 15 | 33 |
| 57 | SB | 178/202 (88%) | 170 (96%) | 8 (4%) | 23 | 47 |
| 58 | SC | 176/184 (96%) | 157 (89%) | 19 (11%) | 5 | 14 |
| 59 | SD | 159/164 (97%) | 146 (92%) | 13 (8%) | 9 | 23 |
| 60 | SE | 216/225 (96%) | 195 (90%) | 21 (10%) | 6 | 18 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|-----|-----|
| 61 | SF | 182/208 (88%) | 173 (95%) | 9 (5%) | 21 | 43 |
| 62 | SG | 190/208 (91%) | 161 (85%) | 29 (15%) | 2 | 6 |
| 63 | SH | 153/159 (96%) | 143 (94%) | 10 (6%) | 14 | 32 |
| 64 | SI | 181/186 (97%) | 166 (92%) | 15 (8%) | 9 | 22 |
| 65 | SJ | 110/111 (99%) | 105 (96%) | 5 (4%) | 23 | 47 |
| 66 | SK | 157/176 (89%) | 142 (90%) | 15 (10%) | 7 | 18 |
| 67 | SL | 116/120 (97%) | 110 (95%) | 6 (5%) | 19 | 41 |
| 68 | SM | 92/104 (88%) | 84 (91%) | 8 (9%) | 8 | 21 |
| 69 | SN | 88/128 (69%) | 81 (92%) | 7 (8%) | 10 | 23 |
| 70 | SO | 104/113 (92%) | 99 (95%) | 5 (5%) | 21 | 44 |
| 71 | SP | 114/117 (97%) | 105 (92%) | 9 (8%) | 10 | 24 |
| 72 | SQ | 57/120 (48%) | 52 (91%) | 5 (9%) | 8 | 21 |
| 73 | SR | 120/130 (92%) | 109 (91%) | 11 (9%) | 7 | 19 |
| 74 | SS | 47/49 (96%) | 44 (94%) | 3 (6%) | 14 | 33 |
| 75 | ST | 126/132 (96%) | 116 (92%) | 10 (8%) | 10 | 24 |
| 76 | SU | 135/152 (89%) | 120 (89%) | 15 (11%) | 5 | 13 |
| 77 | SV | 109/126 (86%) | 102 (94%) | 7 (6%) | 14 | 33 |
| 78 | SW | 98/130 (75%) | 94 (96%) | 4 (4%) | 26 | 50 |
| 79 | SX | 122/131 (93%) | 114 (93%) | 8 (7%) | 14 | 31 |
| 80 | SY | 72/116 (62%) | 67 (93%) | 5 (7%) | 13 | 30 |
| 81 | SZ | 111/118 (94%) | 97 (87%) | 14 (13%) | 3 | 10 |
| 82 | Sa | 83/95 (87%) | 73 (88%) | 10 (12%) | 4 | 11 |
| 83 | Sb | 85/93 (91%) | 78 (92%) | 7 (8%) | 9 | 23 |
| 84 | Sc | 75/76 (99%) | 68 (91%) | 7 (9%) | 7 | 19 |
| 85 | Sd | 52/75 (69%) | 47 (90%) | 5 (10%) | 7 | 18 |
| 86 | Se | 52/54 (96%) | 48 (92%) | 4 (8%) | 10 | 25 |
| 87 | Sf | 70/126 (56%) | 59 (84%) | 11 (16%) | 2 | 5 |
| 88 | Sg | 259/265 (98%) | 237 (92%) | 22 (8%) | 8 | 22 |
| 89 | Sh | 79/177 (45%) | 67 (85%) | 12 (15%) | 2 | 6 |
| All | All | 9711/10798 (90%) | 9066 (93%) | 645 (7%) | 16 | 31 |

5 of 645 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 68 | SM | 110 | SER |
| 82 | Sa | 58 | LYS |
| 71 | SP | 2 | THR |
| 68 | SM | 87 | ASP |
| 76 | SU | 43 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | Lg | 25 | ASN |
| 59 | SD | 3 | ASN |
| 80 | SY | 66 | GLN |
| 23 | LO | 120 | GLN |
| 34 | LZ | 35 | ASN |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | L1 | 1667/1782 (93%) | 447 (26%) | 18 (1%) |
| 2 | L2 | 1148/1526 (75%) | 279 (24%) | 14 (1%) |
| 3 | L3 | 178/216 (82%) | 44 (24%) | 3 (1%) |
| 4 | L4 | 183/184 (99%) | 43 (23%) | 2 (1%) |
| 5 | L5 | 117/135 (86%) | 32 (27%) | 3 (2%) |
| 51 | S1 | 1819/2204 (82%) | 436 (23%) | 26 (1%) |
| 52 | S2 | 74/76 (97%) | 27 (36%) | 8 (10%) |
| 53 | S3 | 74/77 (96%) | 19 (25%) | 2 (2%) |
| 54 | S4 | 72/76 (94%) | 37 (51%) | 1 (1%) |
| 55 | S5 | 11/13 (84%) | 6 (54%) | 0 |
| 6 | L6 | 70/73 (95%) | 32 (45%) | 1 (1%) |
| 7 | L7 | 164/171 (95%) | 40 (24%) | 2 (1%) |
| 8 | L8 | 119/124 (95%) | 19 (15%) | 1 (0%) |
| All | All | 5696/6657 (85%) | 1461 (25%) | 81 (1%) |

5 of 1461 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | L1 | 6 | C |
| 1 | L1 | 7 | C |
| 1 | L1 | 16 | G |
| 1 | L1 | 24 | A |
| 1 | L1 | 29 | C |

5 of 81 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 51 | S1 | 937 | C |
| 52 | S2 | 13 | C |
| 51 | S1 | 1209 | C |
| 51 | S1 | 1858 | G |
| 52 | S2 | 48 | C |

