# wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 09:44 AM JST

| | | |
|---|---|---|
| PDB ID | : | 5GJQ |
| EMDB ID | : | EMD-9511 |
| Title | : | Structure of the human 26S proteasome bound to USP14-UbAl |
| Authors | : | Huang, X.L.; Luan, B.; Wu, J.P.; Shi, Y.G. |
| Deposited on | : | 2016-07-01 |
| Resolution | : | 4.50 Å(reported) |

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

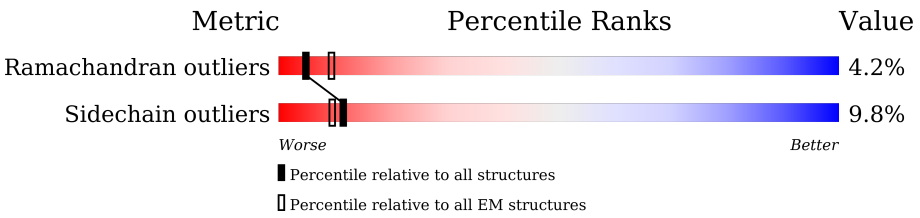
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 | a | 239 | 78% 6% 15% |
| 1 | o | 239 | 75% 10% 15% |
| 2 | B | 246 | 92% 7% |
| 2 | h | 246 | 5% 93% 6% |
| 3 | b | 277 | 76% 21% |
| 3 | p | 277 | 73% 6% 21% |
| 4 | C | 234 | 94% 6% |
| 4 | i | 234 | 87% 12% |
| 5 | c | 205 | 92% 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | q | 205 | 90% 10% |
| 6 | D | 261 | 91% |
| 6 | j | 261 | 89% 7% |
| 7 | d | 201 | 93% 5% |
| 7 | r | 201 | 89% 9% |
| 8 | E | 248 | 8% 90% 8% |
| 8 | k | 248 | 10% 90% 8% |
| 9 | e | 263 | 72% 5% 24% |
| 9 | s | 263 | 71% 6% 24% |
| 10 | F | 241 | 94% |
| 10 | l | 241 | 93% |
| 11 | f | 241 | 84% 5% 12% |
| 11 | t | 241 | 83% 5% 12% |
| 12 | G | 263 | 86% 10% |
| 12 | m | 263 | 82% 9% 10% |
| 13 | g | 264 | 75% 7% 18% |
| 13 | u | 264 | 75% 7% 18% |
| 14 | H | 433 | 15% 67% 18% 12% |
| 15 | I | 440 | 15% 61% 18% 18% |
| 16 | J | 406 | 16% 66% 20% 12% |
| 17 | K | 418 | 11% 65% 23% 9% |
| 18 | L | 389 | 19% 74% 19% |
| 19 | M | 439 | 17% 65% 19% 14% |
| 20 | N | 953 | 49% 80% 5% 14% |
| 21 | X | 255 | 91% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 21 | n | 255 | 89% 5% 5% |
| 22 | O | 376 | 73% 87% 11% |
| 23 | P | 456 | 57% 83% 7% 9% |
| 24 | Q | 422 | 44% 83% 15% |
| 25 | R | 389 | 24% 82% 13% |
| 26 | S | 534 | 52% 69% 26% |
| 27 | T | 350 | 59% 64% 9% 26% |
| 28 | U | 324 | 64% 74% 12% 13% |
| 29 | V | 310 | 52% 69% 12% 17% |
| 30 | W | 377 | 51% 45% 5% 49% |
| 31 | Y | 70 | 60% 70% 14% 16% |
| 32 | Z | 908 | 76% 75% 6% 19% |
| 33 | x | 494 | 39% 55% 15% 28% |
| 34 | y | 76 | 68% 93% 7% |

# 2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 98461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | a | 202 | 1509 | 945 | 258 | 294 | 12 | 0 | 0 |
| 1 | o | 202 | 1509 | 945 | 258 | 294 | 12 | 0 | 0 |

- Molecule 2 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 244 | 1845 | 1171 | 309 | 352 | 13 | 0 | 0 |
| 2 | h | 244 | 1853 | 1177 | 311 | 352 | 13 | 0 | 0 |

- Molecule 3 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | b | 220 | 1643 | 1033 | 280 | 318 | 12 | 0 | 0 |
| 3 | p | 220 | 1643 | 1033 | 280 | 318 | 12 | 0 | 0 |

- Molecule 4 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | C | 233 | 1707 | 1081 | 287 | 334 | 5 | 0 | 0 |
| 4 | i | 231 | 1744 | 1112 | 290 | 336 | 6 | 0 | 0 |

- Molecule 5 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | c | 204 | 1585 | 1010 | 262 | 294 | 19 | 0 | 0 |
| 5 | q | 204 | 1585 | 1010 | 262 | 294 | 19 | 0 | 0 |

- Molecule 6 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | D | 250 | 1912 | 1204 | 329 | 371 | 8 | 0 | 0 |
| 6 | j | 250 | 1913 | 1203 | 330 | 372 | 8 | 0 | 0 |

- Molecule 7 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | d | 199 | 1570 | 1006 | 265 | 290 | 9 | 0 | 0 |
| 7 | r | 199 | 1570 | 1006 | 265 | 290 | 9 | 0 | 0 |

- Molecule 8 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | E | 243 | 1724 | 1068 | 312 | 339 | 5 | 0 | 0 |
| 8 | k | 243 | 1691 | 1051 | 309 | 327 | 4 | 0 | 0 |

- Molecule 9 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | e | 201 | 1548 | 974 | 273 | 292 | 9 | 0 | 0 |
| 9 | s | 201 | 1551 | 977 | 273 | 292 | 9 | 0 | 0 |

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | F | 234 | 1766 | 1108 | 290 | 357 | 11 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | l | 234 | 1726 | 1107 | 291 | 317 | 11 | 0 | 0 |

- Molecule 11 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | f | 213 | 1641 | 1036 | 282 | 313 | 10 | 0 | 0 |
| 11 | t | 213 | 1644 | 1039 | 282 | 313 | 10 | 0 | 0 |

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | G | 238 | 1850 | 1159 | 334 | 346 | 11 | 0 | 0 |
| 12 | m | 238 | 1850 | 1159 | 334 | 346 | 11 | 0 | 0 |

- Molecule 13 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | g | 216 | 1672 | 1055 | 286 | 319 | 12 | 0 | 0 |
| 13 | u | 217 | 1678 | 1058 | 290 | 318 | 12 | 0 | 0 |

- Molecule 14 is a protein called 26S protease regulatory subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | H | 380 | 2879 | 1809 | 513 | 539 | 18 | 0 | 0 |

- Molecule 15 is a protein called 26S protease regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | I | 359 | 2720 | 1708 | 465 | 535 | 12 | 0 | 0 |

- Molecule 16 is a protein called 26S protease regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | J | 358 | 2820 | 1780 | 506 | 518 | 16 | 0 | 0 |

- Molecule 17 is a protein called 26S protease regulatory subunit 6B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | K | 380 | 3039 | 1923 | 524 | 579 | 13 | 0 | 0 |

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | L | 375 | 2860 | 1796 | 512 | 536 | 16 | 0 | 0 |

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | M | 376 | 2858 | 1802 | 496 | 545 | 15 | 0 | 0 |

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | N | 823 | 5462 | 3499 | 933 | 1012 | 18 | 0 | 0 |

- Molecule 21 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | n | 243 | 1873 | 1189 | 317 | 356 | 11 | 0 | 0 |
| 21 | X | 243 | 1873 | 1189 | 317 | 356 | 11 | 0 | 0 |

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | O | 372 | 2372 | 1518 | 405 | 438 | 11 | 0 | 0 |

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | P | 413 | 2828 | 1819 | 489 | 514 | 6 | 0 | 0 |

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | Q | 421 | 2948 | 1864 | 509 | 567 | 8 | 0 | 0 |

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | R | 376 | 2767 | 1794 | 461 | 503 | 9 | 0 | 0 |

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | S | 395 | 2600 | 1662 | 463 | 472 | 3 | 0 | 0 |

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | T | 258 | 1702 | 1102 | 280 | 315 | 5 | 0 | 0 |

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | U | 283 | 2131 | 1370 | 369 | 388 | 4 | 0 | 0 |

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | V | 257 | 2011 | 1276 | 341 | 377 | 17 | 0 | 0 |

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | W | 193 | 1300 | 818 | 228 | 250 | 4 | 0 | 0 |

- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 31 | Y | 59 | 308 | 184 | 60 | 64 | 0 | 0 |

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 32 | Z | 732 | 3608 | 2144 | 732 | 732 | 0 | 0 |

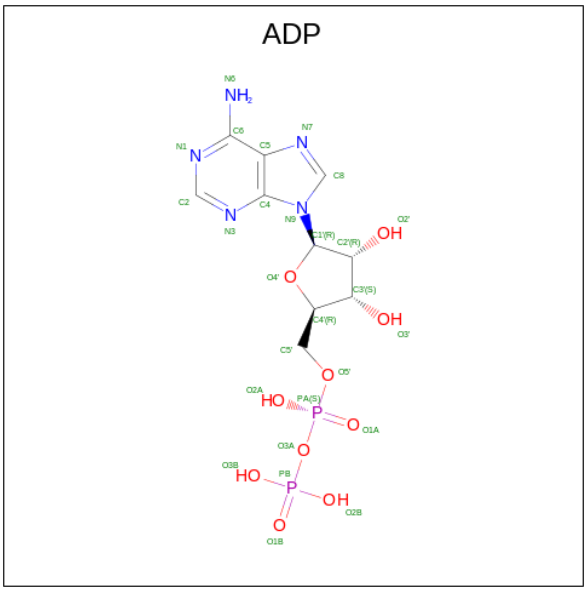
- Molecule 33 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | x | 355 | 2810 | 1782 | 470 | 538 | 20 | 0 | 0 |

- Molecule 34 is a protein called Polyubiquitin-B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | y | 76 | 601 | 378 | 105 | 117 | 1 | 0 | 0 |

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



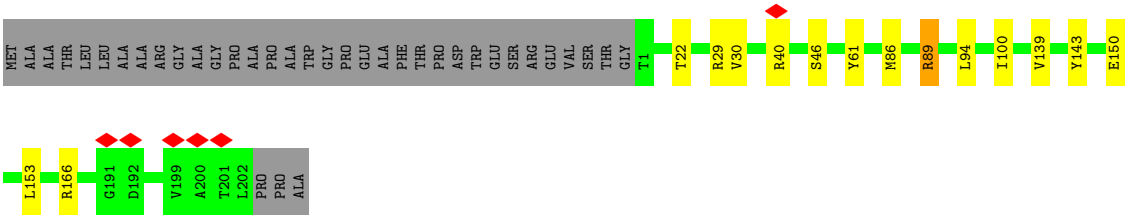

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 35 | H | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 35 | I | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 35 | J | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 35 | K | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 35 | L | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 35 | M | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

# 3 Residue-property plots (i)

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

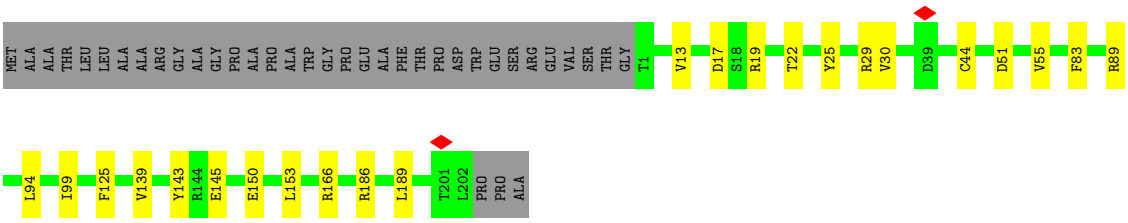
• Molecule 1: Proteasome subunit beta type-6

Chain a:



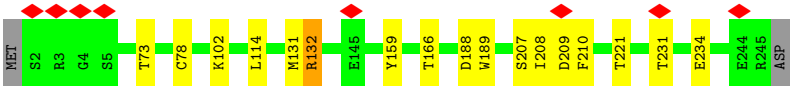

• Molecule 1: Proteasome subunit beta type-6

Chain o:



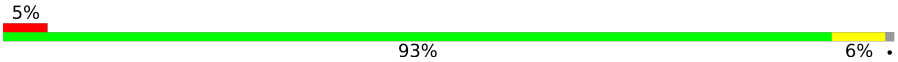

• Molecule 2: Proteasome subunit alpha type-6

Chain B:



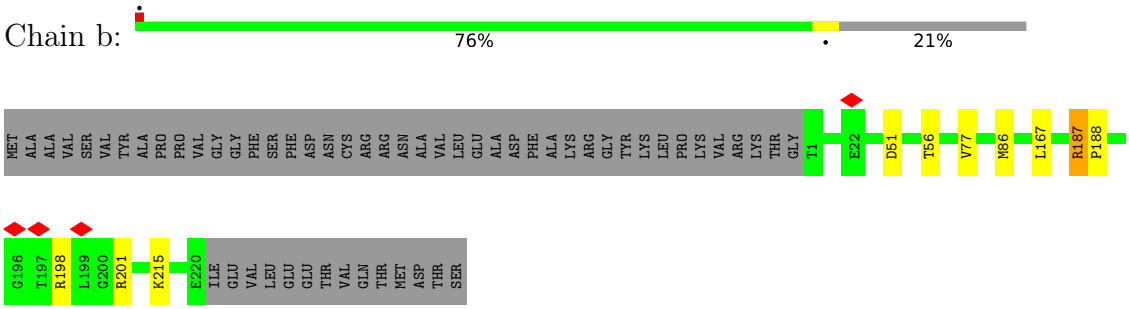

• Molecule 2: Proteasome subunit alpha type-6

Chain h:



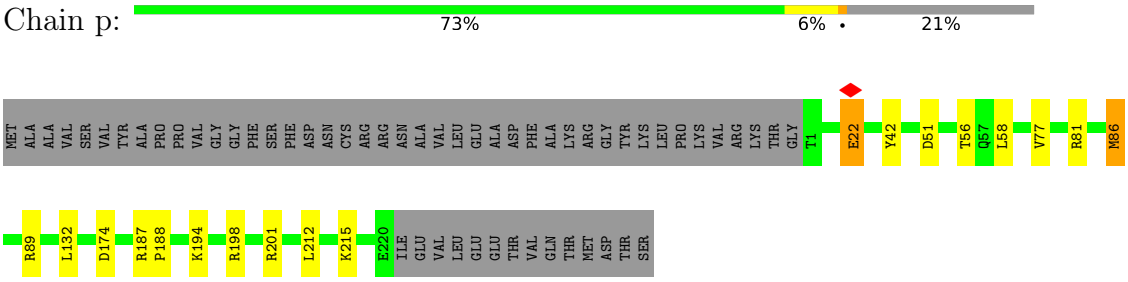
• Molecule 3: Proteasome subunit beta type-7

Chain b:



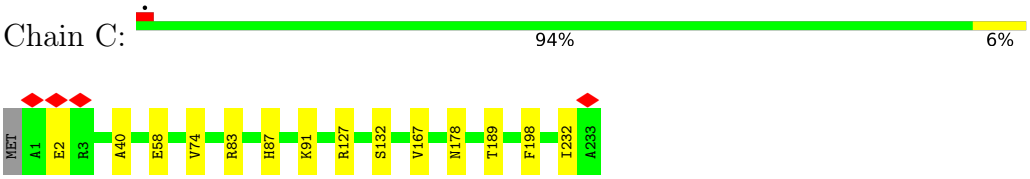

• Molecule 3: Proteasome subunit beta type-7

Chain p:



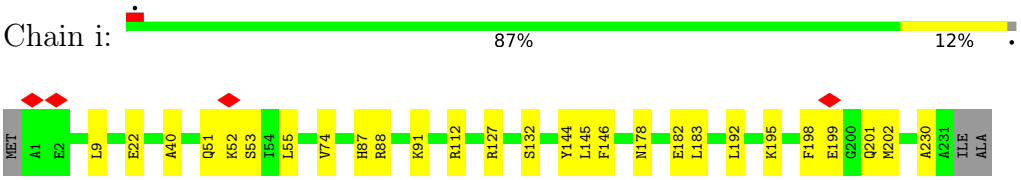

• Molecule 4: Proteasome subunit alpha type-2

Chain C:



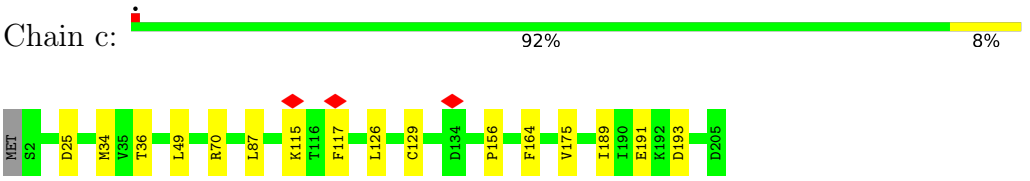

• Molecule 4: Proteasome subunit alpha type-2

Chain i:



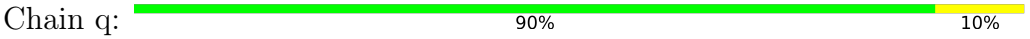

• Molecule 5: Proteasome subunit beta type-3

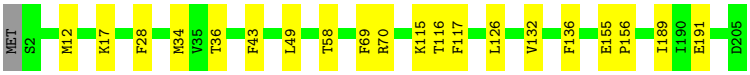
Chain c:




• Molecule 5: Proteasome subunit beta type-3

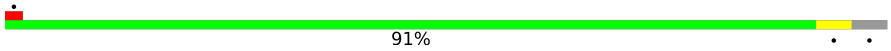
Chain q:





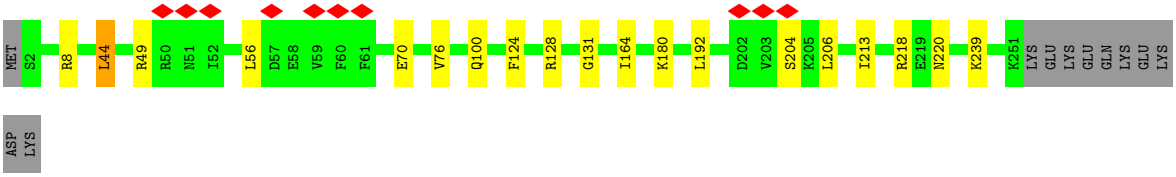

• Molecule 6: Proteasome subunit alpha type-4

Chain D:



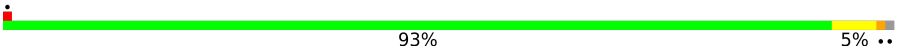
• Molecule 6: Proteasome subunit alpha type-4

