# wwPDB EM Validation Summary Report

Nov 5, 2022 – 09:27 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 5VFU |
| EMDB ID | : | EMD-8668 |
| Title | : | Nucleotide-driven Triple-state Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome |
| Authors | : | Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y. |
| Deposited on | : | 2017-04-09 |
| Resolution | : | 5.80 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 ⓘ symbol.

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

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

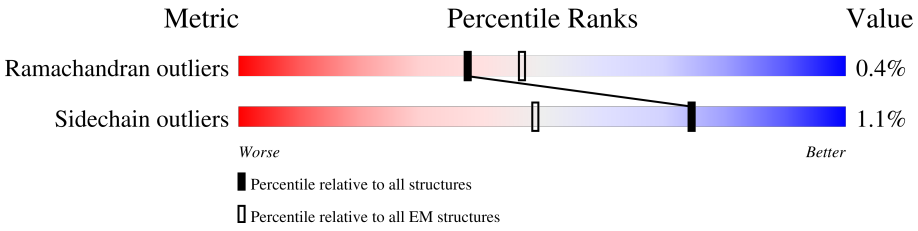
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 5.80 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 | U | 911 | 68% 88% · 12% |
| 2 | V | 480 | 91% 97% · |
| 3 | W | 456 | 94% 97% · |
| 4 | X | 380 | 60% 63% 37% |
| 5 | Y | 378 | 85% 98% · |
| 6 | Z | 286 | 84% 98% · |
| 7 | a | 373 | 94% 99% · |
| 8 | b | 191 | 92% 99% · |
| 9 | c | 287 | 79% 94% · · |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | d | 257 | 95% 98% |
| 11 | e | 70 | 54% 53% 43% |
| 12 | A | 361 | 77% 98% |
| 13 | B | 348 | 87% 96% |
| 14 | C | 384 | 87% 96% |
| 15 | D | 380 | 84% 99% |
| 16 | E | 353 | 81% 99% |
| 17 | F | 377 | 76% 95% |
| 18 | G | 240 | 58% 100% |
| 18 | g | 240 | 58% 100% |
| 19 | H | 232 | 57% 99% |
| 19 | h | 232 | 50% 100% |
| 20 | I | 250 | 62% 99% |
| 20 | i | 250 | 58% 99% |
| 21 | J | 243 | 53% 97% |
| 21 | j | 243 | 57% 98% |
| 22 | K | 234 | 52% 96% |
| 22 | k | 234 | 55% 94% |
| 23 | L | 238 | 50% 98% |
| 23 | l | 238 | 48% 100% |
| 24 | M | 245 | 54% 97% |
| 24 | m | 245 | 56% 97% |
| 25 | N | 191 | 47% 100% |
| 25 | n | 191 | 40% 99% |
| 26 | O | 220 | 45% 100% |

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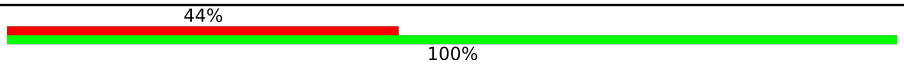
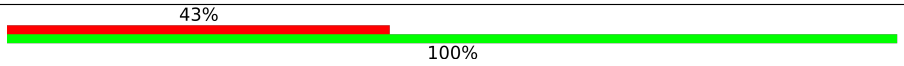
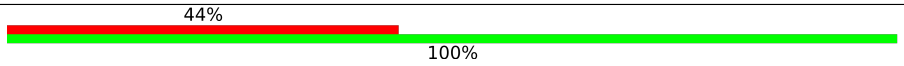
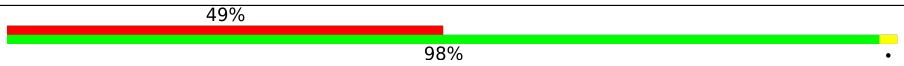
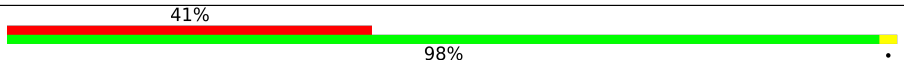
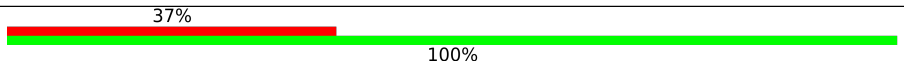
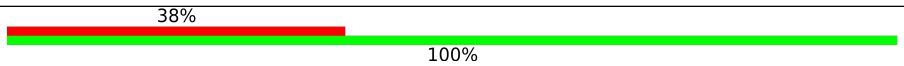
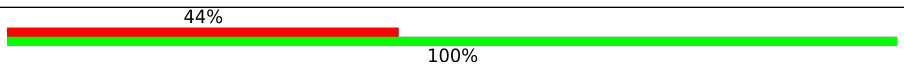
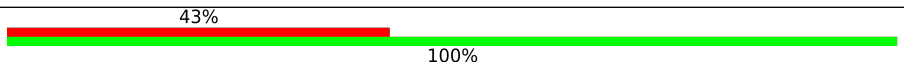
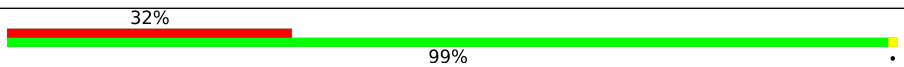
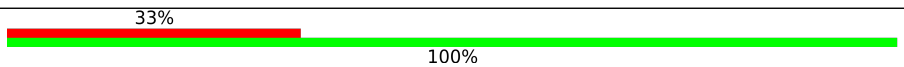
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 26 | o | 220 |   |
| 27 | P | 204 |   |
| 27 | p | 204 |   |
| 28 | Q | 199 |   |
| 28 | q | 199 |   |
| 29 | R | 201 |   |
| 29 | r | 201 |   |
| 30 | S | 213 |   |
| 30 | s | 213 |   |
| 31 | T | 215 |   |
| 31 | t | 215 |   |
| 32 | f | 908 |   |

# 2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 100133 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 26S proteasome non-ATPase regulatory subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | U | 806 | 6287 | 3990 | 1075 | 1178 | 44 | 0 | 0 |

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | V | 480 | 3852 | 2444 | 684 | 710 | 14 | 0 | 0 |

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | W | 456 | 3703 | 2339 | 635 | 704 | 25 | 0 | 0 |

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | X | 241 | 1905 | 1212 | 320 | 365 | 8 | 0 | 0 |

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | Y | 378 | 3115 | 1987 | 533 | 578 | 17 | 0 | 0 |

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | Z | 286 | 2281 | 1457 | 392 | 427 | 5 | 0 | 0 |

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | a | 373 | Total | C | N | O | S | 0 | 0 |
| | | | 2993 | 1910 | 509 | 559 | 15 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| a | 13 | SER | ASN | conflict | UNP Q9UNM6 |

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | b | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1458 | 910 | 261 | 279 | 8 | | |

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | c | 278 | Total | C | N | O | S | 0 | 0 |
| | | | 2187 | 1389 | 374 | 406 | 18 | | |

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | d | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2116 | 1371 | 346 | 390 | 9 | | |

- Molecule 11 is a protein called Sem1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | e | 40 | Total | C | N | O | S | 0 | 0 |
| | | | 334 | 200 | 55 | 77 | 2 | | |

- Molecule 12 is a protein called 26S protease regulatory subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | A | 361 | Total | C | N | O | S | 0 | 0 |
| | | | 2834 | 1788 | 500 | 528 | 18 | | |

- Molecule 13 is a protein called 26S protease regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | B | 348 | Total | C | N | O | S | 0 | 0 |
| | | | 2717 | 1708 | 460 | 537 | 12 | | |

- Molecule 14 is a protein called 26S protease regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | C | 384 | Total | C | N | O | S | 0 | 0 |
| | | | 3015 | 1894 | 540 | 564 | 17 | | |

- Molecule 15 is a protein called 26S protease regulatory subunit 6B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | D | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3040 | 1923 | 524 | 580 | 13 | | |

- Molecule 16 is a protein called 26S protease regulatory subunit 10B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | E | 353 | Total | C | N | O | S | 0 | 0 |
| | | | 2790 | 1755 | 494 | 525 | 16 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | F | 366 | Total | C | N | O | S | 0 | 0 |
| | | | 2863 | 1802 | 496 | 549 | 16 | | |

- Molecule 18 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | G | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1825 | 1160 | 304 | 348 | 13 | | |
| 18 | g | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1826 | 1160 | 305 | 348 | 13 | | |

- Molecule 19 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | H | 232 | Total | C | N | O | S | 0 | 0 |
| | | | 1708 | 1081 | 289 | 333 | 5 | | |
| 19 | h | 232 | Total | C | N | O | S | 0 | 0 |
| | | | 1708 | 1081 | 289 | 333 | 5 | | |

- Molecule 20 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | I | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1912 | 1204 | 329 | 371 | 8 | | |
| 20 | i | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1912 | 1204 | 329 | 371 | 8 | | |

- Molecule 21 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | J | 239 | Total | C | N | O | S | 0 | 0 |
| | | | 1704 | 1056 | 308 | 335 | 5 | | |
| 21 | j | 239 | Total | C | N | O | S | 0 | 0 |
| | | | 1704 | 1056 | 308 | 335 | 5 | | |

- Molecule 22 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | K | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1722 | 1080 | 284 | 348 | 10 | | |
| 22 | k | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1722 | 1080 | 284 | 348 | 10 | | |

- Molecule 23 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | L | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1850 | 1159 | 334 | 346 | 11 | | |
| 23 | l | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1850 | 1159 | 334 | 346 | 11 | | |

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | M | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1856 | 1178 | 314 | 353 | 11 | | |
| 24 | m | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1856 | 1178 | 314 | 353 | 11 | | |

- Molecule 25 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | N | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1430 | 893 | 245 | 280 | 12 | | |
| 25 | n | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1430 | 893 | 245 | 280 | 12 | | |

- Molecule 26 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | O | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1033 | 280 | 318 | 12 | | |
| 26 | o | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1033 | 280 | 318 | 12 | | |

- Molecule 27 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | P | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1585 | 1010 | 262 | 294 | 19 | | |
| 27 | p | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1585 | 1010 | 262 | 294 | 19 | | |

- Molecule 28 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | Q | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1570 | 1006 | 265 | 290 | 9 | | |
| 28 | q | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1570 | 1006 | 265 | 290 | 9 | | |

- Molecule 29 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | R | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1548 | 974 | 273 | 292 | 9 | | |
| 29 | r | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1548 | 974 | 273 | 292 | 9 | | |

- Molecule 30 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | S | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1641 | 1036 | 282 | 313 | 10 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | s | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1641 | 1036 | 282 | 313 | 10 | | |

- Molecule 31 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | T | 215 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1052 | 285 | 318 | 12 | | |
| 31 | t | 215 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1052 | 285 | 318 | 12 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | f | 689 | Total | C | N | O | S | 0 | 0 |
| | | | 5319 | 3343 | 904 | 1037 | 35 | | |

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

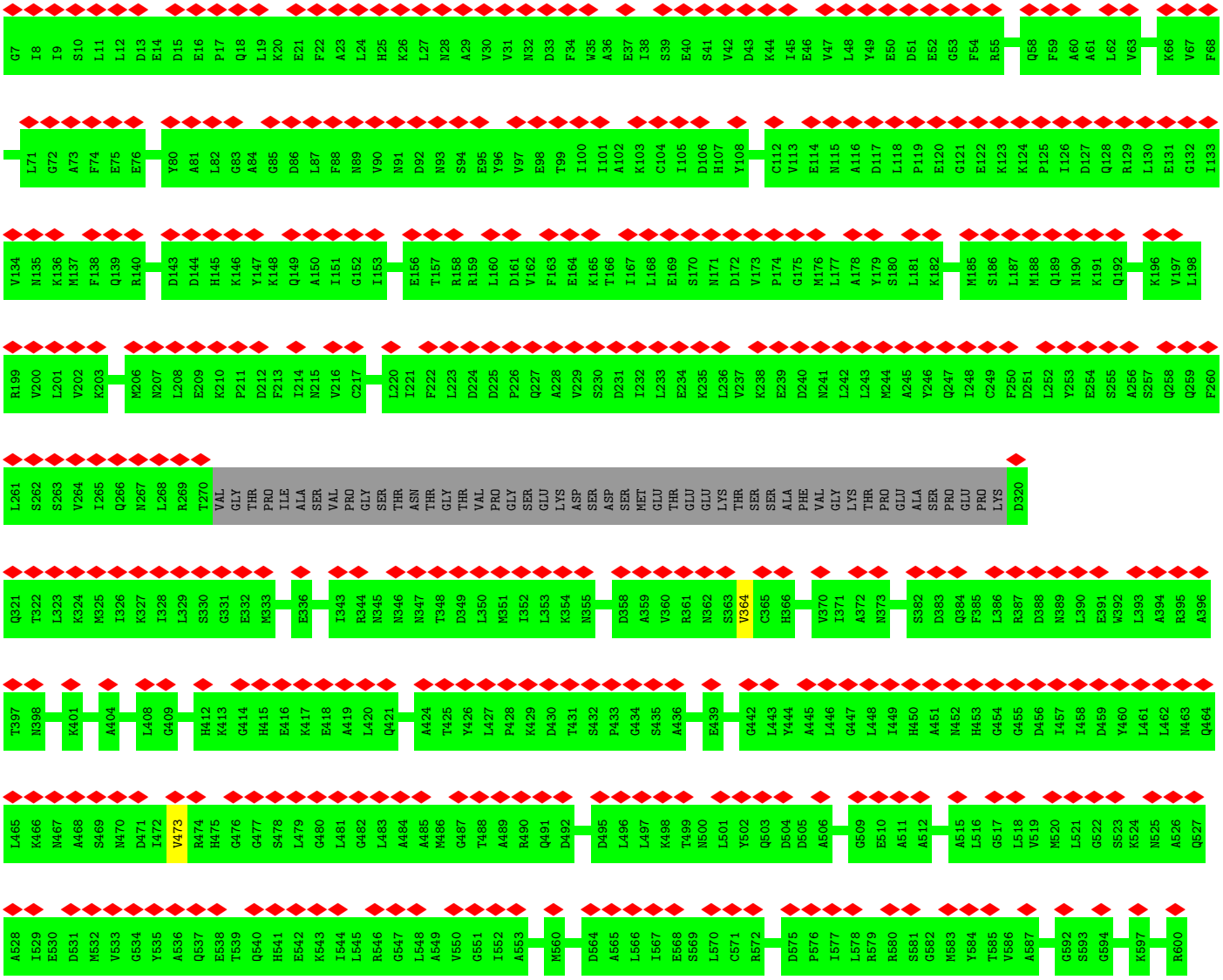
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 33 | c | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

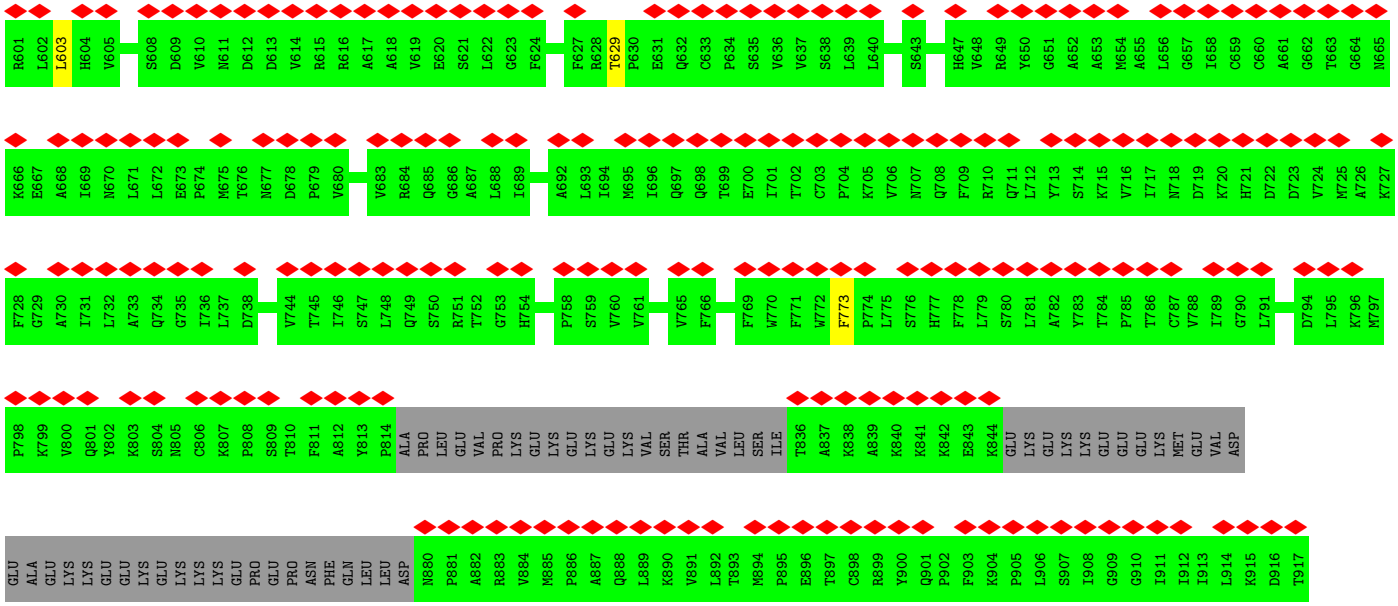
# 3 Residue-property plots (i)

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.

