# wwPDB EM Validation Summary Report (i)

Nov 2, 2024 – 03:39 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 5VFP |
| EMDB ID | : | EMD-8663 |
| 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 | : | 4.20 Å(reported) |

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

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

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

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

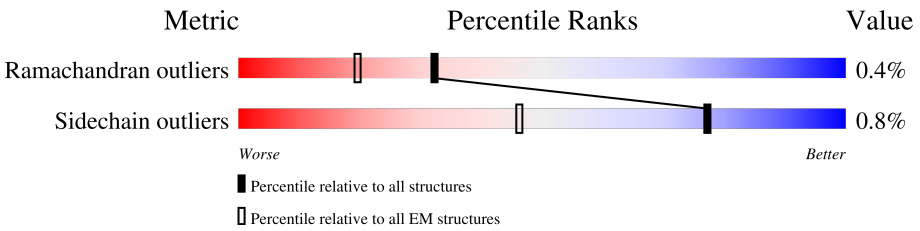
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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 | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 | G | 240 | 25% 99% |
| 1 | g | 240 | 40% 100% |
| 2 | H | 232 | 26% 98% |
| 2 | h | 232 | 42% 100% |
| 3 | I | 250 | 42% 98% |
| 3 | i | 250 | 49% 99% |
| 4 | J | 243 | 46% 97% |
| 4 | j | 243 | 42% 98% |
| 5 | K | 234 | 41% 94% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | k | 234 | 37% 97% |
| 6 | L | 238 | 29% 100% |
| 6 | l | 238 | 32% 100% |
| 7 | M | 245 | 29% 97% |
| 7 | m | 245 | 41% 98% |
| 8 | N | 191 | 13% 99% |
| 8 | n | 191 | 12% 98% |
| 9 | O | 220 | 22% 100% |
| 9 | o | 220 | 25% 100% |
| 10 | P | 204 | 15% 100% |
| 10 | p | 204 | 16% 100% |
| 11 | Q | 199 | 27% 100% |
| 11 | q | 199 | 19% 99% |
| 12 | R | 201 | 17% 100% |
| 12 | r | 201 | 13% 100% |
| 13 | S | 213 | 23% 100% |
| 13 | s | 213 | 19% 100% |
| 14 | T | 215 | 14% 100% |
| 14 | t | 215 | 16% 100% |
| 15 | U | 911 | 59% 87% 12% |
| 16 | V | 480 | 81% 96% |
| 17 | W | 456 | 74% 98% |
| 18 | Y | 378 | 63% 98% |
| 19 | Z | 286 | 72% 97% |
| 20 | a | 373 | 80% 98% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 21 | b | 191 | 87% 98% |
| 22 | c | 287 | 63% 96% |
| 23 | d | 257 | 90% 98% |
| 24 | e | 70 | 51% 56% 43% |
| 25 | X | 380 | 72% 98% |
| 26 | A | 399 | 58% 93% 5% |
| 27 | B | 389 | 71% 93% 5% |
| 28 | C | 392 | 67% 90% 7% |
| 29 | D | 380 | 72% 96% |
| 30 | E | 375 | 61% 98% |
| 31 | F | 396 | 56% 93% 5% |
| 32 | f | 908 | 68% 73% 24% |

# 2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 101342 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 | G | 239 | 1820 | 1157 | 304 | 346 | 13 | 0 | 0 |
| 1 | g | 240 | 1826 | 1160 | 305 | 348 | 13 | 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 | H | 230 | 1688 | 1070 | 284 | 329 | 5 | 0 | 0 |
| 2 | h | 232 | 1708 | 1081 | 289 | 333 | 5 | 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 | I | 248 | 1895 | 1195 | 324 | 368 | 8 | 0 | 0 |
| 3 | i | 250 | 1912 | 1204 | 329 | 371 | 8 | 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 | J | 239 | 1704 | 1056 | 308 | 335 | 5 | 0 | 0 |
| 4 | j | 239 | 1704 | 1056 | 308 | 335 | 5 | 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 | K | 228 | 1729 | 1086 | 284 | 349 | 10 | 0 | 0 |
| 5 | k | 228 | 1722 | 1080 | 284 | 348 | 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 | L | 238 | 1850 | 1159 | 334 | 346 | 11 | 0 | 0 |
| 6 | l | 238 | 1850 | 1159 | 334 | 346 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | M | 240 | 1856 | 1178 | 314 | 353 | 11 | 0 | 0 |
| 7 | m | 240 | 1856 | 1178 | 314 | 353 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | N | 191 | 1430 | 893 | 245 | 280 | 12 | 0 | 0 |
| 8 | n | 191 | 1430 | 893 | 245 | 280 | 12 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | O | 220 | 1643 | 1033 | 280 | 318 | 12 | 0 | 0 |
| 9 | o | 220 | 1643 | 1033 | 280 | 318 | 12 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | P | 204 | 1585 | 1010 | 262 | 294 | 19 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | p | 204 | 1585 | 1010 | 262 | 294 | 19 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | Q | 199 | 1570 | 1006 | 265 | 290 | 9 | 0 | 0 |
| 11 | q | 199 | 1570 | 1006 | 265 | 290 | 9 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | R | 201 | 1548 | 974 | 273 | 292 | 9 | 0 | 0 |
| 12 | r | 201 | 1548 | 974 | 273 | 292 | 9 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | S | 213 | 1641 | 1036 | 282 | 313 | 10 | 0 | 0 |
| 13 | s | 213 | 1641 | 1036 | 282 | 313 | 10 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | T | 215 | 1667 | 1052 | 285 | 318 | 12 | 0 | 0 |
| 14 | t | 215 | 1667 | 1052 | 285 | 318 | 12 | 0 | 0 |

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | U | 806 | 6287 | 3990 | 1075 | 1178 | 44 | 0 | 0 |

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | V | 473 | 3808 | 2418 | 676 | 700 | 14 | 0 | 0 |

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | W | 456 | 3703 | 2339 | 635 | 704 | 25 | 0 | 0 |

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | Y | 378 | 3115 | 1987 | 533 | 578 | 17 | 0 | 0 |

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | Z | 286 | 2281 | 1457 | 392 | 427 | 5 | 0 | 0 |

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | a | 373 | 2995 | 1911 | 510 | 559 | 15 | 0 | 0 |

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | b | 191 | 1458 | 910 | 261 | 279 | 8 | 0 | 0 |

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | c | 278 | 2187 | 1389 | 374 | 406 | 18 | 0 | 0 |

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | d | 257 | 2116 | 1371 | 346 | 390 | 9 | 0 | 0 |

- Molecule 24 is a protein called sem1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | e | 40 | 334 | 200 | 55 | 77 | 2 | 0 | 0 |

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | X | 380 | 3009 | 1918 | 509 | 570 | 12 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | A | 380 | 2893 | 1817 | 515 | 543 | 18 | 0 | 0 |

- Molecule 27 is a protein called 26S proteasome regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | B | 370 | 2806 | 1763 | 478 | 553 | 12 | 0 | 0 |

- Molecule 28 is a protein called 26S proteasome regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | C | 363 | 2859 | 1804 | 513 | 525 | 17 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | D | 380 | 3040 | 1923 | 524 | 580 | 13 | 0 | 0 |

- Molecule 30 is a protein called 26S proteasome regulatory subunit 10B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | E | 375 | 2860 | 1796 | 512 | 536 | 16 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | F | 376 | 2859 | 1802 | 496 | 546 | 15 | 0 | 0 |

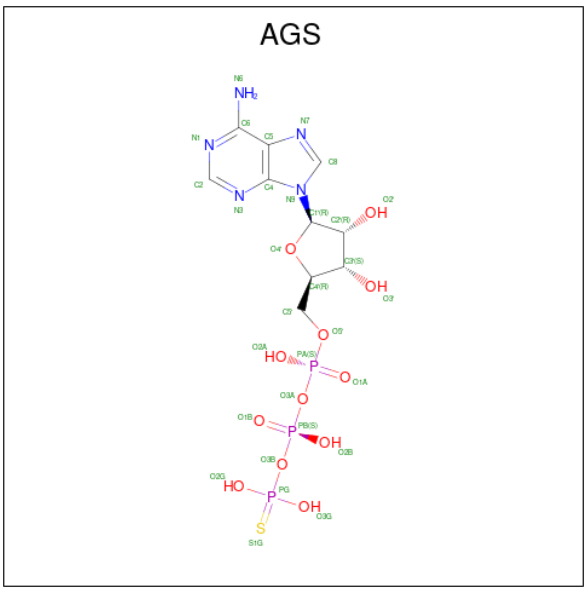
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

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

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

- Molecule 34 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | |
| 34 | A | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 |

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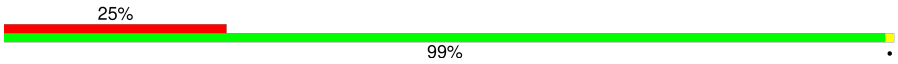
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | |
| 34 | D | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 |
| | | | Total | C | N | O | P | S | |
| 34 | E | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 |
| | | | Total | C | N | O | P | S | |
| 34 | F | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 |

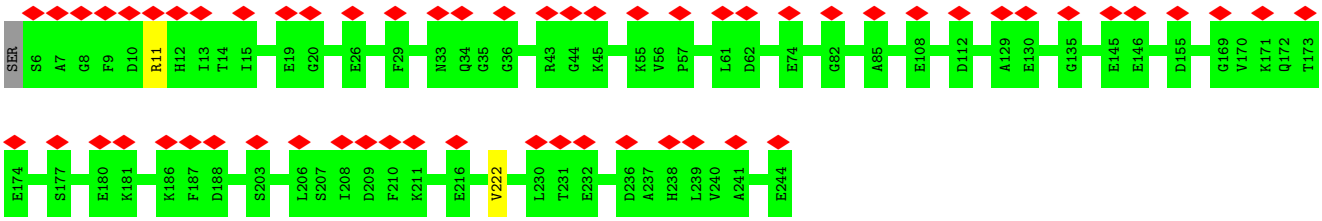
# 3 Residue-property plots (i)

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

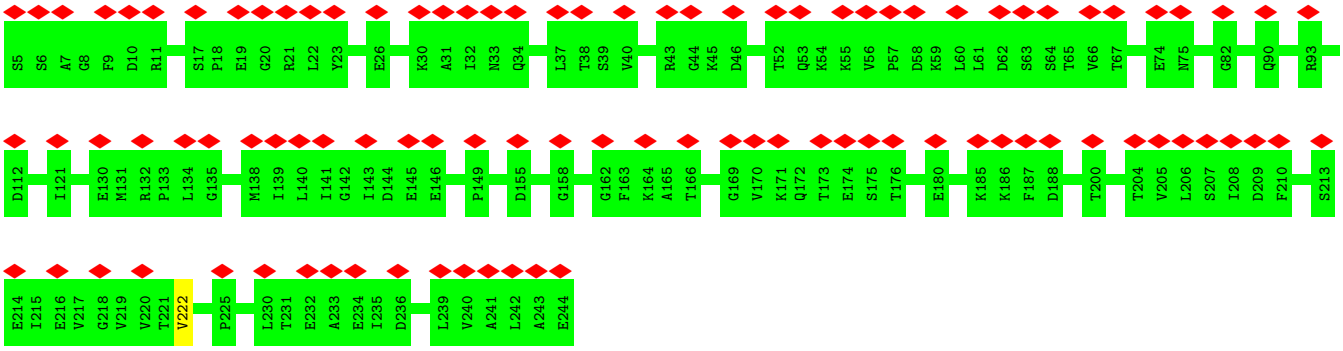
Chain G:



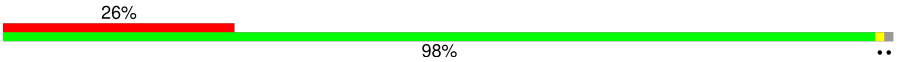

• Molecule 1: Proteasome subunit alpha type-6

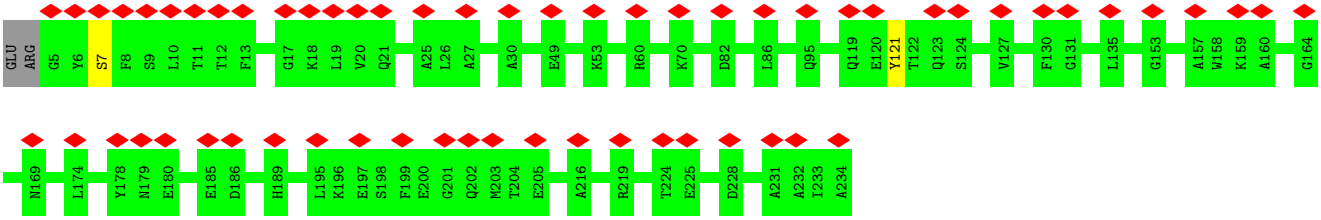
Chain g:




• Molecule 2: Proteasome subunit alpha type-2

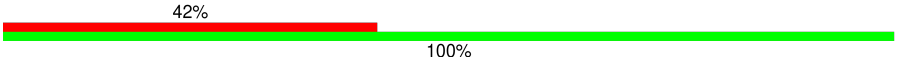
Chain H:

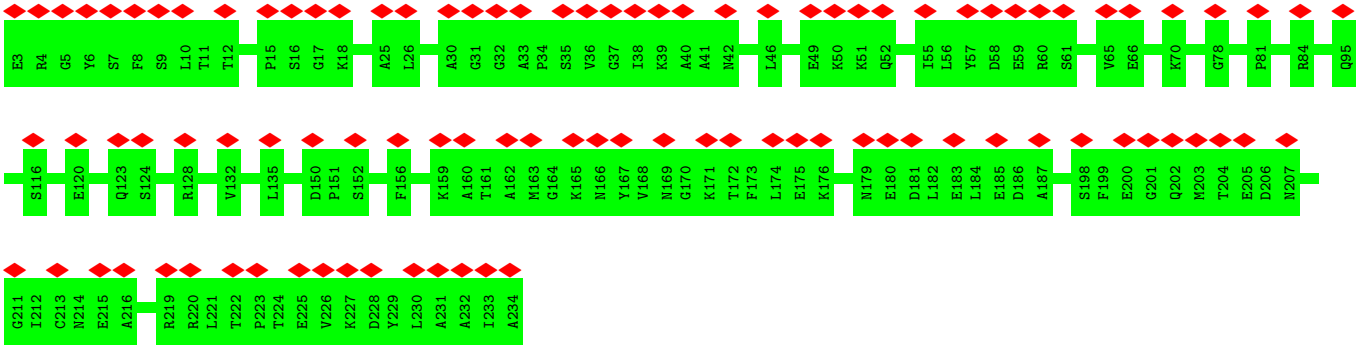


- Molecule 2: Proteasome subunit alpha type-2

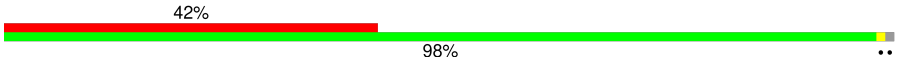
Chain h:

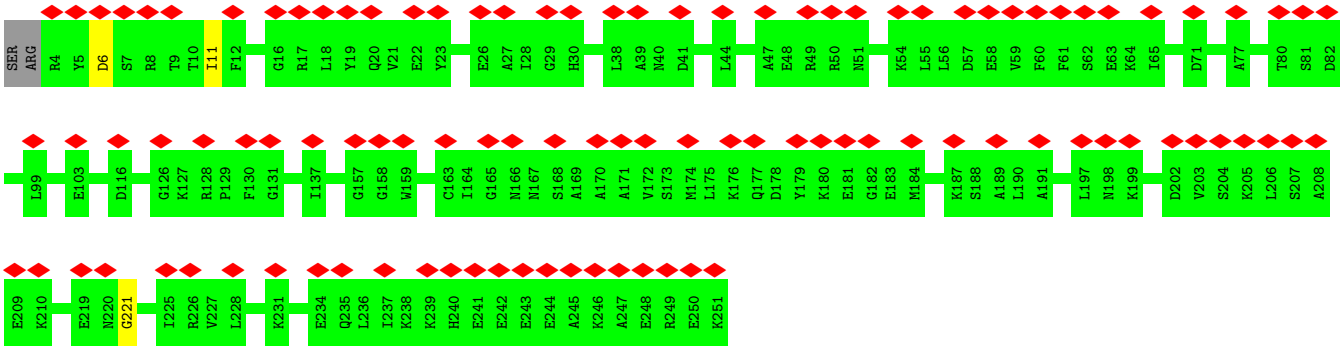



- Molecule 3: Proteasome subunit alpha type-4

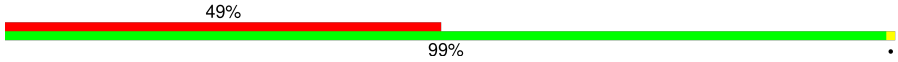
Chain I:

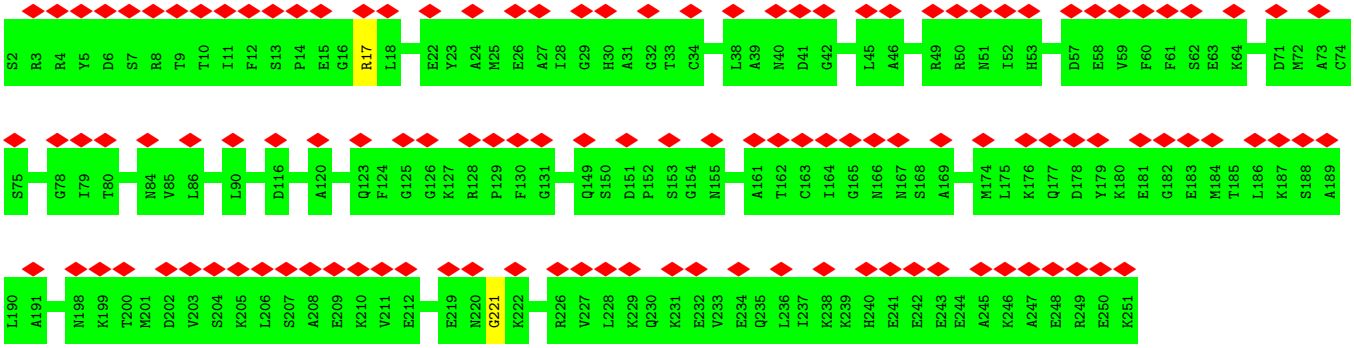



- Molecule 3: Proteasome subunit alpha type-4

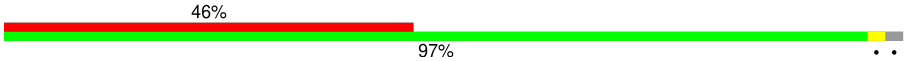
Chain i:

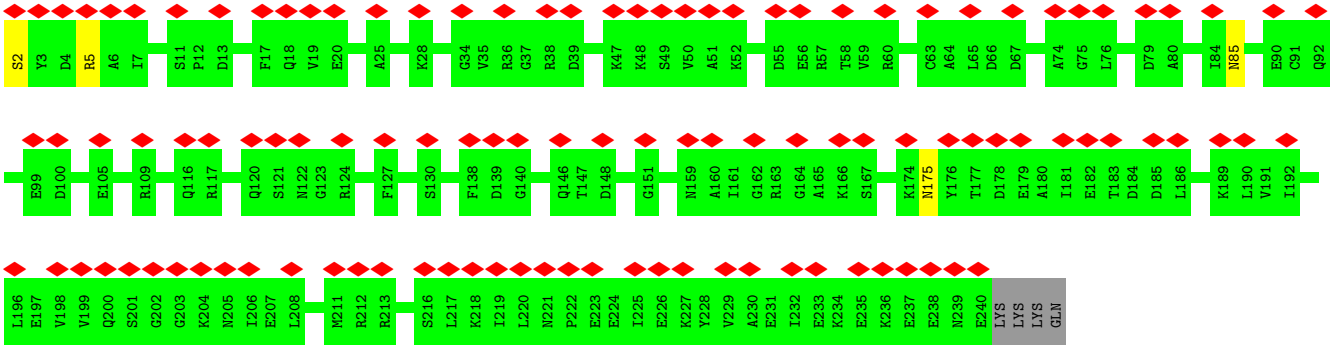



- Molecule 4: Proteasome subunit alpha type-7

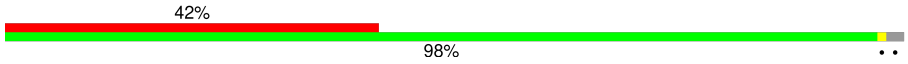
Chain J:

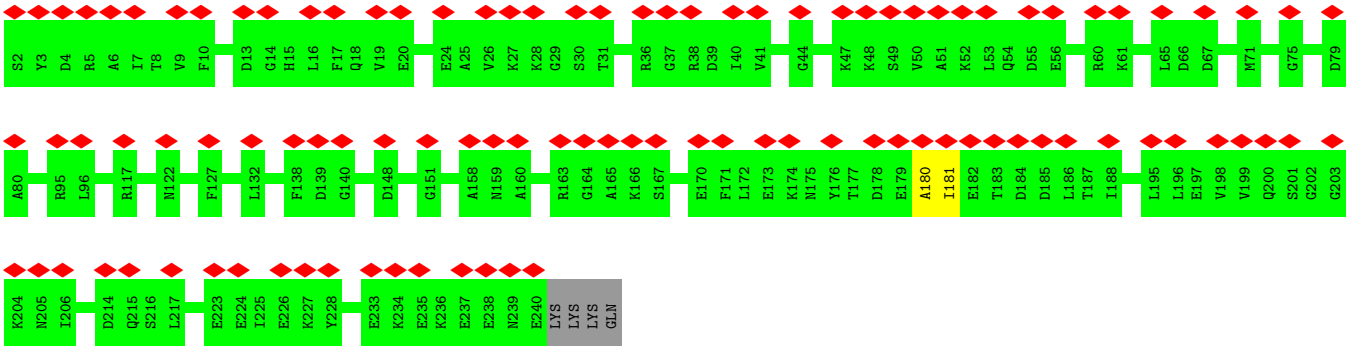





• Molecule 4: Proteasome subunit alpha type-7

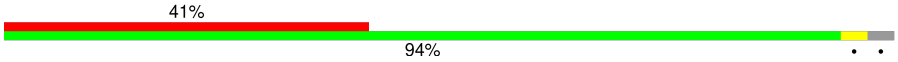
Chain j:

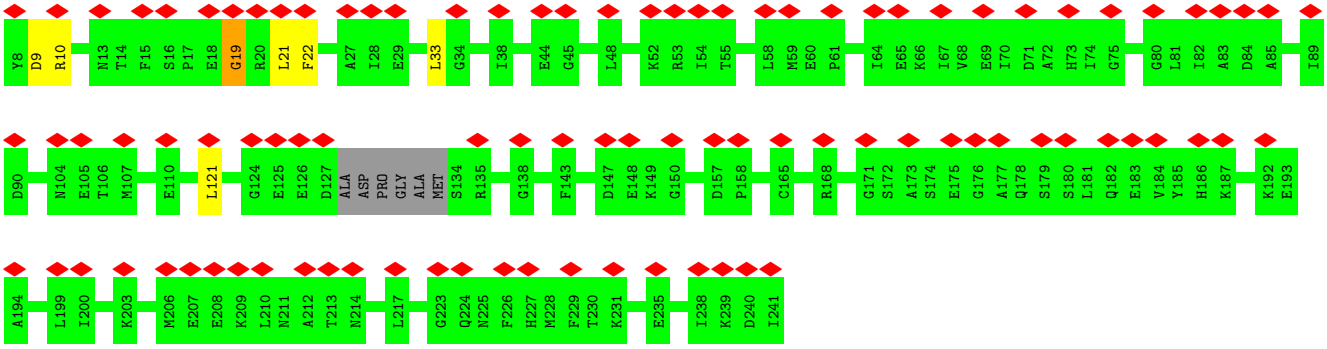



• Molecule 5: Proteasome subunit alpha type-5

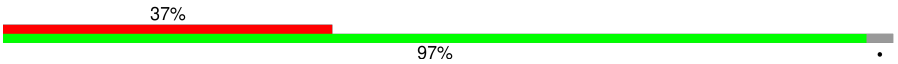
Chain K:

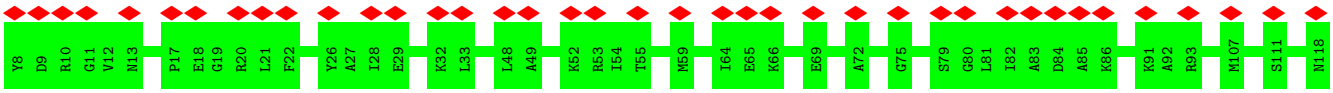


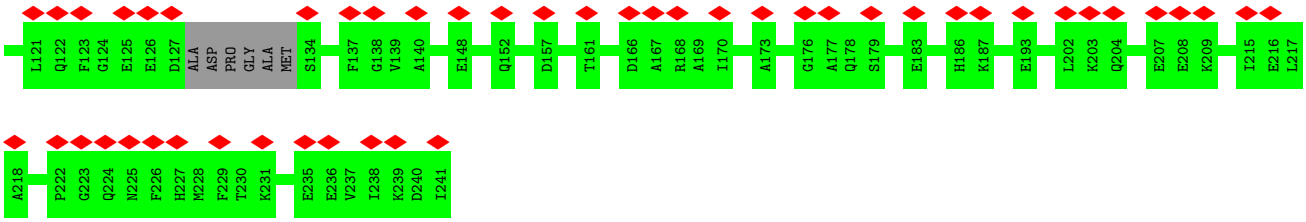




• Molecule 5: Proteasome subunit alpha type-5

Chain k:

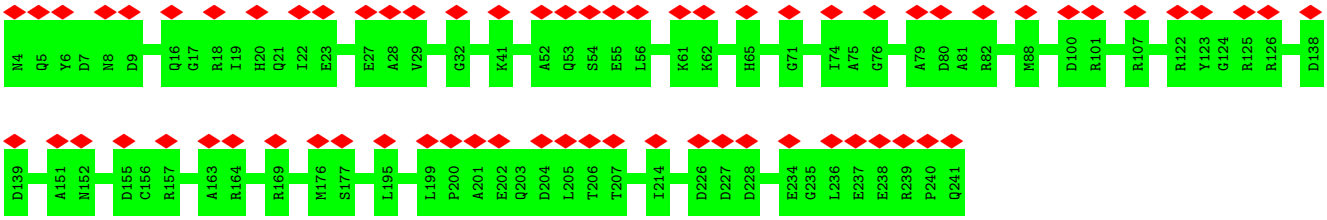




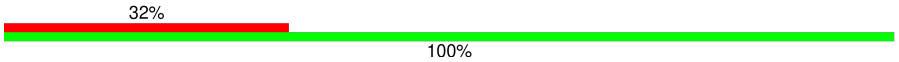

• Molecule 6: Proteasome subunit alpha type-1

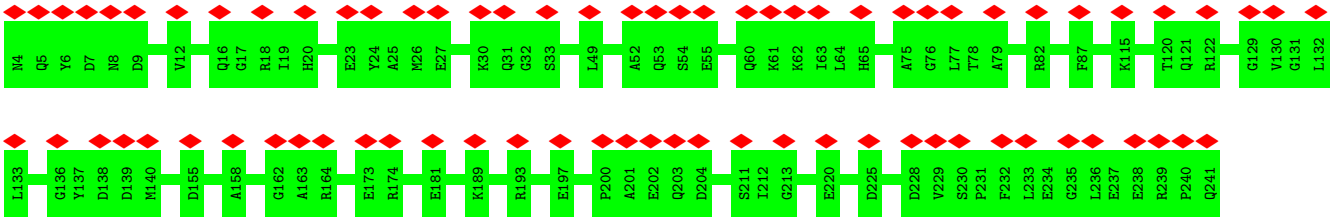
Chain L:




• Molecule 6: Proteasome subunit alpha type-1

Chain l:




• Molecule 7: Proteasome subunit alpha type-3

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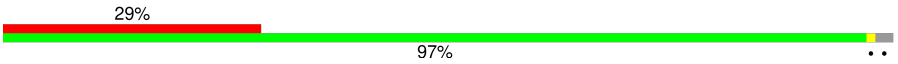
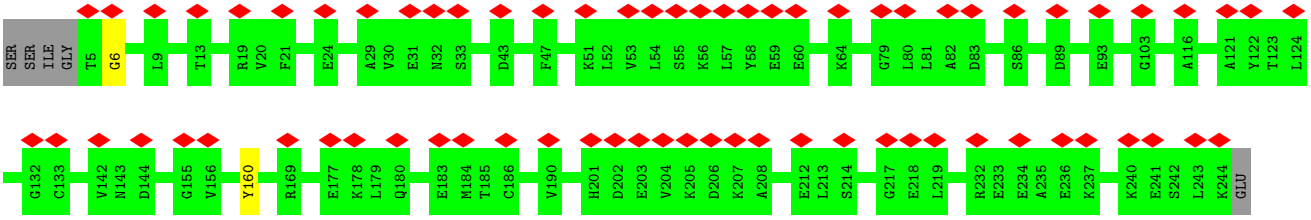
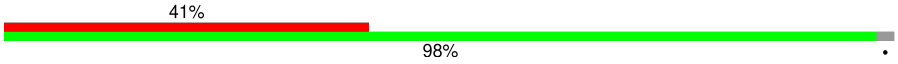
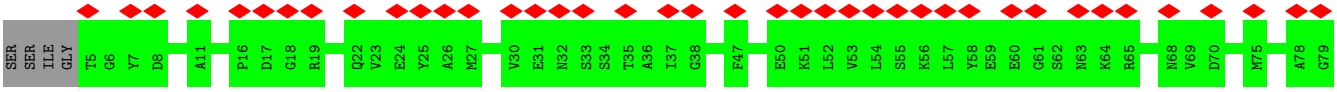


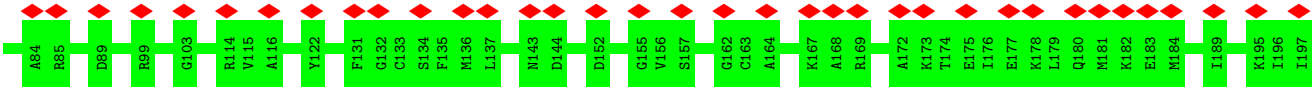



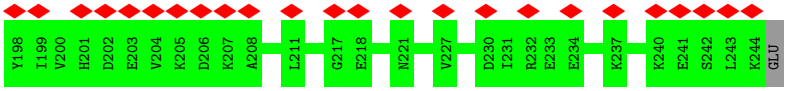

• Molecule 7: Proteasome subunit alpha type-3

Chain m:



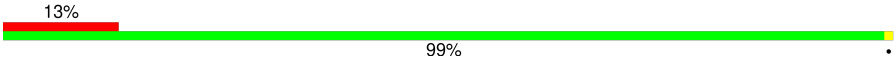



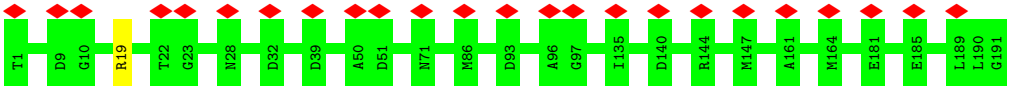



• Molecule 8: Proteasome subunit beta type-6

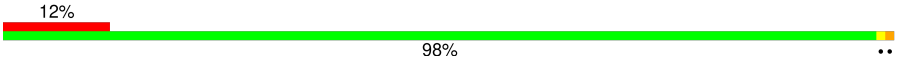
Chain N:

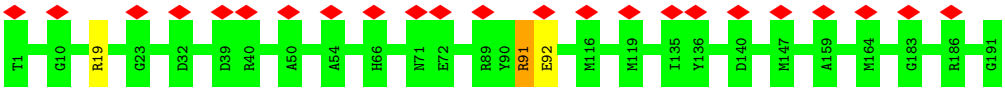



• Molecule 8: Proteasome subunit beta type-6

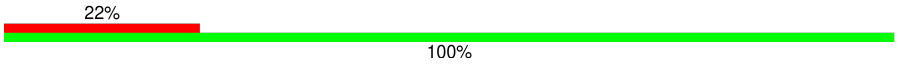
Chain n:

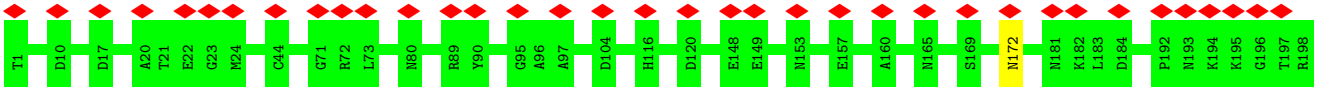


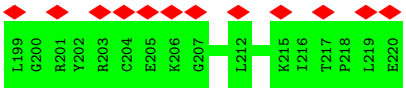




• Molecule 9: Proteasome subunit beta type-7

Chain O:

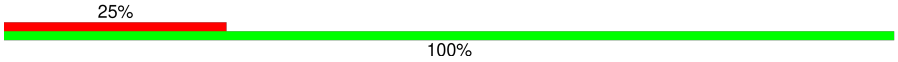


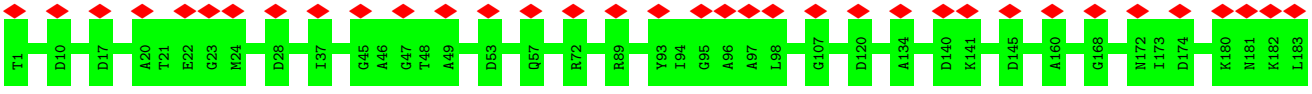



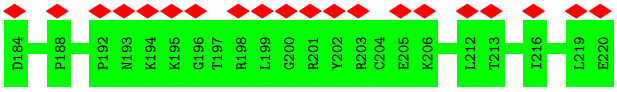




• Molecule 9: Proteasome subunit beta type-7

Chain o:

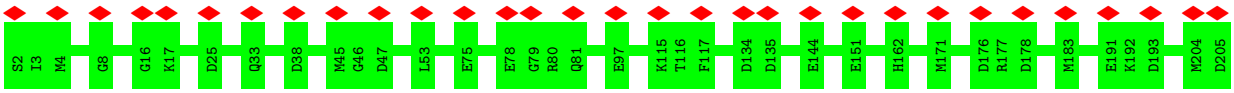


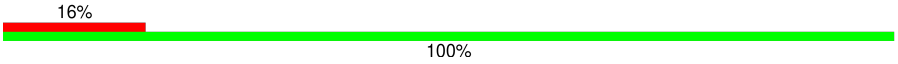

• Molecule 10: Proteasome subunit beta type-3

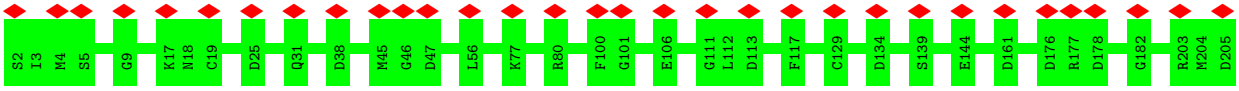
Chain P:




• Molecule 10: Proteasome subunit beta type-3

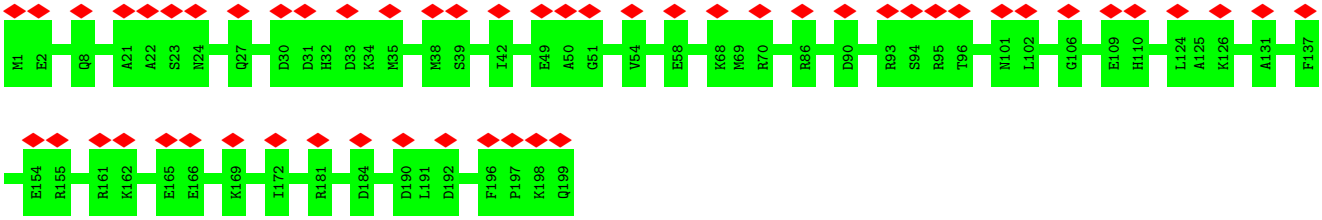
Chain p:



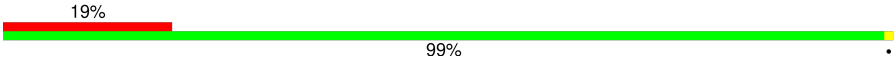

• Molecule 11: Proteasome subunit beta type-2

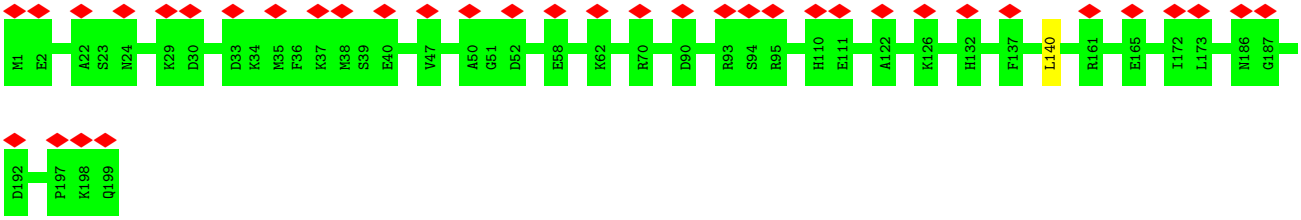
Chain Q:




• Molecule 11: Proteasome subunit beta type-2

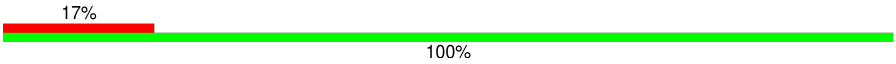
Chain q:

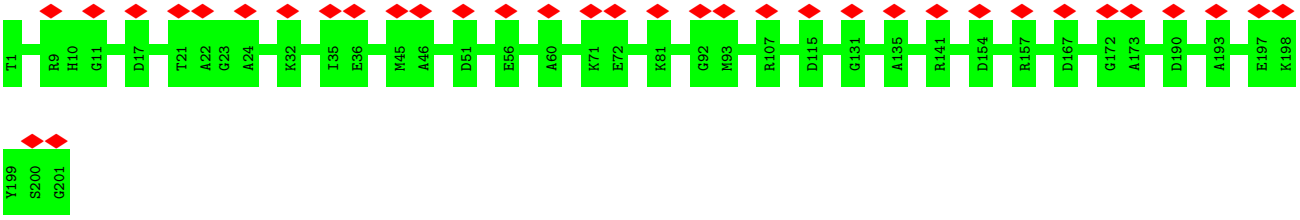



• Molecule 12: Proteasome subunit beta type-5

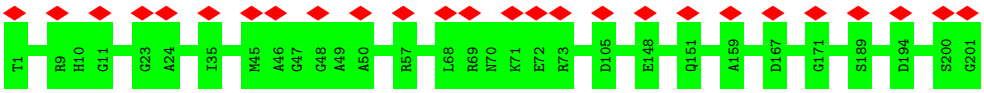
Chain R:



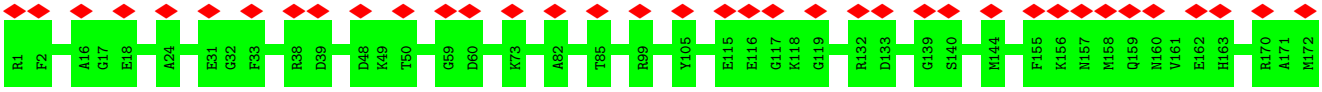

• Molecule 12: Proteasome subunit beta type-5

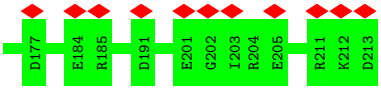
Chain r:




• Molecule 13: Proteasome subunit beta type-1

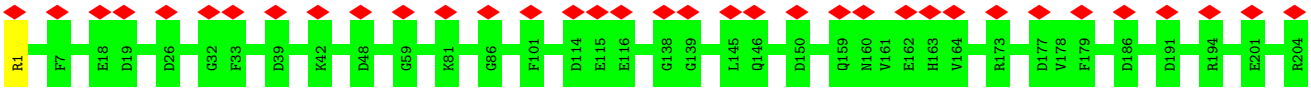
Chain S:

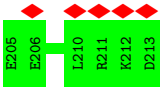



• Molecule 13: Proteasome subunit beta type-1

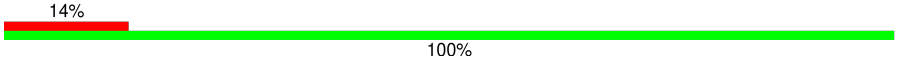
Chain s:

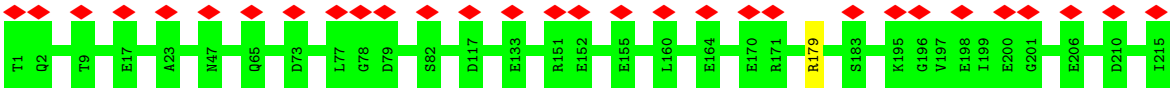



• Molecule 14: Proteasome subunit beta type-4

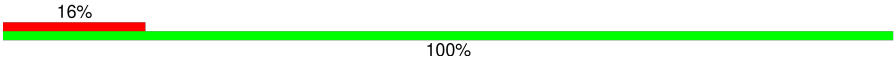
Chain T:

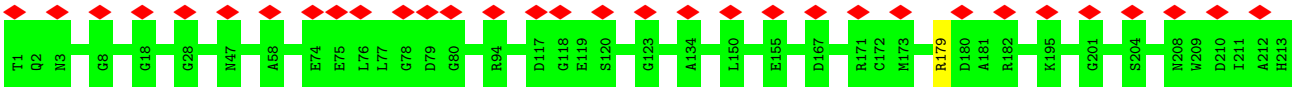



• Molecule 14: Proteasome subunit beta type-4

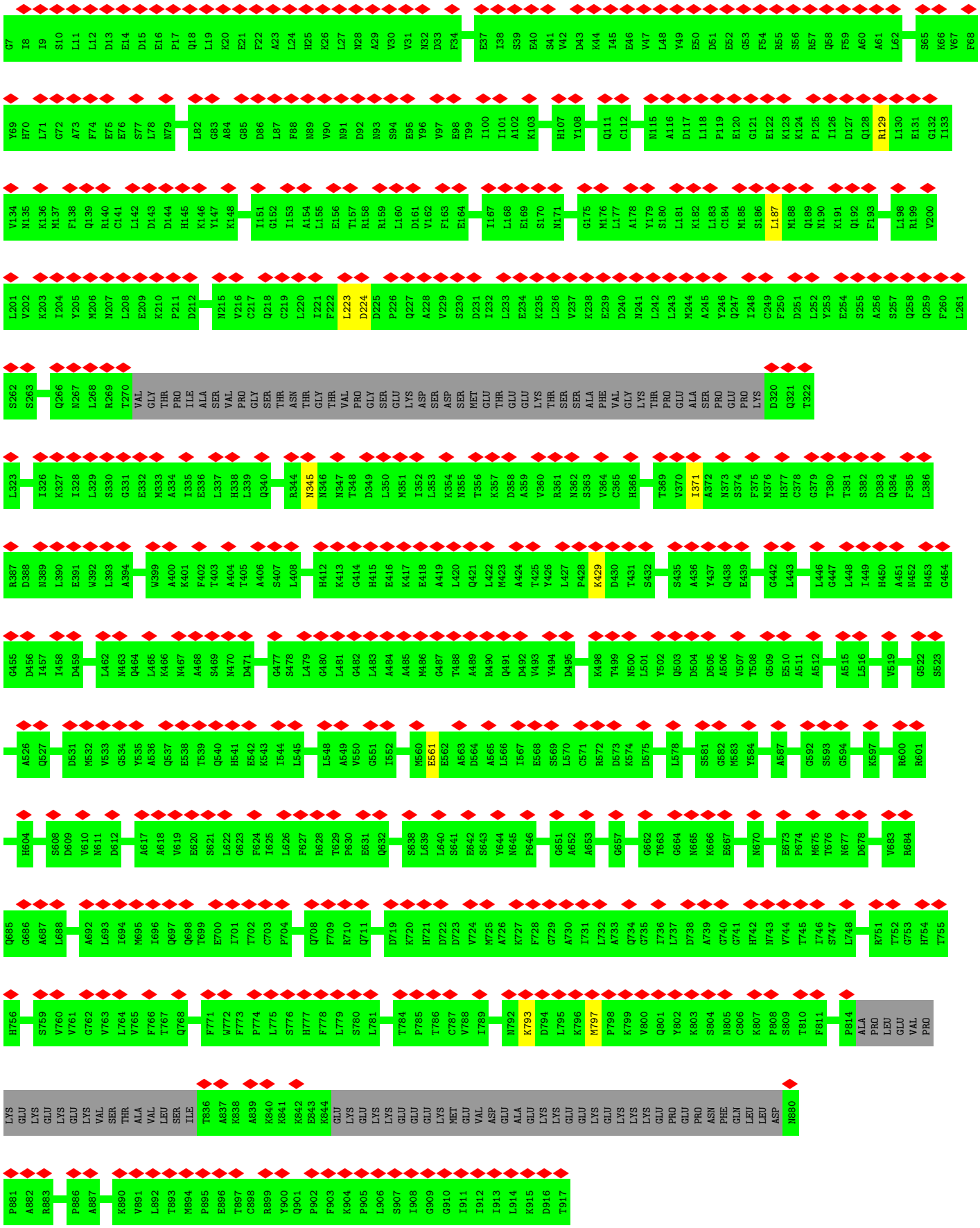
Chain t:



• Molecule 15: 26S proteasome non-ATPase regulatory subunit 1

Chain U: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E37 I38 S39 E40 S41 V42 D43 K44 I45 E46 V47 L48 Y49 E50 D51 E52 G53 F54 R55 S56 R57 Q58 F59 A60 A61 L62
S65 K66 V67 F68
Y69 H70 L71 G72 A73 F74 E75 E76 S77 L78 N79
L82 G83 A84 G85 D86 L87 F88 N89 V90 N91 D92 N93 S94 E95 Y96 V97 E98 T99 I100 I101 A102 K103
H107 Y108
Q111 C112
N115 A116 D117 L118 P119 E120 G121 E122 K123 K124 P125 I126 D127 Q128 R129 L130 E131 G132 I133
V134 N135 K136 M137 F138 Q139 R140 C141 L142 D143 D144 H145 K146 Y147 K148
I151 G152 I153 A154 L155 E156 T157 R158 R159 L160 D161 V162 F163 E164
I167 L168 E169 S170 M171
G175 M176 L177 A178 Y179 S180 L181 K182 L183 C184 M185 S186 L187 M188 Q189 N190 K191 Q192 F193
L198 R199 V200
L201 V202 K203 I204 Y205 M206 N207 L208 E209 K210 P211 D212
N215 V216 C217 Q218 C219 L220 I221 F222 L223 D224 D225 P226 Q227 A228 V229 S230 D231 I232 L233 E234 K235 L236 V237 K238 E239 D240 N241 L242 L243 M244 A245 Y246 Q247 I248 C249 F250 D251 L252 Y253 E254 S255 A256 S257 Q258 Q259 F260 L261
S262 S263
Q266 N267 L268 R269 T270
VAL GLY THR PRO ILE ALA SER VAL PRO GLY SER THR ASN THR GLY THR VAL PRO GLY SER GLU LYS ASP SER ASP SER MET GLU THR GLU GLU LYS THR SER SER ALA PHE VAL GLY LYS THR PRO GLU ALA SER PRO GLU PRO LYS
D320 Q321 T322
L323
I326 K327 I328 L329 S330 G331 E332 M333 A334 I335 E336 L337 H338 L339 Q340
R344 N345 N346 N347 T348 D349 L350 M351 I352 L353 K354 N355 T356 K357 D358 A359 V360 R361 N362 S363 V364 C365 H366
T369 V370 I371 A372 N373 S374 F375 M376 H377 C378 G379 T380 T381 S382 D383 Q384 F385 L386
R387 D388 N389 L390 E391 W392 L393 A394
W399 A400 K401 F402 T403 A404 T405 A406 S407 L408
H412 K413 G414 H415 E416 K417 E418 A419 L420 Q421 L422 M423 A424 T425 Y426 L427 P428 K429 D430 T431 S432
S435 A436 Y437 Q438 E439
G442 L443
L446 G447 L448 I449 H450 A451 N452 H453 G454
G455 D456 I457 I458 D459
L462 N463 Q464 L465 K466 N467 A468 S469 N470 D471
G477 S478 L479 G480 L481 G482 L483 A484 A485 M486 G487 T488 A489 R490 Q491 D492 V493 Y494 D495
K498 T499 N500 L501 Y502 Q503 D504 D505 A506 V507 T508 G509 E510 A511 A512
A515 L516
V519
G522 S523
A526 Q527
D531 M532 V533 G534 Y535 A536 Q537 E538 T539 Q540 H541 E542 K543 I544 L545
L548 A549 V550 G551 I552
M560 E561 E562 A563 D564 A565 L566 I567 E568 S569 L570 C571 R572 D573 K574 D575
L578
S581 G582 M583 Y584
A587
G592 S593 G594
K597
R600 R601
H604
S608 D609 V610 N611 D612
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G651 A652 A653
G657
G662 T663 G664 N665 K666 E667
N670
E673 P674 M675 T676 N677 D678
V683 R684
Q685 G686 A687 L688
A692 L693 I694 M695 I696 Q697 Q698 T699 E700 I701 T702 C703 P704
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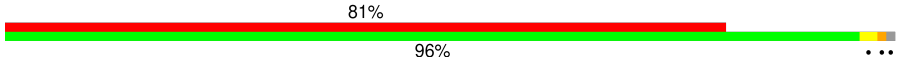
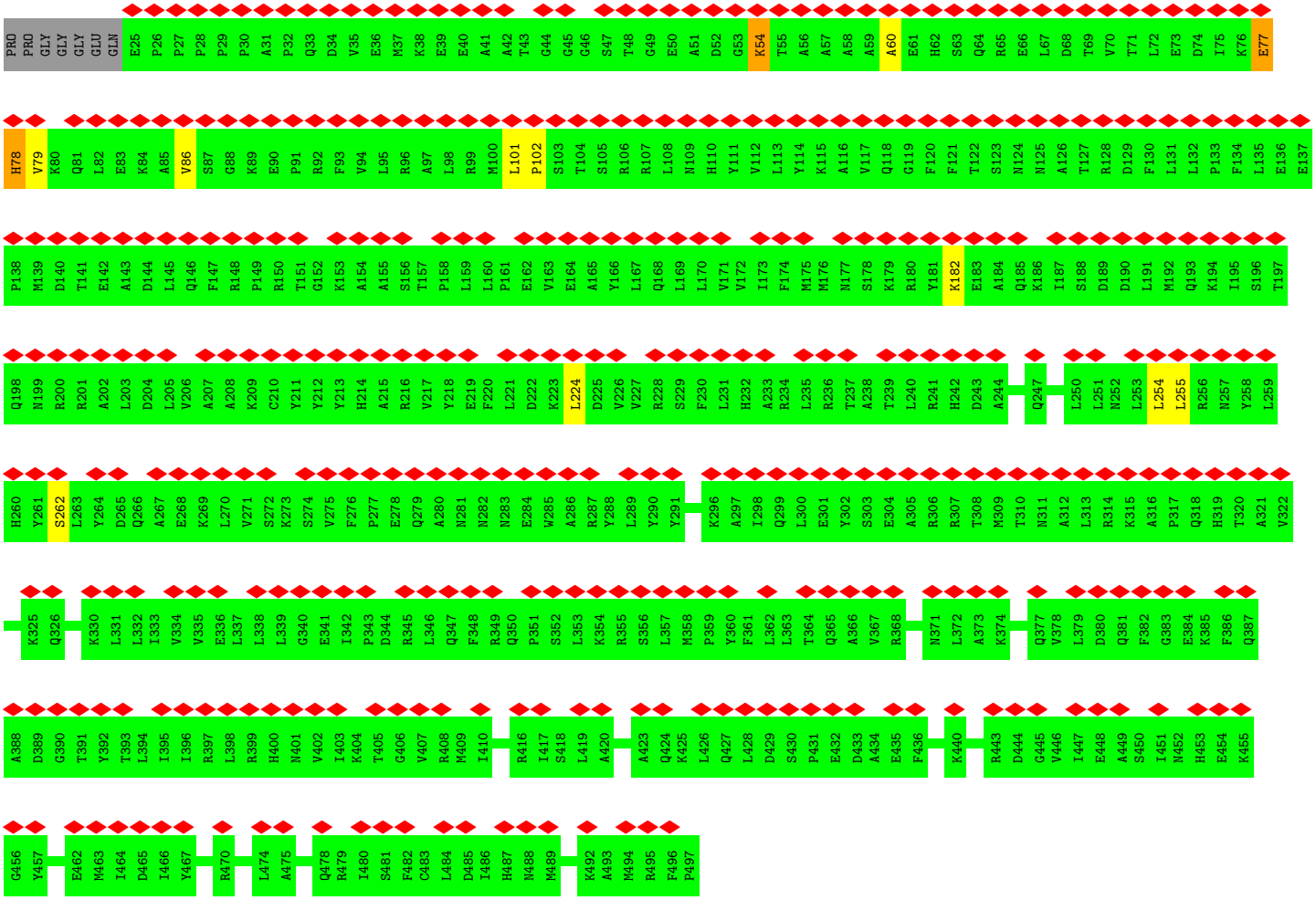
R751 T752 G753 H754 T755
H756
S759 V760 V761 G762 V763 L764 V765 F766 T767 Q768
F771 W772 F773 P774 L775 S776 H777 F778 L779 S780 L781
T784 P785 T786 C787 V788 I789
N792 K793 D794 L795 K796 M797 P798 K799 V800 Q801 Y802 K803 S804 N805 C806 K807 P808 S809 T810 F811
P814
ALA PRO LEU GLU VAL PRO
LYS GLU LYS GLU LYS GLU LYS VAL SER THR ALA VAL LEU SER ILE
T836 A837 K838 A839 K840 K841 K842 E843 K844
GLU LYS LYS GLU LYS LYS GLU GLU GLU LYS MET GLU VAL ASP GLU ALA GLU LYS LYS GLU GLU LYS GLU GLU LYS LYS LYS GLU PRO GLU PRO ASN PHE GLN LEU LEU ASP
N880
P881 A882 R883
P886 A887
K890 V891 L892 T893 M894 P895 E896 T897 C898 R899 Y900 Q901 P902 F903 K904 P905 L906 S907 I908 G909 G910 I911 I912 I913 L914 K915 D916 T917

- Molecule 16: 26S proteasome non-ATPase regulatory subunit 3

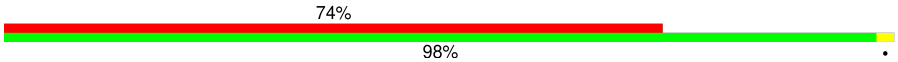
Chain V:

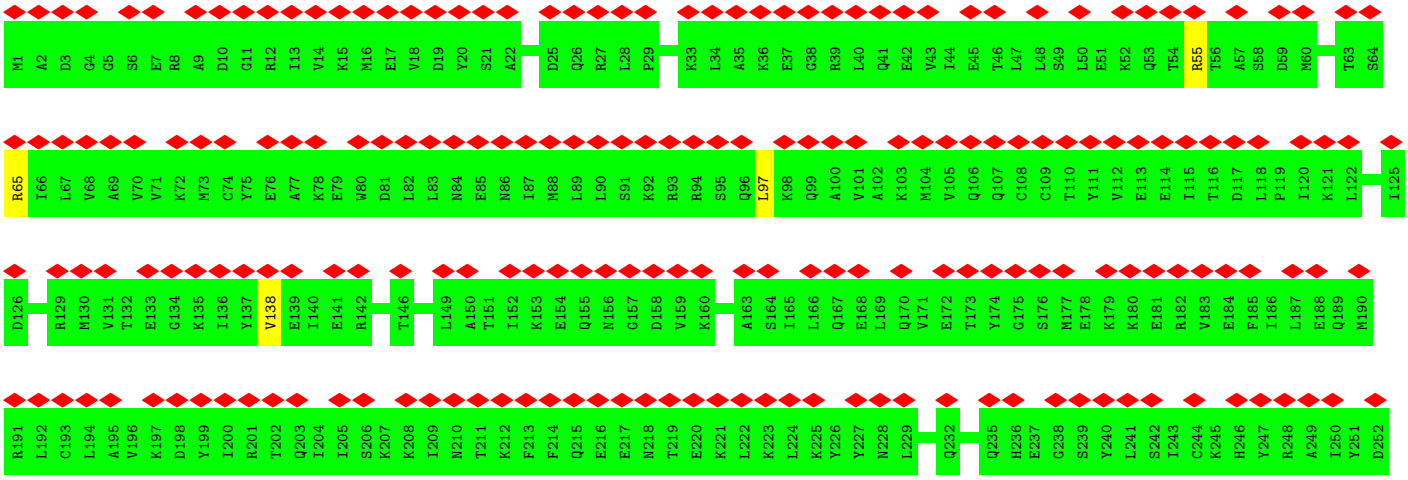



- Molecule 17: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



T253 P254 C255 I256 Q257 A258 E259 S260 E261 Q264 L267 K268 S269 V270 V271 L272 Y273 V274 I275 L276 A277 P278 N281 E282 Q283 S284 D285 H288 R289 I290 S291 G292 D293 K294 K295 L296 E297 E298 I299 P300 K301 Y302 K303 D304 K307 L308 F309 T310 T311 M312 E313 L314 M315 R316 W317

S318 T319 L320 V321 E322 D323 Y324 G325 M326 R329 K330 G331 S332 L333 E334 S335 P336 A337 T338 D339 G342 S343 T344 E345 E346 G347 E348 L354 R357 V358 V359 E360 H361 N362 T365 Y369 Y370 T371 R372 I373 T374 M375 K376 R377 M378 A379 Q380 L381 L382 D383 L384 S385 V386 D387

E388 S389 E390 A391 F392 L393 S394 N395 L396 V397 V398 N399 K400 T401 I402 F403 A404 K405 V406 D407 R408 L409 A410 G411 I412 I413 N414 F415 Q416 R417 P418 K419 D420 P421 M422 M423 W428 S429 Q430 K431 L432 M433 L438 Y439 T442 T443 H444 L445 K448 E449 E450 M451 I452 H453 M454 L455

Q456

- Molecule 18: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 63% 98%

P12 K13 N14 P15 D16 L17 R18 I19 A20 L26 S27 L28 P29 E30 H31 R32 G33 D34 A35 A36 V37 R38 D39 E40 L41 M42 A43 A44 V45 R46 N49 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 L121 T122 A123 F124 R125 K126 T127 Y128 D129 K130 T131 V132 A133 L134 G135 H136 R137

I140 L144 L145 R146 I147 G148 L149 F150 Y151 M152 D153 N154 D155 L156 I157 T158 R159 E162 K163 A164 K165 S166 L167 I168 E169 E170 G171 G172 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 L200 D203 T204

V205 S206 T207 F208 T209 S210 Y211 E212 L213 M214 D215 M228 I229 A230 L236 R237 I241 K242 G243 L250 L253 P254 R257 F261 S262 C266 R267 Y268 S269 V270 F271 F272 E279 Q280 E281 M282 K283 K284 D285 W286 L287 P290 H291 Y292 R293 Y294 R297 H302

Q306 L307 L308 E309 T315 L316 G317 Y318 M319 A320 E321 G324 V325 G326 V327 E328 F329 I330 D331 S335 R336 F337 G341 R342 L343 K346 I347 V350 N351 E352 I353 V354 E355 T356 N357 R358 P359 W364 Q365 Y366 T369 I370 K371 D374 L375 L376 L377 N378 R379 V380

Q381 K382 L383 S384 R385 V386 I387 N388 M389

- Molecule 19: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 72% 97%

A5 V6 Q7 K8 V11 H12 P13 L17 S18 V19 H22 F23 N24 R25 I26 G27 K28 V29 G30 N31 Q32 K33 R34 V35 V36 G37 V38 L39 L40 G41 S42 W43 K46 D49 F54 F57 F58 D59 E60 D61 D62 K63 D64 D65 S66 F69 L70 D71 H72 D73 Y74

M78 Y79 F82 K83 A87 R88 E89 R90 I91 V92 G93 W94 P99 K100 L101 H102 K103 N104 D105 I106 A107 I108 N109 E110 L111 M112 K113 R114 Y115 C116 P117 N118 S119 V120 L121 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 F155 E156 H157 S160 E161 I162 G163 A164 E165 E166 A167 E168 E169 V170 G171 V172 E173 H174 L175 L176 R177 D178 T179 K180 D181 T182 T183 V184 L187 R190 T191 T192 N193 Q194 V195 H196 G197 L198 K199 G200 L201 N202 S203 K204 L205 L206 D207

I208 Y211 L212 E213 K214 V215 A216 T217 G218 K219 L220 P221 I222 N223 H224 Q225 I226 Q229 L230 Q231 D232 V233 F234 N235 P238 D239 V240 S241 L242 Q243 E244 F245 V246 K247 A248 F249 Y250 L251 K252 D255 Q256 V260 Y261 L262 A263 S264 L265 I266 R267 S268 V269 V270 A271 L272 H273