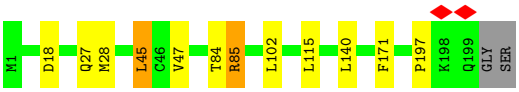
Chain j:




• Molecule 7: Proteasome subunit beta type-2

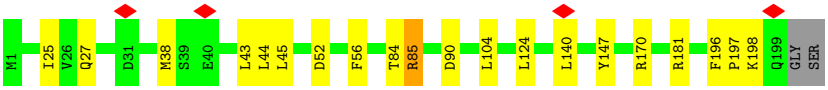
Chain d:



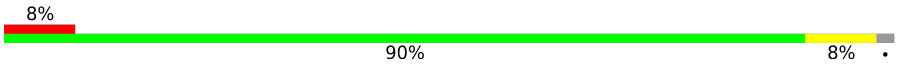

• Molecule 7: Proteasome subunit beta type-2

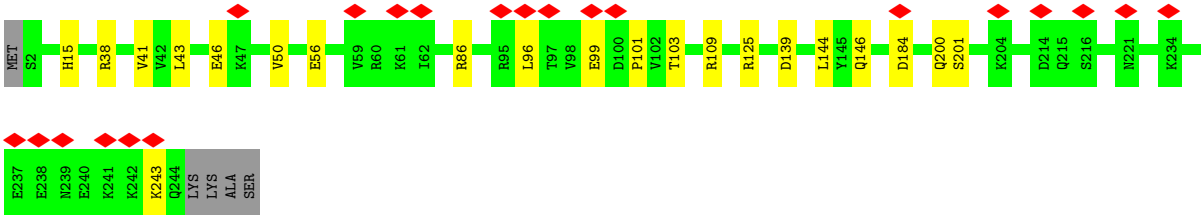
Chain r:




• Molecule 8: Proteasome subunit alpha type-7

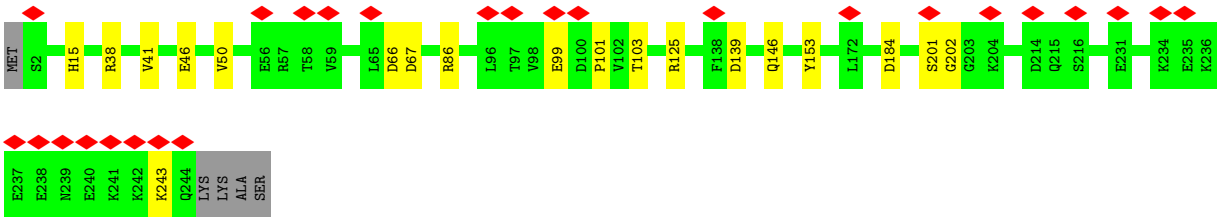
Chain E:



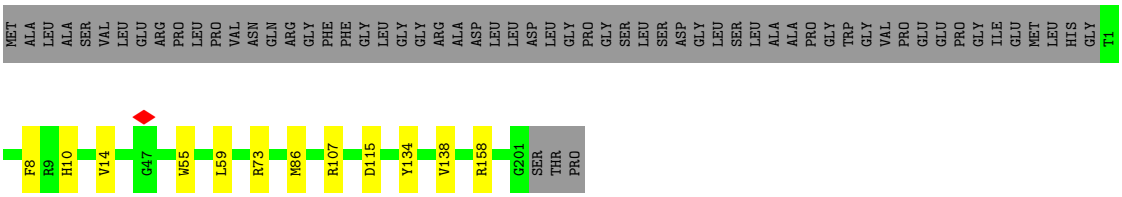

• Molecule 8: Proteasome subunit alpha type-7

Chain k:



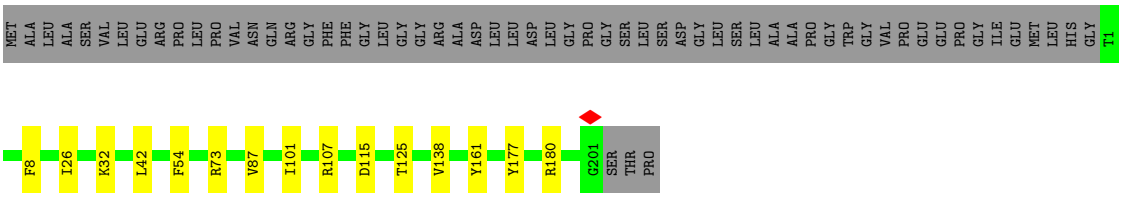

• Molecule 9: Proteasome subunit beta type-5

Chain e:



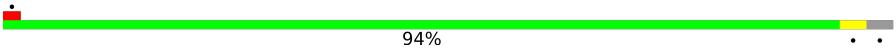

• Molecule 9: Proteasome subunit beta type-5

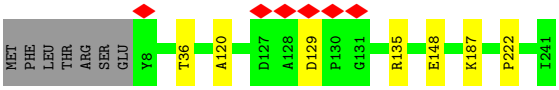
Chain s:




• Molecule 10: Proteasome subunit alpha type-5

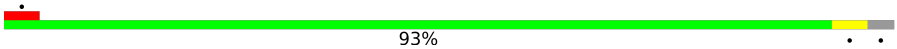
Chain F:

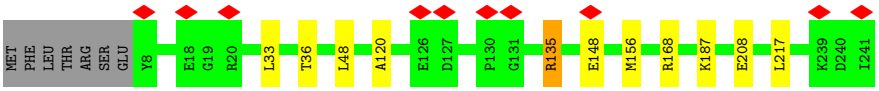



• Molecule 10: Proteasome subunit alpha type-5

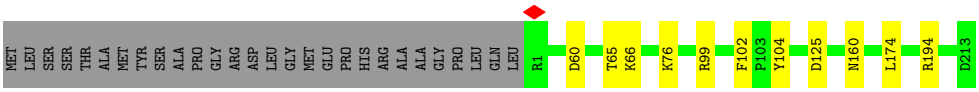
Chain l:



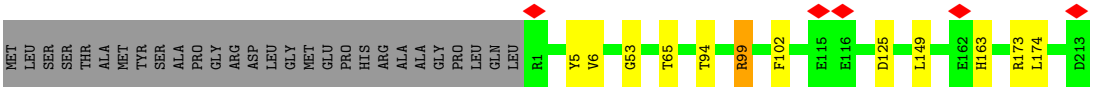

• Molecule 11: Proteasome subunit beta type-1

Chain f:



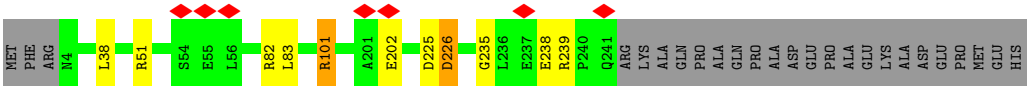
- Molecule 11: Proteasome subunit beta type-1

Chain t:




- Molecule 12: Proteasome subunit alpha type-1

Chain G:

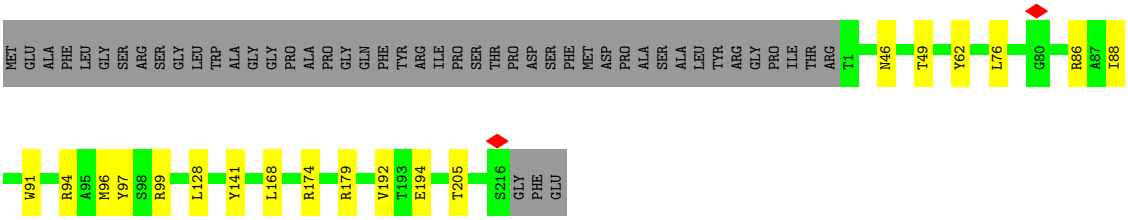



- Molecule 12: Proteasome subunit alpha type-1

Chain m:

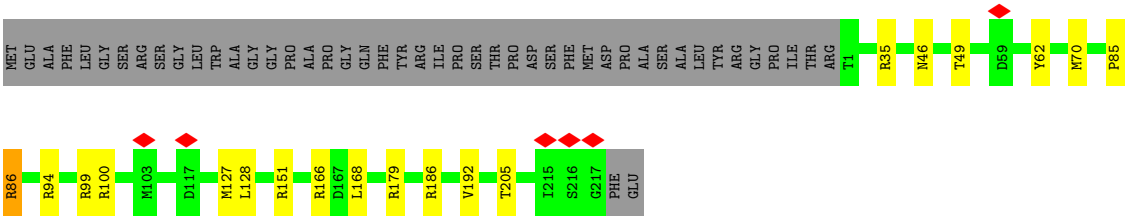
- Molecule 13: Proteasome subunit beta type-4

Chain g:



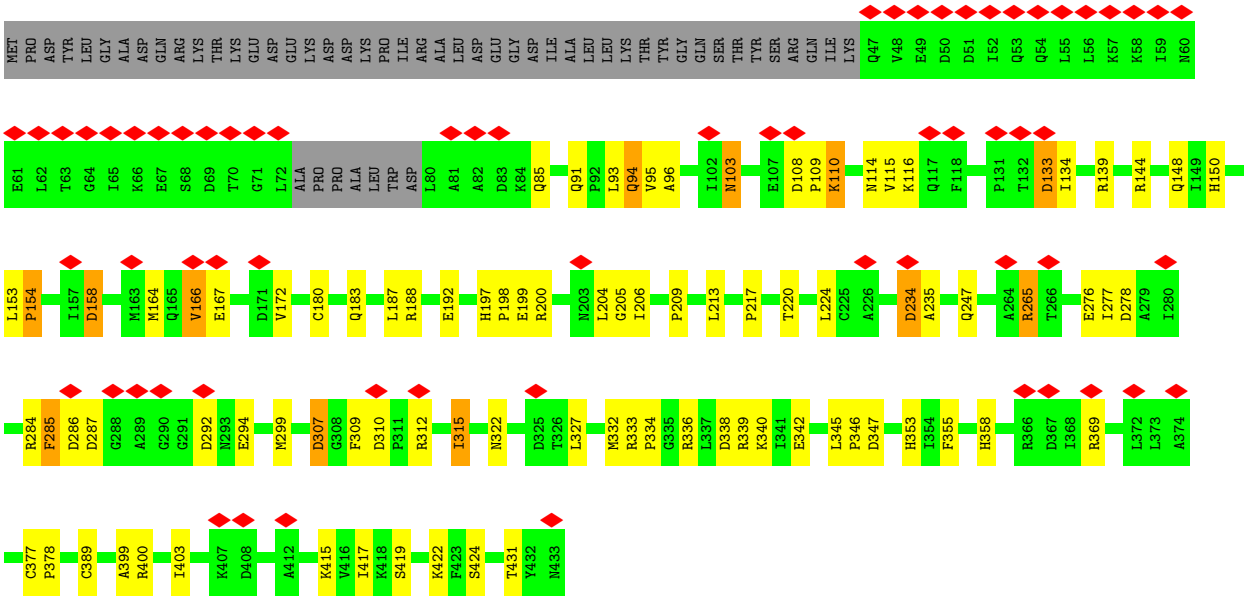

- Molecule 13: Proteasome subunit beta type-4

Chain u:



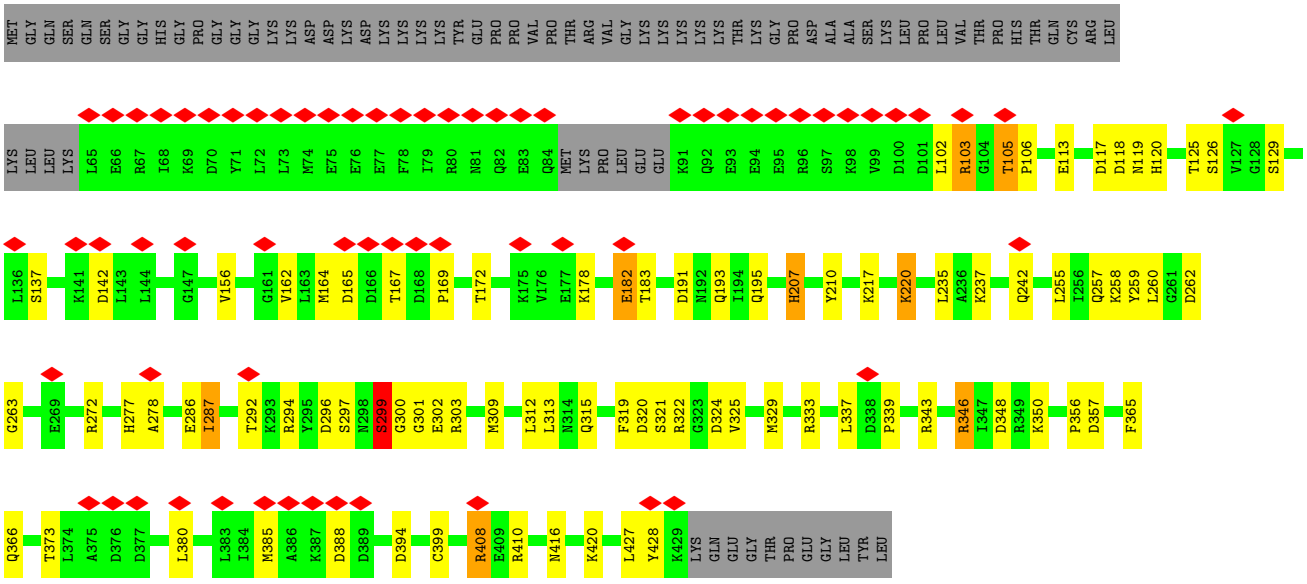

- Molecule 14: 26S protease regulatory subunit 7

Chain H:



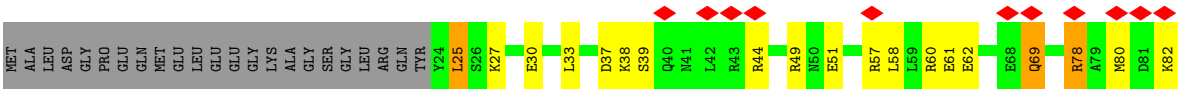

• Molecule 15: 26S protease regulatory subunit 4

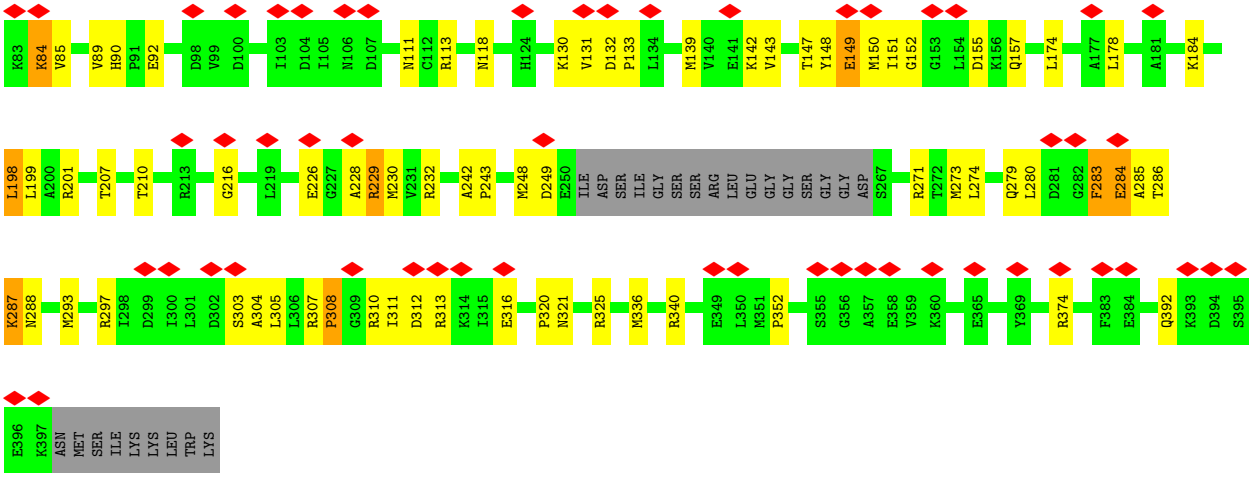
Chain I:




• Molecule 16: 26S protease regulatory subunit 8

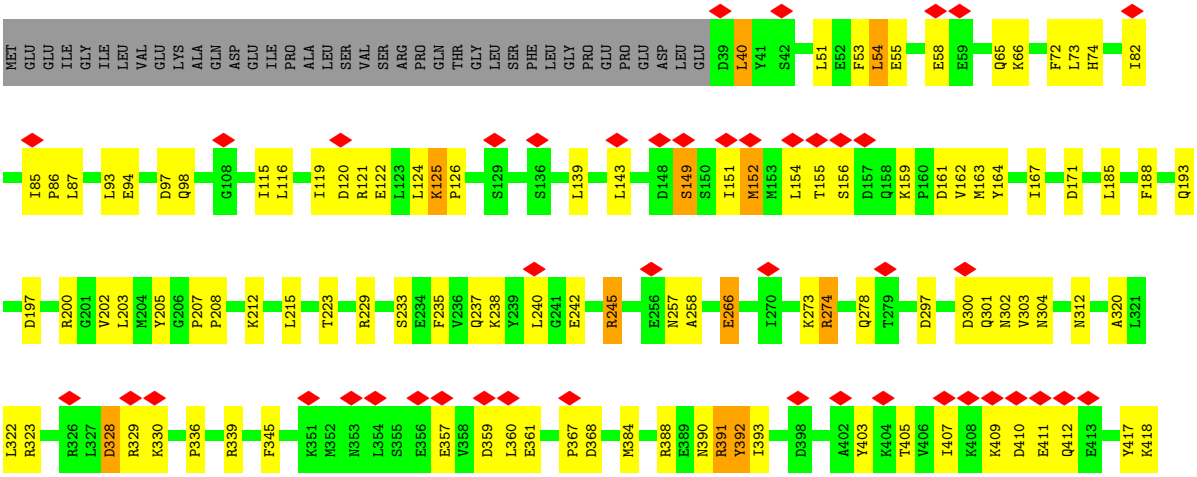
Chain J:





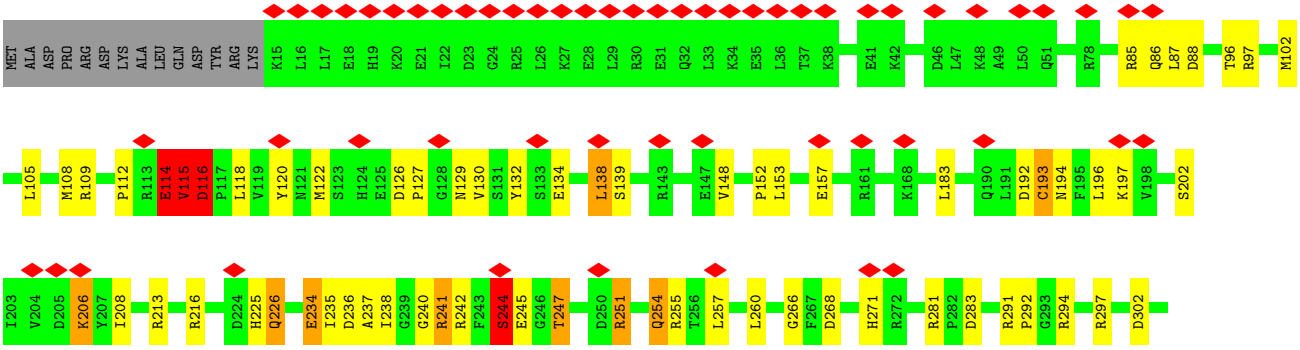

- Molecule 17: 26S protease regulatory subunit 6B

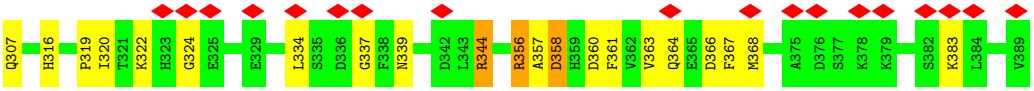
Chain K:




- Molecule 18: 26S protease regulatory subunit 10B

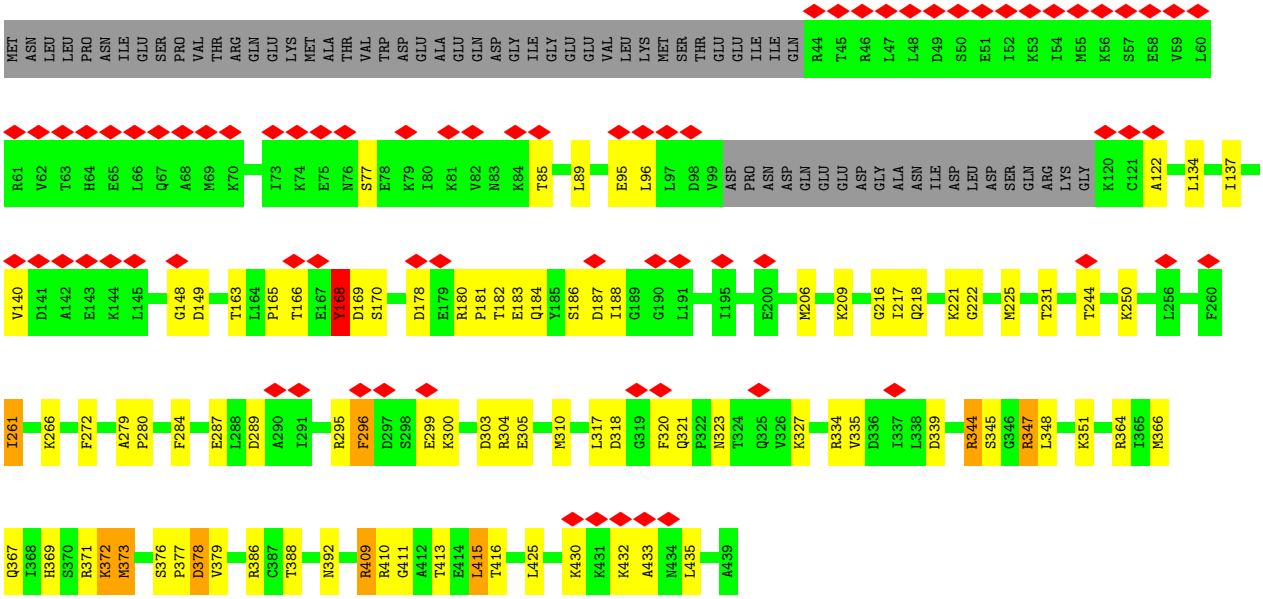
Chain L:





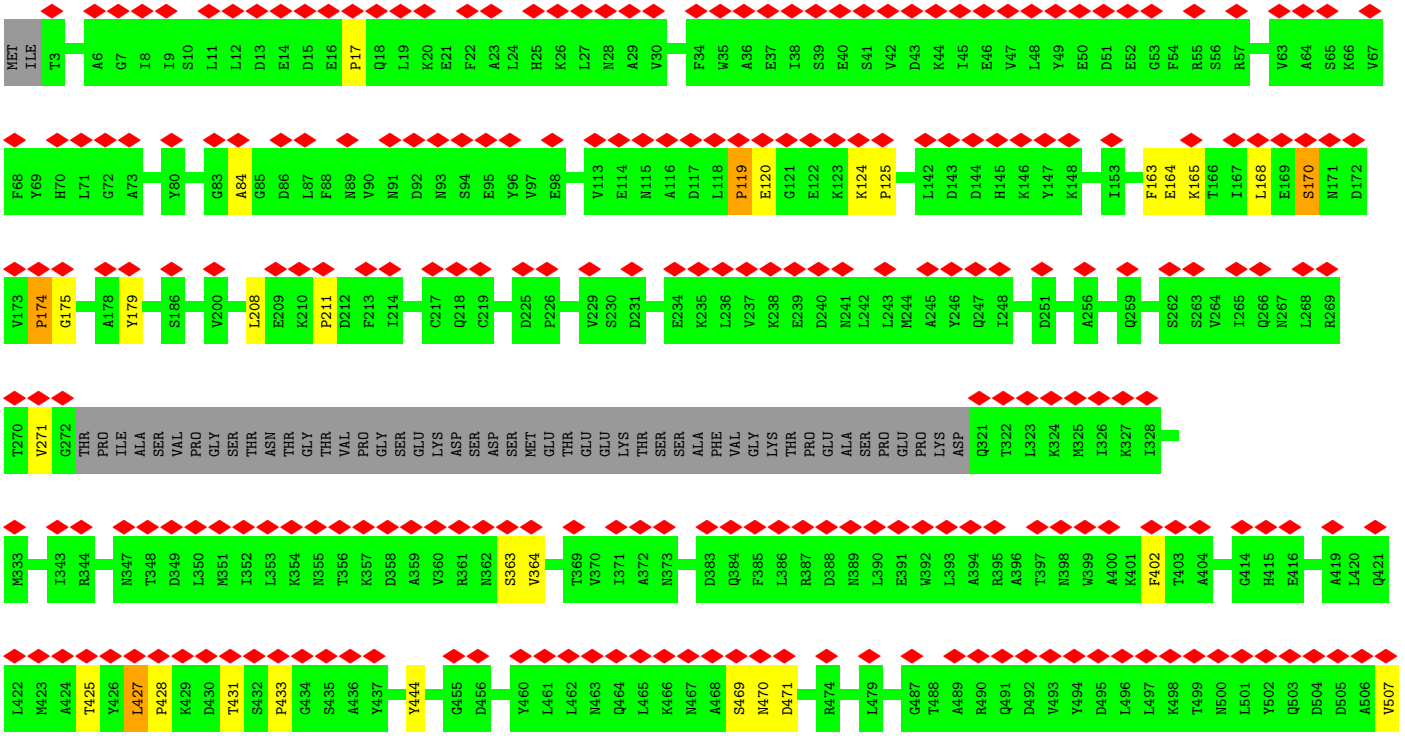

- Molecule 19: 26S protease regulatory subunit 6A

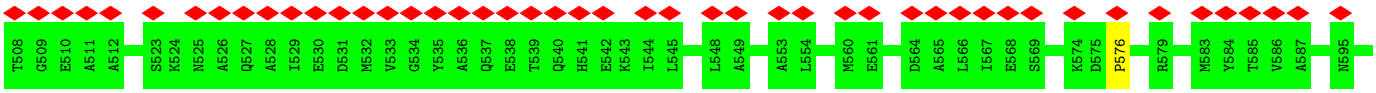
Chain M:

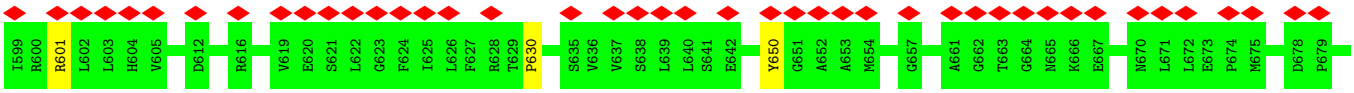


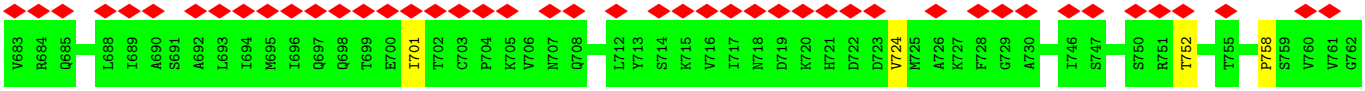

- Molecule 20: 26S proteasome non-ATPase regulatory subunit 1

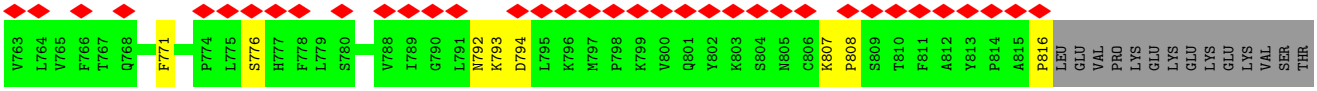
Chain N:

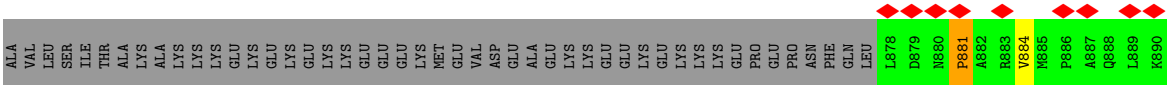


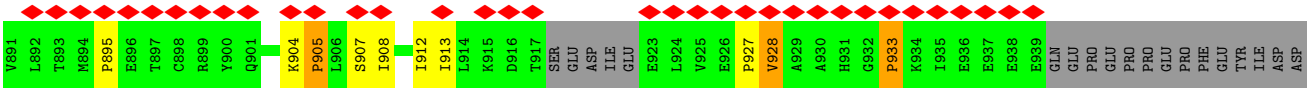


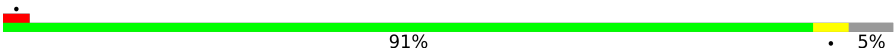




- Molecule 21: Proteasome subunit alpha type-3

Chain n:

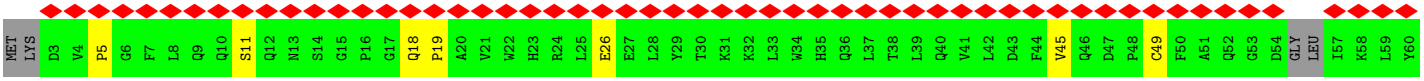
- Molecule 21: Proteasome subunit alpha type-3

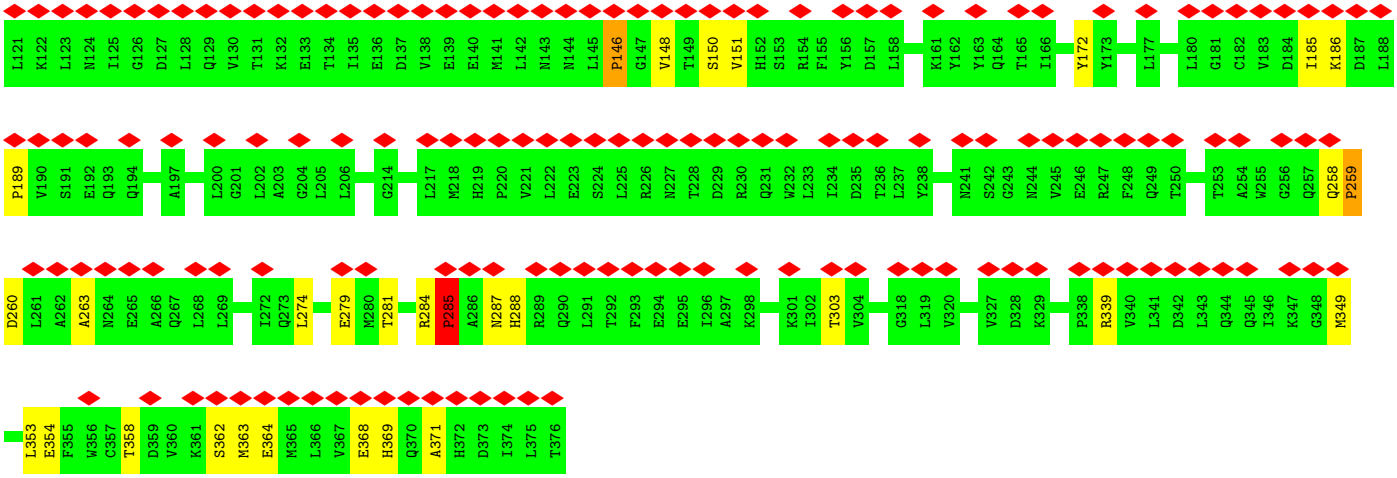
Chain X:



- Molecule 22: 26S proteasome non-ATPase regulatory subunit 13

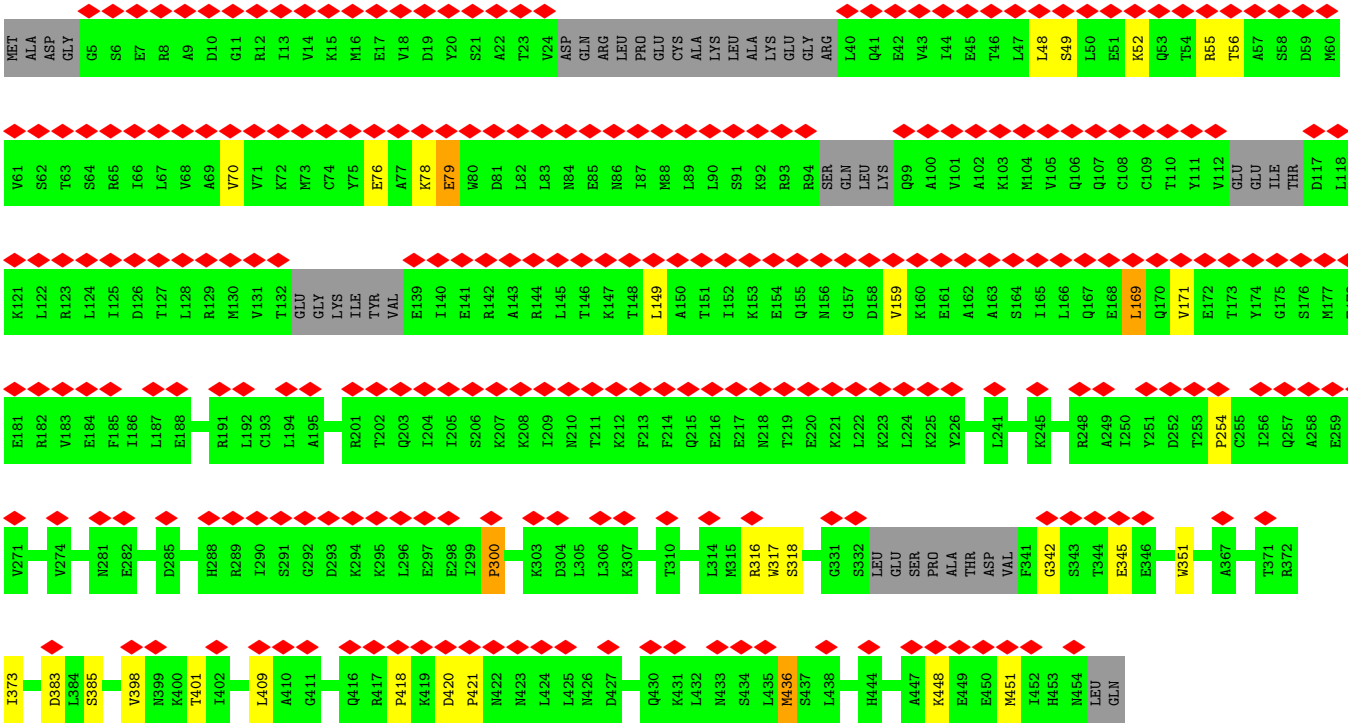
Chain O:





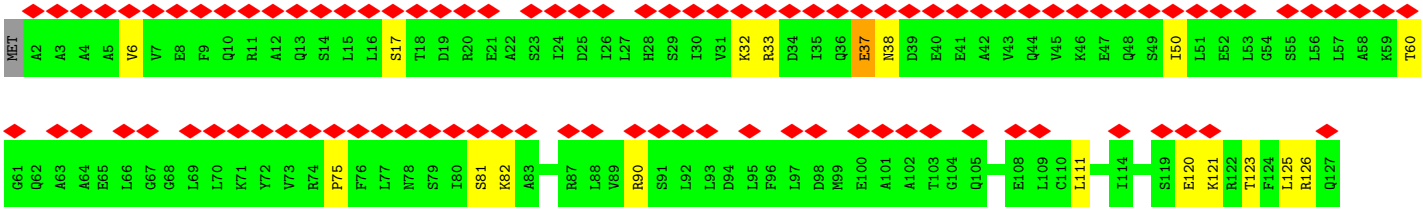

- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

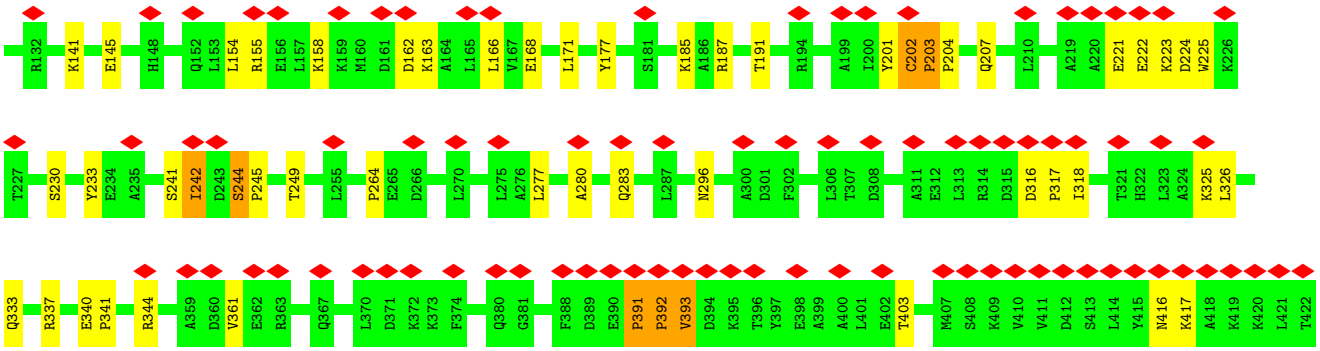
Chain P:




- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

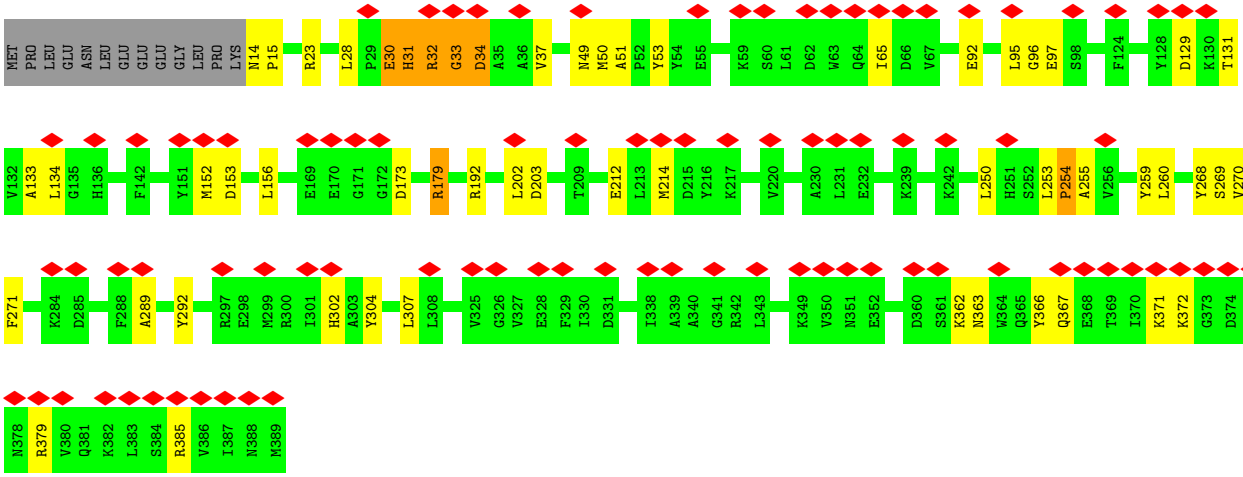
Chain Q:





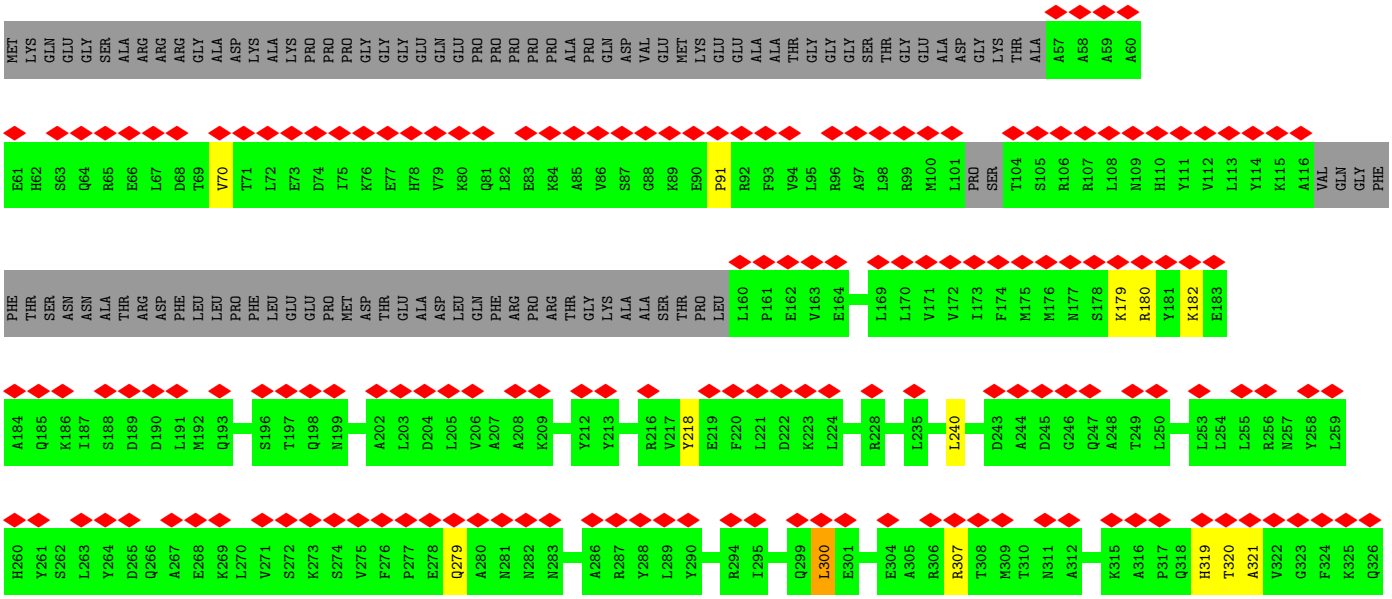

- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain R:



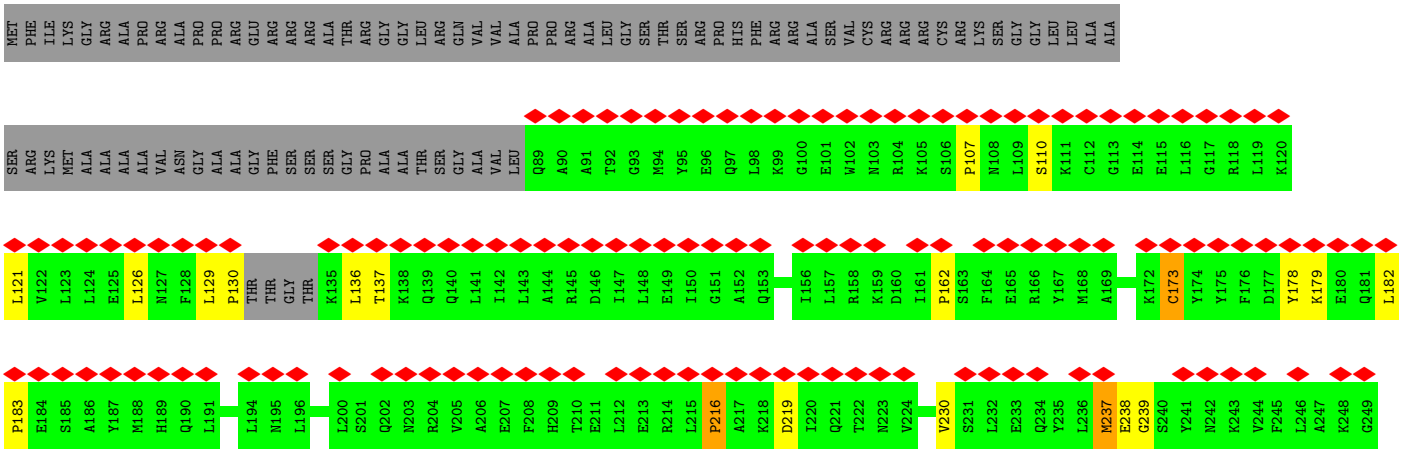

- Molecule 26: 26S proteasome non-ATPase regulatory subunit 3

Chain S:



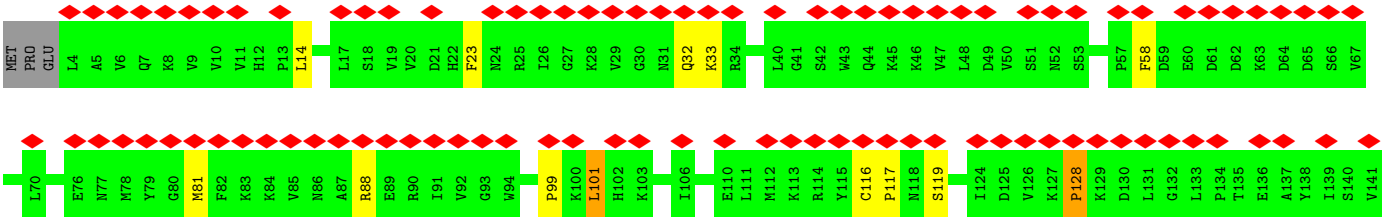
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 8

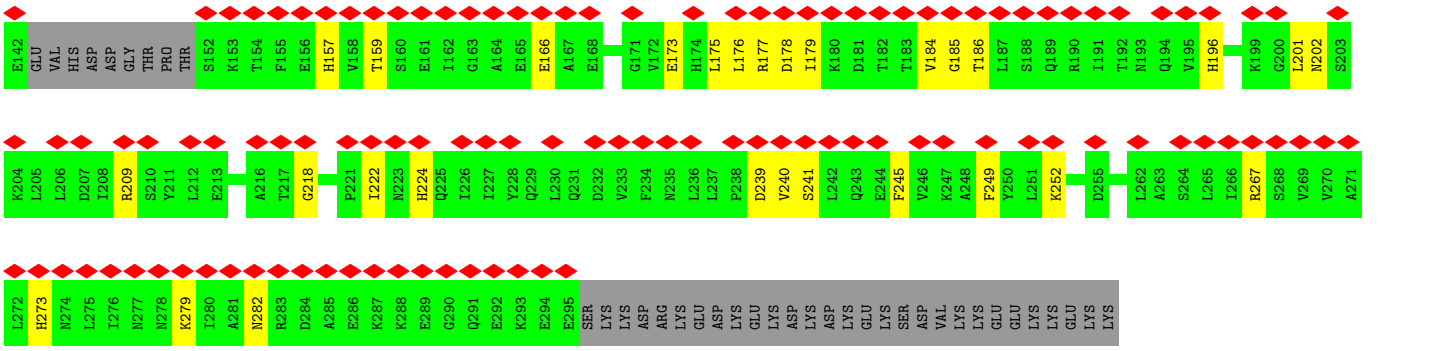
Chain T:




• Molecule 28: 26S proteasome non-ATPase regulatory subunit 7

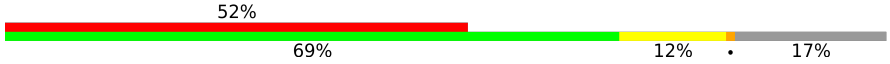
Chain U:

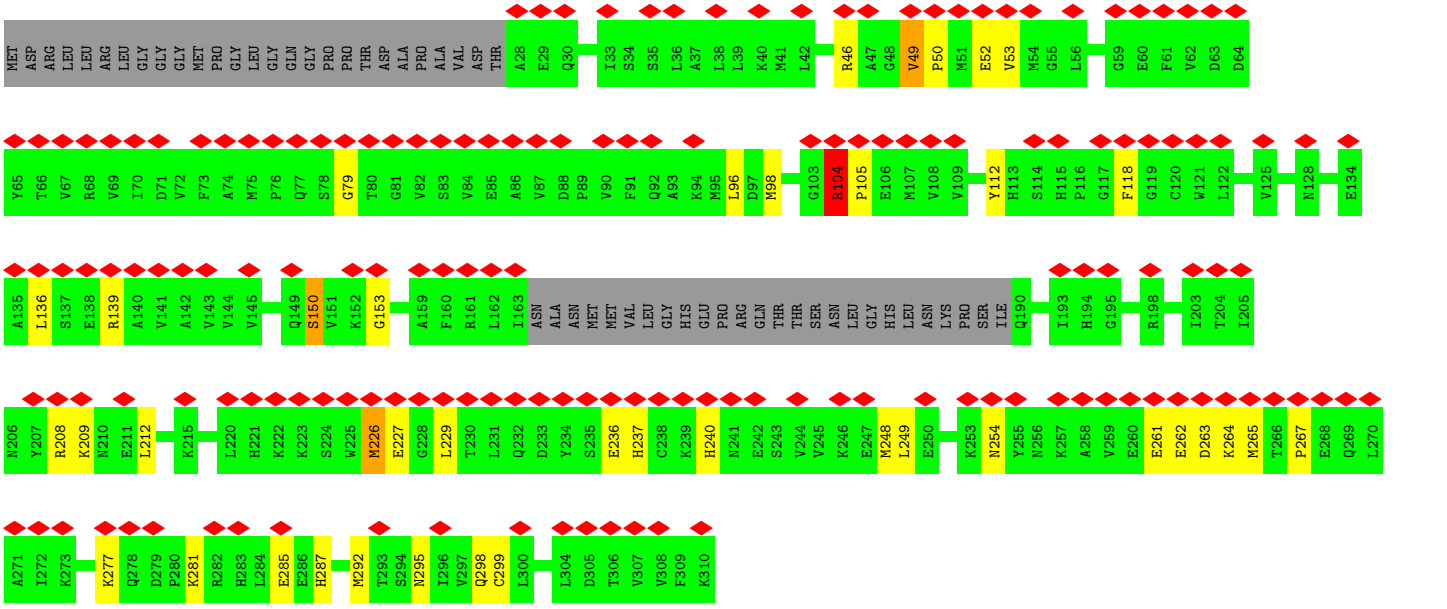





• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

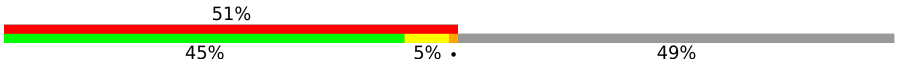
Chain V:

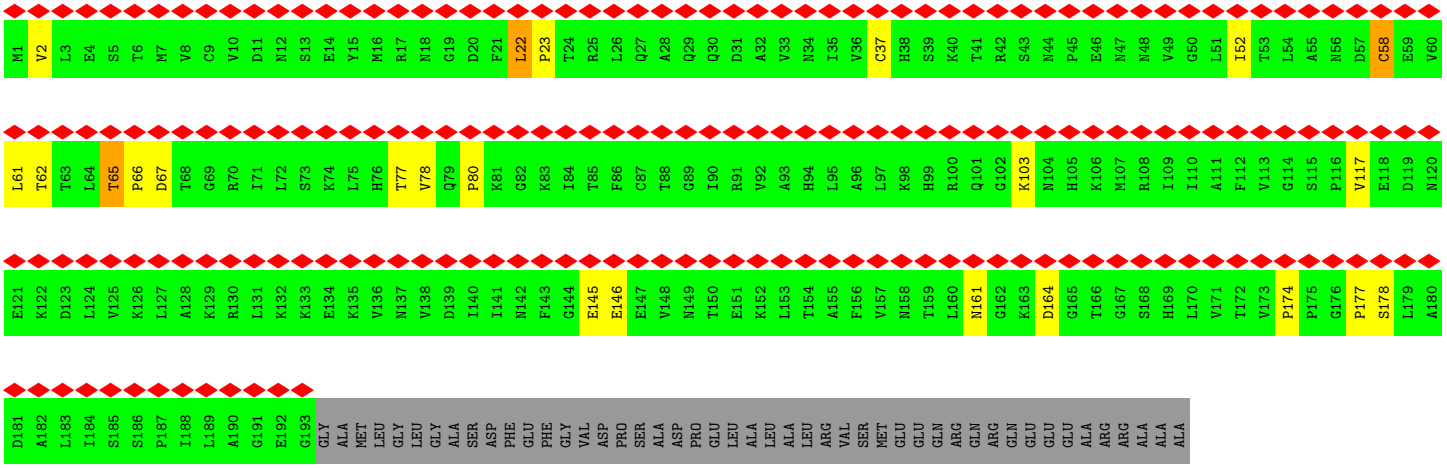



• Molecule 30: 26S proteasome non-ATPase regulatory subunit 4

Chain W:



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

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

SER GLN ALA THR LYS ASP GLY LYS LYS ASP LYS LYS GLU GLU ASP LYS LYS

- Molecule 31: 26S proteasome complex subunit DSS1

Chain Y: 60% 70% 14% 16%

MET SER E3 K4 K5 Q6 P7 V8 D9 L10 G11 L12 L13 E14 E15 D16 D17 E18 F19 E20 E21 F22 P23 A24 E25 D26 W27 ALA GLY LEU ASP GLU ASP GLU D35 A36 H37 V38 W39 E40 D41 N42 W43 D44 D45 D46 N47 V48 E49 H63 G64 Y65 K66 M67 E68 THR SER

- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain Z: 76% 75% 6% 19%

MET GLU GLU GLY GLY ARG ASP LYS ALA PRO VAL GLN PRO GLN GLN SER PRO ALA ALA ALA PRO GLY GLY THR ASP GLU LYS PRO SER GLY LYS GLU ARG ARG ASP ALA GLY ASP LYS ASP LYS GLU GLN GLU LEU SER GLU GLU ASP LYS GLN LEU GLN ASP GLU LEU GLU MET LEU VAL

GLU ARG LEU GLY GLU LYS ASP THR SER LEU TYR ARG PRO ALA LEU GLU GLU LEU ARG ARG GLN ILE ARG SER SER THR THR SER MET THR SER VAL PRO LYS PRO LEU LYS PHE LEU ARG PRO HIS TYR GLY LYS L106 K107 E108 I109 Y110 E111 N112 M113 A114 P115 G116 E117 N118 K119 R120

F121 A122 A123 D124 I125 I126 S127 V128 L129 A130 M131 T132 M133 S134 G135 E136 R137 E138 C139 L140 K141 Y142 R143 L144 V145 G146 S147 Q148 E149 E150 L151 A152 S153 W154 G155 H156 E157 Y158 V159 R160 H161 L162 A163 G164 E165 V166 A167 K168 E169 W170 GLN GLU LEU ASP ASP ALA GLU LYS V179 Q180

R181 E182 P183 L184 L185 T186 L187 V188 K189 E190 I191 V192 P193 Y194 N195 M196 A197 H198 N199 A200 E201 H202 E203 A204 C205 D206 L207 L208 M209 E210 I211 E212 Q213 V214 D215 M216 L217 E218 K219 D220 I221 D222 E223 N224 A225 Y226 A227 K228 Y229 C230 L231 Y232 L233 T234 S235 C236 V237 N238 Y239 V240

P241 E242 P243 E244 N245 S246 A247 L248 L249 R250 C251 A252 L253 G254 V255 F256 R257 K258 F259 S260 R261 F262 P263 E264 A265 L266 R267 L268 A269 L270 M271 L272 N273 D274 M275 E276 L277 V278 E279 D280 I281 F282 T283 S284 C285 K286 V289 V290 Q291 K292 Q293 M294 A295 F296 M297 L298 G299 R300 H301

