wwPDB EM Validation Summary Report

Aug 15, 2022 – 10:20 am BST

PDB ID	:	8AMZ
EMDB ID	:	EMD-14175
Title	:	Spinach 19S proteasome
Authors	:	Kandolf, S.; Grishkovskaya, I.; Meinhart, A.; Haselbach, D.
Deposited on	:	2022-08-04
Resolution	:	3.30 Å(reported)
Based on initial model	:	6MSB

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

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

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

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

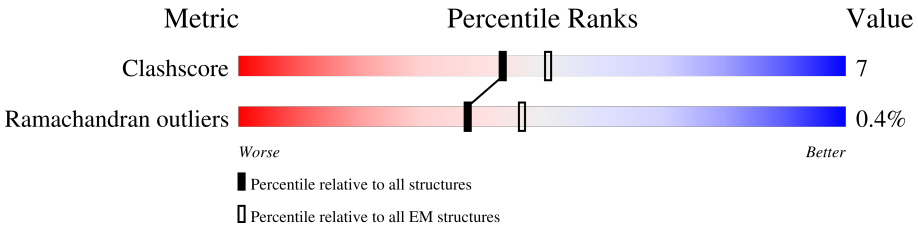
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 3.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	H	426	8% 81% 12% 8%
2	I	444	13% 75% 12% 14%
3	J	404	7% 77% 13% 10%
4	K	420	77% 13% 10%
5	L	397	9% 80% 14% 6%
6	M	427	7% 77% 11% 12%
7	V	309	12% 92% 7%
8	S	487	9% 66% 16% 17%
9	T	267	25% 93% 7%

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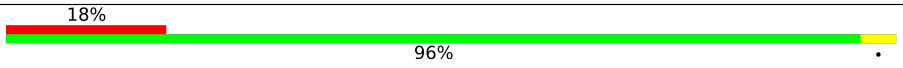
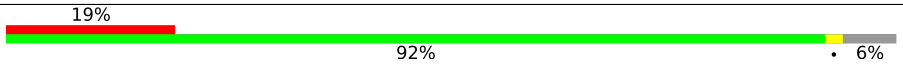
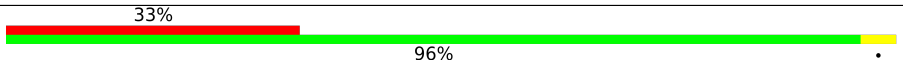
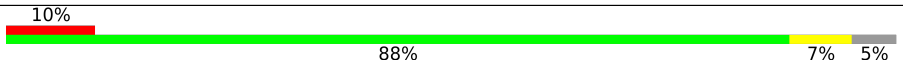
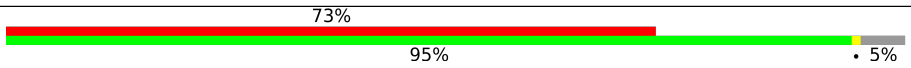
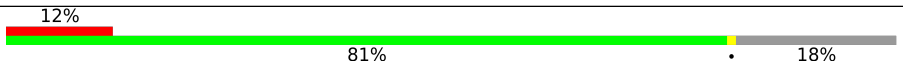
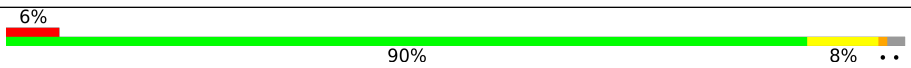
Mol	Chain	Length	Quality of chain
10	W	403	
11	O	386	
12	U	304	
13	Q	421	
14	P	442	
15	Z	895	
16	N	1000	
17	R	386	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 34609 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 regulatory subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	H	394	1941	1153	394	394	0	0

- Molecule 2 is a protein called AAA domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	I	384	1897	1129	384	384	0	0

- Molecule 3 is a protein called AAA domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	J	362	1788	1064	362	362	0	0

- Molecule 4 is a protein called AAA domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	K	380	1879	1119	380	380	0	0

- Molecule 5 is a protein called AAA domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	L	375	1849	1099	375	375	0	0

- Molecule 6 is a protein called AAA domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	M	376	1859	1107	376	376	0	0

- Molecule 7 is a protein called 26S proteasome regulatory subunit RPN11.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	V	287	Total	C	N	O	0	0
			1416	842	287	287		

- Molecule 8 is a protein called PCI domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	405	Total	C	N	O	0	0
			2007	1197	405	405		

- Molecule 9 is a protein called PCI domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	267	Total	C	N	O	0	0
			1330	796	267	267		

- Molecule 10 is a protein called VWFA domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	192	Total	C	N	O	0	0
			942	558	192	192		