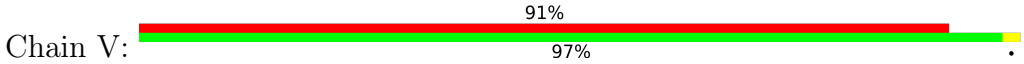
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1

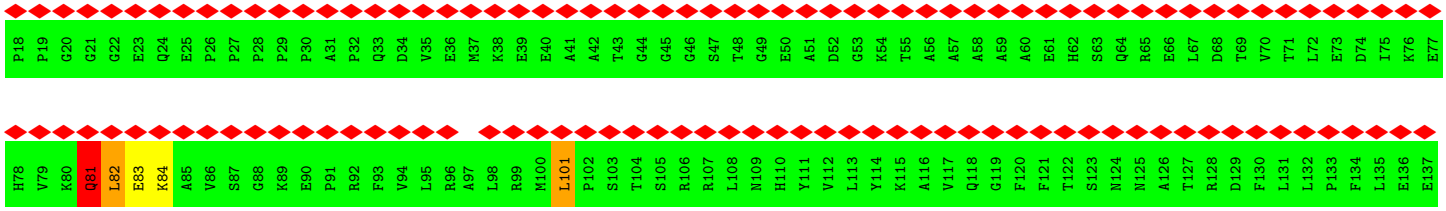
Chain U:



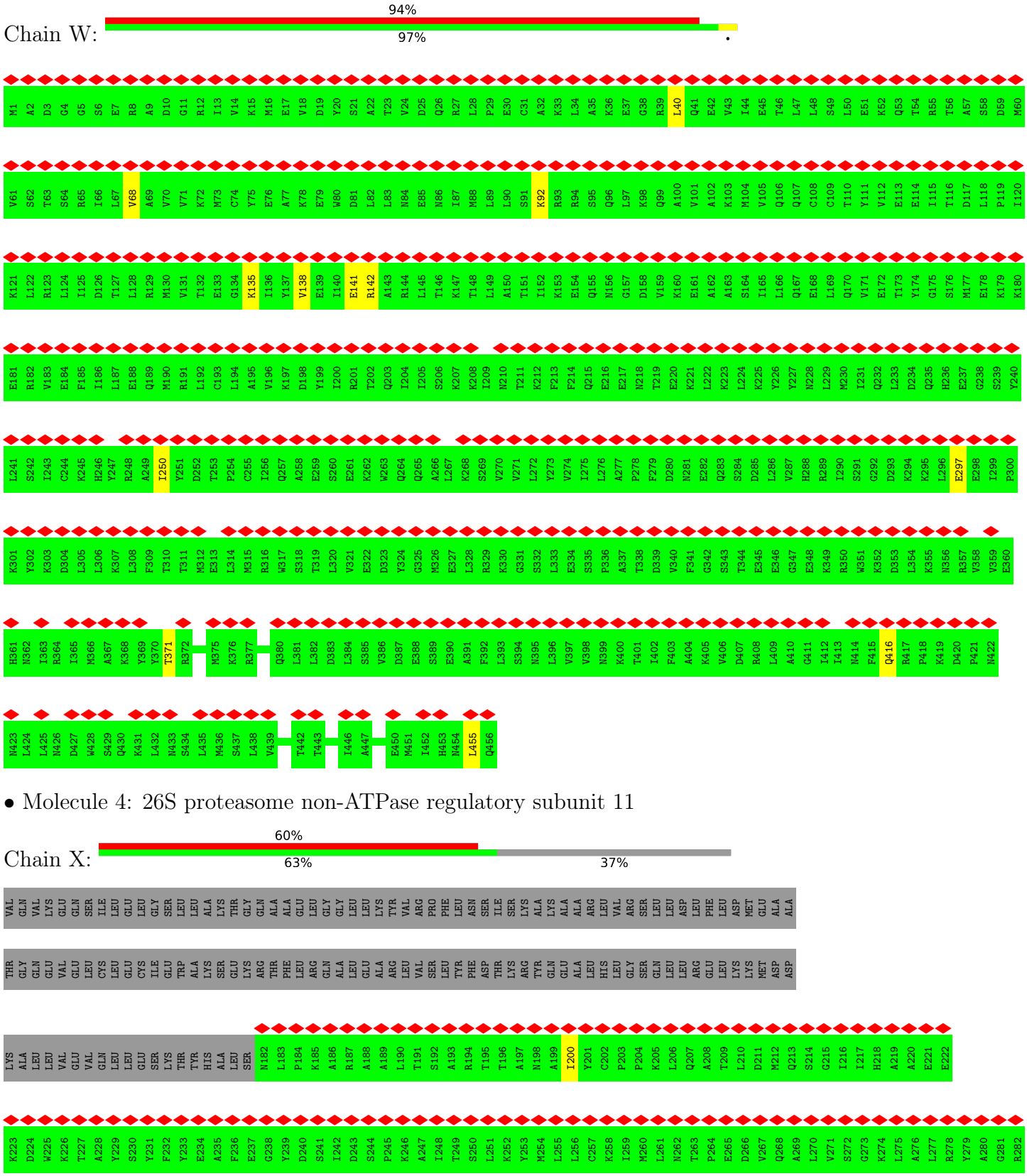

• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3



• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

Chain W:




• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X:

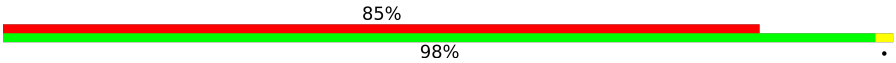
Q283 T284 E285 A286 L287 K288 C289 V290 A291 Q292 A293 S294 K295 N296 R297 S298 L299 A300 D301 F302 E303 K304 A305 L306 T307 D308 Y309 R310 A311 E312 L313 R314 D315 D316 P317 I318 I319 S320 T321 H322 L323 A324 K325 L326 Y327 D328 N329 L330 L331 E332 Q333 N334 L335 I336 R337 V338 I339 E340 P341 F342

S343 R344 V345 Q346 I347 E348 H349 I350 S351 S352 L353 I354 K355 L356 S357 K358 A359 D360 V361 E362 R363 K364 L365 S366 Q367 M368 I369 L370 D371 K372 K373 F374 H375 G376 I377 L378 D379 Q380 G381 E382 G383 V384 L385 I386 I387 F388 D389 E390 P391 P392 V393 D394 K395 T396 Y397 E398 A399 A400 L401 E402

T403 I404 Q405 N406 M407 S408 K409 V410 V411 D412 S413 L414 Y415 N416 K417 A418 K419 K420 L421 T422

• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:




P12 K13 N14 P15 D16 L17 R18 I19 A20 Q21 L22 R23 F24 L25 L26 S27 L28 P29 E30 H31 R32 G33 D34 A35 A36 V37 R38 D39 E40 L41 M42 A43 A44 V45 R46 D47 N48 N49 M50 A51 P52 Y53 Y54 E55 A56 L57 C58 K59 S60 L61 D62 W63 Q64 I65 D66 V67 D68 L69 L70 N71

K72 M73 K74 K75 A76 N77 E78 D79 E80 L81 K82 R83 L84 D85 E86 E87 L88 E89 D90 A91 E92 K93 N94 L95 G96 E97 S98 E99 I100 R101 D102 A103 M104 M105 A106 K107 A108 E109 Y110 L111 C112 R113 I114 G115 D116 K117 E118 G119 A120 L121 T122 A123 F124 R125 K126 T127 Y128 D129 K130 T131

V132 A133 L134 D139 I140 V141 F142 Y143 L144 L145 R146 I147 G148 L149 F150 Y151 M152 D153 N154 D155 L156 I157 T158 R159 N160 T161 E162 K163 A164 K165 S166 L167 I168 E169 E170 G171 C172 D173 W174 D175 R176 R177 N178 R179 L180 K181 V182 Y183 Q184 G185 L186 Y187 C188 V189 A190 I191 R192 D193 F194

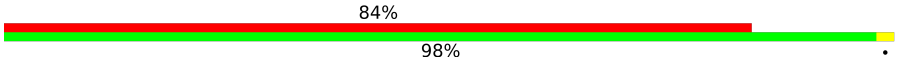
K195 Q196 A197 A198 E199 L200 F201 L202 D203 T204 V205 S206 T207 F208 T209 S210 Y211 E212 L213 M214 D215 Y216 K217 T218 Y222 V226 I229 A230 L231 E232 R233 P234 D235 E238 K239 V240 I241 K242 G243 A244 E245 I246 L247 E248 V249 L250 H251 S252 L253 P254 A255 V256 R257 Q258 Y264

E265 C266 R267 Y268 S269 V270 Q273 A276 V277 V278 E279 Q280 E281 M282 K283 K284 D285 W286 L287 F288 A289 P290 H291 Y292 R293 Y294 R297 E298 M299 R300 I301 H302 A303 Y304 S305 Q306 L307 L308 E309 S310 Y311 R312 S313 L314 T315 L316 G317 Y318 M319 A320 E321 A322 V325 G326 V327 E328

F329 I330 D331 Q332 R336 F337 I338 A339 A340 G341 R342 L343 H344 C345 K346 I347 D348 K349 V350 N351 E352 I353 T356 N357 R358 P359 D360 S361 K362 N363 W364 Q365 Y366 Q367 E368 T369 I370 K371 K372 G373 D374 L375 L376 L377 N378 R379 V380 Q381 K382 L383 S384 R385 V386 I387 N388 M389

• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:



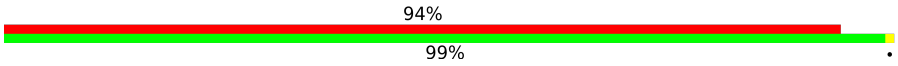

A5 V6 Q7 K8 V9 V10 V11 H12 P13 L14 V15 S18 V19 V20 D21 H22 F23 N24 R25 I26 G27 K28 V29 G30 N31 Q32 K33 R34 V35 V36 G37 V38 L39 L40 G41 S42 W43 Q44 K45 K46 V47 L48 S51 N52 S53 F54 A55 V56 P57 F58 D59 E60 D61 D62 K63 D64 D65 S66

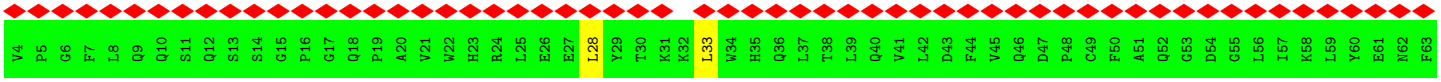
V67 W68 F69 L70 D71 H72 D73 E76 N77 G80 M81 F82 K83 K84 V85 N86 A87 R88 E89 R90 I91 V92 G93 W94 P99 K100 L101 H102 K103 N104 A107 I108 N109 E110 L111 M112 K113 R114 Y115 C116 P117 N118 S119 V120 I124 D125 V126 K127 P128 K129 D130 L131 G132 L133 P134

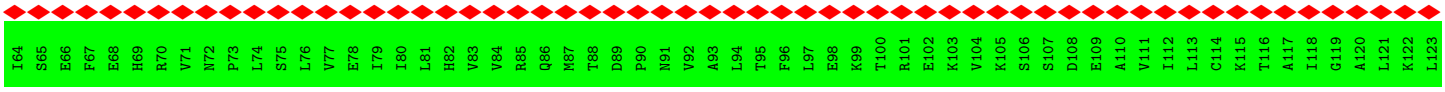
T135 E136 A137 Y138 I139 S140 V141 E142 E143 V144 H145 D146 D147 G148 T149 P150 T151 S152 K153 T154 T159 S160 E161 I162 G163 A164 E165 E166 A167 E168 E169 V170 G171 V172 E173 H174 L175 L176 R177 D178 I179 K180 D181 T182 T183 V184 G185 T186 L187 S188 Q189 R190 I191 T192 N193 Q194 V195 H196 G197

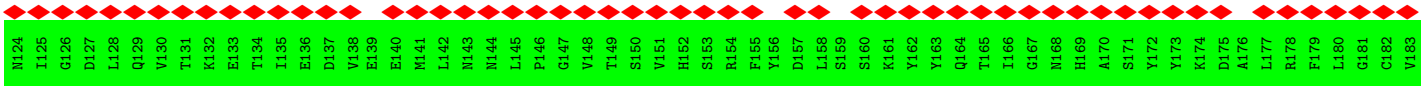

• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

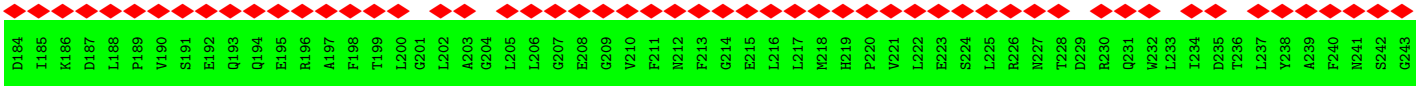
Chain a:

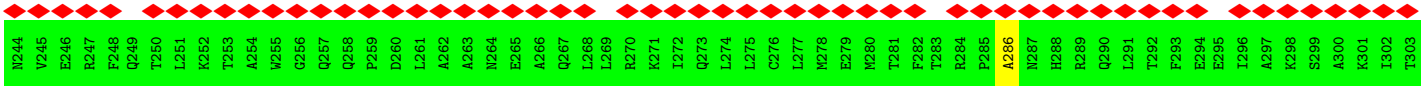


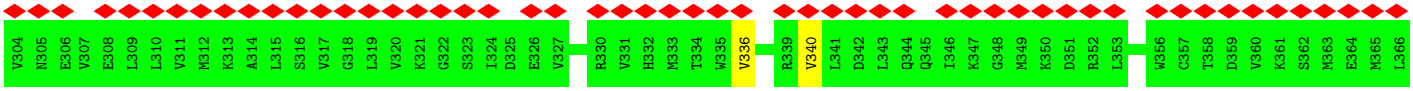



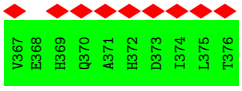



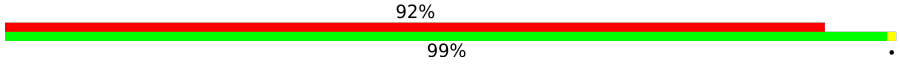



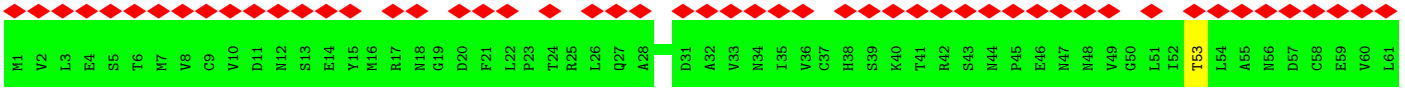



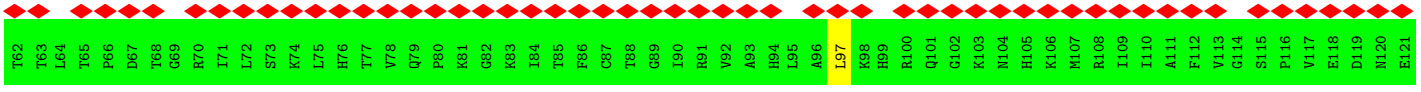



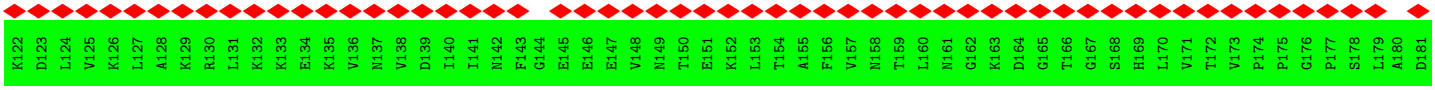

• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

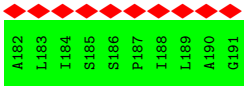
Chain b:



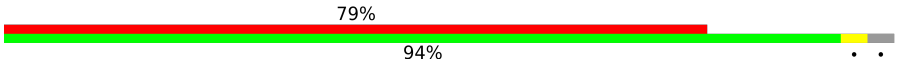



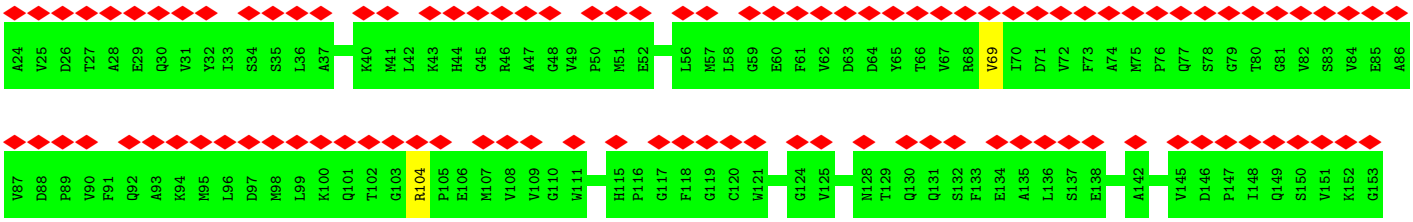






• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

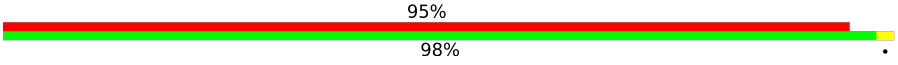
Chain c:

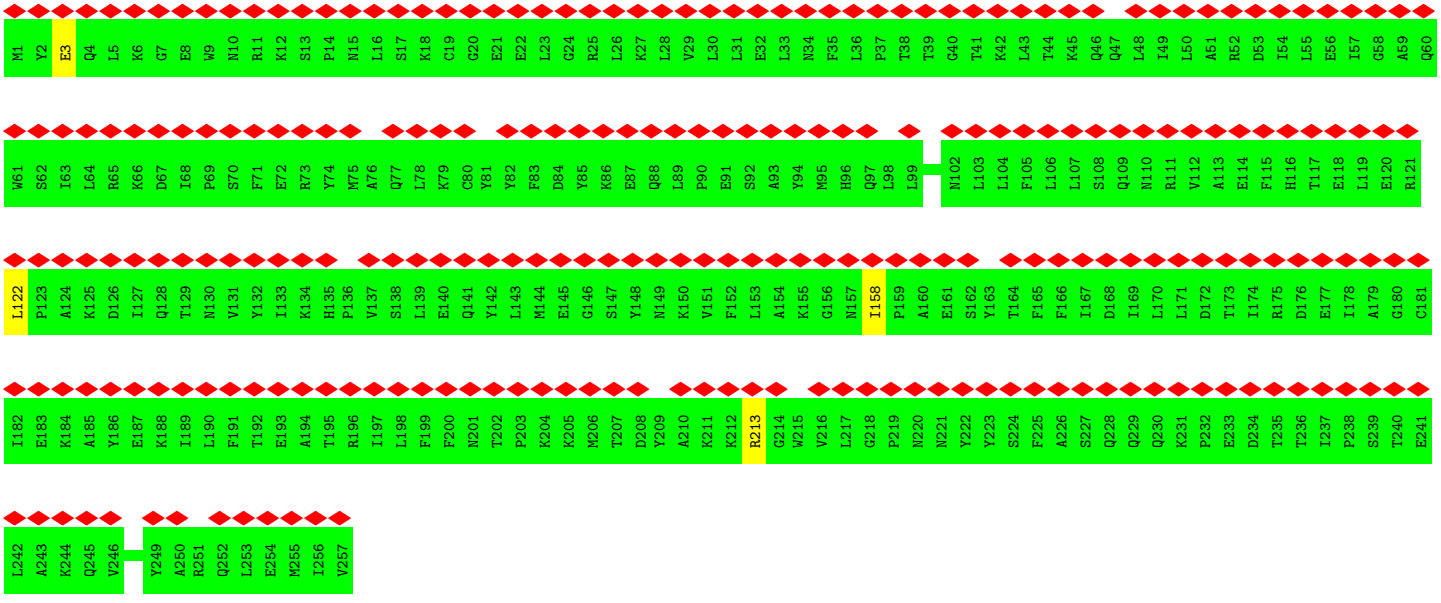



• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

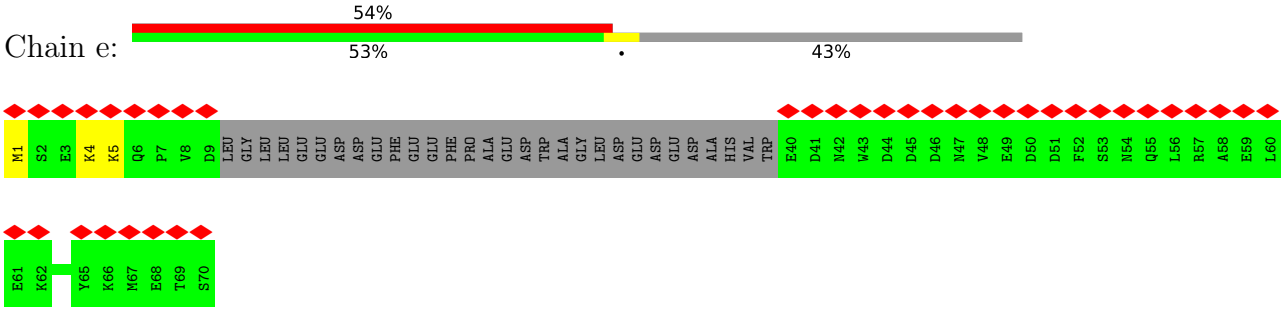
Chain d:



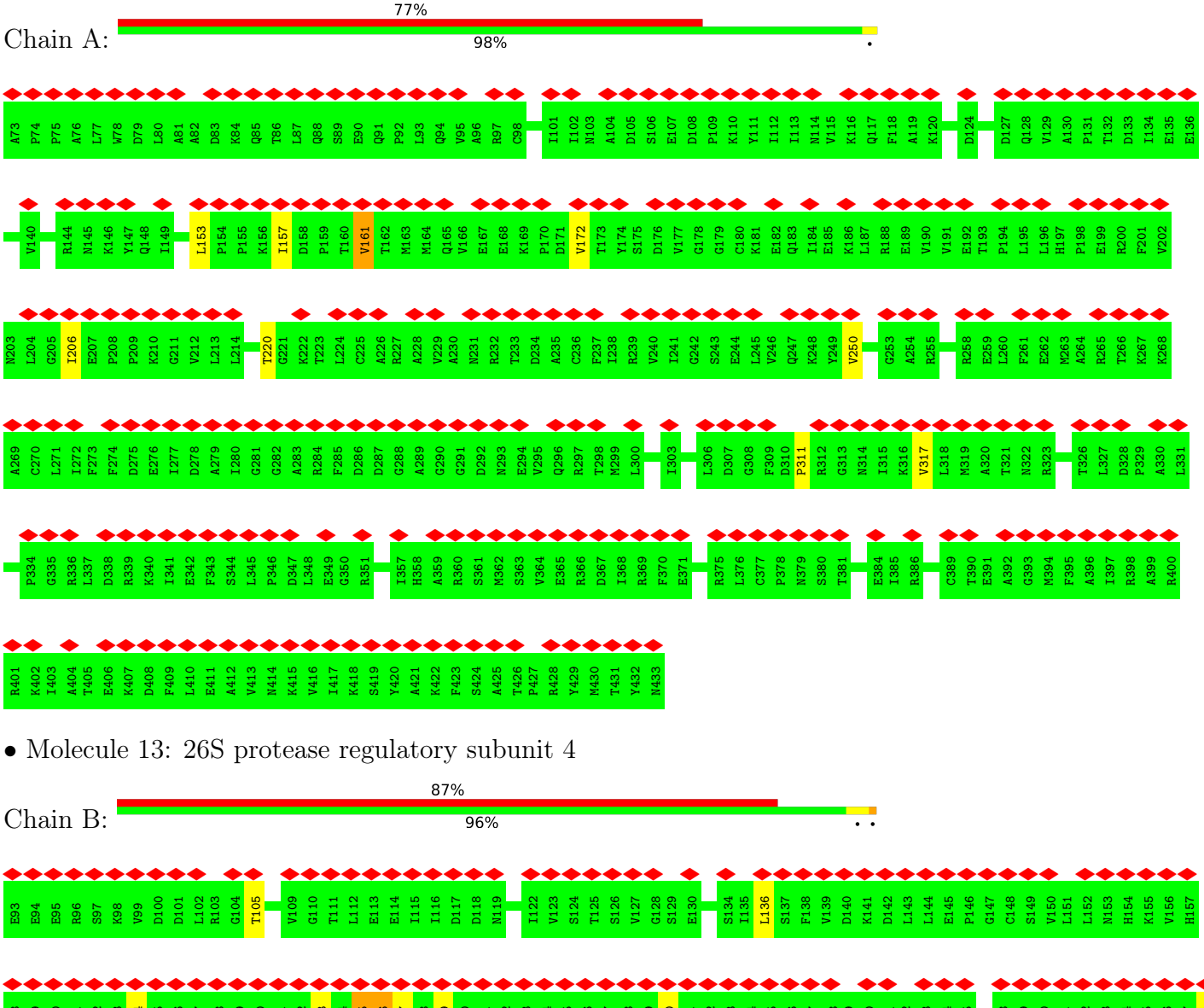

• Molecule 11: Sem1

Chain e:



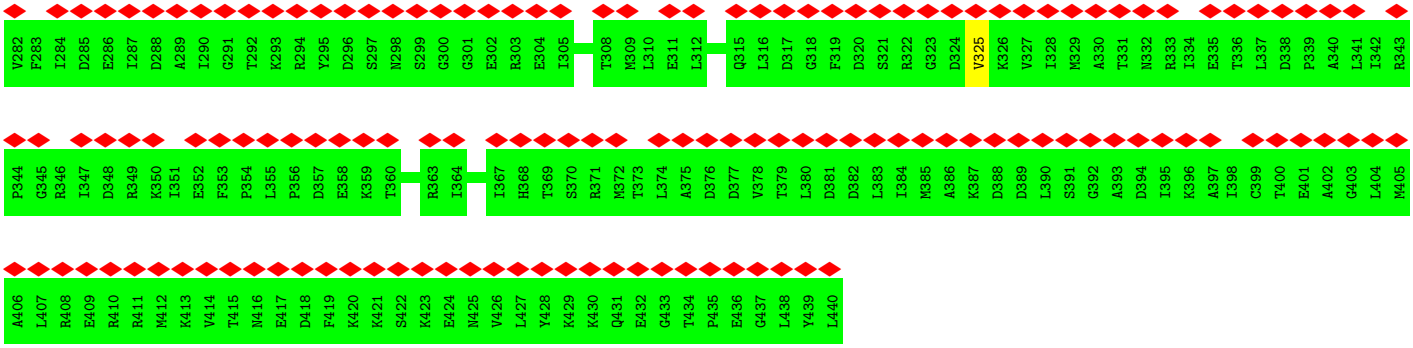

• Molecule 12: 26S protease regulatory subunit 7

Chain A:



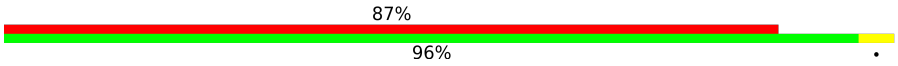

• Molecule 13: 26S protease regulatory subunit 4

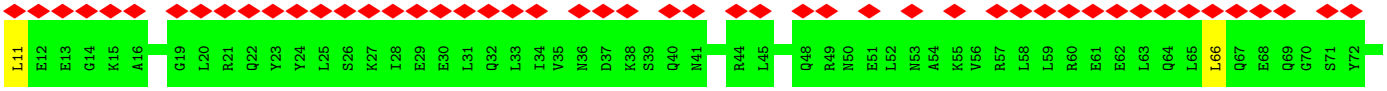
Chain B:

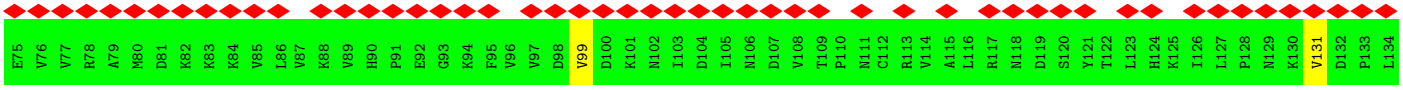


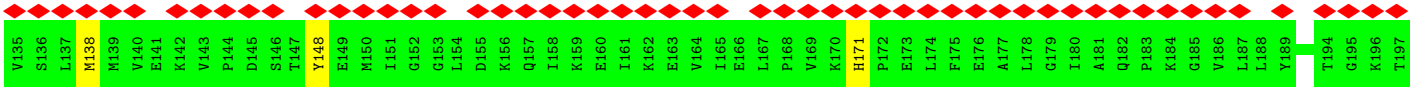

• Molecule 14: 26S protease regulatory subunit 8

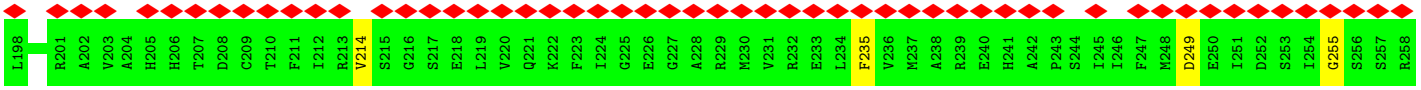
Chain C:

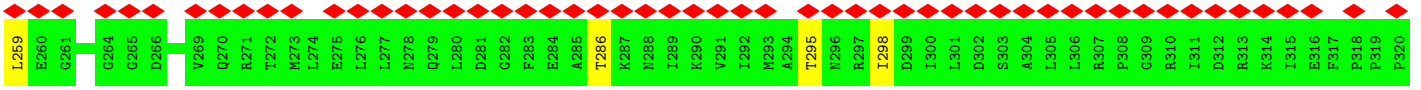


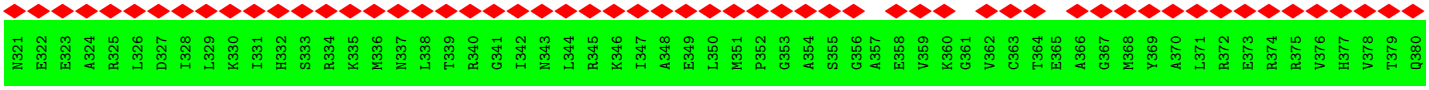



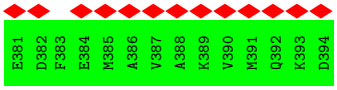



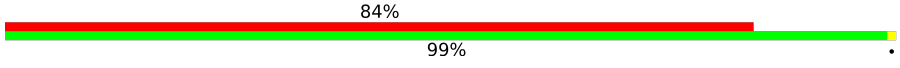



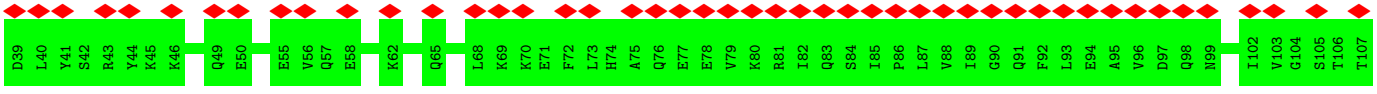



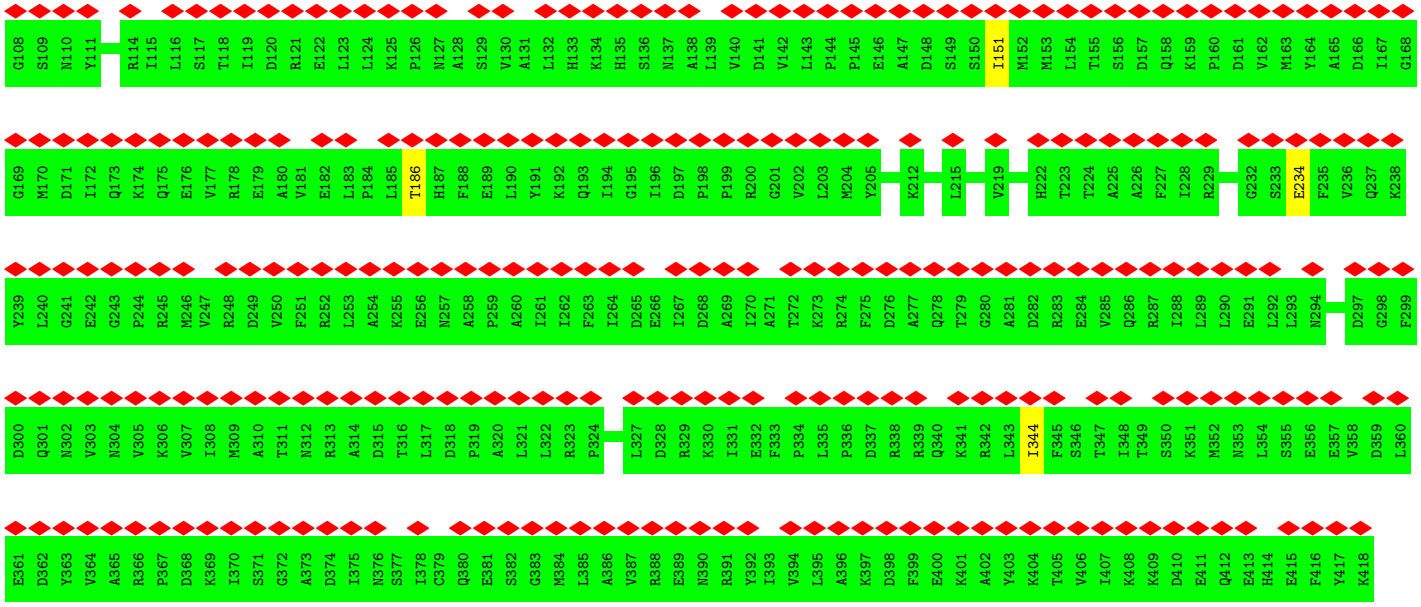




• Molecule 15: 26S protease regulatory subunit 6B

Chain D:

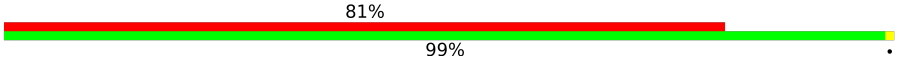


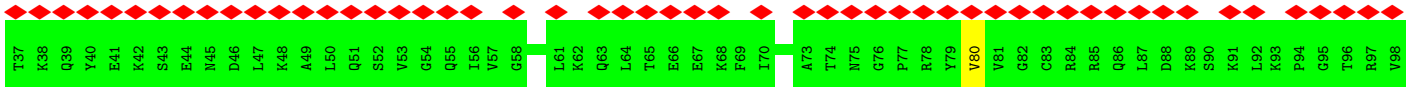






• Molecule 16: 26S protease regulatory subunit 10B

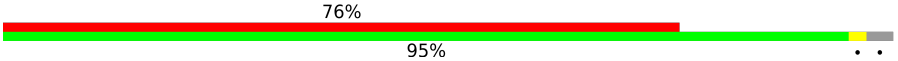
Chain E:

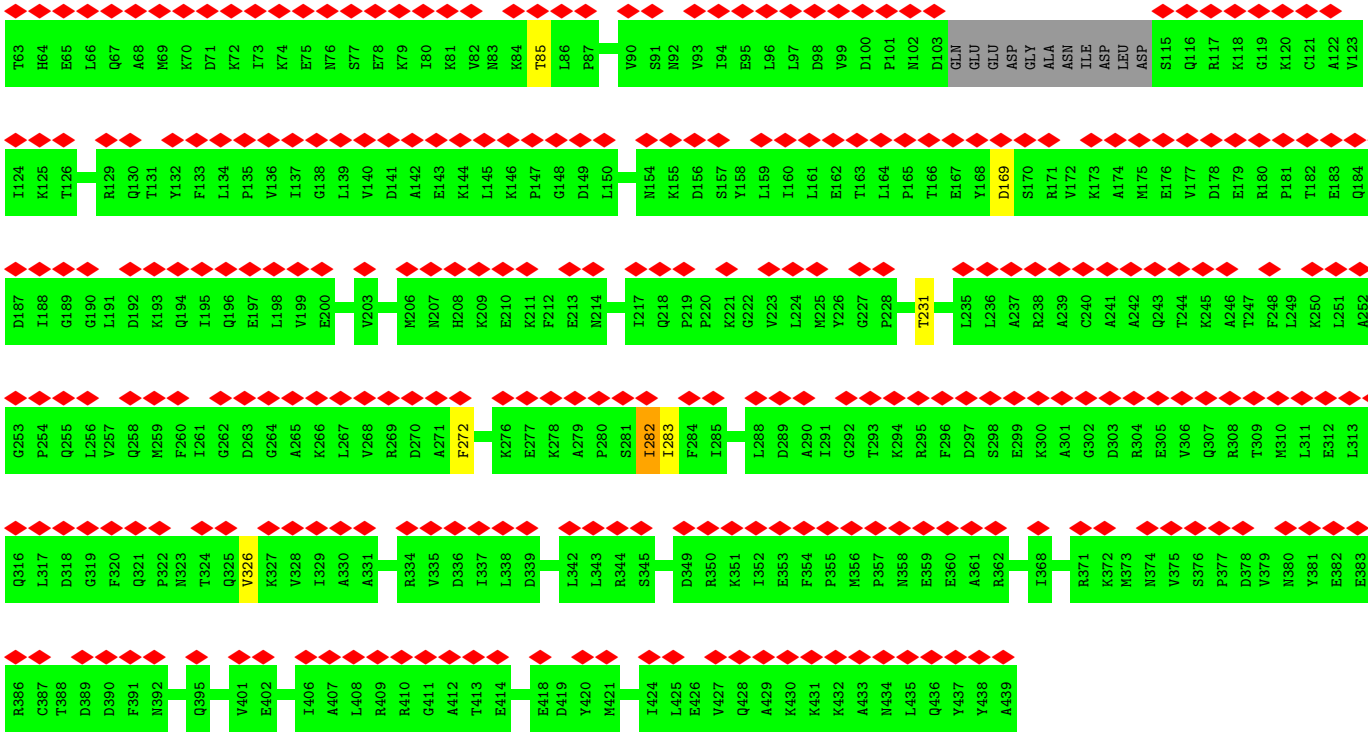



• Molecule 17: 26S protease regulatory subunit 6A

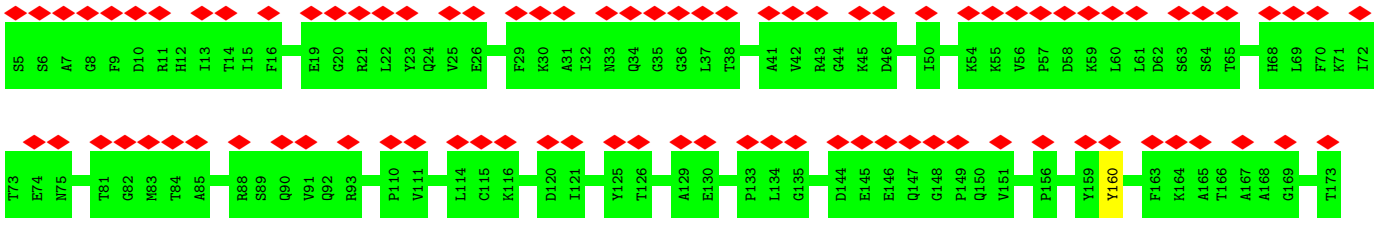
Chain F:





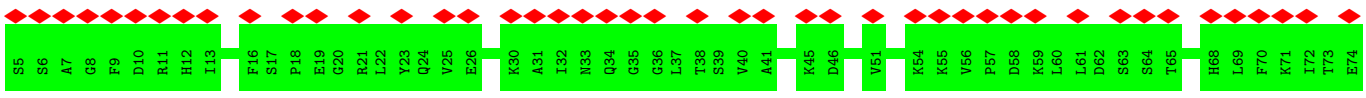

• Molecule 18: Proteasome subunit alpha type-6

Chain G:

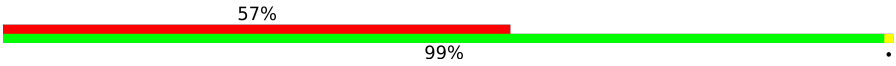

• Molecule 18: Proteasome subunit alpha type-6

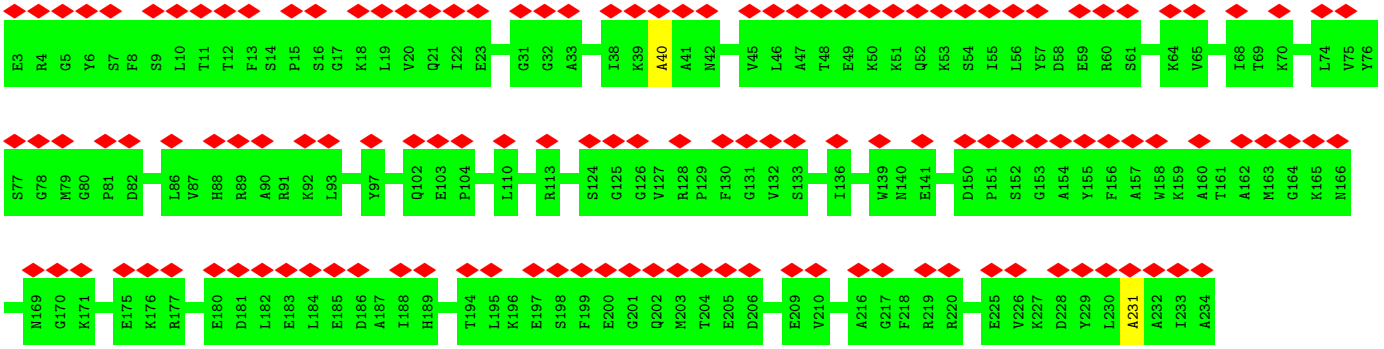
Chain g:


• Molecule 19: Proteasome subunit alpha type-2

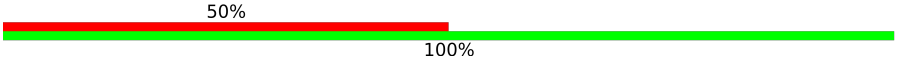
Chain H:

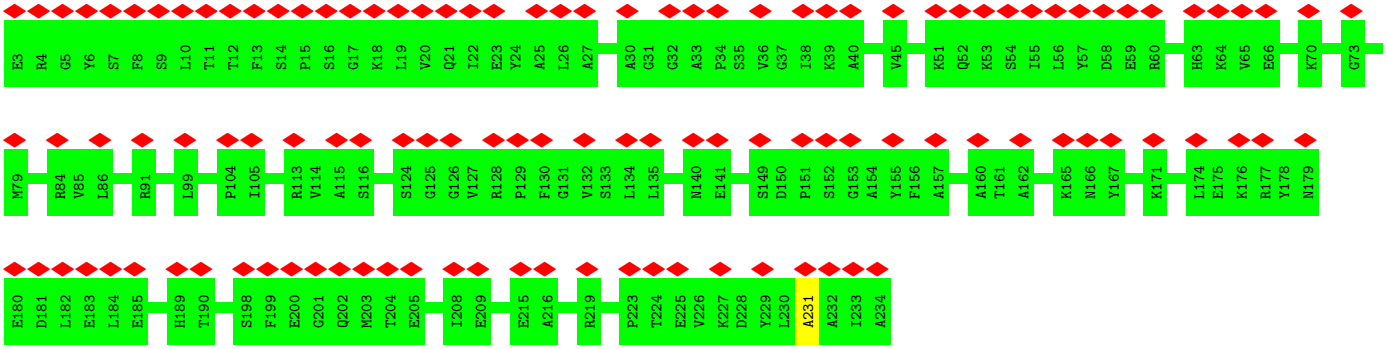



• Molecule 19: Proteasome subunit alpha type-2

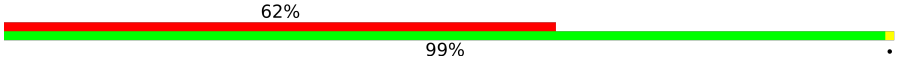
Chain h:

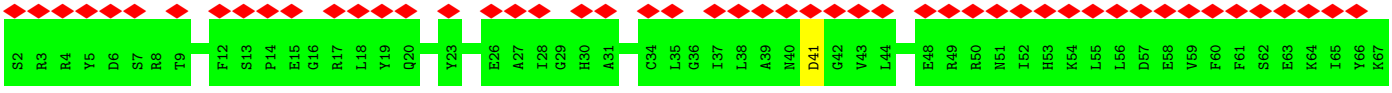


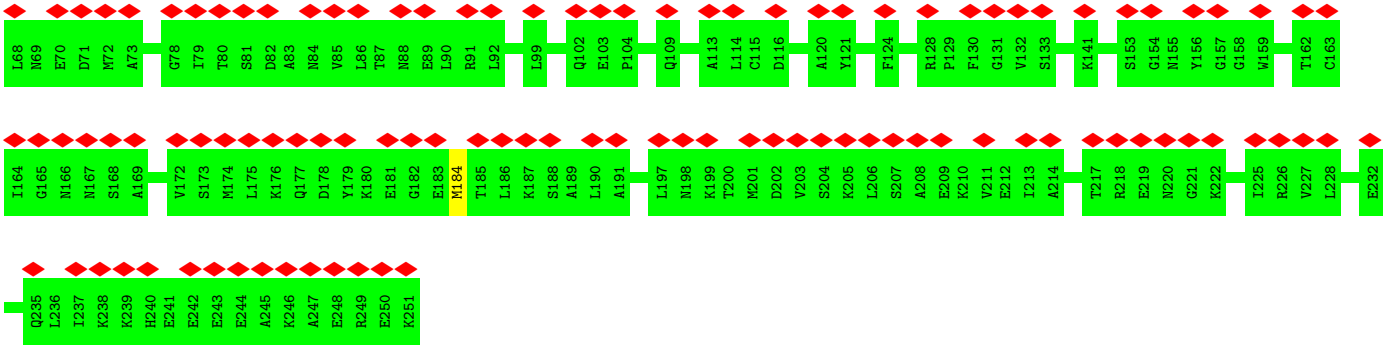




• Molecule 20: Proteasome subunit alpha type-4

Chain I:

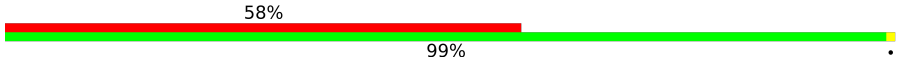


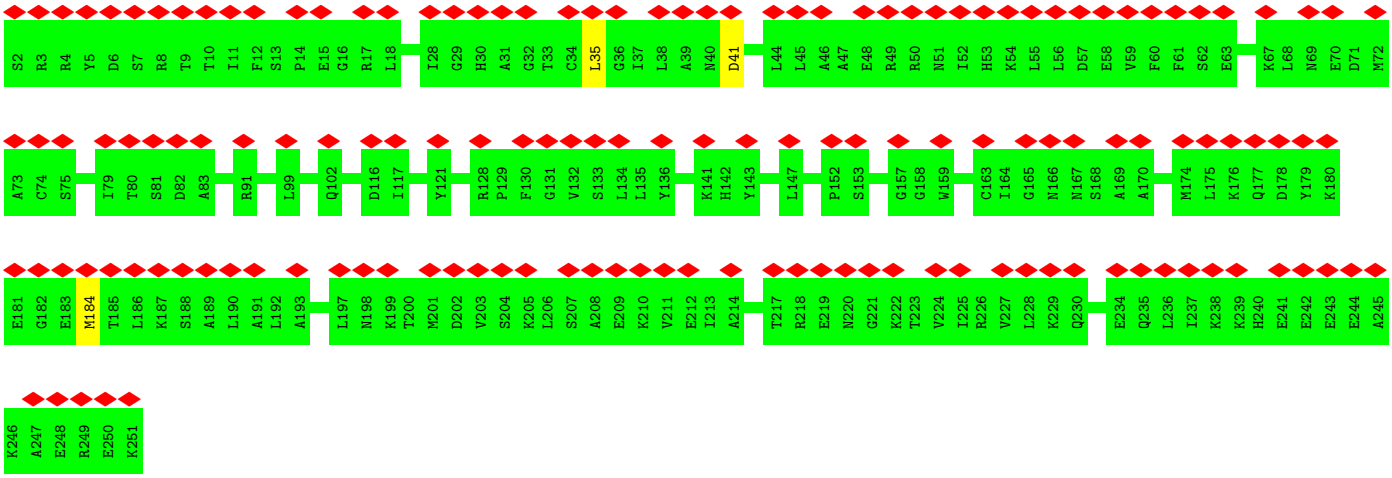






• Molecule 20: Proteasome subunit alpha type-4

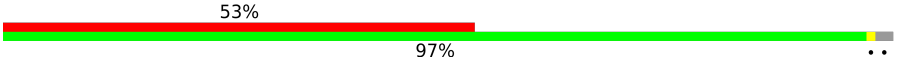
Chain i:

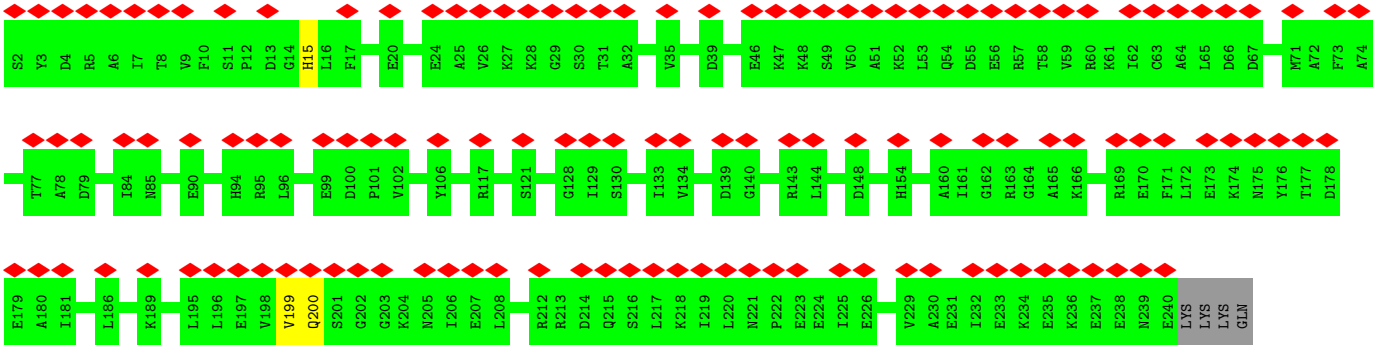



• Molecule 21: Proteasome subunit alpha type-7

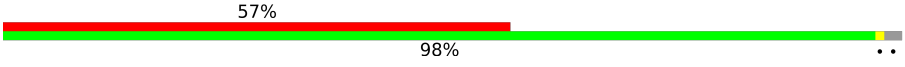
Chain J:

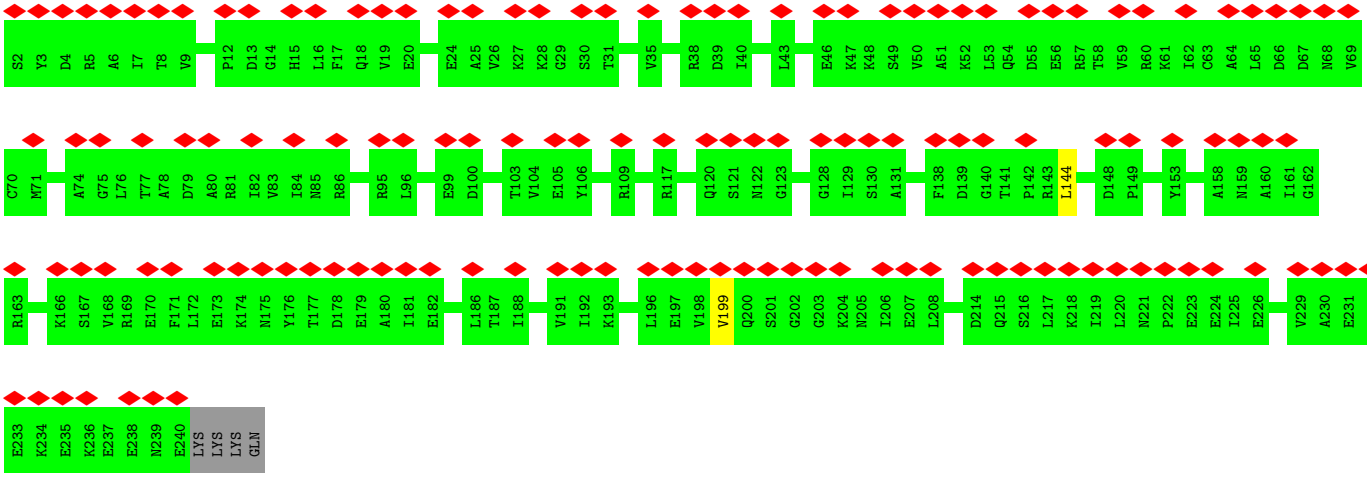



• Molecule 21: Proteasome subunit alpha type-7

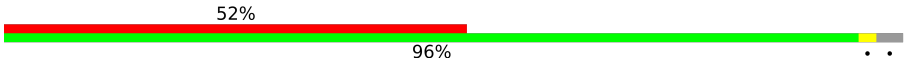
Chain j:

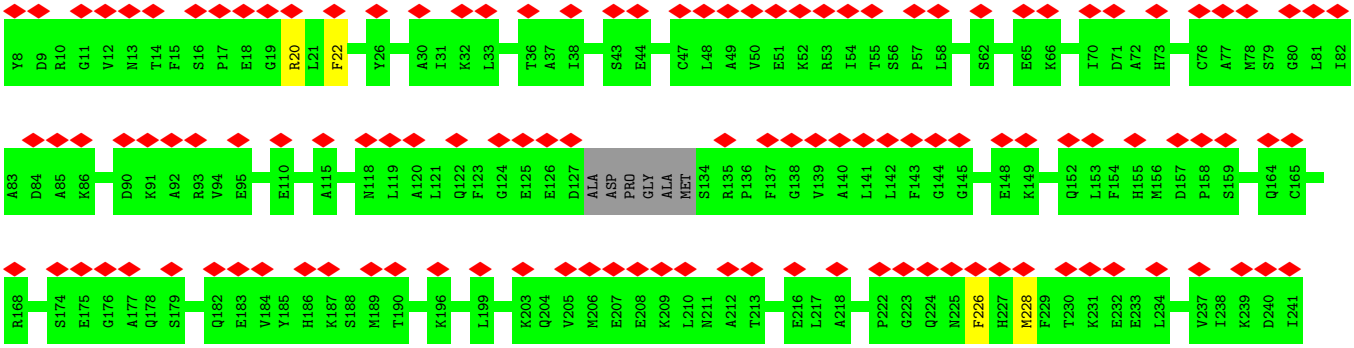





• Molecule 22: Proteasome subunit alpha type-5

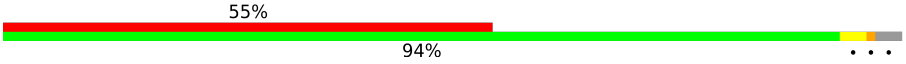
Chain K:

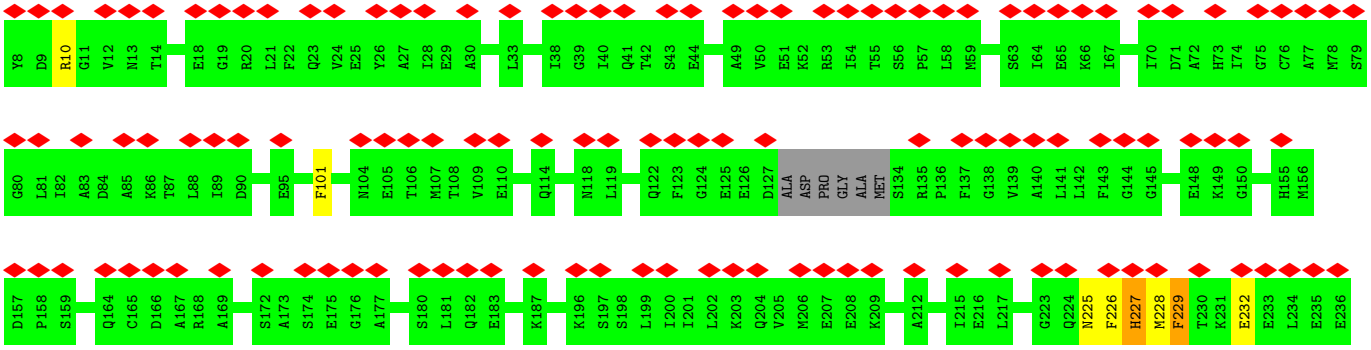



• Molecule 22: Proteasome subunit alpha type-5

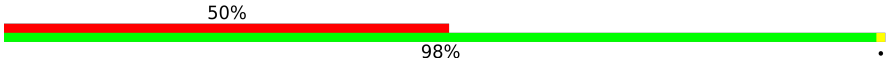
Chain k:

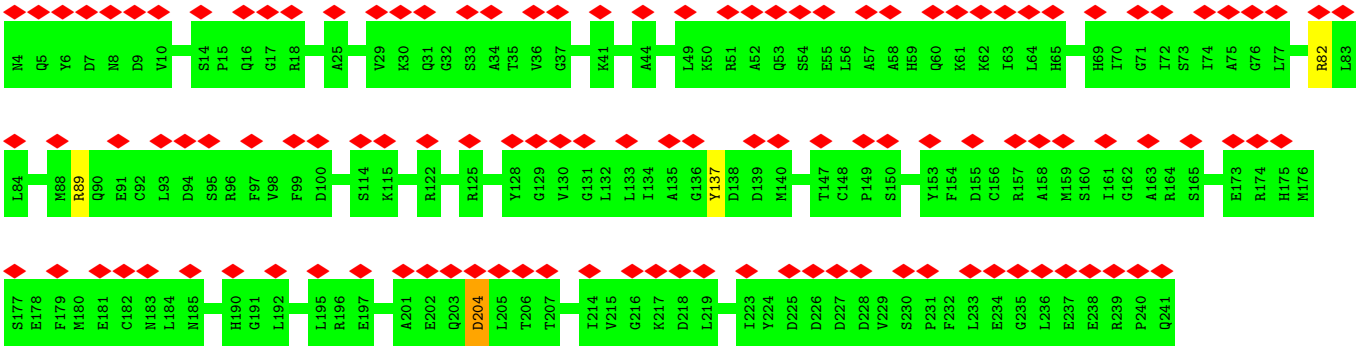



• Molecule 23: Proteasome subunit alpha type-1

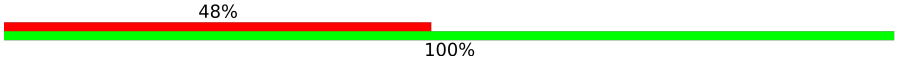
Chain L:

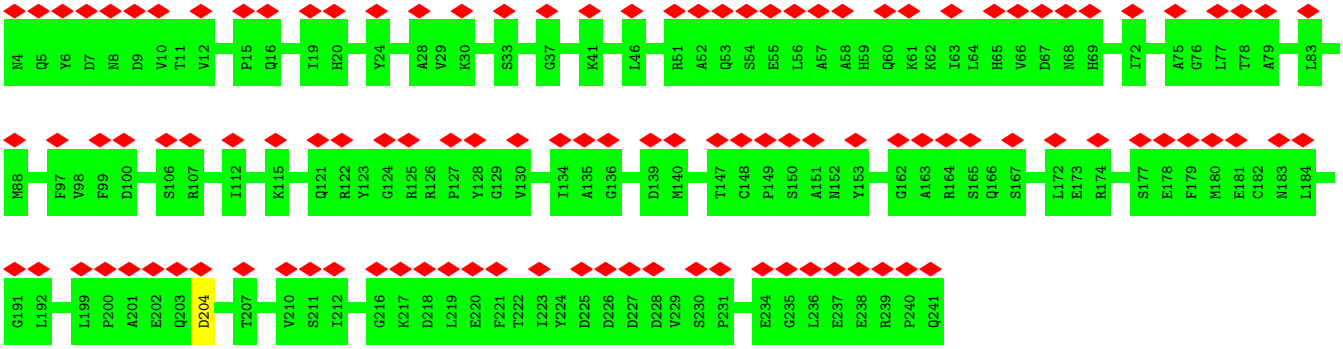



• Molecule 23: Proteasome subunit alpha type-1

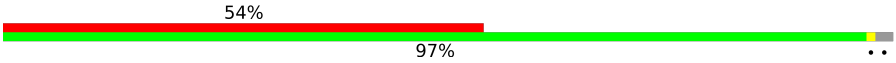
Chain l:

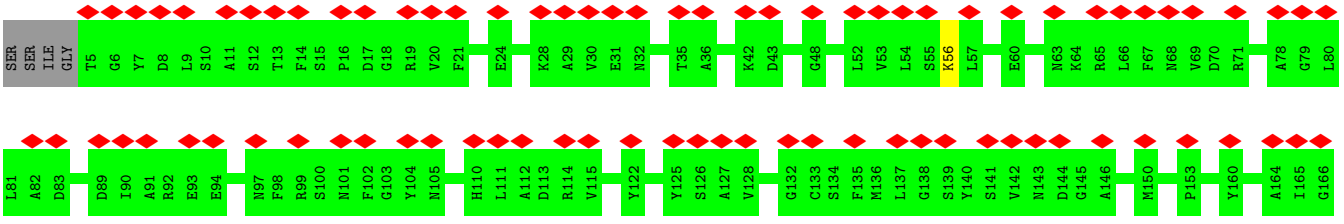



• Molecule 24: Proteasome subunit alpha type-3

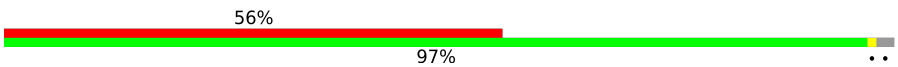
Chain M:

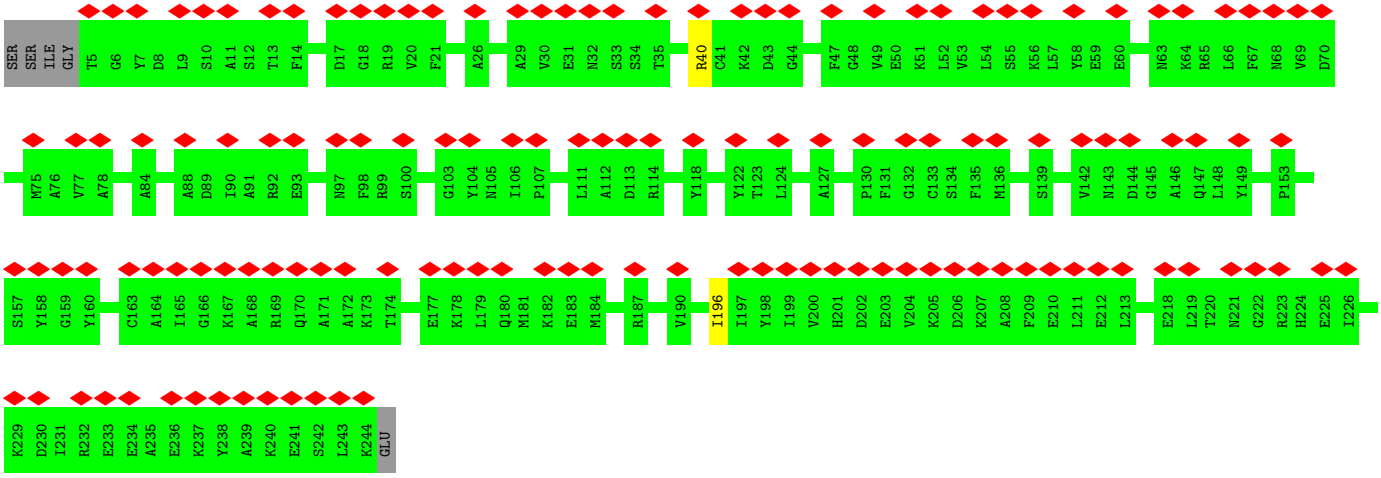


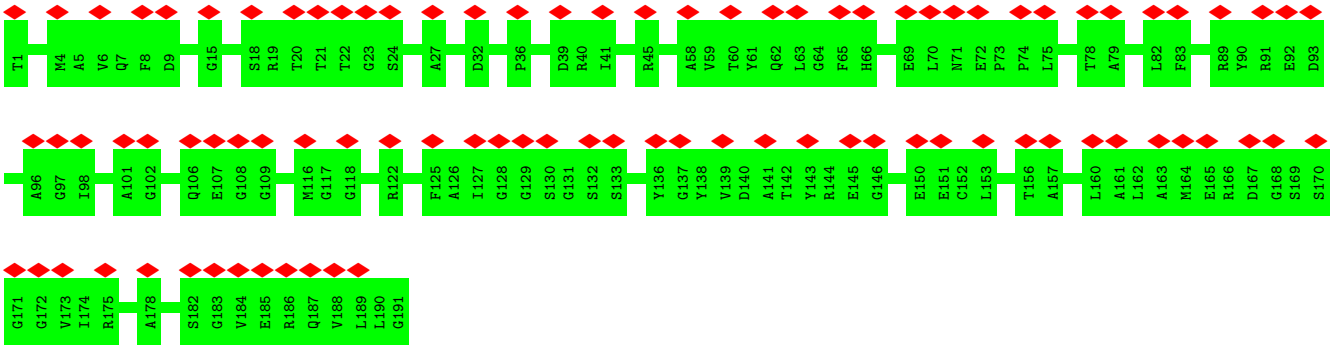

• Molecule 24: Proteasome subunit alpha type-3

Chain m:

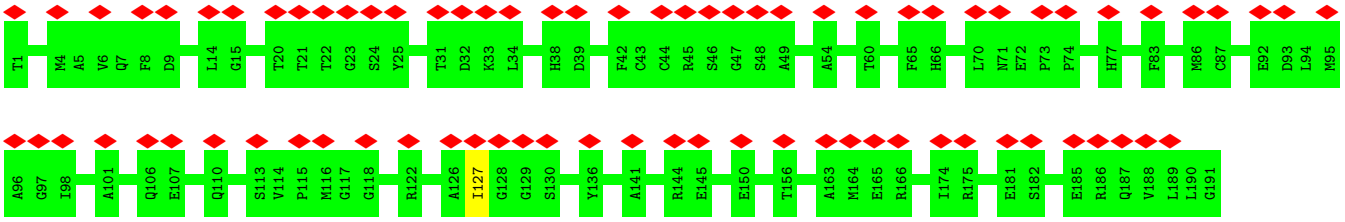




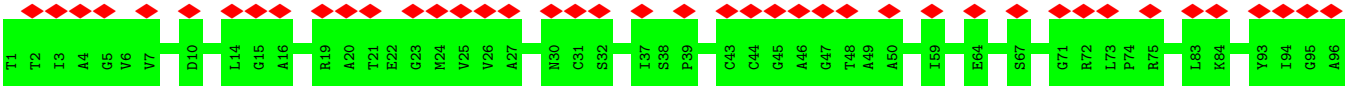

• Molecule 25: Proteasome subunit beta type-6

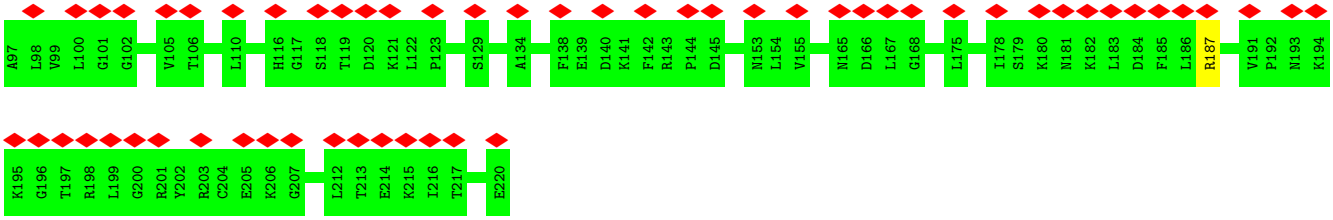




• Molecule 25: Proteasome subunit beta type-6

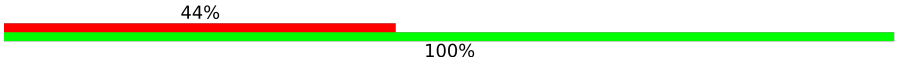

• Molecule 26: Proteasome subunit beta type-7

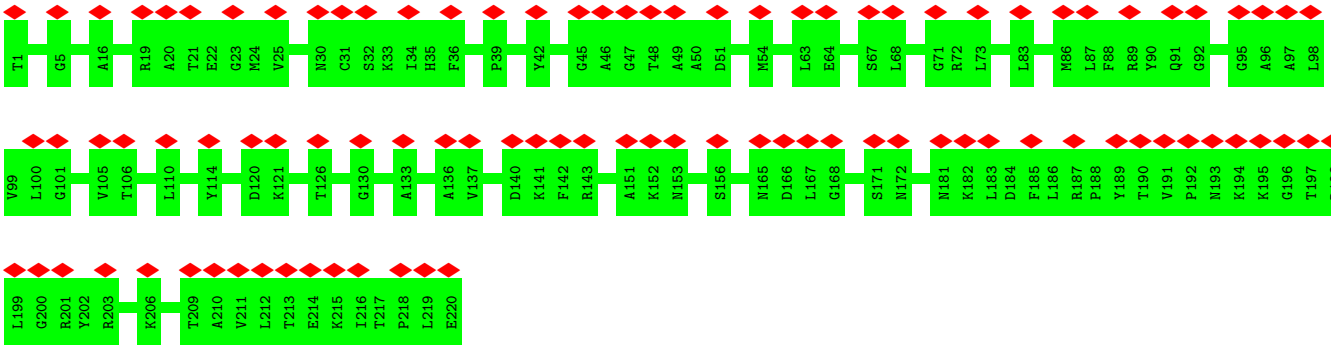






• Molecule 26: Proteasome subunit beta type-7

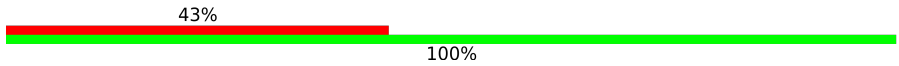
Chain o:

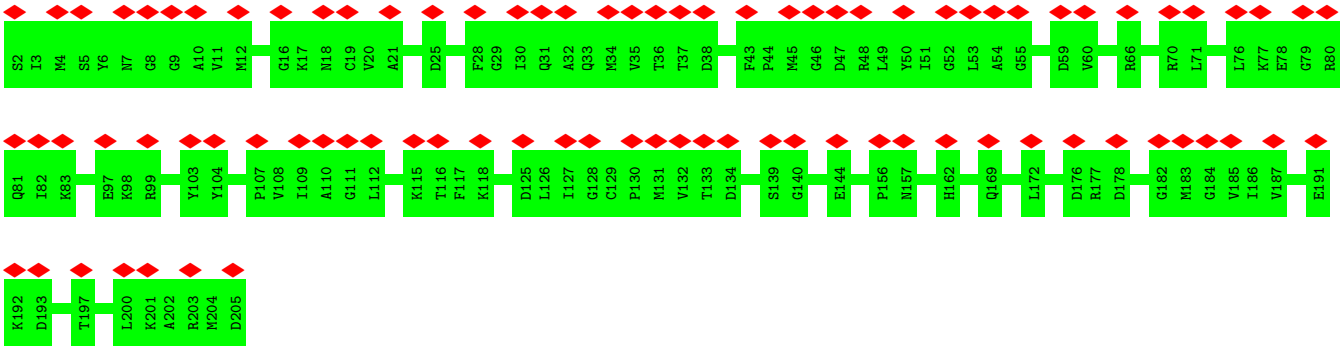



• Molecule 27: Proteasome subunit beta type-3

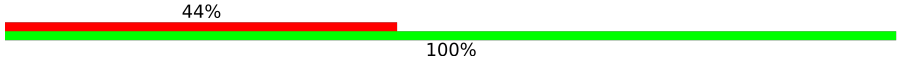
Chain P:

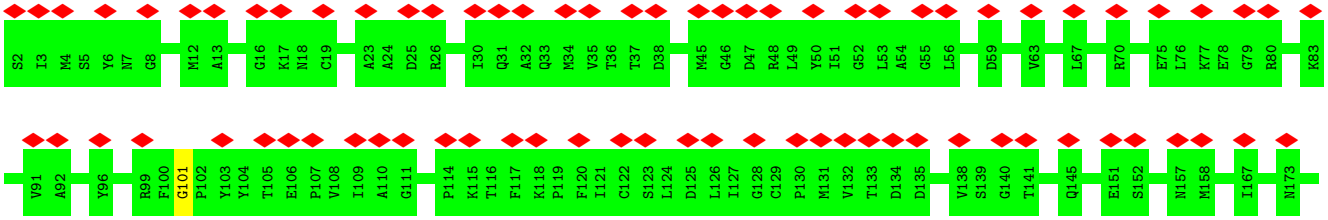


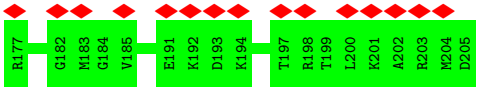




• Molecule 27: Proteasome subunit beta type-3

Chain p:

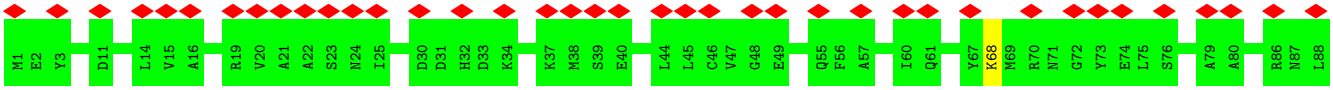


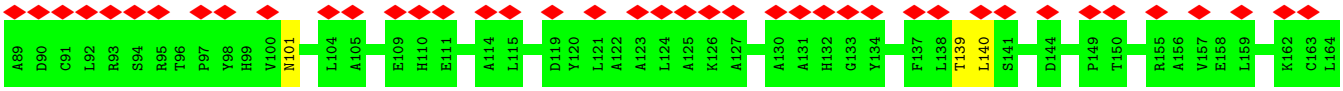



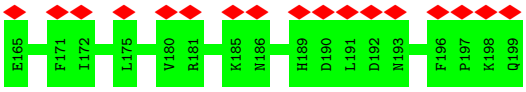



• Molecule 28: Proteasome subunit beta type-2

Chain Q:

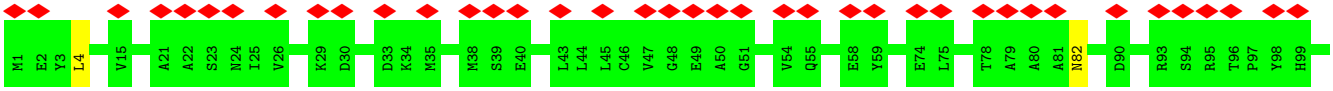



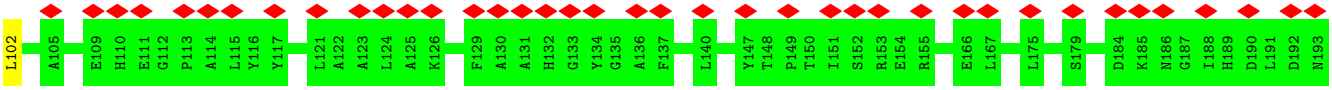




• Molecule 28: Proteasome subunit beta type-2

Chain q:

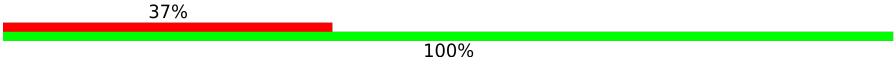



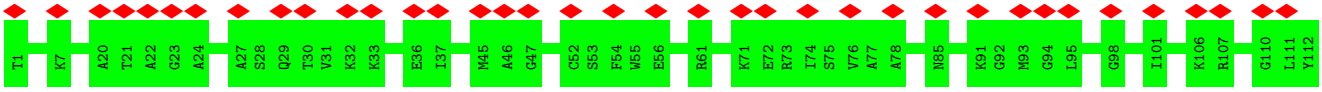



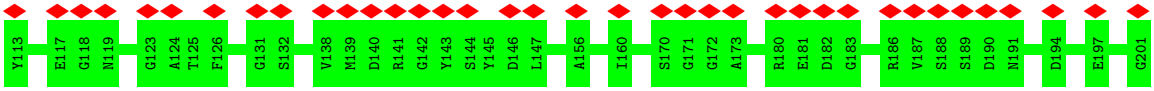


• Molecule 29: Proteasome subunit beta type-5

Chain R:

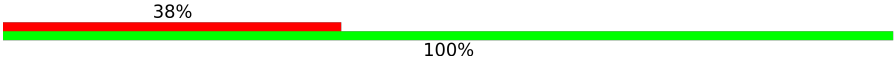


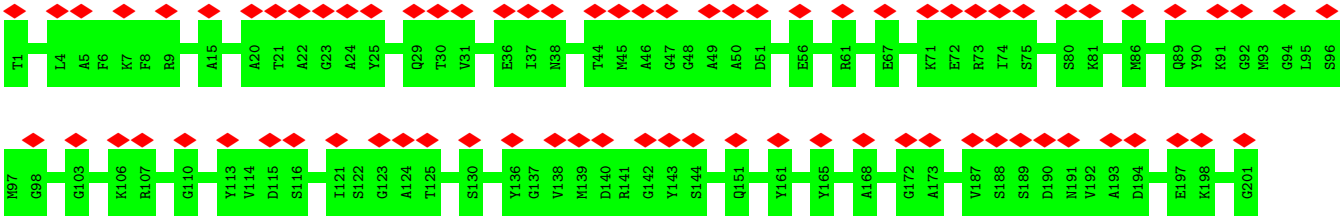



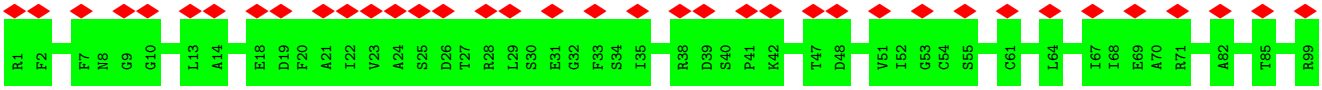

• Molecule 29: Proteasome subunit beta type-5

Chain r:

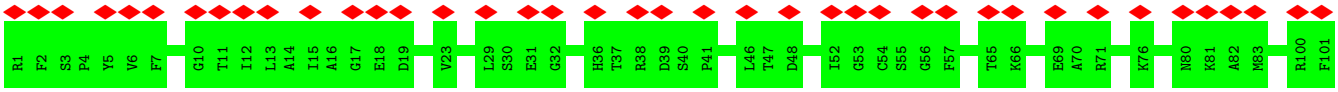




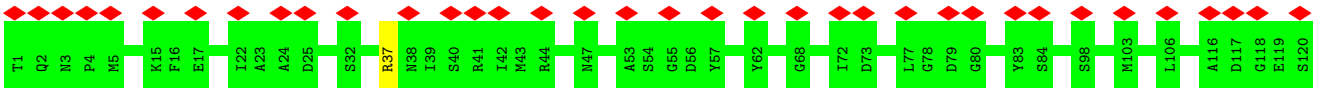

• Molecule 30: Proteasome subunit beta type-1


• Molecule 30: Proteasome subunit beta type-1

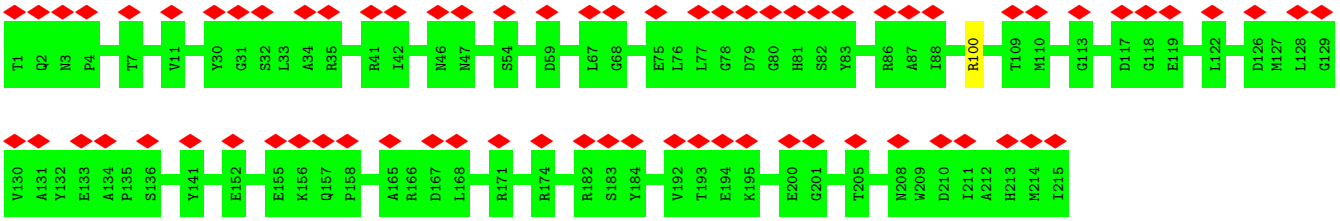




• Molecule 31: Proteasome subunit beta type-4

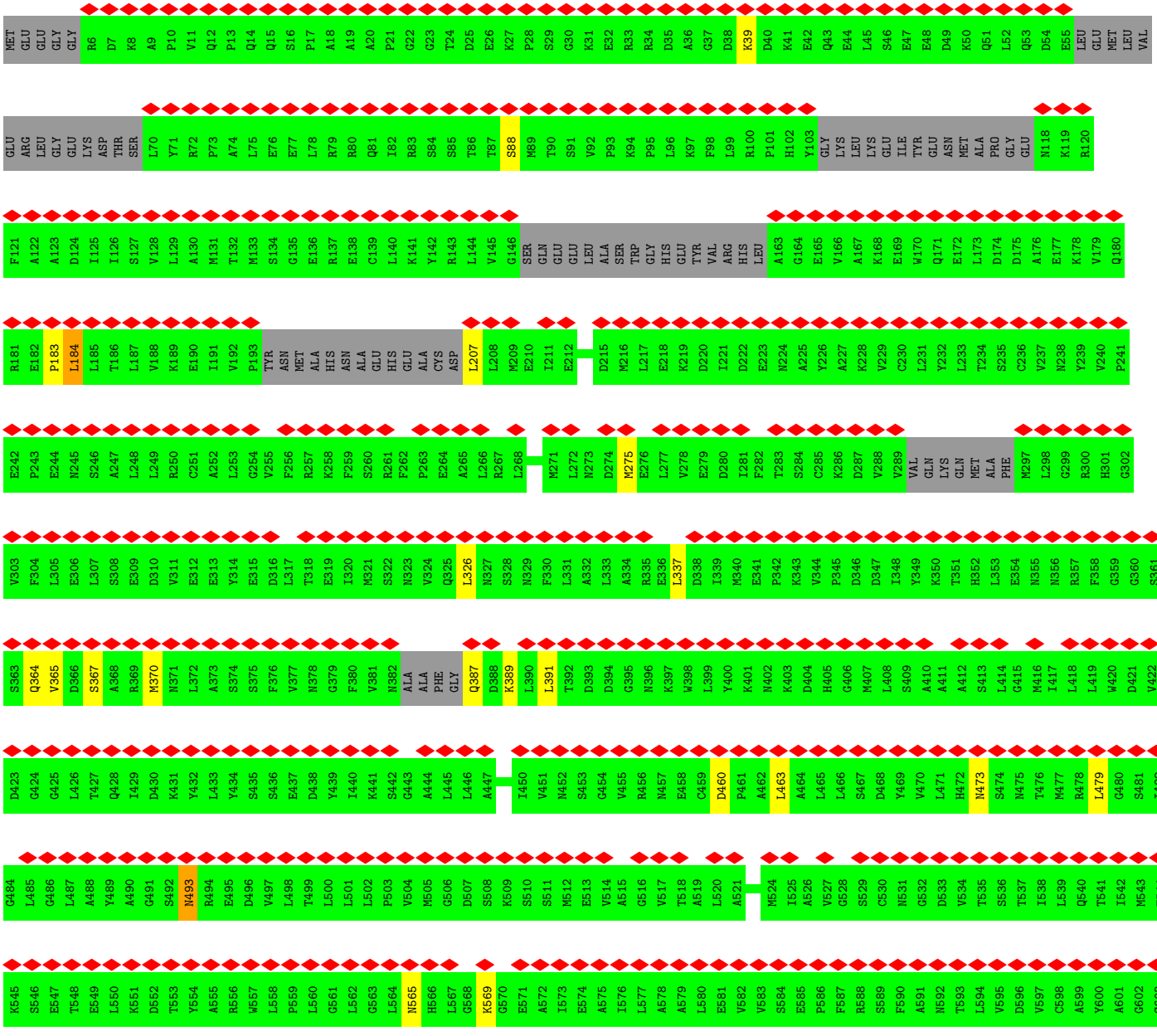

• Molecule 31: Proteasome subunit beta type-4

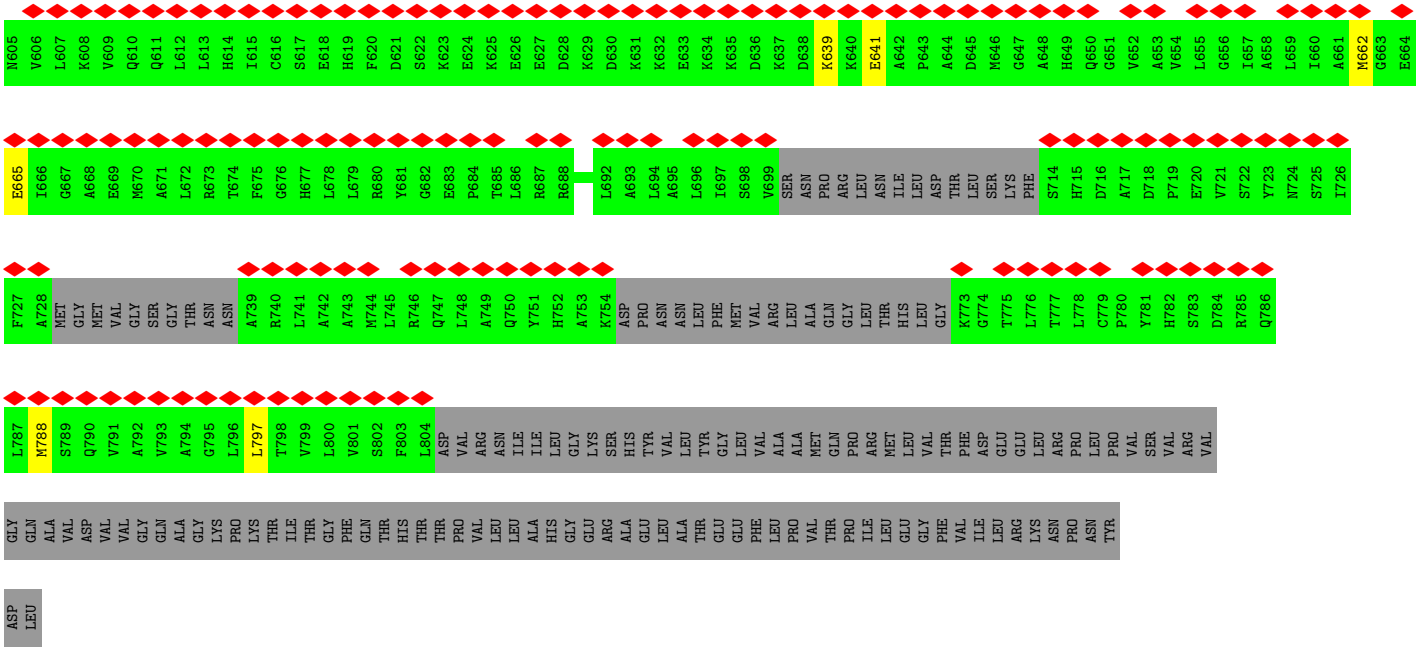
Chain t:


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

Chain f:


N605 V606 L607 K608 V609 Q610 Q611 L612 L613 H614 I615 C616 S617 E618 H619 F620 D621 S622 K623 E624 K625 E626 E627 D628 K629 D630 K631 K632 E633 K634 K635 D636 K637 D638 K639 K640 E641 A642 P643 A644 D645 M646 G647 A648 H649 Q650 G651 V652 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 L692 A693 L694 A695 L696 I697 S698 V699 SER ASN PRO ARG LEU ASN ILE LEU ASP THR LEU SER LYS PHE S714 H715 D716 A717 D718 P719 E720 V721 S722 Y723 N724 S725 I726
F727 A728 MET GLY MET VAL GLY SER GLY THR ASN ASN A739 R740 L741 A742 A743 M744 L745 R746 Q747 L748 A749 Q750 Y751 H752 A753 K754 ASP PRO ASN ASN LEU PHE MET VAL ARG LEU ALA GLN GLY LEU THR HIS LEU GLY 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 ASP VAL ARG ASN ILE ILE LEU GLY LYS SER HIS TYR VAL LEU TYR GLY LEU VAL ALA ALA MET GLN PRO ARG MET LEU VAL THR PHE ASP GLU GLU LEU ARG PRO LEU PRO VAL SER VAL ARG VAL
GLY GLN ALA VAL ASP VAL VAL GLY GLN ALA GLY LYS PRO LYS THR ILE THR GLY PHE GLN THR HIS THR THR PRO VAL LEU LEU ALA HIS GLY GLU ARG ALA GLU LEU ALA THR GLU GLU PHE LEU PRO VAL THR PRO ILE LEU GLU GLY PHE VAL ILE LEU ARG LYS ASN PRO ASN TYR
ASP LEU

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 23567 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TECNAI ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 30 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.009 | Depositor |
| Minimum map value | -0.004 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.004 | Depositor |
| Map size (Å) | 420.0, 420.0, 420.0 | wwPDB |
| Map dimensions | 560, 560, 560 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.75, 0.75, 0.75 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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 | U | 0.23 | 0/6396 | 0.41 | 0/8646 |
| 2 | V | 0.25 | 0/3929 | 0.49 | 0/5309 |
| 3 | W | 0.24 | 0/3751 | 0.46 | 2/5042 (0.0%) |
| 4 | X | 0.23 | 0/1936 | 0.43 | 0/2614 |
| 5 | Y | 0.24 | 0/3173 | 0.45 | 0/4273 |
| 6 | Z | 0.24 | 0/2324 | 0.49 | 0/3150 |
| 7 | a | 0.23 | 0/3051 | 0.43 | 0/4130 |
| 8 | b | 0.25 | 0/1478 | 0.44 | 0/2001 |
| 9 | c | 0.28 | 1/2226 (0.0%) | 0.48 | 0/3007 |
| 10 | d | 0.25 | 0/2162 | 0.50 | 0/2919 |
| 11 | e | 0.24 | 0/338 | 0.47 | 0/450 |
| 12 | A | 0.25 | 0/2885 | 0.48 | 0/3897 |
| 13 | B | 0.26 | 0/2757 | 0.55 | 0/3724 |
| 14 | C | 0.26 | 0/3054 | 0.48 | 0/4107 |
| 15 | D | 0.24 | 0/3090 | 0.46 | 0/4168 |
| 16 | E | 0.24 | 0/2835 | 0.44 | 0/3821 |
| 17 | F | 0.25 | 0/2903 | 0.48 | 0/3912 |
| 18 | G | 0.36 | 0/1858 | 0.59 | 0/2521 |
| 18 | g | 0.33 | 0/1859 | 0.58 | 0/2523 |
| 19 | H | 0.37 | 0/1743 | 0.59 | 0/2372 |
| 19 | h | 0.35 | 0/1743 | 0.59 | 1/2372 (0.0%) |
| 20 | I | 0.36 | 0/1942 | 0.62 | 2/2628 (0.1%) |
| 20 | i | 0.34 | 0/1942 | 0.63 | 3/2628 (0.1%) |
| 21 | J | 0.38 | 0/1728 | 0.60 | 0/2358 |
| 21 | j | 0.34 | 0/1728 | 0.57 | 1/2358 (0.0%) |
| 22 | K | 0.35 | 0/1747 | 0.59 | 0/2364 |
| 22 | k | 0.33 | 0/1747 | 0.60 | 0/2364 |
| 23 | L | 0.37 | 0/1885 | 0.59 | 1/2552 (0.0%) |
| 23 | l | 0.33 | 0/1885 | 0.58 | 0/2552 |
| 24 | M | 0.38 | 0/1891 | 0.58 | 0/2552 |
| 24 | m | 0.34 | 0/1891 | 0.57 | 0/2552 |
| 25 | N | 0.35 | 0/1454 | 0.53 | 0/1967 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 25 | n | 0.35 | 0/1454 | 0.55 | 0/1967 |
| 26 | O | 0.34 | 0/1670 | 0.53 | 0/2265 |
| 26 | o | 0.34 | 0/1670 | 0.53 | 0/2265 |
| 27 | P | 0.35 | 0/1614 | 0.53 | 0/2177 |
| 27 | p | 0.34 | 0/1614 | 0.53 | 0/2177 |
| 28 | Q | 0.38 | 0/1603 | 0.60 | 0/2174 |
| 28 | q | 0.40 | 0/1603 | 0.65 | 1/2174 (0.0%) |
| 29 | R | 0.38 | 0/1579 | 0.52 | 0/2134 |
| 29 | r | 0.36 | 0/1579 | 0.51 | 0/2134 |
| 30 | S | 0.35 | 0/1671 | 0.54 | 0/2253 |
| 30 | s | 0.34 | 0/1671 | 0.55 | 0/2253 |
| 31 | T | 0.37 | 0/1700 | 0.55 | 0/2305 |
| 31 | t | 0.36 | 0/1700 | 0.53 | 0/2305 |
| 32 | f | 0.32 | 0/5393 | 0.68 | 1/7271 (0.0%) |
| All | All | 0.31 | 1/101852 (0.0%) | 0.53 | 12/137687 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | V | 0 | 3 |
| 3 | W | 0 | 1 |
| 5 | Y | 0 | 2 |
| 7 | a | 0 | 1 |
| 10 | d | 0 | 1 |
| 11 | e | 0 | 1 |
| 12 | A | 0 | 1 |
| 13 | B | 0 | 1 |
| 14 | C | 0 | 2 |
| 18 | G | 0 | 1 |
| 19 | H | 0 | 2 |
| 21 | J | 0 | 2 |
| 21 | j | 0 | 1 |
| 22 | K | 0 | 1 |
| 22 | k | 0 | 3 |
| 23 | L | 0 | 2 |
| 23 | l | 0 | 1 |
| 24 | M | 0 | 1 |
| 26 | O | 0 | 1 |
| 27 | p | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 28 | Q | 0 | 2 |
| 28 | q | 0 | 1 |
| 30 | s | 0 | 1 |
| All | All | 0 | 33 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | c | 104 | ARG | C-N | 6.63 | 1.46 | 1.34 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | i | 35 | LEU | CA-CB-CG | 6.85 | 131.05 | 115.30 |
| 19 | h | 231 | ALA | C-N-CA | 5.71 | 135.96 | 121.70 |
| 28 | q | 4 | LEU | CB-CG-CD2 | 5.69 | 120.67 | 111.00 |
| 20 | i | 41 | ASP | CB-CG-OD1 | 5.61 | 123.35 | 118.30 |
| 32 | f | 493 | ASN | N-CA-C | -5.58 | 95.92 | 111.00 |

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | V | 101 | LEU | Peptide |
| 2 | V | 319 | HIS | Peptide |
| 2 | V | 81 | GLN | Peptide |
| 3 | W | 416 | GLN | Peptide |
| 5 | Y | 63 | TRP | Peptide |

