# wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 05:54 PM EST

| | | |
|---|---|---|
| PDB ID | : | 6MSH |
| EMDB ID | : | EMD-9220 |
| Title | : | Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome |
| Authors | : | Mao, Y.D. |
| Deposited on | : | 2018-10-16 |
| Resolution | : | 3.60 Å(reported) |

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

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

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

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

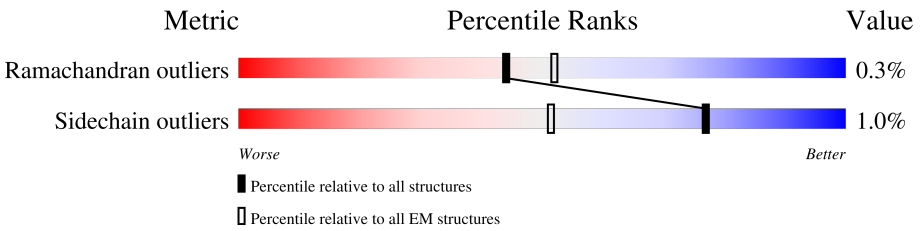
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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 | 953 | 64% 85% • 14% |
| 2 | V | 533 | 75% 89% • 10% |
| 3 | W | 456 | 71% 97% • |
| 4 | X | 422 | 17% 90% 10% |
| 5 | Y | 389 | 27% 96% • • |
| 6 | Z | 324 | 67% 83% 5% • 12% |
| 7 | a | 376 | 82% 98% • • |
| 8 | b | 377 | 50% 51% 49% |
| 9 | c | 309 | 61% 90% • 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | d | 349 | 71% 73% 26% |
| 11 | e | 70 | 40% 54% 43% |
| 12 | f | 892 | 99% 94% |
| 13 | A | 433 | 45% 80% 18% |
| 14 | B | 440 | 58% 78% 20% |
| 15 | C | 398 | 45% 97% |
| 16 | D | 418 | 27% 88% 9% |
| 17 | E | 403 | 33% 94% |
| 18 | F | 439 | 39% 87% 10% |
| 19 | v | 22 | 95% 100% |
| 20 | G | 245 | 6% 98% |
| 20 | g | 245 | 16% 98% |
| 21 | H | 233 | 99% |
| 21 | h | 233 | 14% 99% |
| 22 | I | 260 | 8% 96% |
| 22 | i | 260 | 27% 96% |
| 23 | J | 247 | 13% 97% |
| 23 | j | 247 | 36% 97% |
| 24 | K | 240 | 9% 95% 5% |
| 24 | k | 240 | 15% 95% 5% |
| 25 | L | 268 | 88% 11% |
| 25 | l | 268 | 11% 88% 11% |
| 26 | M | 254 | 7% 94% 6% |
| 26 | m | 254 | 15% 94% 6% |
| 27 | N | 238 | 80% 20% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 27 | n | 238 | 80% 20% |
| 28 | O | 276 | 80% 20% |
| 28 | o | 276 | 5% 80% 20% |
| 29 | P | 204 | 100% |
| 29 | p | 204 | 100% |
| 30 | Q | 201 | 98% |
| 30 | q | 201 | 98% |
| 31 | R | 262 | 76% 23% |
| 31 | r | 262 | 76% 23% |
| 32 | S | 240 | 5% 89% 11% |
| 32 | s | 240 | 89% 11% |
| 33 | T | 263 | 82% 18% |
| 33 | t | 263 | 82% 18% |

# 2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 103729 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 | 820 | 6398 | 4062 | 1086 | 1206 | 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 | 380 | 3009 | 1918 | 509 | 570 | 12 | 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 |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | a | 373 | 2995 | 1911 | 510 | 559 | 15 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | c | 287 | 2260 | 1430 | 389 | 422 | 19 | 0 | 0 |

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

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

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

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | f | 886 | 6840 | 4300 | 1171 | 1324 | 45 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | A | 356 | 2767 | 1741 | 488 | 521 | 17 | 0 | 0 |

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | B | 350 | 2706 | 1703 | 458 | 533 | 12 | 0 | 0 |

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | C | 396 | 3105 | 1954 | 558 | 576 | 17 | 0 | 0 |

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | D | 380 | 3040 | 1923 | 524 | 580 | 13 | 0 | 0 |

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | E | 389 | 3097 | 1947 | 552 | 581 | 17 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | F | 395 | 3098 | 1951 | 533 | 596 | 18 | 0 | 0 |

- Molecule 19 is a protein called substrate.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 19 | v | 22 | 110 | 66 | 22 | 22 | 0 | 0 |

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | G | 240 | 1826 | 1160 | 305 | 348 | 13 | 0 | 0 |
| 20 | g | 240 | 1826 | 1160 | 305 | 348 | 13 | 0 | 0 |

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | H | 232 | 1708 | 1081 | 289 | 333 | 5 | 0 | 0 |
| 21 | h | 232 | 1708 | 1081 | 289 | 333 | 5 | 0 | 0 |

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | I | 250 | 1912 | 1204 | 329 | 371 | 8 | 0 | 0 |
| 22 | i | 250 | 1912 | 1204 | 329 | 371 | 8 | 0 | 0 |

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | J | 239 | 1704 | 1056 | 308 | 335 | 5 | 0 | 0 |
| 23 | j | 239 | 1704 | 1056 | 308 | 335 | 5 | 0 | 0 |

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | K | 228 | 1722 | 1080 | 284 | 348 | 10 | 0 | 0 |
| 24 | k | 228 | 1722 | 1080 | 284 | 348 | 10 | 0 | 0 |

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | L | 238 | 1850 | 1159 | 334 | 346 | 11 | 0 | 0 |
| 25 | l | 238 | 1850 | 1159 | 334 | 346 | 11 | 0 | 0 |

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | M | 240 | 1856 | 1178 | 314 | 353 | 11 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | m | 240 | 1856 | 1178 | 314 | 353 | 11 | 0 | 0 |

- Molecule 27 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | N | 191 | 1430 | 893 | 245 | 280 | 12 | 0 | 0 |
| 27 | n | 191 | 1430 | 893 | 245 | 280 | 12 | 0 | 0 |

- Molecule 28 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | O | 220 | 1643 | 1033 | 280 | 318 | 12 | 0 | 0 |
| 28 | o | 220 | 1643 | 1033 | 280 | 318 | 12 | 0 | 0 |

- Molecule 29 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | P | 204 | 1585 | 1010 | 262 | 294 | 19 | 0 | 0 |
| 29 | p | 204 | 1585 | 1010 | 262 | 294 | 19 | 0 | 0 |

- Molecule 30 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | Q | 199 | 1570 | 1006 | 265 | 290 | 9 | 0 | 0 |
| 30 | q | 199 | 1570 | 1006 | 265 | 290 | 9 | 0 | 0 |

- Molecule 31 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | R | 201 | 1548 | 974 | 273 | 292 | 9 | 0 | 0 |
| 31 | r | 201 | 1548 | 974 | 273 | 292 | 9 | 0 | 0 |

- Molecule 32 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | S | 213 | 1641 | 1036 | 282 | 313 | 10 | 0 | 0 |
| 32 | s | 213 | 1641 | 1036 | 282 | 313 | 10 | 0 | 0 |

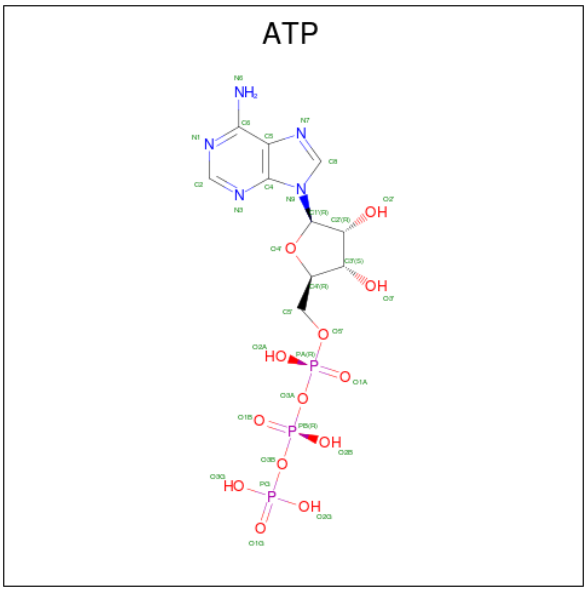
- Molecule 33 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | T | 215 | 1667 | 1052 | 285 | 318 | 12 | 0 | 0 |
| 33 | t | 215 | 1667 | 1052 | 285 | 318 | 12 | 0 | 0 |

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 34 | c | 1 | 1 | 1 | 0 |

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 35 | C | 1 | 31 | 10 | 5 | 13 | 3 | 0 |

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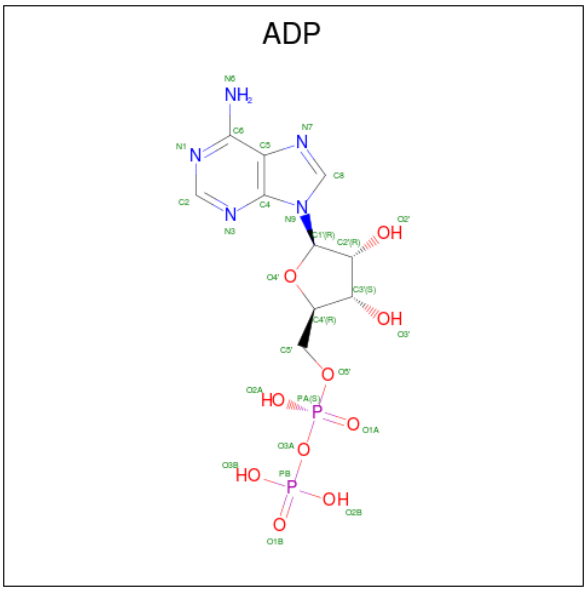
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 35 | D | 1 | 31 | 10 | 5 | 13 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 35 | E | 1 | 31 | 10 | 5 | 13 | 3 | 0 |

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



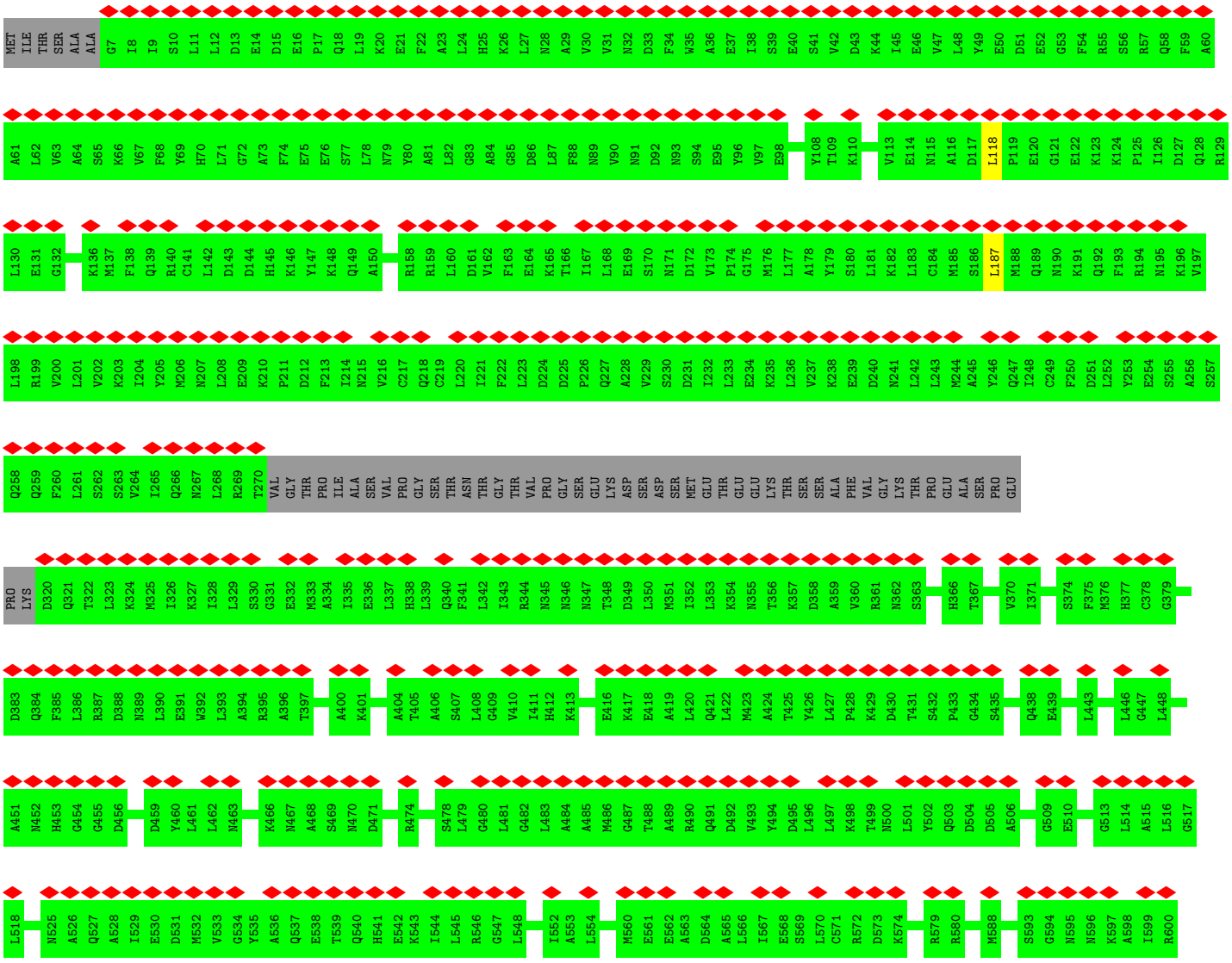

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 36 | F | 1 | 27 | 10 | 5 | 10 | 2 | 0 |

# 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: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 64% 85% 14%



L603 H604 S608 D609 V610 N611 D612 D613 R616 A617 A618 V619 E620 S621 L622 G623 F624 I625 L626 F627 R628 T629 P630 E631 Q632 S635 V636 V637 S638 L639 L640 S641 E642 G651 A652 A653 L656 G657 I658 C659 C660 A661 G662 T663 G664 N665 K666 I669 N670 L671 L672 E673 P674

M675 T676 N677 D678 F679 V680 N681 A687 L688 I689 A690 S691 A692 L693 I694 M695 I696 Q697 Q698 T699 E700 I701 P704 K705 V706 N707 Q708 F709 R710 Q711 L712 K715 V716 I717 N718 D719 K720 H721 D722 D723 V724 M725 A726 K727 L732 A733 Q734 G735 I736 L737 D738 V744 T745 I746 S747

L748 Q749 S750 R751 T752 G753 H754 T755 H756 S759 V760 V761 G762 V763 L764 V765 F766 T767 F771 W772 F773 P774 L775 S776 H777 F778 L781 A782 Y783 T784 P785 T786 C787 V788 I789 G790 L791 N792 K793 D794 L795 K796 M797 P798 K799 V800 Q801 Y802 K803 S804 N805 P808 S809 T810 Y813

P814 A815 P816 L817 E818 V819 P820 LYS GLU LYS GLU LYS GLU LYS VAL SER THR ALA VAL LEU SER ILE THR ALA LYS ALA LYS LYS LYS LYS GLU LYS GLU LYS GLU LYS GLU LYS LYS LYS GLU GLU LYS MET GLU VAL ASP GLU ALA GLU LYS LYS GLU LYS LYS LYS LYS GLU PRO GLU P873

N874 F875 Q876 L877 L878 D879 N880 P881 A882 R883 P886 A887 Q888 L889 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 S918 E919 D920 I921 E922 E923 L924 V925 E926 P927 VAL ALA ALA HIS GLY PRO LYS

ILE GLU GLU GLU GLU GLN GLU PRO GLU PRO PRO GLU PRO PHE GLU TYR ILE ASP ASP

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

Chain V:

LYS GLN GLU GLY SER ALA ARG ARG ARG GLY ALA ASP LYS ALA LYS PRO P18 P19 G20 G21 G22 E23 Q24 E25 P26 P27 P28 P29 P30 A31 P32 Q33 D34 V35 E36 M37 K38 E39 E40 A41 A42 T43 G44 G45 G46 S47 T48 G49 E50 A51 D52 G53 K54 T55 A56 A57 A58 A59 A60 E61

H62 S63 Q64 R65 E66 L67 D68 T69 V70 T71 L72 E73 D74 I75 K76 E77 H78 V79 K80 Q81 L82 E83 K84 A85 V86 S87 G88 K89 E90 P91 R92 F93 V94 L95 R96 A97 L98 R99 M100 L101 P102 S103 T104 S105 R106 R107 L108 N109 H110 Y111 V112 L113 Y114 K115 A116 V117 Q118 G119 F120 F121

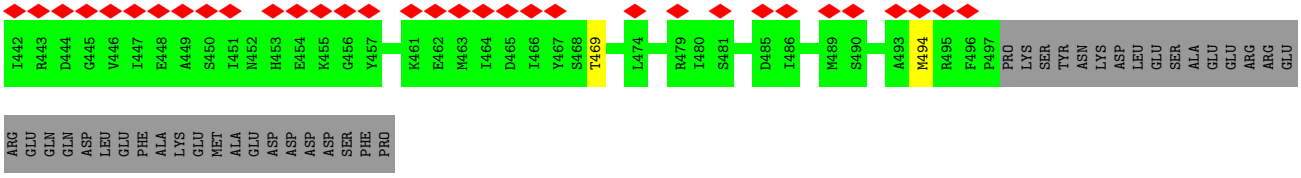
T122 S123 N124 N125 A126 T127 R128 D129 F130 L131 L132 P133 F134 L135 E136 E137 P138 M139 D140 T141 E142 A143 D144 L145 Q146 F147 R148 P149 R150 T151 G152 K153 A154 A155 S156 T157 P158 L159 L160 P161 E162 V163 E164 A165 Y166 L167 Q168 L169 L170 V171 V172 I173 F174 M175 M176 N177 S178 K179 R180 Y181