- Molecule 11 is a protein called PCI domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	386	Total	C	N	O	0	0
			1916	1144	386	386		

- Molecule 12 is a protein called MPN domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	286	Total	C	N	O	0	0
			1420	848	286	286		

- Molecule 13 is a protein called PCI domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Q	421	Total	C	N	O	0	0
			2095	1253	421	421		

- Molecule 14 is a protein called PCI domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	P	421	Total	C	N	O	0	0
			2091	1249	421	421		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Z	854	Total	C	N	O	0	0
			4212	2504	854	854		

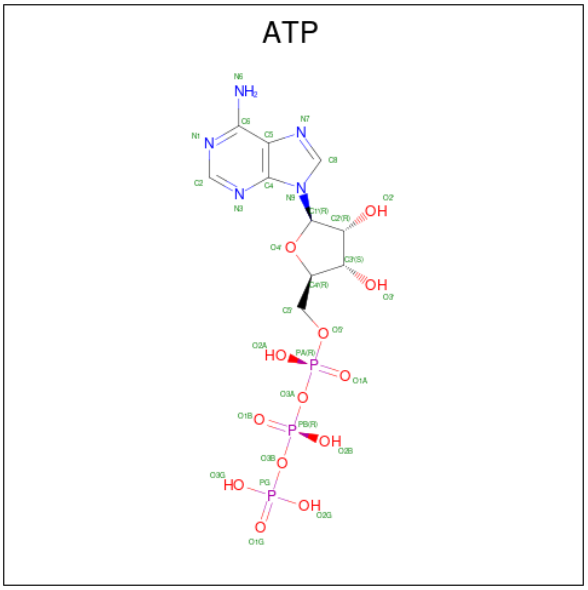
- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	N	816	Total	C	N	O	0	0
			4024	2392	816	816		

- Molecule 17 is a protein called PCI domain-containing protein.

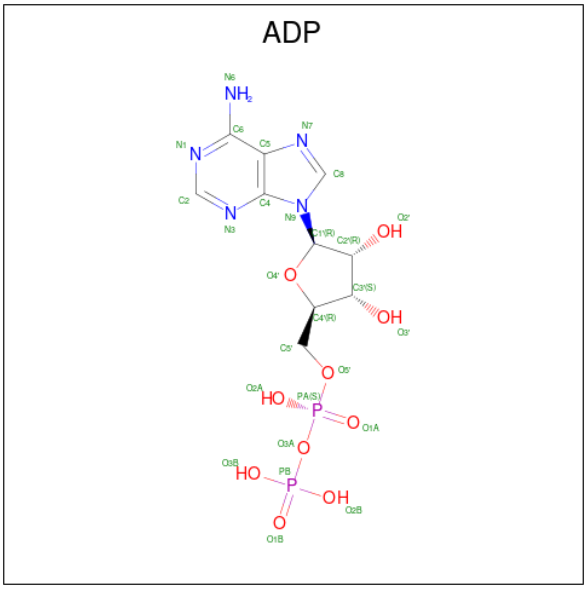
Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	380	Total	C	N	O	0	0
			1885	1125	380	380		

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
18	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



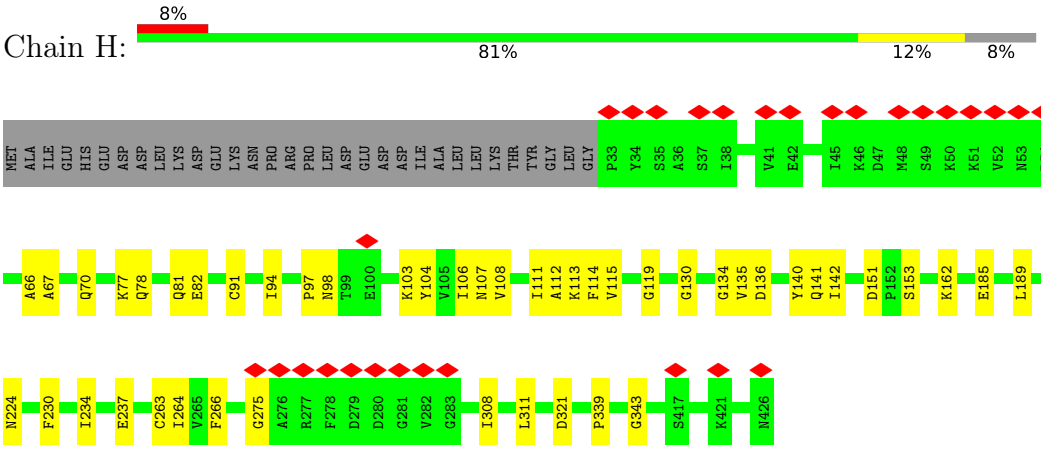
Mol	Chain	Residues	Atoms					AltConf
19	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