GLY VAL PHE LEU GLU LEU SER E309 D310 V311 E312 E313 Y314 E315 D316 L317 T318 E319 I320 M321 S322 N323 V324 Q325 L326 N327 S328 N329 F330 L331 A332 L333 A334 R335 E336 L337 D338 I339 M340 K343 V344 P345 D346 D347 I348 Y349 K350 T351 H352 L353 E354 N355 N356 R357 F358 G359 G360 S361 G362

S363 Q364 V365 D366 S367 A368 R369 M370 N371 L372 A373 S374 S375 F376 V377 N378 G379 F380 V381 N382 A383 A384 F385 G386 Q387 D388 K389 L390 L391 T392 D393 D394 G395 N396 K397 W398 L399 Y400 K401 N402 K403 D404 H405 G406 S409 A410 A411 A412 S413 L414 G415 M416 I417 L418 L419 W420 D421 V422 D423

G424 G425 L426 T427 Q428 I429 D430 K431 Y432 L433 Y434 S435 S436 E437 D438 Y439 I440 K441 S442 G443 A444 L445 L446 A447 C448 G449 I450 V451 N452 S453 G454 V455 R456 N457 E458 C459 D460 P461 A462 L463 A464 L465 L466 S467 D468 Y469 V470 L471 H472 N473 S474 N475 T476 M477 R478 L479 G480 S481 I482 F483

G484 L485 G486 L487 A488 Y489 S492 N493 R494 E495 D496 V497 L498 T499 L500 L501 L502 P503 V504 M505 G506 D507 S508 K509 S510 S511 M512 E513 V514 A515 G516 V517 T518 A519 L520 A521 C522 G523 M524 I525 G528 S529 C530 D533 V534 T535 S536 T537 I538 L539 Q540 T541 I542 M543 E544 K545 S546

E547 T548 E549 L550 K551 D552 T553 Y554 A555 R556 W557 L558 P559 L560 G561 L562 G563 L564 N565 H566 L567 G568 K569 G570 E571 A572 I573 E574 A575 I576 L577 A578 A579 L580 E581 V582 V583 S584 E585 P586 F587 R588 S589 F590 A591 N592 T593 L594 V595 D596 V597 C598 A599 Y600 A601 G602 S603 G604 N605 V606

L607 K608 V609 Q610 Q611 L612 L613 H614 I615 G616 S617 E618 HIS PHE ASP SER LYS GLU LYS GLU GLU ASP LYS ASP LYS LYS GLU LYS LYS ASP LYS ASP LYS LYS GLU ALA PRO ALA ASP MET GLY HIS GLN GLY VAL A653 V654 L655 G656 I657 A658 L659 I660 A661 M662 G663 E664 E665 I666

G667 A668 E669 M670 A671 L672 R673 T674 F675 G676 H677 L678 L679 R680 Y681 G682 E683 P684 T685 L686 R687 R688 A689 V690 P691 L692 A693 L694 A695 L696 I697 S700 N701 P702 R703 L704 N705 T706 L707 D708 T709 L710 S711 K712 F713 S714 H715 D716 A717 D718 P719 E720 V721 S722 Y723 N724 S725 I726 F727

A728 M729 G730 M731 V732 G733 S734 G735 T736 N737 N738 A739 R740 L741 A742 A743 M744 L745 R746 Q747 L748 A749 Q750 Y751 H752 A753 K754 D755 P756 N757 N758 L759 F760 M761 V762 R763 L764 A765 Q766 G767 L768 T769 H770 L771 G772 K773 G774 T775 L776 T777 L778 C779 P780 Y781 H782 S783 D784 R785 Q786 L787

M788 S789 Q790 V791 A792 V793 A794 G795 L796 L797 T798 V799 L800 V801 S802 F803 L804 D805 V806 R807 N808 I809 I810 L811 G812 K813 S814 H815 Y816 V817 L818 Y819 G820 L821 V822 A823 Q826 P827 R828 M829 L830 V831 T832 F833 D834 E835 E836 L837 R838 P839 L840 P841 V842 S843 V844 R845 V846 G847 Q848

ALA VAL ASP VAL VAL GLY GLN ALA GLY LYS PRO LYS THR ILE THR GLY PHE GLN THR HIS THR THR P871 V872 L873 L874 A875 H876 G877 E878 R879 A880 E881 L882 A883 T884 E885 E886 F887 L888 P889 V890 T891 P892 I893 L894 E895 G896 F897 V898 I899 L900 R901 K902 N903 P904 N905 Y906 D907 L908

- Molecule 33: Ubiquitin carboxyl-terminal hydrolase 14

Chain x:

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

ILE LYS ILE LYS ASN GLY MET THR LEU LEU MET MET GLY SER ALA ASP ALA LEU PRO GLU GLU GLU PRO SER ALA LYS THR VAL PHE VAL GLU ASP MET THR GLU GLU GLN LEU A97 S98 A99 M100 E101 L102 P103 C104 N108 L109 G110 N111 Y114 M115 N116 A117 C121 P126

D130 K133 R134 Y135 A136 G137 A138 L139 R140 A141 S142 G143 E144 M145 A146 S147 Y150 L155 R156 D160 D163 K164 T165 S166 S167 S168 I172 I173 L174 L175 Q176 F177 M180 A181 F182 P183 Q184 F185 A186 E187 K188 G189 E190 Q191 G192 Q193 Y194 L195 Q196 Q197 D198 C202

Q205 M206 M207 R208 V209 L210 Q211 Q212 K213 L214 E215 A216 I217 E218 D219 D220 SER VAL LYS GLU THR ASP SER SER SER ALA SER ALA ALA T234 P235 S236 K237 K238 K239 S240 L241 E249 F250 E251 T252 T253 M254 K255 C256 T257 E258 S259 E260 E261 E262 E263 V264 T265 K266 G267 K268 E269

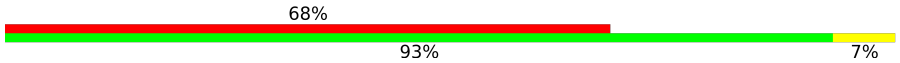
N270 Q271 L272 Q273 L274 S275 C276 F277 I278 N279 Q280 E281 V282 K283 Y284 L285 F286 T287 G288 L291 R292 E295 E296 I297 T298 K299 Q300 S301 P302 T303 L304 Q305 R306 N307 A308 L309 Y310 I311 K312 S313 S314 K315 I316 S317 R318 T324 M327 V328 R329 F330 F331 Y332 K333 E334 K335 E336

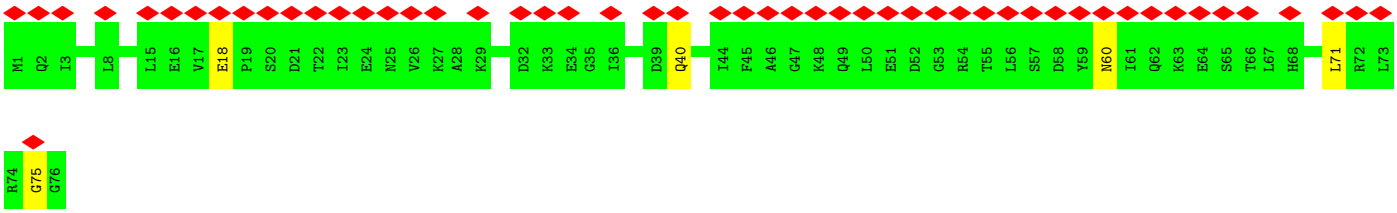
S337 V338 N339 A340 K341 V342 L343 K344 D345 V346 K347 F348 P349 L350 M351 L352 D353 M354 Y355 E356 L357 C358 T359 P360 E361 E364 K365 S368 F369 R370 S371 K372 F373 K374 D375 L376 E377 D378 LYS LYS VAL ASN GLN GLN PRO ASN THR SER ASP LYS LYS SER SER PRO GLN LYS E397 Y398

E401 P402 A406 D407 D408 I409 D418 L423 T424 H425 Q426 G427 R428 S429 S430 S431 H434 Y435 V436 R441 K442 Q443 D444 E445 F449 D450 D451 D452 K453 V454 S455 I456 V457 E460 D461 I462 L463 R464 L465 S466 G467 G468 G469 D470 W471 P481 R482 VAL GLU ILE

• Molecule 34: Polyubiquitin-B

Chain y:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 141293 | 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 ($e^-/Å^2$) | 37 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.171 | Depositor |
| Minimum map value | -0.078 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.006 | Depositor |
| Recommended contour level | 0.033 | Depositor |
| Map size (Å) | 547.84, 547.84, 547.84 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.07, 1.07, 1.07 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLZ, ADP

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 | a | 1.10 | 3/1535 (0.2%) | 1.10 | 6/2078 (0.3%) |
| 1 | o | 1.13 | 4/1535 (0.3%) | 1.18 | 13/2078 (0.6%) |
| 2 | B | 0.83 | 1/1878 (0.1%) | 0.88 | 2/2549 (0.1%) |
| 2 | h | 1.01 | 0/1886 | 1.00 | 2/2557 (0.1%) |
| 3 | b | 0.98 | 0/1670 | 1.06 | 2/2265 (0.1%) |
| 3 | p | 1.06 | 2/1670 (0.1%) | 1.15 | 8/2265 (0.4%) |
| 4 | C | 0.82 | 0/1742 | 0.89 | 4/2372 (0.2%) |
| 4 | i | 1.11 | 5/1780 (0.3%) | 1.10 | 7/2417 (0.3%) |
| 5 | c | 1.08 | 2/1614 (0.1%) | 1.11 | 6/2177 (0.3%) |
| 5 | q | 1.21 | 5/1614 (0.3%) | 1.19 | 4/2177 (0.2%) |
| 6 | D | 0.81 | 2/1942 (0.1%) | 0.89 | 1/2628 (0.0%) |
| 6 | j | 0.99 | 1/1943 (0.1%) | 1.04 | 7/2629 (0.3%) |
| 7 | d | 0.99 | 0/1603 | 1.09 | 6/2174 (0.3%) |
| 7 | r | 1.12 | 2/1603 (0.1%) | 1.17 | 10/2174 (0.5%) |
| 8 | E | 0.78 | 0/1748 | 0.88 | 5/2386 (0.2%) |
| 8 | k | 0.95 | 2/1716 (0.1%) | 1.04 | 5/2347 (0.2%) |
| 9 | e | 1.08 | 2/1579 (0.1%) | 1.11 | 7/2134 (0.3%) |
| 9 | s | 1.13 | 4/1582 (0.3%) | 1.10 | 6/2138 (0.3%) |
| 10 | F | 0.76 | 0/1794 | 0.84 | 0/2430 |
| 10 | l | 0.95 | 1/1753 (0.1%) | 1.01 | 4/2346 (0.2%) |
| 11 | f | 1.03 | 1/1671 (0.1%) | 1.05 | 2/2253 (0.1%) |
| 11 | t | 1.08 | 2/1674 (0.1%) | 1.14 | 4/2257 (0.2%) |
| 12 | G | 0.77 | 0/1885 | 0.88 | 3/2552 (0.1%) |
| 12 | m | 0.95 | 1/1885 (0.1%) | 1.01 | 4/2552 (0.2%) |
| 13 | g | 1.01 | 3/1705 (0.2%) | 1.06 | 7/2312 (0.3%) |
| 13 | u | 1.04 | 1/1711 (0.1%) | 1.10 | 9/2319 (0.4%) |
| 14 | H | 0.82 | 1/2925 (0.0%) | 1.09 | 8/3952 (0.2%) |
| 15 | I | 0.80 | 1/2756 (0.0%) | 1.01 | 8/3727 (0.2%) |
| 16 | J | 0.77 | 0/2857 | 0.95 | 4/3844 (0.1%) |
| 17 | K | 0.81 | 1/3089 (0.0%) | 0.99 | 7/4168 (0.2%) |
| 18 | L | 0.79 | 4/2904 (0.1%) | 1.09 | 12/3924 (0.3%) |
| 19 | M | 0.75 | 0/2896 | 0.91 | 3/3912 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 20 | N | 0.41 | 1/5520 (0.0%) | 0.60 | 1/7446 (0.0%) |
| 21 | X | 0.83 | 0/1908 | 0.87 | 1/2575 (0.0%) |
| 21 | n | 0.93 | 2/1908 (0.1%) | 0.98 | 4/2575 (0.2%) |
| 22 | O | 0.56 | 0/2387 | 0.74 | 3/3211 (0.1%) |
| 23 | P | 0.54 | 0/2857 | 0.72 | 4/3855 (0.1%) |
| 24 | Q | 0.62 | 1/2981 (0.0%) | 0.76 | 4/4045 (0.1%) |
| 25 | R | 0.65 | 1/2817 (0.0%) | 0.80 | 6/3811 (0.2%) |
| 26 | S | 0.57 | 0/2623 | 0.70 | 2/3545 (0.1%) |
| 27 | T | 0.56 | 0/1716 | 0.68 | 3/2310 (0.1%) |
| 28 | U | 0.58 | 0/2167 | 0.75 | 2/2936 (0.1%) |
| 29 | V | 0.60 | 0/2047 | 0.83 | 4/2763 (0.1%) |
| 30 | W | 0.52 | 0/1312 | 0.76 | 3/1769 (0.2%) |
| 31 | Y | 0.58 | 0/307 | 0.84 | 1/424 (0.2%) |
| 32 | Z | 0.32 | 0/3603 | 0.53 | 1/5005 (0.0%) |
| 33 | x | 0.67 | 0/2860 | 0.90 | 2/3852 (0.1%) |
| 34 | y | 0.60 | 0/603 | 0.75 | 0/811 |
| All | All | 0.83 | 56/99761 (0.1%) | 0.94 | 217/135026 (0.2%) |

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 |
|---|---|---|---|
| 3 | b | 0 | 2 |
| 4 | i | 0 | 1 |
| 6 | j | 0 | 1 |
| 7 | r | 0 | 1 |
| 14 | H | 0 | 1 |
| 15 | I | 0 | 4 |
| 16 | J | 0 | 1 |
| 17 | K | 0 | 1 |
| 18 | L | 0 | 4 |
| 19 | M | 0 | 2 |
| 20 | N | 0 | 3 |
| 22 | O | 0 | 2 |
| 23 | P | 0 | 2 |
| 24 | Q | 0 | 6 |
| 25 | R | 0 | 5 |
| 27 | T | 0 | 1 |
| 28 | U | 0 | 1 |
| 29 | V | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 30 | W | 0 | 7 |
| 31 | Y | 0 | 2 |
| 32 | Z | 0 | 7 |
| 34 | y | 0 | 2 |
| All | All | 0 | 59 |

The worst 5 of 56 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | q | 155 | GLU | CD-OE2 | 13.15 | 1.40 | 1.25 |
| 18 | L | 116 | ASP | N-CA | -10.28 | 1.25 | 1.46 |
| 4 | i | 22 | GLU | CG-CD | 8.89 | 1.65 | 1.51 |
| 3 | p | 81 | ARG | CZ-NH2 | 8.66 | 1.44 | 1.33 |
| 5 | c | 164 | PHE | CG-CD1 | -8.04 | 1.26 | 1.38 |

The worst 5 of 217 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | L | 115 | VAL | CA-C-N | -22.22 | 68.32 | 117.20 |
| 14 | H | 336 | ARG | NE-CZ-NH1 | -21.51 | 109.54 | 120.30 |
| 18 | L | 115 | VAL | C-N-CA | -18.03 | 76.64 | 121.70 |
| 14 | H | 336 | ARG | NE-CZ-NH2 | 16.39 | 128.50 | 120.30 |
| 17 | K | 200 | ARG | NE-CZ-NH1 | 14.57 | 127.59 | 120.30 |

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | H | 154 | PRO | Peptide |
| 15 | I | 105 | THR | Peptide |
| 15 | I | 137 | SER | Peptide |
| 15 | I | 299 | SER | Mainchain |
| 3 | b | 187 | ARG | Peptide,Mainchain |