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

170 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 | $\#|Z| > 2$ |
| 2 | A2M | L2 | 591 | 2,92 | 18,25,26 | 4.26 | 7 (38%) | 18,36,39 | 2.60 | 3 (16%) |
| 1 | OMU | L1 | 48 | 1 | 19,22,23 | 0.35 | 0 | 26,31,34 | 1.03 | 2 (7%) |
| 51 | OMU | S1 | 1621 | 90,51 | 19,22,23 | 3.02 | 8 (42%) | 26,31,34 | 1.72 | 5 (19%) |
| 51 | PSU | S1 | 2046 | 51 | 18,21,22 | 4.47 | 7 (38%) | 22,30,33 | 1.82 | 5 (22%) |
| 2 | A2M | L2 | 570 | 1,2 | 18,25,26 | 4.24 | 6 (33%) | 18,36,39 | 2.75 | 3 (16%) |
| 51 | PSU | S1 | 1192 | 51 | 18,21,22 | 4.46 | 7 (38%) | 22,30,33 | 1.72 | 5 (22%) |
| 2 | PSU | L2 | 1060 | 2 | 18,21,22 | 4.44 | 7 (38%) | 22,30,33 | 1.93 | 5 (22%) |
| 51 | OMG | S1 | 1623 | 51,91 | 18,26,27 | 2.55 | 8 (44%) | 19,38,41 | 1.52 | 4 (21%) |
| 1 | A2M | L1 | 955 | 1 | 18,25,26 | 0.63 | 1 (5%) | 18,36,39 | 0.77 | 1 (5%) |
| 51 | A2M | S1 | 479 | 51 | 18,25,26 | 4.24 | 7 (38%) | 18,36,39 | 2.66 | 3 (16%) |
| 51 | OMG | S1 | 2151 | 51 | 18,26,27 | 2.53 | 8 (44%) | 19,38,41 | 1.57 | 5 (26%) |
| 1 | OMU | L1 | 845 | 1 | 19,22,23 | 0.35 | 0 | 26,31,34 | 0.84 | 0 |
| 1 | PSU | L1 | 510 | 1 | 18,21,22 | 0.90 | 1 (5%) | 22,30,33 | 0.64 | 0 |
| 1 | PSU | L1 | 940 | 1 | 18,21,22 | 4.45 | 7 (38%) | 22,30,33 | 1.80 | 5 (22%) |
| 2 | OMG | L2 | 1078 | 2 | 18,26,27 | 2.50 | 8 (44%) | 19,38,41 | 1.72 | 5 (26%) |
| 1 | PSU | L1 | 313 | 1 | 18,21,22 | 4.44 | 7 (38%) | 22,30,33 | 1.71 | 4 (18%) |
| 2 | PSU | L2 | 1144 | 2 | 18,21,22 | 4.44 | 7 (38%) | 22,30,33 | 1.88 | 5 (22%) |
| 2 | A2M | L2 | 572 | 2 | 18,25,26 | 4.26 | 7 (38%) | 18,36,39 | 2.66 | 3 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|---------|--------|------|---------|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 51 | A2M | S1 | 2021 | 51 | 18,25,26 | 0.61 | 0 | 18,36,39 | 0.81 | 1 (5%) |
| 51 | PSU | S1 | 1292 | 90,51,91 | 18,21,22 | 4.42 | 7 (38%) | 22,30,33 | 1.77 | 5 (22%) |
| 1 | OMG | L1 | 856 | 1 | 18,26,27 | 2.53 | 8 (44%) | 19,38,41 | 1.55 | 5 (26%) |
| 1 | PSU | L1 | 1529 | 1 | 18,21,22 | 4.44 | 7 (38%) | 22,30,33 | 1.81 | 5 (22%) |
| 2 | OMC | L2 | 1159 | 2 | 19,22,23 | 0.29 | 0 | 26,31,34 | 0.49 | 0 |
| 2 | OMG | L2 | 71 | 2,92 | 18,26,27 | 2.58 | 8 (44%) | 19,38,41 | 1.60 | 4 (21%) |
| 2 | A2M | L2 | 1067 | 2 | 18,25,26 | 0.64 | 1 (5%) | 18,36,39 | 0.75 | 1 (5%) |
| 51 | OMU | S1 | 1833 | 51 | 19,22,23 | 3.02 | 8 (42%) | 26,31,34 | 1.81 | 5 (19%) |
| 2 | A2M | L2 | 628 | 2 | 18,25,26 | 0.63 | 1 (5%) | 18,36,39 | 0.73 | 1 (5%) |
| 2 | OMG | L2 | 1253 | 2 | 18,26,27 | 2.47 | 8 (44%) | 19,38,41 | 1.59 | 5 (26%) |
| 1 | OMG | L1 | 1190 | 1,90 | 18,26,27 | 2.51 | 8 (44%) | 19,38,41 | 1.69 | 5 (26%) |
| 1 | A2M | L1 | 407 | 1 | 18,25,26 | 4.25 | 6 (33%) | 18,36,39 | 2.64 | 3 (16%) |
| 2 | OMG | L2 | 641 | 2 | 18,26,27 | 2.52 | 8 (44%) | 19,38,41 | 1.60 | 5 (26%) |
| 2 | PSU | L2 | 1213 | 2 | 18,21,22 | 4.43 | 7 (38%) | 22,30,33 | 1.84 | 5 (22%) |
| 51 | 7MG | S1 | 1995 | 51,53 | 22,26,27 | 4.24 | 10 (45%) | 29,39,42 | 2.06 | 9 (31%) |
| 2 | PSU | L2 | 472 | 2 | 18,21,22 | 4.45 | 7 (38%) | 22,30,33 | 1.76 | 5 (22%) |
| 2 | PSU | L2 | 1194 | 2 | 18,21,22 | 4.46 | 7 (38%) | 22,30,33 | 1.77 | 4 (18%) |
| 51 | OMC | S1 | 2140 | 51 | 19,22,23 | 3.02 | 8 (42%) | 26,31,34 | 0.78 | 0 |
| 7 | PSU | L7 | 101 | 7 | 18,21,22 | 4.40 | 8 (44%) | 22,30,33 | 1.81 | 6 (27%) |
| 51 | 5MC | S1 | 2061 | 51 | 18,22,23 | 3.48 | 7 (38%) | 26,32,35 | 0.94 | 1 (3%) |
| 51 | A2M | S1 | 897 | 51 | 18,25,26 | 4.25 | 6 (33%) | 18,36,39 | 2.71 | 3 (16%) |
| 1 | PSU | L1 | 774 | 1 | 18,21,22 | 0.87 | 1 (5%) | 22,30,33 | 0.79 | 1 (4%) |
| 2 | PSU | L2 | 662 | 90,2 | 18,21,22 | 4.40 | 7 (38%) | 22,30,33 | 1.75 | 5 (22%) |
| 1 | OMU | L1 | 1107 | 1 | 19,22,23 | 3.01 | 8 (42%) | 26,31,34 | 1.75 | 4 (15%) |
| 2 | OMC | L2 | 1397 | 2 | 19,22,23 | 2.93 | 8 (42%) | 26,31,34 | 0.79 | 0 |
| 51 | PSU | S1 | 1533 | 51 | 18,21,22 | 4.49 | 7 (38%) | 22,30,33 | 1.81 | 5 (22%) |
| 2 | PSU | L2 | 437 | 2 | 18,21,22 | 0.85 | 1 (5%) | 22,30,33 | 0.67 | 0 |
| 51 | OMG | S1 | 1550 | 51 | 18,26,27 | 1.02 | 3 (16%) | 19,38,41 | 0.68 | 0 |
| 2 | A2M | L2 | 665 | 2 | 18,25,26 | 4.23 | 7 (38%) | 18,36,39 | 2.69 | 3 (16%) |
| 2 | OMU | L2 | 1077 | 2 | 19,22,23 | 3.01 | 8 (42%) | 26,31,34 | 1.70 | 4 (15%) |
| 51 | OMC | S1 | 38 | 51 | 19,22,23 | 3.00 | 8 (42%) | 26,31,34 | 0.84 | 0 |
| 7 | PSU | L7 | 166 | 1,7 | 18,21,22 | 4.49 | 7 (38%) | 22,30,33 | 1.81 | 5 (22%) |
| 1 | PSU | L1 | 1528 | 1 | 18,21,22 | 4.46 | 7 (38%) | 22,30,33 | 1.80 | 5 (22%) |
| 4 | OMG | L4 | 74 | 4 | 18,26,27 | 1.03 | 3 (16%) | 19,38,41 | 0.65 | 0 |
| 1 | A2M | L1 | 1373 | 1 | 18,25,26 | 4.22 | 6 (33%) | 18,36,39 | 2.70 | 3 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 1 | PSU | L1 | 1526 | 1 | 18,21,22 | 4.46 | 8 (44%) | 22,30,33 | 1.85 | 6 (27%) |
| 1 | PSU | L1 | 672 | 1,90 | 18,21,22 | 0.85 | 1 (5%) | 22,30,33 | 0.61 | 0 |
| 51 | PSU | S1 | 455 | 51 | 18,21,22 | 4.53 | 7 (38%) | 22,30,33 | 1.72 | 4 (18%) |
| 2 | A2M | L2 | 1185 | 2 | 18,25,26 | 4.19 | 6 (33%) | 18,36,39 | 2.72 | 3 (16%) |
| 1 | A2M | L1 | 697 | 1 | 18,25,26 | 4.24 | 7 (38%) | 18,36,39 | 2.65 | 3 (16%) |
| 51 | PSU | S1 | 12 | 51 | 18,21,22 | 0.88 | 1 (5%) | 22,30,33 | 0.63 | 0 |
| 2 | PSU | L2 | 1318 | 2 | 18,21,22 | 4.44 | 7 (38%) | 22,30,33 | 1.85 | 5 (22%) |
| 2 | PSU | L2 | 1303 | 2 | 18,21,22 | 4.48 | 7 (38%) | 22,30,33 | 1.86 | 6 (27%) |
| 52 | MIA | S2 | 37 | 52 | 24,31,32 | 2.43 | 3 (12%) | 26,44,47 | 4.88 | 10 (38%) |
| 1 | A2M | L1 | 235 | 1 | 18,25,26 | 4.24 | 7 (38%) | 18,36,39 | 2.67 | 3 (16%) |
| 1 | PSU | L1 | 1017 | 1,91 | 18,21,22 | 4.43 | 7 (38%) | 22,30,33 | 1.82 | 5 (22%) |
| 51 | A2M | S1 | 668 | 90,51 | 18,25,26 | 4.14 | 7 (38%) | 18,36,39 | 2.75 | 4 (22%) |
| 51 | A2M | S1 | 28 | 51 | 18,25,26 | 4.27 | 7 (38%) | 18,36,39 | 2.58 | 3 (16%) |
| 51 | PSU | S1 | 1539 | 51 | 18,21,22 | 4.48 | 7 (38%) | 22,30,33 | 1.79 | 5 (22%) |
| 2 | OMC | L2 | 359 | 2 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 0.70 | 0 |
| 1 | A2M | L1 | 1539 | 1,90,2 | 18,25,26 | 4.22 | 7 (38%) | 18,36,39 | 2.73 | 3 (16%) |
| 2 | A2M | L2 | 604 | 1,2 | 18,25,26 | 4.26 | 6 (33%) | 18,36,39 | 2.63 | 3 (16%) |
| 1 | A2M | L1 | 858 | 1 | 18,25,26 | 4.23 | 6 (33%) | 18,36,39 | 2.70 | 3 (16%) |
| 7 | OMG | L7 | 75 | 7 | 18,26,27 | 2.56 | 8 (44%) | 19,38,41 | 1.53 | 4 (21%) |
| 2 | 5MC | L2 | 524 | 90,2 | 18,22,23 | 0.34 | 0 | 26,32,35 | 0.53 | 0 |
| 51 | MA6 | S1 | 2184 | 51 | 18,26,27 | 1.16 | 2 (11%) | 19,38,41 | 2.91 | 2 (10%) |
| 51 | OMC | S1 | 1866 | 51 | 19,22,23 | 2.96 | 8 (42%) | 26,31,34 | 0.79 | 0 |
| 2 | PSU | L2 | 1403 | 2 | 18,21,22 | 4.47 | 7 (38%) | 22,30,33 | 1.87 | 6 (27%) |
| 2 | PSU | L2 | 1265 | 2 | 18,21,22 | 4.45 | 7 (38%) | 22,30,33 | 1.70 | 4 (18%) |
| 1 | OMG | L1 | 1540 | 1,2 | 18,26,27 | 1.04 | 3 (16%) | 19,38,41 | 0.67 | 0 |
| 2 | OMG | L2 | 1360 | 2,52 | 18,26,27 | 2.55 | 8 (44%) | 19,38,41 | 1.49 | 4 (21%) |
| 1 | PSU | L1 | 1177 | 1 | 18,21,22 | 4.46 | 7 (38%) | 22,30,33 | 1.73 | 5 (22%) |
| 1 | PSU | L1 | 1181 | 1 | 18,21,22 | 4.47 | 7 (38%) | 22,30,33 | 1.81 | 5 (22%) |
| 51 | PSU | S1 | 1246 | 51 | 18,21,22 | 4.49 | 7 (38%) | 22,30,33 | 1.82 | 5 (22%) |
| 1 | OMU | L1 | 1659 | 1,90 | 19,22,23 | 2.97 | 8 (42%) | 26,31,34 | 1.68 | 4 (15%) |
| 2 | PSU | L2 | 504 | 2 | 18,21,22 | 4.52 | 7 (38%) | 22,30,33 | 1.84 | 5 (22%) |
| 2 | 5MC | L2 | 1308 | 2 | 18,22,23 | 4.65 | 12 (66%) | 26,32,35 | 1.26 | 2 (7%) |
| 2 | OMC | L2 | 443 | 90,2,91 | 19,22,23 | 0.37 | 0 | 26,31,34 | 0.58 | 0 |
| 51 | PSU | S1 | 1566 | 51 | 18,21,22 | 4.52 | 8 (44%) | 22,30,33 | 1.72 | 4 (18%) |
| 2 | PSU | L2 | 1152 | 2 | 18,21,22 | 4.45 | 7 (38%) | 22,30,33 | 1.93 | 5 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 2 | OMG | L2 | 1231 | 2 | 18,26,27 | 2.52 | 8 (44%) | 19,38,41 | 1.54 | 5 (26%) |
| 2 | OMU | L2 | 560 | 2 | 19,22,23 | 0.26 | 0 | 26,31,34 | 1.21 | 3 (11%) |
| 51 | OMC | S1 | 18 | 51 | 19,22,23 | 2.93 | 8 (42%) | 26,31,34 | 0.80 | 0 |
| 1 | A2M | L1 | 927 | 1 | 18,25,26 | 4.23 | 7 (38%) | 18,36,39 | 2.60 | 3 (16%) |
| 2 | PSU | L2 | 1284 | 2 | 18,21,22 | 4.50 | 7 (38%) | 22,30,33 | 1.80 | 5 (22%) |
| 2 | A2M | L2 | 527 | 90,2 | 18,25,26 | 4.09 | 7 (38%) | 18,36,39 | 2.77 | 4 (22%) |
| 7 | A2M | L7 | 162 | 1,7 | 18,25,26 | 4.27 | 6 (33%) | 18,36,39 | 2.62 | 3 (16%) |
| 1 | OMC | L1 | 695 | 1 | 19,22,23 | 2.90 | 8 (42%) | 26,31,34 | 0.70 | 0 |
| 51 | A2M | S1 | 512 | 51 | 18,25,26 | 4.27 | 7 (38%) | 18,36,39 | 2.61 | 3 (16%) |
| 3 | OMU | L3 | 13 | 3 | 19,22,23 | 3.01 | 8 (42%) | 26,31,34 | 1.76 | 4 (15%) |
| 2 | PSU | L2 | 597 | 2 | 18,21,22 | 4.42 | 7 (38%) | 22,30,33 | 1.78 | 5 (22%) |
| 51 | OMU | S1 | 1662 | 51 | 19,22,23 | 3.02 | 8 (42%) | 26,31,34 | 1.68 | 4 (15%) |
| 51 | PSU | S1 | 2202 | 51 | 18,21,22 | 4.43 | 8 (44%) | 22,30,33 | 1.71 | 5 (22%) |
| 2 | OMC | L2 | 583 | 2 | 19,22,23 | 2.93 | 8 (42%) | 26,31,34 | 0.70 | 0 |
| 2 | OMG | L2 | 1046 | 90,2,53 | 18,26,27 | 2.53 | 8 (44%) | 19,38,41 | 1.50 | 4 (21%) |
| 2 | OMU | L2 | 1359 | 2,92 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 1.68 | 4 (15%) |
| 51 | OMG | S1 | 1865 | 51 | 18,26,27 | 2.59 | 8 (44%) | 19,38,41 | 1.57 | 4 (21%) |
| 1 | A2M | L1 | 678 | 1,2 | 18,25,26 | 0.63 | 1 (5%) | 18,36,39 | 0.77 | 1 (5%) |
| 2 | PSU | L2 | 626 | 2 | 18,21,22 | 4.43 | 7 (38%) | 22,30,33 | 1.71 | 4 (18%) |
| 1 | PSU | L1 | 1011 | 1,2 | 18,21,22 | 0.79 | 1 (5%) | 22,30,33 | 0.75 | 0 |
| 2 | OMG | L2 | 686 | 2 | 18,26,27 | 2.57 | 8 (44%) | 19,38,41 | 1.55 | 5 (26%) |
| 51 | OMU | S1 | 1979 | 51 | 19,22,23 | 3.05 | 8 (42%) | 26,31,34 | 1.71 | 4 (15%) |
| 51 | PSU | S1 | 33 | 51 | 18,21,22 | 4.52 | 7 (38%) | 22,30,33 | 1.80 | 5 (22%) |
| 51 | OMG | S1 | 1647 | 51 | 18,26,27 | 2.58 | 8 (44%) | 19,38,41 | 1.62 | 4 (21%) |
| 2 | PSU | L2 | 1264 | 2,91 | 18,21,22 | 4.41 | 8 (44%) | 22,30,33 | 1.70 | 4 (18%) |
| 2 | PSU | L2 | 593 | 2,92 | 18,21,22 | 4.41 | 7 (38%) | 22,30,33 | 1.70 | 5 (22%) |
| 2 | OMC | L2 | 1248 | 2 | 19,22,23 | 2.97 | 8 (42%) | 26,31,34 | 0.86 | 0 |
| 2 | OMC | L2 | 14 | 1,2 | 19,22,23 | 0.30 | 0 | 26,31,34 | 0.65 | 1 (3%) |
| 2 | PSU | L2 | 1413 | 2 | 18,21,22 | 4.37 | 7 (38%) | 22,30,33 | 1.82 | 5 (22%) |
| 2 | A2M | L2 | 382 | 2 | 18,25,26 | 4.27 | 6 (33%) | 18,36,39 | 2.64 | 3 (16%) |
| 1 | OMC | L1 | 1527 | 1,90 | 19,22,23 | 2.95 | 8 (42%) | 26,31,34 | 0.79 | 0 |
| 51 | OMU | S1 | 29 | 51 | 19,22,23 | 3.04 | 8 (42%) | 26,31,34 | 1.71 | 5 (19%) |
| 2 | PSU | L2 | 1361 | 2,92,52 | 18,21,22 | 4.48 | 7 (38%) | 22,30,33 | 1.80 | 5 (22%) |
| 51 | PSU | S1 | 1657 | 51 | 18,21,22 | 4.46 | 7 (38%) | 22,30,33 | 1.77 | 5 (22%) |
| 1 | OMU | L1 | 847 | 1 | 19,22,23 | 0.23 | 0 | 26,31,34 | 0.62 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\|>2 | Counts | RMSZ | #\|Z\|>2 |
| 1 | PSU | L1 | 1533 | 1,2 | 18,21,22 | 4.45 | 7 (38%) | 22,30,33 | 1.87 | 5 (22%) |
| 2 | PSU | L2 | 802 | 2 | 18,21,22 | 4.49 | 7 (38%) | 22,30,33 | 1.81 | 6 (27%) |
| 2 | A2M | L2 | 95 | 2 | 18,25,26 | 4.25 | 7 (38%) | 18,36,39 | 2.68 | 3 (16%) |
| 2 | OMG | L2 | 655 | 2 | 18,26,27 | 2.55 | 8 (44%) | 19,38,41 | 1.63 | 6 (31%) |
| 2 | OMU | L2 | 1419 | 2 | 19,22,23 | 2.97 | 8 (42%) | 26,31,34 | 1.67 | 4 (15%) |
| 1 | OMG | L1 | 959 | 1 | 18,26,27 | 1.03 | 3 (16%) | 19,38,41 | 0.98 | 1 (5%) |
| 51 | B8N | S1 | 1543 | - | 24,29,30 | 4.25 | 14 (58%) | 29,42,45 | 2.00 | 7 (24%) |
| 1 | PSU | L1 | 239 | 1 | 18,21,22 | 0.88 | 1 (5%) | 22,30,33 | 0.65 | 0 |
| 2 | OMU | L2 | 667 | 2 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 1.72 | 4 (15%) |
| 51 | A2M | S1 | 98 | 90,51 | 18,25,26 | 4.26 | 7 (38%) | 18,36,39 | 2.60 | 3 (16%) |
| 2 | OMG | L2 | 534 | 2 | 18,26,27 | 2.53 | 8 (44%) | 19,38,41 | 1.48 | 4 (21%) |
| 2 | A2M | L2 | 1384 | 90,2 | 18,25,26 | 4.24 | 6 (33%) | 18,36,39 | 2.66 | 3 (16%) |
| 7 | A2M | L7 | 43 | 90,7 | 18,25,26 | 4.26 | 6 (33%) | 18,36,39 | 2.82 | 3 (16%) |
| 2 | PSU | L2 | 1058 | 2 | 18,21,22 | 4.46 | 7 (38%) | 22,30,33 | 1.95 | 5 (22%) |
| 51 | OMU | S1 | 8 | 51 | 19,22,23 | 0.24 | 0 | 26,31,34 | 0.60 | 1 (3%) |
| 2 | A2M | L2 | 647 | 2 | 18,25,26 | 4.19 | 8 (44%) | 18,36,39 | 2.68 | 3 (16%) |
| 2 | A2M | L2 | 502 | 2 | 18,25,26 | 4.22 | 8 (44%) | 18,36,39 | 2.71 | 3 (16%) |
| 51 | MA6 | S1 | 2185 | 90,51 | 18,26,27 | 1.11 | 1 (5%) | 19,38,41 | 3.17 | 2 (10%) |
| 1 | A2M | L1 | 69 | 1 | 18,25,26 | 4.14 | 6 (33%) | 18,36,39 | 2.82 | 5 (27%) |
| 51 | 5MC | S1 | 1544 | 51 | 18,22,23 | 0.32 | 0 | 26,32,35 | 0.52 | 0 |
| 51 | OMC | S1 | 2059 | 51 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 1.22 | 2 (7%) |
| 2 | OMU | L2 | 73 | 2,92 | 19,22,23 | 3.02 | 8 (42%) | 26,31,34 | 1.67 | 4 (15%) |
| 1 | PSU | L1 | 1664 | 1 | 18,21,22 | 0.89 | 1 (5%) | 22,30,33 | 0.65 | 0 |
| 2 | PSU | L2 | 78 | 2 | 18,21,22 | 4.43 | 7 (38%) | 22,30,33 | 1.81 | 5 (22%) |
| 2 | PSU | L2 | 512 | 2 | 18,21,22 | 4.49 | 7 (38%) | 22,30,33 | 1.78 | 5 (22%) |
| 51 | OMG | S1 | 1829 | 90,51 | 18,26,27 | 1.03 | 3 (16%) | 19,38,41 | 0.64 | 0 |
| 1 | OMC | L1 | 1010 | 1,90,91 | 19,22,23 | 0.31 | 0 | 26,31,34 | 0.44 | 0 |
| 51 | OMG | S1 | 600 | 51 | 18,26,27 | 2.55 | 8 (44%) | 19,38,41 | 1.52 | 4 (21%) |
| 2 | PSU | L2 | 510 | 2 | 18,21,22 | 4.45 | 7 (38%) | 22,30,33 | 1.77 | 5 (22%) |
| 51 | OMU | S1 | 661 | 51 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 1.67 | 5 (19%) |
| 2 | OMG | L2 | 1229 | 2 | 18,26,27 | 2.55 | 8 (44%) | 19,38,41 | 1.53 | 4 (21%) |