K182 E183 A184 Q185 K186 I187 S188 D189 D190 L191 M192 Q193 K194 I195 S196 T197 Q198 N199 R200 R201 A202 L203 D204 L205 V206 A207 A208 K209 C210 Y211 Y212 Y213 H214 A215 R216 V217 Y218 E219 F220 L221 D222 K223 L224 D225 V226 V227 R228 S229 F230 L231 H232 A233 R234 L235 R236 T237 A238 T239 L240 R241

H242 D243 A244 D245 G246 Q247 A248 T249 L250 L251 N252 L253 L254 L255 R256 N257 Y258 L259 H260 Y261 S262 L263 Y264 D265 Q266 A267 E268 K269 L270 V271 S272 K273 S274 V275 F276 P277 E278 Q279 A280 N281 N282 N283 E284 W285 A286 R287 Y288 L289 Y290 Y291 T292 G293 R294 I295 K296 A297 I298 Q299 L300 E301

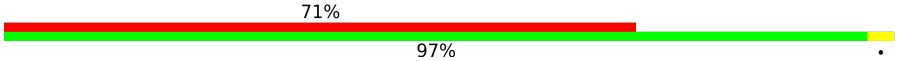
Y302 S303 E304 A305 R306 R307 T308 M309 T310 N311 A312 L313 R314 K315 A316 P317 Q318 H319 T320 A321 V322 G323 F324 K325 H329 K330 L331 L332 I333 V334 V335 E336 L337 L338 L339 G340 E341 I342 P343 D344 R345 L346 Q347 F348 R349 Q350 P351 S352 L353 K354 R355 S356 L357 M358 F361 L362 L363 T364

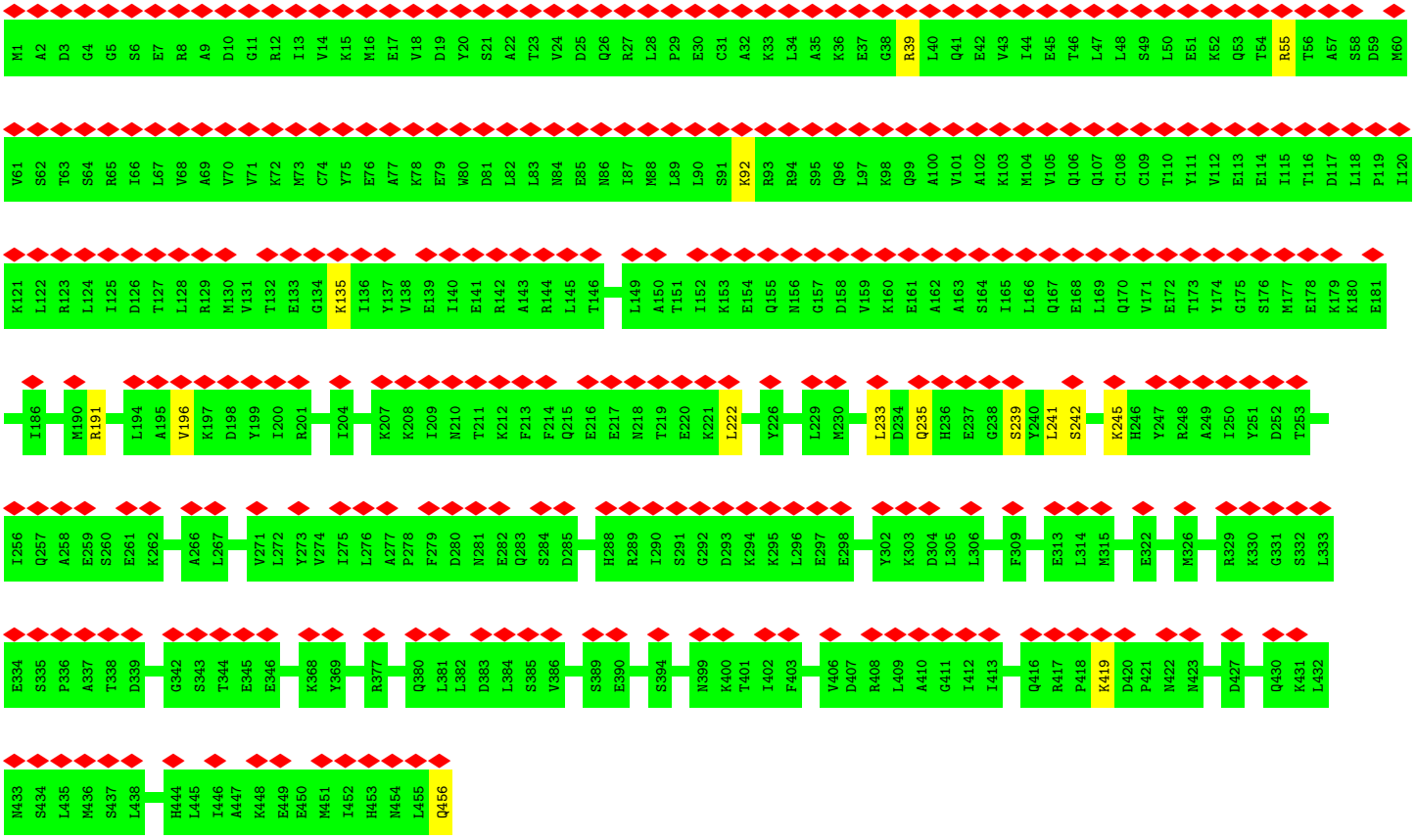
Q365 A366 V367 R368 T369 G370 N371 L372 A373 K374 L379 F382 K385 F386 Q387 A388 D389 G390 T391 Y392 I395 I396 R397 L398 R399 H400 N401 V402 I403 K404 T405 G406 V407 R416 A420 D421 I422 A423 Q424 Q427 L428 D429 S430 P431 E432 D433 A434 E435 F436 A439 K440 A441




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

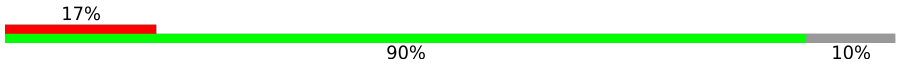
Chain W:

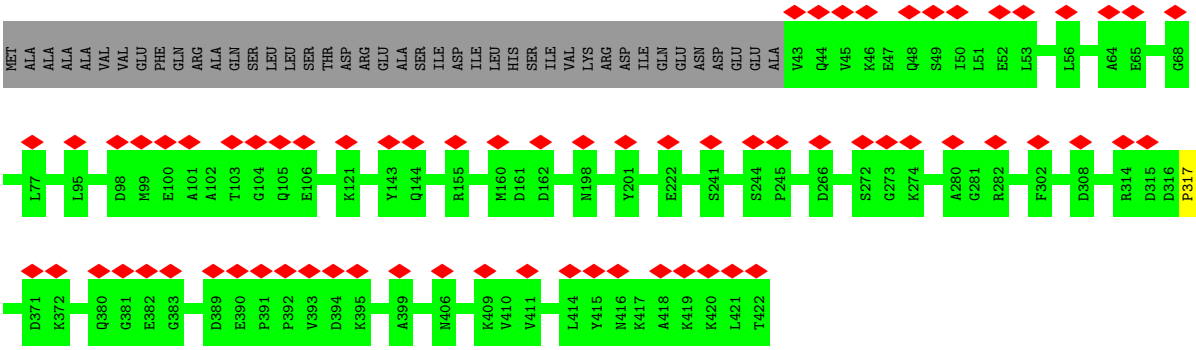



• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

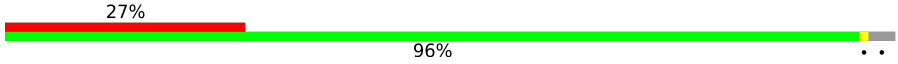
Chain X:

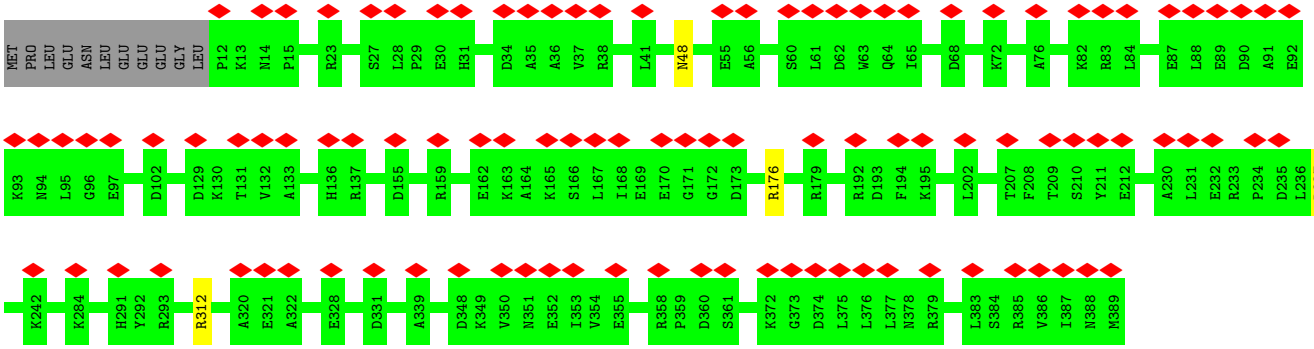


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

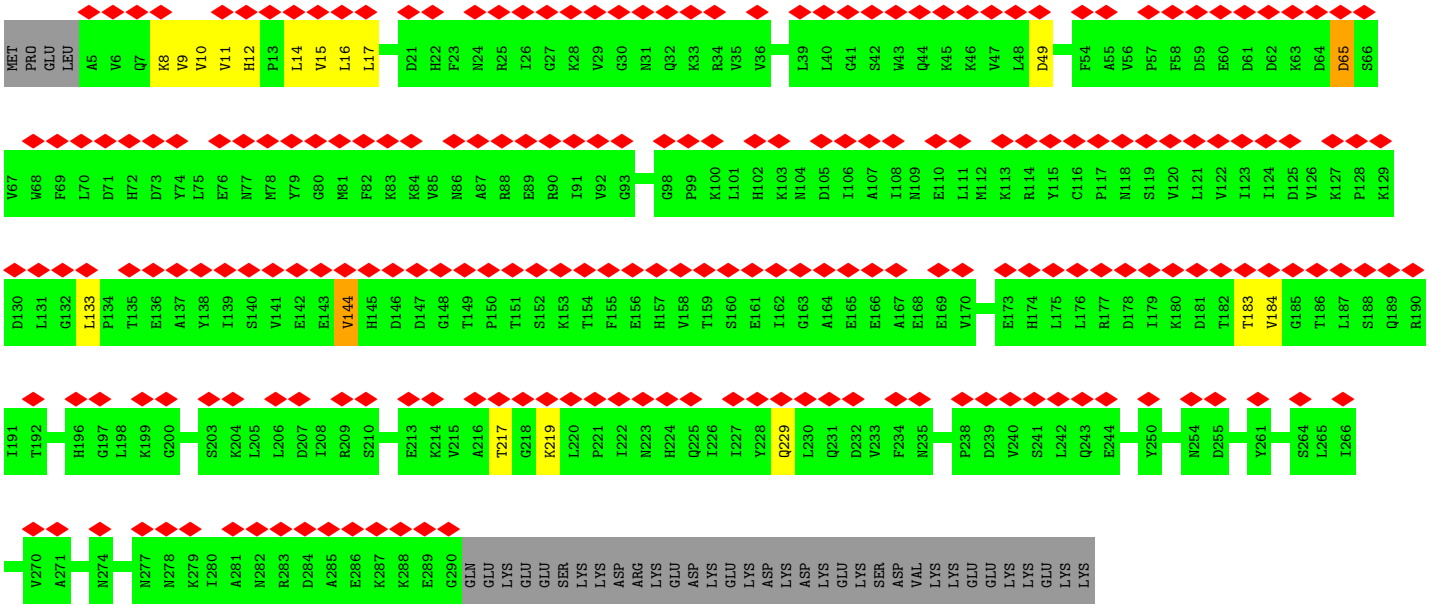
Chain Y:



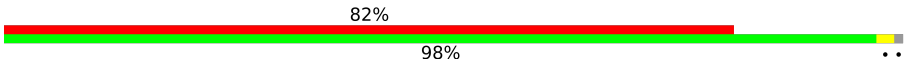

- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

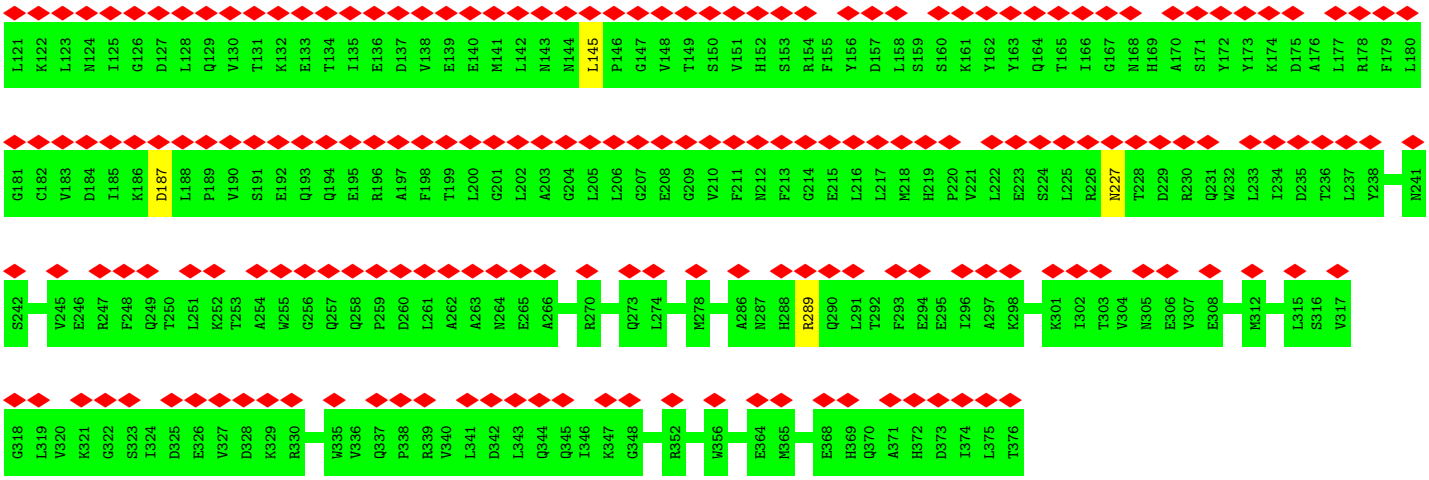
Chain Z:




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

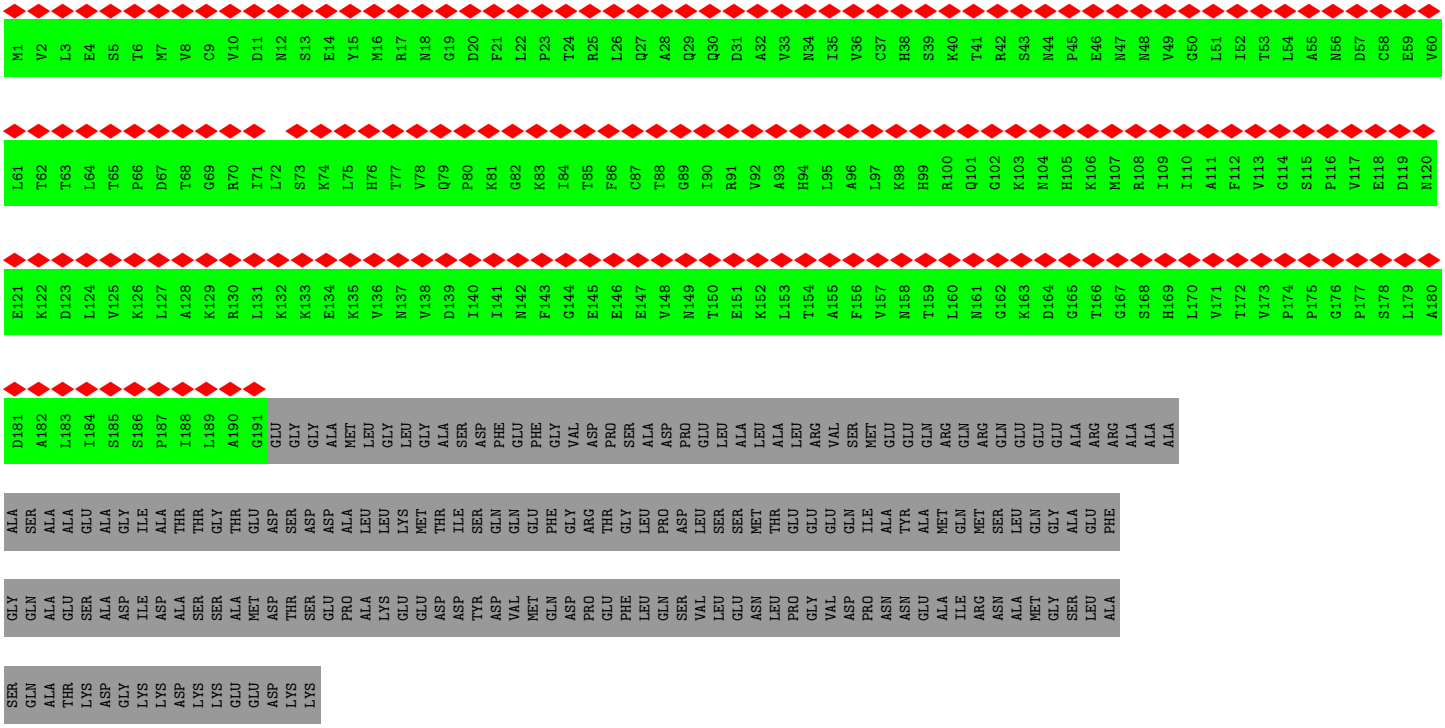
Chain a:





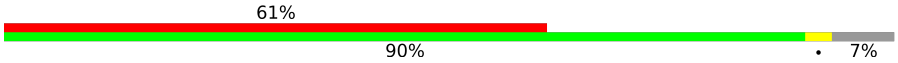

- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

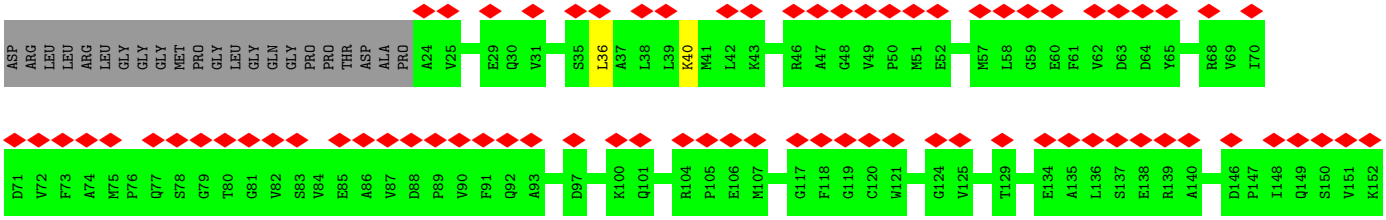
Chain b:

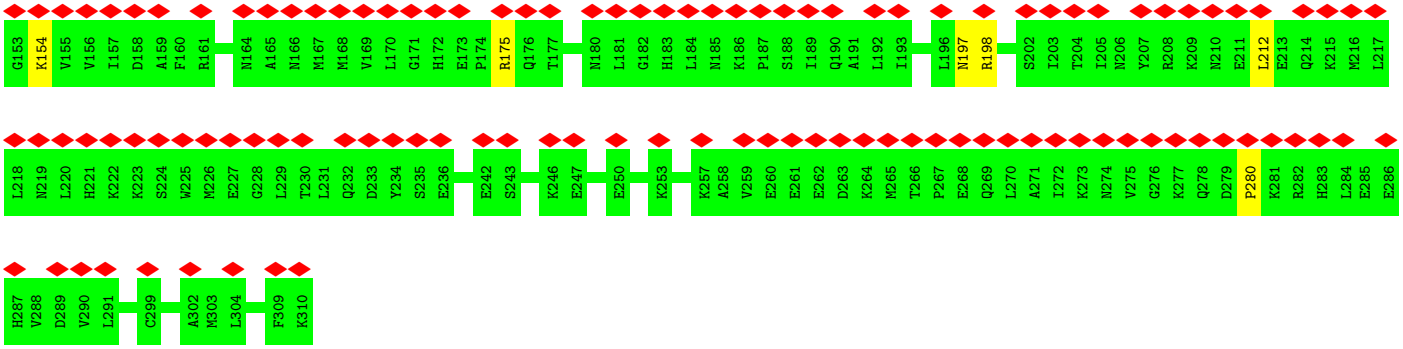



- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain c:

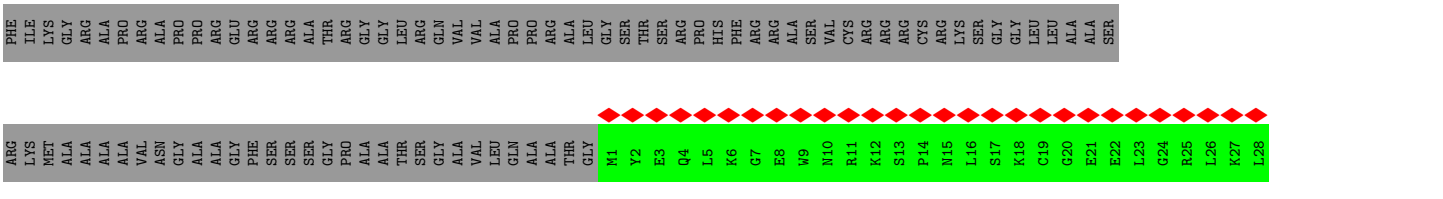




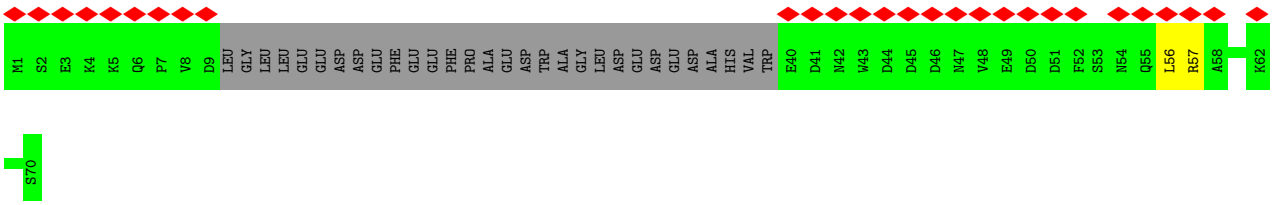

- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



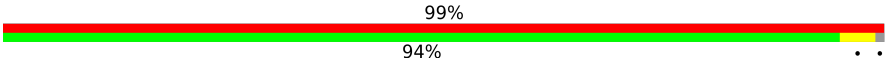

- Molecule 11: 26S proteasome complex subunit SEM1

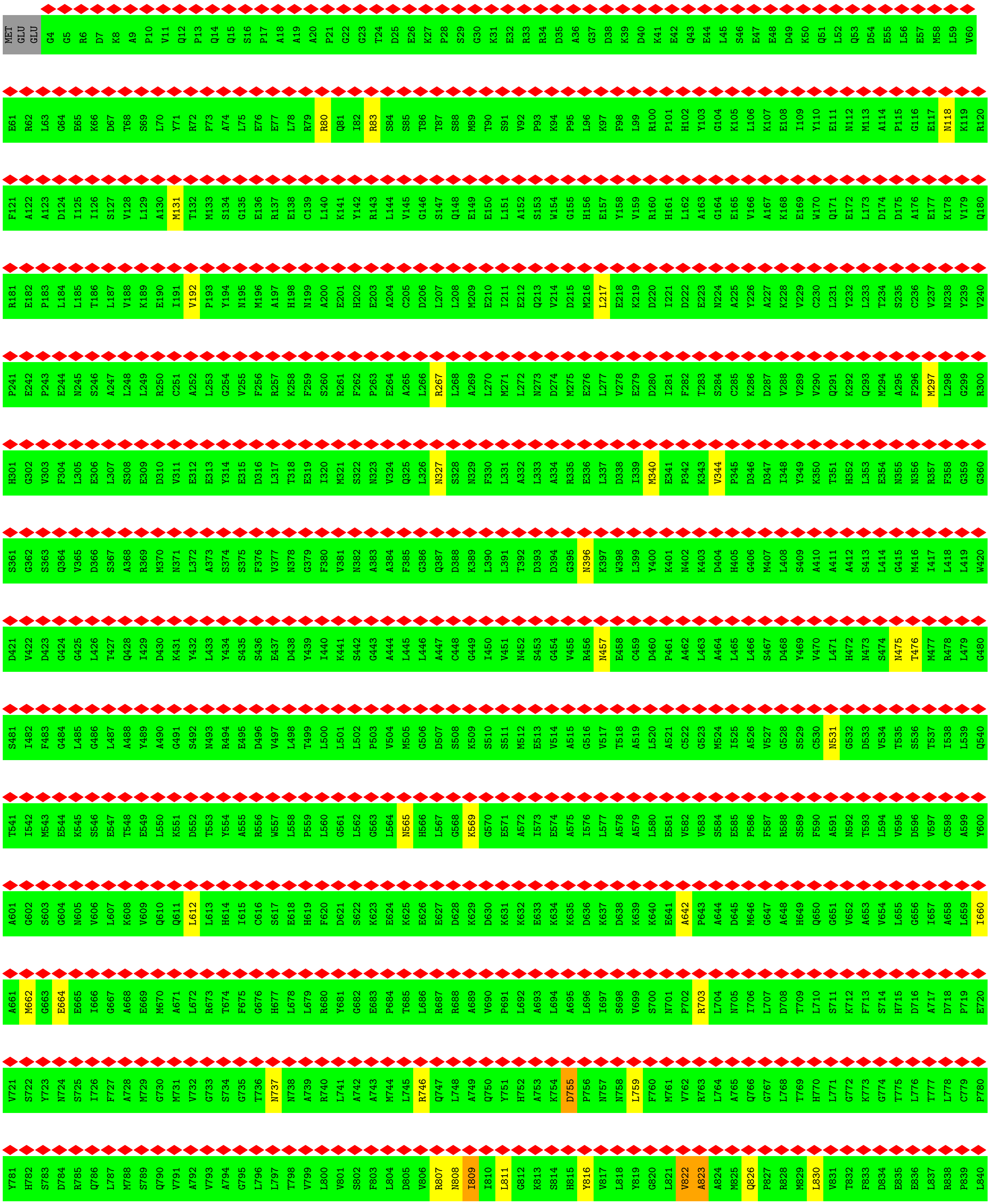
Chain e:




- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain f:




MET GLU GLU G4 G5 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 L56 E57 M58 L59 V60
E61 R62 L63 G64 E65 K66 D67 T68 S69 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 G104 K105 L106 K107 E108 I109 Y110 E111 N112 M113 A114 P115 G116 E117 N118 K119 R120
F121 A122 A123 D124 I125 I126 S127 V128 L129 A130 M131 T132 M133 S134 G135 E136 R137 E138 C139 L140 K141 Y142 R143 L144 V145 G146 S147 Q148 E149 E150 L151 A152 S153 W154 G155 H156 E157 Y158 V159 R160 H161 L162 A163 G164 E165 V166 A167 K168 E169 W170 Q171 E172 L173 D174 D175 A176 E177 K178 V179 Q180
R181 E182 P183 L184 L185 T186 L187 V188 K189 E190 I191 V192 P193 Y194 N195 M196 A197 H198 N199 A200 E201 H202 E203 A204 C205 D206 L207 L208 M209 E210 I211 E212 Q213 V214 D215 M216 L217 E218 K219 D220 I221 D222 E223 N224 A225 Y226 A227 K228 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 F256 R257 K258 F259 S260 R261 F262 P263 E264 A265 L266 R267 L268 A269 L270 M271 L272 N273 D274 M275 E276 L277 V278 E279 D280 I281 F282 T283 S284 C285 K286 D287 V288 V289 V290 Q291 K292 Q293 M294 A295 F296 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 Q325 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 A383 A384 F385 G386 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 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 A689 V690 P691 L692 A693 L694 A695 L696 I697 S698 V699 S700 N701 P702 R703 L704 N705 I706 L707 D708 T709 L710 S711 K712 F713 S714 H715 D716 A717 D718 P719 E720
V721 S722 Y723 N724 S725 I726 F727 A728 M729 G730 M731 V732 G733 S734 G735 T736 N737 N738 A739 R740 L741 A742 A743 M744 L745 R746 Q747 L748 A749 Q750 Y751 H752 A753 K754 D755 P756 N757 N758 L759 F760 M761 V762 R763 L764 A765 Q766 G767 L768 T769 H770 L771 G772 K773 G774 T775 L776 T777 L778 C779 P780
Y781 H782 S783 D784 R785 Q786 L787 M788 S789 Q790 V791 A792 V793 A794 G795 L796 L797 T798 V799 L800 V801 S802 F803 L804 D805 V806 R807 N808 I809 I810 L811 G812 K813 S814 H815 Y816 V817 L818 Y819 G820 L821 V822 A823 A824 M825 Q826 P827 R828 M829 L830 V831 T832 F833 D834 E835 E836 L837 R838 P839 L840

P841 V842 S843 V844 R845 V846 G847 Q848 A849 V850 D851 V852 V853 G854 Q855 A856 G857 K858 P859 K860 T861 I862 T863 G864 F865 Q866 T867 H868 T869 T870 P871 V872 L873 L874 A875 H876 G877 E878 R879 A880 E881 L882 A883 T884 E885 E886 F887 L888 P889 VAL THR PRO

- Molecule 13: 26S proteasome regulatory subunit 7

Chain A: 45% 80% • 18%

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

GLU LEU THR GLY ILE LYS E67 S68 D69 T70 G71 L72 A73 P74 P75 A76 L77 W78 D79 L80 A81 A82 D83 K84 Q85 T86 L87 Q88 S89 E90 Q91 P92 L93 Q94 I102 D105 S106 E107 D108 P109 K116 Q117 F118 A119 K120 D127 Q128 V129 A130 P131 T132 D133 I134 E135 E136

R139 V140 R144 N145 P154 P155 K156 I157 D158 P159 T160 V161 T162 M163 M164 Q165 V166 E167 E168 K169 P170 D171 V172 T173 Y174 S175 G178 G179 C180 K181 E182 Q183 R188 V191 E192 T193 P194 L195 L196 F201 V202 N203 E207 P208 P209 K210 G211 L214 L224 R227

D234 A235 R239 V240 I241 G242 S243 E244 L245 V246 Q247 K248 Y249 V250 G251 E252 G253 A254 R255 M256 E259 L260 F261 E262 M263 A264 R265 T266 K267 K268 A269 C270 L271 I272 F273 F274 D275 E276 I277 D278 A279 I280 G281 G282 A283 R284 F285 D286 D287 G288 A289 G290 G291 D292 N293 E294 V295

Q296 R297 L300 N304 G308 F309 D310 P311 R312 G313 N314 I315 K316 V317 L318 M319 N322 R323 P324 D325 T326 L327 D328 P329 A330 L331 M332 R333 P334 G335 R336 L337 D338 R339 K340 I341 S344 L345 P346 D347 H353 R360 S361 E365 R366 D367 I368 R369 F370 L373

R386 I397 R398 A399 R400 R401 K402 I403 K407 K418 S419 Y420 A421 K422 PHE SER ALA THR PRO ARG TYR MET THR TYR ASN

- Molecule 14: 26S proteasome regulatory subunit 4

Chain B: 58% 78% • 20%

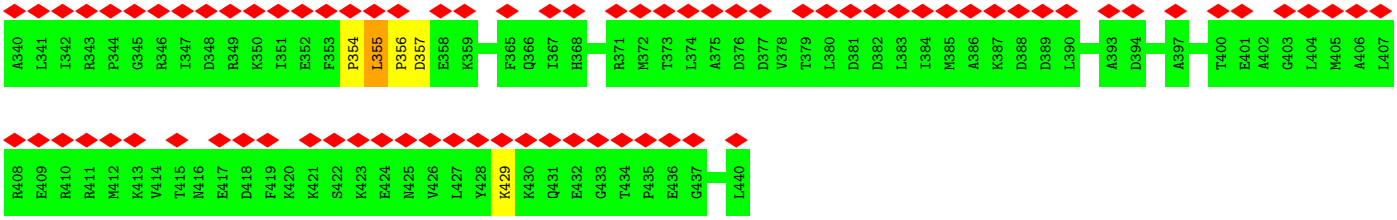
MET GLY GLN SER GLN SER GLY GLY HIS GLY PRO GLY GLY GLY LYS LYS ASP ASP LYS ASP LYS LYS LYS LYS TYR GLU PRO PRO VAL PRO THR ARG VAL GLY LYS LYS LYS LYS LYS THR LYS GLY PRO ASP ALA ALA SER LYS LEU PRO LEU VAL THR PRO HIS THR GLN CYS ARG LEU

LYS LEU LEU LYS LEU GLU ARG ILE LYS ASP TYR LEU LEU MET GLU GLU GLU PHE ILE ARG ASN GLN GLU GLN MET LYS PRO LEU GLU GLU K91 Q92 E93 E94 E95 R96 S97 K98 V99 D100 D101 L102 R103 G104 T105 G110 E113 E114 I115 I116 D117 D118 N119 H120 A121 T125 S126

V127 G128 S129 L136 V139 D140 K141 D142 L143 L144 E145 P146 G147 C148 S149 V150 K155 G161 V162 L163 M164 D165 D166 T167 D168 P169 L170 V171 T172 V173 M174 K175 V176 E177 K178 A179 P180 Q181 E182 T183 Y184 A185 D186 I187 G188 G189 L190 D191 N192 I197 K198 V201 E202 L203

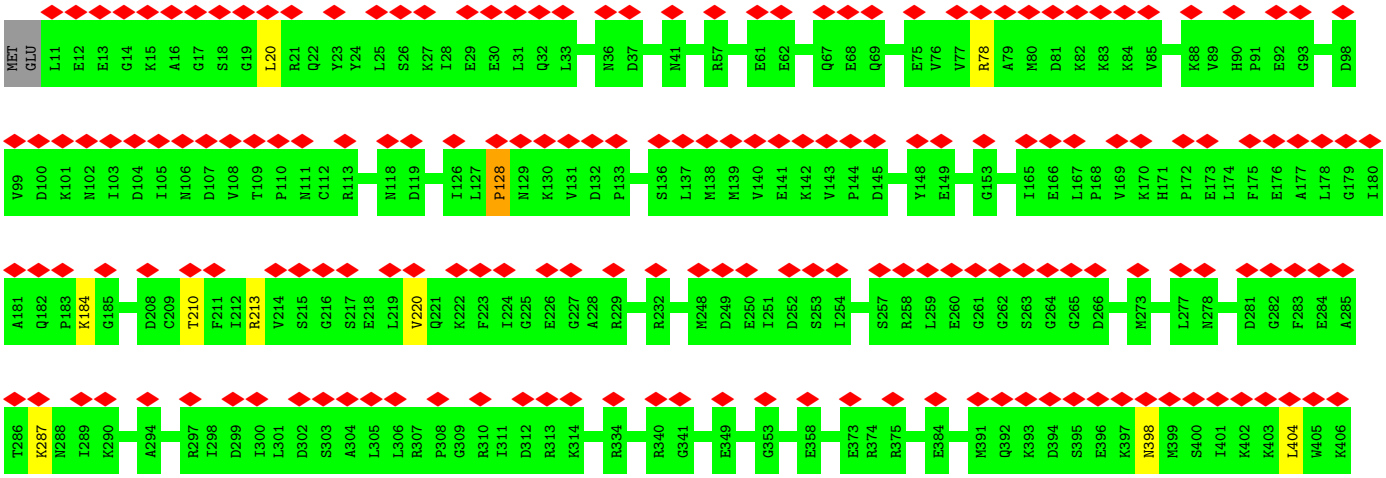
P204 L205 T206 H207 P208 E209 Y210 Y211 E212 E213 M214 G215 I216 K220 G221 G226 P227 P228 K237 A240 N241 S244 A245 T246 F247 L248 R249 V250 V251 G252 S253 E254 L255 I256 Q257 K258 Y259 L260 G261 D262 G263 P264 K265 R268 E269 L270 F271 R272 V273 A274 E275 E276 H277 A278