## 5.2 Too-close contacts (i)

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

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | a | 200/239 (84%) | 195 (98%) | 4 (2%) | 1 (0%) | 29 | 68 |
| 1 | o | 200/239 (84%) | 195 (98%) | 4 (2%) | 1 (0%) | 29 | 68 |
| 2 | B | 242/246 (98%) | 228 (94%) | 9 (4%) | 5 (2%) | 7 | 39 |
| 2 | h | 242/246 (98%) | 230 (95%) | 12 (5%) | 0 | 100 | 100 |
| 3 | b | 218/277 (79%) | 210 (96%) | 7 (3%) | 1 (0%) | 29 | 68 |
| 3 | p | 218/277 (79%) | 207 (95%) | 9 (4%) | 2 (1%) | 17 | 56 |
| 4 | C | 231/234 (99%) | 204 (88%) | 24 (10%) | 3 (1%) | 12 | 48 |
| 4 | i | 229/234 (98%) | 202 (88%) | 24 (10%) | 3 (1%) | 12 | 48 |
| 5 | c | 202/205 (98%) | 189 (94%) | 11 (5%) | 2 (1%) | 15 | 54 |
| 5 | q | 202/205 (98%) | 188 (93%) | 11 (5%) | 3 (2%) | 10 | 46 |
| 6 | D | 248/261 (95%) | 236 (95%) | 11 (4%) | 1 (0%) | 34 | 72 |
| 6 | j | 248/261 (95%) | 233 (94%) | 12 (5%) | 3 (1%) | 13 | 50 |
| 7 | d | 197/201 (98%) | 186 (94%) | 10 (5%) | 1 (0%) | 29 | 68 |
| 7 | r | 197/201 (98%) | 186 (94%) | 9 (5%) | 2 (1%) | 15 | 54 |
| 8 | E | 241/248 (97%) | 223 (92%) | 12 (5%) | 6 (2%) | 5 | 35 |
| 8 | k | 241/248 (97%) | 224 (93%) | 11 (5%) | 6 (2%) | 5 | 35 |
| 9 | e | 199/263 (76%) | 195 (98%) | 4 (2%) | 0 | 100 | 100 |
| 9 | s | 199/263 (76%) | 191 (96%) | 8 (4%) | 0 | 100 | 100 |
| 10 | F | 232/241 (96%) | 216 (93%) | 14 (6%) | 2 (1%) | 17 | 56 |
| 10 | l | 232/241 (96%) | 215 (93%) | 15 (6%) | 2 (1%) | 17 | 56 |
| 11 | f | 211/241 (88%) | 205 (97%) | 6 (3%) | 0 | 100 | 100 |
| 11 | t | 211/241 (88%) | 202 (96%) | 9 (4%) | 0 | 100 | 100 |
| 12 | G | 236/263 (90%) | 223 (94%) | 10 (4%) | 3 (1%) | 12 | 48 |
| 12 | m | 236/263 (90%) | 222 (94%) | 10 (4%) | 4 (2%) | 9 | 43 |
| 13 | g | 214/264 (81%) | 203 (95%) | 10 (5%) | 1 (0%) | 29 | 68 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 13 | u | 215/264 (81%) | 205 (95%) | 9 (4%) | 1 (0%) | 29 | 68 |
| 14 | H | 376/433 (87%) | 254 (68%) | 81 (22%) | 41 (11%) | 0 | 8 |
| 15 | I | 355/440 (81%) | 264 (74%) | 63 (18%) | 28 (8%) | 1 | 14 |
| 16 | J | 354/406 (87%) | 253 (72%) | 68 (19%) | 33 (9%) | 0 | 12 |
| 17 | K | 378/418 (90%) | 260 (69%) | 73 (19%) | 45 (12%) | 0 | 6 |
| 18 | L | 373/389 (96%) | 268 (72%) | 69 (18%) | 36 (10%) | 0 | 11 |
| 19 | M | 372/439 (85%) | 257 (69%) | 72 (19%) | 43 (12%) | 0 | 6 |
| 20 | N | 815/953 (86%) | 610 (75%) | 176 (22%) | 29 (4%) | 3 | 28 |
| 21 | X | 241/255 (94%) | 233 (97%) | 5 (2%) | 3 (1%) | 13 | 50 |
| 21 | n | 241/255 (94%) | 232 (96%) | 7 (3%) | 2 (1%) | 19 | 60 |
| 22 | O | 368/376 (98%) | 292 (79%) | 55 (15%) | 21 (6%) | 1 | 20 |
| 23 | P | 401/456 (88%) | 333 (83%) | 55 (14%) | 13 (3%) | 4 | 30 |
| 24 | Q | 419/422 (99%) | 324 (77%) | 67 (16%) | 28 (7%) | 1 | 18 |
| 25 | R | 374/389 (96%) | 292 (78%) | 60 (16%) | 22 (6%) | 1 | 20 |
| 26 | S | 389/534 (73%) | 332 (85%) | 42 (11%) | 15 (4%) | 3 | 26 |
| 27 | T | 254/350 (73%) | 191 (75%) | 44 (17%) | 19 (8%) | 1 | 15 |
| 28 | U | 279/324 (86%) | 224 (80%) | 42 (15%) | 13 (5%) | 2 | 24 |
| 29 | V | 253/310 (82%) | 210 (83%) | 32 (13%) | 11 (4%) | 2 | 25 |
| 30 | W | 191/377 (51%) | 143 (75%) | 38 (20%) | 10 (5%) | 2 | 22 |
| 31 | Y | 55/70 (79%) | 36 (66%) | 12 (22%) | 7 (13%) | 0 | 5 |
| 32 | Z | 722/908 (80%) | 560 (78%) | 113 (16%) | 49 (7%) | 1 | 17 |
| 33 | x | 349/494 (71%) | 245 (70%) | 62 (18%) | 42 (12%) | 0 | 6 |
| 34 | y | 74/76 (97%) | 71 (96%) | 3 (4%) | 0 | 100 | 100 |
| All | All | 13374/15440 (87%) | 11297 (84%) | 1514 (11%) | 563 (4%) | 5 | 25 |

5 of 563 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | F | 120 | ALA |
| 12 | G | 238 | GLU |
| 14 | H | 95 | VAL |
| 14 | H | 108 | ASP |
| 14 | H | 109 | PRO |

### 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 | |
|---|---|---|---|---|---|---|
| 1 | a | 155/181 (86%) | 148 (96%) | 7 (4%) | 27 | 54 |
| 1 | o | 155/181 (86%) | 148 (96%) | 7 (4%) | 27 | 54 |
| 2 | B | 193/210 (92%) | 182 (94%) | 11 (6%) | 20 | 48 |
| 2 | h | 195/210 (93%) | 183 (94%) | 12 (6%) | 18 | 45 |
| 3 | b | 177/228 (78%) | 170 (96%) | 7 (4%) | 31 | 56 |
| 3 | p | 177/228 (78%) | 168 (95%) | 9 (5%) | 24 | 50 |
| 4 | C | 163/191 (85%) | 155 (95%) | 8 (5%) | 25 | 51 |
| 4 | i | 177/191 (93%) | 163 (92%) | 14 (8%) | 12 | 38 |
| 5 | c | 172/174 (99%) | 163 (95%) | 9 (5%) | 23 | 50 |
| 5 | q | 172/174 (99%) | 163 (95%) | 9 (5%) | 23 | 50 |
| 6 | D | 193/221 (87%) | 182 (94%) | 11 (6%) | 20 | 48 |
| 6 | j | 193/221 (87%) | 183 (95%) | 10 (5%) | 23 | 50 |
| 7 | d | 164/171 (96%) | 156 (95%) | 8 (5%) | 25 | 51 |
| 7 | r | 164/171 (96%) | 157 (96%) | 7 (4%) | 29 | 55 |
| 8 | E | 152/211 (72%) | 142 (93%) | 10 (7%) | 16 | 43 |
| 8 | k | 142/211 (67%) | 134 (94%) | 8 (6%) | 21 | 48 |
| 9 | e | 153/202 (76%) | 149 (97%) | 4 (3%) | 46 | 67 |
| 9 | s | 154/202 (76%) | 148 (96%) | 6 (4%) | 32 | 57 |
| 10 | F | 190/203 (94%) | 185 (97%) | 5 (3%) | 46 | 67 |
| 10 | l | 191/203 (94%) | 185 (97%) | 6 (3%) | 40 | 63 |
| 11 | f | 174/199 (87%) | 166 (95%) | 8 (5%) | 27 | 53 |
| 11 | t | 175/199 (88%) | 168 (96%) | 7 (4%) | 31 | 56 |
| 12 | G | 198/224 (88%) | 191 (96%) | 7 (4%) | 36 | 60 |
| 12 | m | 198/224 (88%) | 183 (92%) | 15 (8%) | 13 | 40 |
| 13 | g | 175/215 (81%) | 166 (95%) | 9 (5%) | 24 | 50 |
| 13 | u | 175/215 (81%) | 164 (94%) | 11 (6%) | 18 | 44 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 14 | H | 292/372 (78%) | 238 (82%) | 54 (18%) | 1 | 10 |
| 15 | I | 291/385 (76%) | 231 (79%) | 60 (21%) | 1 | 7 |
| 16 | J | 310/352 (88%) | 246 (79%) | 64 (21%) | 1 | 7 |
| 17 | K | 333/366 (91%) | 268 (80%) | 65 (20%) | 1 | 9 |
| 18 | L | 298/341 (87%) | 239 (80%) | 59 (20%) | 1 | 9 |
| 19 | M | 296/379 (78%) | 240 (81%) | 56 (19%) | 1 | 9 |
| 20 | N | 377/816 (46%) | 345 (92%) | 32 (8%) | 10 | 36 |
| 21 | X | 193/212 (91%) | 186 (96%) | 7 (4%) | 35 | 60 |
| 21 | n | 193/212 (91%) | 184 (95%) | 9 (5%) | 26 | 52 |
| 22 | O | 144/336 (43%) | 119 (83%) | 25 (17%) | 2 | 12 |
| 23 | P | 202/416 (49%) | 182 (90%) | 20 (10%) | 8 | 28 |
| 24 | Q | 249/362 (69%) | 207 (83%) | 42 (17%) | 2 | 13 |
| 25 | R | 226/344 (66%) | 196 (87%) | 30 (13%) | 4 | 20 |
| 26 | S | 163/460 (35%) | 153 (94%) | 10 (6%) | 18 | 46 |
| 27 | T | 109/294 (37%) | 92 (84%) | 17 (16%) | 2 | 16 |
| 28 | U | 212/295 (72%) | 184 (87%) | 28 (13%) | 4 | 20 |
| 29 | V | 219/268 (82%) | 188 (86%) | 31 (14%) | 3 | 18 |
| 30 | W | 109/312 (35%) | 102 (94%) | 7 (6%) | 17 | 44 |
| 31 | Y | 4/63 (6%) | 4 (100%) | 0 | 100 | 100 |
| 33 | x | 305/439 (70%) | 254 (83%) | 51 (17%) | 2 | 14 |
| 34 | y | 68/68 (100%) | 64 (94%) | 4 (6%) | 19 | 47 |
| All | All | 9120/12352 (74%) | 8224 (90%) | 896 (10%) | 11 | 28 |

5 of 896 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | M | 168 | TYR |
| 33 | x | 431 | SER |
| 22 | O | 65 | SER |
| 33 | x | 337 | SER |
| 29 | V | 98 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | W | 169 | HIS |
| 33 | x | 197 | GLN |
| 34 | y | 25 | ASN |
| 17 | K | 302 | ASN |
| 17 | K | 286 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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 | $\#\|Z\| > 2$ |
| 34 | GLZ | y | 76 | 34 | 3,3,3 | 0.74 | 0 | 0,2,2 | - | - |

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 |
|---|---|---|---|---|---|---|---|
| 34 | GLZ | y | 76 | 34 | - | 0/0/1/1 | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

6 ligands 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 | $\#\|Z\| > 2$ |
| 35 | ADP | H | 501 | - | 24,29,29 | 1.58 | 4 (16%) | 29,45,45 | 2.76 | 10 (34%) |
| 35 | ADP | L | 401 | - | 24,29,29 | 1.02 | 1 (4%) | 29,45,45 | 1.74 | 8 (27%) |
| 35 | ADP | I | 501 | - | 24,29,29 | 1.47 | 3 (12%) | 29,45,45 | 1.90 | 6 (20%) |
| 35 | ADP | K | 501 | - | 24,29,29 | 1.34 | 3 (12%) | 29,45,45 | 1.92 | 11 (37%) |
| 35 | ADP | J | 501 | - | 24,29,29 | 1.35 | 4 (16%) | 29,45,45 | 2.15 | 9 (31%) |
| 35 | ADP | M | 501 | - | 24,29,29 | 1.16 | 3 (12%) | 29,45,45 | 1.81 | 10 (34%) |

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 |
|---|---|---|---|---|---|---|---|
| 35 | ADP | H | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 35 | ADP | L | 401 | - | - | 2/12/32/32 | 0/3/3/3 |
| 35 | ADP | I | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 35 | ADP | K | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 35 | ADP | J | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 35 | ADP | M | 501 | - | - | 3/12/32/32 | 0/3/3/3 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 35 | H | 501 | ADP | O4'-C1' | 4.76 | 1.47 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 35 | I | 501 | ADP | C5-C4 | 4.40 | 1.52 | 1.40 |
| 35 | J | 501 | ADP | C2'-C1' | -2.91 | 1.49 | 1.53 |
| 35 | H | 501 | ADP | C6-C5 | 2.90 | 1.54 | 1.43 |
| 35 | K | 501 | ADP | O4'-C1' | 2.80 | 1.45 | 1.41 |

The worst 5 of 54 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | H | 501 | ADP | C3'-C2'-C1' | 7.83 | 112.77 | 100.98 |
| 35 | H | 501 | ADP | O4'-C1'-C2' | -5.76 | 98.51 | 106.93 |
| 35 | I | 501 | ADP | C3'-C2'-C1' | 5.66 | 109.49 | 100.98 |
| 35 | H | 501 | ADP | C4-C5-N7 | -5.00 | 104.19 | 109.40 |
| 35 | J | 501 | ADP | N3-C2-N1 | -4.59 | 121.50 | 128.68 |

There are no chirality outliers.

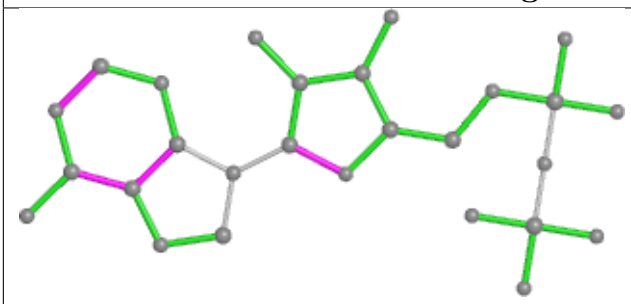
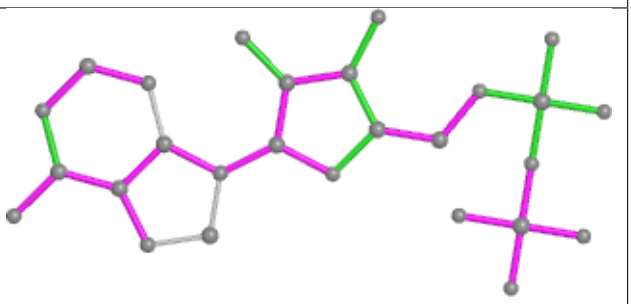
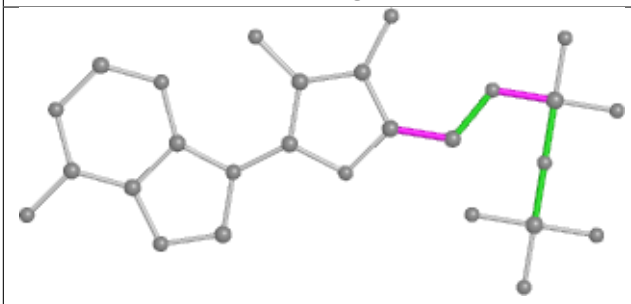
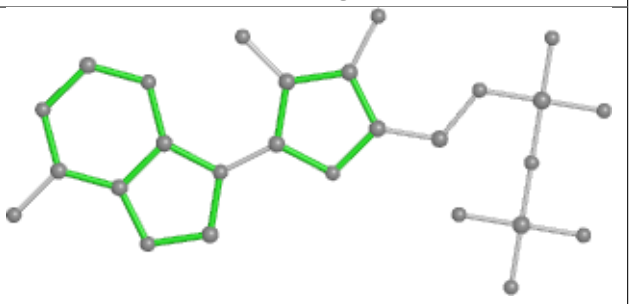
5 of 20 torsion outliers are listed below:

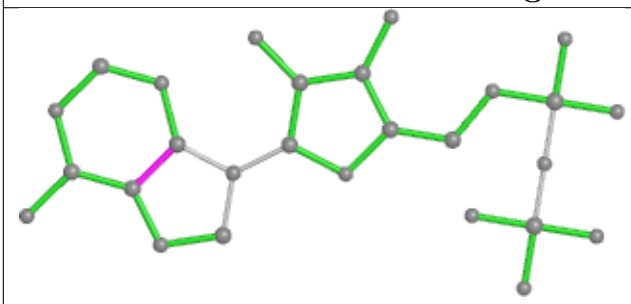
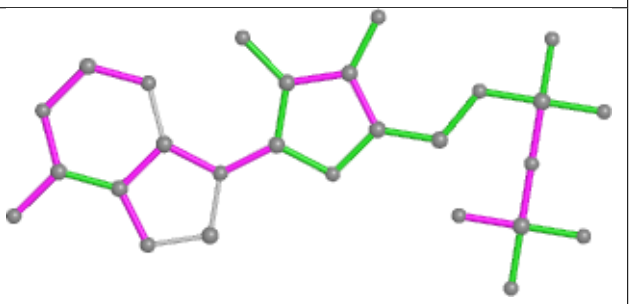
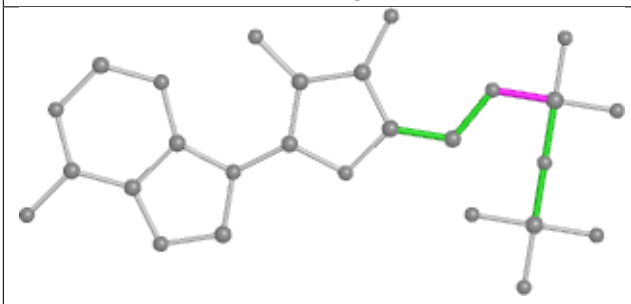
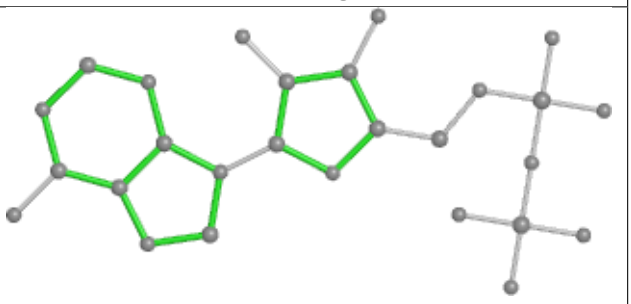
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 35 | H | 501 | ADP | O4'-C4'-C5'-O5' |
| 35 | I | 501 | ADP | O4'-C4'-C5'-O5' |
| 35 | J | 501 | ADP | C5'-O5'-PA-O1A |
| 35 | J | 501 | ADP | C5'-O5'-PA-O2A |
| 35 | J | 501 | ADP | C5'-O5'-PA-O3A |

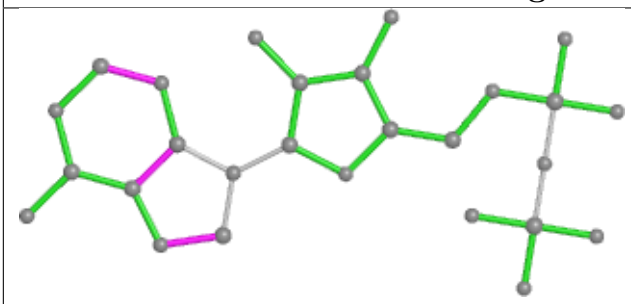
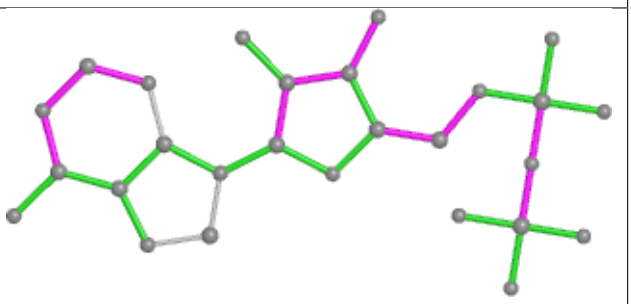
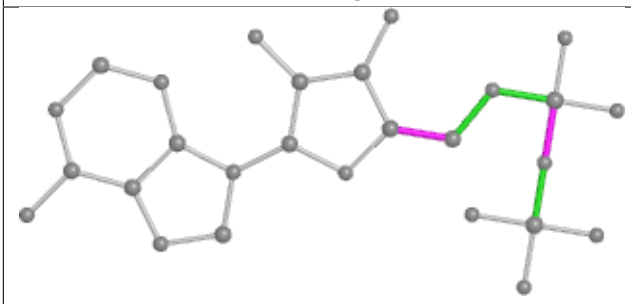
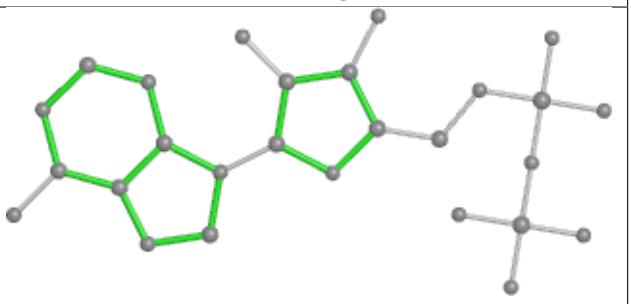
There are no ring outliers.