| 1 | OMG | L1 | 1626 | 1 | 18,26,27 | 1.01 | 3 (16%) | 19,38,41 | 0.83 | 1 (5%) |
| 2 | PSU | L2 | 500 | 2 | 18,21,22 | 4.47 | 7 (38%) | 22,30,33 | 1.80 | 5 (22%) |
| 2 | A2M | L2 | 1372 | 2 | 18,25,26 | 4.25 | 6 (33%) | 18,36,39 | 2.72 | 3 (16%) |
| 1 | A2M | L1 | 681 | 1 | 18,25,26 | 0.60 | 0 | 18,36,39 | 0.74 | 1 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 7 | PSU | L7 | 74 | 7 | 18,21,22 | 4.49 | 7 (38%) | 22,30,33 | 1.82 | 5 (22%) |
| 51 | PSU | S1 | 2048 | 51 | 18,21,22 | 0.87 | 1 (5%) | 22,30,33 | 0.75 | 0 |
| 1 | A2M | L1 | 305 | 1 | 18,25,26 | 4.17 | 8 (44%) | 18,36,39 | 2.76 | 5 (27%) |
| 51 | OMG | S1 | 1478 | 51 | 18,26,27 | 2.53 | 8 (44%) | 19,38,41 | 1.59 | 5 (26%) |
| 1 | PSU | L1 | 1171 | 1,91 | 18,21,22 | 4.46 | 8 (44%) | 22,30,33 | 1.77 | 4 (18%) |
| 1 | OMG | L1 | 1524 | 1 | 18,26,27 | 2.56 | 8 (44%) | 19,38,41 | 1.74 | 6 (31%) |
| 2 | OMU | L2 | 56 | 1,2 | 19,22,23 | 3.01 | 8 (42%) | 26,31,34 | 1.72 | 4 (15%) |
| 7 | PSU | L7 | 69 | 90,7 | 18,21,22 | 4.44 | 7 (38%) | 22,30,33 | 1.82 | 6 (27%) |
| 1 | OMU | L1 | 1371 | 1 | 19,22,23 | 3.08 | 8 (42%) | 26,31,34 | 1.87 | 6 (23%) |
| 1 | PSU | L1 | 422 | 1 | 18,21,22 | 4.47 | 7 (38%) | 22,30,33 | 1.73 | 5 (22%) |
| 2 | OMC | L2 | 1317 | 2 | 19,22,23 | 2.92 | 8 (42%) | 26,31,34 | 0.75 | 0 |
| 2 | PSU | L2 | 565 | 2 | 18,21,22 | 0.87 | 1 (5%) | 22,30,33 | 0.72 | 1 (4%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | A2M | L2 | 591 | 2,92 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMU | L1 | 48 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 51 | OMU | S1 | 1621 | 90,51 | - | 0/9/27/28 | 0/2/2/2 |
| 51 | PSU | S1 | 2046 | 51 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | L2 | 570 | 1,2 | - | 0/5/27/28 | 0/3/3/3 |
| 51 | PSU | S1 | 1192 | 51 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 1060 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | OMG | S1 | 1623 | 51,91 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | L1 | 955 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 51 | A2M | S1 | 479 | 51 | - | 0/5/27/28 | 0/3/3/3 |
| 51 | OMG | S1 | 2151 | 51 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | OMU | L1 | 845 | 1 | - | 3/9/27/28 | 0/2/2/2 |
| 1 | PSU | L1 | 510 | 1 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | PSU | L1 | 940 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMG | L2 | 1078 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | PSU | L1 | 313 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 1144 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | L2 | 572 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 51 | A2M | S1 | 2021 | 51 | - | 1/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 51 | PSU | S1 | 1292 | 90,51,91 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | L1 | 856 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | L1 | 1529 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMC | L2 | 1159 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMG | L2 | 71 | 2,92 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | A2M | L2 | 1067 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 51 | OMU | S1 | 1833 | 51 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | A2M | L2 | 628 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | L2 | 1253 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMG | L1 | 1190 | 1,90 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | L1 | 407 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | L2 | 641 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | L2 | 1213 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | 7MG | S1 | 1995 | 51,53 | - | 2/7/37/38 | 0/3/3/3 |
| 2 | PSU | L2 | 472 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 1194 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | OMC | S1 | 2140 | 51 | - | 3/9/27/28 | 0/2/2/2 |
| 7 | PSU | L7 | 101 | 7 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | 5MC | S1 | 2061 | 51 | - | 2/7/25/26 | 0/2/2/2 |
| 51 | A2M | S1 | 897 | 51 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | L1 | 774 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 662 | 90,2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | L1 | 1107 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMC | L2 | 1397 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 51 | PSU | S1 | 1533 | 51 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 437 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | OMG | S1 | 1550 | 51 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | A2M | L2 | 665 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | OMU | L2 | 1077 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 51 | OMC | S1 | 38 | 51 | - | 0/9/27/28 | 0/2/2/2 |
| 7 | PSU | L7 | 166 | 1,7 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | L1 | 1528 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 4 | OMG | L4 | 74 | 4 | - | 3/5/27/28 | 0/3/3/3 |
| 1 | A2M | L1 | 1373 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | L1 | 1526 | 1 | - | 4/7/25/26 | 0/2/2/2 |
| 1 | PSU | L1 | 672 | 1,90 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | PSU | S1 | 455 | 51 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | A2M | L2 | 1185 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | A2M | L1 | 697 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 51 | PSU | S1 | 12 | 51 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 2 | PSU | L2 | 1318 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 1303 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 52 | MIA | S2 | 37 | 52 | - | 0/11/33/34 | 0/3/3/3 |
| 1 | A2M | L1 | 235 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | L1 | 1017 | 1,91 | - | 2/7/25/26 | 0/2/2/2 |
| 51 | A2M | S1 | 668 | 90,51 | - | 3/5/27/28 | 0/3/3/3 |
| 51 | A2M | S1 | 28 | 51 | - | 0/5/27/28 | 0/3/3/3 |
| 51 | PSU | S1 | 1539 | 51 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMC | L2 | 359 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | A2M | L1 | 1539 | 1,90,2 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | A2M | L2 | 604 | 1,2 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | L1 | 858 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 7 | OMG | L7 | 75 | 7 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | 5MC | L2 | 524 | 90,2 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | MA6 | S1 | 2184 | 51 | - | 0/7/29/30 | 0/3/3/3 |
| 51 | OMC | S1 | 1866 | 51 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | PSU | L2 | 1403 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 1265 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | L1 | 1540 | 1,2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | OMG | L2 | 1360 | 2,52 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | L1 | 1177 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | L1 | 1181 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | PSU | S1 | 1246 | 51 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | L1 | 1659 | 1,90 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | PSU | L2 | 504 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 5MC | L2 | 1308 | 2 | - | 4/7/25/26 | 0/2/2/2 |
| 2 | OMC | L2 | 443 | 90,2,91 | - | 4/9/27/28 | 0/2/2/2 |
| 51 | PSU | S1 | 1566 | 51 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 1152 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMG | L2 | 1231 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMU | L2 | 560 | 2 | - | 3/9/27/28 | 0/2/2/2 |
| 51 | OMC | S1 | 18 | 51 | - | 1/9/27/28 | 0/2/2/2 |
| 1 | A2M | L1 | 927 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | L2 | 1284 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | L2 | 527 | 90,2 | - | 3/5/27/28 | 0/3/3/3 |
| 7 | A2M | L7 | 162 | 1,7 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | OMC | L1 | 695 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 51 | A2M | S1 | 512 | 51 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | OMU | L3 | 13 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | PSU | L2 | 597 | 2 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 51 | OMU | S1 | 1662 | 51 | - | 1/9/27/28 | 0/2/2/2 |
| 51 | PSU | S1 | 2202 | 51 | - | 1/7/25/26 | 0/2/2/2 |
| 2 | OMC | L2 | 583 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMG | L2 | 1046 | 90,2,53 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | OMU | L2 | 1359 | 2,92 | - | 0/9/27/28 | 0/2/2/2 |
| 51 | OMG | S1 | 1865 | 51 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | L1 | 678 | 1,2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | L2 | 626 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | L1 | 1011 | 1,2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMG | L2 | 686 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 51 | OMU | S1 | 1979 | 51 | - | 1/9/27/28 | 0/2/2/2 |
| 51 | PSU | S1 | 33 | 51 | - | 2/7/25/26 | 0/2/2/2 |
| 51 | OMG | S1 | 1647 | 51 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | L2 | 1264 | 2,91 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 593 | 2,92 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMC | L2 | 1248 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | OMC | L2 | 14 | 1,2 | - | 2/9/27/28 | 0/2/2/2 |
| 2 | PSU | L2 | 1413 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | L2 | 382 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMC | L1 | 1527 | 1,90 | - | 1/9/27/28 | 0/2/2/2 |
| 51 | OMU | S1 | 29 | 51 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | PSU | L2 | 1361 | 2,92,52 | - | 5/7/25/26 | 0/2/2/2 |
| 51 | PSU | S1 | 1657 | 51 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | OMU | L1 | 847 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | L1 | 1533 | 1,2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 802 | 2 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | A2M | L2 | 95 | 2 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | OMG | L2 | 655 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMU | L2 | 1419 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMG | L1 | 959 | 1 | - | 3/5/27/28 | 0/3/3/3 |
| 51 | B8N | S1 | 1543 | - | - | 10/16/34/35 | 0/2/2/2 |
| 1 | PSU | L1 | 239 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | L2 | 667 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 51 | A2M | S1 | 98 | 90,51 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | OMG | L2 | 534 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | A2M | L2 | 1384 | 90,2 | - | 0/5/27/28 | 0/3/3/3 |
| 7 | A2M | L7 | 43 | 90,7 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | L2 | 1058 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | OMU | S1 | 8 | 51 | - | 7/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 2 | A2M | L2 | 647 | 2 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | A2M | L2 | 502 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 51 | MA6 | S1 | 2185 | 90,51 | - | 1/7/29/30 | 0/3/3/3 |
| 1 | A2M | L1 | 69 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 51 | 5MC | S1 | 1544 | 51 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | OMC | S1 | 2059 | 51 | - | 3/9/27/28 | 0/2/2/2 |
| 2 | OMU | L2 | 73 | 2,92 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | L1 | 1664 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 78 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | L2 | 512 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | OMG | S1 | 1829 | 90,51 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | OMC | L1 | 1010 | 1,90,91 | - | 2/9/27/28 | 0/2/2/2 |
| 51 | OMG | S1 | 600 | 51 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | PSU | L2 | 510 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | OMU | S1 | 661 | 51 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMG | L2 | 1229 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | OMG | L1 | 1626 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | L2 | 500 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | L2 | 1372 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | L1 | 681 | 1 | - | 4/5/27/28 | 0/3/3/3 |
| 7 | PSU | L7 | 74 | 7 | - | 0/7/25/26 | 0/2/2/2 |
| 51 | PSU | S1 | 2048 | 51 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | A2M | L1 | 305 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 51 | OMG | S1 | 1478 | 51 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | PSU | L1 | 1171 | 1,91 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | OMG | L1 | 1524 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | OMU | L2 | 56 | 1,2 | - | 1/9/27/28 | 0/2/2/2 |
| 7 | PSU | L7 | 69 | 90,7 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | L1 | 1371 | 1 | - | 3/9/27/28 | 0/2/2/2 |
| 1 | PSU | L1 | 422 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMC | L2 | 1317 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | PSU | L2 | 565 | 2 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 1036 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 51 | S1 | 512 | A2M | O4'-C1' | 15.43 | 1.62 | 1.41 |
| 51 | S1 | 28 | A2M | O4'-C1' | 15.40 | 1.62 | 1.41 |
| 2 | L2 | 572 | A2M | O4'-C1' | 15.37 | 1.62 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 2 | L2 | 604 | A2M | O4'-C1' | 15.34 | 1.62 | 1.41 |
| 1 | L1 | 407 | A2M | O4'-C1' | 15.34 | 1.62 | 1.41 |