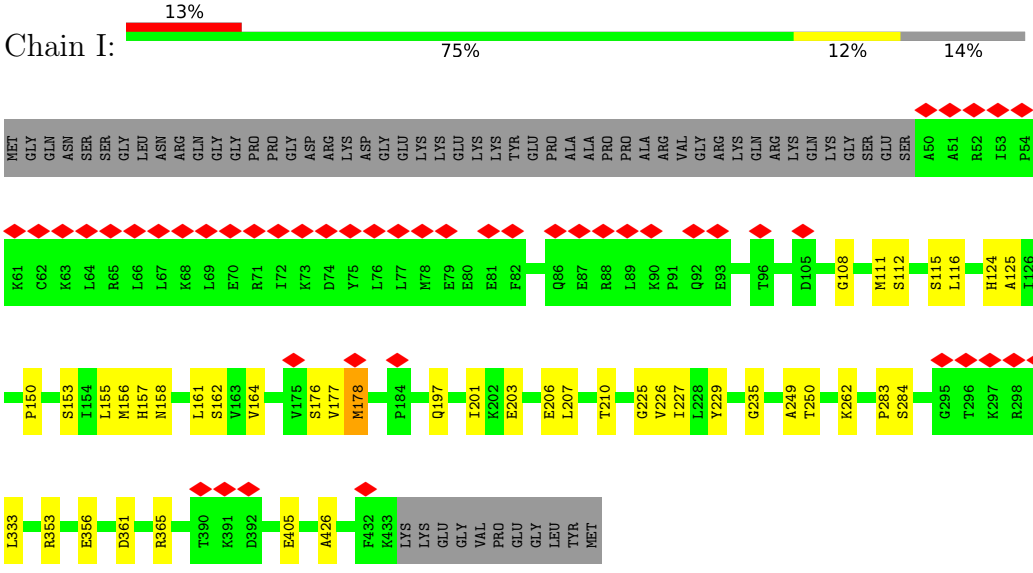
• Molecule 1: 26S proteasome regulatory subunit 7

Chain H:



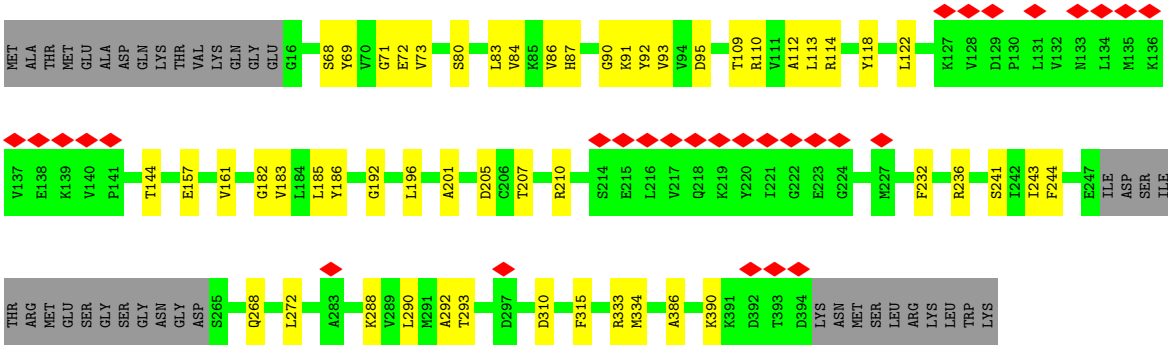
• Molecule 2: AAA domain-containing protein

Chain I:



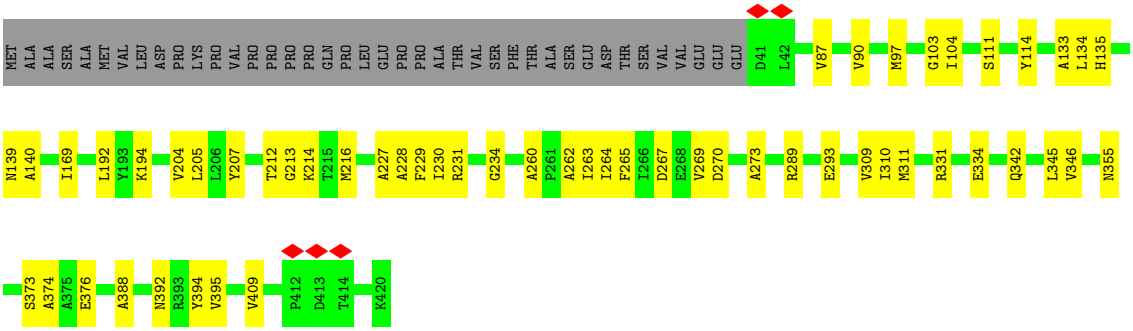
• Molecule 3: AAA domain-containing protein