P279 S280 I281 V282 F283 I284 D285 E286 I287 D288 A289 I290 G291 T292 K293 R294 Y295 D296 S297 N298 S299 G300 G301 E302 R303 E304 I305 Q306 R307 T308 M309 L310 E311 L312 L313 N314 Q315 L316 D317 G318 F319 D320 S321 R322 G323 D324 V325 K326 V327 I328 T331 N332 R333 I334 E335 T336 L337 D338 P339



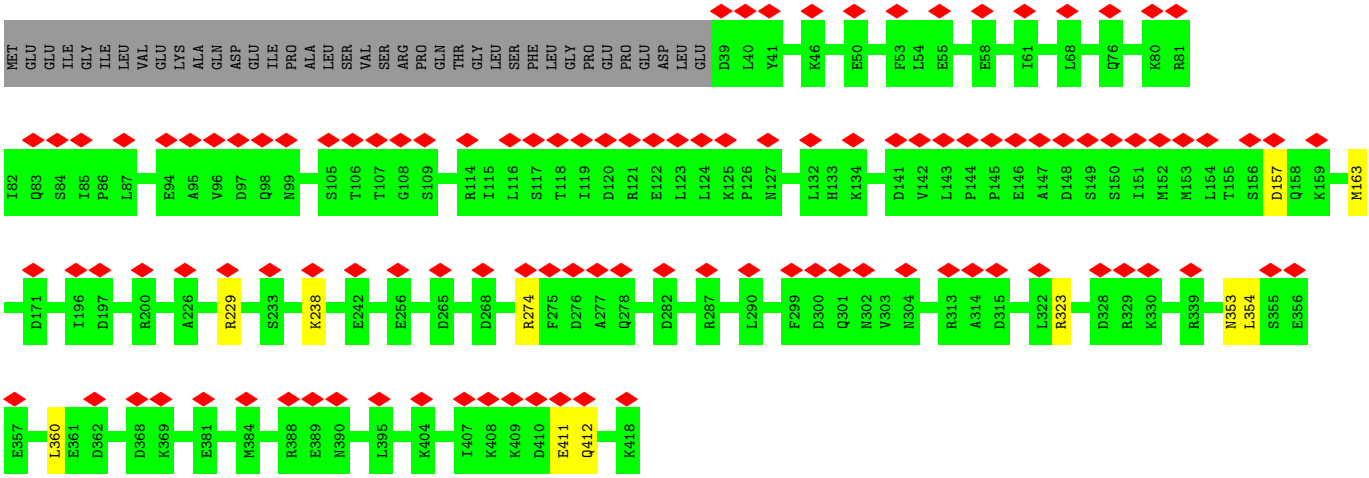

• Molecule 15: 26S proteasome regulatory subunit 8

Chain C: 45% 97%



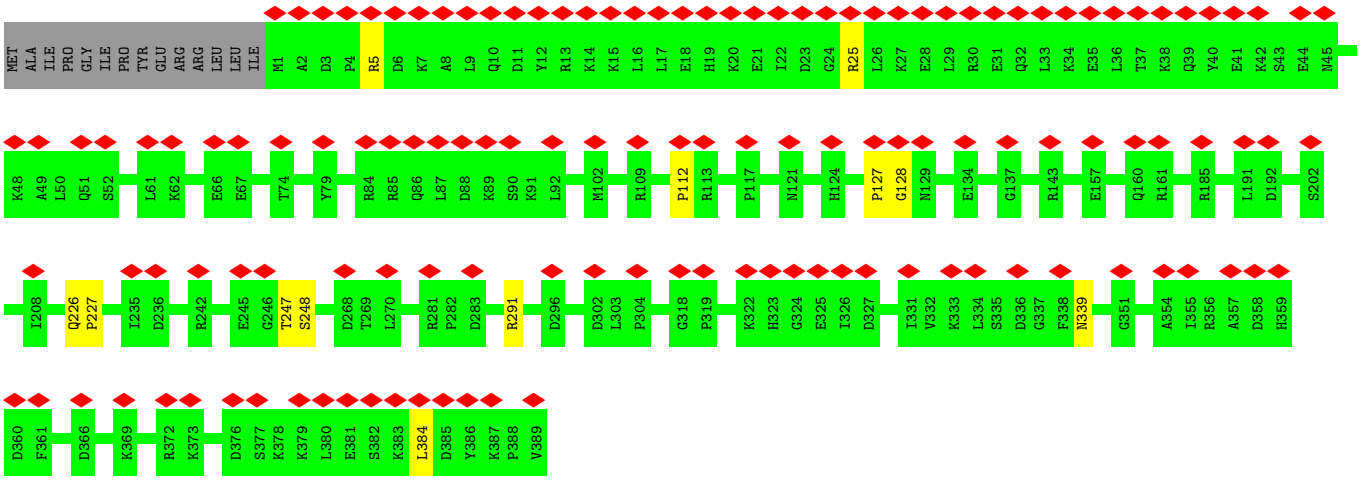

• Molecule 16: 26S proteasome regulatory subunit 6B

Chain D: 27% 88% 9%



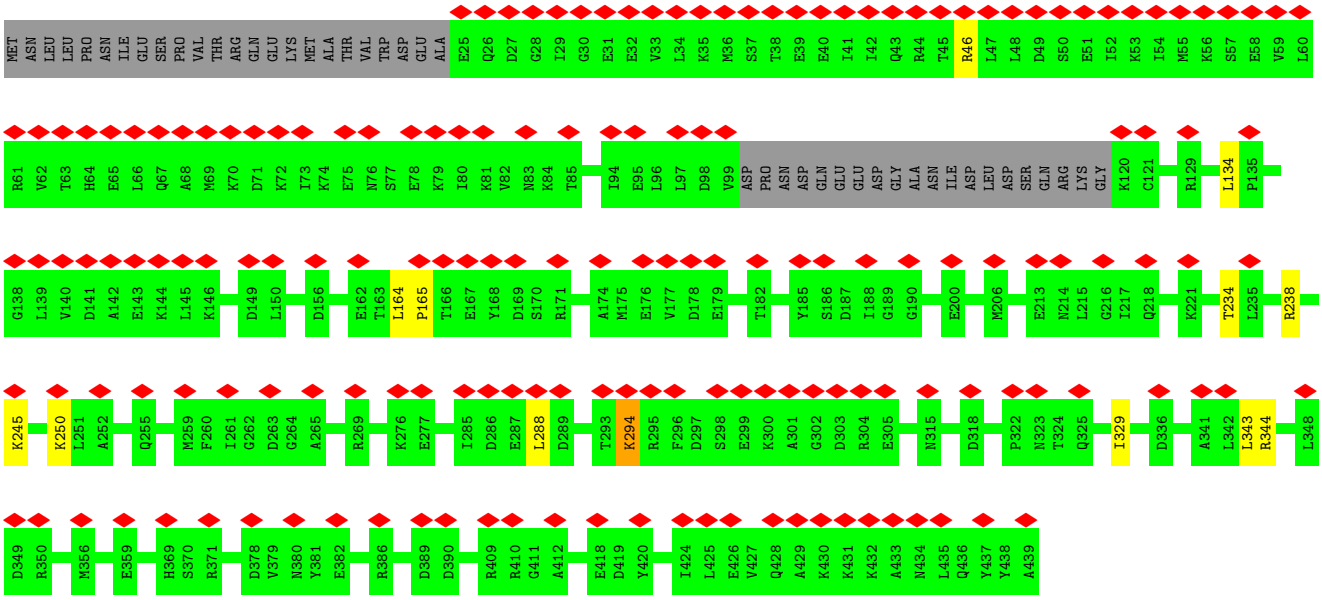

• Molecule 17: 26S proteasome regulatory subunit 10B

Chain E: 33% 94%



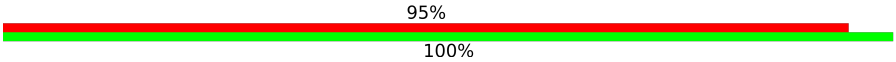

- Molecule 18: 26S proteasome regulatory subunit 6A

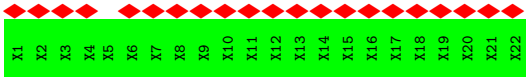
Chain F:




- Molecule 19: substrate

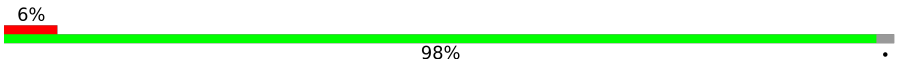
Chain v:

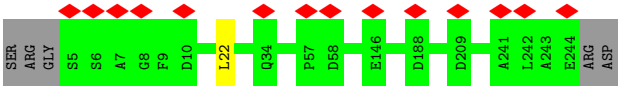



- Molecule 20: Proteasome subunit alpha type-6

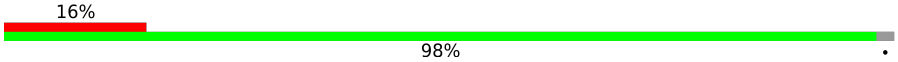
Chain G:

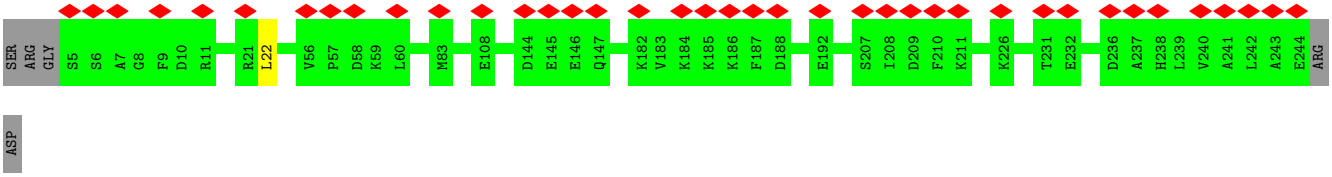


- Molecule 20: Proteasome subunit alpha type-6

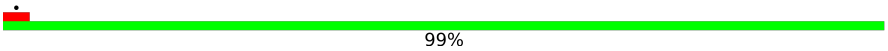
Chain g:

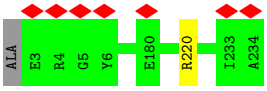



- Molecule 21: Proteasome subunit alpha type-2

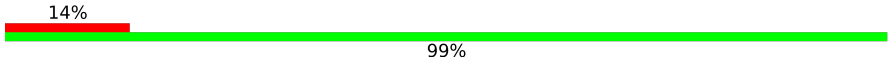
Chain H:

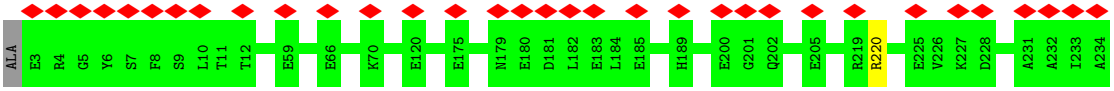



- Molecule 21: Proteasome subunit alpha type-2

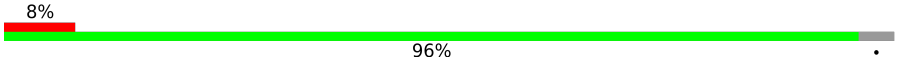
Chain h:

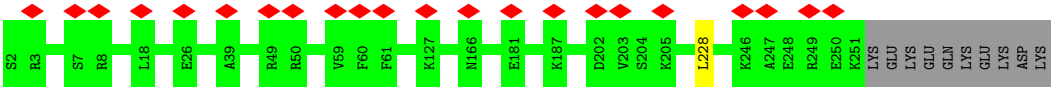



- Molecule 22: Proteasome subunit alpha type-4

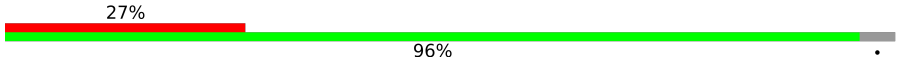
Chain I:

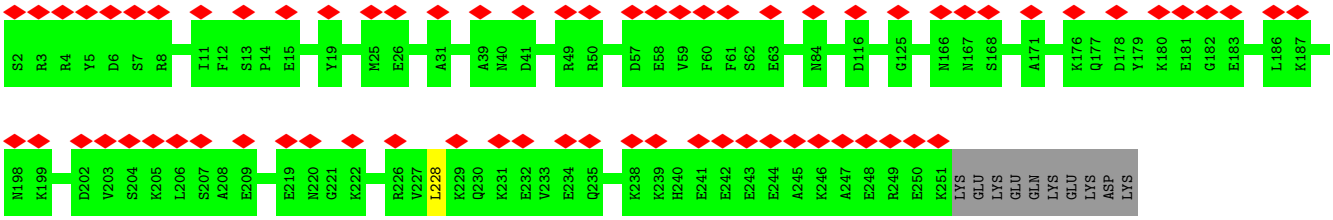



- Molecule 22: Proteasome subunit alpha type-4

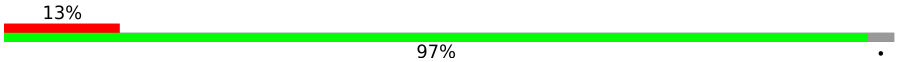
Chain i:

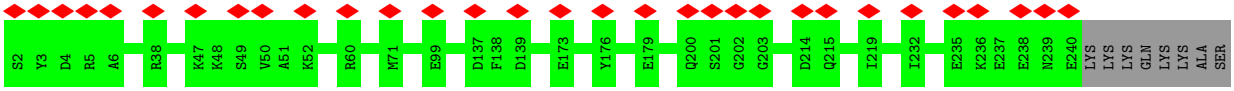



- Molecule 23: Proteasome subunit alpha type-7

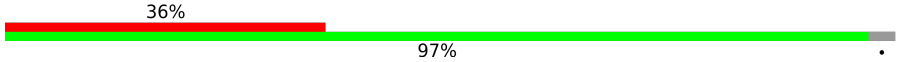
Chain J:

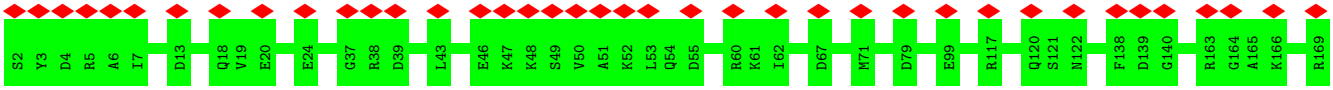


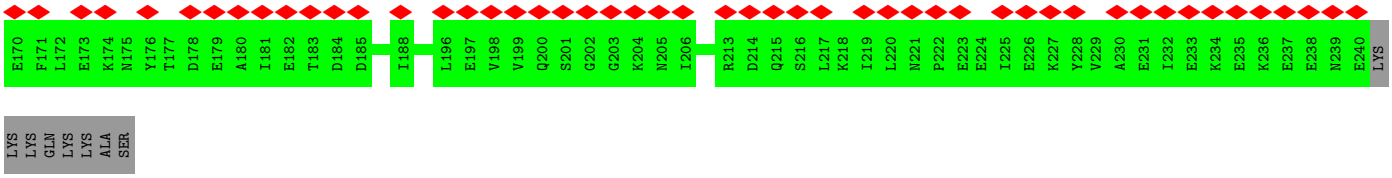



• Molecule 23: Proteasome subunit alpha type-7

Chain j:

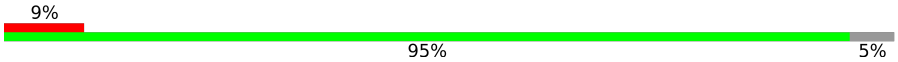


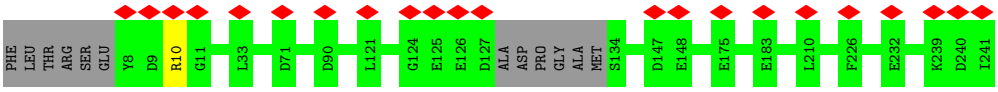




• Molecule 24: Proteasome subunit alpha type-5

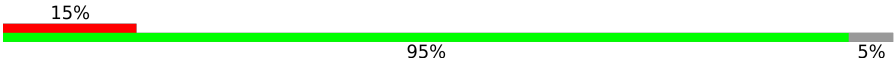
Chain K:

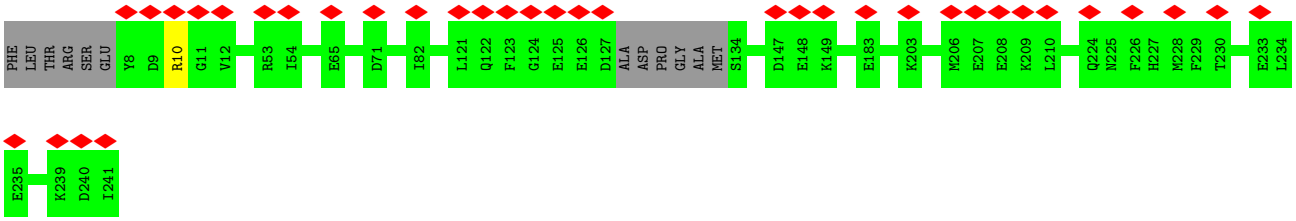



• Molecule 24: Proteasome subunit alpha type-5

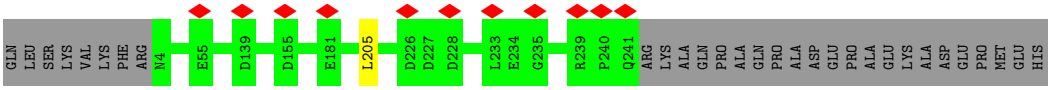
Chain k:



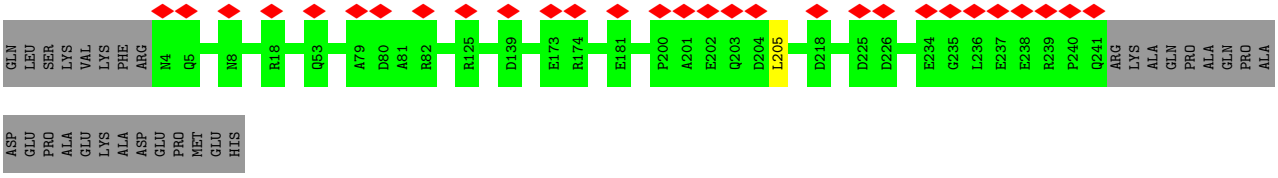

• Molecule 25: Proteasome subunit alpha type-1

Chain L:



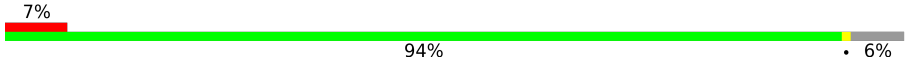

• Molecule 25: Proteasome subunit alpha type-1

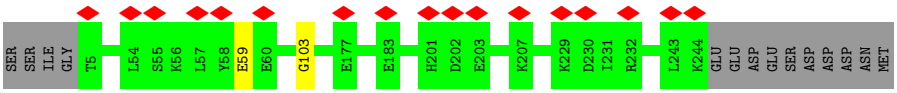
Chain l:




• Molecule 26: Proteasome subunit alpha type-3

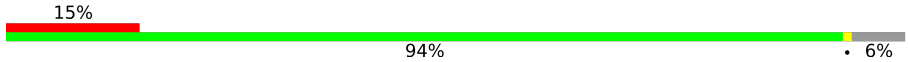
Chain M:

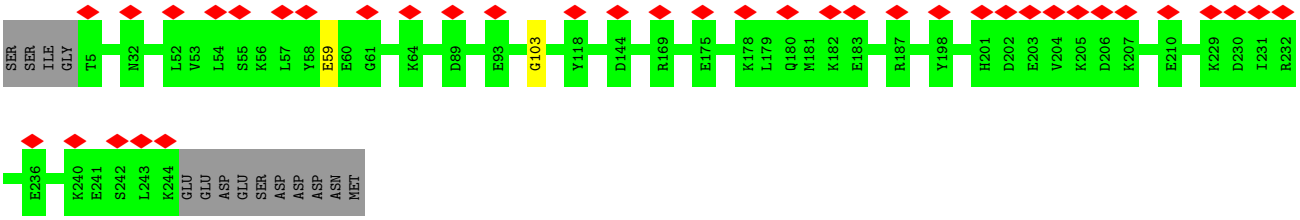



• Molecule 26: Proteasome subunit alpha type-3

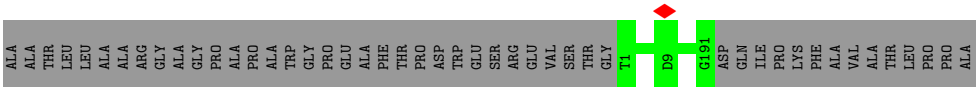
Chain m:



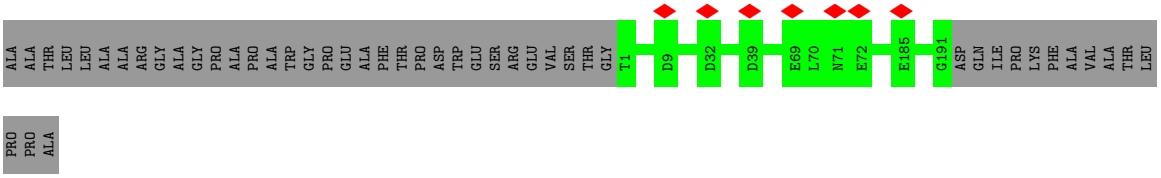

• Molecule 27: Proteasome subunit beta type-6

Chain N:



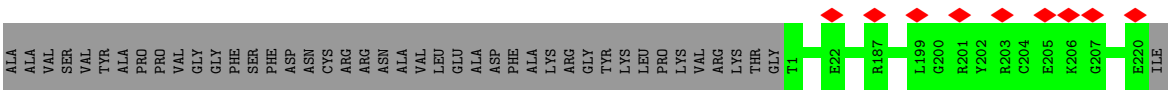

• Molecule 27: Proteasome subunit beta type-6

Chain n:



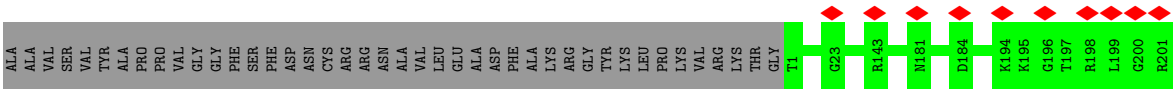

• Molecule 28: Proteasome subunit beta type-7

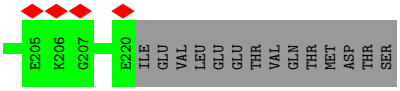
Chain O:



• Molecule 28: Proteasome subunit beta type-7

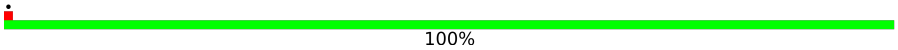
Chain o:

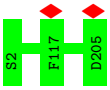



• Molecule 29: Proteasome subunit beta type-3

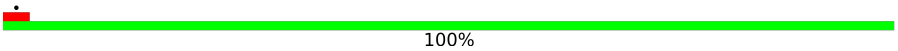
Chain P:

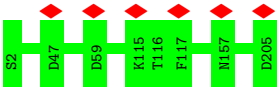



• Molecule 29: Proteasome subunit beta type-3

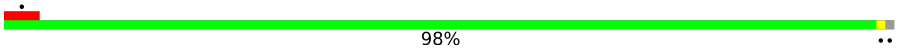
Chain p:

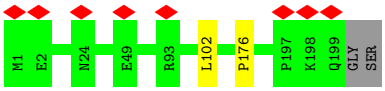



• Molecule 30: Proteasome subunit beta type-2

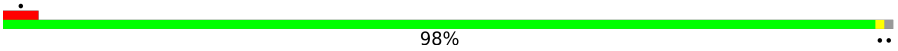
Chain Q:

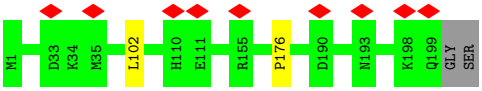



• Molecule 30: Proteasome subunit beta type-2

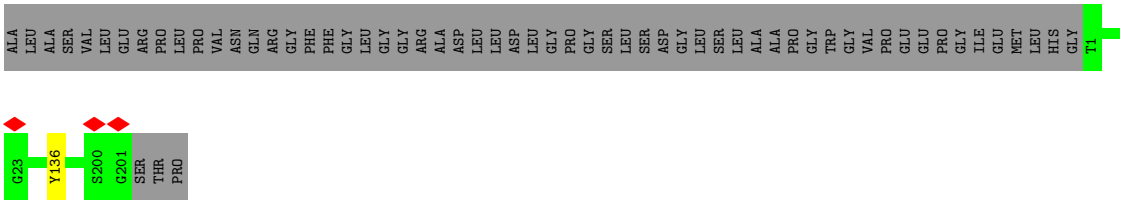
Chain q:



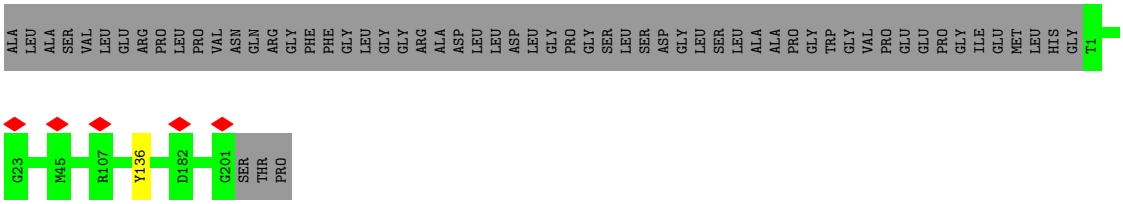

• Molecule 31: Proteasome subunit beta type-5

Chain R:



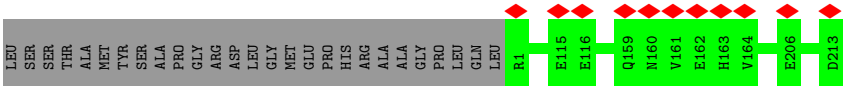

• Molecule 31: Proteasome subunit beta type-5

Chain r:



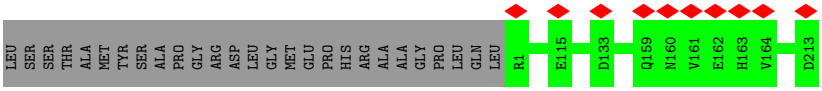

• Molecule 32: Proteasome subunit beta type-1

Chain S:



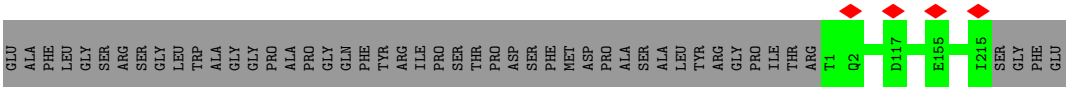

• Molecule 32: Proteasome subunit beta type-1

Chain s:



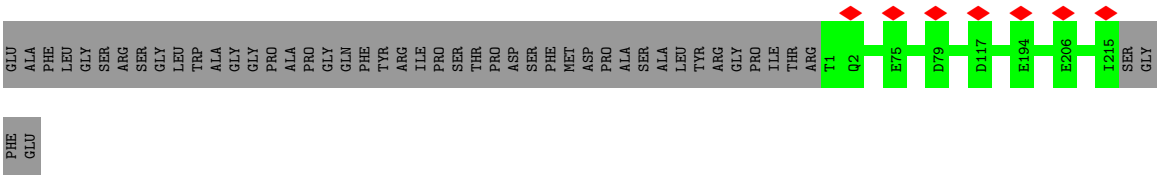

• Molecule 33: Proteasome subunit beta type-4

Chain T:




• Molecule 33: Proteasome subunit beta type-4

Chain t:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 71651 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 44 | 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 | 0.016 | Depositor |
| Minimum map value | -0.006 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.006 | Depositor |
| Map size (Å) | 411.0, 411.0, 411.0 | wwPDB |
| Map dimensions | 600, 600, 600 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.685, 0.685, 0.685 | 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: ATP, ADP, 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 | 0.31 | 0/6513 | 0.56 | 1/8816 (0.0%) |
| 2 | V | 0.34 | 0/3929 | 0.63 | 0/5309 |
| 3 | W | 0.31 | 0/3751 | 0.59 | 1/5042 (0.0%) |
| 4 | X | 0.39 | 0/3053 | 0.57 | 0/4115 |
| 5 | Y | 0.38 | 0/3173 | 0.61 | 0/4273 |
| 6 | Z | 0.30 | 0/2324 | 0.61 | 2/3150 (0.1%) |
| 7 | a | 0.31 | 0/3053 | 0.59 | 1/4133 (0.0%) |
| 8 | b | 0.29 | 0/1478 | 0.58 | 0/2001 |
| 9 | c | 0.33 | 0/2302 | 0.63 | 1/3110 (0.0%) |
| 10 | d | 0.32 | 0/2162 | 0.59 | 0/2919 |
| 11 | e | 0.32 | 0/338 | 0.65 | 1/450 (0.2%) |
| 12 | f | 0.33 | 1/6954 (0.0%) | 0.71 | 6/9399 (0.1%) |
| 13 | A | 0.34 | 0/2814 | 0.55 | 0/3801 |
| 14 | B | 0.32 | 0/2745 | 0.57 | 0/3709 |
| 15 | C | 0.35 | 0/3146 | 0.60 | 1/4226 (0.0%) |
| 16 | D | 0.41 | 0/3090 | 0.63 | 1/4168 (0.0%) |
| 17 | E | 0.37 | 0/3145 | 0.62 | 1/4233 (0.0%) |
| 18 | F | 0.37 | 0/3137 | 0.63 | 3/4223 (0.1%) |
| 20 | G | 0.47 | 0/1859 | 0.57 | 0/2523 |
| 20 | g | 0.47 | 0/1859 | 0.57 | 0/2523 |
| 21 | H | 0.50 | 0/1743 | 0.59 | 1/2372 (0.0%) |
| 21 | h | 0.50 | 0/1743 | 0.59 | 1/2372 (0.0%) |
| 22 | I | 0.43 | 0/1942 | 0.59 | 0/2628 |
| 22 | i | 0.43 | 0/1942 | 0.59 | 0/2628 |
| 23 | J | 0.41 | 0/1728 | 0.54 | 0/2358 |
| 23 | j | 0.41 | 0/1728 | 0.54 | 0/2358 |
| 24 | K | 0.39 | 0/1747 | 0.56 | 0/2364 |
| 24 | k | 0.39 | 0/1747 | 0.56 | 0/2364 |
| 25 | L | 0.43 | 0/1885 | 0.59 | 0/2552 |
| 25 | l | 0.43 | 0/1885 | 0.59 | 0/2552 |
| 26 | M | 0.46 | 0/1891 | 0.59 | 0/2552 |
| 26 | m | 0.46 | 0/1891 | 0.59 | 0/2552 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 27 | N | 0.43 | 0/1454 | 0.53 | 0/1967 |
| 27 | n | 0.43 | 0/1454 | 0.53 | 0/1967 |
| 28 | O | 0.42 | 0/1670 | 0.55 | 0/2265 |
| 28 | o | 0.42 | 0/1670 | 0.55 | 0/2265 |
| 29 | P | 0.45 | 0/1614 | 0.54 | 0/2177 |
| 29 | p | 0.45 | 0/1614 | 0.54 | 0/2177 |
| 30 | Q | 0.47 | 0/1603 | 0.62 | 0/2174 |
| 30 | q | 0.47 | 0/1603 | 0.62 | 0/2174 |
| 31 | R | 0.46 | 0/1579 | 0.52 | 0/2134 |
| 31 | r | 0.46 | 0/1579 | 0.52 | 0/2134 |
| 32 | S | 0.42 | 0/1671 | 0.54 | 0/2253 |
| 32 | s | 0.42 | 0/1671 | 0.54 | 0/2253 |
| 33 | T | 0.44 | 0/1700 | 0.53 | 0/2305 |
| 33 | t | 0.44 | 0/1700 | 0.53 | 0/2305 |
| All | All | 0.39 | 1/105279 (0.0%) | 0.59 | 21/142325 (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 | 1 |
| 6 | Z | 0 | 2 |
| 7 | a | 0 | 1 |
| 10 | d | 0 | 1 |
| 12 | f | 0 | 12 |
| 13 | A | 0 | 2 |
| 15 | C | 0 | 2 |
| 16 | D | 0 | 2 |
| 17 | E | 0 | 1 |
| 18 | F | 0 | 1 |
| All | All | 0 | 25 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | f | 192 | VAL | C-N | 5.92 | 1.45 | 1.34 |

The worst 5 of 21 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 12 | f | 830 | LEU | CA-CB-CG | 7.96 | 133.61 | 115.30 |
| 18 | F | 343 | LEU | CA-CB-CG | 7.43 | 132.40 | 115.30 |
| 11 | e | 56 | LEU | CA-CB-CG | 7.33 | 132.15 | 115.30 |
| 12 | f | 759 | LEU | CA-CB-CG | 6.76 | 130.84 | 115.30 |
| 12 | f | 612 | LEU | CA-CB-CG | 6.74 | 130.79 | 115.30 |