The worst 5 of 568 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 52 | S2 | 37 | MIA | C1'-N9-C4 | 17.12 | 156.72 | 126.64 |
| 51 | S1 | 2185 | MA6 | N1-C6-N6 | -12.27 | 104.14 | 117.06 |
| 52 | S2 | 37 | MIA | C11-S10-C2 | 11.54 | 110.89 | 102.27 |
| 51 | S1 | 2184 | MA6 | N1-C6-N6 | -11.14 | 105.33 | 117.06 |
| 52 | S2 | 37 | MIA | S10-C2-N3 | 8.91 | 147.02 | 116.10 |

There are no chirality outliers.

5 of 157 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 7 | L7 | 162 | A2M | C1'-C2'-O2'-CM' |
| 1 | L1 | 48 | OMU | O4'-C1'-N1-C2 |
| 1 | L1 | 48 | OMU | O4'-C1'-N1-C6 |
| 1 | L1 | 305 | A2M | O4'-C4'-C5'-O5' |
| 1 | L1 | 510 | PSU | C2'-C1'-C5-C6 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 520 ligands modelled in this entry, 519 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|----------|--------|------|----------|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 93 | A1H4F | L2 | 1601 | - | 32,32,32 | 4.25 | 11 (34%) | 37,42,42 | 1.42 | 5 (13%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 93 | A1H4F | L2 | 1601 | - | - | 9/26/39/39 | 0/2/2/2 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 93 | L2 | 1601 | A1H4F | C03-C02 | -16.85 | 1.28 | 1.53 |
| 93 | L2 | 1601 | A1H4F | C27-C05 | -11.96 | 1.29 | 1.53 |
| 93 | L2 | 1601 | A1H4F | C13-N14 | 6.04 | 1.46 | 1.34 |
| 93 | L2 | 1601 | A1H4F | C02-C27 | 5.95 | 1.65 | 1.53 |
| 93 | L2 | 1601 | A1H4F | O28-C29 | 3.78 | 1.43 | 1.35 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|------|------------|---------|
| 93 | L2 | 1601 | A1H4F | O28-C29-C30 | 5.01 | 120.30 | 111.09 |
| 93 | L2 | 1601 | A1H4F | C12-C13-N14 | 3.01 | 121.61 | 116.37 |
| 93 | L2 | 1601 | A1H4F | C12-O11-C10 | -2.90 | 112.57 | 117.67 |
| 93 | L2 | 1601 | A1H4F | O23-C21-C15 | 2.26 | 120.92 | 113.40 |
| 93 | L2 | 1601 | A1H4F | O23-C21-O22 | -2.08 | 119.36 | 124.09 |

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 93 | L2 | 1601 | A1H4F | C12-C13-N14-C15 |
| 93 | L2 | 1601 | A1H4F | O24-C13-N14-C15 |
| 93 | L2 | 1601 | A1H4F | C09-C10-O11-C12 |
| 93 | L2 | 1601 | A1H4F | C25-C10-O11-C12 |
| 93 | L2 | 1601 | A1H4F | N14-C15-C16-C17 |

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 then 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.



Ligand A1H4F L2 1601

Bond lengths

Bond angles

Torsions

Rings
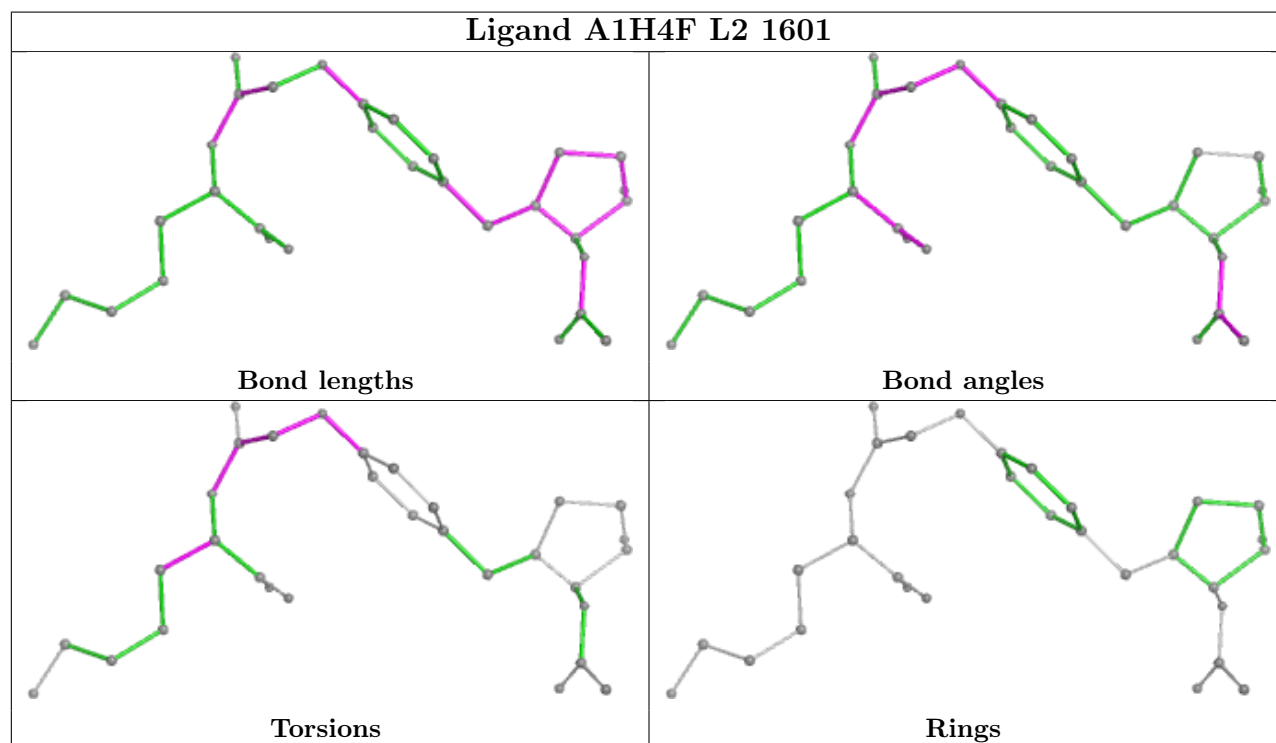
## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 51  | S1    | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 1 | S1 | 1543:B8N | O3' | 1544:5MC | P | 3.54 |
| 1 | S1 | 1542:C | O3' | 1543:B8N | P | 2.98 |