Chain J:



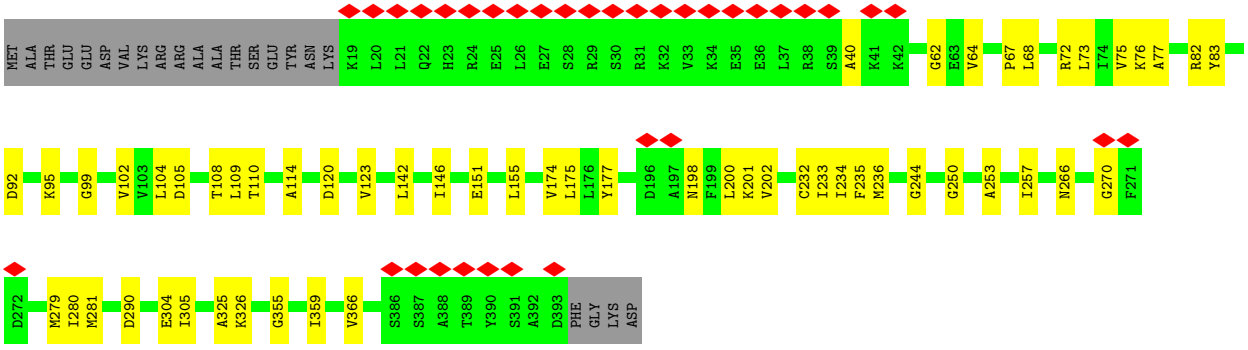
• Molecule 4: AAA domain-containing protein

Chain K:



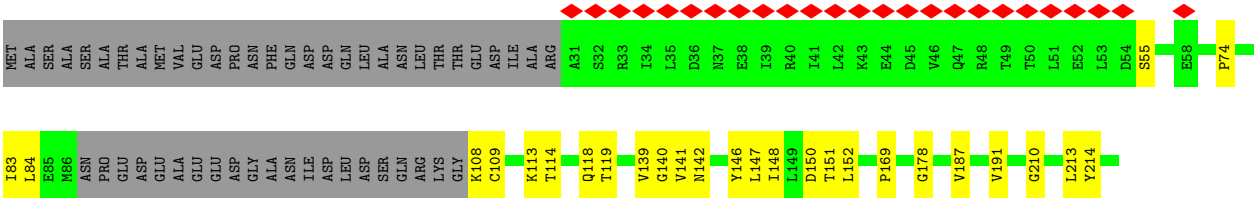
• Molecule 5: AAA domain-containing protein

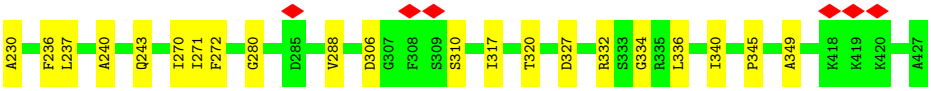
Chain L:



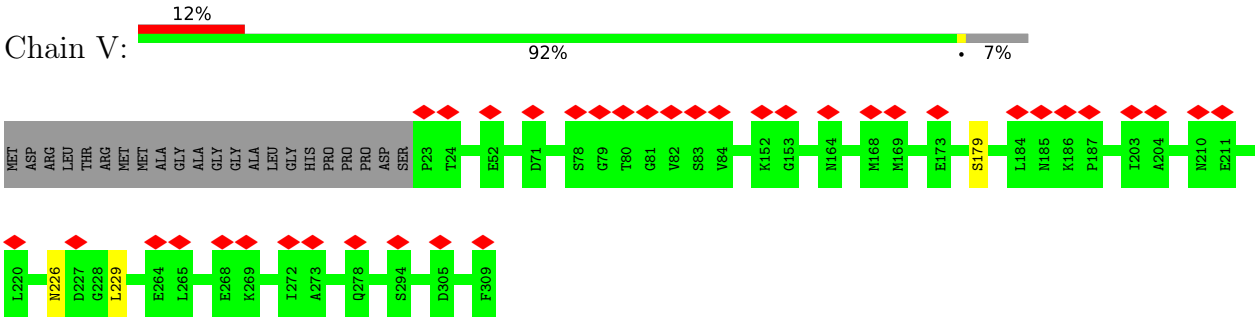
• Molecule 6: AAA domain-containing protein

