# wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 09:12 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 6EPE |
| EMDB ID | : | EMD-3915 |
| Title | : | Substrate processing state 26S proteasome (SPS2) |
| Authors | : | Guo, Q.; Lehmer, C.; Martinez-Sanchez, A.; Rudack, T.; Beck, F.; Hartmann, H.; Hipp, M.S.; Hartl, F.U.; Edbauer, D.; Baumeister, W.; Fernandez-Busna diego, R. |
| Deposited on | : | 2017-10-11 |
| Resolution | : | 12.80 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 (i)) were used in the production of this report:

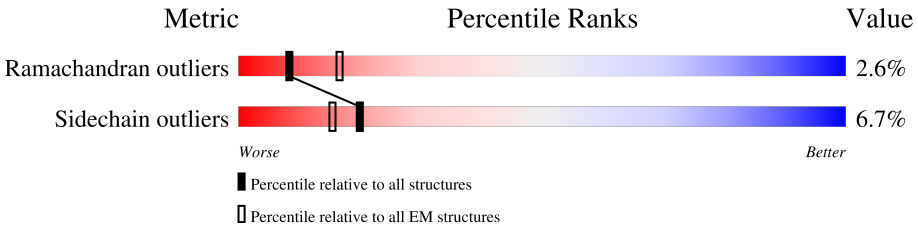
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 12.80 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 | 246 | 11% 76% 22% |
| 2 | B | 234 | 11% 73% 25% |
| 3 | C | 261 | 13% 74% 18% 5% |
| 4 | D | 254 | 14% 67% 25% |
| 5 | E | 241 | 5% 78% 16% |
| 6 | F | 263 | 70% 17% 10% |
| 7 | G | 255 | 9% 73% 20% |
| 8 | 1 | 238 | 10% 57% 23% 15% |
| 9 | 2 | 277 | 17% 53% 21% 5% 21% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | 3 | 205 | 13% 66% 27% 6% |
| 11 | 4 | 201 | 17% 64% 27% 6% |
| 12 | 5 | 263 | 10% 50% 22% 24% |
| 13 | 6 | 240 | 18% 63% 23% 11% |
| 14 | 7 | 263 | 15% 53% 24% 5% 18% |
| 15 | W | 377 | 16% 40% 11% 48% |
| 16 | V | 310 | 8% 74% 17% 7% |
| 17 | T | 353 | 18% 55% 15% 5% 25% |
| 18 | Y | 70 | 9% 27% 7% 66% |
| 19 | Z | 908 | 39% 75% 21% |
| 20 | N | 953 | 18% 74% 18% 5% |
| 21 | S | 530 | 17% 68% 17% 5% 10% |
| 22 | P | 456 | 28% 78% 19% |
| 23 | Q | 422 | 22% 74% 23% |
| 24 | R | 389 | 21% 73% 24% |
| 25 | U | 320 | 17% 68% 17% 5% 10% |
| 26 | O | 376 | 37% 76% 20% |
| 27 | H | 433 | 12% 69% 18% 9% |
| 28 | I | 440 | 14% 67% 17% 12% |
| 29 | K | 418 | 15% 70% 20% 6% |
| 30 | L | 403 | 21% 70% 23% |
| 31 | M | 442 | 18% 71% 20% 6% |
| 32 | J | 406 | 12% 73% 23% |

# 2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 82758 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 alpha type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 246 | 1920 | 1215 | 322 | 369 | 14 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 234 | 1828 | 1166 | 311 | 344 | 7 | 0 | 0 |

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 249 | 1960 | 1238 | 337 | 374 | 11 | 0 | 0 |

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 246 | 1926 | 1209 | 340 | 371 | 6 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 233 | 1778 | 1114 | 296 | 358 | 10 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 238 | 1871 | 1170 | 337 | 353 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 245 | Total | C | N | O | S | 0 | 0 |
| | | | 1912 | 1212 | 326 | 362 | 12 | | |

- Molecule 8 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | 1 | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1516 | 948 | 259 | 297 | 12 | | |

- Molecule 9 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | 2 | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1651 | 1042 | 281 | 316 | 12 | | |

- Molecule 10 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | 3 | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1600 | 1018 | 266 | 296 | 20 | | |

- Molecule 11 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | 4 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1572 | 1007 | 267 | 289 | 9 | | |

- Molecule 12 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | 5 | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1560 | 984 | 272 | 295 | 9 | | |

- Molecule 13 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | 6 | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1659 | 1050 | 284 | 315 | 10 | | |

- Molecule 14 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | 7 | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1686 | 1065 | 292 | 317 | 12 | | |

- Molecule 15 is a protein called 26S proteasome subunit S5a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | W | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 922 | 265 | 285 | 8 | | |

- Molecule 16 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | V | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2272 | 1438 | 391 | 424 | 19 | | |

- Molecule 17 is a protein called Proteasome 26S subunit, non-ATPase 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | T | 263 | Total | C | N | O | S | 0 | 0 |
| | | | 2149 | 1390 | 351 | 398 | 10 | | |

- Molecule 18 is a protein called RCG28037.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | Y | 24 | Total | C | N | O | S | 0 | 0 |
| | | | 199 | 120 | 34 | 44 | 1 | | |

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | Z | 896 | Total | C | N | O | S | 0 | 0 |
| | | | 6913 | 4342 | 1178 | 1346 | 47 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | N | 905 | Total | C | N | O | S | 0 | 0 |
| | | | 7082 | 4487 | 1193 | 1356 | 46 | | |

- Molecule 21 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | S | 476 | Total | C | N | O | S | 0 | 0 |
| | | | 3844 | 2438 | 685 | 707 | 14 | | |

- Molecule 22 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | P | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3706 | 2338 | 635 | 709 | 24 | | |

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | Q | 422 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2116 | 567 | 639 | 13 | | |

- Molecule 24 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | R | 389 | Total | C | N | O | S | 0 | 0 |
| | | | 3204 | 2042 | 542 | 600 | 20 | | |

- Molecule 25 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 7 (Predicted).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | U | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2299 | 1470 | 395 | 428 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | O | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 3011 | 1918 | 514 | 564 | 15 | | |

- Molecule 27 is a protein called 26S proteasome regulatory subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | H | 396 | Total | C | N | O | S | 0 | 0 |
| | | | 3113 | 1960 | 546 | 589 | 18 | | |

- Molecule 28 is a protein called 26S proteasome regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | I | 385 | Total | C | N | O | S | 0 | 0 |
| | | | 3042 | 1913 | 516 | 598 | 15 | | |

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | K | 391 | Total | C | N | O | S | 0 | 0 |
| | | | 3126 | 1978 | 535 | 600 | 13 | | |

- Molecule 30 is a protein called Proteasome 26S subunit, ATPase 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | L | 389 | Total | C | N | O | S | 0 | 0 |
| | | | 3098 | 1947 | 552 | 582 | 17 | | |

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | M | 415 | Total | C | N | O | S | 0 | 0 |
| | | | 3252 | 2038 | 561 | 635 | 18 | | |

- Molecule 32 is a protein called 26S proteasome regulatory subunit 8.

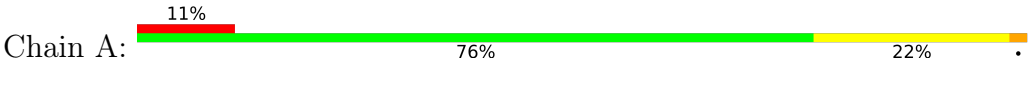
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | J | 406 | Total | C | N | O | S | 0 | 0 |
| | | | 3194 | 2006 | 569 | 599 | 20 | | |

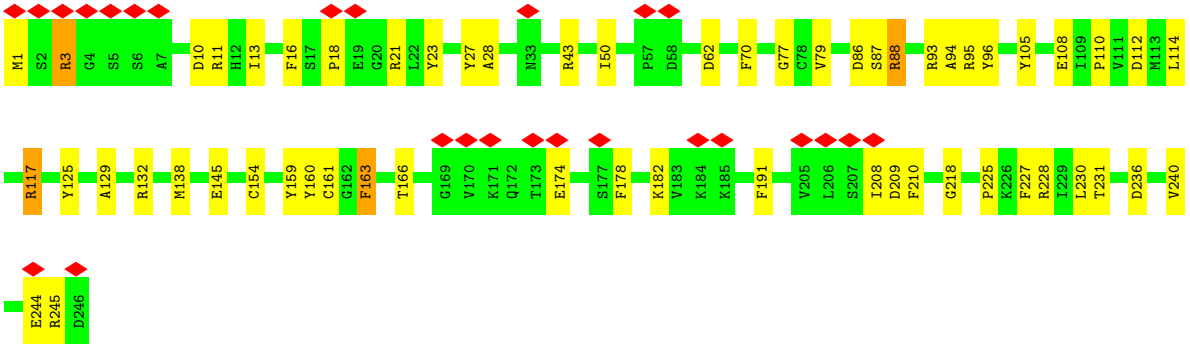
# 3 Residue-property plots (i)

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 alpha type-6

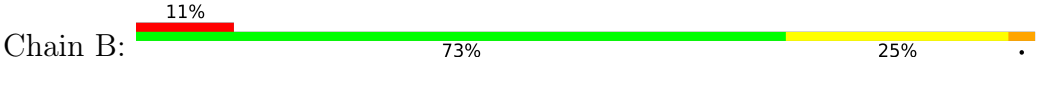
Chain A:

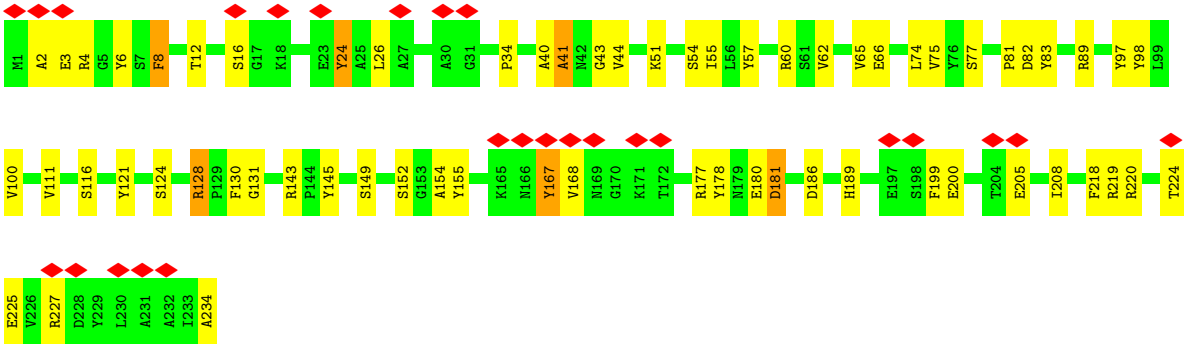



• Molecule 2: Proteasome subunit alpha type-2

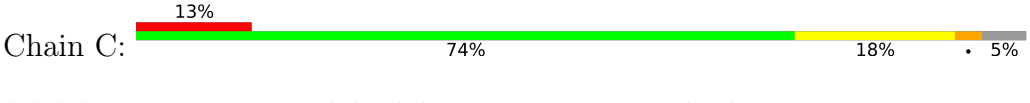
Chain B:

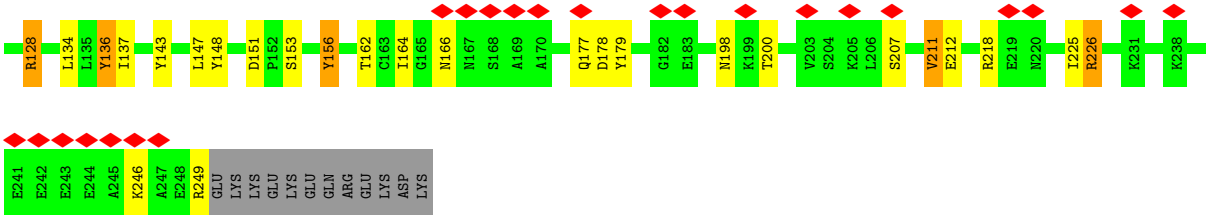


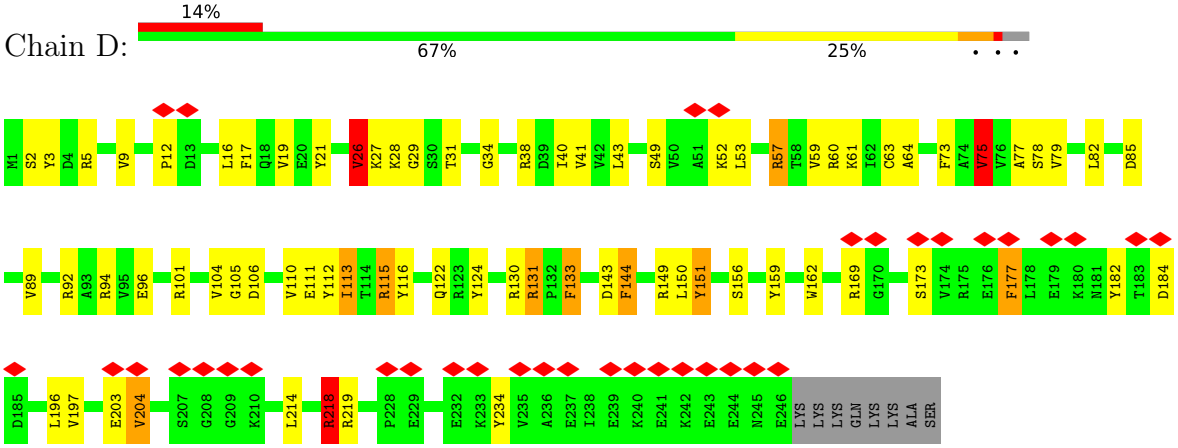

• Molecule 3: Proteasome subunit alpha type-4

Chain C:

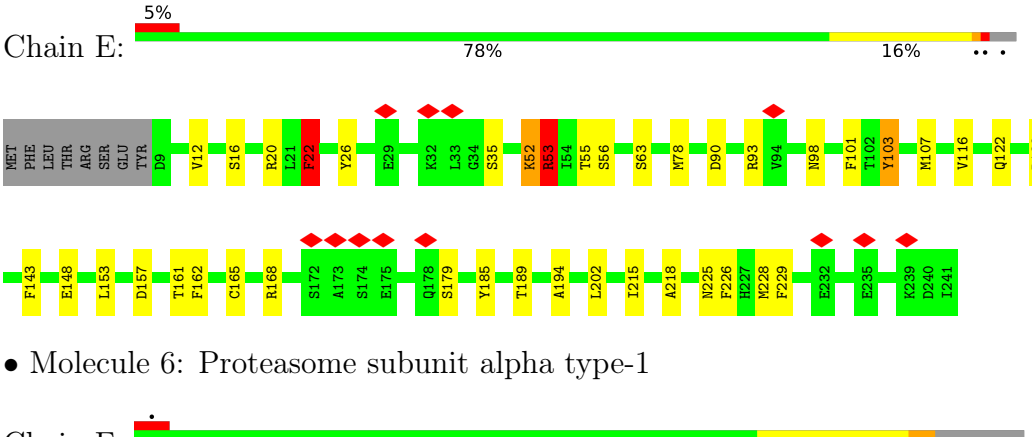


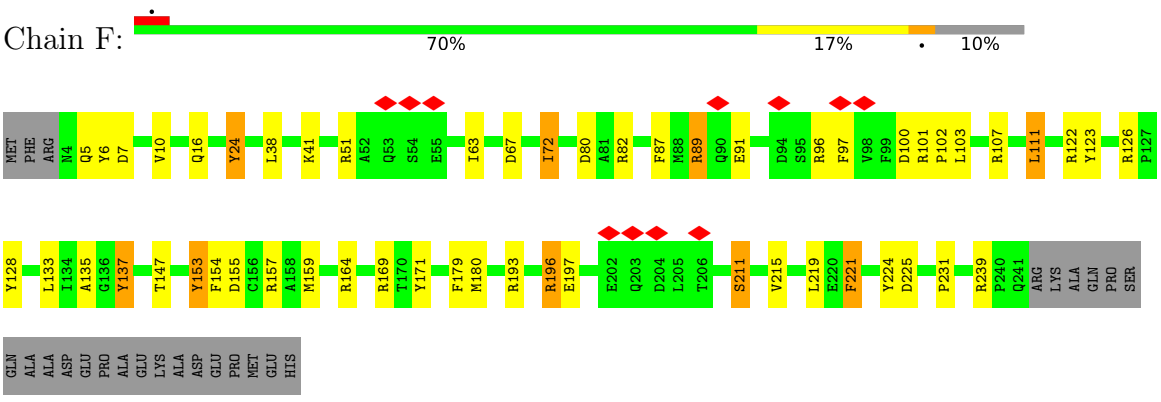

• Molecule 4: Proteasome subunit alpha type-7



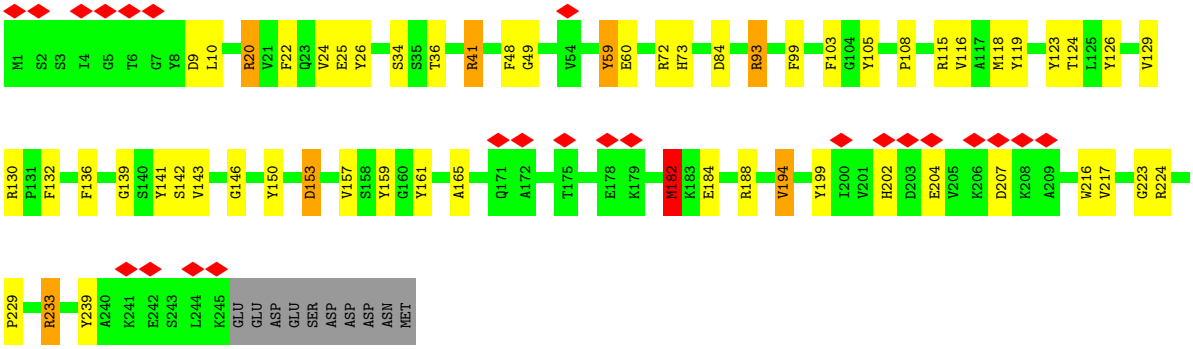

• Molecule 5: Proteasome subunit alpha type-5



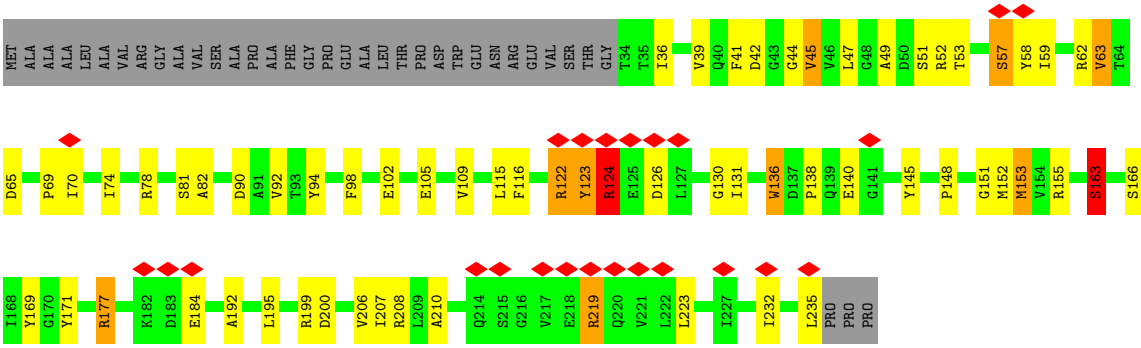

• Molecule 6: Proteasome subunit alpha type-1



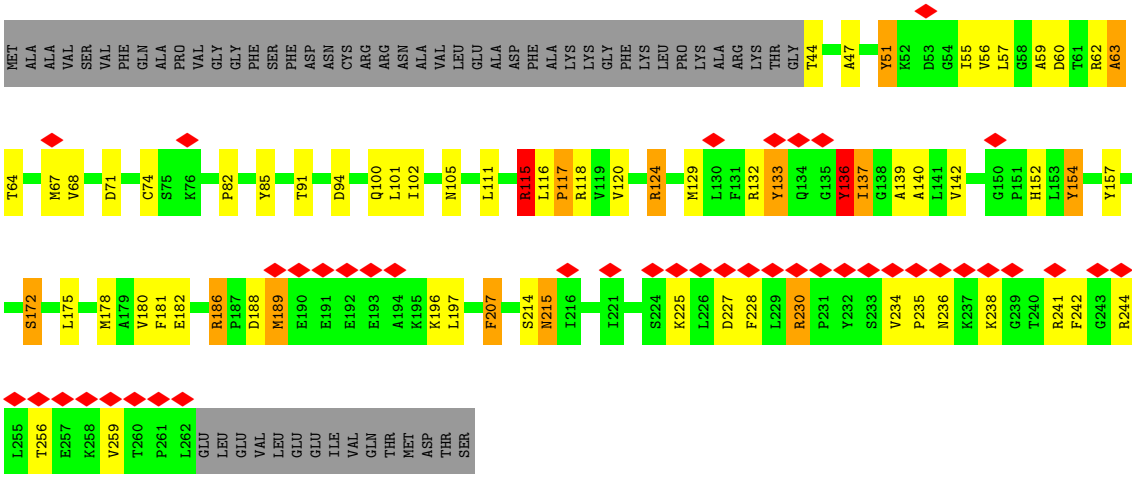

• Molecule 7: Proteasome subunit alpha type-3



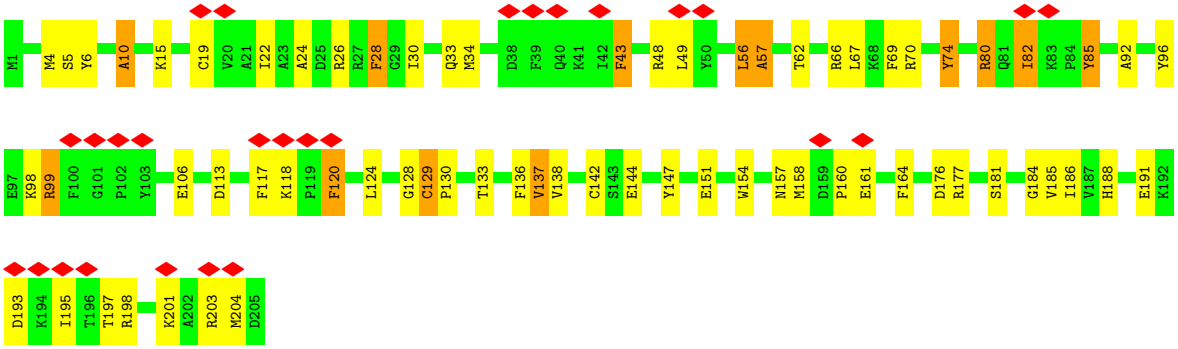

• Molecule 8: Proteasome subunit beta type-6

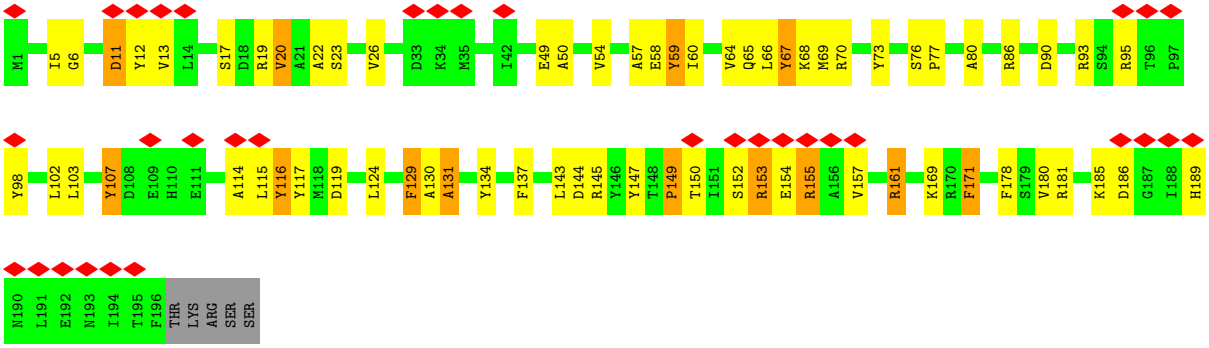

• Molecule 9: Proteasome subunit beta type-7

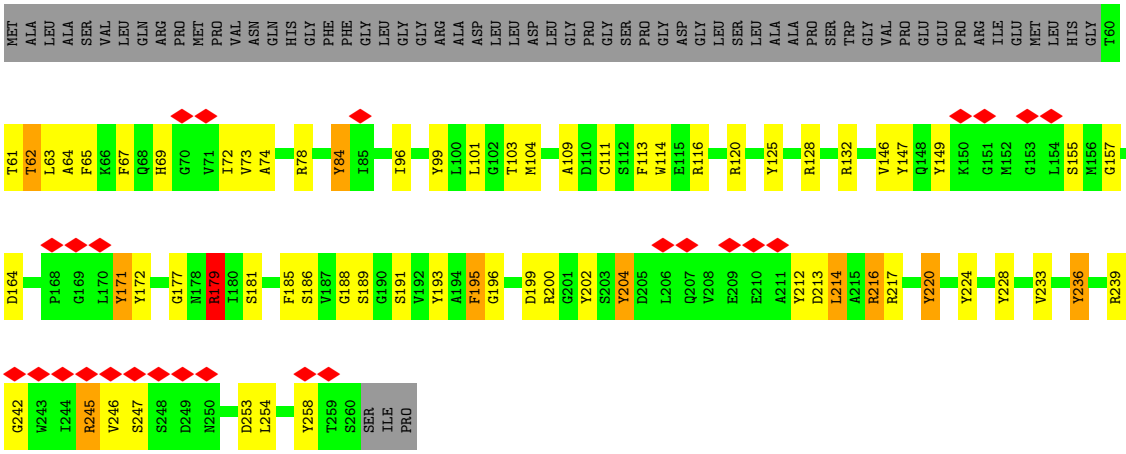

• Molecule 10: Proteasome subunit beta type-3



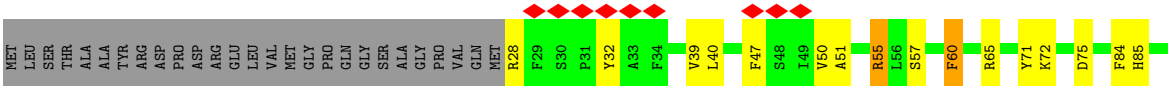

• Molecule 11: Proteasome subunit beta type-2

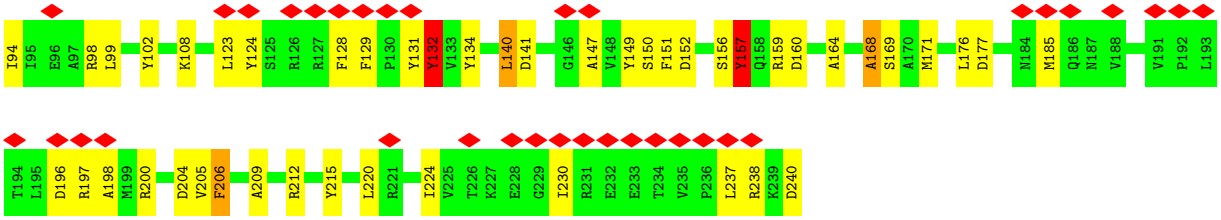




• Molecule 12: Proteasome subunit beta type-5


• Molecule 13: Proteasome subunit beta type-1

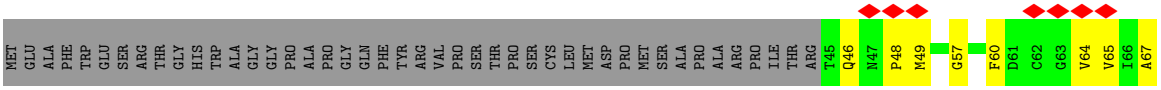



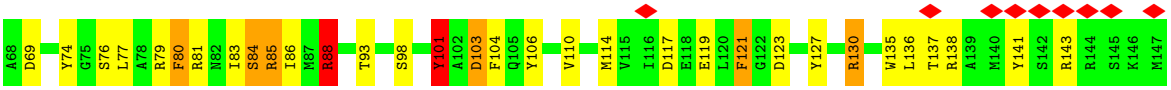


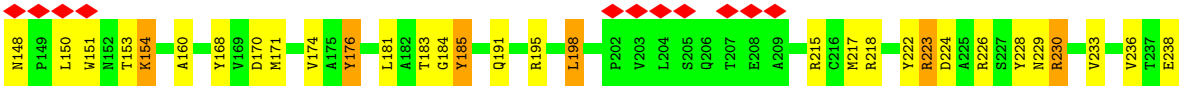


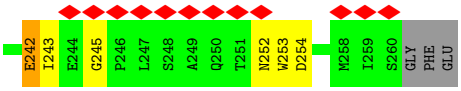
• Molecule 14: Proteasome subunit beta type-4

Chain 7:

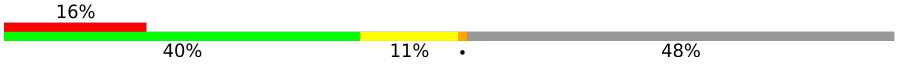


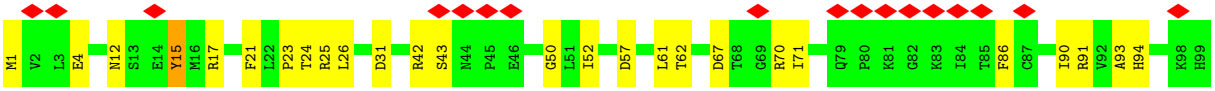


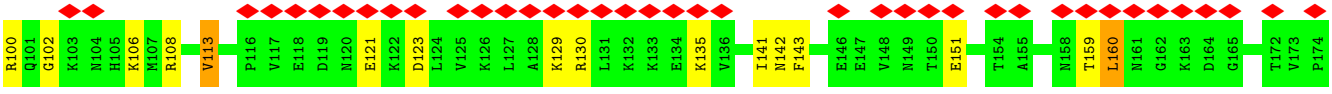


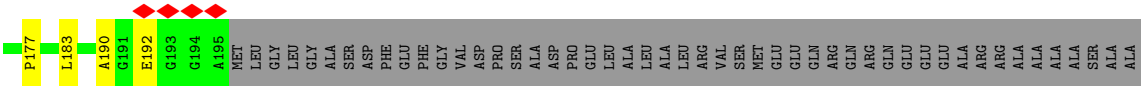
• Molecule 15: 26S proteasome subunit S5a