# 6  Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-19576. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

## 6.1  Orthogonal projections ⓘ
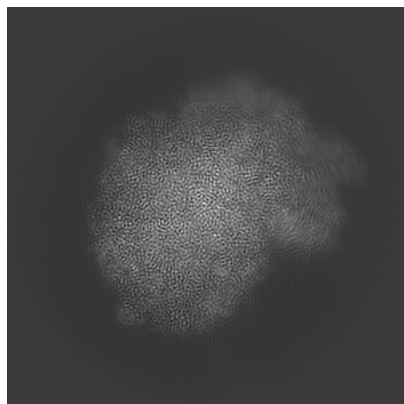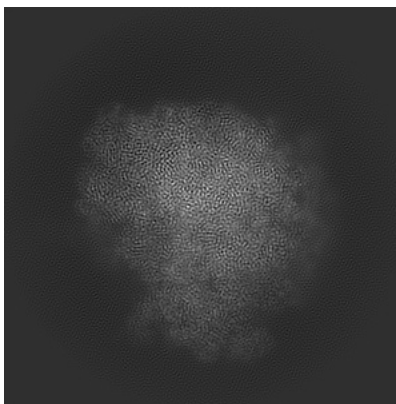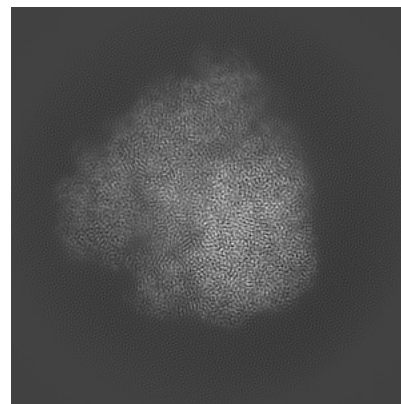
### 6.1.1  Primary map



|     |     |     |
|:---:|:---:|:---:|
| X | Y | Z |

### 6.1.2  Raw map



|     |     |     |
|:---:|:---:|:---:|
| X | Y | Z |
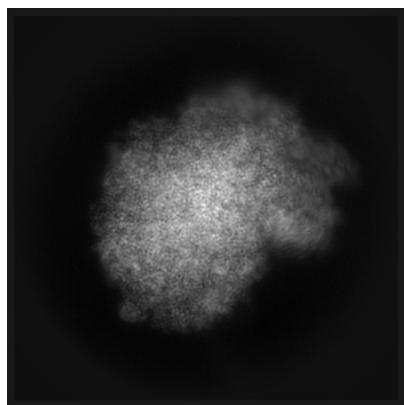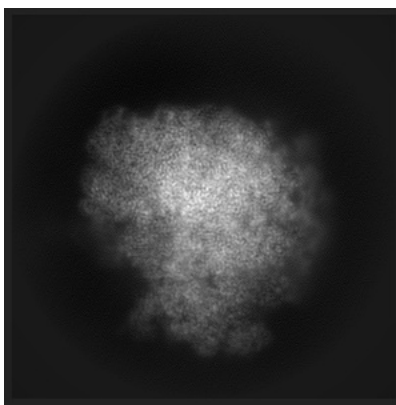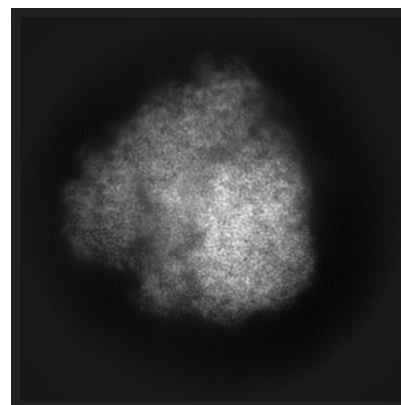
The images above show the map projected in three orthogonal directions.

## 6.2   Central slices   ⓘ
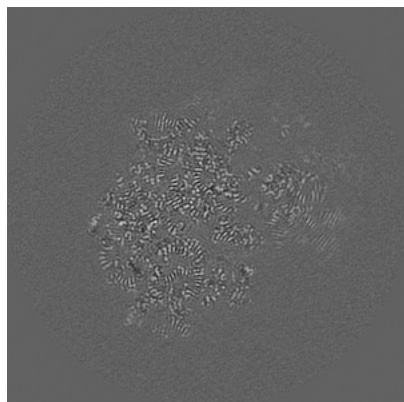
### 6.2.1   Primary map
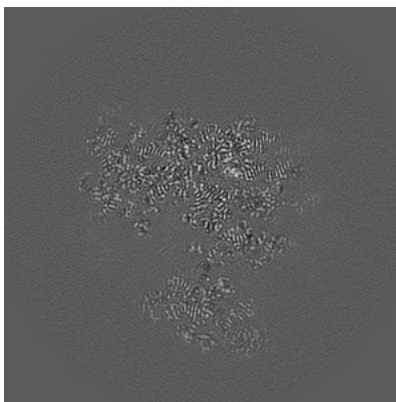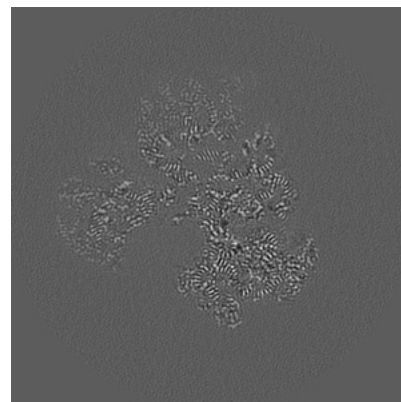


X Index: 240        Y Index: 240        Z Index: 240

### 6.2.2   Raw map
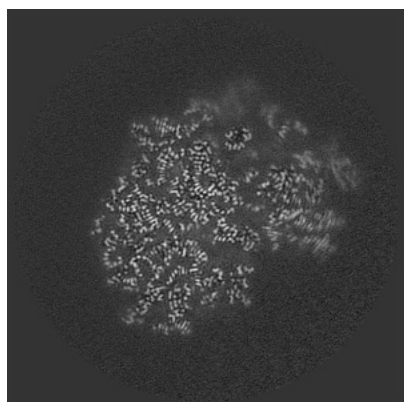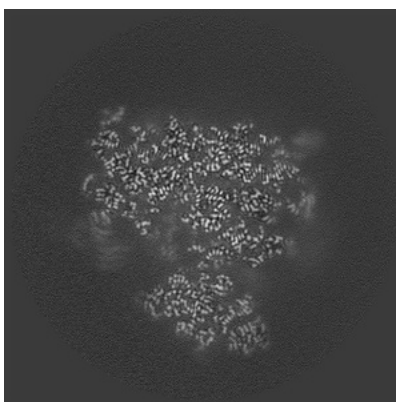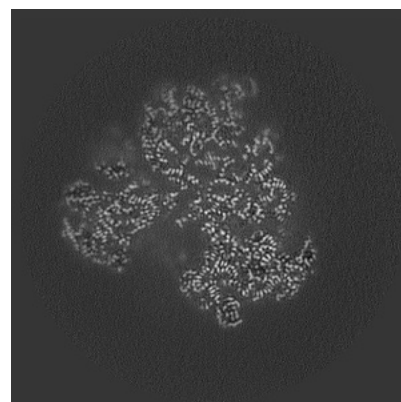


X Index: 240        Y Index: 240        Z Index: 240

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

## 6.3    Largest variance slices ⓘ

### 6.3.1    Primary map
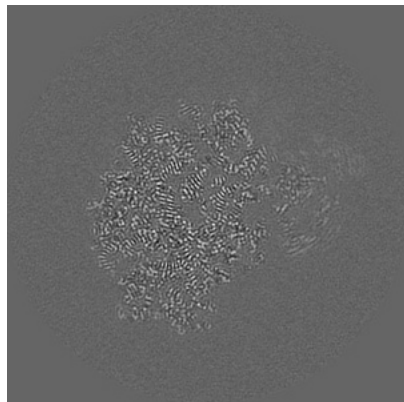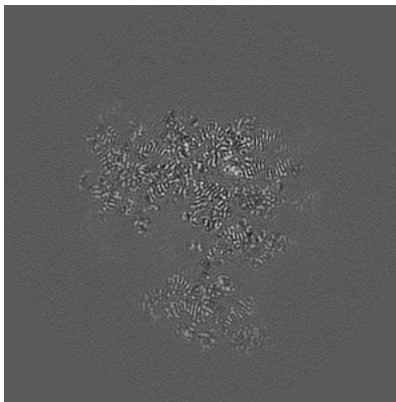


X Index: 270        Y Index: 240        Z Index: 259
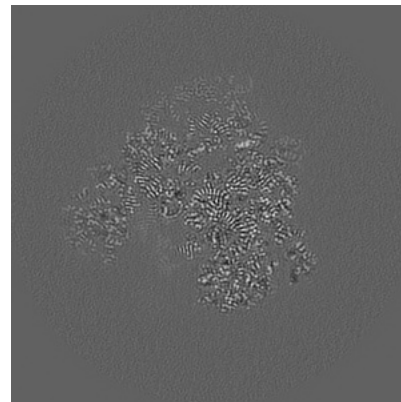
### 6.3.2    Raw map
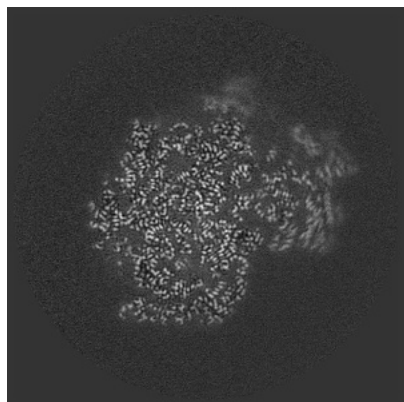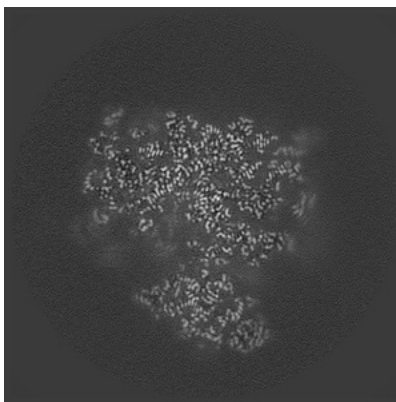