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | V | 29 | PRO | Peptide |
| 6 | Z | 144 | VAL | Peptide |
| 6 | Z | 183 | THR | Peptide |
| 7 | a | 18 | GLN | Peptide |
| 10 | d | 199 | PHE | 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 | 814/953 (85%) | 760 (93%) | 53 (6%) | 1 (0%) | 51 83 |
| 2 | V | 478/533 (90%) | 436 (91%) | 41 (9%) | 1 (0%) | 47 79 |
| 3 | W | 454/456 (100%) | 420 (92%) | 34 (8%) | 0 | 100 100 |
| 4 | X | 378/422 (90%) | 355 (94%) | 22 (6%) | 1 (0%) | 41 75 |
| 5 | Y | 376/389 (97%) | 340 (90%) | 36 (10%) | 0 | 100 100 |
| 6 | Z | 284/324 (88%) | 240 (84%) | 38 (13%) | 6 (2%) | 7 40 |
| 7 | a | 371/376 (99%) | 338 (91%) | 32 (9%) | 1 (0%) | 41 75 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 8 | b | 189/377 (50%) | 171 (90%) | 18 (10%) | 0 | 100 | 100 |
| 9 | c | 285/309 (92%) | 241 (85%) | 43 (15%) | 1 (0%) | 34 | 71 |
| 10 | d | 255/349 (73%) | 216 (85%) | 38 (15%) | 1 (0%) | 34 | 71 |
| 11 | e | 36/70 (51%) | 31 (86%) | 5 (14%) | 0 | 100 | 100 |
| 12 | f | 884/892 (99%) | 709 (80%) | 164 (19%) | 11 (1%) | 13 | 51 |
| 13 | A | 354/433 (82%) | 310 (88%) | 42 (12%) | 2 (1%) | 25 | 64 |
| 14 | B | 348/440 (79%) | 300 (86%) | 44 (13%) | 4 (1%) | 14 | 53 |
| 15 | C | 394/398 (99%) | 342 (87%) | 51 (13%) | 1 (0%) | 41 | 75 |
| 16 | D | 378/418 (90%) | 335 (89%) | 42 (11%) | 1 (0%) | 41 | 75 |
| 17 | E | 387/403 (96%) | 338 (87%) | 43 (11%) | 6 (2%) | 9 | 46 |
| 18 | F | 391/439 (89%) | 350 (90%) | 40 (10%) | 1 (0%) | 41 | 75 |
| 20 | G | 238/245 (97%) | 228 (96%) | 10 (4%) | 0 | 100 | 100 |
| 20 | g | 238/245 (97%) | 228 (96%) | 10 (4%) | 0 | 100 | 100 |
| 21 | H | 230/233 (99%) | 216 (94%) | 14 (6%) | 0 | 100 | 100 |
| 21 | h | 230/233 (99%) | 216 (94%) | 14 (6%) | 0 | 100 | 100 |
| 22 | I | 248/260 (95%) | 230 (93%) | 18 (7%) | 0 | 100 | 100 |
| 22 | i | 248/260 (95%) | 230 (93%) | 18 (7%) | 0 | 100 | 100 |
| 23 | J | 237/247 (96%) | 223 (94%) | 14 (6%) | 0 | 100 | 100 |
| 23 | j | 237/247 (96%) | 223 (94%) | 14 (6%) | 0 | 100 | 100 |
| 24 | K | 224/240 (93%) | 212 (95%) | 12 (5%) | 0 | 100 | 100 |
| 24 | k | 224/240 (93%) | 212 (95%) | 12 (5%) | 0 | 100 | 100 |
| 25 | L | 236/268 (88%) | 223 (94%) | 13 (6%) | 0 | 100 | 100 |
| 25 | l | 236/268 (88%) | 223 (94%) | 13 (6%) | 0 | 100 | 100 |
| 26 | M | 238/254 (94%) | 216 (91%) | 20 (8%) | 2 (1%) | 19 | 59 |
| 26 | m | 238/254 (94%) | 216 (91%) | 20 (8%) | 2 (1%) | 19 | 59 |
| 27 | N | 189/238 (79%) | 183 (97%) | 6 (3%) | 0 | 100 | 100 |
| 27 | n | 189/238 (79%) | 183 (97%) | 6 (3%) | 0 | 100 | 100 |
| 28 | O | 218/276 (79%) | 209 (96%) | 9 (4%) | 0 | 100 | 100 |
| 28 | o | 218/276 (79%) | 209 (96%) | 9 (4%) | 0 | 100 | 100 |
| 29 | P | 202/204 (99%) | 191 (95%) | 11 (5%) | 0 | 100 | 100 |
| 29 | p | 202/204 (99%) | 191 (95%) | 11 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 30 | Q | 197/201 (98%) | 181 (92%) | 15 (8%) | 1 (0%) | 29 | 68 |
| 30 | q | 197/201 (98%) | 181 (92%) | 15 (8%) | 1 (0%) | 29 | 68 |
| 31 | R | 199/262 (76%) | 190 (96%) | 9 (4%) | 0 | 100 | 100 |
| 31 | r | 199/262 (76%) | 190 (96%) | 9 (4%) | 0 | 100 | 100 |
| 32 | S | 211/240 (88%) | 202 (96%) | 9 (4%) | 0 | 100 | 100 |
| 32 | s | 211/240 (88%) | 202 (96%) | 9 (4%) | 0 | 100 | 100 |
| 33 | T | 213/263 (81%) | 198 (93%) | 15 (7%) | 0 | 100 | 100 |
| 33 | t | 213/263 (81%) | 198 (93%) | 15 (7%) | 0 | 100 | 100 |
| All | All | 13216/14843 (89%) | 12036 (91%) | 1136 (9%) | 44 (0%) | 44 | 75 |

5 of 44 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Z | 217 | THR |
| 10 | d | 200 | PHE |
| 12 | f | 808 | ASN |
| 12 | f | 853 | VAL |
| 14 | B | 354 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | U | 700/816 (86%) | 696 (99%) | 4 (1%) | 86 | 94 |
| 2 | V | 414/459 (90%) | 411 (99%) | 3 (1%) | 84 | 93 |
| 3 | W | 416/416 (100%) | 402 (97%) | 14 (3%) | 37 | 69 |
| 4 | X | 327/362 (90%) | 327 (100%) | 0 | 100 | 100 |
| 5 | Y | 334/344 (97%) | 330 (99%) | 4 (1%) | 71 | 87 |
| 6 | Z | 257/295 (87%) | 247 (96%) | 10 (4%) | 32 | 65 |
| 7 | a | 333/336 (99%) | 330 (99%) | 3 (1%) | 78 | 90 |
| 8 | b | 167/312 (54%) | 167 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 9 | c | 252/267 (94%) | 246 (98%) | 6 (2%) | 49 | 75 |
| 10 | d | 231/293 (79%) | 231 (100%) | 0 | 100 | 100 |
| 11 | e | 38/63 (60%) | 37 (97%) | 1 (3%) | 46 | 74 |
| 12 | f | 742/748 (99%) | 724 (98%) | 18 (2%) | 49 | 75 |
| 13 | A | 298/372 (80%) | 293 (98%) | 5 (2%) | 60 | 82 |
| 14 | B | 300/385 (78%) | 297 (99%) | 3 (1%) | 76 | 88 |
| 15 | C | 340/346 (98%) | 333 (98%) | 7 (2%) | 53 | 78 |
| 16 | D | 333/366 (91%) | 326 (98%) | 7 (2%) | 53 | 78 |
| 17 | E | 341/353 (97%) | 337 (99%) | 4 (1%) | 71 | 87 |
| 18 | F | 340/379 (90%) | 331 (97%) | 9 (3%) | 46 | 74 |
| 20 | G | 193/209 (92%) | 192 (100%) | 1 (0%) | 88 | 95 |
| 20 | g | 193/209 (92%) | 192 (100%) | 1 (0%) | 88 | 95 |
| 21 | H | 164/190 (86%) | 164 (100%) | 0 | 100 | 100 |
| 21 | h | 164/190 (86%) | 164 (100%) | 0 | 100 | 100 |
| 22 | I | 193/220 (88%) | 192 (100%) | 1 (0%) | 88 | 95 |
| 22 | i | 193/220 (88%) | 192 (100%) | 1 (0%) | 88 | 95 |
| 23 | J | 152/210 (72%) | 152 (100%) | 0 | 100 | 100 |
| 23 | j | 152/210 (72%) | 152 (100%) | 0 | 100 | 100 |
| 24 | K | 186/202 (92%) | 185 (100%) | 1 (0%) | 88 | 95 |
| 24 | k | 186/202 (92%) | 185 (100%) | 1 (0%) | 88 | 95 |
| 25 | L | 198/229 (86%) | 197 (100%) | 1 (0%) | 88 | 95 |
| 25 | l | 198/229 (86%) | 197 (100%) | 1 (0%) | 88 | 95 |
| 26 | M | 192/211 (91%) | 192 (100%) | 0 | 100 | 100 |
| 26 | m | 192/211 (91%) | 192 (100%) | 0 | 100 | 100 |
| 27 | N | 148/180 (82%) | 148 (100%) | 0 | 100 | 100 |
| 27 | n | 148/180 (82%) | 148 (100%) | 0 | 100 | 100 |
| 28 | O | 177/227 (78%) | 177 (100%) | 0 | 100 | 100 |
| 28 | o | 177/227 (78%) | 177 (100%) | 0 | 100 | 100 |
| 29 | P | 172/173 (99%) | 172 (100%) | 0 | 100 | 100 |
| 29 | p | 172/173 (99%) | 172 (100%) | 0 | 100 | 100 |
| 30 | Q | 164/171 (96%) | 163 (99%) | 1 (1%) | 86 | 94 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 30 | q | 164/171 (96%) | 163 (99%) | 1 (1%) | 86 94 |
| 31 | R | 153/201 (76%) | 152 (99%) | 1 (1%) | 84 93 |
| 31 | r | 153/201 (76%) | 152 (99%) | 1 (1%) | 84 93 |
| 32 | S | 174/198 (88%) | 174 (100%) | 0 | 100 100 |
| 32 | s | 174/198 (88%) | 174 (100%) | 0 | 100 100 |
| 33 | T | 175/214 (82%) | 175 (100%) | 0 | 100 100 |
| 33 | t | 175/214 (82%) | 175 (100%) | 0 | 100 100 |
| All | All | 11045/12582 (88%) | 10935 (99%) | 110 (1%) | 77 88 |

5 of 110 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | f | 660 | ILE |
| 15 | C | 20 | LEU |
| 31 | r | 136 | TYR |
| 22 | I | 228 | LEU |
| 12 | f | 703 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | B | 277 | HIS |
| 17 | E | 271 | HIS |
| 30 | q | 82 | ASN |
| 14 | B | 416 | ASN |
| 16 | D | 187 | HIS |

### 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 monosaccharides 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 | $\#\|Z\| > 2$ |
| 36 | ADP | F | 501 | - | 24,29,29 | 0.91 | 1 (4%) | 29,45,45 | 1.55 | 5 (17%) |
| 35 | ATP | E | 401 | - | 26,33,33 | 0.96 | 1 (3%) | 31,52,52 | 1.88 | 8 (25%) |
| 35 | ATP | C | 501 | - | 26,33,33 | 0.89 | 1 (3%) | 31,52,52 | 1.67 | 7 (22%) |
| 35 | ATP | D | 501 | - | 26,33,33 | 0.94 | 1 (3%) | 31,52,52 | 1.66 | 5 (16%) |

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 |
|---|---|---|---|---|---|---|---|
| 36 | ADP | F | 501 | - | - | 7/12/32/32 | 0/3/3/3 |
| 35 | ATP | E | 401 | - | - | 1/18/38/38 | 0/3/3/3 |
| 35 | ATP | C | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 35 | ATP | D | 501 | - | - | 7/18/38/38 | 0/3/3/3 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 35 | E | 401 | ATP | C5-C4 | 2.43 | 1.47 | 1.40 |
| 35 | D | 501 | ATP | C5-C4 | 2.33 | 1.47 | 1.40 |
| 35 | C | 501 | ATP | C5-C4 | 2.17 | 1.46 | 1.40 |
| 36 | F | 501 | ADP | C5-C4 | 2.12 | 1.46 | 1.40 |

The worst 5 of 25 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 401 | ATP | PA-O3A-PB | -5.60 | 113.59 | 132.83 |
| 35 | C | 501 | ATP | PB-O3B-PG | -4.05 | 118.91 | 132.83 |
| 36 | F | 501 | ADP | PA-O3A-PB | -3.95 | 119.28 | 132.83 |
| 35 | C | 501 | ATP | C3'-C2'-C1' | 3.87 | 106.81 | 100.98 |
| 35 | E | 401 | ATP | C3'-C2'-C1' | 3.87 | 106.80 | 100.98 |

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

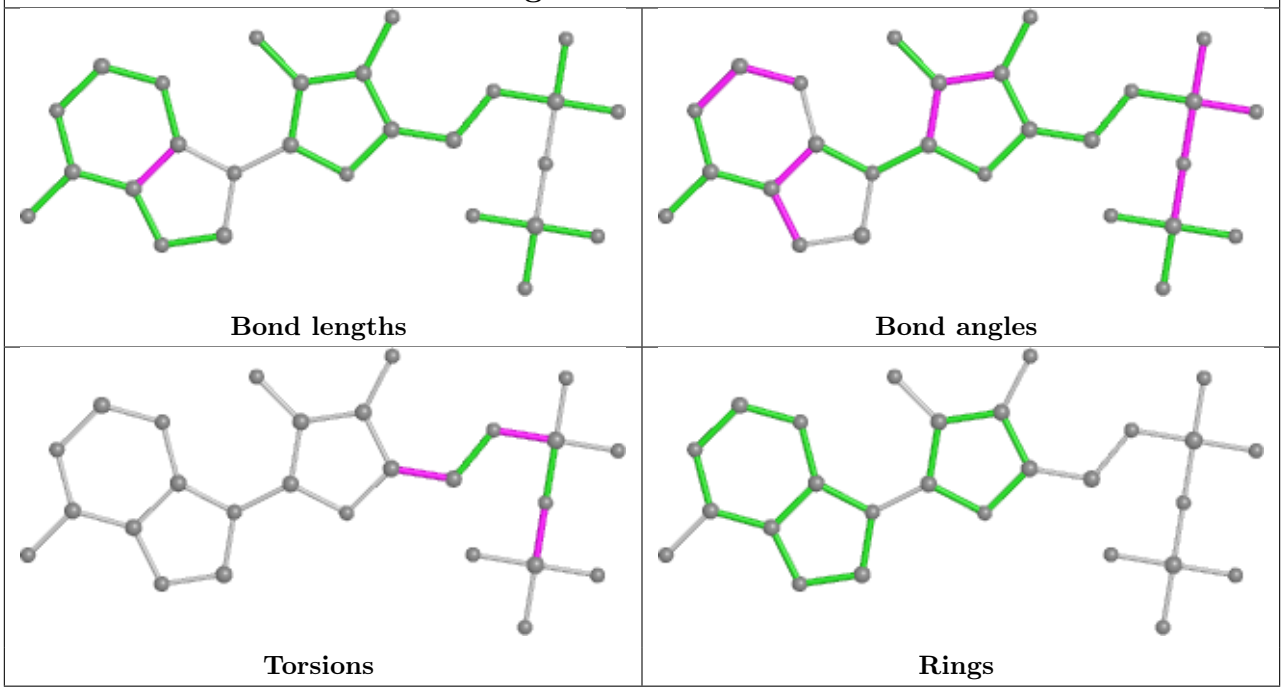
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 35 | D | 501 | ATP | C5'-O5'-PA-O1A |
| 35 | D | 501 | ATP | C5'-O5'-PA-O2A |
| 36 | F | 501 | ADP | PA-O3A-PB-O2B |
| 36 | F | 501 | ADP | PA-O3A-PB-O3B |
| 36 | F | 501 | ADP | C5'-O5'-PA-O1A |

There are no ring outliers.

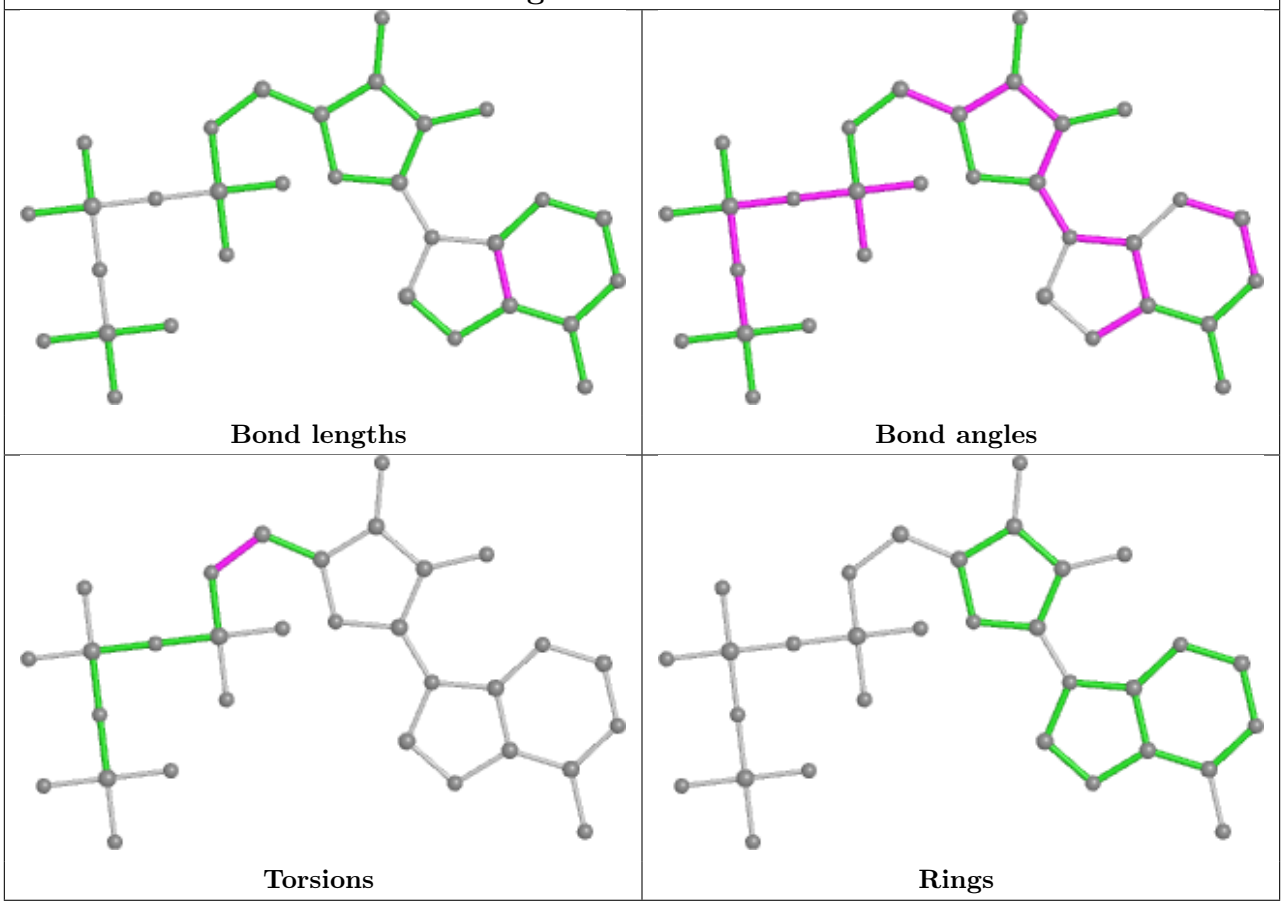
No monomer is involved in short contacts.

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.