N274 L275 I276 N277 N278 K279 I280 A281 N282 R283 D284 A285 E286 K287 K288 E289 G290

- Molecule 20: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 80% 98%

V4 P5 G6 F7 L8 Q9 Q10 S11 Q12 N13 S14 G15 P16 G17 Q18 P19 A20 V21 W22 H23 R24 L25 E26 E27 L28 Y29 T30 K31 K32 L33 W34 H35 Q36 L37 T38 L39 Q40 V41 L42 D43 F44 V45 Q46 D47 P48 C49 F50 A51 Q52 G53 D54 G55 L56 I57 K58 L59 Y60 E61 N62 F63

I64 S65 E66 F67 E68 H69 R70 V71 L74 S75 L76 V77 E78 I79 I80 L81 H82 V83 V84 R85 Q86 M87 T88 D89 P90 N91 V92 A93 L94 T95 F96 L97 E98 K99 T100 R101 E102 K103 V104 K105 S106 S107 D108 E109 A110 V111 I112 L113 C114 K115 T116 A117 I118 G119 A120 L121 K122 L123 N124

I125 G126 D127 L128 Q129 V130 T131 T134 I135 E136 D137 V138 E139 E140 M141 L142 N143 N144 L145 P146 G147 V148 T149 S150 S153 R154 D157 L158 K161 Y162 Y163 Q164 T165 I166 G167 N168 H169 A170 S171 Y172 Y173 K174 D175 A176 L177 R178 F179 L180 G181 C182 V183 D184 I185 K186 D187 L188

P189 V190 S191 E192 Q193 Q194 E195 R196 A197 F198 T199 L200 G201 L202 A203 G204 L205 L206 G207 E208 G209 V210 F211 N212 F213 G214 E215 L216 L217 M218 H219 P220 V221 L222 E223 S224 L225 R226 N227 T228 D229 R230 Q231 W232 L233 I234 D235 Y238 A239 S242 G243 N244 V245 E246 R247 F248 Q249 T250

L251 K252 T253 A254 W255 G256 Q257 Q258 L261 A262 A263 N264 E265 A266 Q267 I268 L269 R270 K271 I272 Q273 L274 L275 C276 E279 M280 T281 F282 T283 R284 P285 A286 N287 H288 R289 Q290 L291 T292 F293 E294 E295 I296 A297 K298 S299 A300 K301 I302 T303 V304 N305 E306 V307 L310 V311 M312 K313

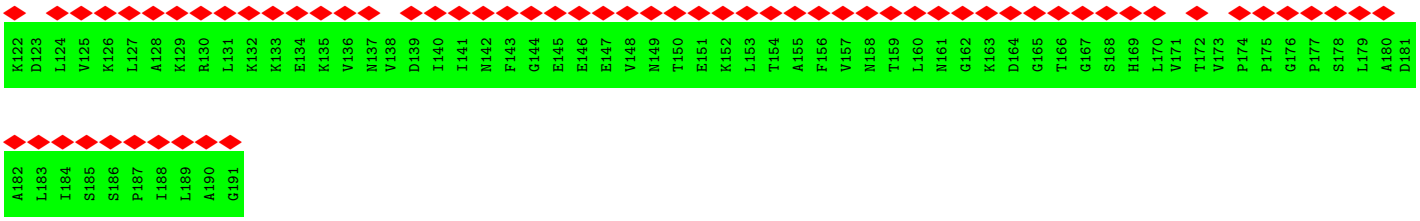
A314 L315 S316 V317 G318 L319 V320 K321 G322 S323 E326 V327 D328 K329 R330 V331 H332 M333 Q337 P338 R339 V340 L341 D342 L343 Q344 Q345 I346 K347 G348 M349 K350 D351 R352 F355 W356 C357 T358 D359 V360 K361 S362 M363 E364 M365 I366 V367 E368 H369 Q370 A371 H372 D373 I374 L375 T376

- Molecule 21: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 87% 98%

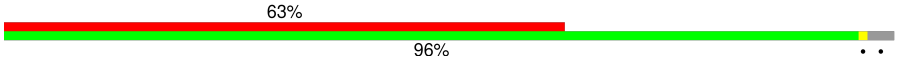
M1 V2 L3 E4 S5 T6 M7 V8 C9 V10 D11 N12 S13 E14 Y15 M16 R17 D20 F21 L22 P23 T24 R25 L26 Q27 A28 Q29 Q30 D31 A32 V33 M34 I35 V36 C37 H38 S39 K40 T41 R42 S43 N44 P45 E46 M47 N48 V49 G50 L51 I52 T53 L54 A55 N56 D57 C58 E59 V60 L61

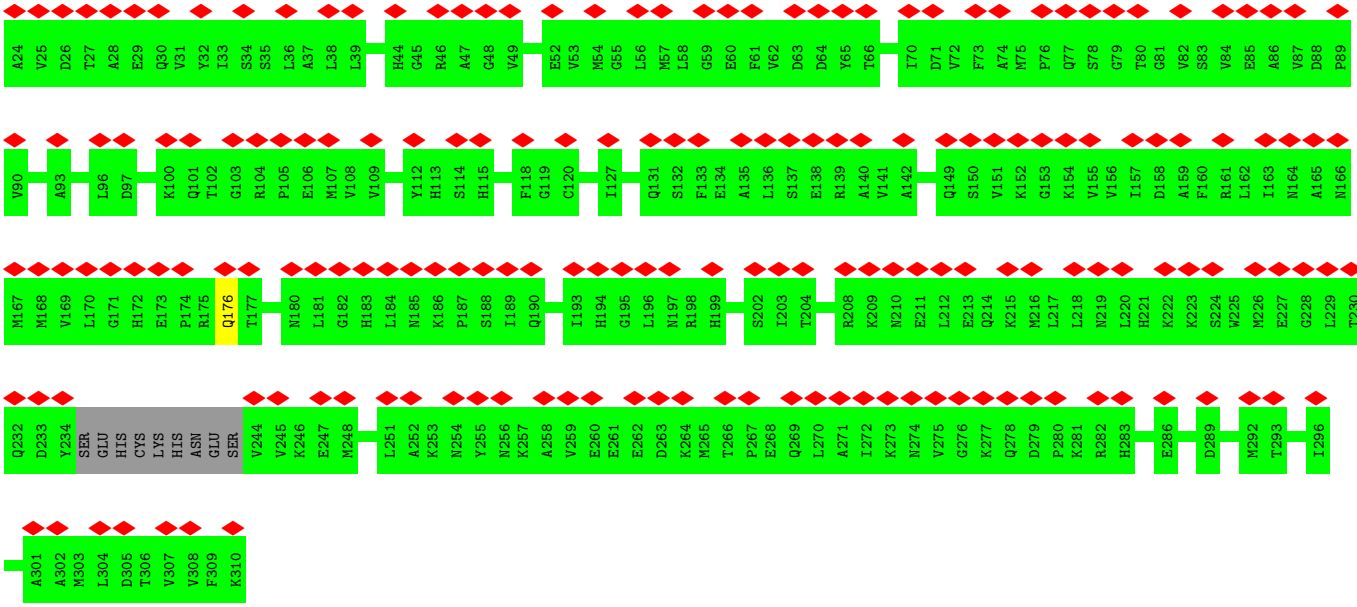
T62 T63 L64 T65 P66 D67 T68 G69 R70 I71 L72 S73 K74 L75 H76 T77 V78 Q79 P80 K81 G82 K83 I84 T85 F86 C87 T88 G89 I90 R91 V92 A93 H94 L95 A96 L97 K98 H99 R100 Q101 G102 K103 N104 H105 K106 M107 R108 I109 I110 A111 F112 V113 G114 S115 P116 V117 E118 D119 N120 E121




• Molecule 22: 26S proteasome non-ATPase regulatory subunit 14

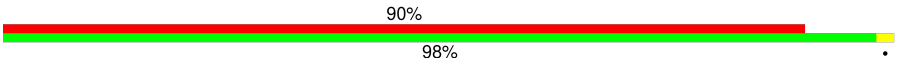
Chain c:

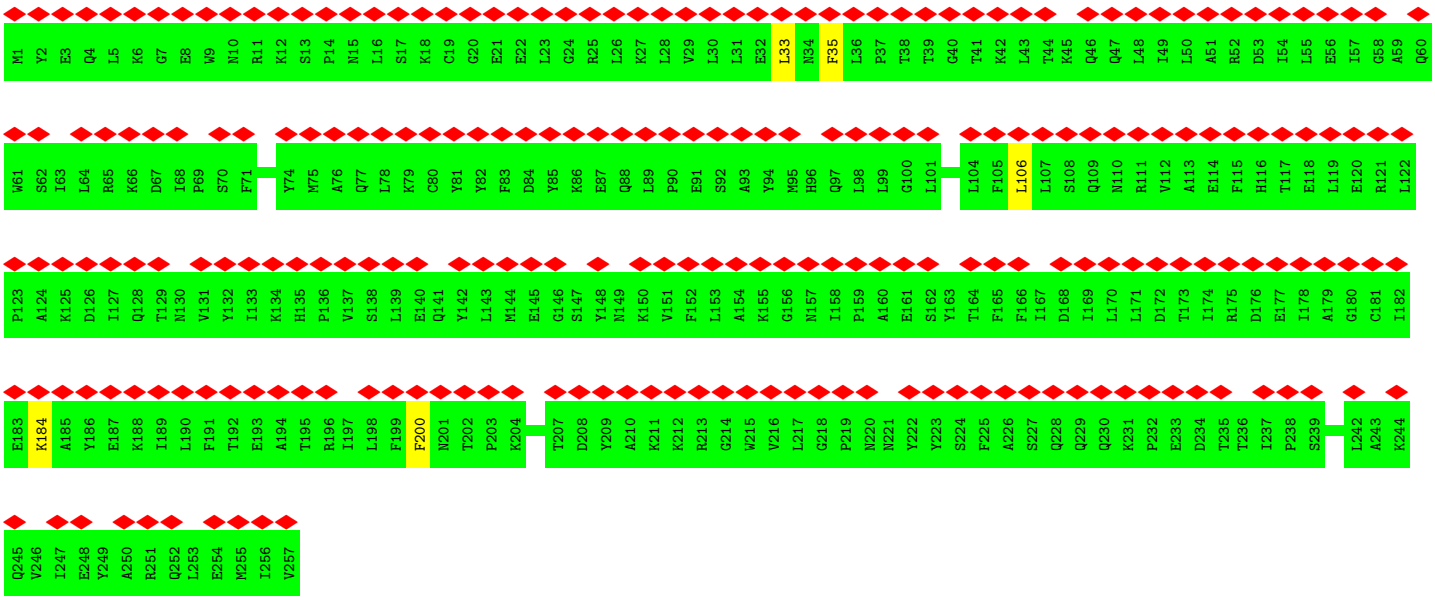


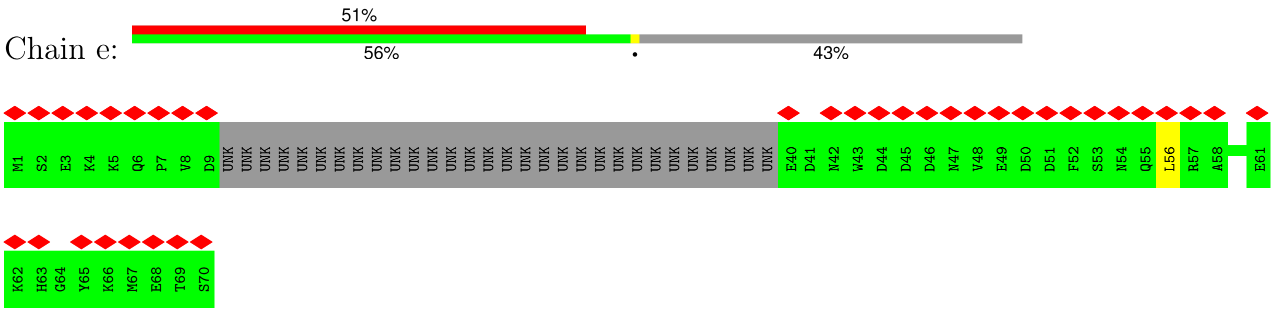

• Molecule 23: 26S proteasome non-ATPase regulatory subunit 8

Chain d:

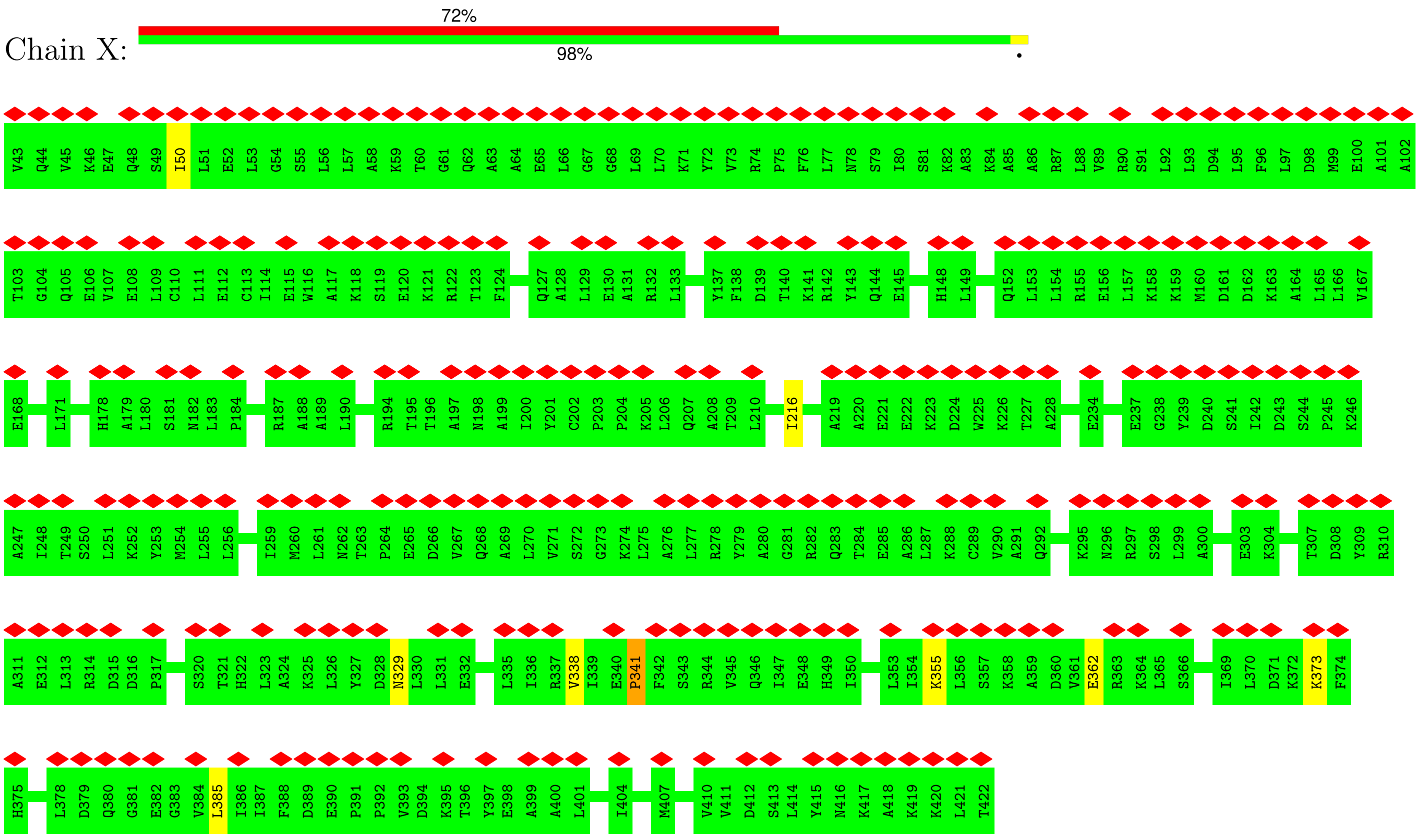


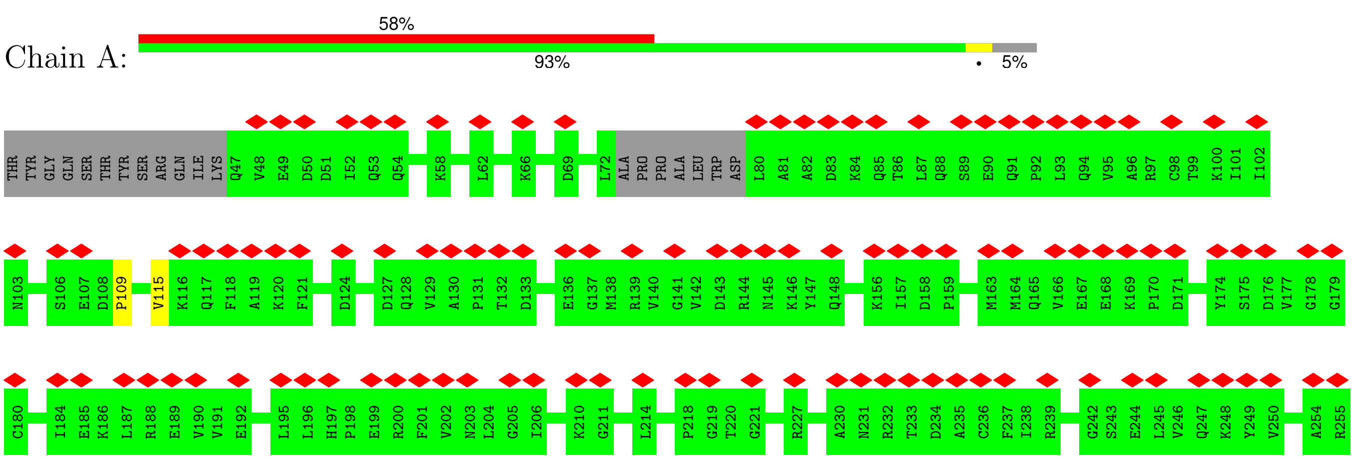
- Molecule 24: sem1

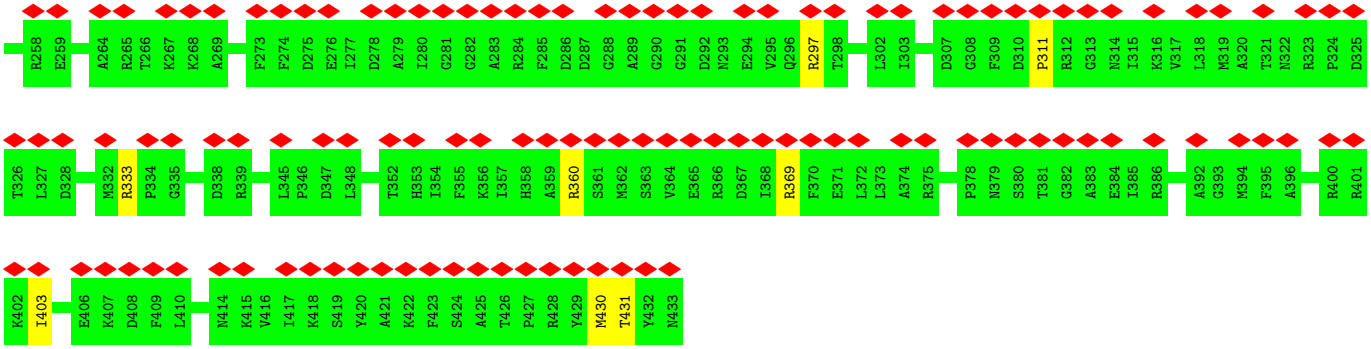



- Molecule 25: 26S proteasome non-ATPase regulatory subunit 11



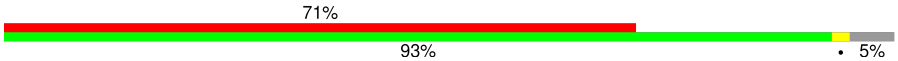

- Molecule 26: 26S proteasome regulatory subunit 7

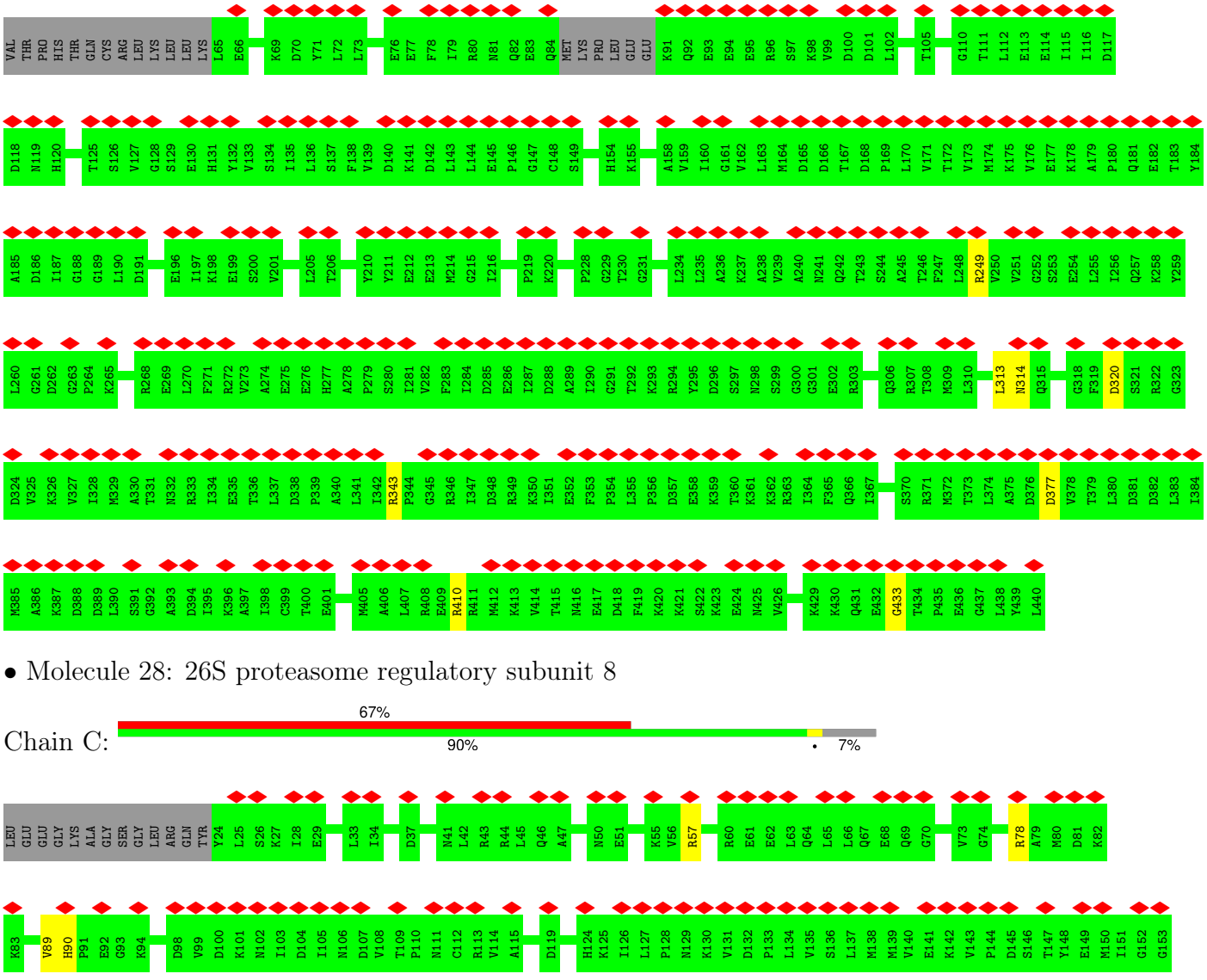





- Molecule 27: 26S proteasome regulatory subunit 4

Chain B:




- Molecule 28: 26S proteasome regulatory subunit 8

Chain C:

L154 D155 K156 K159 E160 I161 K162 E163 V164 I165 E166 L167 P168 V169 K170 H171 L174 F175 E176 A177 L178 G179 I180 A181 K184 G185 V186 L187 L188 Y189 G190 P191 P192 G193 T194 G195 K196 T197 A200 R201 A202 V203 A204 H205 D208 C209 T210 F211 I212 R213 V214 S215 G216 S217 E218

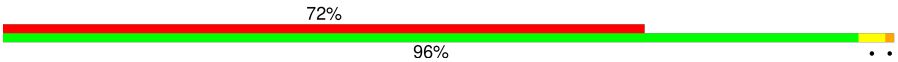
L219 V220 Q221 K222 F223 I224 G225 E226 G227 A228 R229 M230 V231 R232 E233 L234 F235 V236 M237 A238 R239 E240 H241 A242 P243 S244 I245 I246 F247 M248 D249 E250 ILE ASP SER ILE GLY SER SER ARG LEU GLU GLY GLY SER GLY GLY ASP S267 E268 V269 Q270 R271 T272 M273 L274 E275 L276 L277 N278

Q279 L280 D281 G282 F283 E284 A285 T286 K287 N288 I289 K290 V291 I292 M293 A294 T295 N296 R297 I298 D299 I300 L301 D302 S303 A304 L305 L306 R307 P308 G309 R310 I311 D312 R313 K314 I315 E316 F317 P318 P319 P320 N321 R325 L326 D327 I328 L329 K330 I331 H332 S333 R334 K335 L338 T339 R340 G341

I342 N343 L344 R345 K346 I347 A348 E349 L350 M351 P352 G353 A354 S355 G356 A357 K360 T364 E365 A366 G367 M368 Y369 A370 L371 R372 E373 R374 R375 V376 H377 V378 T379 Q380 E381 D382 F383 E384 M385 A386 V387 A388 K389 V390 M391 Q392 K393 D394 S395 E396 K397 N398 M399 S400 I401 K402

- Molecule 29: 26S proteasome regulatory subunit 6B

Chain D:




D39 L40 Y41 L47 Q48 Q49 E50 L51 E52 F53 L54 E55 E58 E59 Y60 I61 K62 D63 E64 Q65 H74 E77 E78 V79 K80 R81 I82 Q83 S84 I85 P86 L87 G90 L93 E94 A95 V96 D97 Q98 N99 T100 S105 T106 T107 G108 R114 I115 L116 S117 T118 I119 D120

R121 E122 L123 L124 K125 P126 A131 L132 H133 K134 H135 D141 V142 L143 E146 A147 D148 S149 S150 I151 M152 M153 L154 T155 S156 D157 Q158 K159 P160 D161 V162 M163 Y164 A165 D166 I167 G168 G169 M170 D171 I172 Q173 K174 Q175 E176 V177 R178 E179 A180 V181 E182 L183 P184 L185 T186 H187 F188

E189 L190 Y191 K192 Q193 I194 G195 I196 D197 P198 P199 R200 G201 V202 L203 M204 Y205 C210 G211 K212 L215 A216 K217 A218 V219 A220 H221 H222 T223 T224 A225 A226 F227 I228 R229 V230 V231 G232 S233 E234 F235 V236 Q237 K238 Y239 L240 G241 E242 G243 P244 R245 M246 V247 R248 D249 V250 F251 R252

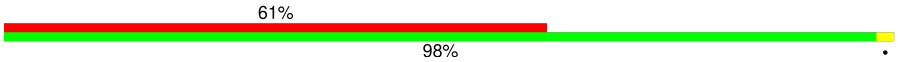
L253 A254 K255 E256 N257 A258 P259 A260 I261 I262 F263 I264 D265 E266 I267 D268 A269 I270 A271 T272 K273 R274 F275 D276 A277 Q278 T279 D282 R283 E284 R287 L290 E291 L292 L293 N294 Q295 M296 D297 G298 F299 D300 Q301 N302 V303 N304 V307 I308 M309 A310 T311 N312 R313 A314 D315 T316

L317 D318 P319 A320 L321 L322 R323 P324 G325 R326 L327 D328 R329 K330 I331 E332 F333 P334 L335 P336 D337 R338 R339 Q340 K341 R342 F345 S346 T347 I348 T349 S350 K351 M352 N353 L354 S355 E356 E357 V358 D359 L360 E361 D362 Y363 V364 A365 R366 P367 D368 K369 I370 S371 N376 S377 I378 E381

S382 G383 M384 L385 A386 V387 R388 E389 N390 R391 Y392 I393 V394 L395 D398 F399 E400 Y403 K404 I407 K408 K409 D410 E411 Q412 E413 H414 E415 F416 Y417 K418

- Molecule 30: 26S proteasome regulatory subunit 10B

Chain E:




K15 L16 L17 E18 H19 K20 E21 I22 D23 L26 K27 E28 L29 R30 E31 Q32 L33 K34 E35 L36 T37 K38 Q39 Y40 E41 K42 N45 D46 L47 K48 Q51 S52 V53 E59 K62 Q63 L64 T65 E66 E67 K68 F69 I70 N75 G76 P77 R78 Y79 R84 R85 Q86 L87 D88

K89 S90 K91 L92 K93 P94 R97 L100 D101 M102 L105 M108 R109 R113 E114 V115 D116 N121 M122 S123 H124 E125 D126 P127 G128 N129 V130 S131 Y132 S133 E134 I135 G136 G137 L138 S139 E140 R143 E144 L145 R146 E147 V148 I149 E150 L151 P152 L153 T154 N155 P156 E157 L158

F159 Q160 R161 V162 G163 I164 I165 C170 L171 G174 A188 S189 Q190 L191 D192 C193 N194 F195 L196 K197 S201 V204 D205 K206 Y207 I208 G209 E210 S211 A212 R213 L214 I215 R216 F219 R223 D224 H225 Q226 M232 D233 E234 I235 D236 A237 I238 G239 G240 R241 R242 F243 S244

E245 G246 T247 S248 A249 D250 R251 E252 I253 Q254 R255 T256 L257 M258 E259 L260 L261 N262 Q263 M264 D265 G266 F267 D268 T269 L270 H271 R272 V273 K274 M277 A278 T279 N280 D283 T284 L285 D286 P287 A288 L289 L290 G293 R294 L295 D296 R297 K298 D302 N305 E306 Q307 A308 R309 L310

D311 K314 P319 I320 T321 K322 H323 G324 E325 I326 D327 Y328 E329 A330 I331 V332 K333 L334 S335 D336 G337 F338 A341 E349 F353 A354 I355 R356 A357 D358 H359 Q364 E365 D366 F367 M368 K369 R372 A375 D376 S377 K378 K379 L380 E381 S382 K383 L384 D385 Y386 K387 P388

V389

- Molecule 31: 26S proteasome regulatory subunit 6A

Chain F: 56% 93% • 5%

R44 T45 R46 L47 L48 D49 S50 E51 I52 K53 I54 M55 K56 S57 E58 V59 L60 R61 V62 T63 H64 E65 L66 Q67 A68 M69 K70 D71 K72 I73 K74 E75 N76 S77 E78 K79 I80 K81 V82 N83 K84 T85 Y88 N92 V93 I94 E95 L96 L97 D98 V99 ASP PRO ASN ASP GLN GLU GLU

ASP GLY ALA ASN ILE ASP LEU ASP SER GLN ARG LYS GLY K120 C121 A122 S127 F133 L134 P135 V136 I137 G138 L139 V140 D141 A142 E143 K144 L145 K146 L150 V151 G152 V153 N154 K155 D156 S157 Y158 L159 I160 L161 E162 T163 L164 P165 T166 E167 Y168 D169 S170 R171 V172 K173 A174 M175

E176 V177 D178 E179 R180 P181 T182 E183 Q184 Y185 S186 D187 G190 L191 Q194 I195 Q196 E197 L198 V199 E200 A201 L204 N207 H208 K209 E210 E213 N214 L215 G216 I217 Q218 P219 G222 V223 L224 R238 A239 C240 A241 A242 Q243 T244 K245 A246 T247 F248 L249 K250 G253 P254

Q255 L256 V257 Q258 M259 F260 I261 G262 D263 G264 A265 K266 L267 V268 R269 D270 A273 E277 K278 A279 E287 L288 D289 A290 I291 K294 R295 F296 D297 S298 E299 K300 A301 G302 D303 R304 E305 R308 T309 M310 L311 E312 N315 Q316 L317 D318 G319 F320 Q321 T324 Q325 V326 K327

A330 A331 R334 V335 D336 I337 L338 D339 P340 A341 L342 L343 R344 S345 D349 R350 K351 F354 N358 A361 M366 H369 S370 R371 K372 M373 N374 V375 S376 P377 D378 V379 N380 Y381 E382 E383 L384 A385 R386 C387 T388 D389 D390 G393 V399 R409 R410 G411 A412

T413 E414 L415 T416 H417 E418 D419 Y420 M421 E422 L425 E426 V427 Q428 A429 K430 K431 K432 A433 N434 L435 Q436 A439

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

Chain f: 68% 73% • 24%

MET GLU GLU GLY GLY R6 D7 K8 A9 P10 V11 Q12 P13 Q14 Q15 S16 P17 A18 A19 A20 P21 G22 G23 T24 D25 E26 K27 P28 S29 G30 K31 E32 R33 R34 D35 A36 G37 D38 K39 D40 K41 E42 Q43 E44 L45 S46 E47 E48 D49 K50 Q51 L52 Q53 D54 E55 LEU GLU MET LEU VAL

GLU ARG LEU GLY GLU LYS ASP THR SER L70 Y71 R72 P73 A74 L75 E76 E77 L78 R79 R80 Q81 I82 R83 S84 S85 T86 T87 S88 M89 T90 S91 V92 P93 K94 P95 L96 K97 F98 L99 R100 P101 H102 Y103 GLY LYS LEU LYS GLU ILE TYR GLU ASN MET ALA PRO GLY GLU N118 K119 R120

F121 A122 A123 D124 I125 I126 S127 V128 L129 A130 M131 T132 M133 E136 R137 E138 C139 L140 K141 Y142 R143 L144 V145 G146 SER GLN GLU GLU LEU ALA SER TRP GLY HIS GLU TYR VAL ARG HIS LEU A163 G164 E165 V166 A167 K168 E169 W170 Q171 E172 L173 D174 D175 A176 E177 K178 V179 Q180 R181

E182 P183 L184 L185 T186 L187 V188 K189 E190 I191 V192 P193 TYR ASN MET ALA HIS ASN ALA GLU HIS GLU ALA CYS ASP L207 L208 M209 E210 I211 E212 Q213 V214 D215 M216 L217 E218 K219 D220 I221 D222 E223 N224 A225 Y226 A227 K228 V229 C230 L231 Y232 L233 T234 S235 C236 V237 N238 Y239 V240 P241

E242 P243 E244 N245 S246 A247 L248 L249 R250 C251 A252 L253 G254 V255 K258 F259 S260 R261 F262 P263 E264 A265 L266 R267 L268 A269 L270 M271 L272 N273 D274 M275 E276 L277 V278 E279 D280 I281 F282 T283 S284 C285 K286 D287 V288 V289 VAL GLN LYS GLN MET ALA PHE M297 L298 G299 R300 H301 G302

V303 F304 L305 E306 L307 S308 E309 D310 V311 E312 E313 Y314 E315 D316 L317 T318 E319 I320 M321 S322 N323 V324 G325 L326 N327 S328 N329 F330 L331 A332 L333 A334 R335 E336 L337 D338 I339 M340 E341 P342 K343 V344 P345 D346 D347 I348 Y349 K350 T351 H352 L353 E354 N355 N356 R357 F358 G359 G360 S361 G362

S363 Q364 V365 D366 S367 A368 R369 M370 N371 L372 A373 S374 S375 F376 V377 N378 G379 F380 V381 N382 ALA ALA PHE GLY Q387 D388 K389 L390 L391 T392 D393 D394 G395 N396 K397 W398 L399 Y400 K401 N402 K403 D404 H405 G406 M407 L408 S409 A410 A411 A412 S413 L414 G415 M416 I417 L418 L419 W420 D421 V422

D423 G424 G425 L426 T427 Q428 I429 D430 K431 Y432 L433 Y434 S435 S436 E437 D438 Y439 I440 K441 S442 G443 A444 L445 L446 A447 C448 G449 I450 V451 N452 S453 G454 V455 R456 N457 E458 C459 D460 P461 A462 L463 A464 L465 L466 S467 D468 Y469 V470 L471 H472 N473 S474 N475 T476 M477 R478 L479 G480 S481 I482

F483 G484 L485 G486 L487 A488 Y489 A490 G491 S492 N493 R494 E495 D496 V497 L498 T499 L500 L501 L502 P503 V504 M505 G506 D507 S508 K509 S510 S511 M512 E513 V514 A515 G516 V517 T518 A519 L520 A521 C522 G523 M524 I525 A526 V527 G528 S529 C530 N531 G532 D533 V534 T535 S536 T537 I538 L539 Q540 T541 I542

M543 E544 K545 S546 E547 T548 E549 L550 K551 D552 T553 Y554 A555 R556 W557 L558 P559 L560 G561 L562 G563 L564 N565 H566 L567 G568 K569 G570 E571 A572 I573 E574 A575 I576 L577 A578 A579 L580 E581 V582 V583 S584 E585 P586 F587 R588 S589 F590 A591 N592 T593 L594 V595 D596 V597 C598 A599 Y600 A601 G602

S603 G604 N605 V606 L607 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 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 A689 V690 P691 L692 A693 L694 A695 L696 I697 S698 V699 SER ASN PRO ARG LEU ASN ILE LEU 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 | 66246 | 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 ($e^-/Å^2$) | 10 | 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 | 0.023 | Depositor |
| Minimum map value | -0.010 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.008 | 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 (i)

## 5.1 Standard geometry (i)

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

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 | G | 0.37 | 0/1853 | 0.60 | 0/2515 |
| 1 | g | 0.36 | 0/1859 | 0.58 | 0/2523 |
| 2 | H | 0.38 | 0/1723 | 0.60 | 1/2346 (0.0%) |
| 2 | h | 0.35 | 0/1743 | 0.56 | 0/2372 |
| 3 | I | 0.37 | 0/1925 | 0.65 | 0/2606 |
| 3 | i | 0.36 | 0/1942 | 0.64 | 0/2628 |
| 4 | J | 0.37 | 0/1728 | 0.59 | 0/2358 |
| 4 | j | 0.35 | 0/1728 | 0.58 | 0/2358 |
| 5 | K | 0.35 | 0/1755 | 0.66 | 2/2375 (0.1%) |
| 5 | k | 0.34 | 0/1747 | 0.58 | 0/2364 |
| 6 | L | 0.38 | 0/1885 | 0.60 | 0/2552 |
| 6 | l | 0.36 | 0/1885 | 0.59 | 0/2552 |
| 7 | M | 0.39 | 0/1891 | 0.60 | 1/2552 (0.0%) |
| 7 | m | 0.39 | 0/1891 | 0.58 | 0/2552 |
| 8 | N | 0.39 | 0/1454 | 0.55 | 0/1967 |
| 8 | n | 0.38 | 0/1454 | 0.57 | 0/1967 |
| 9 | O | 0.36 | 0/1670 | 0.57 | 0/2265 |
| 9 | o | 0.36 | 0/1670 | 0.57 | 0/2265 |
| 10 | P | 0.37 | 0/1614 | 0.54 | 0/2177 |
| 10 | p | 0.37 | 0/1614 | 0.55 | 0/2177 |
| 11 | Q | 0.40 | 0/1603 | 0.62 | 0/2174 |
| 11 | q | 0.42 | 0/1603 | 0.64 | 0/2174 |
| 12 | R | 0.39 | 0/1579 | 0.53 | 0/2134 |
| 12 | r | 0.38 | 0/1579 | 0.52 | 0/2134 |
| 13 | S | 0.36 | 0/1671 | 0.54 | 0/2253 |
| 13 | s | 0.37 | 0/1671 | 0.55 | 0/2253 |
| 14 | T | 0.39 | 0/1700 | 0.56 | 0/2305 |
| 14 | t | 0.37 | 0/1700 | 0.55 | 0/2305 |
| 15 | U | 0.34 | 0/6396 | 0.66 | 4/8646 (0.0%) |
| 16 | V | 0.37 | 0/3883 | 0.72 | 3/5247 (0.1%) |
| 17 | W | 0.34 | 0/3751 | 0.69 | 3/5042 (0.1%) |
| 18 | Y | 0.36 | 0/3173 | 0.71 | 1/4273 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 19 | Z | 0.35 | 0/2324 | 0.73 | 4/3150 (0.1%) |
| 20 | a | 0.32 | 0/3053 | 0.68 | 4/4133 (0.1%) |
| 21 | b | 0.33 | 0/1478 | 0.70 | 1/2001 (0.0%) |
| 22 | c | 0.36 | 0/2226 | 0.70 | 1/3007 (0.0%) |
| 23 | d | 0.35 | 0/2162 | 0.72 | 1/2919 (0.0%) |
| 24 | e | 0.38 | 0/338 | 0.78 | 1/450 (0.2%) |
| 25 | X | 0.33 | 0/3053 | 0.62 | 0/4115 |
| 26 | A | 0.34 | 0/2939 | 0.61 | 0/3970 |
| 27 | B | 0.33 | 0/2844 | 0.63 | 2/3846 (0.1%) |
| 28 | C | 0.33 | 0/2896 | 0.65 | 1/3895 (0.0%) |
| 29 | D | 0.37 | 0/3090 | 0.71 | 4/4168 (0.1%) |
| 30 | E | 0.32 | 0/2904 | 0.57 | 1/3924 (0.0%) |
| 31 | F | 0.35 | 0/2897 | 0.64 | 3/3912 (0.1%) |
| 32 | f | 0.31 | 0/5393 | 0.68 | 1/7271 (0.0%) |
| All | All | 0.36 | 0/102937 | 0.63 | 39/139172 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | G | 0 | 1 |
| 1 | g | 0 | 1 |
| 3 | I | 0 | 1 |
| 4 | J | 0 | 1 |
| 4 | j | 0 | 1 |
| 5 | K | 0 | 4 |
| 7 | M | 0 | 1 |
| 8 | n | 0 | 1 |
| 9 | O | 0 | 1 |
| 15 | U | 0 | 2 |
| 16 | V | 0 | 3 |
| 19 | Z | 0 | 2 |
| 20 | a | 0 | 2 |
| 21 | b | 0 | 1 |
| 23 | d | 0 | 2 |
| 25 | X | 0 | 2 |
| 26 | A | 0 | 1 |
| 28 | C | 0 | 2 |
| 29 | D | 0 | 6 |
| All | All | 0 | 35 |