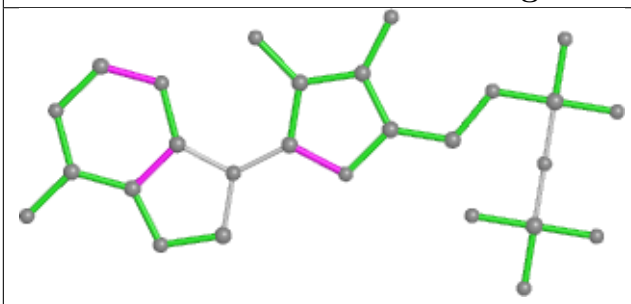
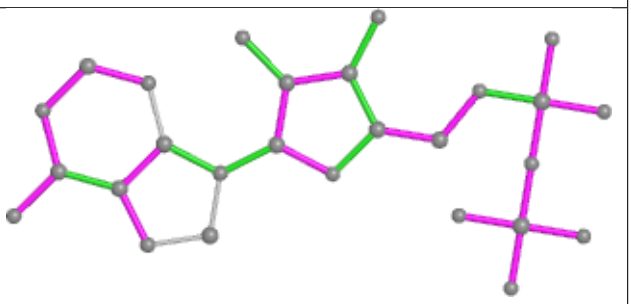
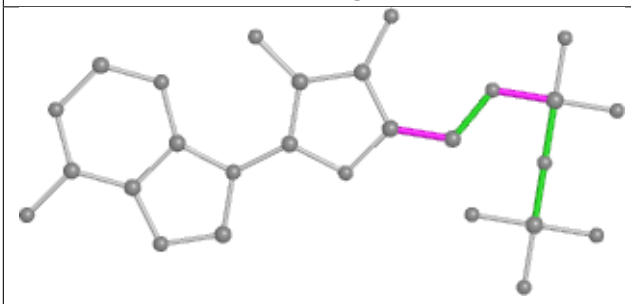
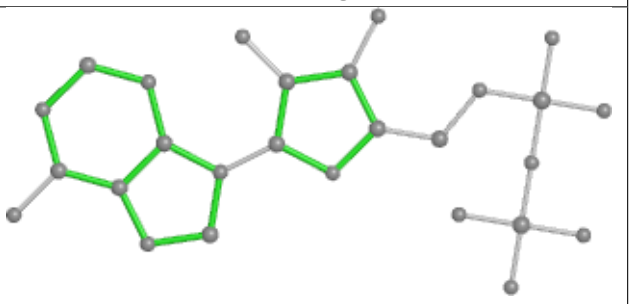
No monomer is involved in short contacts.

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.

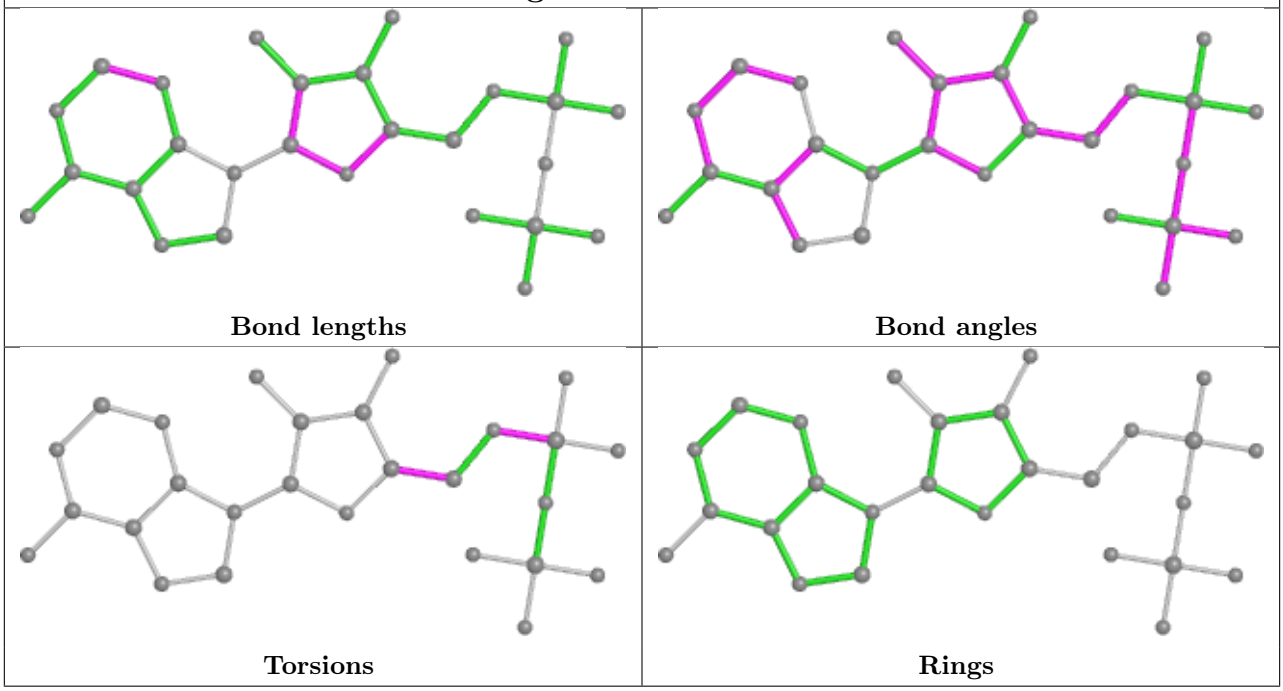
| Ligand ADP H 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP L 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

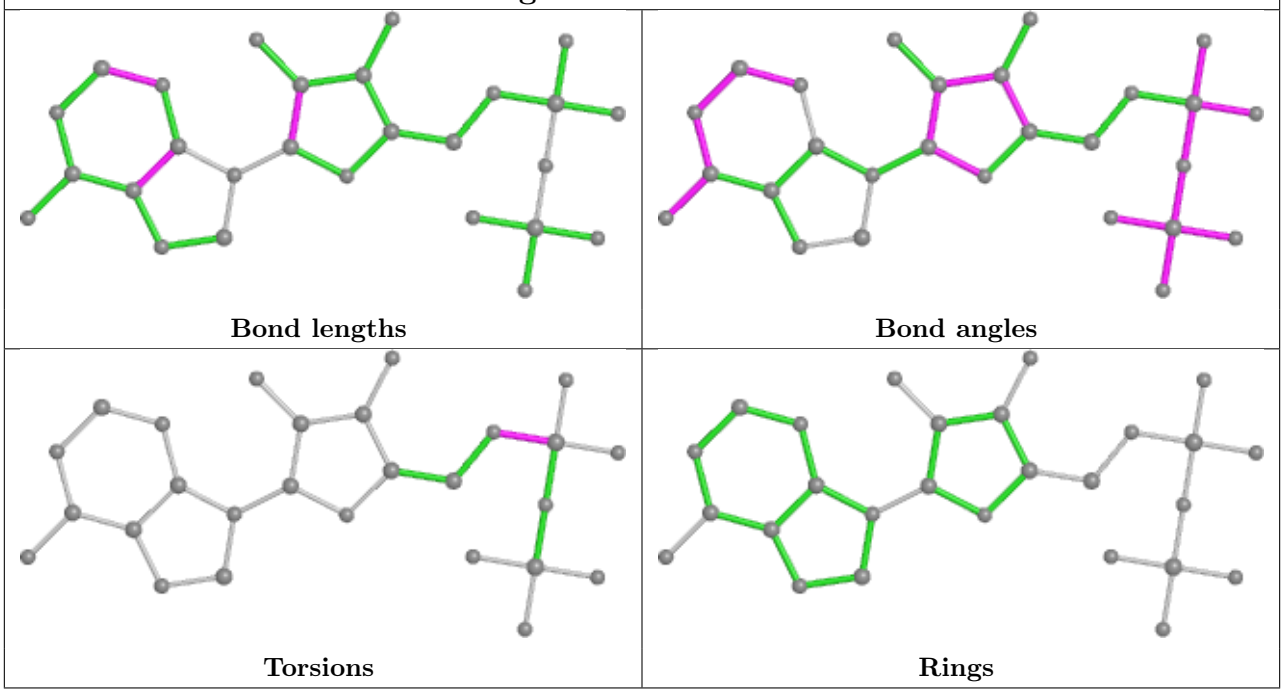
| Ligand ADP I 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP K 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

**Ligand ADP J 501**




**Ligand ADP M 501**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

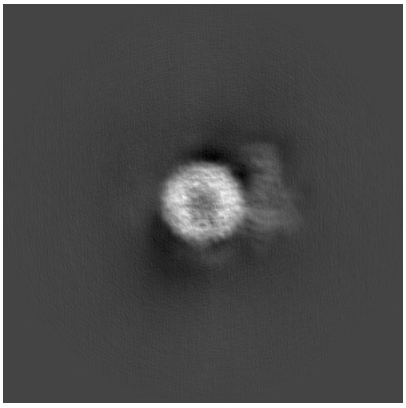
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9511. These allow visual inspection of the internal detail of the map and identification of artifacts.

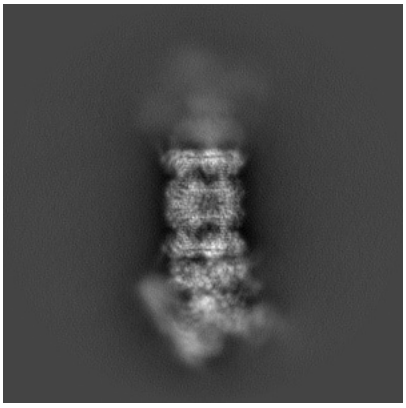
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

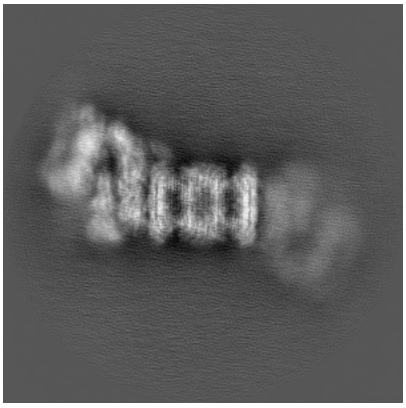
### 6.1.1 Primary map



X



Y

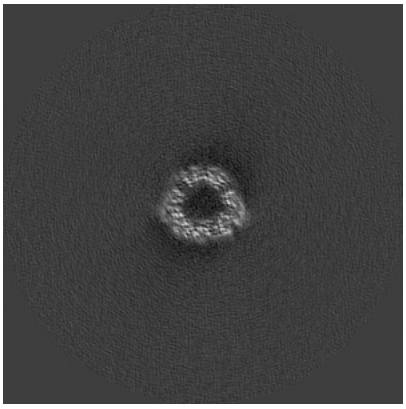


Z

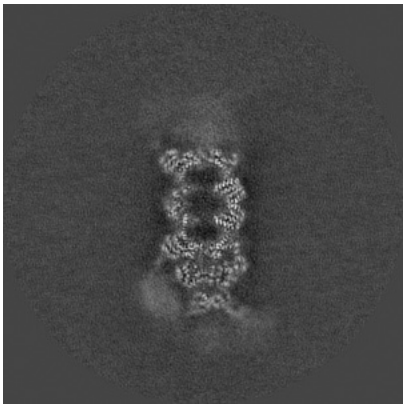
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

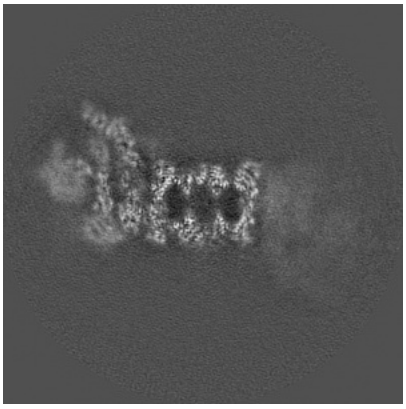
### 6.2.1 Primary map



X Index: 256



Y Index: 256

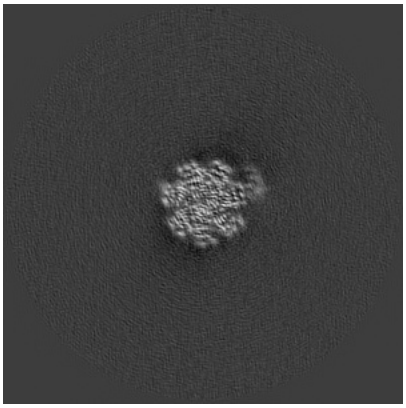


Z Index: 256

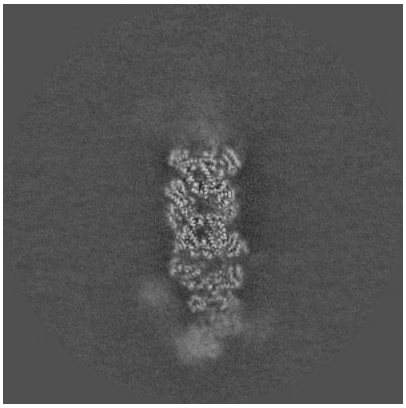
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

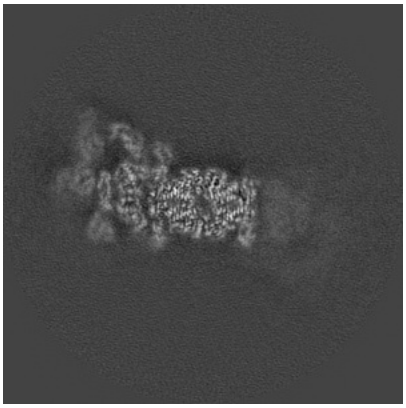
### 6.3.1 Primary map



X Index: 202



Y Index: 278

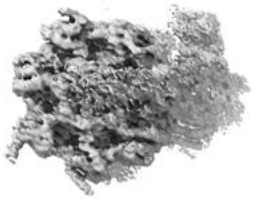


Z Index: 280

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

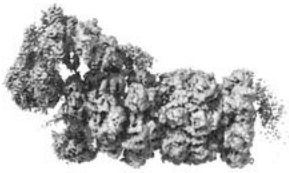
## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

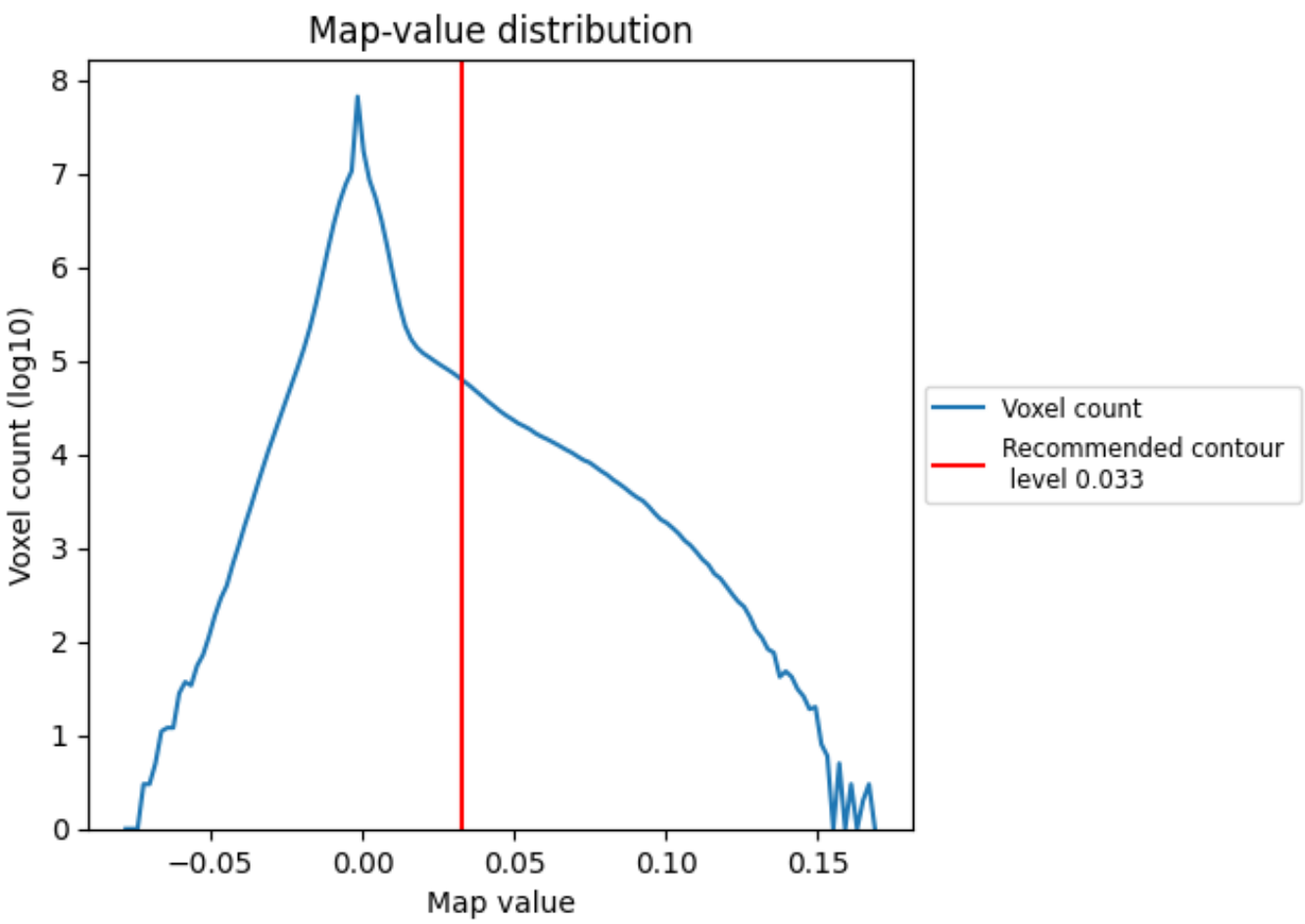
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