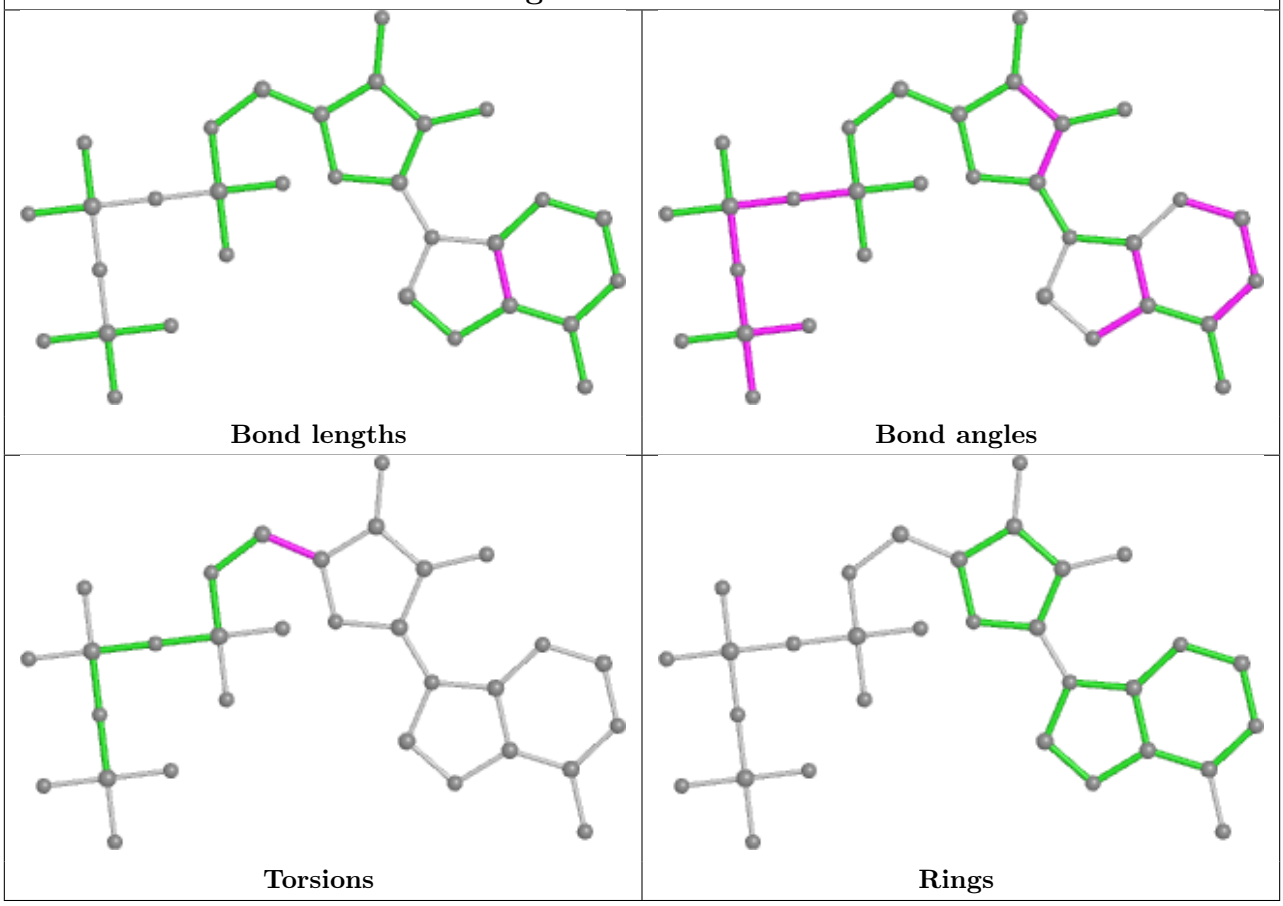
## Ligand ADP F 501

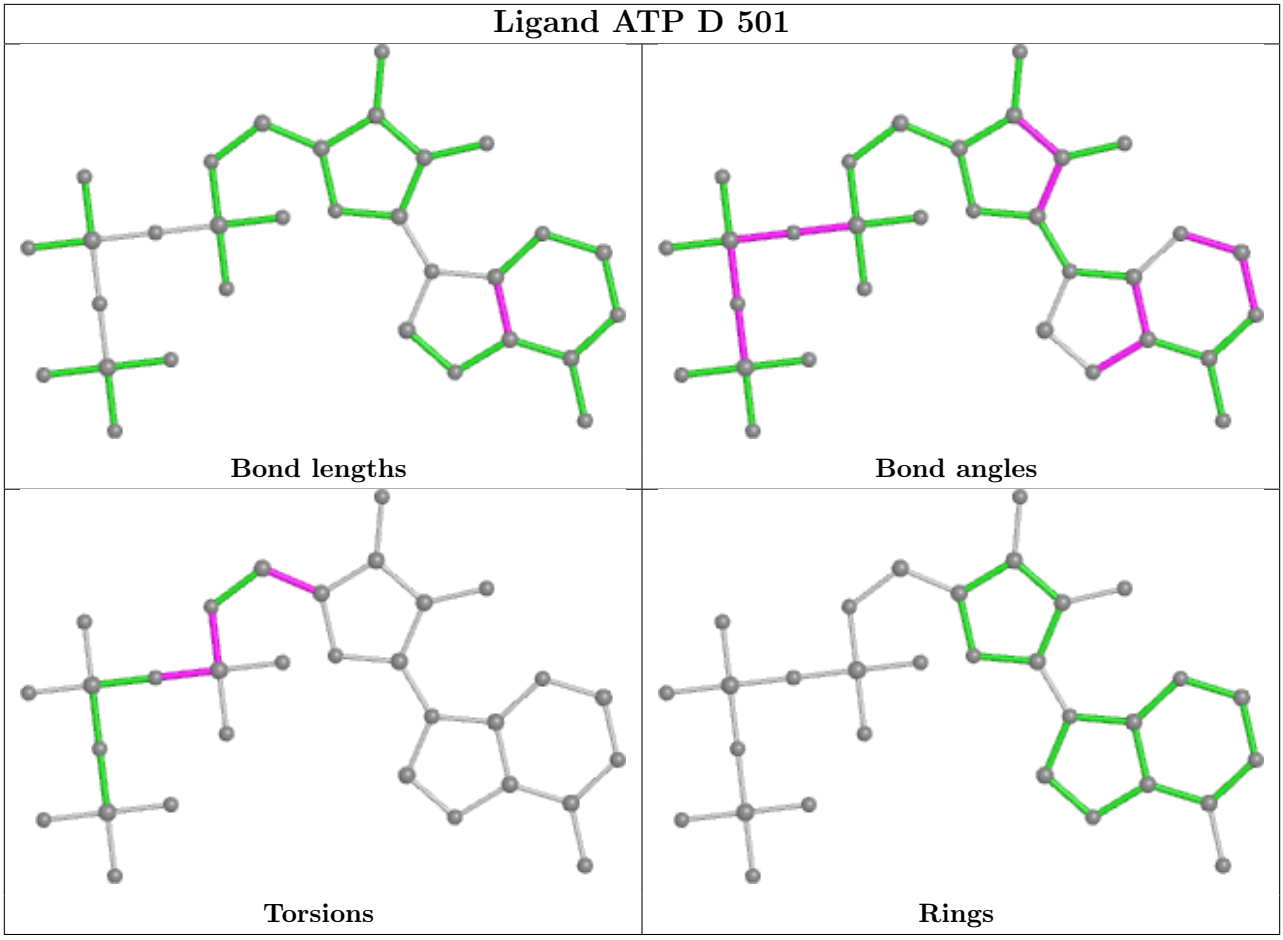



## Ligand ATP E 401



**Ligand ATP C 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.

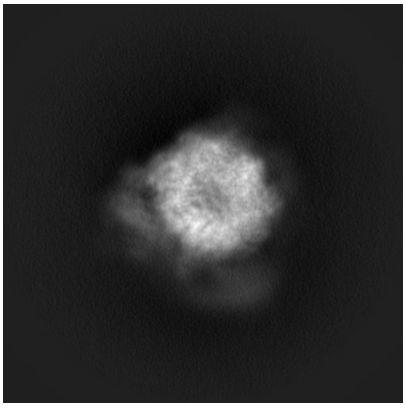
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9220. These allow visual inspection of the internal detail of the map and identification of artifacts.

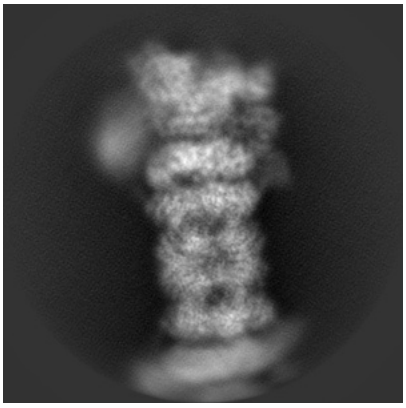
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

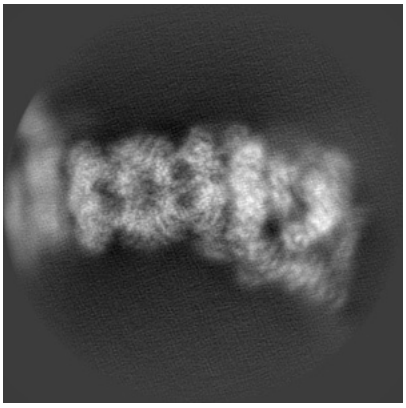
### 6.1.1 Primary map



X



Y

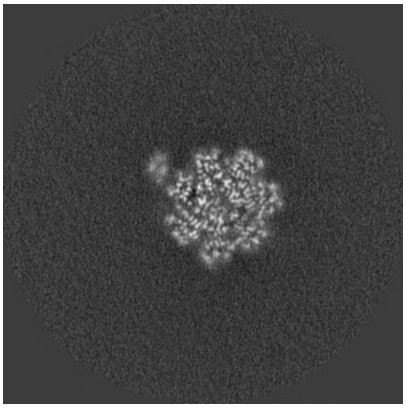


Z

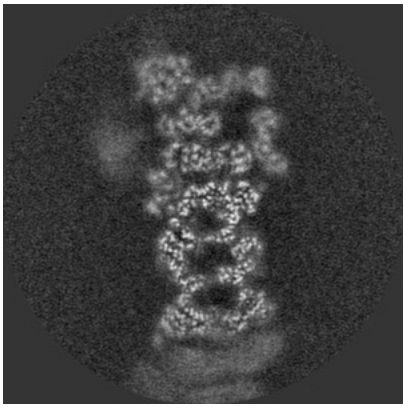
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

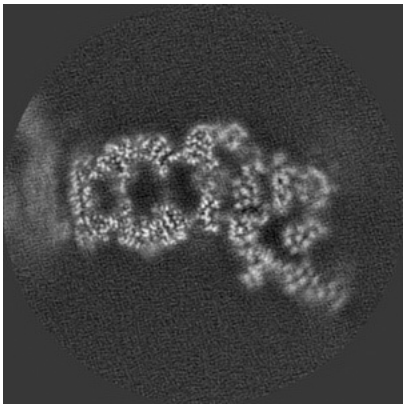
### 6.2.1 Primary map



X Index: 300



Y Index: 300

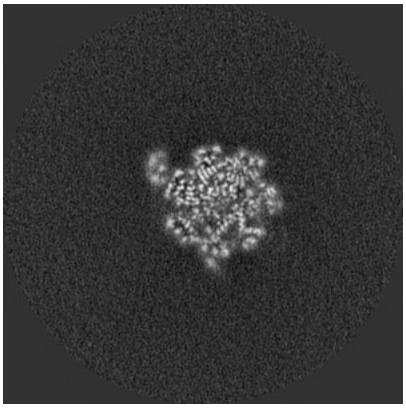


Z Index: 300

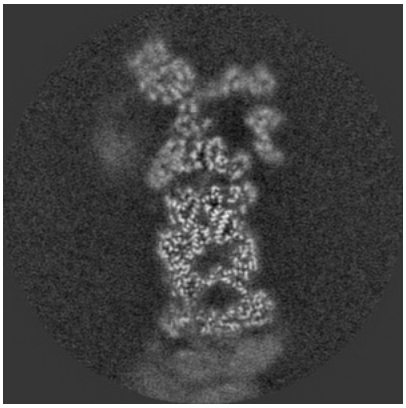
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

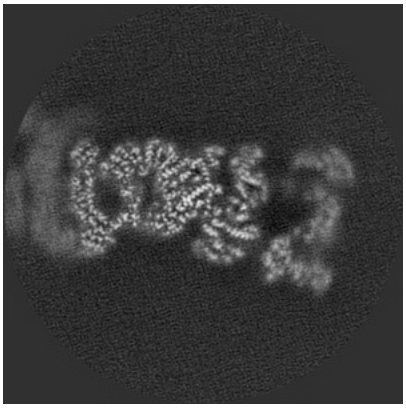
### 6.3.1 Primary map



X Index: 307



Y Index: 287



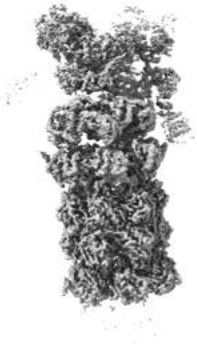
Z Index: 343

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

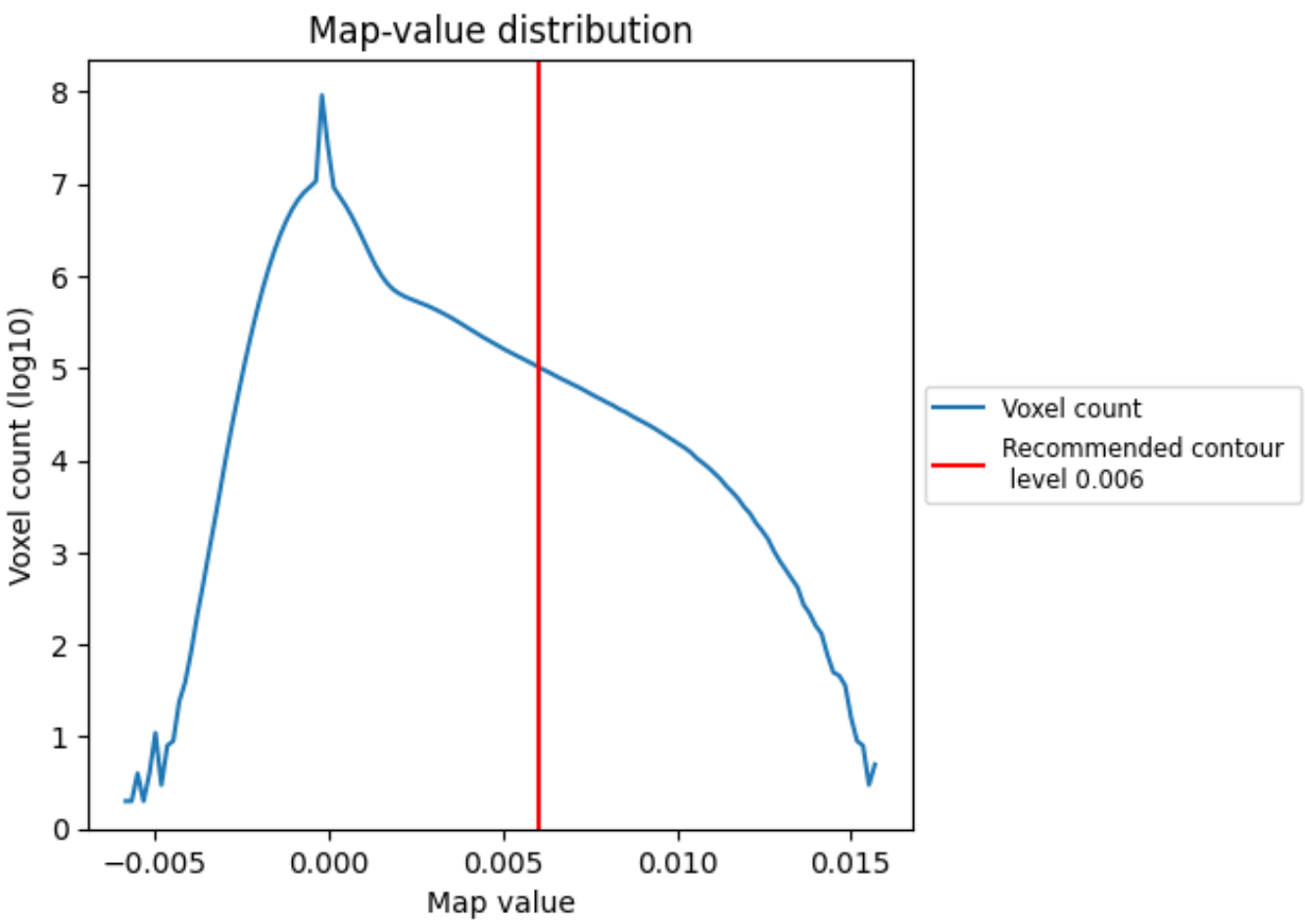
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