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | b | 21 | PHE | C-N-CA | 8.09 | 141.92 | 121.70 |
| 29 | D | 368 | ASP | C-N-CA | 7.78 | 141.14 | 121.70 |
| 24 | e | 56 | LEU | CA-CB-CG | 7.42 | 132.36 | 115.30 |
| 20 | a | 180 | LEU | CA-CB-CG | 7.18 | 131.82 | 115.30 |
| 18 | Y | 287 | LEU | CA-CB-CG | 7.11 | 131.64 | 115.30 |

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | G | 222 | VAL | Peptide |
| 3 | I | 6 | ASP | Peptide |
| 4 | J | 2 | SER | Peptide |
| 5 | K | 19 | GLY | Peptide |
| 5 | K | 9 | ASP | 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 | G | 237/240 (99%) | 210 (89%) | 27 (11%) | 0 | 100 | 100 |
| 1 | g | 238/240 (99%) | 218 (92%) | 20 (8%) | 0 | 100 | 100 |
| 2 | H | 228/232 (98%) | 213 (93%) | 15 (7%) | 0 | 100 | 100 |
| 2 | h | 230/232 (99%) | 226 (98%) | 4 (2%) | 0 | 100 | 100 |
| 3 | I | 246/250 (98%) | 226 (92%) | 19 (8%) | 1 (0%) | 30 | 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | i | 248/250 (99%) | 227 (92%) | 20 (8%) | 1 (0%) | 30 | 67 |
| 4 | J | 237/243 (98%) | 218 (92%) | 19 (8%) | 0 | 100 | 100 |
| 4 | j | 237/243 (98%) | 216 (91%) | 20 (8%) | 1 (0%) | 30 | 67 |
| 5 | K | 224/234 (96%) | 205 (92%) | 18 (8%) | 1 (0%) | 30 | 67 |
| 5 | k | 224/234 (96%) | 206 (92%) | 18 (8%) | 0 | 100 | 100 |
| 6 | L | 236/238 (99%) | 225 (95%) | 11 (5%) | 0 | 100 | 100 |
| 6 | l | 236/238 (99%) | 224 (95%) | 12 (5%) | 0 | 100 | 100 |
| 7 | M | 238/245 (97%) | 221 (93%) | 17 (7%) | 0 | 100 | 100 |
| 7 | m | 238/245 (97%) | 222 (93%) | 16 (7%) | 0 | 100 | 100 |
| 8 | N | 189/191 (99%) | 180 (95%) | 8 (4%) | 1 (0%) | 25 | 62 |
| 8 | n | 189/191 (99%) | 178 (94%) | 8 (4%) | 3 (2%) | 8 | 38 |
| 9 | O | 218/220 (99%) | 207 (95%) | 11 (5%) | 0 | 100 | 100 |
| 9 | o | 218/220 (99%) | 207 (95%) | 11 (5%) | 0 | 100 | 100 |
| 10 | P | 202/204 (99%) | 193 (96%) | 9 (4%) | 0 | 100 | 100 |
| 10 | p | 202/204 (99%) | 190 (94%) | 12 (6%) | 0 | 100 | 100 |
| 11 | Q | 197/199 (99%) | 178 (90%) | 19 (10%) | 0 | 100 | 100 |
| 11 | q | 197/199 (99%) | 177 (90%) | 20 (10%) | 0 | 100 | 100 |
| 12 | R | 199/201 (99%) | 187 (94%) | 12 (6%) | 0 | 100 | 100 |
| 12 | r | 199/201 (99%) | 189 (95%) | 10 (5%) | 0 | 100 | 100 |
| 13 | S | 211/213 (99%) | 205 (97%) | 6 (3%) | 0 | 100 | 100 |
| 13 | s | 211/213 (99%) | 204 (97%) | 7 (3%) | 0 | 100 | 100 |
| 14 | T | 213/215 (99%) | 206 (97%) | 7 (3%) | 0 | 100 | 100 |
| 14 | t | 213/215 (99%) | 204 (96%) | 9 (4%) | 0 | 100 | 100 |
| 15 | U | 798/911 (88%) | 721 (90%) | 77 (10%) | 0 | 100 | 100 |
| 16 | V | 471/480 (98%) | 411 (87%) | 55 (12%) | 5 (1%) | 12 | 46 |
| 17 | W | 454/456 (100%) | 400 (88%) | 51 (11%) | 3 (1%) | 19 | 56 |
| 18 | Y | 376/378 (100%) | 325 (86%) | 48 (13%) | 3 (1%) | 16 | 54 |
| 19 | Z | 284/286 (99%) | 246 (87%) | 35 (12%) | 3 (1%) | 12 | 46 |
| 20 | a | 371/373 (100%) | 331 (89%) | 39 (10%) | 1 (0%) | 37 | 71 |
| 21 | b | 189/191 (99%) | 170 (90%) | 17 (9%) | 2 (1%) | 12 | 46 |
| 22 | c | 274/287 (96%) | 235 (86%) | 38 (14%) | 1 (0%) | 30 | 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 23 | d | 255/257 (99%) | 219 (86%) | 35 (14%) | 1 (0%) | 30 | 67 |
| 24 | e | 36/70 (51%) | 29 (81%) | 7 (19%) | 0 | 100 | 100 |
| 25 | X | 378/380 (100%) | 341 (90%) | 35 (9%) | 2 (0%) | 25 | 62 |
| 26 | A | 376/399 (94%) | 327 (87%) | 45 (12%) | 4 (1%) | 12 | 46 |
| 27 | B | 366/389 (94%) | 322 (88%) | 42 (12%) | 2 (0%) | 25 | 62 |
| 28 | C | 359/392 (92%) | 320 (89%) | 36 (10%) | 3 (1%) | 16 | 54 |
| 29 | D | 378/380 (100%) | 323 (85%) | 49 (13%) | 6 (2%) | 8 | 38 |
| 30 | E | 373/375 (100%) | 340 (91%) | 33 (9%) | 0 | 100 | 100 |
| 31 | F | 372/396 (94%) | 337 (91%) | 33 (9%) | 2 (0%) | 25 | 62 |
| 32 | f | 669/908 (74%) | 579 (86%) | 82 (12%) | 8 (1%) | 11 | 44 |
| All | All | 12934/13558 (95%) | 11738 (91%) | 1142 (9%) | 54 (0%) | 32 | 67 |

5 of 54 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | V | 78 | HIS |
| 16 | V | 262 | SER |
| 17 | W | 314 | LEU |
| 18 | Y | 283 | LYS |
| 18 | Y | 284 | LYS |

### 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 | G | 192/205 (94%) | 191 (100%) | 1 (0%) | 86 | 90 |
| 1 | g | 193/205 (94%) | 193 (100%) | 0 | 100 | 100 |
| 2 | H | 162/190 (85%) | 161 (99%) | 1 (1%) | 84 | 88 |
| 2 | h | 164/190 (86%) | 164 (100%) | 0 | 100 | 100 |
| 3 | I | 191/210 (91%) | 190 (100%) | 1 (0%) | 86 | 90 |
| 3 | i | 193/210 (92%) | 192 (100%) | 1 (0%) | 86 | 90 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | J | 152/207 (73%) | 149 (98%) | 3 (2%) | 50 | 68 |
| 4 | j | 152/207 (73%) | 152 (100%) | 0 | 100 | 100 |
| 5 | K | 187/196 (95%) | 186 (100%) | 1 (0%) | 86 | 90 |
| 5 | k | 186/196 (95%) | 186 (100%) | 0 | 100 | 100 |
| 6 | L | 198/204 (97%) | 198 (100%) | 0 | 100 | 100 |
| 6 | l | 198/204 (97%) | 198 (100%) | 0 | 100 | 100 |
| 7 | M | 192/202 (95%) | 192 (100%) | 0 | 100 | 100 |
| 7 | m | 192/202 (95%) | 192 (100%) | 0 | 100 | 100 |
| 8 | N | 148/148 (100%) | 148 (100%) | 0 | 100 | 100 |
| 8 | n | 148/148 (100%) | 148 (100%) | 0 | 100 | 100 |
| 9 | O | 177/181 (98%) | 177 (100%) | 0 | 100 | 100 |
| 9 | o | 177/181 (98%) | 177 (100%) | 0 | 100 | 100 |
| 10 | P | 172/173 (99%) | 172 (100%) | 0 | 100 | 100 |
| 10 | p | 172/173 (99%) | 172 (100%) | 0 | 100 | 100 |
| 11 | Q | 164/170 (96%) | 164 (100%) | 0 | 100 | 100 |
| 11 | q | 164/170 (96%) | 163 (99%) | 1 (1%) | 84 | 88 |
| 12 | R | 153/156 (98%) | 153 (100%) | 0 | 100 | 100 |
| 12 | r | 153/156 (98%) | 153 (100%) | 0 | 100 | 100 |
| 13 | S | 174/178 (98%) | 174 (100%) | 0 | 100 | 100 |
| 13 | s | 174/178 (98%) | 173 (99%) | 1 (1%) | 84 | 88 |
| 14 | T | 175/178 (98%) | 174 (99%) | 1 (1%) | 84 | 88 |
| 14 | t | 175/178 (98%) | 174 (99%) | 1 (1%) | 84 | 88 |
| 15 | U | 685/779 (88%) | 681 (99%) | 4 (1%) | 84 | 88 |
| 16 | V | 410/414 (99%) | 405 (99%) | 5 (1%) | 67 | 78 |
| 17 | W | 416/416 (100%) | 410 (99%) | 6 (1%) | 62 | 75 |
| 18 | Y | 334/334 (100%) | 332 (99%) | 2 (1%) | 84 | 88 |
| 19 | Z | 257/257 (100%) | 253 (98%) | 4 (2%) | 58 | 73 |
| 20 | a | 333/333 (100%) | 332 (100%) | 1 (0%) | 91 | 92 |
| 21 | b | 167/167 (100%) | 167 (100%) | 0 | 100 | 100 |
| 22 | c | 243/252 (96%) | 243 (100%) | 0 | 100 | 100 |
| 23 | d | 231/231 (100%) | 230 (100%) | 1 (0%) | 89 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 24 | e | 38/38 (100%) | 38 (100%) | 0 | 100 | 100 |
| 25 | X | 327/327 (100%) | 321 (98%) | 6 (2%) | 54 | 71 |
| 26 | A | 298/343 (87%) | 293 (98%) | 5 (2%) | 56 | 72 |
| 27 | B | 300/345 (87%) | 296 (99%) | 4 (1%) | 65 | 76 |
| 28 | C | 315/340 (93%) | 312 (99%) | 3 (1%) | 73 | 81 |
| 29 | D | 333/333 (100%) | 330 (99%) | 3 (1%) | 75 | 83 |
| 30 | E | 298/329 (91%) | 292 (98%) | 6 (2%) | 50 | 68 |
| 31 | F | 296/340 (87%) | 295 (100%) | 1 (0%) | 91 | 92 |
| 32 | f | 580/763 (76%) | 559 (96%) | 21 (4%) | 30 | 52 |
| All | All | 10739/11537 (93%) | 10655 (99%) | 84 (1%) | 77 | 84 |

5 of 84 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | E | 161 | ARG |
| 32 | f | 391 | LEU |
| 30 | E | 255 | ARG |
| 32 | f | 184 | LEU |
| 32 | f | 479 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | E | 194 | ASN |
| 31 | F | 333 | ASN |
| 32 | f | 752 | HIS |
| 18 | Y | 306 | GLN |
| 18 | Y | 178 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 34 | AGS | E | 401 | - | 28,33,33 | 1.11 | 2 (7%) | 31,52,52 | 1.20 | 3 (9%) |
| 34 | AGS | A | 501 | - | 28,33,33 | 1.01 | 2 (7%) | 31,52,52 | 1.31 | 3 (9%) |
| 34 | AGS | F | 501 | - | 28,33,33 | 1.20 | 2 (7%) | 31,52,52 | 1.53 | 4 (12%) |
| 34 | AGS | D | 501 | - | 28,33,33 | 0.97 | 3 (10%) | 31,52,52 | 1.41 | 4 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 34 | AGS | E | 401 | - | - | 6/17/38/38 | 0/3/3/3 |
| 34 | AGS | A | 501 | - | - | 5/17/38/38 | 0/3/3/3 |
| 34 | AGS | F | 501 | - | - | 6/17/38/38 | 0/3/3/3 |
| 34 | AGS | D | 501 | - | - | 8/17/38/38 | 0/3/3/3 |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 34 | E | 401 | AGS | PA-O3A | -3.47 | 1.55 | 1.59 |
| 34 | F | 501 | AGS | PB-O3B | -3.28 | 1.56 | 1.59 |
| 34 | F | 501 | AGS | PB-O3A | -3.16 | 1.56 | 1.59 |
| 34 | D | 501 | AGS | PB-O3B | -2.88 | 1.56 | 1.59 |
| 34 | E | 401 | AGS | PB-O3A | -2.33 | 1.57 | 1.59 |

The worst 5 of 14 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | F | 501 | AGS | PB-O3B-PG | -5.95 | 111.39 | 133.17 |
| 34 | D | 501 | AGS | PB-O3B-PG | -5.72 | 112.25 | 133.17 |
| 34 | A | 501 | AGS | PB-O3B-PG | -4.36 | 117.21 | 133.17 |
| 34 | E | 401 | AGS | PB-O3B-PG | -3.84 | 119.12 | 133.17 |
| 34 | E | 401 | AGS | O3A-PA-O1A | -2.70 | 102.58 | 110.70 |

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

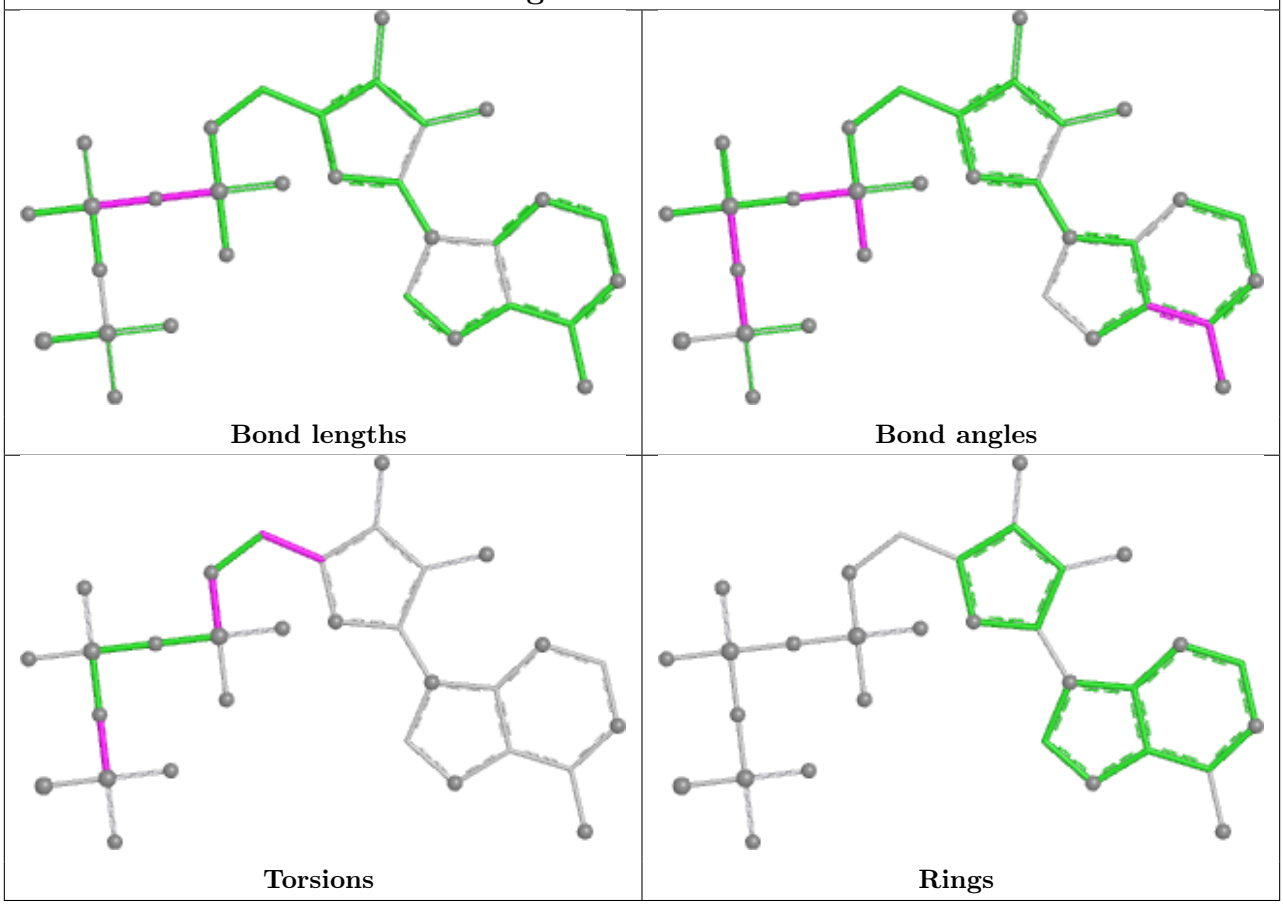
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 34 | A | 501 | AGS | C5'-O5'-PA-O1A |
| 34 | D | 501 | AGS | C5'-O5'-PA-O1A |
| 34 | D | 501 | AGS | C5'-O5'-PA-O3A |
| 34 | E | 401 | AGS | PB-O3B-PG-O2G |
| 34 | E | 401 | AGS | C5'-O5'-PA-O1A |

There are no ring outliers.