## 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 | U | 798/911 (88%) | 735 (92%) | 62 (8%) | 1 (0%) | 51 | 85 |
| 2 | V | 478/480 (100%) | 413 (86%) | 59 (12%) | 6 (1%) | 12 | 48 |
| 3 | W | 454/456 (100%) | 406 (89%) | 45 (10%) | 3 (1%) | 22 | 62 |
| 4 | X | 239/380 (63%) | 213 (89%) | 26 (11%) | 0 | 100 | 100 |
| 5 | Y | 376/378 (100%) | 333 (89%) | 38 (10%) | 5 (1%) | 12 | 48 |
| 6 | Z | 284/286 (99%) | 253 (89%) | 30 (11%) | 1 (0%) | 34 | 72 |
| 7 | a | 371/373 (100%) | 331 (89%) | 38 (10%) | 2 (0%) | 29 | 69 |
| 8 | b | 189/191 (99%) | 174 (92%) | 15 (8%) | 0 | 100 | 100 |
| 9 | c | 274/287 (96%) | 242 (88%) | 28 (10%) | 4 (2%) | 10 | 45 |
| 10 | d | 255/257 (99%) | 227 (89%) | 27 (11%) | 1 (0%) | 34 | 72 |
| 11 | e | 36/70 (51%) | 30 (83%) | 6 (17%) | 0 | 100 | 100 |
| 12 | A | 359/361 (99%) | 312 (87%) | 43 (12%) | 4 (1%) | 14 | 51 |
| 13 | B | 346/348 (99%) | 295 (85%) | 46 (13%) | 5 (1%) | 11 | 46 |
| 14 | C | 382/384 (100%) | 339 (89%) | 41 (11%) | 2 (0%) | 29 | 69 |
| 15 | D | 378/380 (100%) | 333 (88%) | 44 (12%) | 1 (0%) | 41 | 76 |
| 16 | E | 351/353 (99%) | 321 (92%) | 29 (8%) | 1 (0%) | 41 | 76 |
| 17 | F | 362/377 (96%) | 322 (89%) | 38 (10%) | 2 (1%) | 25 | 66 |
| 18 | G | 238/240 (99%) | 224 (94%) | 14 (6%) | 0 | 100 | 100 |
| 18 | g | 238/240 (99%) | 226 (95%) | 12 (5%) | 0 | 100 | 100 |
| 19 | H | 230/232 (99%) | 213 (93%) | 17 (7%) | 0 | 100 | 100 |
| 19 | h | 230/232 (99%) | 215 (94%) | 15 (6%) | 0 | 100 | 100 |
| 20 | I | 248/250 (99%) | 236 (95%) | 12 (5%) | 0 | 100 | 100 |
| 20 | i | 248/250 (99%) | 228 (92%) | 20 (8%) | 0 | 100 | 100 |
| 21 | J | 237/243 (98%) | 216 (91%) | 20 (8%) | 1 (0%) | 34 | 72 |
| 21 | j | 237/243 (98%) | 222 (94%) | 15 (6%) | 0 | 100 | 100 |
| 22 | K | 224/234 (96%) | 205 (92%) | 19 (8%) | 0 | 100 | 100 |
| 22 | k | 224/234 (96%) | 203 (91%) | 18 (8%) | 3 (1%) | 12 | 48 |
| 23 | L | 236/238 (99%) | 224 (95%) | 12 (5%) | 0 | 100 | 100 |
| 23 | l | 236/238 (99%) | 222 (94%) | 14 (6%) | 0 | 100 | 100 |
| 24 | M | 238/245 (97%) | 221 (93%) | 17 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 24 | m | 238/245 (97%) | 220 (92%) | 18 (8%) | 0 | 100 | 100 |
| 25 | N | 189/191 (99%) | 179 (95%) | 10 (5%) | 0 | 100 | 100 |
| 25 | n | 189/191 (99%) | 181 (96%) | 8 (4%) | 0 | 100 | 100 |
| 26 | O | 218/220 (99%) | 210 (96%) | 8 (4%) | 0 | 100 | 100 |
| 26 | o | 218/220 (99%) | 211 (97%) | 7 (3%) | 0 | 100 | 100 |
| 27 | P | 202/204 (99%) | 194 (96%) | 8 (4%) | 0 | 100 | 100 |
| 27 | p | 202/204 (99%) | 186 (92%) | 16 (8%) | 0 | 100 | 100 |
| 28 | Q | 197/199 (99%) | 179 (91%) | 18 (9%) | 0 | 100 | 100 |
| 28 | q | 197/199 (99%) | 177 (90%) | 20 (10%) | 0 | 100 | 100 |
| 29 | R | 199/201 (99%) | 189 (95%) | 10 (5%) | 0 | 100 | 100 |
| 29 | r | 199/201 (99%) | 191 (96%) | 8 (4%) | 0 | 100 | 100 |
| 30 | S | 211/213 (99%) | 203 (96%) | 8 (4%) | 0 | 100 | 100 |
| 30 | s | 211/213 (99%) | 201 (95%) | 10 (5%) | 0 | 100 | 100 |
| 31 | T | 213/215 (99%) | 204 (96%) | 9 (4%) | 0 | 100 | 100 |
| 31 | t | 213/215 (99%) | 201 (94%) | 12 (6%) | 0 | 100 | 100 |
| 32 | f | 669/908 (74%) | 579 (86%) | 82 (12%) | 8 (1%) | 13 | 49 |
| All | All | 12761/13430 (95%) | 11639 (91%) | 1072 (8%) | 50 (0%) | 38 | 72 |

5 of 50 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | U | 364 | VAL |
| 2 | V | 82 | LEU |
| 2 | V | 83 | GLU |
| 2 | V | 84 | LYS |
| 3 | W | 68 | VAL |

### 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 | U | 685/779 (88%) | 681 (99%) | 4 (1%) | 86 92 |
| 2 | V | 414/414 (100%) | 406 (98%) | 8 (2%) | 57 75 |
| 3 | W | 416/416 (100%) | 410 (99%) | 6 (1%) | 67 80 |
| 4 | X | 208/327 (64%) | 207 (100%) | 1 (0%) | 88 93 |
| 5 | Y | 334/334 (100%) | 332 (99%) | 2 (1%) | 86 92 |
| 6 | Z | 257/257 (100%) | 252 (98%) | 5 (2%) | 57 75 |
| 7 | a | 333/333 (100%) | 331 (99%) | 2 (1%) | 86 92 |
| 8 | b | 167/167 (100%) | 165 (99%) | 2 (1%) | 71 83 |
| 9 | c | 243/252 (96%) | 240 (99%) | 3 (1%) | 71 83 |
| 10 | d | 231/231 (100%) | 229 (99%) | 2 (1%) | 78 87 |
| 11 | e | 38/63 (60%) | 36 (95%) | 2 (5%) | 22 47 |
| 12 | A | 308/308 (100%) | 303 (98%) | 5 (2%) | 62 79 |
| 13 | B | 304/304 (100%) | 295 (97%) | 9 (3%) | 41 63 |
| 14 | C | 332/332 (100%) | 321 (97%) | 11 (3%) | 38 61 |
| 15 | D | 333/333 (100%) | 330 (99%) | 3 (1%) | 78 87 |
| 16 | E | 308/308 (100%) | 306 (99%) | 2 (1%) | 86 92 |
| 17 | F | 312/321 (97%) | 306 (98%) | 6 (2%) | 57 75 |
| 18 | G | 192/205 (94%) | 192 (100%) | 0 | 100 100 |
| 18 | g | 193/205 (94%) | 193 (100%) | 0 | 100 100 |
| 19 | H | 164/190 (86%) | 164 (100%) | 0 | 100 100 |
| 19 | h | 164/190 (86%) | 164 (100%) | 0 | 100 100 |
| 20 | I | 193/210 (92%) | 193 (100%) | 0 | 100 100 |
| 20 | i | 193/210 (92%) | 193 (100%) | 0 | 100 100 |
| 21 | J | 152/207 (73%) | 152 (100%) | 0 | 100 100 |
| 21 | j | 152/207 (73%) | 152 (100%) | 0 | 100 100 |
| 22 | K | 186/196 (95%) | 183 (98%) | 3 (2%) | 62 79 |
| 22 | k | 186/196 (95%) | 182 (98%) | 4 (2%) | 52 71 |
| 23 | L | 198/204 (97%) | 196 (99%) | 2 (1%) | 76 86 |
| 23 | l | 198/204 (97%) | 198 (100%) | 0 | 100 100 |
| 24 | M | 192/202 (95%) | 191 (100%) | 1 (0%) | 88 93 |
| 24 | m | 192/202 (95%) | 190 (99%) | 2 (1%) | 76 86 |
| 25 | N | 148/148 (100%) | 148 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 25 | n | 148/148 (100%) | 147 (99%) | 1 (1%) | 84 90 |
| 26 | O | 177/181 (98%) | 177 (100%) | 0 | 100 100 |
| 26 | o | 177/181 (98%) | 177 (100%) | 0 | 100 100 |
| 27 | P | 172/173 (99%) | 172 (100%) | 0 | 100 100 |
| 27 | p | 172/173 (99%) | 172 (100%) | 0 | 100 100 |
| 28 | Q | 164/170 (96%) | 162 (99%) | 2 (1%) | 71 83 |
| 28 | q | 164/170 (96%) | 163 (99%) | 1 (1%) | 86 92 |
| 29 | R | 153/156 (98%) | 153 (100%) | 0 | 100 100 |
| 29 | r | 153/156 (98%) | 153 (100%) | 0 | 100 100 |
| 30 | S | 174/178 (98%) | 174 (100%) | 0 | 100 100 |
| 30 | s | 174/178 (98%) | 174 (100%) | 0 | 100 100 |
| 31 | T | 175/178 (98%) | 173 (99%) | 2 (1%) | 73 84 |
| 31 | t | 175/178 (98%) | 174 (99%) | 1 (1%) | 86 92 |
| 32 | f | 580/763 (76%) | 559 (96%) | 21 (4%) | 35 59 |
| All | All | 10684/11438 (93%) | 10571 (99%) | 113 (1%) | 74 84 |

5 of 113 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | C | 235 | PHE |
| 32 | f | 662 | MET |
| 17 | F | 282 | ILE |
| 32 | f | 641 | GLU |
| 32 | f | 389 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | D | 302 | ASN |
| 20 | I | 95 | GLN |
| 31 | t | 81 | HIS |
| 15 | D | 412 | GLN |
| 17 | F | 323 | ASN |

#### 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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

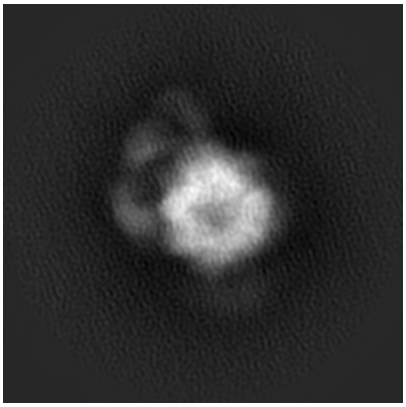
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8668. 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.

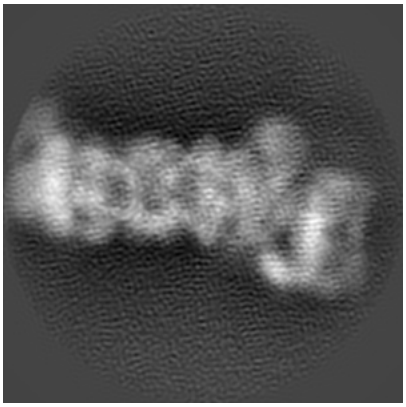
## 6.1 Orthogonal projections

### 6.1.1 Primary map



X

Y

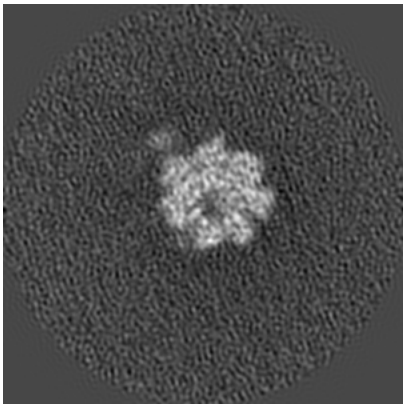


Z

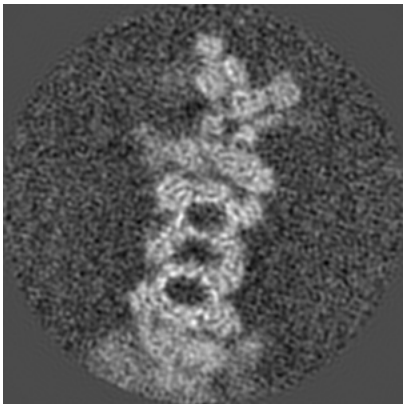
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

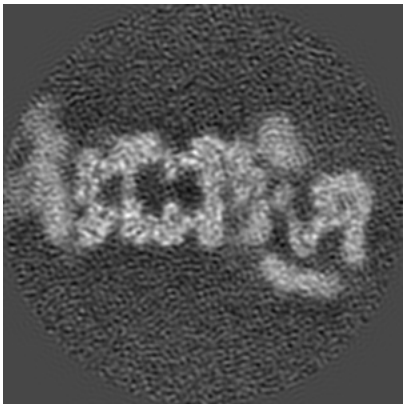
### 6.2.1 Primary map



X Index: 280



Y Index: 280

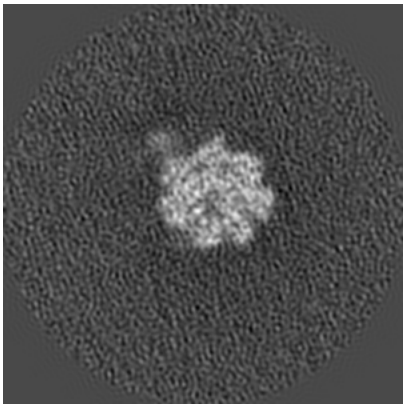


Z Index: 280

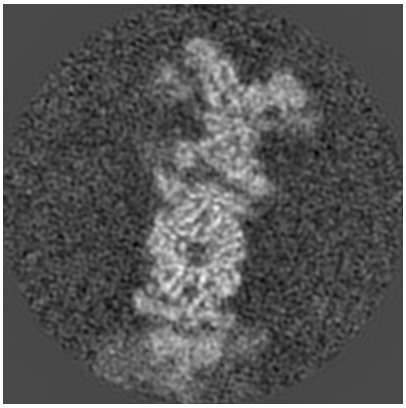
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

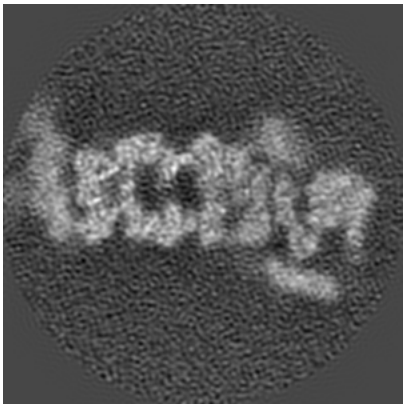
### 6.3.1 Primary map



X Index: 282



Y Index: 264



Z Index: 286

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 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

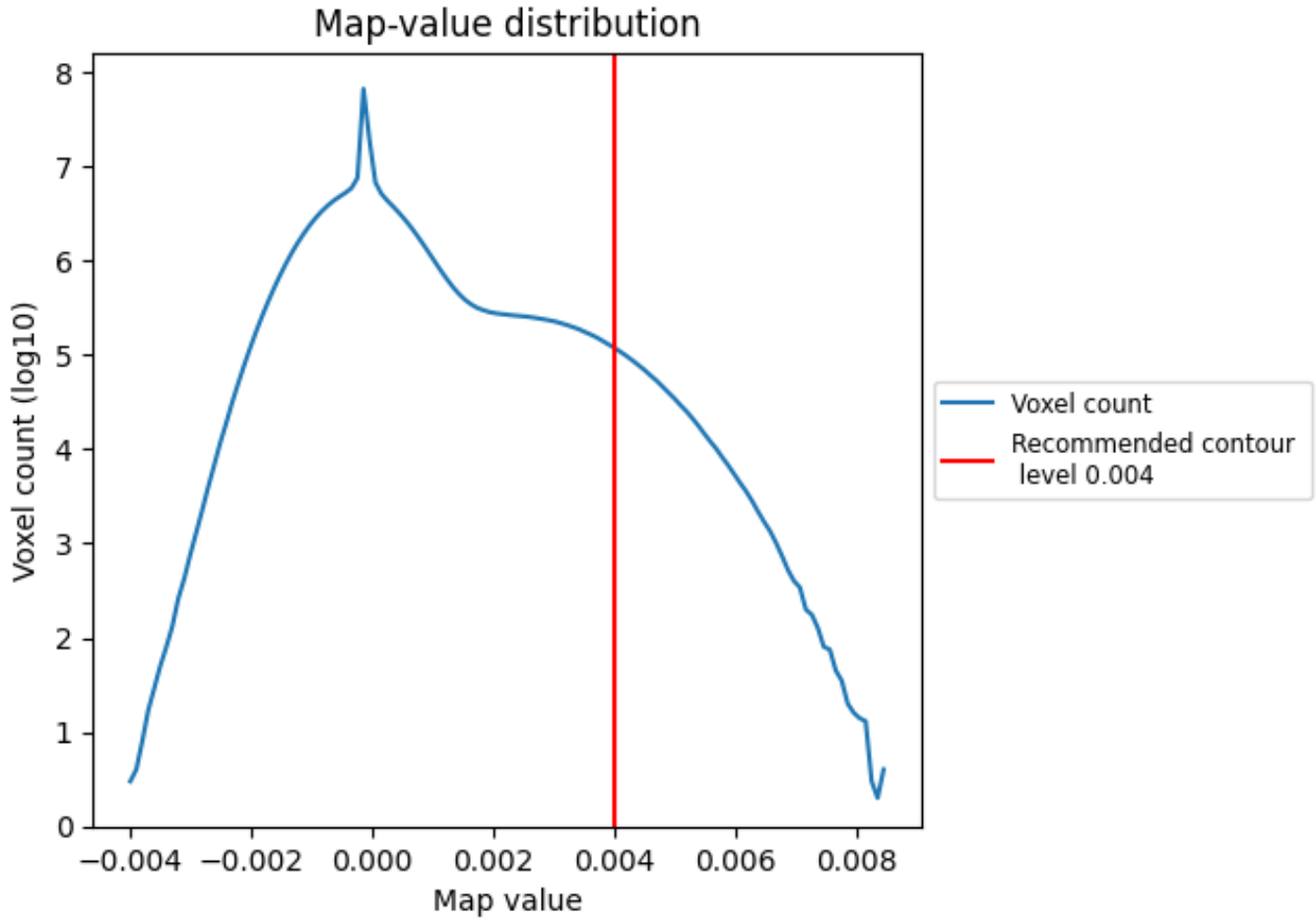
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