X Index: 255        Y Index: 236        Z Index: 259
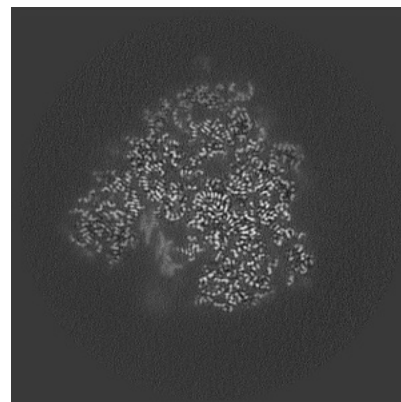
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



| X | Y | Z |

### 6.4.2 Raw map



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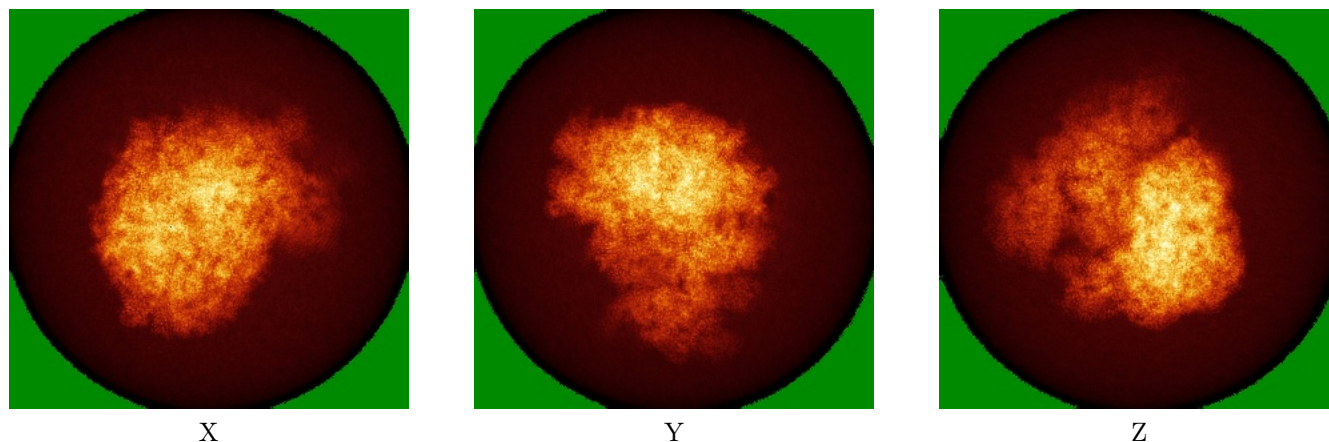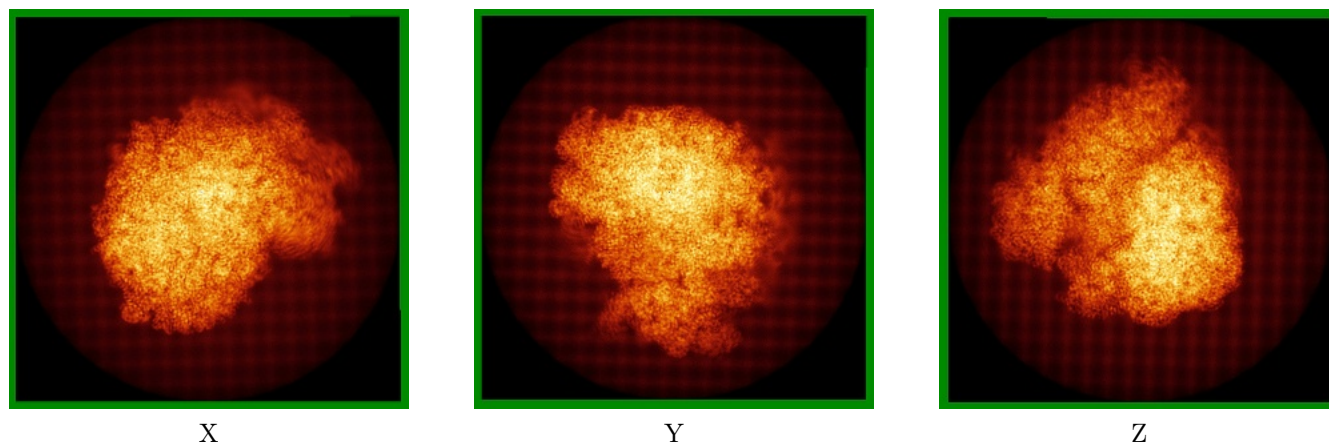
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views ⓘ

### 6.5.1 Primary map



|     |     |     |
| --- | --- | --- |
| X   | Y   | Z   |
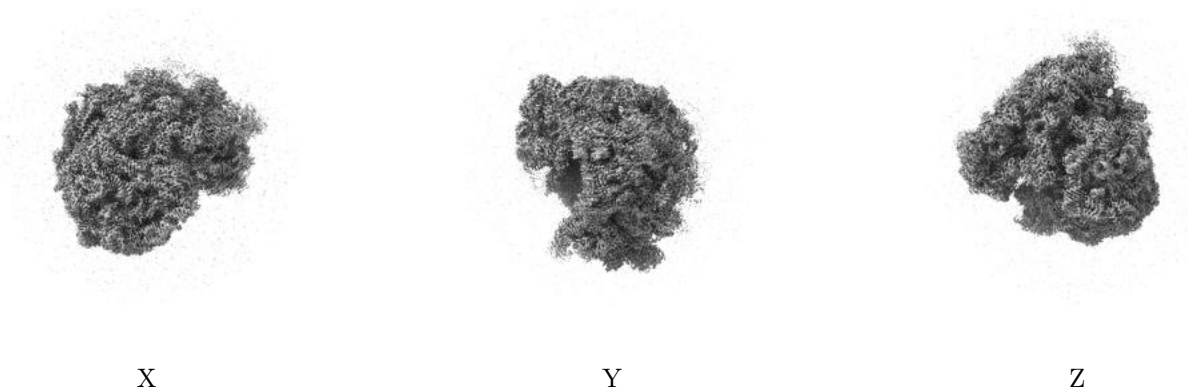
The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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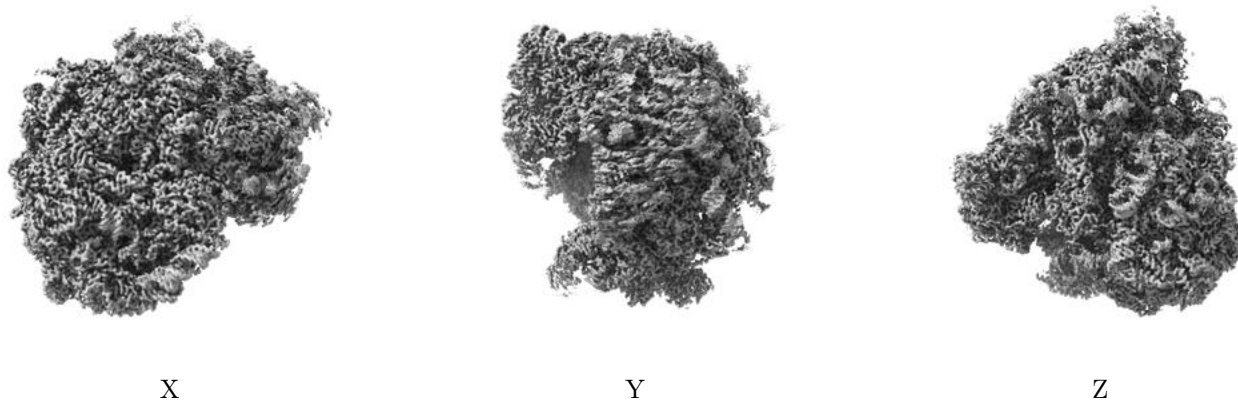
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation ⓘ

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

# 7 Map analysis ⓘ

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

## 7.1 Map-value distribution ⓘ
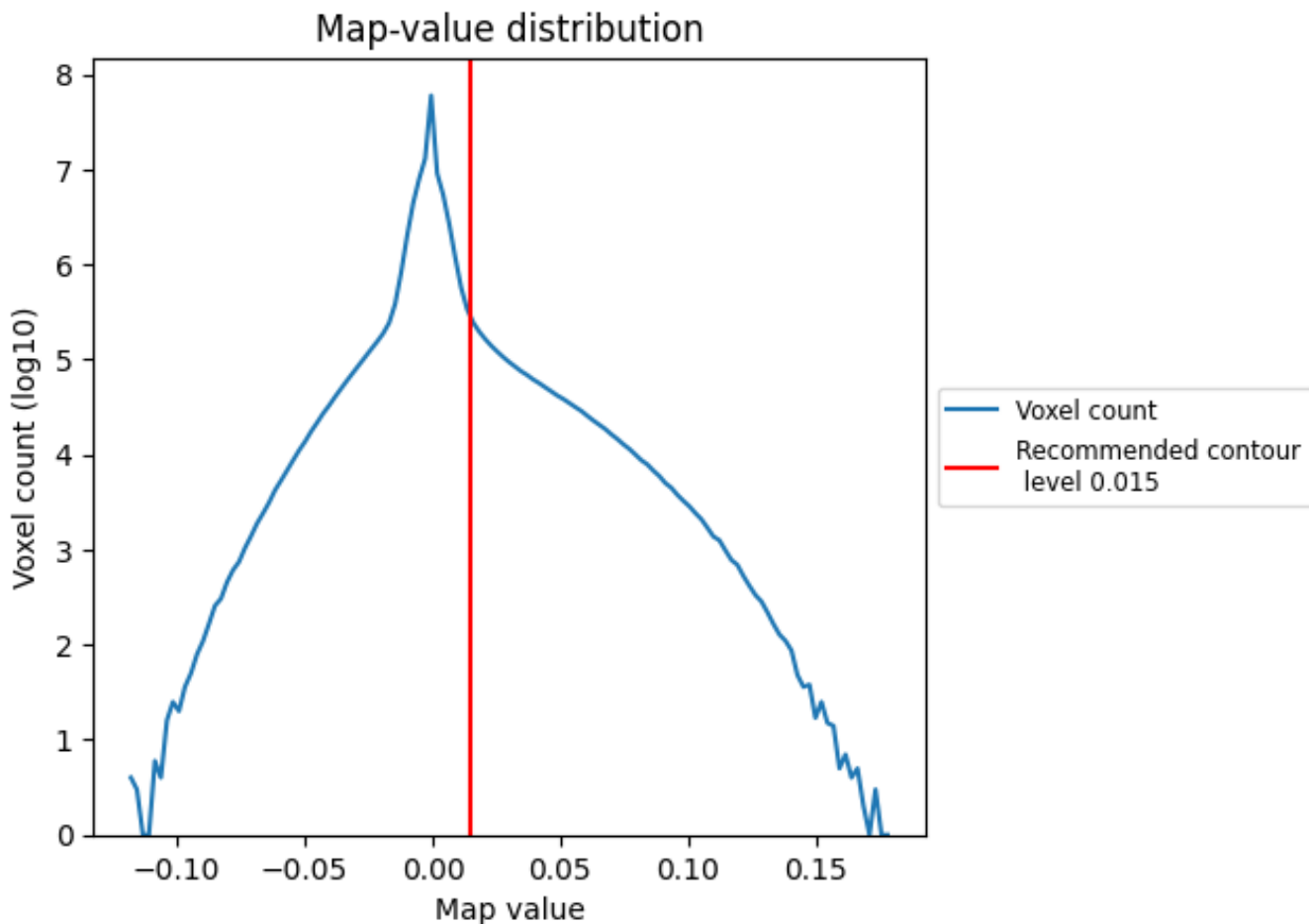


The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2　Volume estimate ⓘ
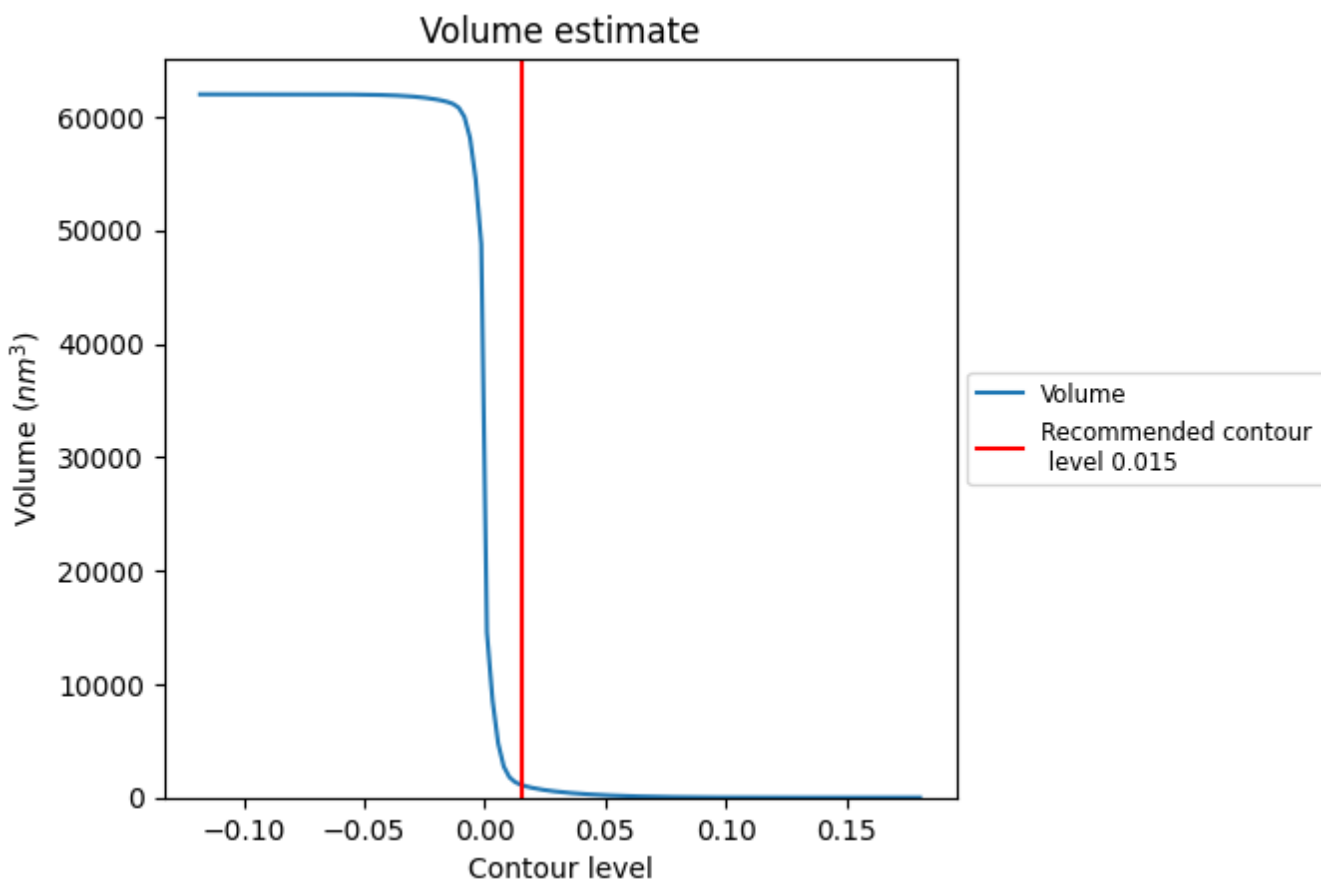