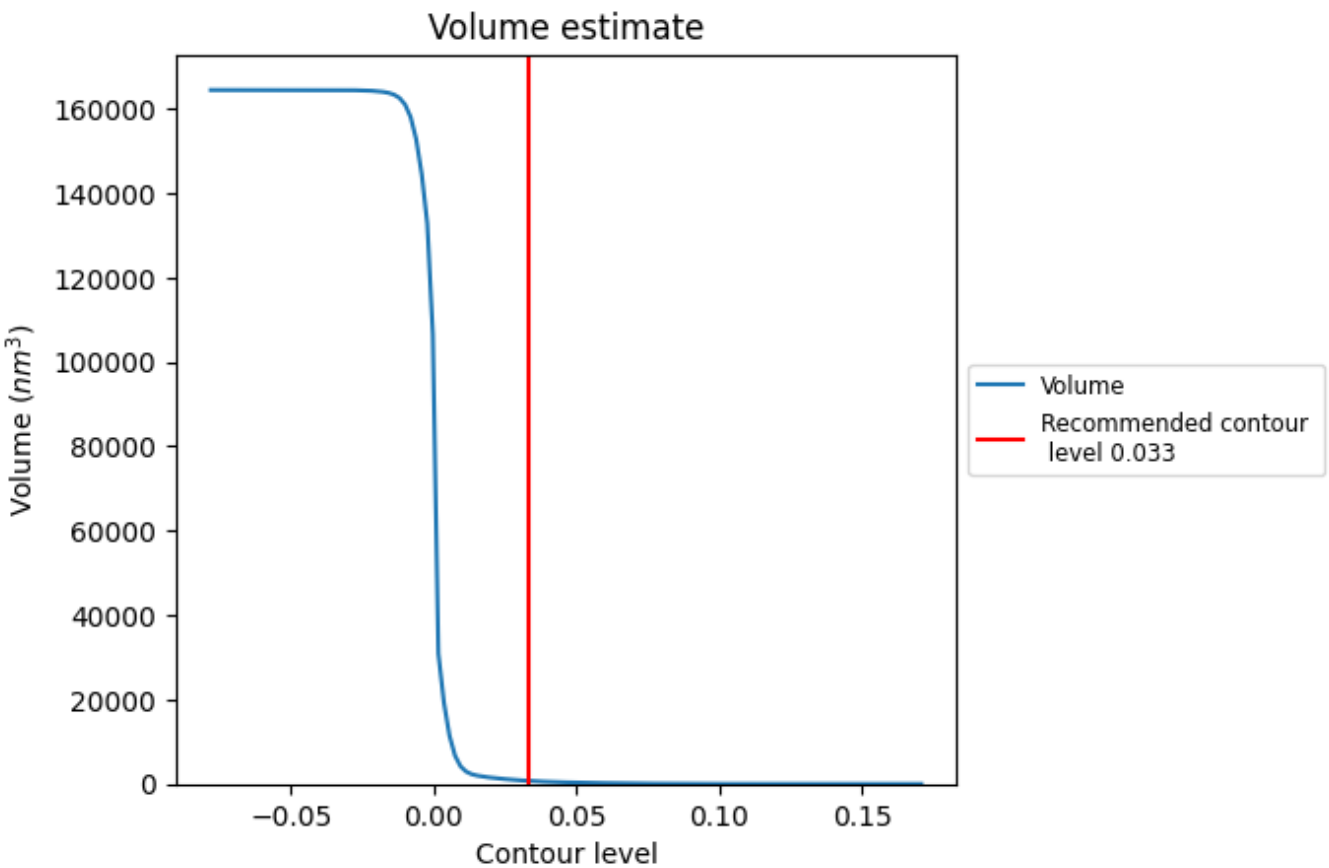
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

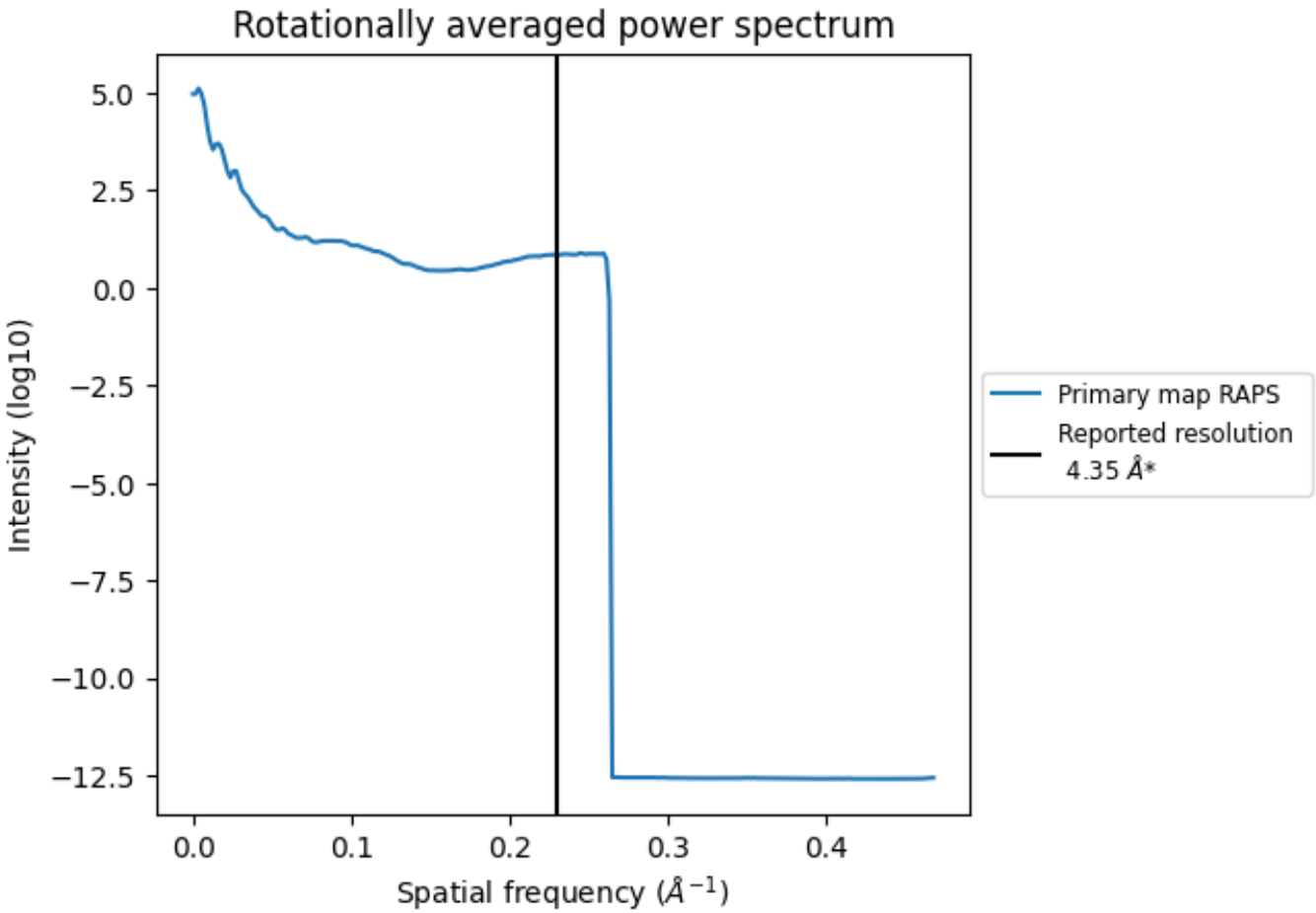
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 752 $nm^3$; this corresponds to an approximate mass of 679 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 (i)




*Reported resolution corresponds to spatial frequency of 0.230 Å$^{-1}$

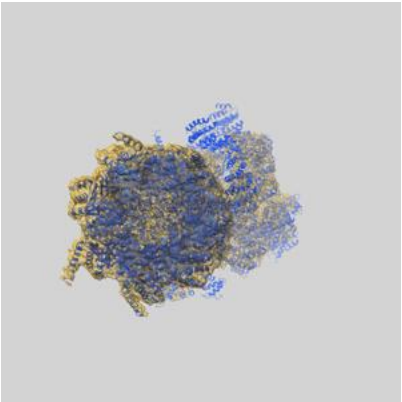
# 8 Fourier-Shell correlation (i)

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

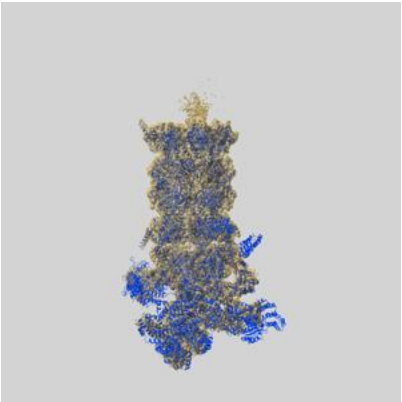
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9511 and PDB model 5GJQ. Per-residue inclusion information can be found in section 3 on page 12.

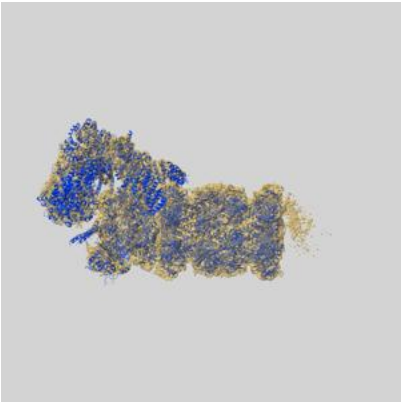
## 9.1 Map-model overlay (i)



X



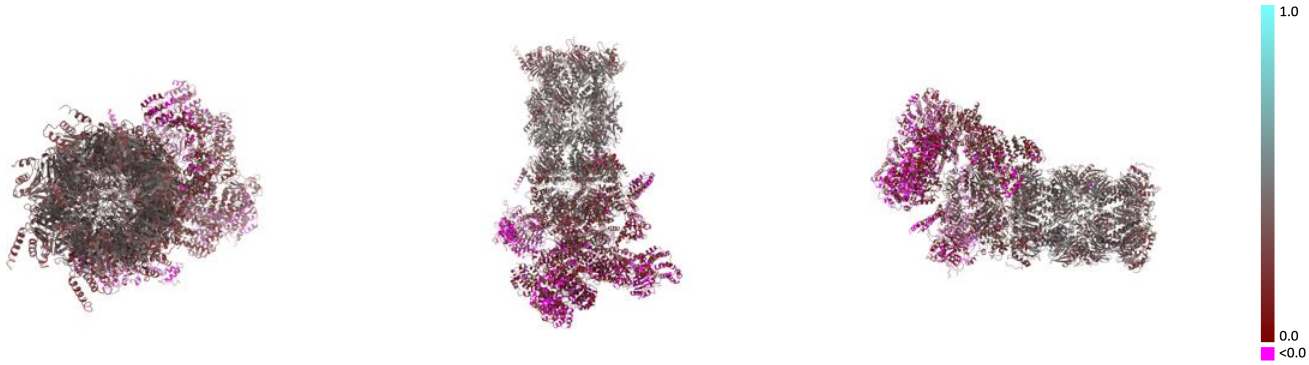
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

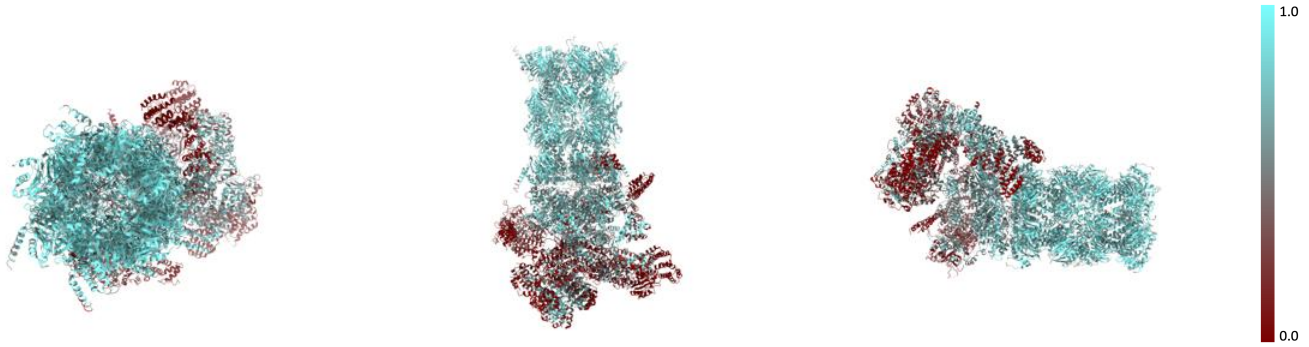
## 9.2 Q-score mapped to coordinate model (i)




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.

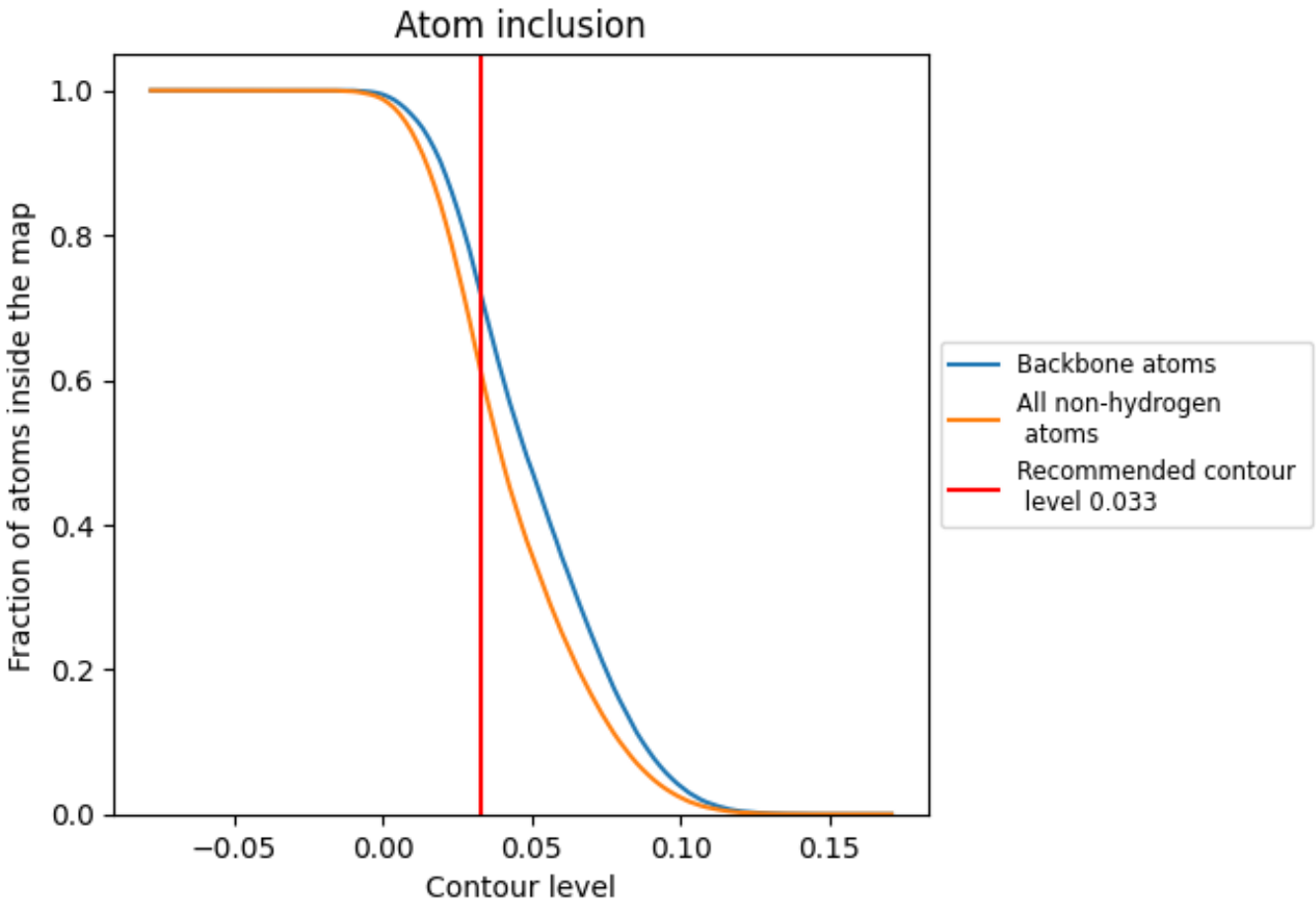
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.033).

## 9.4 Atom inclusion (i)




At the recommended contour level, 72% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.033) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6086 | 0.2740 |
| B | 0.7939 | 0.3520 |
| C | 0.8172 | 0.3590 |
| D | 0.8031 | 0.3480 |
| E | 0.7651 | 0.3130 |
| F | 0.7885 | 0.3570 |
| G | 0.8008 | 0.3490 |
| H | 0.6429 | 0.3090 |
| I | 0.6237 | 0.3070 |
| J | 0.6241 | 0.2940 |
| K | 0.6551 | 0.2840 |
| L | 0.6175 | 0.2840 |
| M | 0.6228 | 0.2930 |
| N | 0.3863 | 0.0710 |
| O | 0.2563 | 0.1060 |
| P | 0.3282 | 0.1410 |
| Q | 0.4816 | 0.2210 |
| R | 0.5944 | 0.2160 |
| S | 0.2863 | 0.1500 |
| T | 0.1912 | 0.1140 |
| U | 0.2700 | 0.1230 |
| V | 0.3095 | 0.1700 |
| W | 0.0054 | 0.0270 |
| X | 0.8119 | 0.3640 |
| Y | 0.2760 | 0.2040 |
| Z | 0.0793 | 0.0230 |
| a | 0.8084 | 0.3870 |
| b | 0.8042 | 0.3810 |
| c | 0.8055 | 0.3870 |
| d | 0.8300 | 0.3760 |
| e | 0.8264 | 0.3890 |
| f | 0.8467 | 0.3860 |
| g | 0.8618 | 0.4020 |
| h | 0.7822 | 0.3800 |
| i | 0.7943 | 0.3970 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| j | 0.7643 | 0.3570 |
| k | 0.7647 | 0.3420 |
| l | 0.7860 | 0.3670 |
| m | 0.8124 | 0.3770 |
| n | 0.7874 | 0.3670 |
| o | 0.8395 | 0.3930 |
| p | 0.8346 | 0.3940 |
| q | 0.8350 | 0.4030 |
| r | 0.8143 | 0.3910 |
| s | 0.8594 | 0.3920 |
| t | 0.7998 | 0.3950 |
| u | 0.8162 | 0.3960 |
| x | 0.3774 | 0.1260 |
| y | 0.2703 | 0.0860 |