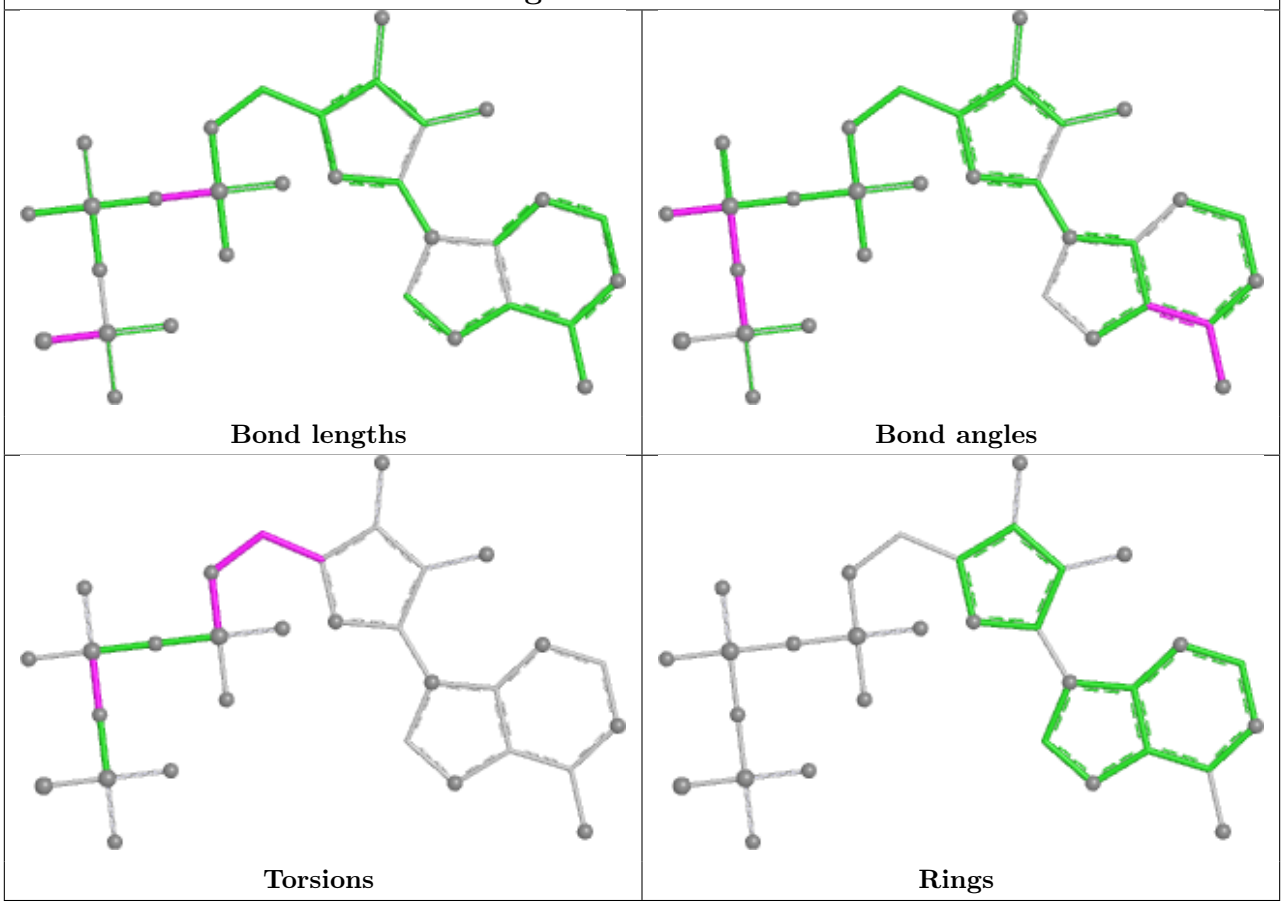
No monomer is involved in short contacts.

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

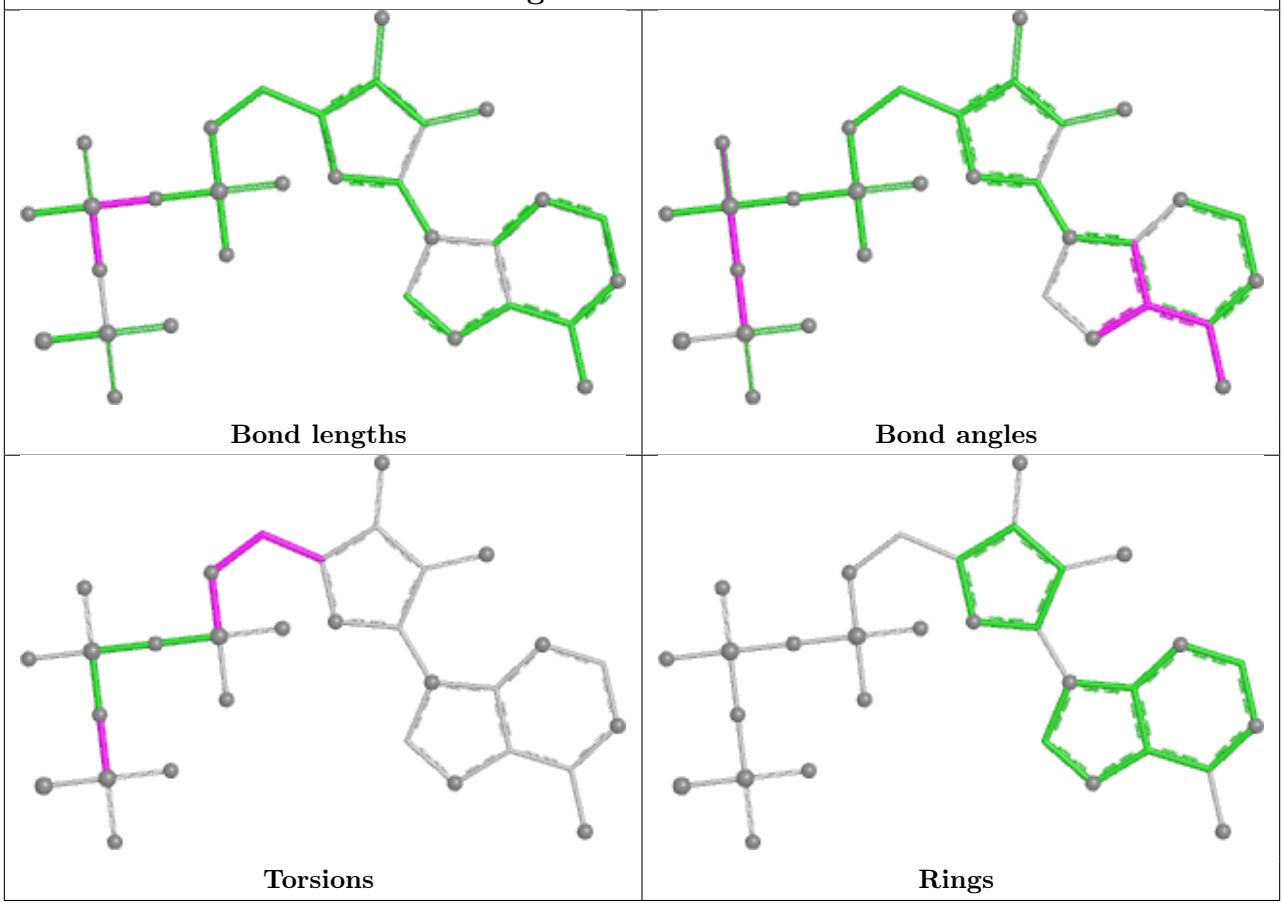
**Ligand AGS E 401**

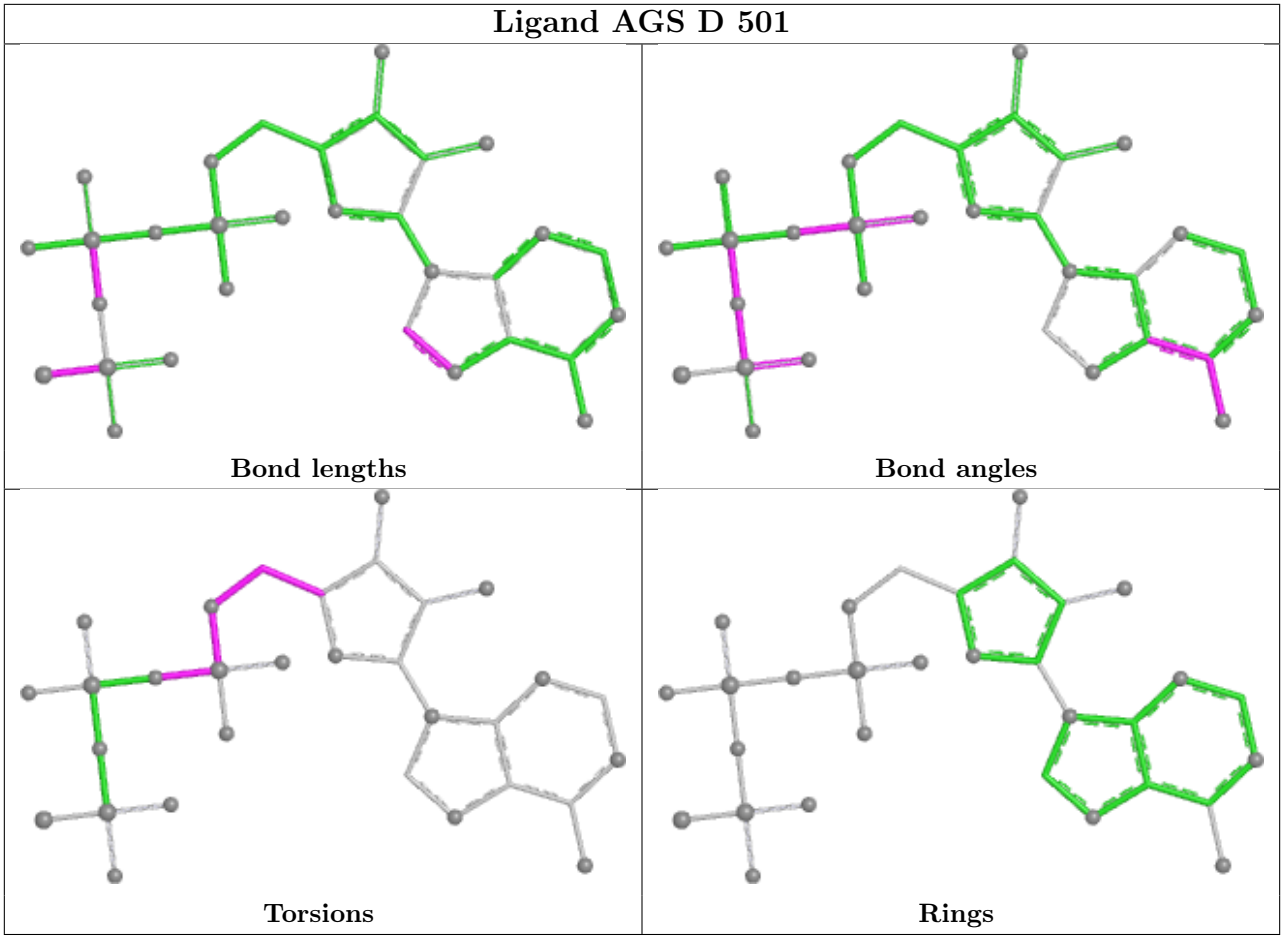


**Ligand AGS A 501**



**Ligand AGS F 501**






## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

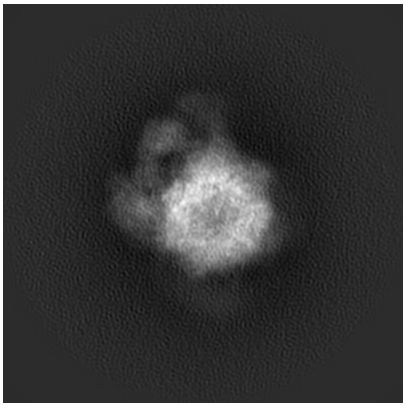
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8663. These allow visual inspection of the internal detail of the map and identification of artifacts.

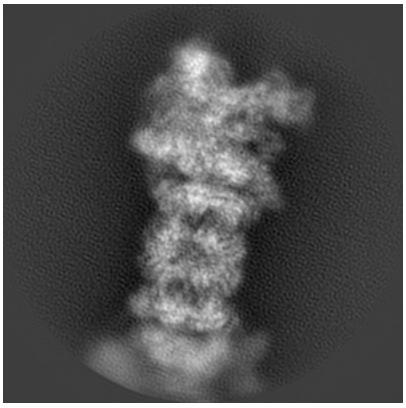
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

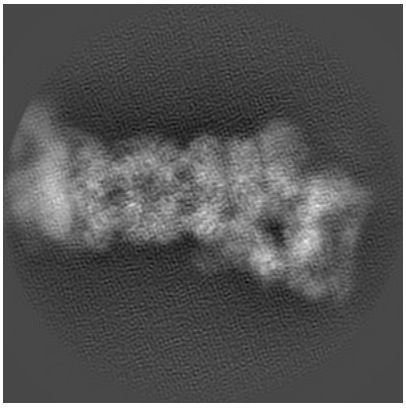
### 6.1.1 Primary map



X



Y

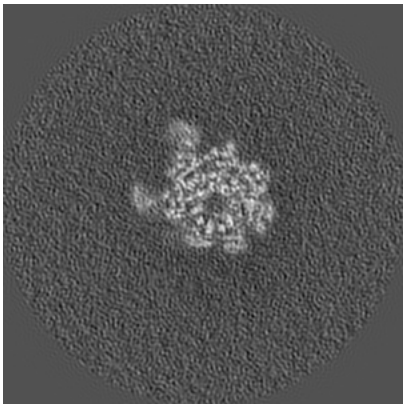


Z

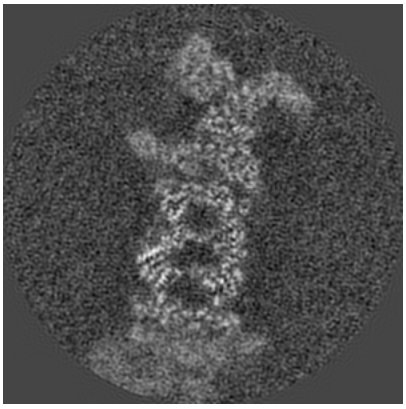
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

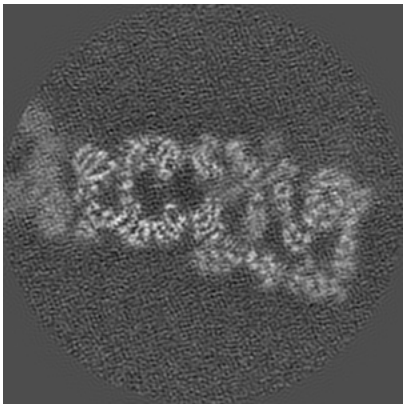
### 6.2.1 Primary map



X Index: 280



Y Index: 280

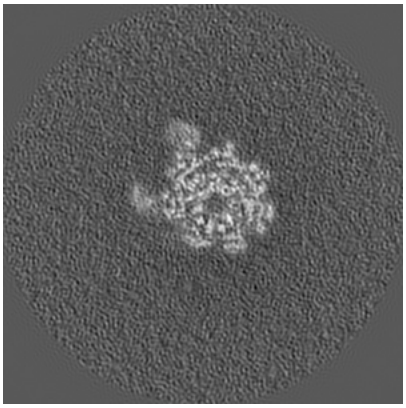


Z Index: 280

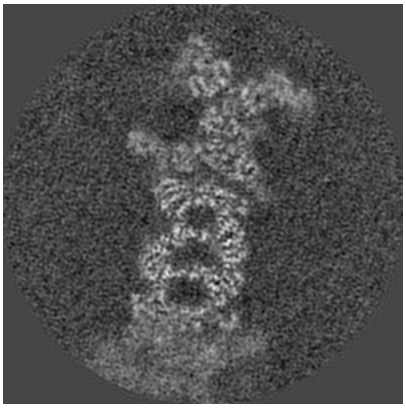
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

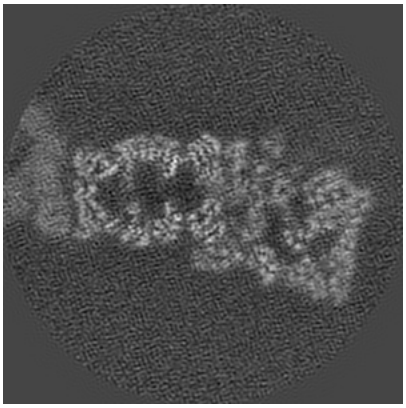
### 6.3.1 Primary map



X Index: 281



Y Index: 277

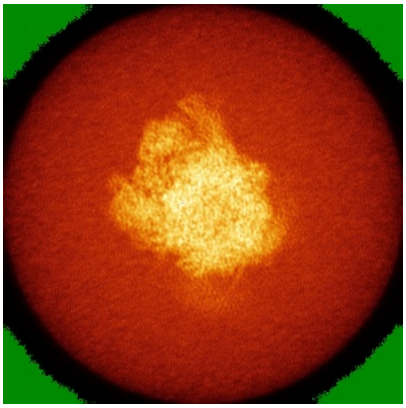


Z Index: 275

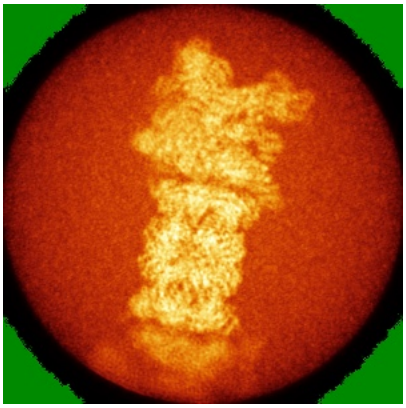
The images above show the largest variance slices of the map in three orthogonal directions.

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

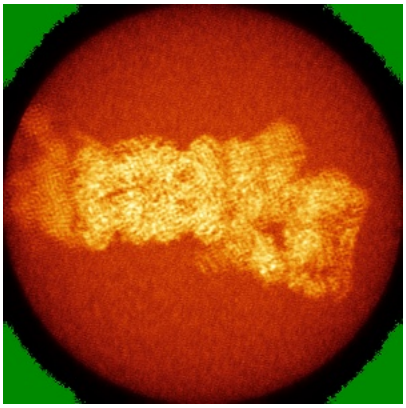
### 6.4.1 Primary map



X



Y

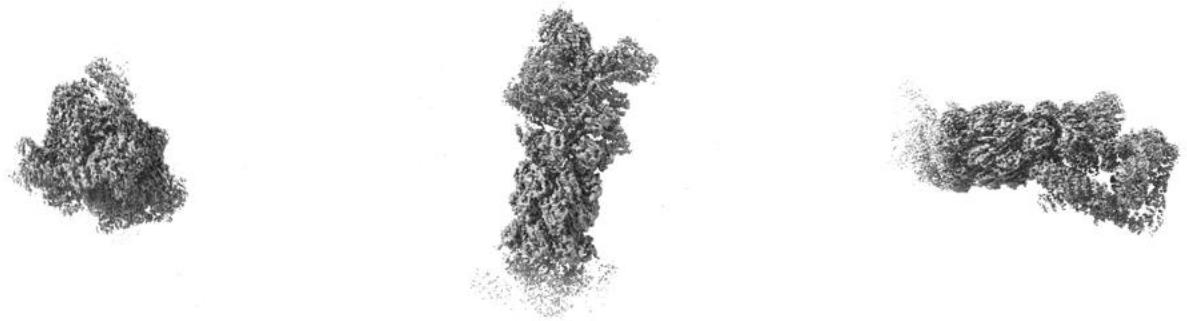


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

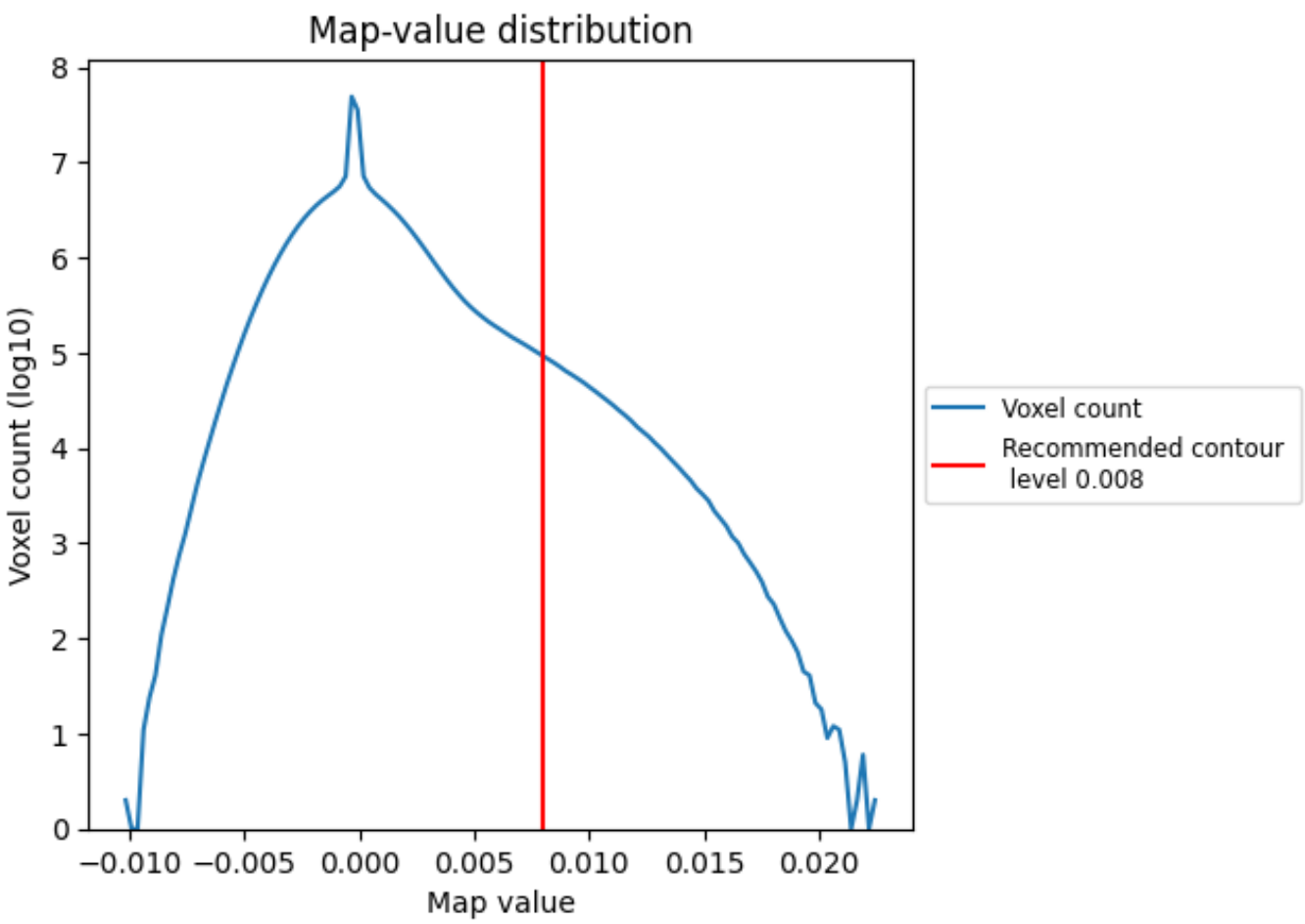
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