The volume at the recommended contour level is 1131 nm$^3$; this corresponds to an approximate mass of 1022 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3　Rotationally averaged power spectrum ⓘ
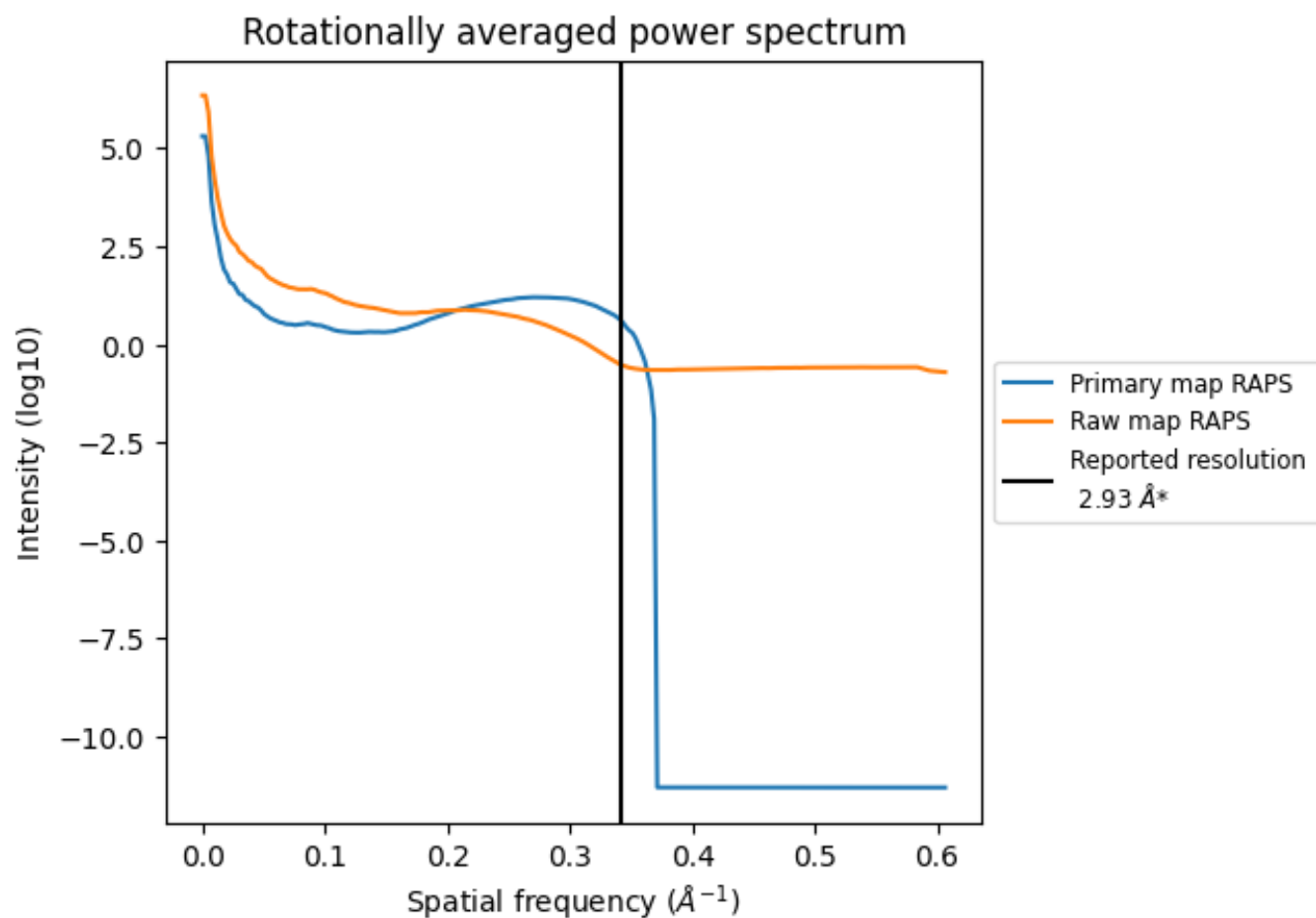


*Reported resolution corresponds to spatial frequency of 0.341 Å$^{-1}$

# 8   Fourier-Shell correlation ⓘ

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

## 8.1   FSC ⓘ
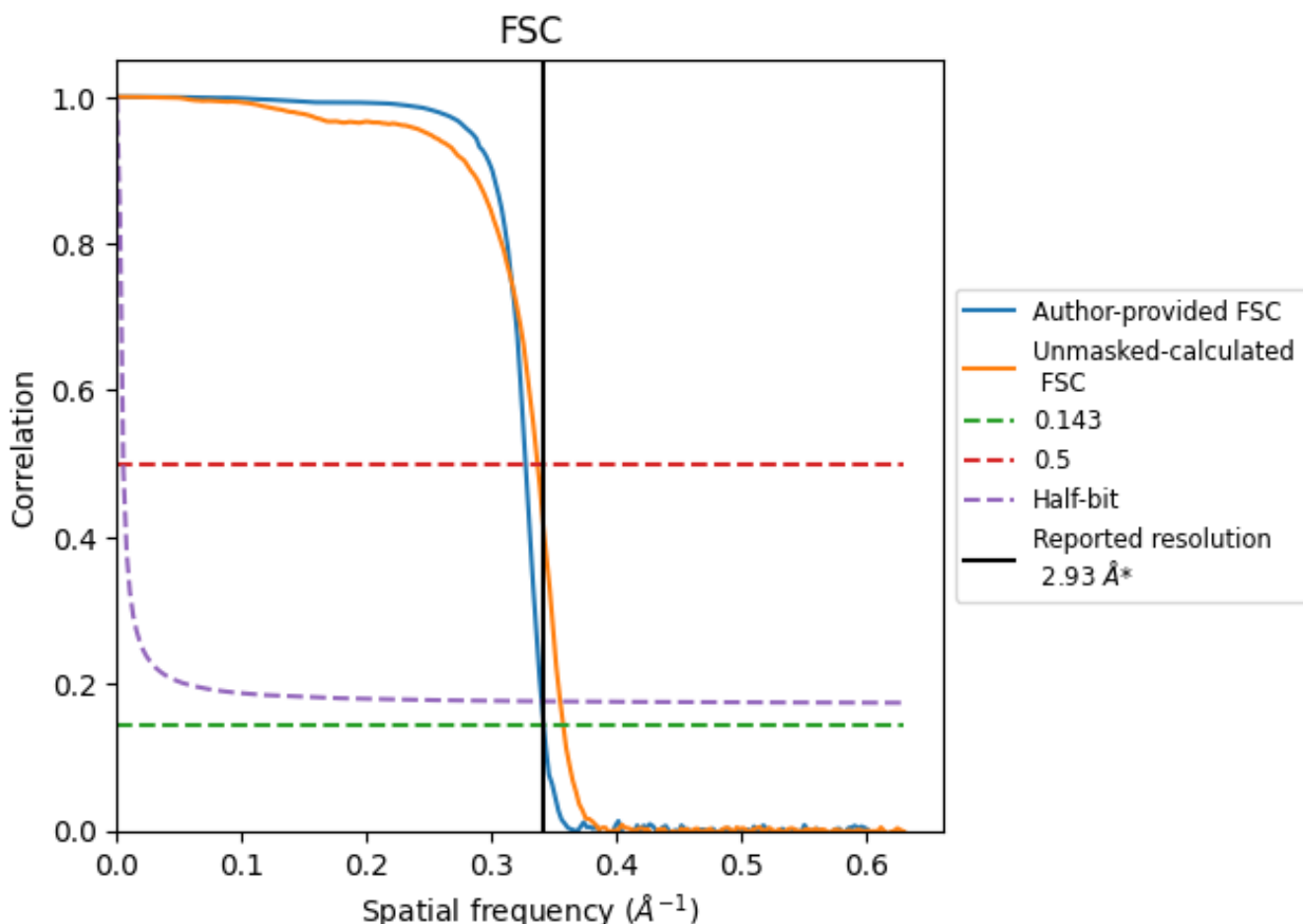


*Reported resolution corresponds to spatial frequency of 0.341 $\mathring{A}^{-1}$

## 8.2   Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.93 | - | - |
| Author-provided FSC curve | 2.92 | 3.05 | 2.94 |
| Unmasked-calculated* | 2.80 | 2.97 | 2.82 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

# 9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-19576 and PDB model 8RXH. Per-residue inclusion information can be found in section 3 on page 25.

## 9.1   Map-model overlay ⓘ



X                Y                Z
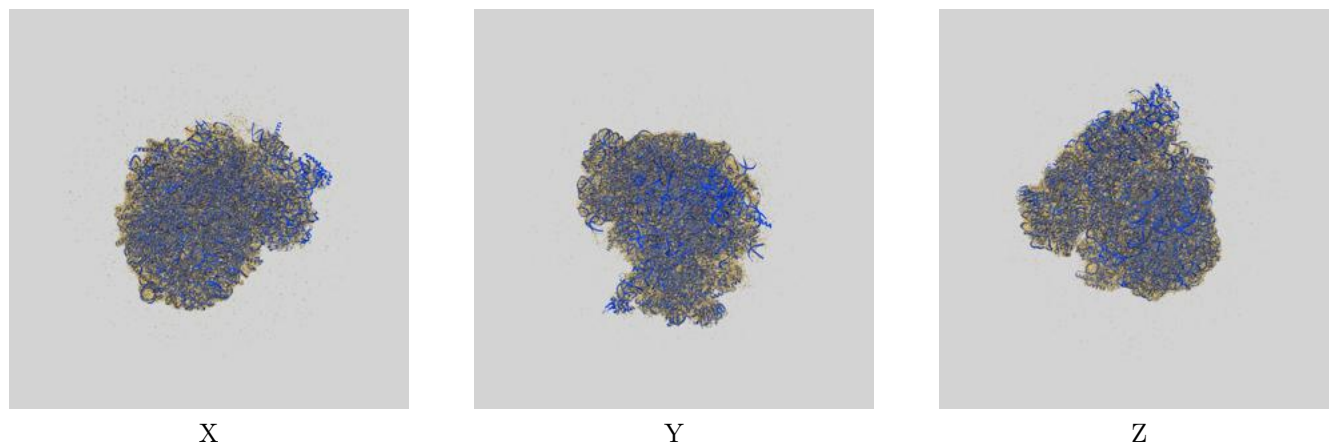
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2   Q-score mapped to coordinate model ⓘ