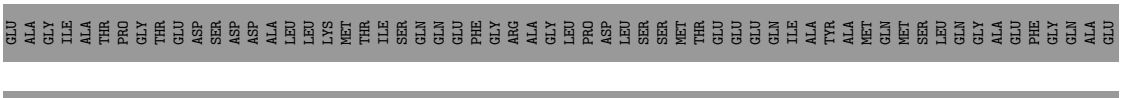
Chain W:

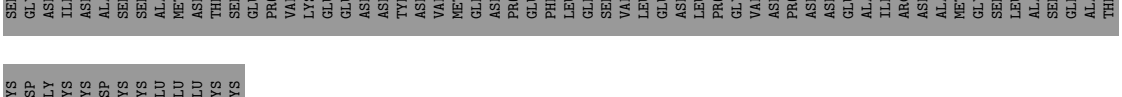


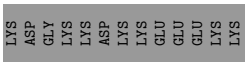







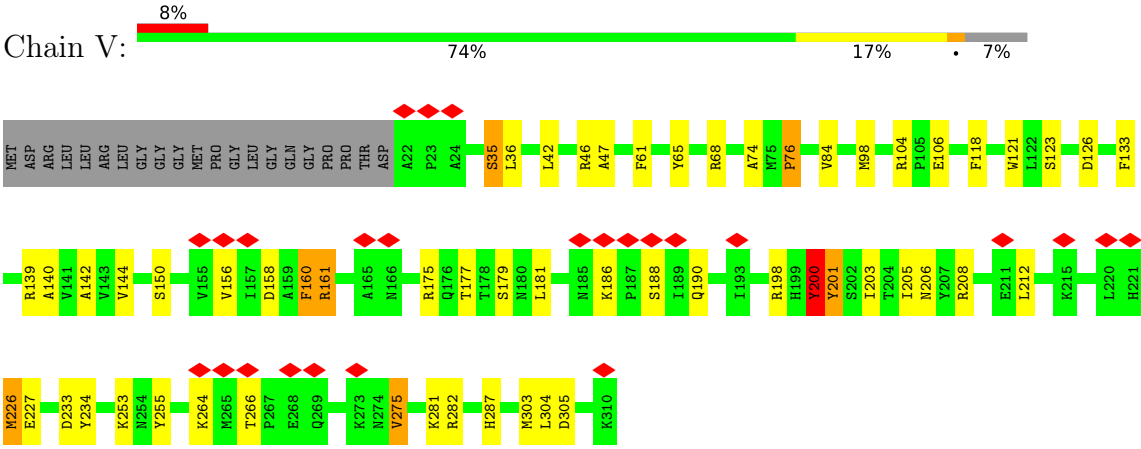






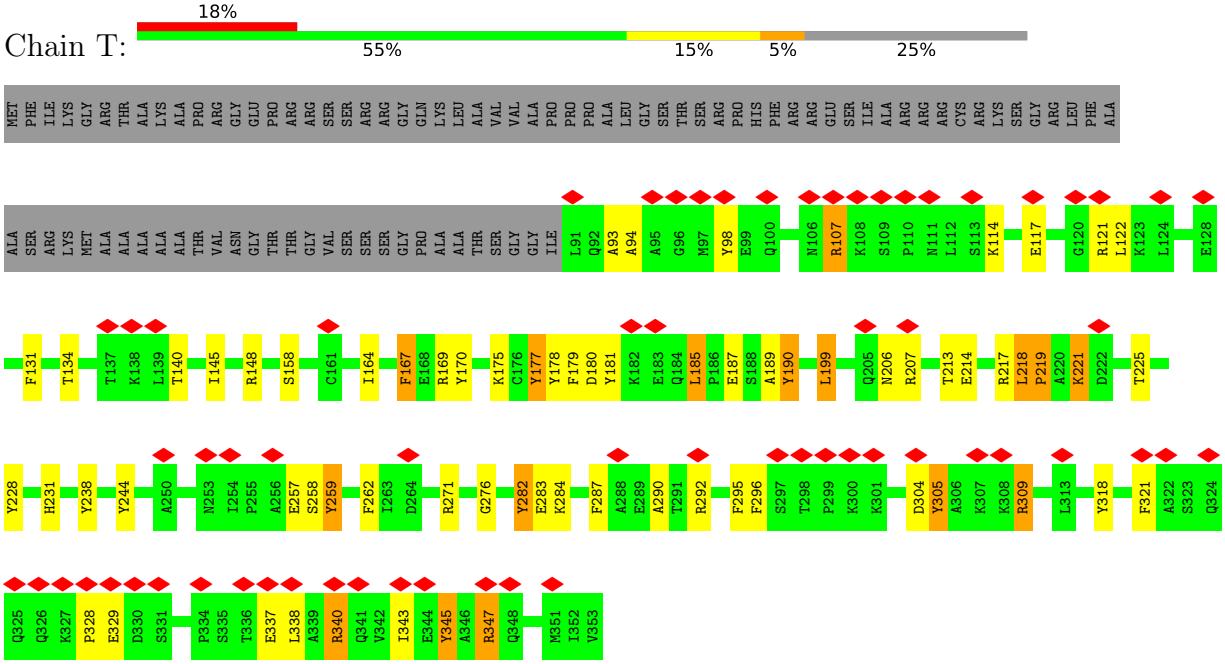
• Molecule 16: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 14

Chain V:



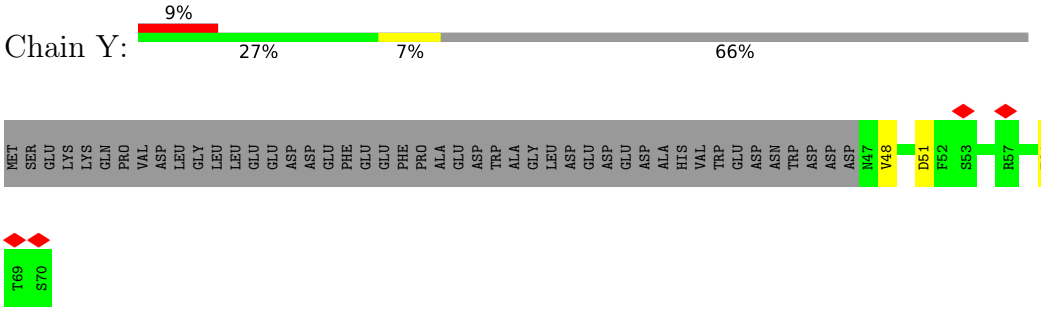

• Molecule 17: Proteasome 26S subunit, non-ATPase 8

Chain T:



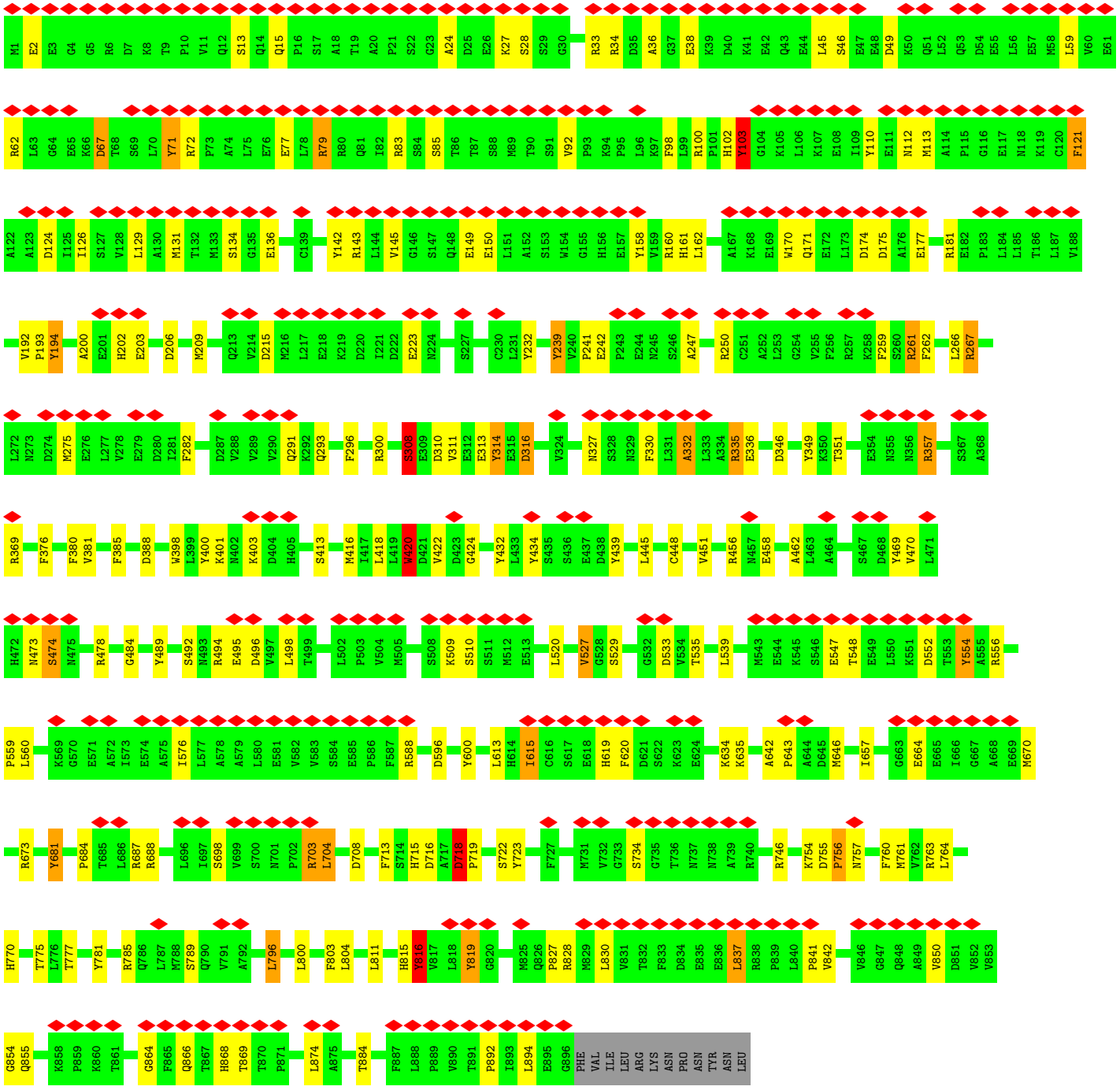

• Molecule 18: RCG28037

Chain Y:



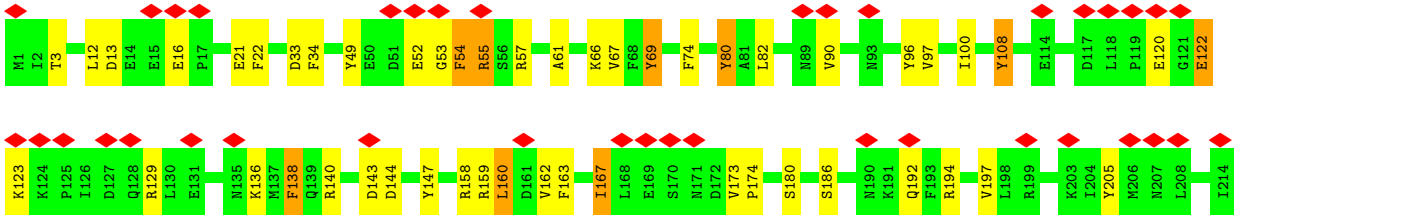

• Molecule 19: 26S proteasome non-ATPase regulatory subunit 2

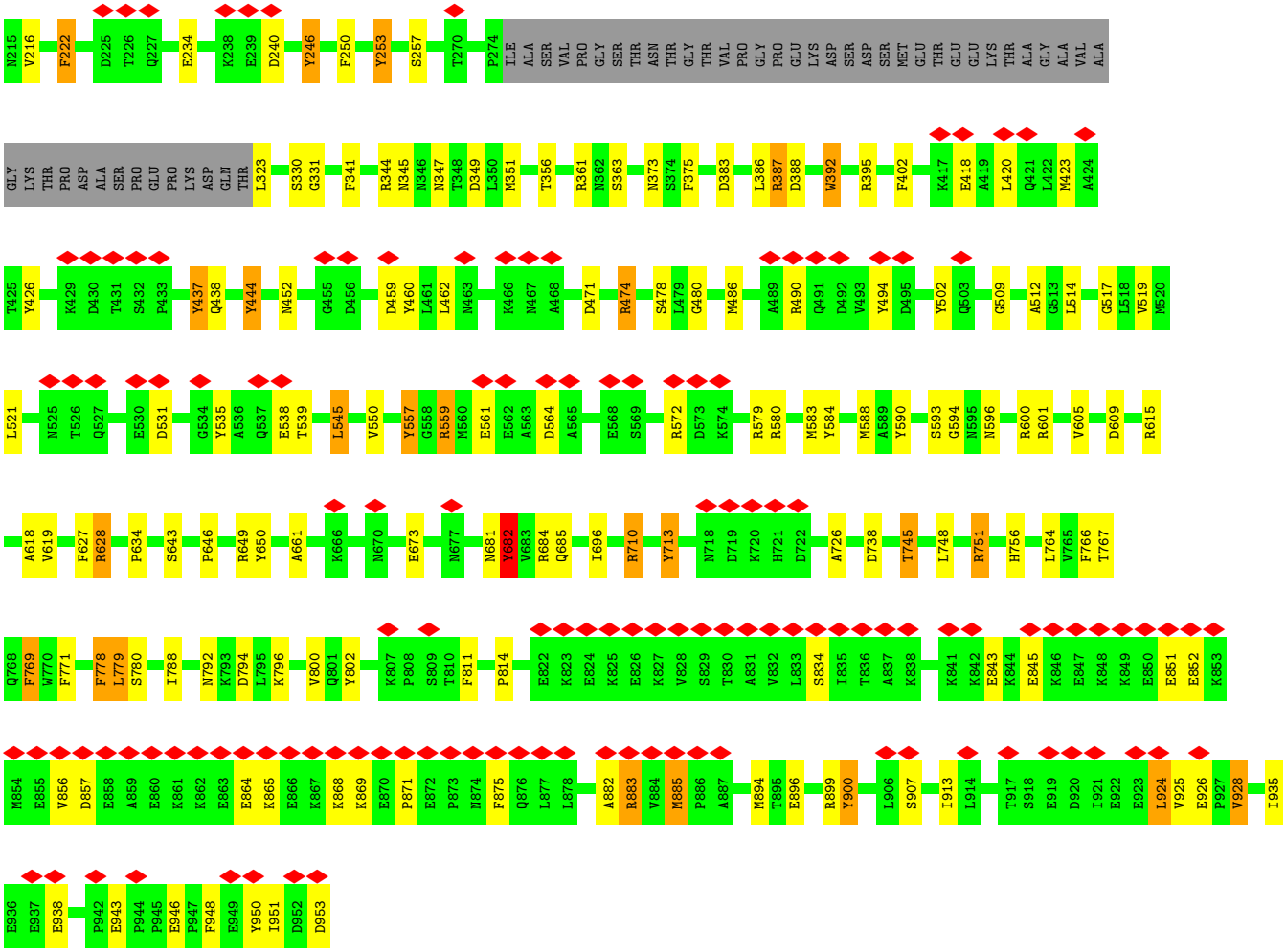
Chain Z:



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

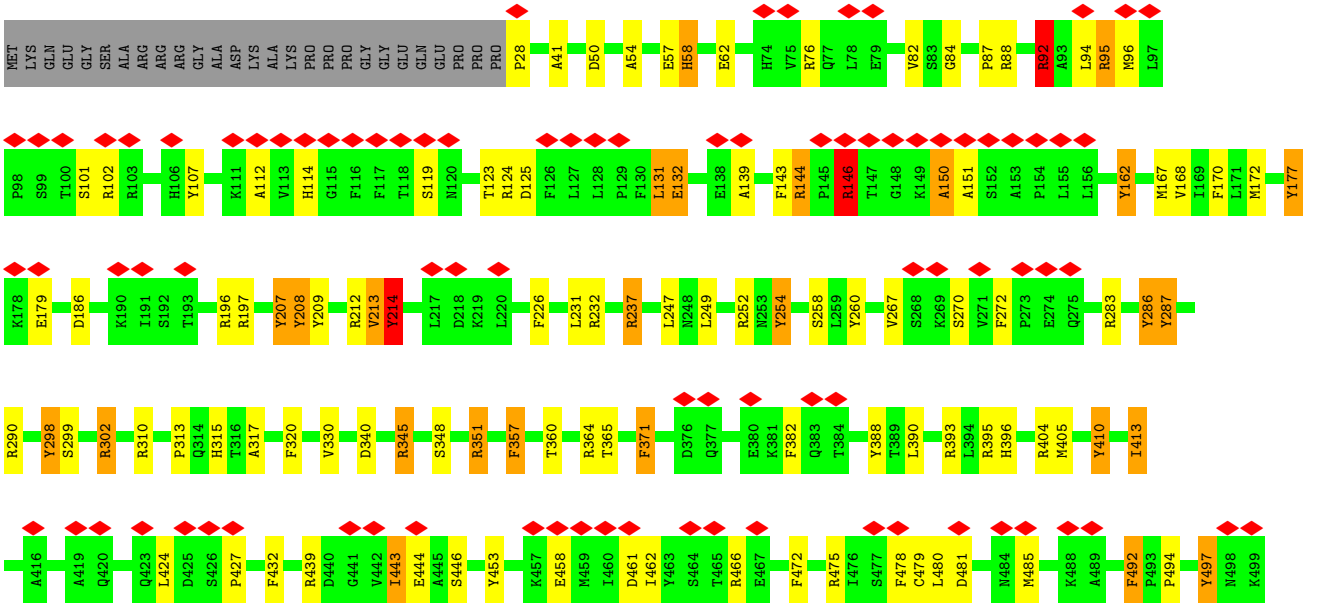
Chain N:

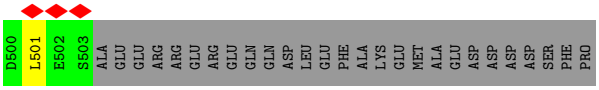





• Molecule 21: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 3

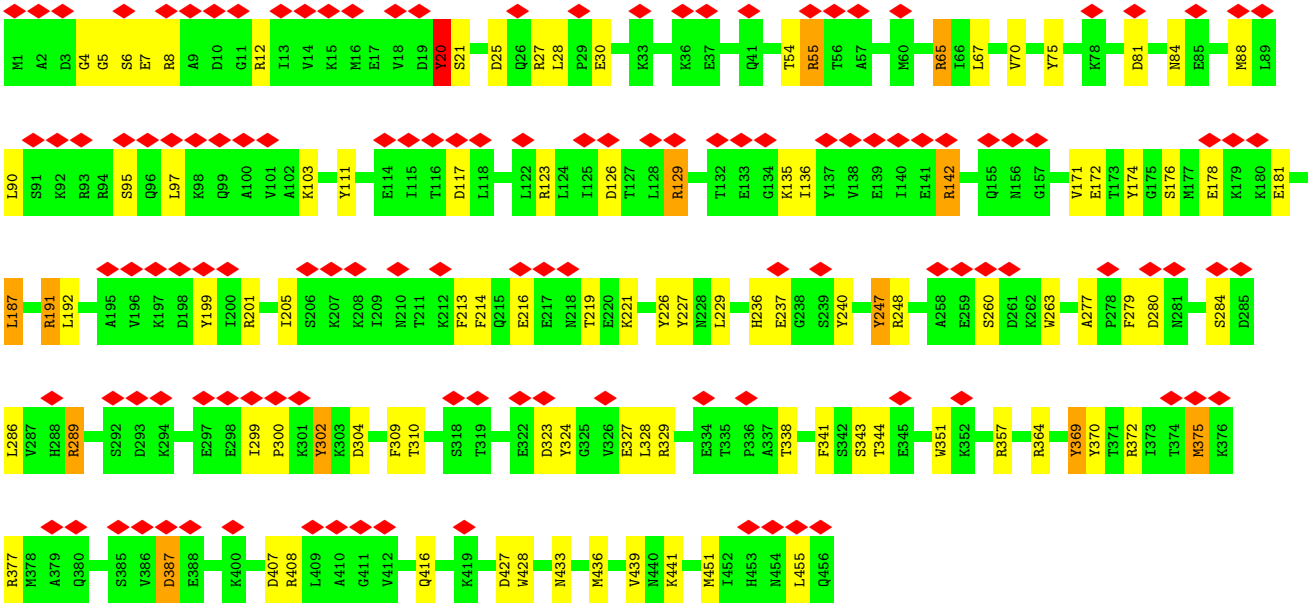
Chain S:



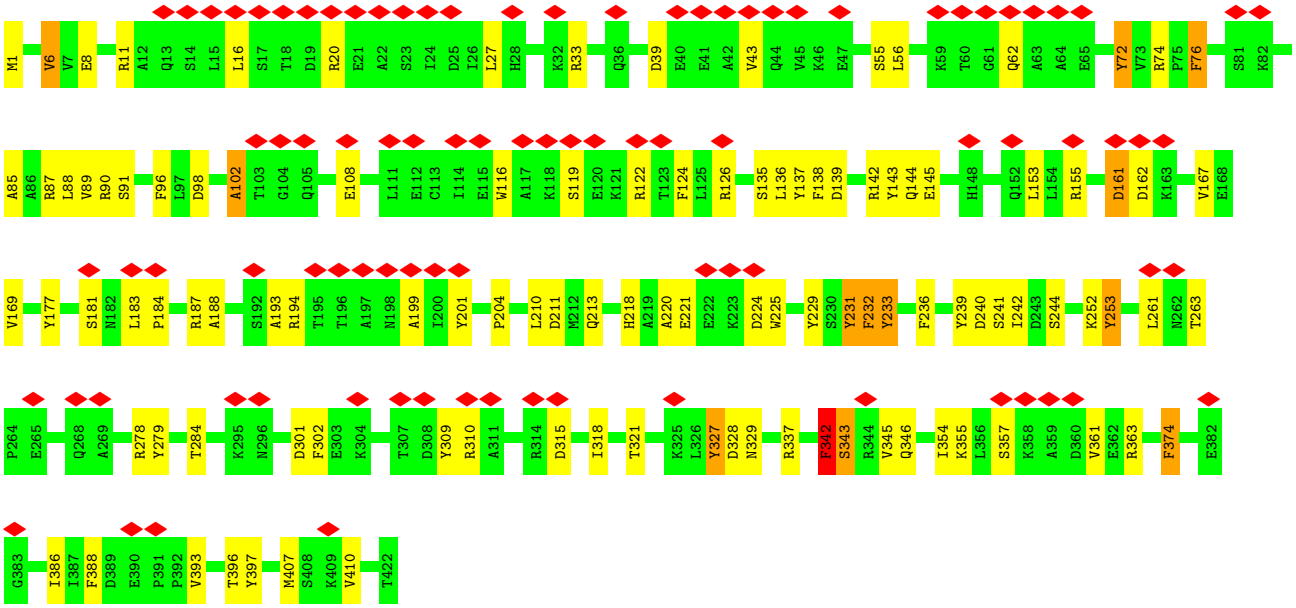
• Molecule 22: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 12

Chain P:

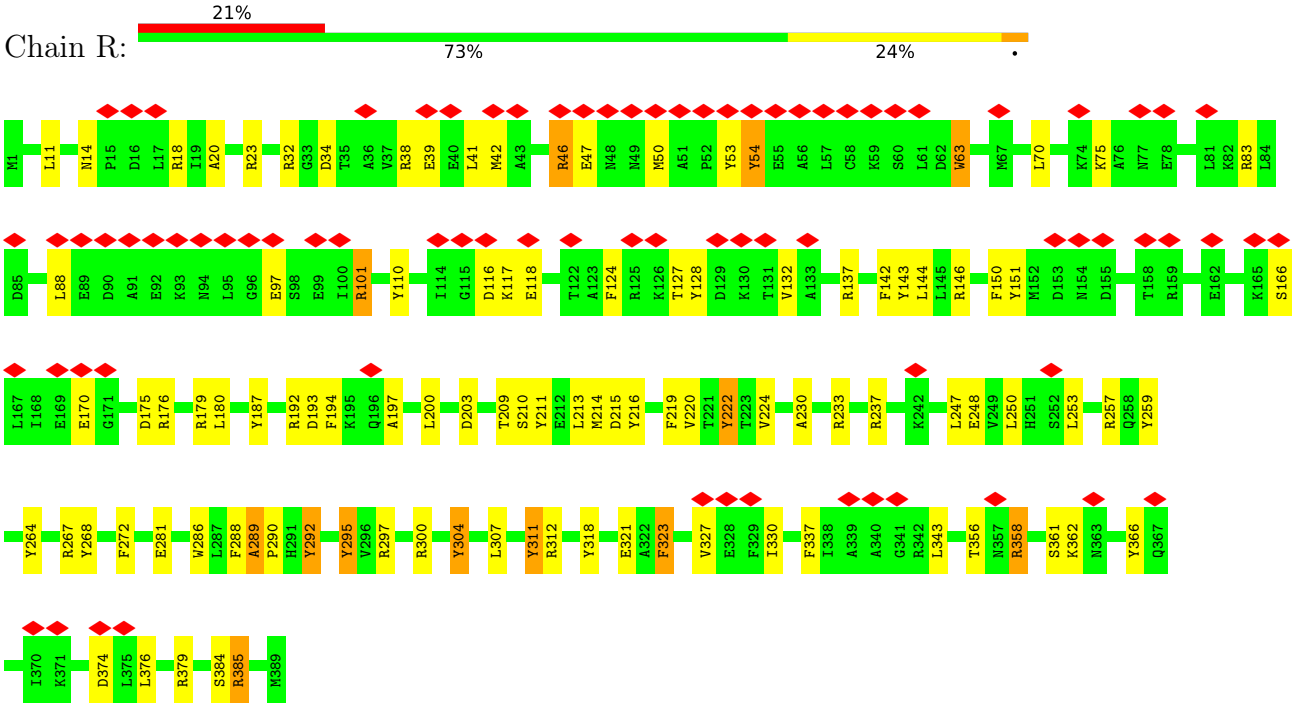
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 11

Chain Q:

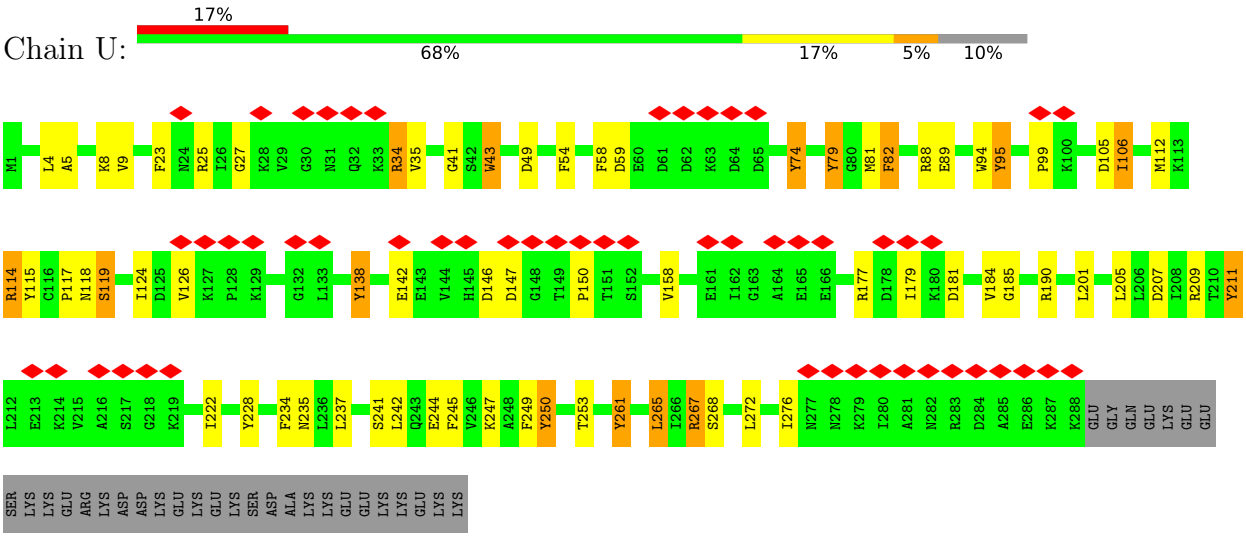
• Molecule 24: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 6

Chain R:



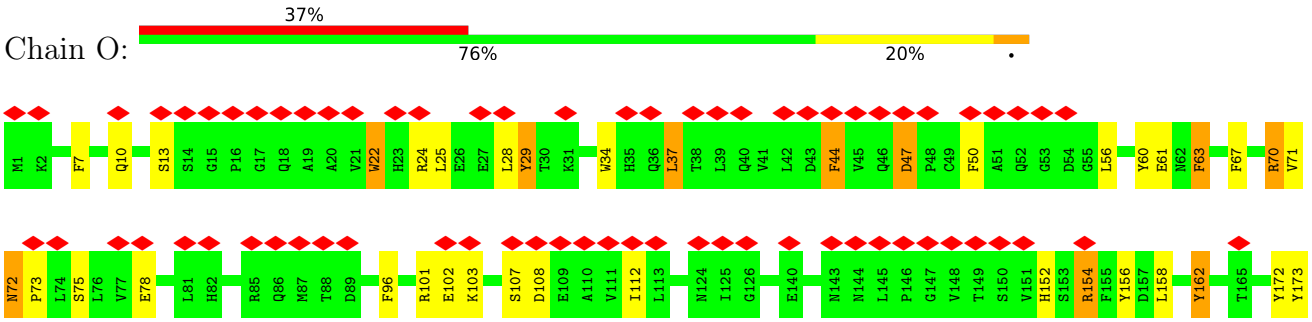

• Molecule 25: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 7 (Predicted)