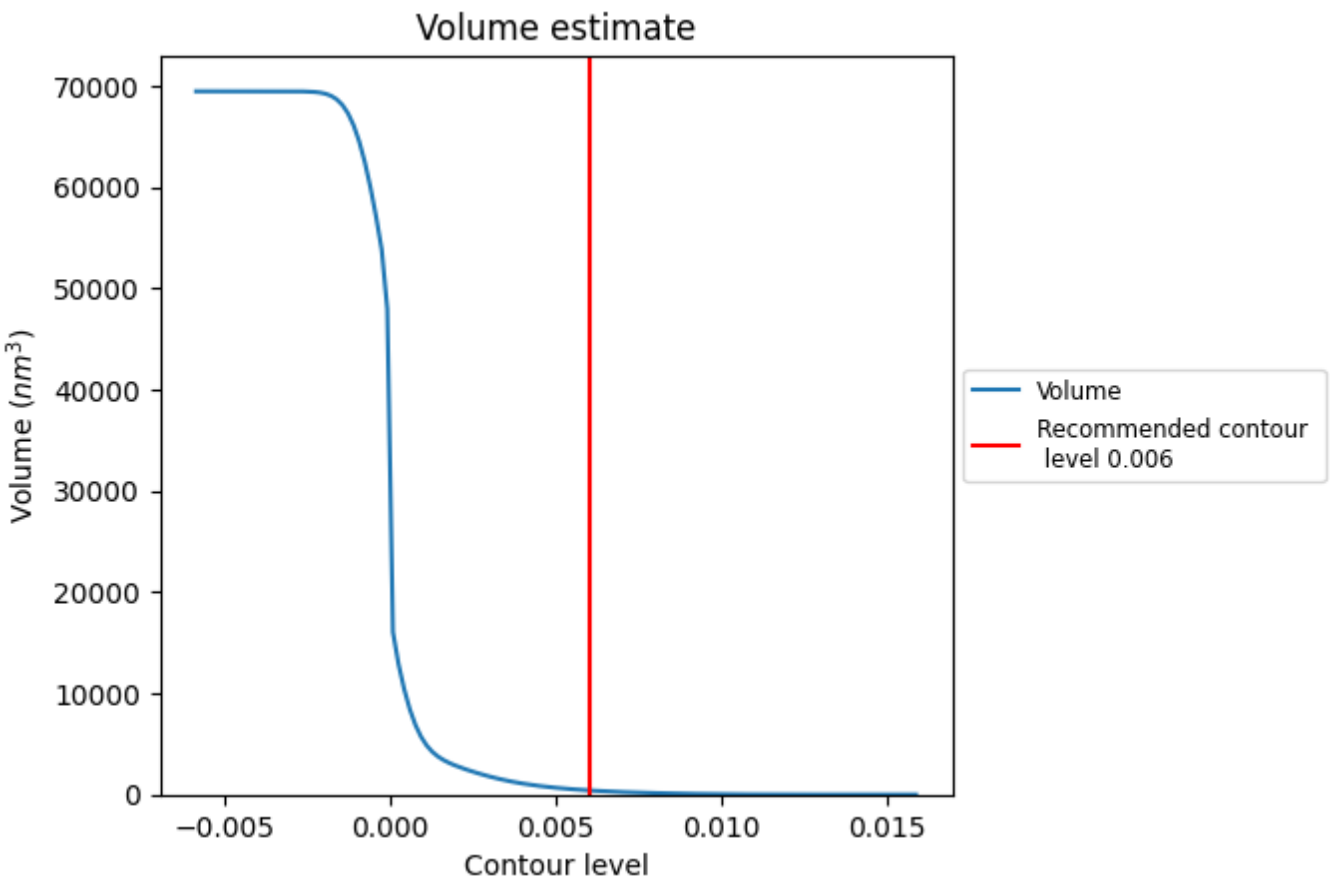
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

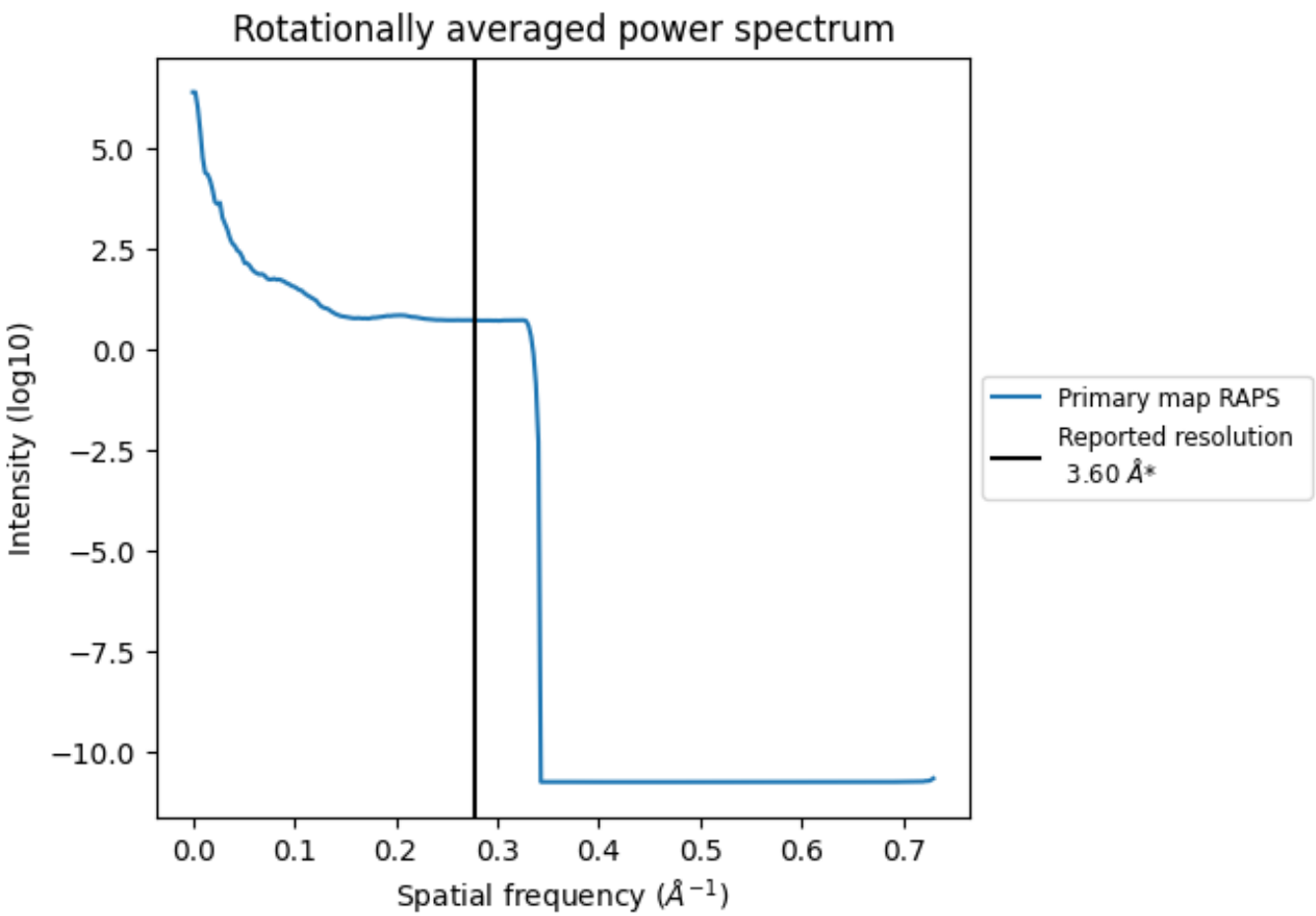
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 414 $nm^3$; this corresponds to an approximate mass of 374 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 0.278 Å$^{-1}$

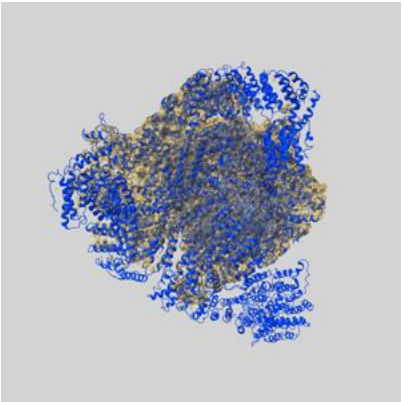
# 8 Fourier-Shell correlation (i)

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

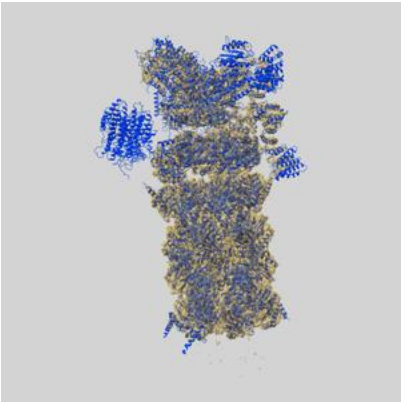
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9220 and PDB model 6MSH. Per-residue inclusion information can be found in section 3 on page 12.

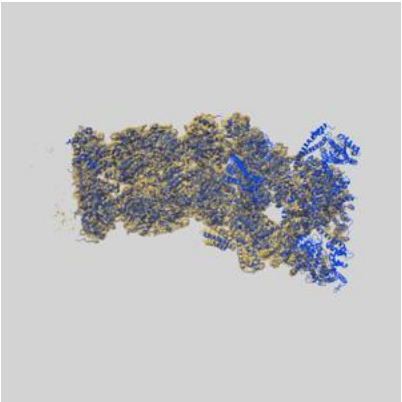
## 9.1 Map-model overlay (i)



X



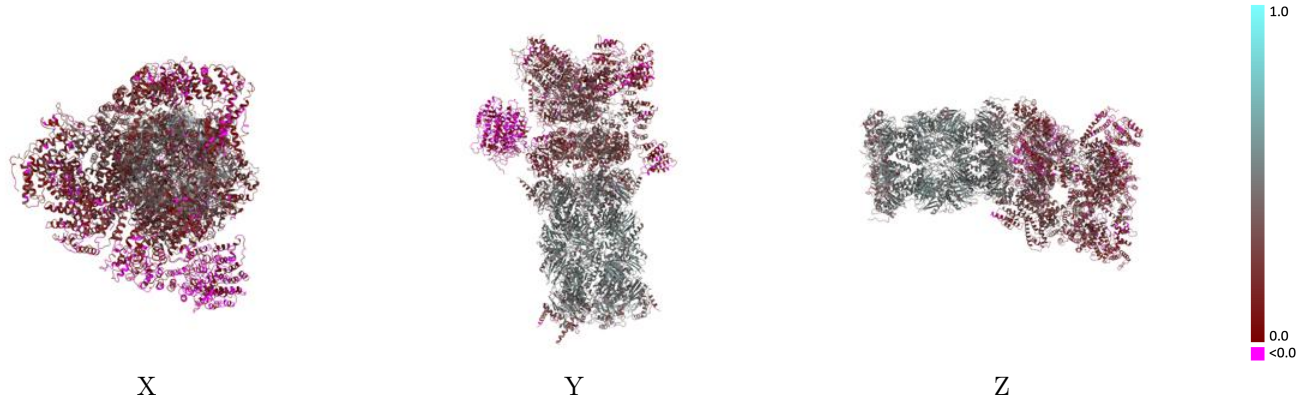
Y



Z

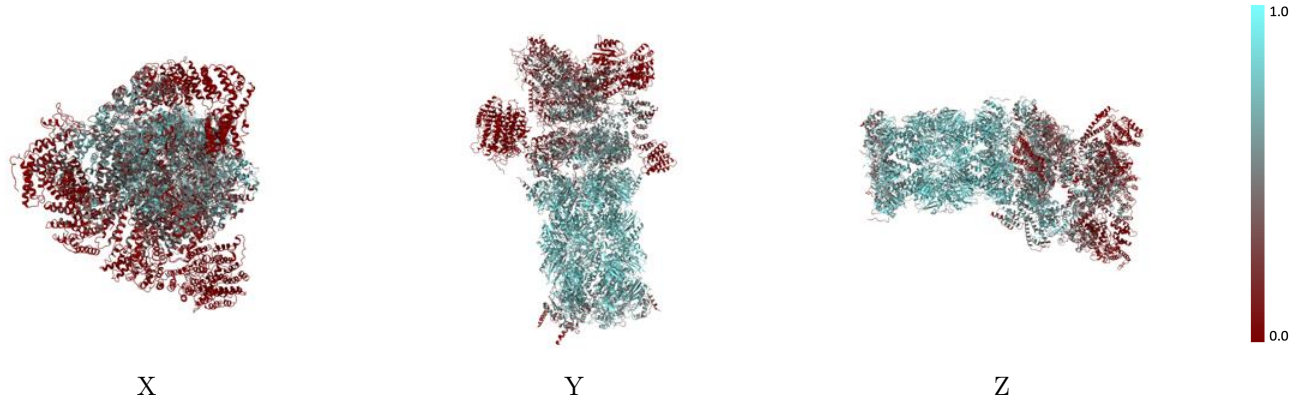
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



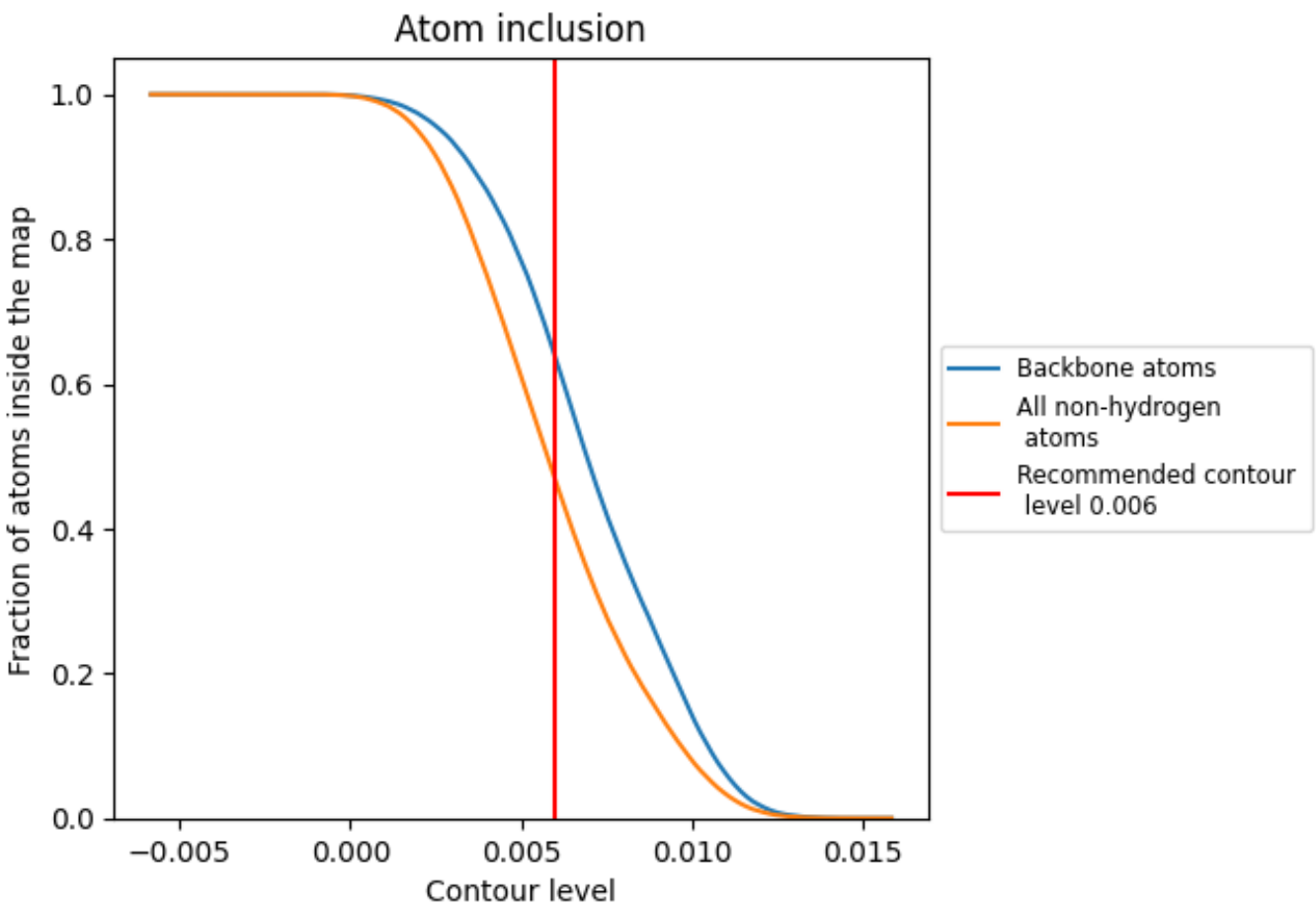

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

## 9.4 Atom inclusion (i)




At the recommended contour level, 64% of all backbone atoms, 47% 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 (0.006) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4683 | 0.3220 |
| A | 0.3547 | 0.2230 |
| B | 0.2201 | 0.1930 |
| C | 0.4112 | 0.2770 |
| D | 0.5106 | 0.3430 |
| E | 0.4629 | 0.3010 |
| F | 0.4253 | 0.2540 |
| G | 0.7227 | 0.4480 |
| H | 0.7700 | 0.4580 |
| I | 0.6948 | 0.4170 |
| J | 0.6639 | 0.4090 |
| K | 0.6589 | 0.4270 |
| L | 0.7161 | 0.4530 |
| M | 0.6962 | 0.4230 |
| N | 0.7811 | 0.4940 |
| O | 0.7639 | 0.4890 |
| P | 0.7683 | 0.4970 |
| Q | 0.7498 | 0.4730 |
| R | 0.7844 | 0.5020 |
| S | 0.7252 | 0.4900 |
| T | 0.7677 | 0.4990 |
| U | 0.2318 | 0.2070 |
| V | 0.1614 | 0.1790 |
| W | 0.2424 | 0.1690 |
| X | 0.5599 | 0.2920 |
| Y | 0.5318 | 0.2640 |
| Z | 0.2610 | 0.2130 |
| a | 0.1624 | 0.1660 |
| b | 0.0215 | 0.1490 |
| c | 0.3065 | 0.2540 |
| d | 0.0727 | 0.1700 |
| e | 0.2576 | 0.1920 |
| f | 0.0001 | 0.0170 |
| g | 0.6013 | 0.4430 |
| h | 0.6156 | 0.4520 |

*Continued on next page...*

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| i | 0.5363 | 0.4160 |
| j | 0.4982 | 0.3920 |
| k | 0.5686 | 0.4300 |
| l | 0.6779 | 0.4630 |
| m | 0.6225 | 0.4350 |
| n | 0.7575 | 0.5040 |
| o | 0.7218 | 0.4950 |
| p | 0.7368 | 0.5030 |
| q | 0.7316 | 0.4850 |
| r | 0.7784 | 0.5130 |
| s | 0.7452 | 0.4980 |
| t | 0.7794 | 0.5080 |
| v | 0.0727 | 0.2000 |