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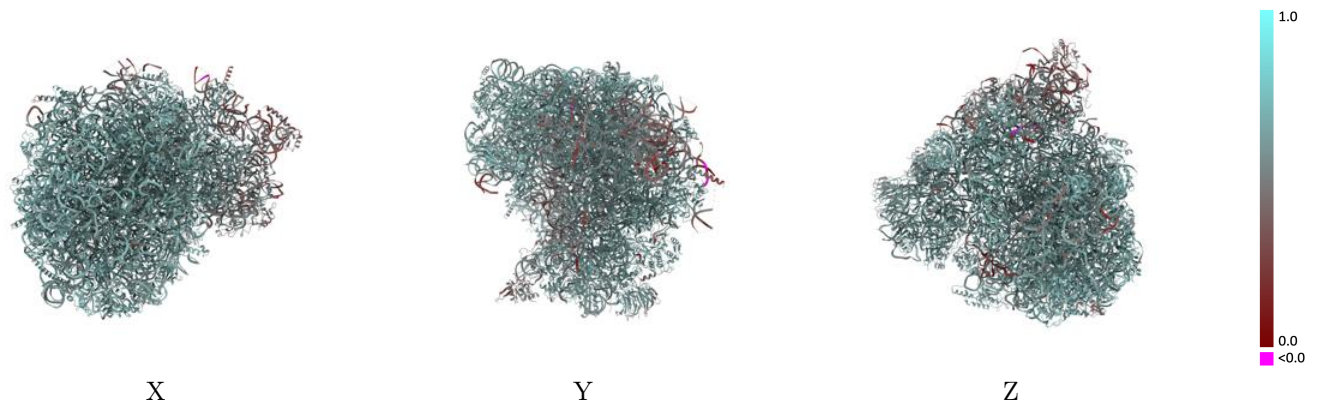
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3   Atom inclusion mapped to coordinate model ⓘ



X            Y            Z
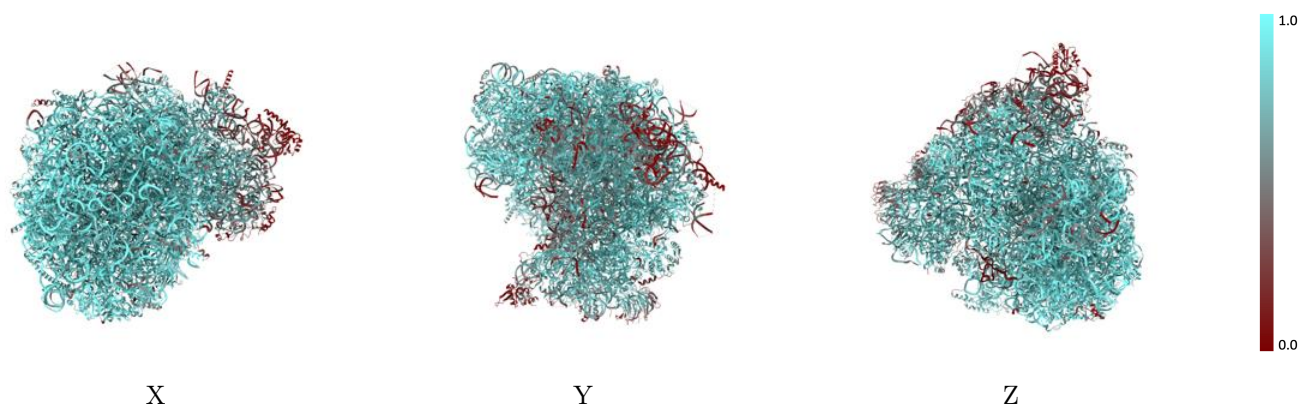
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

## 9.4 Atom inclusion ⓘ
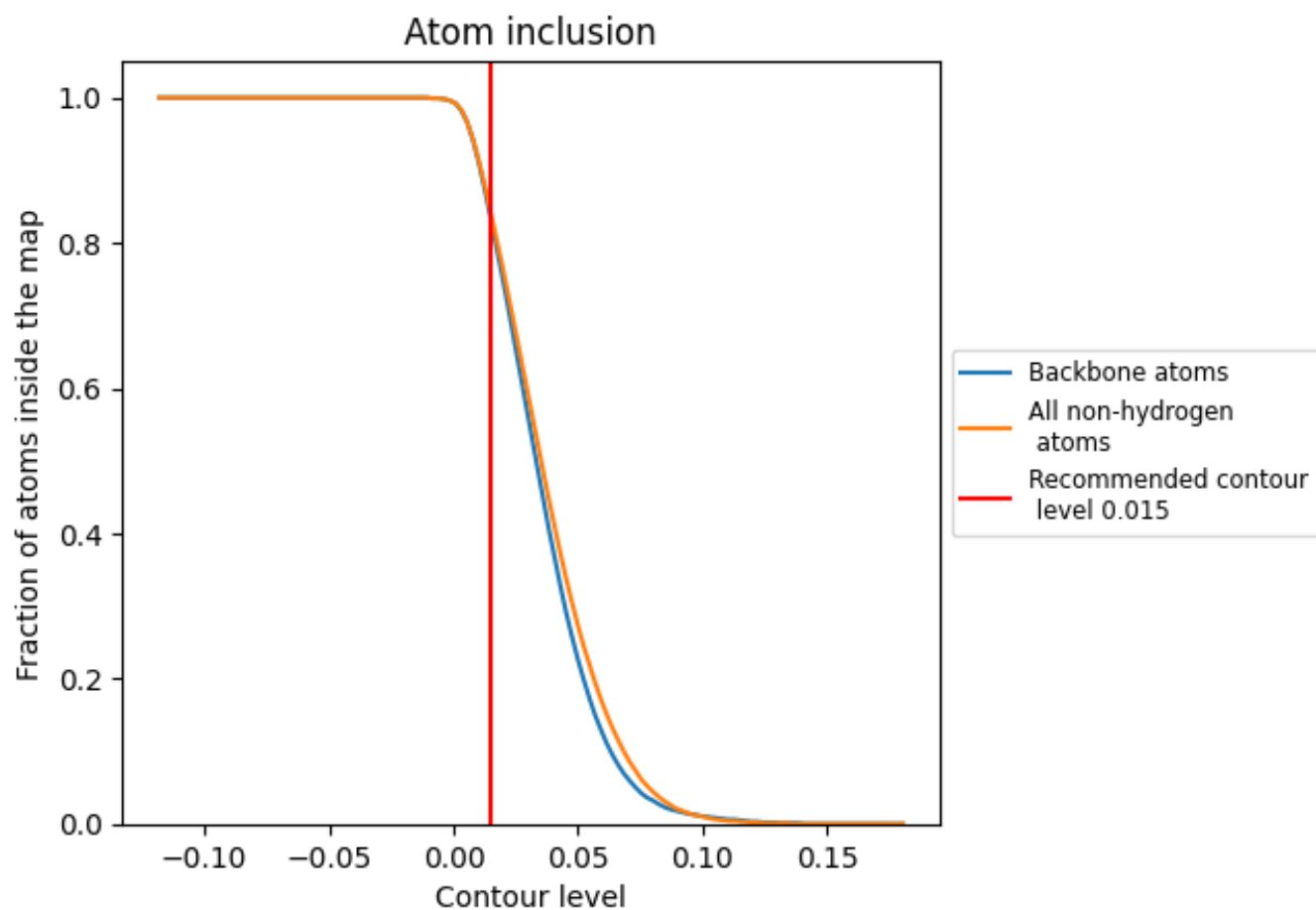


At the recommended contour level, 83% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5   Map-model fit summary   ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| All | 0.8420 | 0.6030 |
| L1 | 0.9320 | 0.6220 |
| L2 | 0.9180 | 0.6170 |
| L3 | 0.8960 | 0.6070 |
| L4 | 0.9590 | 0.6350 |
| L5 | 0.8820 | 0.6040 |
| L6 | 0.8930 | 0.6060 |
| L7 | 0.9420 | 0.6280 |
| L8 | 0.9610 | 0.6320 |
| LA | 0.9610 | 0.6540 |
| LB | 0.9350 | 0.6480 |
| LC | 0.9460 | 0.6480 |
| LD | 0.7950 | 0.6200 |
| LE | 0.9070 | 0.6430 |
| LF | 0.8420 | 0.6220 |
| LG | 0.8390 | 0.6190 |
| LH | 0.9400 | 0.6510 |
| LI | 0.8920 | 0.6400 |
| LJ | 0.9370 | 0.6450 |
| LK | 0.8420 | 0.6300 |
| LL | 0.9530 | 0.6560 |
| LM | 0.9800 | 0.6600 |
| LN | 0.8920 | 0.6370 |
| LO | 0.8180 | 0.6190 |
| LP | 0.9580 | 0.6520 |
| LQ | 0.7810 | 0.6070 |
| LR | 0.9520 | 0.6510 |
| LS | 0.9180 | 0.6380 |
| LT | 0.9700 | 0.6580 |
| LU | 0.6830 | 0.6010 |
| LV | 0.9440 | 0.6490 |
| LW | 0.9420 | 0.6530 |
| LX | 0.7440 | 0.5880 |
| LY | 0.8830 | 0.6370 |
| LZ | 0.9170 | 0.6470 |

1.0

0.0
<0.0

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W O R L D W I D E
**wwPDB**
PROTEIN DATA BANK

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| La | 0.9080 | 0.6420 |
| Lb | 0.9470 | 0.6470 |
| Lc | 0.9490 | 0.6530 |
| Ld | 0.8790 | 0.6220 |
| Le | 0.8420 | 0.6300 |
| Lf | 0.9300 | 0.6430 |
| Lg | 0.9470 | 0.6540 |
| Lh | 0.8720 | 0.6250 |
| Li | 0.8480 | 0.6220 |
| Lj | 0.9760 | 0.6570 |
| Lk | 0.8260 | 0.6310 |
| Ll | 0.9600 | 0.6520 |
| Lm | 0.9080 | 0.6390 |
| Ln | 0.9080 | 0.6330 |
| Lo | 0.9340 | 0.6380 |
| Lp | 0.9490 | 0.6520 |
| S1 | 0.7820 | 0.5580 |
| S2 | 0.2470 | 0.3850 |
| S3 | 0.6870 | 0.5430 |
| S4 | 0.3680 | 0.3940 |
| S5 | 0.8180 | 0.5790 |
| SA | 0.8530 | 0.6310 |
| SB | 0.8440 | 0.6220 |
| SC | 0.7350 | 0.6070 |
| SD | 0.5680 | 0.5300 |
| SE | 0.5580 | 0.5210 |
| SF | 0.8710 | 0.6360 |
| SG | 0.4640 | 0.5130 |
| SH | 0.8320 | 0.6220 |
| SI | 0.8130 | 0.6140 |
| SJ | 0.9330 | 0.6430 |
| SK | 0.7710 | 0.5930 |
| SL | 0.8580 | 0.6210 |
| SM | 0.6760 | 0.5900 |
| SN | 0.6840 | 0.5830 |
| SO | 0.9080 | 0.6360 |
| SP | 0.7980 | 0.5820 |
| SQ | 0.1990 | 0.4560 |
| SR | 0.7420 | 0.6060 |
| SS | 0.8920 | 0.6250 |
| ST | 0.9080 | 0.6310 |
| SU | 0.8270 | 0.6090 |

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| Chain | Atom inclusion | Q-score |
|-------|---------------|---------|
| SV | 0.6950 | 0.6010 |
| SW | 0.7130 | 0.6020 |
| SX | 0.8310 | 0.6170 |
| SY | 0.8420 | 0.6210 |
| SZ | 0.3880 | 0.4940 |
| Sa | 0.6330 | 0.5710 |
| Sb | 0.9210 | 0.6410 |
| Sc | 0.8460 | 0.6120 |
| Sd | 0.7370 | 0.6000 |
| Se | 0.5230 | 0.4940 |
| Sf | 0.2880 | 0.4960 |
| Sg | 0.5490 | 0.5650 |
| Sh | 0.0860 | 0.4150 |