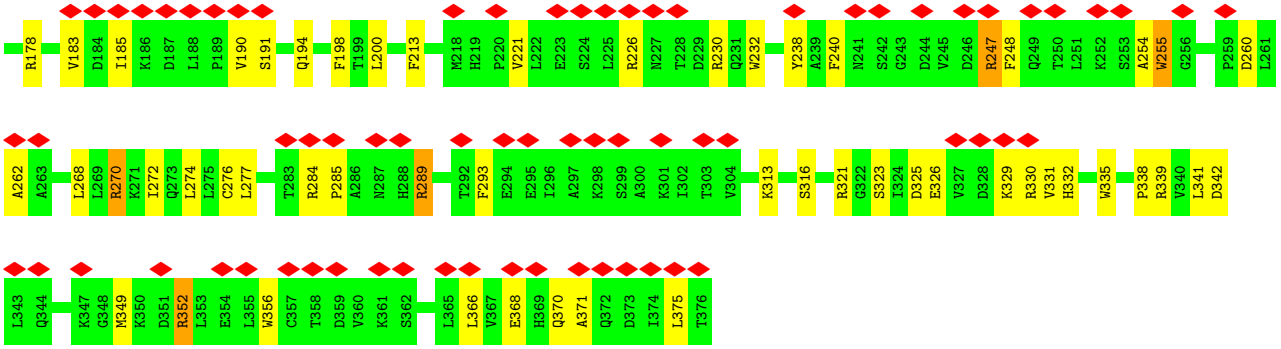
Chain U:




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

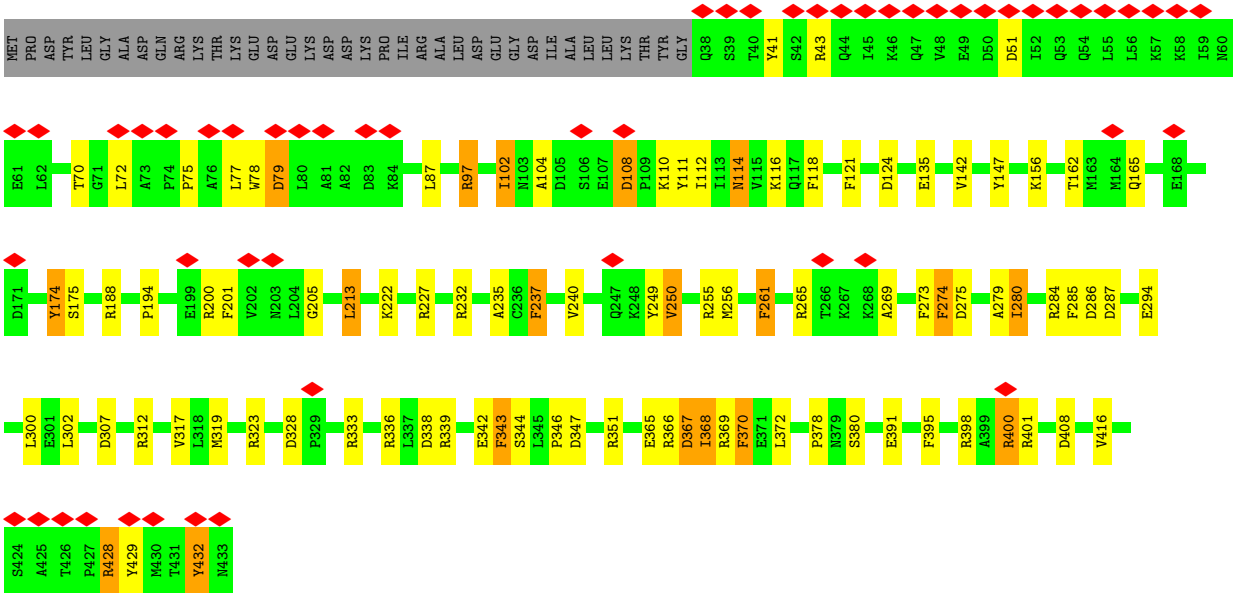
Chain O:





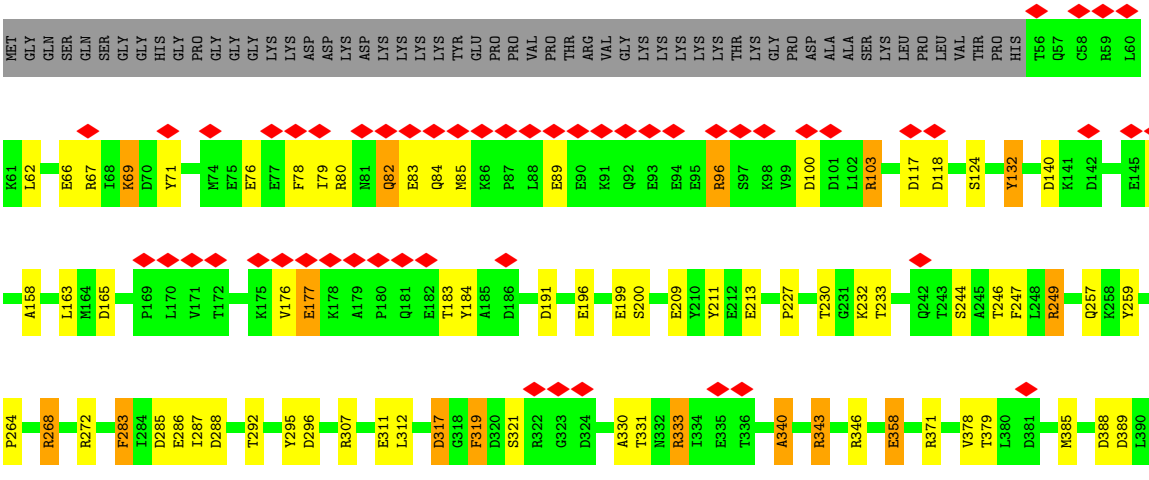

• Molecule 27: 26S proteasome regulatory subunit 7

Chain H:

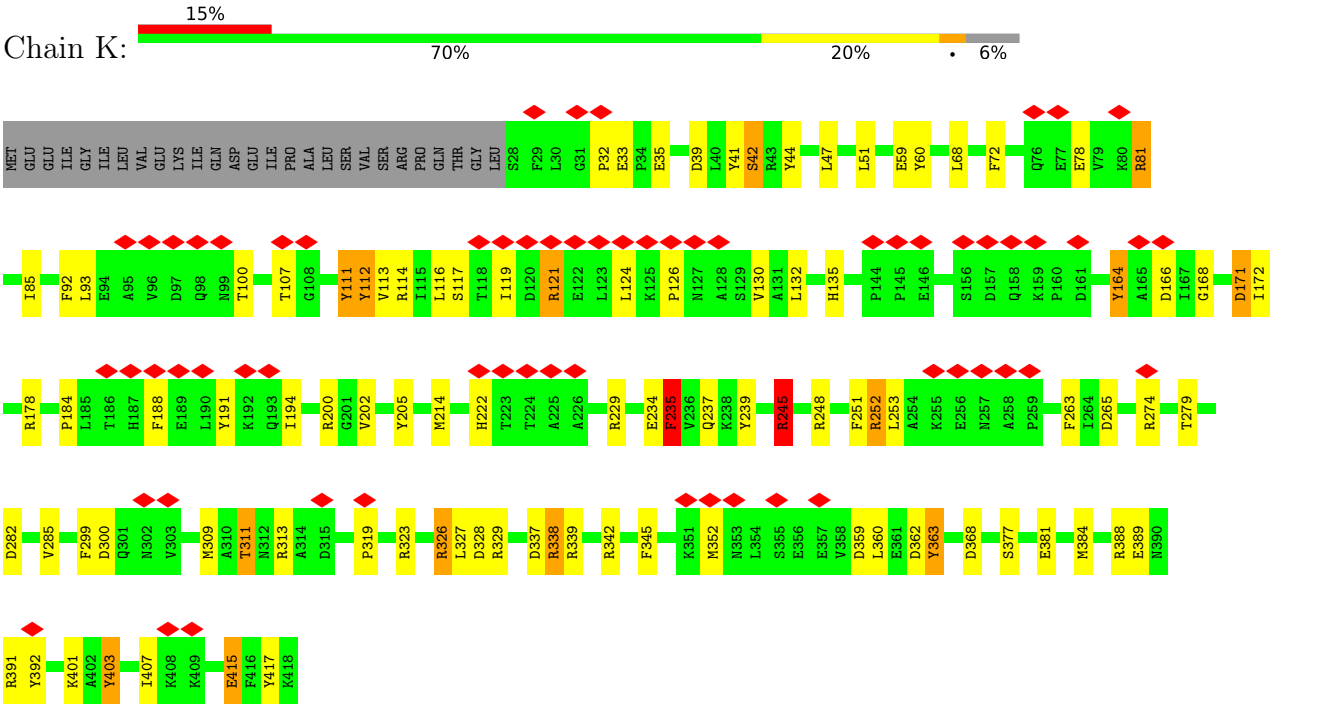




• Molecule 28: 26S proteasome regulatory subunit 4

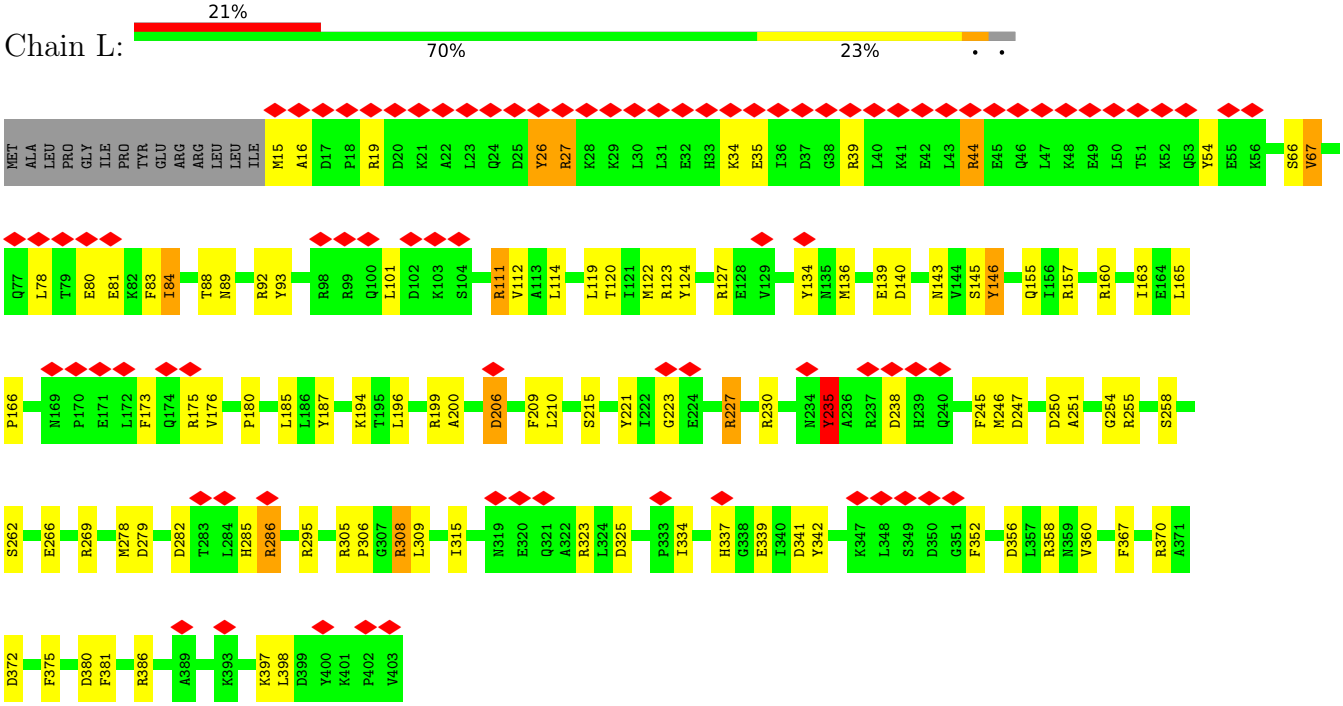
Chain I:


• Molecule 29: 26S proteasome regulatory subunit 6B

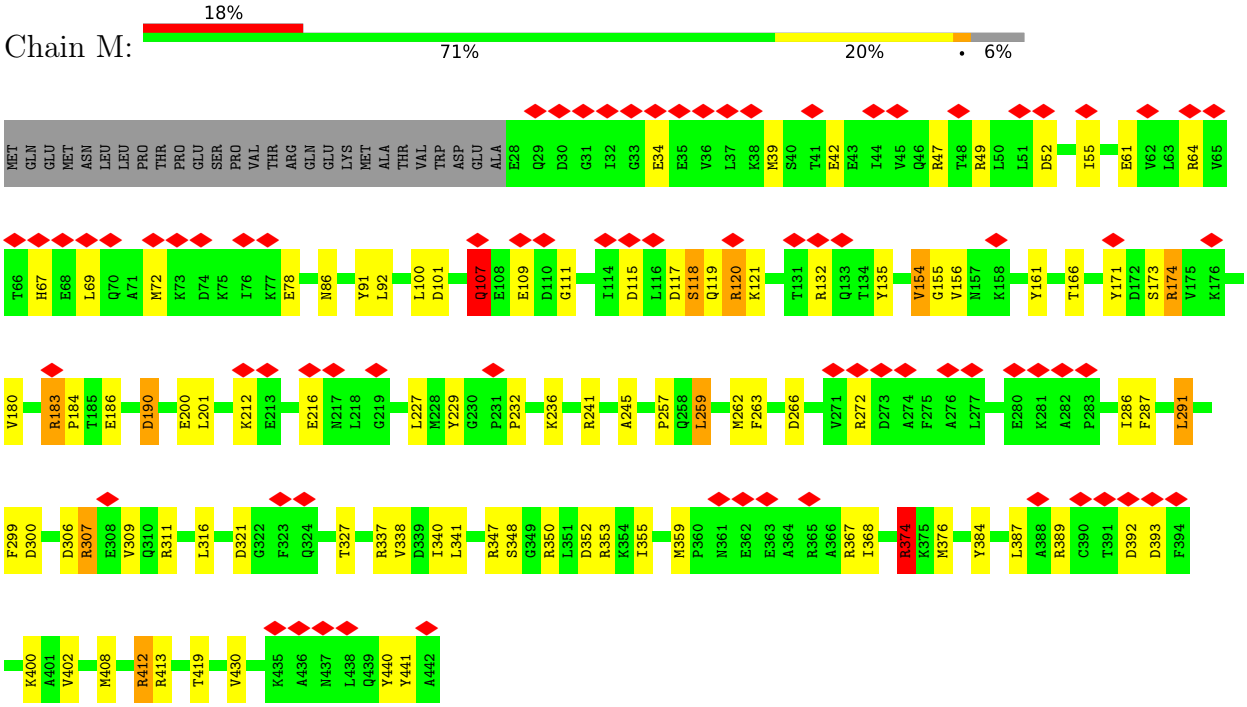



• Molecule 30: Proteasome 26S subunit, ATPase 6



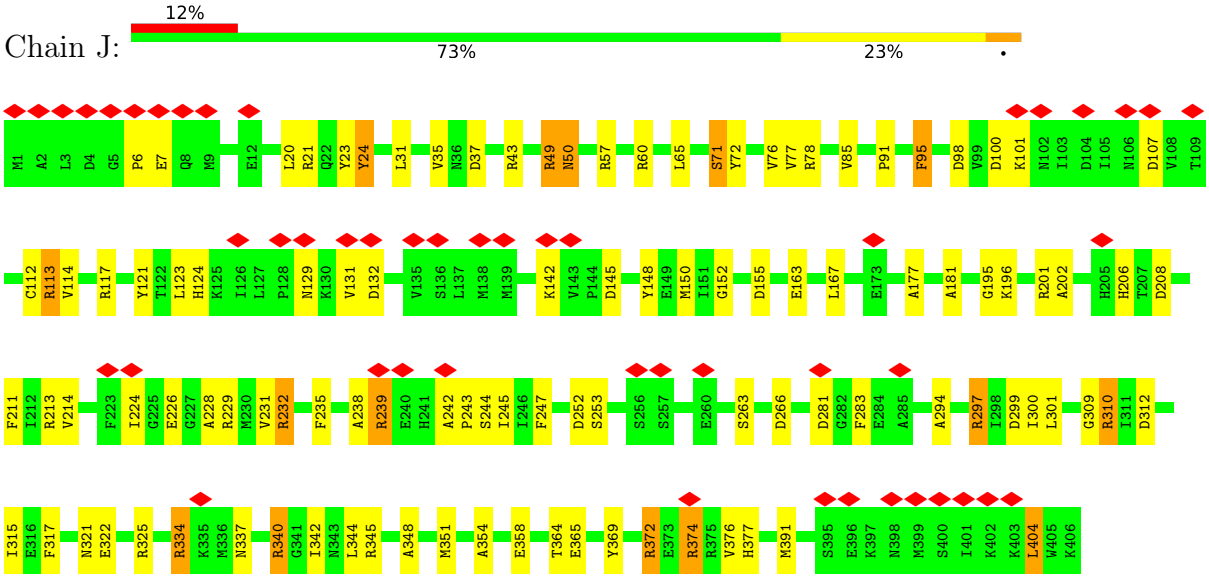

• Molecule 31: 26S proteasome regulatory subunit 6A

Chain M:




• Molecule 32: 26S proteasome regulatory subunit 8

Chain J:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of subtomograms used | 3482 | 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 ($e^-/Å^2$) | 1.8 | Depositor |
| Minimum defocus (nm) | 5000 | Depositor |
| Maximum defocus (nm) | 7000 | Depositor |
| Magnification | 42000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.748 | Depositor |
| Minimum map value | -0.362 | Depositor |
| Average map value | -0.005 | Depositor |
| Map value standard deviation | 0.162 | Depositor |
| Recommended contour level | 0.4 | Depositor |
| Map size (Å) | 307.80002, 307.80002, 307.80002 | wwPDB |
| Map dimensions | 90, 90, 90 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 3.4200003, 3.4200003, 3.4200003 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 | 1.72 | 16/1954 (0.8%) | 2.01 | 53/2638 (2.0%) |
| 2 | B | 1.81 | 27/1867 (1.4%) | 1.87 | 44/2527 (1.7%) |
| 3 | C | 1.73 | 17/1990 (0.9%) | 1.92 | 40/2680 (1.5%) |
| 4 | D | 1.72 | 20/1953 (1.0%) | 1.95 | 51/2637 (1.9%) |
| 5 | E | 1.70 | 15/1806 (0.8%) | 1.86 | 26/2439 (1.1%) |
| 6 | F | 1.74 | 16/1906 (0.8%) | 2.04 | 51/2577 (2.0%) |
| 7 | G | 1.77 | 22/1947 (1.1%) | 1.99 | 50/2620 (1.9%) |
| 8 | 1 | 1.73 | 13/1542 (0.8%) | 2.07 | 52/2089 (2.5%) |
| 9 | 2 | 1.72 | 16/1679 (1.0%) | 2.11 | 55/2271 (2.4%) |
| 10 | 3 | 1.71 | 15/1629 (0.9%) | 2.06 | 54/2195 (2.5%) |
| 11 | 4 | 1.73 | 11/1604 (0.7%) | 1.96 | 40/2170 (1.8%) |
| 12 | 5 | 1.81 | 21/1592 (1.3%) | 2.25 | 57/2152 (2.6%) |
| 13 | 6 | 1.75 | 16/1690 (0.9%) | 2.10 | 51/2278 (2.2%) |
| 14 | 7 | 1.76 | 16/1720 (0.9%) | 2.10 | 58/2327 (2.5%) |
| 15 | W | 1.62 | 12/1500 (0.8%) | 1.88 | 36/2030 (1.8%) |
| 16 | V | 1.70 | 18/2315 (0.8%) | 1.94 | 48/3129 (1.5%) |
| 17 | T | 1.72 | 25/2195 (1.1%) | 1.98 | 51/2964 (1.7%) |
| 18 | Y | 1.69 | 0/201 | 1.79 | 4/266 (1.5%) |
| 19 | Z | 1.74 | 71/7026 (1.0%) | 1.97 | 168/9495 (1.8%) |
| 20 | N | 1.69 | 50/7207 (0.7%) | 1.95 | 157/9741 (1.6%) |
| 21 | S | 1.77 | 45/3918 (1.1%) | 1.90 | 85/5287 (1.6%) |
| 22 | P | 1.70 | 31/3754 (0.8%) | 1.91 | 84/5049 (1.7%) |
| 23 | Q | 1.70 | 29/3381 (0.9%) | 1.95 | 89/4558 (2.0%) |
| 24 | R | 1.80 | 40/3263 (1.2%) | 1.96 | 77/4393 (1.8%) |
| 25 | U | 1.67 | 17/2344 (0.7%) | 1.94 | 59/3178 (1.9%) |
| 26 | O | 1.74 | 31/3066 (1.0%) | 1.93 | 79/4148 (1.9%) |
| 27 | H | 1.72 | 27/3166 (0.9%) | 1.95 | 78/4275 (1.8%) |
| 28 | I | 1.72 | 23/3085 (0.7%) | 1.94 | 68/4158 (1.6%) |
| 29 | K | 1.74 | 29/3179 (0.9%) | 1.97 | 79/4290 (1.8%) |
| 30 | L | 1.71 | 32/3146 (1.0%) | 1.93 | 91/4233 (2.1%) |
| 31 | M | 1.73 | 38/3293 (1.2%) | 1.90 | 69/4436 (1.6%) |
| 32 | J | 1.76 | 31/3236 (1.0%) | 1.91 | 82/4347 (1.9%) |
| All | All | 1.73 | 790/84154 (0.9%) | 1.96 | 2086/113577 (1.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 6 |
| 2 | B | 0 | 4 |
| 3 | C | 0 | 6 |
| 4 | D | 0 | 9 |
| 5 | E | 0 | 3 |
| 6 | F | 0 | 9 |
| 7 | G | 0 | 6 |
| 8 | 1 | 0 | 5 |
| 9 | 2 | 0 | 6 |
| 10 | 3 | 0 | 4 |
| 11 | 4 | 0 | 9 |
| 12 | 5 | 0 | 11 |
| 13 | 6 | 0 | 3 |
| 14 | 7 | 0 | 10 |
| 15 | W | 0 | 3 |
| 16 | V | 0 | 5 |
| 17 | T | 0 | 12 |
| 19 | Z | 0 | 14 |
| 20 | N | 0 | 21 |
| 21 | S | 0 | 17 |
| 22 | P | 0 | 14 |
| 23 | Q | 0 | 14 |
| 24 | R | 0 | 12 |
| 25 | U | 0 | 10 |
| 26 | O | 0 | 9 |
| 27 | H | 0 | 10 |
| 28 | I | 0 | 12 |
| 29 | K | 0 | 20 |
| 30 | L | 0 | 11 |
| 31 | M | 0 | 7 |
| 32 | J | 0 | 9 |
| All | All | 0 | 291 |

The worst 5 of 790 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | N | 57 | ARG | CZ-NH2 | 9.37 | 1.45 | 1.33 |
| 31 | M | 161 | TYR | CB-CG | 8.74 | 1.64 | 1.51 |
| 19 | Z | 746 | ARG | CD-NE | 8.63 | 1.61 | 1.46 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | 5 | 200 | ARG | NE-CZ | 8.61 | 1.44 | 1.33 |
| 13 | 6 | 206 | PHE | CG-CD1 | 8.59 | 1.51 | 1.38 |

The worst 5 of 2086 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | 5 | 239 | ARG | NE-CZ-NH2 | -19.68 | 110.46 | 120.30 |
| 20 | N | 684 | ARG | NE-CZ-NH2 | -18.89 | 110.86 | 120.30 |
| 29 | K | 339 | ARG | NE-CZ-NH1 | 18.36 | 129.48 | 120.30 |
| 9 | 2 | 244 | ARG | NE-CZ-NH2 | -18.19 | 111.20 | 120.30 |
| 27 | H | 43 | ARG | NE-CZ-NH1 | 17.85 | 129.22 | 120.30 |

There are no chirality outliers.

5 of 291 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 11 | ARG | Mainchain |
| 1 | A | 117 | ARG | Sidechain |
| 1 | A | 163 | PHE | Sidechain |
| 1 | A | 3 | ARG | Sidechain |
| 1 | A | 88 | ARG | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1920 | 0 | 1927 | 0 | 0 |
| 2 | B | 1828 | 0 | 1823 | 0 | 0 |
| 3 | C | 1960 | 0 | 1983 | 0 | 0 |
| 4 | D | 1926 | 0 | 1955 | 0 | 0 |
| 5 | E | 1778 | 0 | 1756 | 0 | 0 |
| 6 | F | 1871 | 0 | 1856 | 0 | 0 |
| 7 | G | 1912 | 0 | 1907 | 0 | 0 |
| 8 | 1 | 1516 | 0 | 1485 | 0 | 0 |
| 9 | 2 | 1651 | 0 | 1674 | 0 | 0 |
| 10 | 3 | 1600 | 0 | 1621 | 0 | 0 |
| 11 | 4 | 1572 | 0 | 1575 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 12 | 5 | 1560 | 0 | 1519 | 0 | 0 |
| 13 | 6 | 1659 | 0 | 1654 | 0 | 0 |
| 14 | 7 | 1686 | 0 | 1662 | 0 | 0 |
| 15 | W | 1480 | 0 | 1522 | 0 | 0 |
| 16 | V | 2272 | 0 | 2288 | 0 | 0 |
| 17 | T | 2149 | 0 | 2170 | 0 | 0 |
| 18 | Y | 199 | 0 | 180 | 0 | 0 |
| 19 | Z | 6913 | 0 | 6910 | 0 | 0 |
| 20 | N | 7082 | 0 | 7122 | 0 | 0 |
| 21 | S | 3844 | 0 | 3888 | 0 | 0 |
| 22 | P | 3706 | 0 | 3817 | 0 | 0 |
| 23 | Q | 3335 | 0 | 3435 | 0 | 0 |
| 24 | R | 3204 | 0 | 3204 | 0 | 0 |
| 25 | U | 2299 | 0 | 2334 | 0 | 0 |
| 26 | O | 3011 | 0 | 3042 | 0 | 0 |
| 27 | H | 3113 | 0 | 3162 | 0 | 0 |
| 28 | I | 3042 | 0 | 3098 | 0 | 0 |
| 29 | K | 3126 | 0 | 3151 | 0 | 0 |
| 30 | L | 3098 | 0 | 3171 | 0 | 0 |
| 31 | M | 3252 | 0 | 3321 | 0 | 0 |
| 32 | J | 3194 | 0 | 3311 | 0 | 0 |
| All | All | 82758 | 0 | 83523 | 0 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 244/246 (99%) | 229 (94%) | 13 (5%) | 2 (1%) | 19 60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 2 | B | 232/234 (99%) | 214 (92%) | 14 (6%) | 4 (2%) | 9 42 |
| 3 | C | 247/261 (95%) | 231 (94%) | 13 (5%) | 3 (1%) | 13 50 |
| 4 | D | 244/254 (96%) | 221 (91%) | 13 (5%) | 10 (4%) | 3 23 |
| 5 | E | 231/241 (96%) | 214 (93%) | 12 (5%) | 5 (2%) | 6 35 |
| 6 | F | 236/263 (90%) | 216 (92%) | 18 (8%) | 2 (1%) | 19 60 |
| 7 | G | 243/255 (95%) | 225 (93%) | 14 (6%) | 4 (2%) | 9 44 |
| 8 | 1 | 200/238 (84%) | 174 (87%) | 14 (7%) | 12 (6%) | 1 17 |
| 9 | 2 | 217/277 (78%) | 184 (85%) | 18 (8%) | 15 (7%) | 1 15 |
| 10 | 3 | 203/205 (99%) | 160 (79%) | 27 (13%) | 16 (8%) | 1 13 |
| 11 | 4 | 194/201 (96%) | 167 (86%) | 14 (7%) | 13 (7%) | 1 15 |
| 12 | 5 | 199/263 (76%) | 173 (87%) | 17 (8%) | 9 (4%) | 2 22 |
| 13 | 6 | 211/240 (88%) | 178 (84%) | 26 (12%) | 7 (3%) | 4 26 |
| 14 | 7 | 214/263 (81%) | 187 (87%) | 18 (8%) | 9 (4%) | 3 22 |
| 15 | W | 193/377 (51%) | 179 (93%) | 12 (6%) | 2 (1%) | 15 55 |
| 16 | V | 287/310 (93%) | 264 (92%) | 17 (6%) | 6 (2%) | 7 36 |
| 17 | T | 261/353 (74%) | 229 (88%) | 26 (10%) | 6 (2%) | 6 34 |
| 18 | Y | 22/70 (31%) | 22 (100%) | 0 | 0 | 100 100 |
| 19 | Z | 894/908 (98%) | 800 (90%) | 62 (7%) | 32 (4%) | 3 25 |
| 20 | N | 903/953 (95%) | 833 (92%) | 52 (6%) | 18 (2%) | 7 38 |
| 21 | S | 474/530 (89%) | 416 (88%) | 43 (9%) | 15 (3%) | 4 26 |
| 22 | P | 454/456 (100%) | 428 (94%) | 20 (4%) | 6 (1%) | 12 48 |
| 23 | Q | 420/422 (100%) | 389 (93%) | 20 (5%) | 11 (3%) | 5 31 |
| 24 | R | 387/389 (100%) | 360 (93%) | 20 (5%) | 7 (2%) | 8 40 |
| 25 | U | 286/320 (89%) | 262 (92%) | 15 (5%) | 9 (3%) | 4 27 |
| 26 | O | 374/376 (100%) | 347 (93%) | 22 (6%) | 5 (1%) | 12 48 |
| 27 | H | 394/433 (91%) | 361 (92%) | 24 (6%) | 9 (2%) | 6 34 |
| 28 | I | 383/440 (87%) | 353 (92%) | 23 (6%) | 7 (2%) | 8 40 |
| 29 | K | 389/418 (93%) | 361 (93%) | 25 (6%) | 3 (1%) | 19 60 |
| 30 | L | 387/403 (96%) | 369 (95%) | 14 (4%) | 4 (1%) | 15 55 |
| 31 | M | 413/442 (93%) | 380 (92%) | 27 (6%) | 6 (2%) | 10 46 |
| 32 | J | 404/406 (100%) | 364 (90%) | 30 (7%) | 10 (2%) | 5 32 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 10440/11447 (91%) | 9490 (91%) | 683 (6%) | 267 (3%) | 8 31 |

5 of 267 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 41 | ALA |
| 4 | D | 9 | VAL |
| 8 | 1 | 53 | THR |
| 8 | 1 | 207 | ILE |
| 8 | 1 | 232 | ILE |