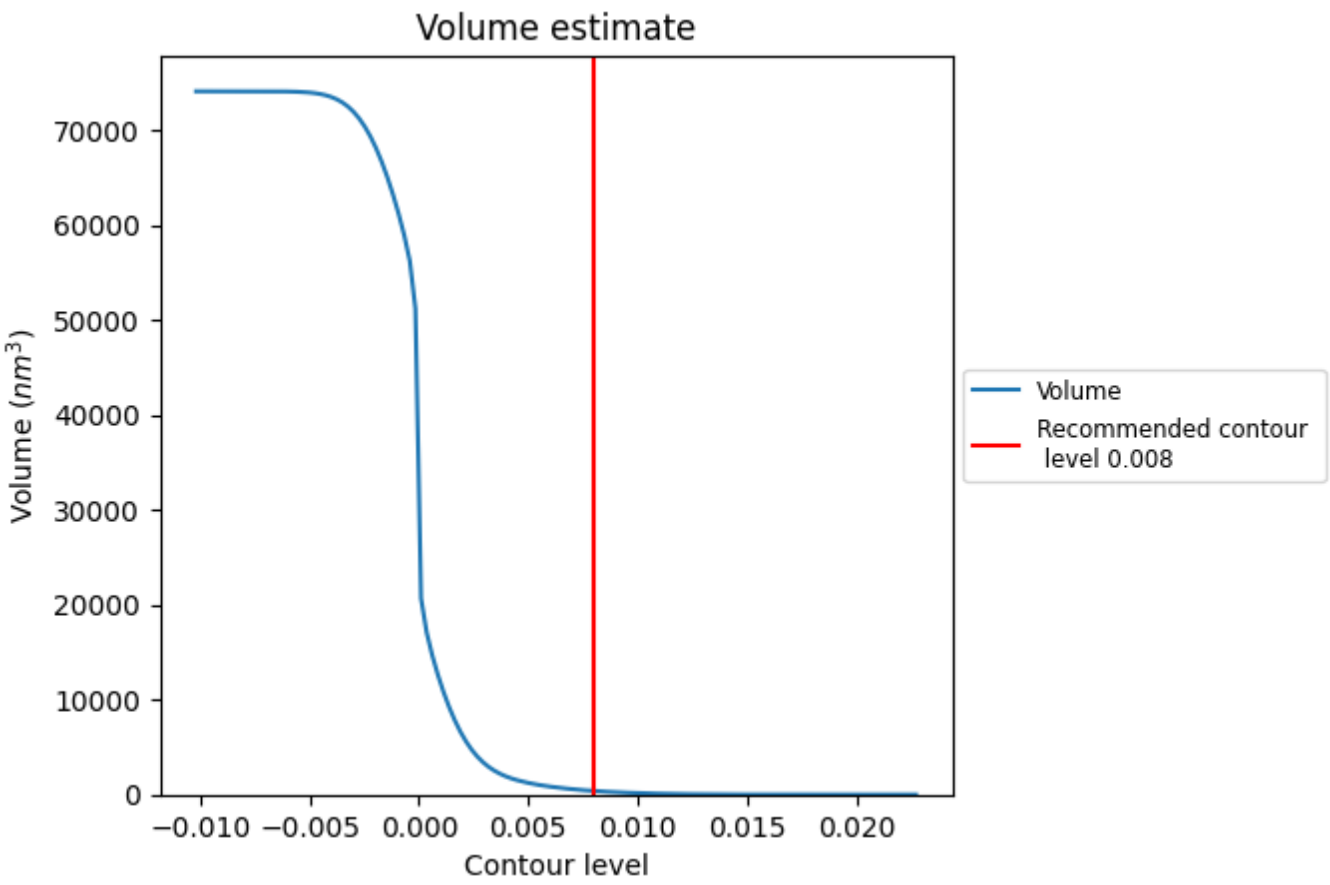
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

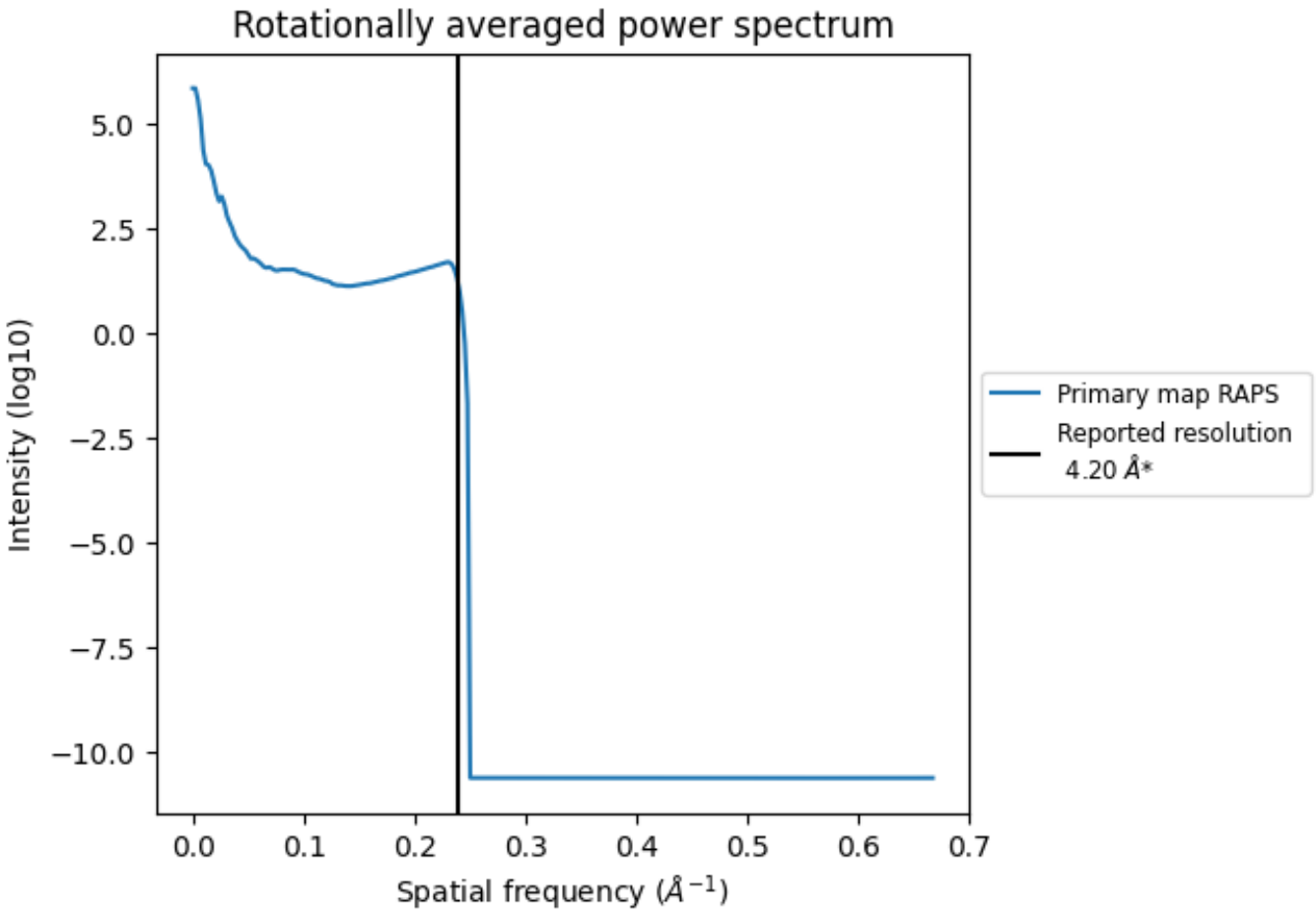
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 381 $nm^3$; this corresponds to an approximate mass of 344 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 0.238 Å$^{-1}$

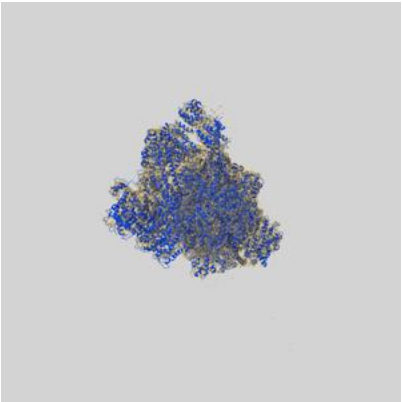
# 8 Fourier-Shell correlation (i)

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

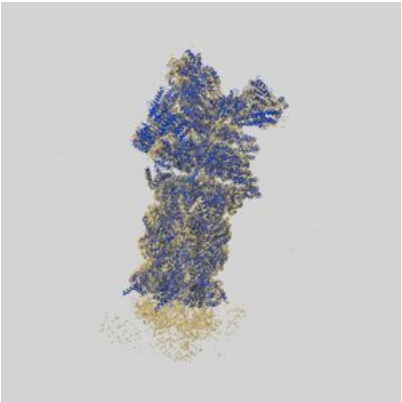
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8663 and PDB model 5VFP. Per-residue inclusion information can be found in section 3 on page 12.

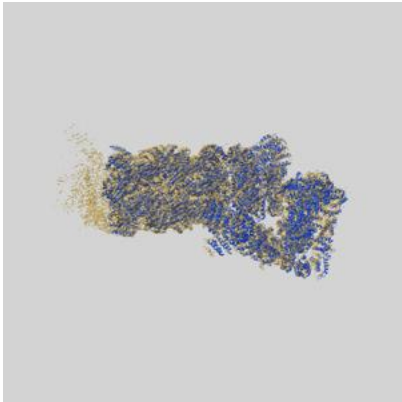
## 9.1 Map-model overlay (i)



X



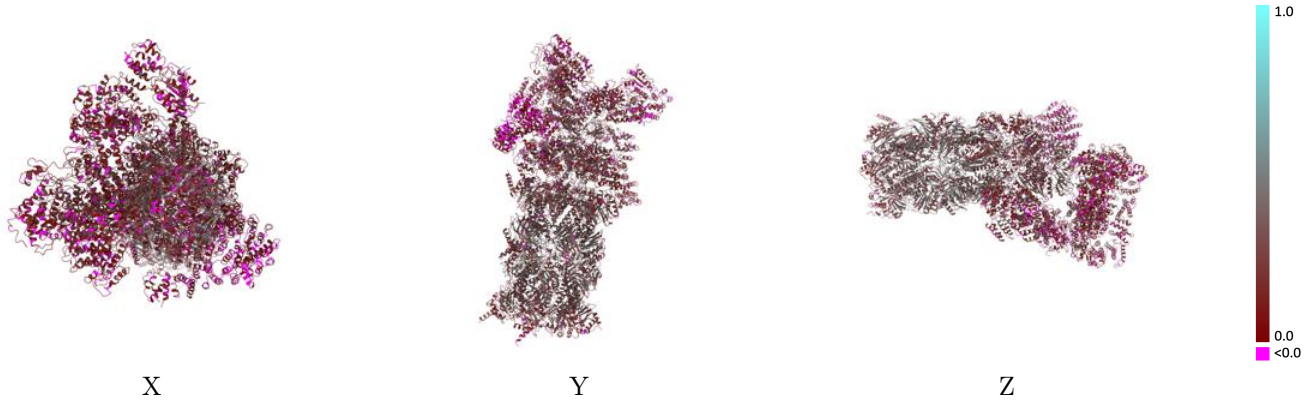
Y



Z

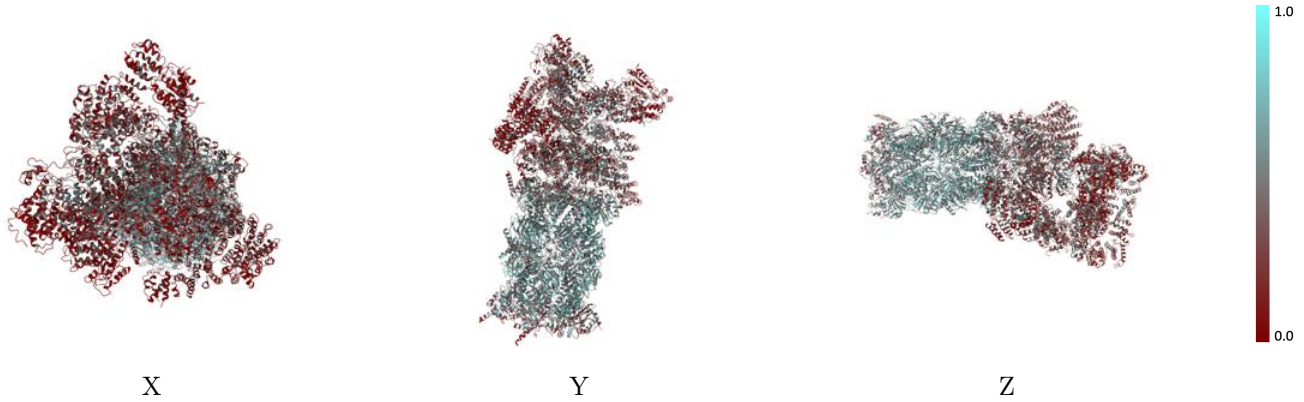
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



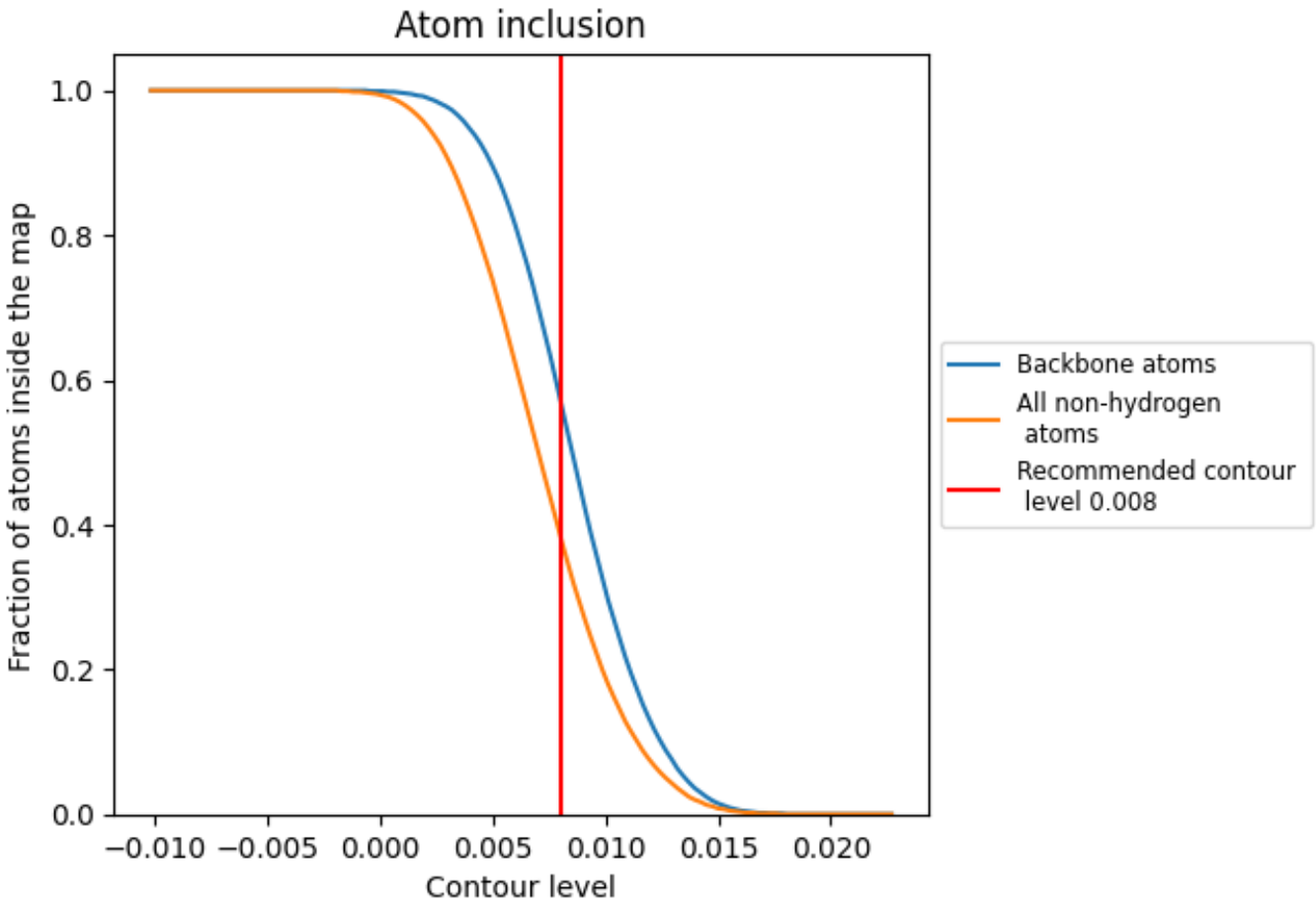

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)




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 (0.008).

## 9.4 Atom inclusion (i)




At the recommended contour level, 57% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.3840 | 0.2500 |
| A | 0.3480 | 0.2590 |
| B | 0.2810 | 0.2520 |
| C | 0.2830 | 0.2300 |
| D | 0.2940 | 0.2570 |
| E | 0.3560 | 0.2650 |
| F | 0.3600 | 0.2590 |
| G | 0.5150 | 0.3320 |
| H | 0.5350 | 0.3240 |
| I | 0.4580 | 0.2840 |
| J | 0.4330 | 0.2700 |
| K | 0.4490 | 0.2760 |
| L | 0.5040 | 0.3020 |
| M | 0.5070 | 0.3020 |
| N | 0.6130 | 0.3610 |
| O | 0.5520 | 0.3400 |
| P | 0.5710 | 0.3530 |
| Q | 0.5420 | 0.3170 |
| R | 0.5980 | 0.3540 |
| S | 0.5440 | 0.3410 |
| T | 0.5950 | 0.3570 |
| U | 0.3000 | 0.1860 |
| V | 0.2060 | 0.1670 |
| W | 0.2570 | 0.1650 |
| X | 0.2740 | 0.2240 |
| Y | 0.3160 | 0.1800 |
| Z | 0.2810 | 0.1930 |
| a | 0.2280 | 0.1600 |
| b | 0.1570 | 0.1470 |
| c | 0.3050 | 0.1920 |
| d | 0.1330 | 0.1380 |
| e | 0.1790 | 0.1800 |
| f | 0.1530 | 0.0730 |
| g | 0.4370 | 0.2810 |
| h | 0.4470 | 0.2890 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| i | 0.4190 | 0.2660 |
| j | 0.4480 | 0.2800 |
| k | 0.4550 | 0.2810 |
| l | 0.5090 | 0.2900 |
| m | 0.4570 | 0.2710 |
| n | 0.6040 | 0.3600 |
| o | 0.5340 | 0.3320 |
| p | 0.5670 | 0.3490 |
| q | 0.5730 | 0.3350 |
| r | 0.6060 | 0.3570 |
| s | 0.5740 | 0.3460 |
| t | 0.6140 | 0.3510 |