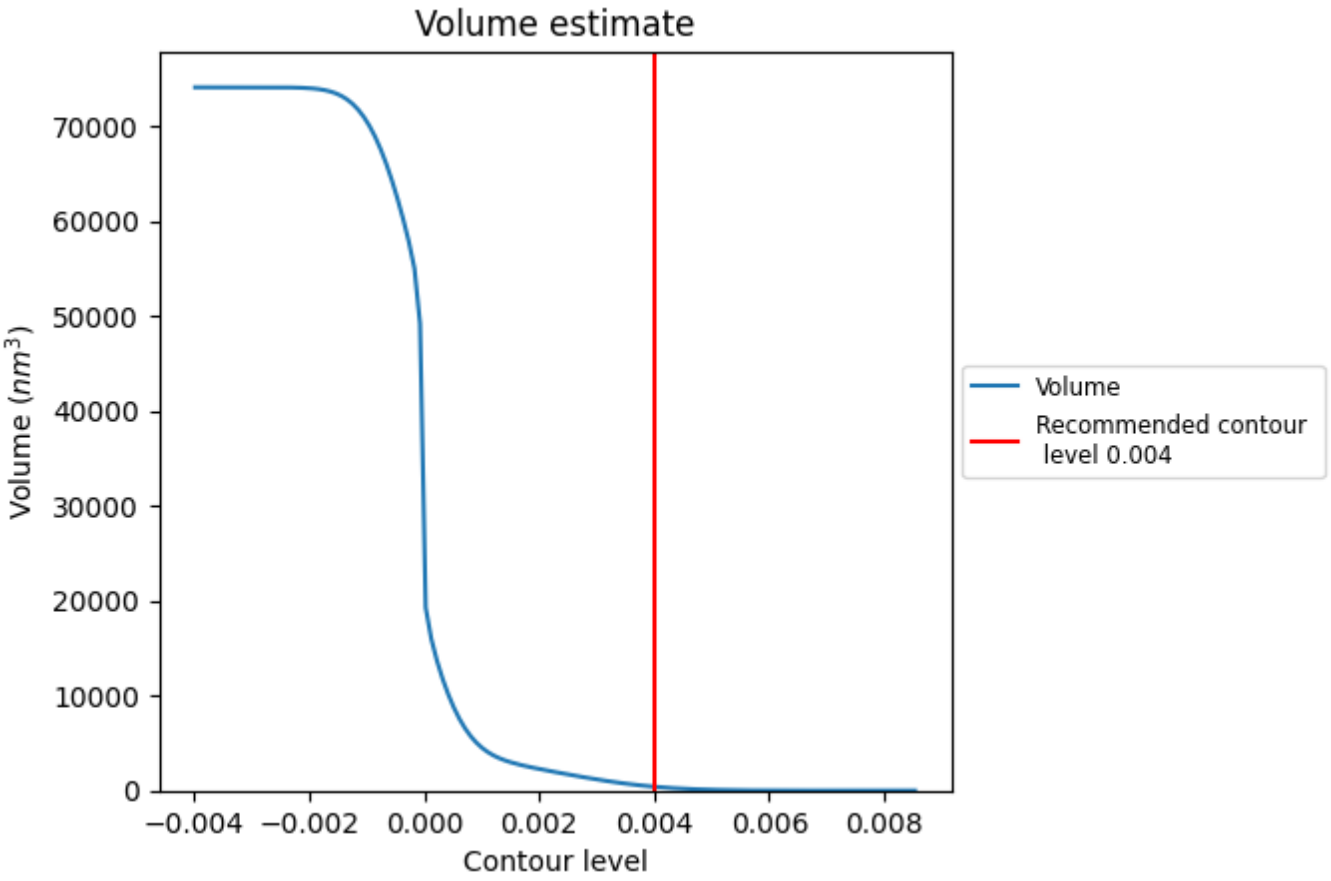
This section contains the results of statistical analysis of the map.

## 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.

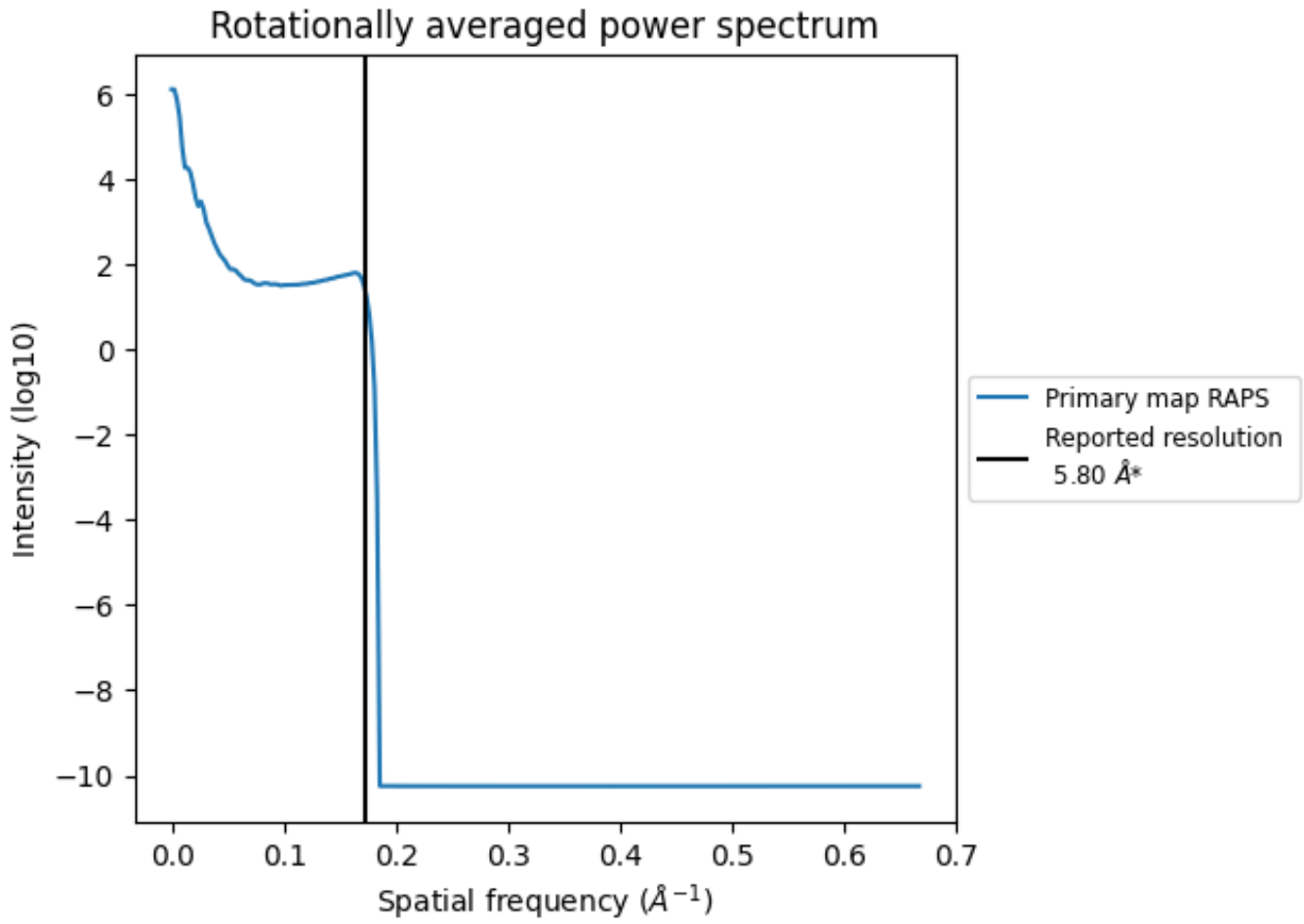
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 405 $nm^3$; this corresponds to an approximate mass of 366 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 0.172 Å$^{-1}$

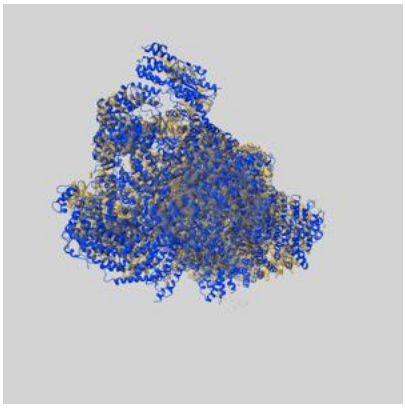
# 8 Fourier-Shell correlation (i)

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

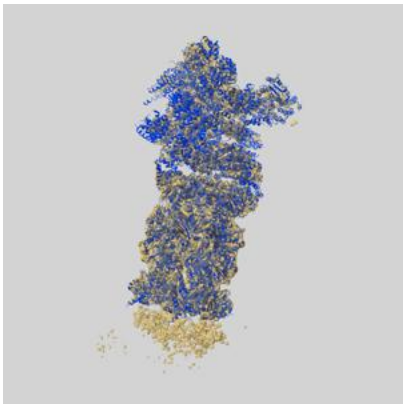
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8668 and PDB model 5VFU. Per-residue inclusion information can be found in section 3 on page 11.

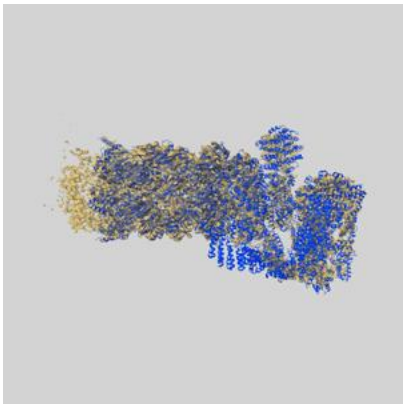
## 9.1 Map-model overlay



X



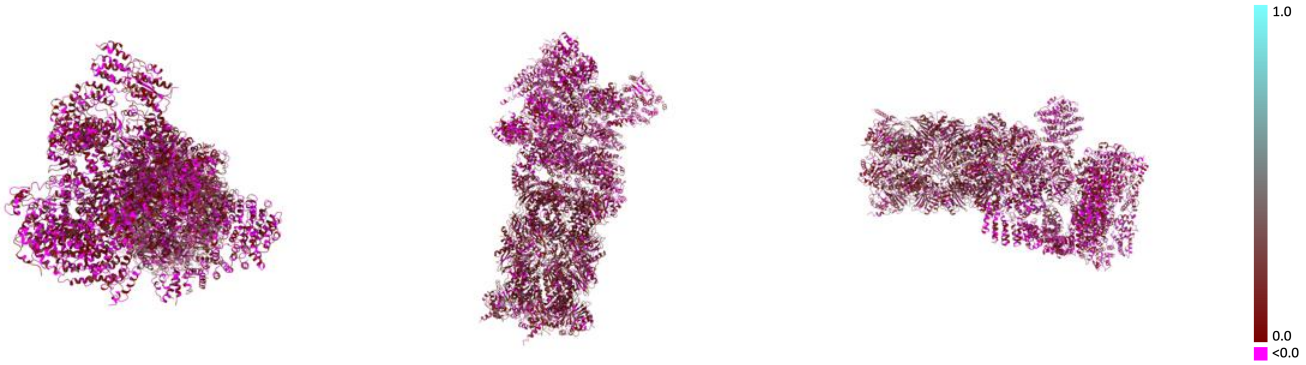
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

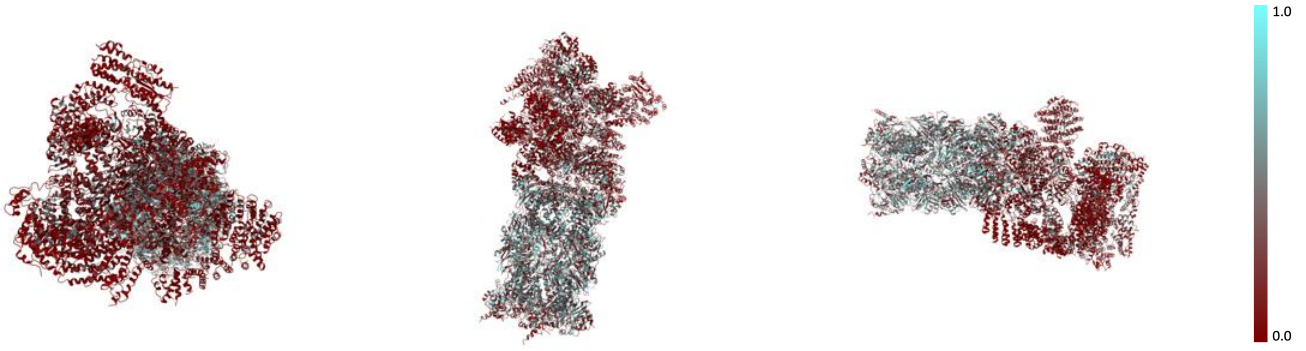
## 9.2 Q-score mapped to coordinate model




X Y Z

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

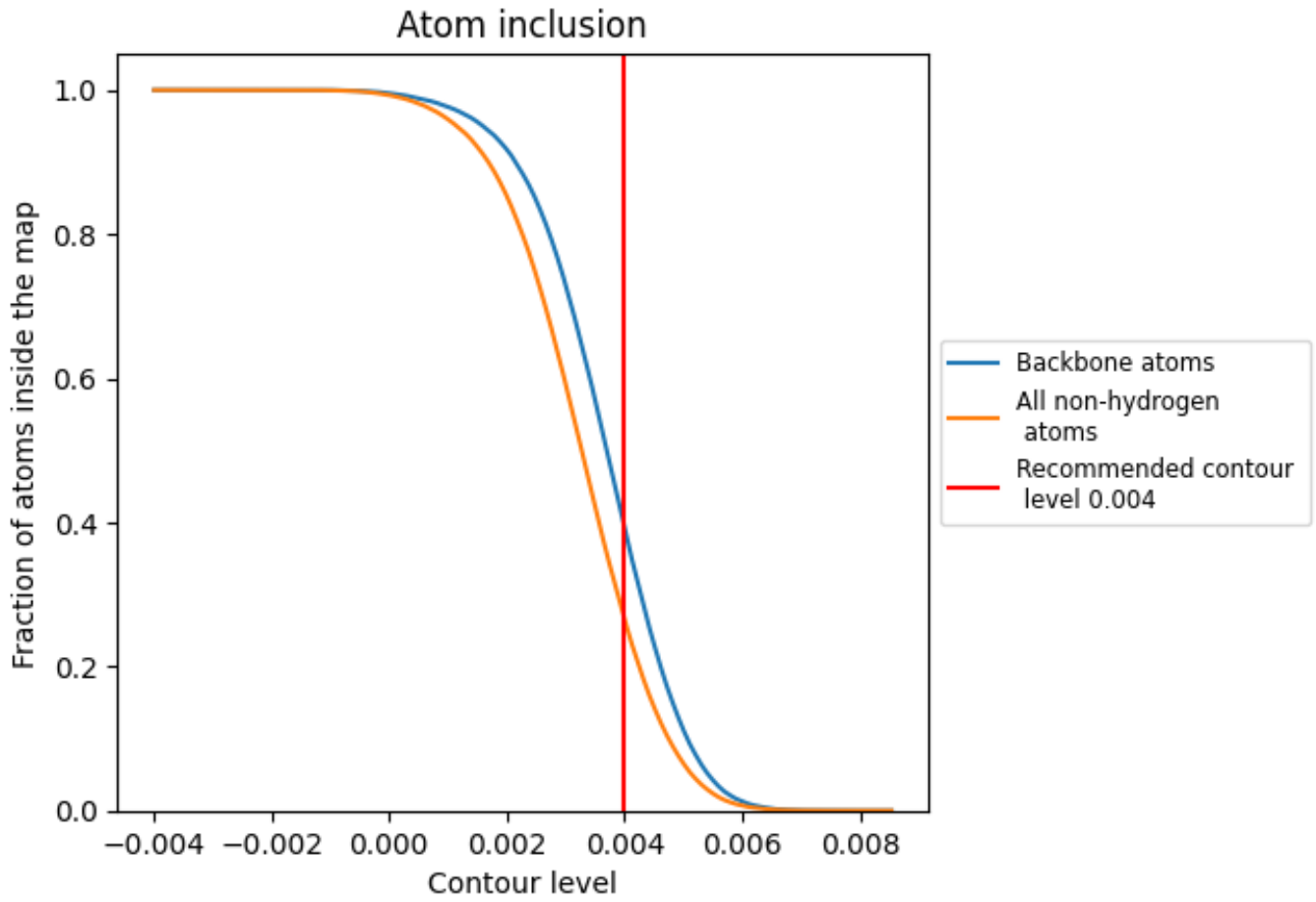
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

## 9.4 Atom inclusion (i)




At the recommended contour level, 39% of all backbone atoms, 27% 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 (0.004) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.2657 | 0.0980 |
| A | 0.2199 | 0.0990 |
| B | 0.1392 | 0.0780 |
| C | 0.1391 | 0.0700 |
| D | 0.1580 | 0.0620 |
| E | 0.1749 | 0.0740 |
| F | 0.1897 | 0.0820 |
| G | 0.3343 | 0.1230 |
| H | 0.3594 | 0.1240 |
| I | 0.3244 | 0.1260 |
| J | 0.3836 | 0.1400 |
| K | 0.3605 | 0.1350 |
| L | 0.4079 | 0.1320 |
| M | 0.3726 | 0.1270 |
| N | 0.4328 | 0.1320 |
| O | 0.4281 | 0.1470 |
| P | 0.4557 | 0.1280 |
| Q | 0.4326 | 0.1480 |
| R | 0.4853 | 0.1440 |
| S | 0.4386 | 0.1460 |
| T | 0.4966 | 0.1530 |
| U | 0.2193 | 0.0670 |
| V | 0.1151 | 0.0620 |
| W | 0.0592 | 0.0590 |
| X | 0.0577 | 0.0180 |
| Y | 0.1646 | 0.0630 |
| Z | 0.1761 | 0.0760 |
| a | 0.0835 | 0.0600 |
| b | 0.0791 | 0.0550 |
| c | 0.2015 | 0.0920 |
| d | 0.0785 | 0.0290 |
| e | 0.0606 | 0.0310 |
| f | 0.0637 | 0.0400 |
| g | 0.3653 | 0.1320 |
| h | 0.3975 | 0.1420 |


*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| i | 0.3314 | 0.1280 |
| j | 0.3487 | 0.1290 |
| k | 0.3652 | 0.1410 |
| l | 0.4023 | 0.1280 |
| m | 0.3610 | 0.1150 |
| n | 0.4621 | 0.1440 |
| o | 0.4442 | 0.1520 |
| p | 0.4519 | 0.1350 |
| q | 0.4456 | 0.1370 |
| r | 0.4673 | 0.1380 |
| s | 0.4492 | 0.1400 |
| t | 0.4978 | 0.1630 |