### 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 | 210/210 (100%) | 203 (97%) | 7 (3%) | 38 61 |
| 2 | B | 191/191 (100%) | 179 (94%) | 12 (6%) | 18 43 |
| 3 | C | 209/221 (95%) | 197 (94%) | 12 (6%) | 20 45 |
| 4 | D | 208/215 (97%) | 188 (90%) | 20 (10%) | 8 27 |
| 5 | E | 195/203 (96%) | 184 (94%) | 11 (6%) | 21 46 |
| 6 | F | 204/224 (91%) | 195 (96%) | 9 (4%) | 28 53 |
| 7 | G | 202/212 (95%) | 188 (93%) | 14 (7%) | 15 40 |
| 8 | 1 | 160/185 (86%) | 138 (86%) | 22 (14%) | 3 17 |
| 9 | 2 | 180/227 (79%) | 160 (89%) | 20 (11%) | 6 22 |
| 10 | 3 | 175/175 (100%) | 159 (91%) | 16 (9%) | 9 29 |
| 11 | 4 | 167/172 (97%) | 147 (88%) | 20 (12%) | 5 20 |
| 12 | 5 | 158/205 (77%) | 142 (90%) | 16 (10%) | 7 25 |
| 13 | 6 | 179/200 (90%) | 162 (90%) | 17 (10%) | 8 27 |
| 14 | 7 | 178/215 (83%) | 154 (86%) | 24 (14%) | 4 17 |
| 15 | W | 168/312 (54%) | 160 (95%) | 8 (5%) | 25 51 |
| 16 | V | 253/268 (94%) | 236 (93%) | 17 (7%) | 16 41 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 17 | T | 233/298 (78%) | 220 (94%) | 13 (6%) | 21 | 46 |
| 18 | Y | 22/63 (35%) | 21 (96%) | 1 (4%) | 27 | 52 |
| 19 | Z | 753/765 (98%) | 705 (94%) | 48 (6%) | 17 | 42 |
| 20 | N | 776/814 (95%) | 729 (94%) | 47 (6%) | 18 | 44 |
| 21 | S | 414/458 (90%) | 385 (93%) | 29 (7%) | 15 | 40 |
| 22 | P | 419/419 (100%) | 400 (96%) | 19 (4%) | 27 | 52 |
| 23 | Q | 362/362 (100%) | 345 (95%) | 17 (5%) | 26 | 51 |
| 24 | R | 345/345 (100%) | 322 (93%) | 23 (7%) | 16 | 41 |
| 25 | U | 259/289 (90%) | 247 (95%) | 12 (5%) | 27 | 52 |
| 26 | O | 334/334 (100%) | 316 (95%) | 18 (5%) | 22 | 47 |
| 27 | H | 341/372 (92%) | 317 (93%) | 24 (7%) | 15 | 40 |
| 28 | I | 341/385 (89%) | 321 (94%) | 20 (6%) | 19 | 45 |
| 29 | K | 343/367 (94%) | 322 (94%) | 21 (6%) | 18 | 44 |
| 30 | L | 341/353 (97%) | 318 (93%) | 23 (7%) | 16 | 41 |
| 31 | M | 357/382 (94%) | 334 (94%) | 23 (6%) | 17 | 42 |
| 32 | J | 352/352 (100%) | 331 (94%) | 21 (6%) | 19 | 44 |
| All | All | 9029/9793 (92%) | 8425 (93%) | 604 (7%) | 20 | 41 |

5 of 604 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | O | 158 | LEU |
| 31 | M | 327 | THR |
| 27 | H | 114 | ASN |
| 26 | O | 154 | ARG |
| 29 | K | 113 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

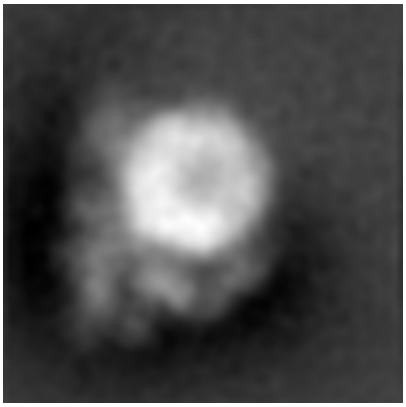
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3915. These allow visual inspection of the internal detail of the map and identification of artifacts.

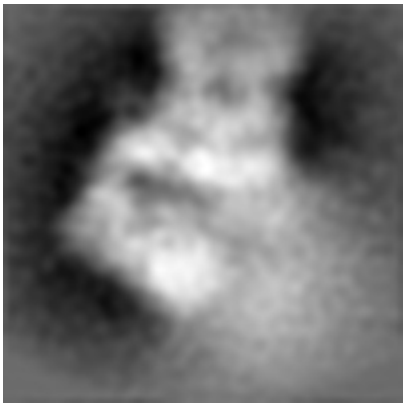
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

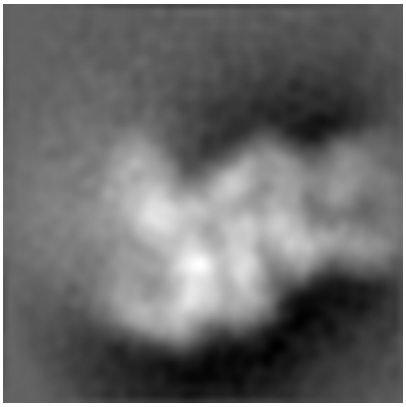
### 6.1.1 Primary map



X



Y



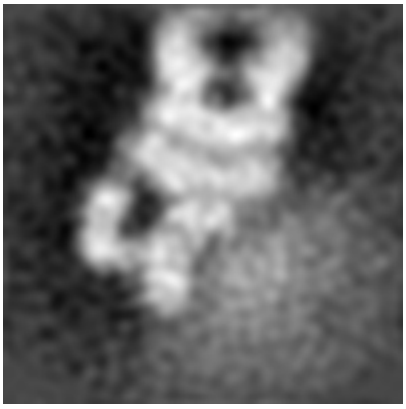
Z

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

## 6.2 Central slices

### 6.2.1 Primary map

X Index: 45



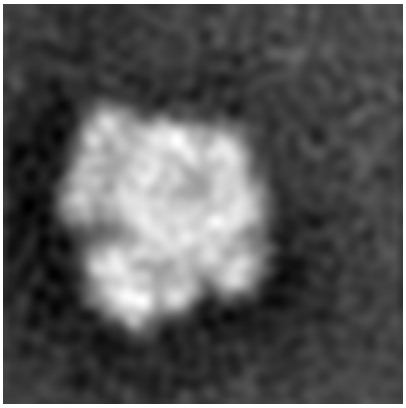
Y Index: 45

Z Index: 45

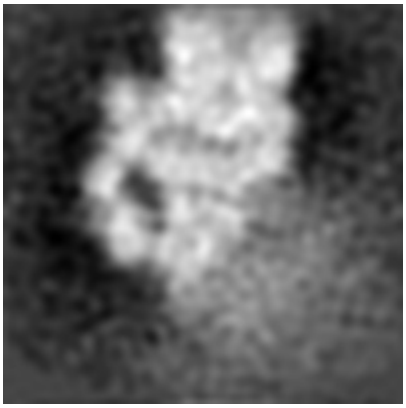
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

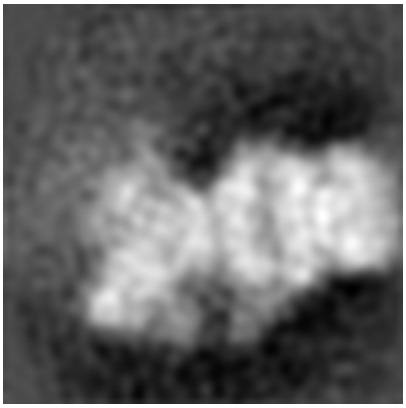
### 6.3.1 Primary map



X Index: 54



Y Index: 36

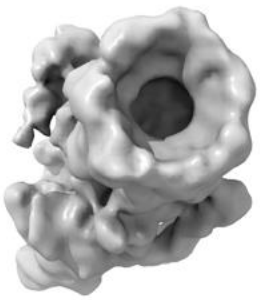


Z Index: 40

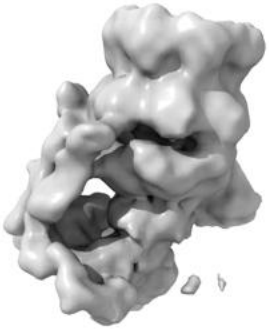
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

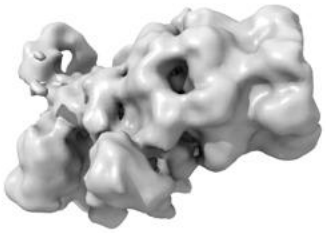
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

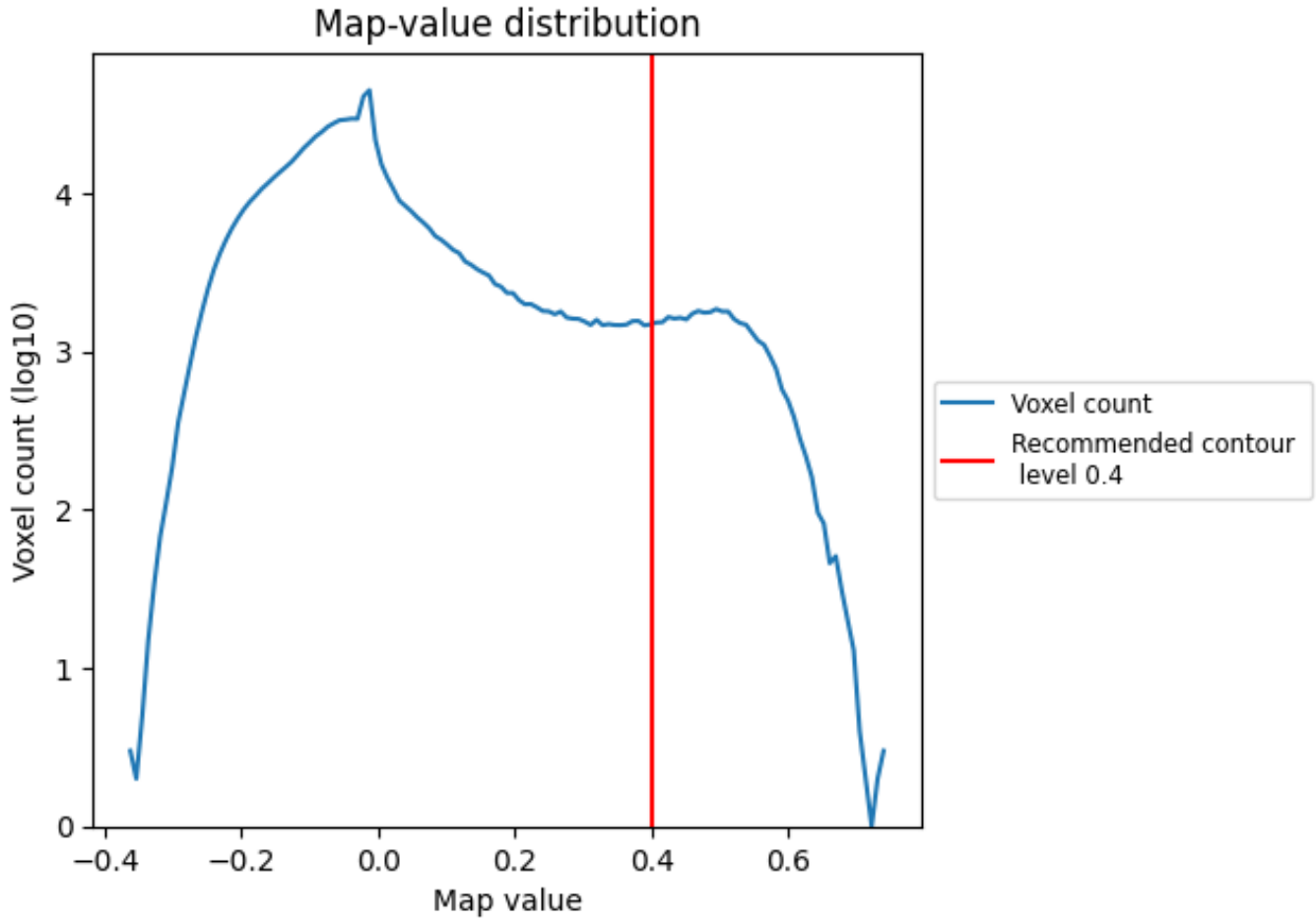
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

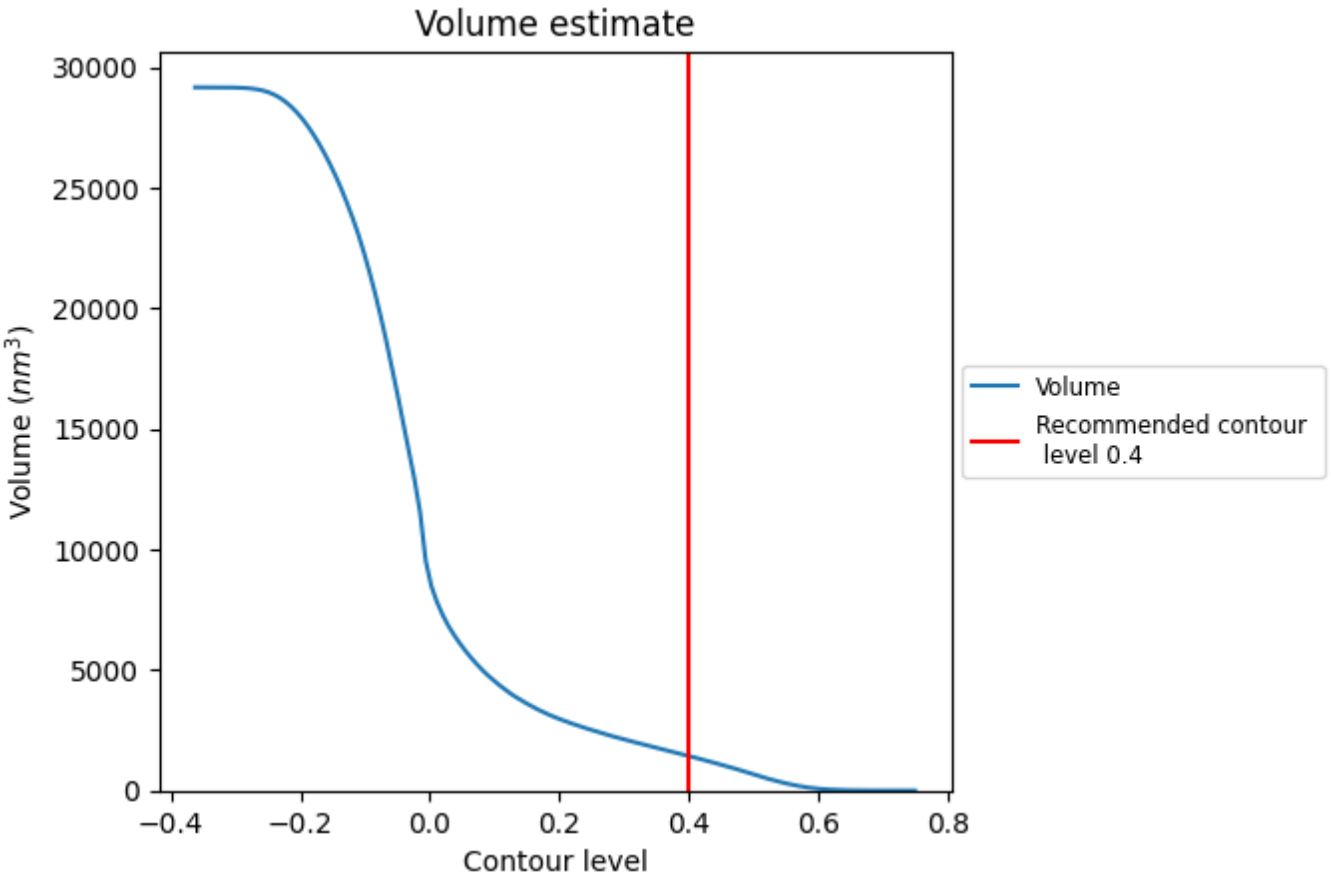
This section contains the results of statistical analysis of the map.

## 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.

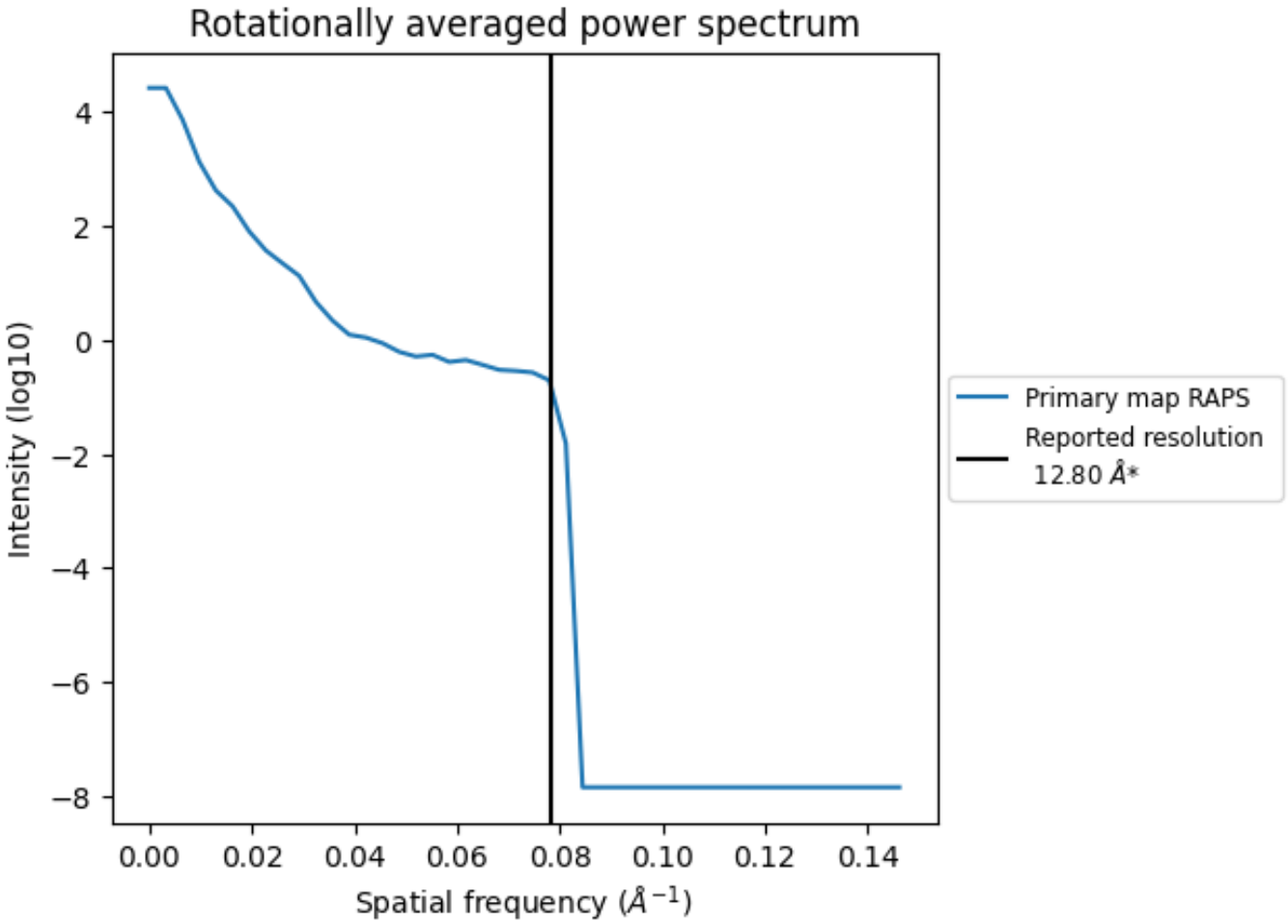
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1428 $nm^3$; this corresponds to an approximate mass of 1290 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 0.078 Å$^{-1}$

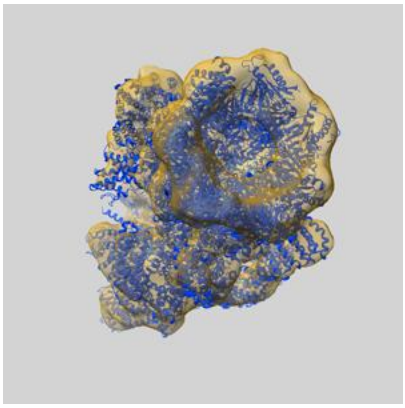
# 8 Fourier-Shell correlation (i)

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

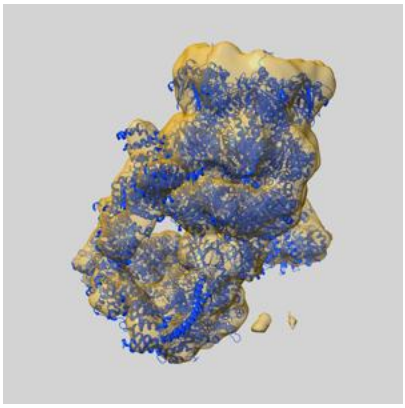
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3915 and PDB model 6EPE. Per-residue inclusion information can be found in section 3 on page 9.

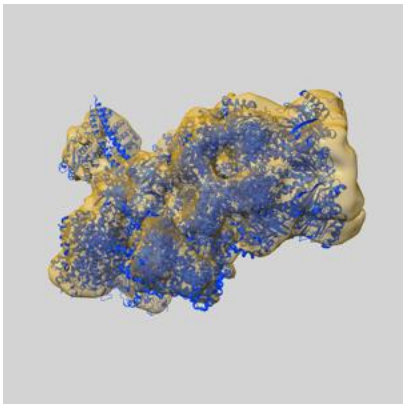
## 9.1 Map-model overlay



X



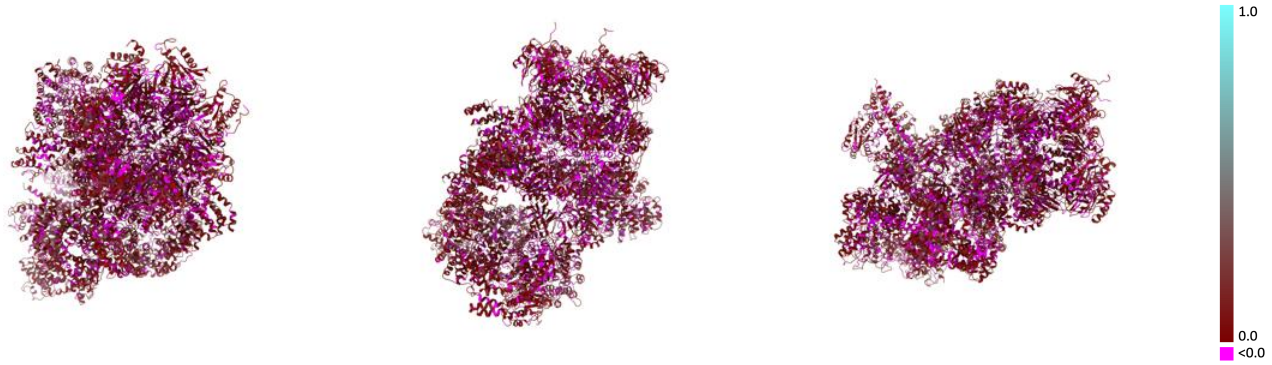
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

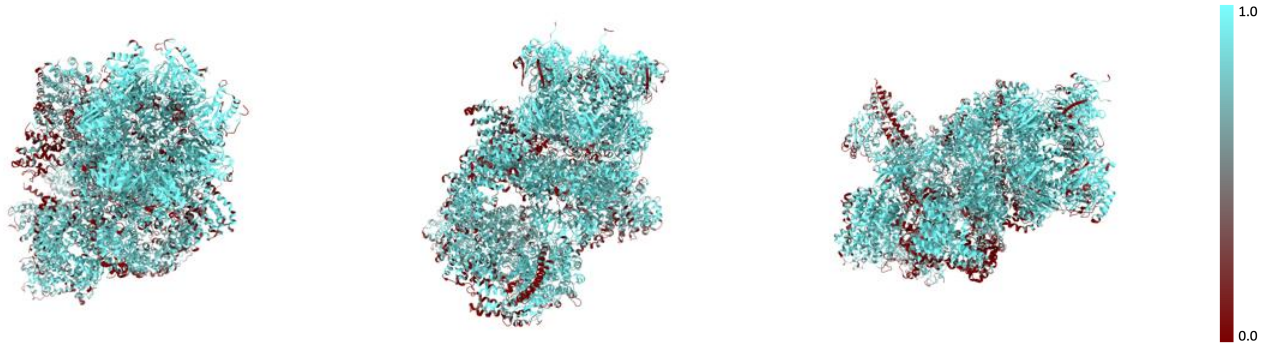
## 9.2 Q-score mapped to coordinate model (i)




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.

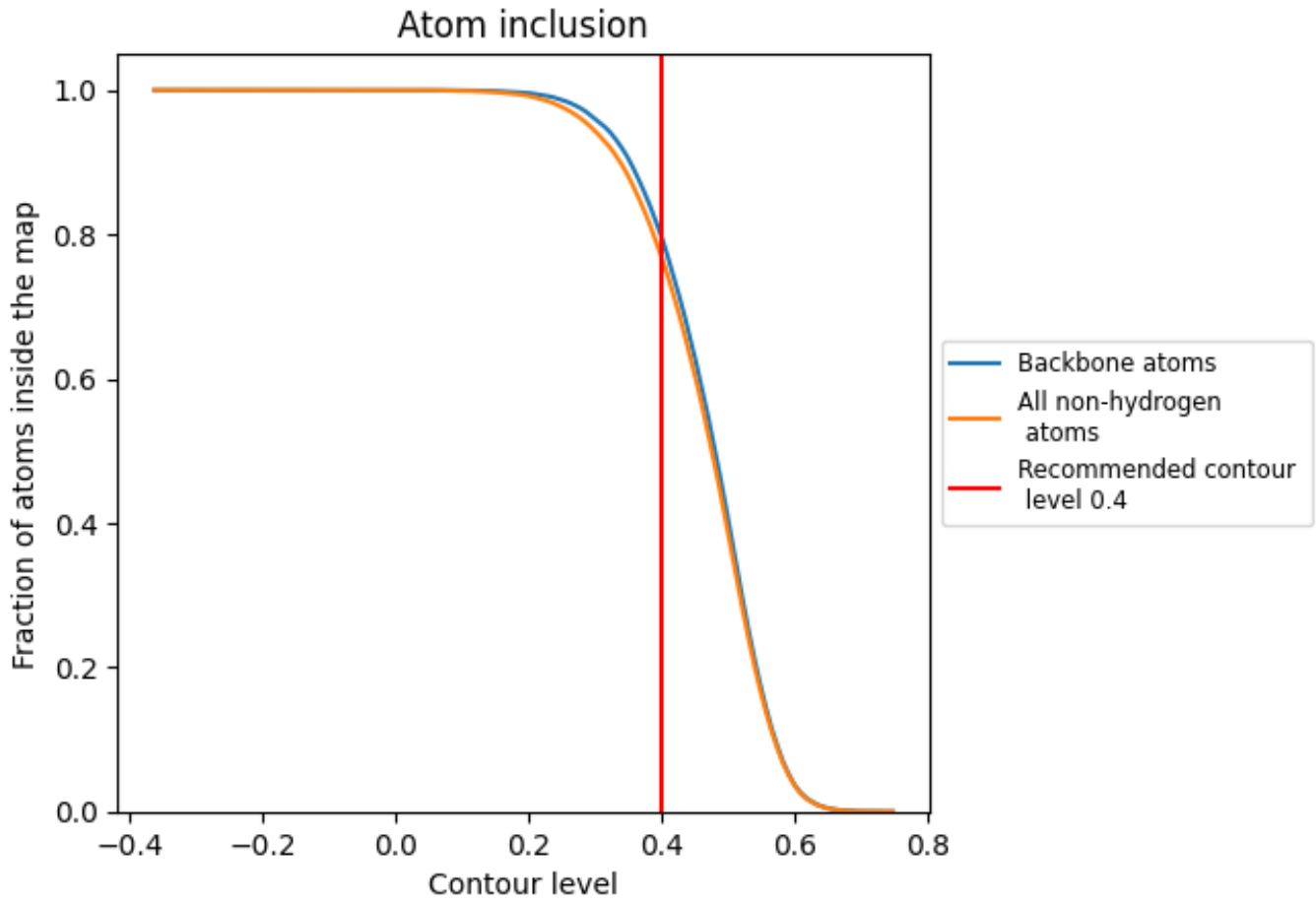
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.4).

## 9.4 Atom inclusion (i)




At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7703 | 0.0530 |
| 1 | 0.8580 | 0.0500 |
| 2 | 0.7485 | 0.0540 |
| 3 | 0.8205 | 0.0380 |
| 4 | 0.7941 | 0.0600 |
| 5 | 0.8453 | 0.0550 |
| 6 | 0.7609 | 0.0480 |
| 7 | 0.7976 | 0.0540 |
| A | 0.8743 | 0.0390 |
| B | 0.8635 | 0.0370 |
| C | 0.8356 | 0.0540 |
| D | 0.8330 | 0.0510 |
| E | 0.9268 | 0.0450 |
| F | 0.9272 | 0.0510 |
| G | 0.8733 | 0.0410 |
| H | 0.8340 | 0.0450 |
| I | 0.7993 | 0.0510 |
| J | 0.8295 | 0.0600 |
| K | 0.7985 | 0.0480 |
| L | 0.7327 | 0.0450 |
| M | 0.7805 | 0.0290 |
| N | 0.7718 | 0.0550 |
| O | 0.6061 | 0.0690 |
| P | 0.6854 | 0.0700 |
| Q | 0.7317 | 0.0500 |
| R | 0.7553 | 0.0700 |
| S | 0.7845 | 0.0630 |
| T | 0.7150 | 0.0750 |
| U | 0.7843 | 0.0570 |
| V | 0.8836 | 0.0440 |
| W | 0.6528 | 0.0600 |
| Y | 0.6888 | 0.0570 |
| Z | 0.5840 | 0.0460 |