Chain M:

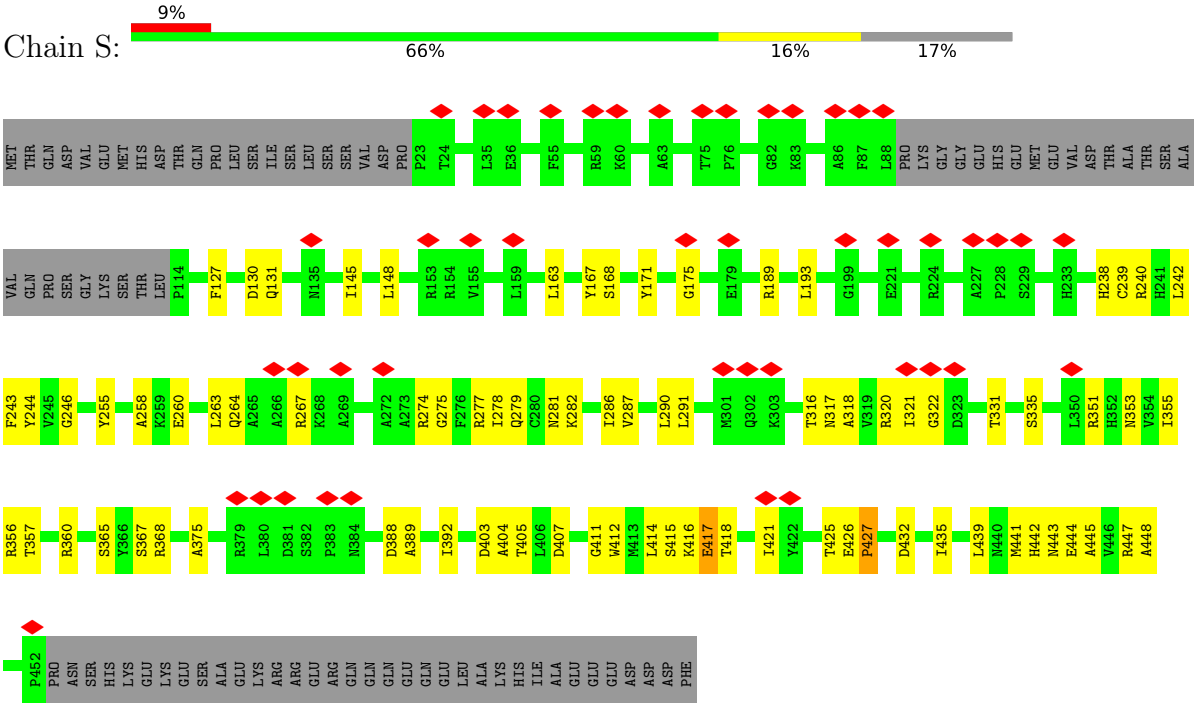




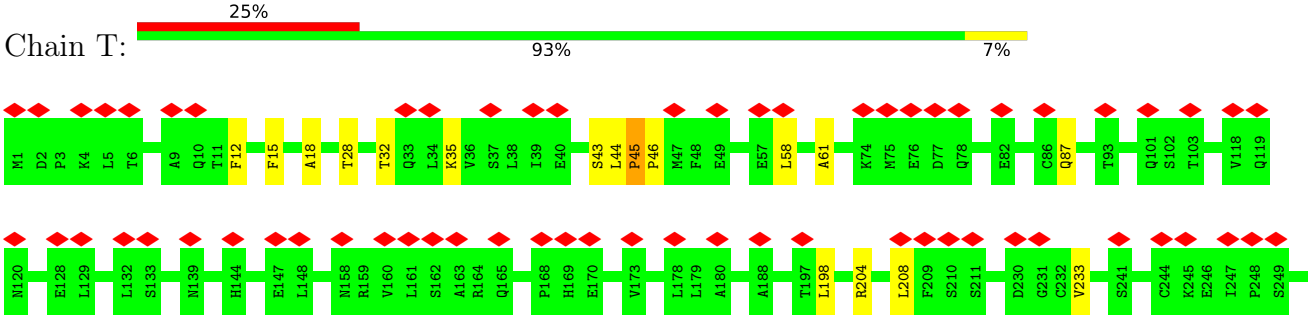
• Molecule 7: 26S proteasome regulatory subunit RPN11

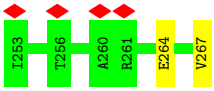


• Molecule 8: PCI domain-containing protein



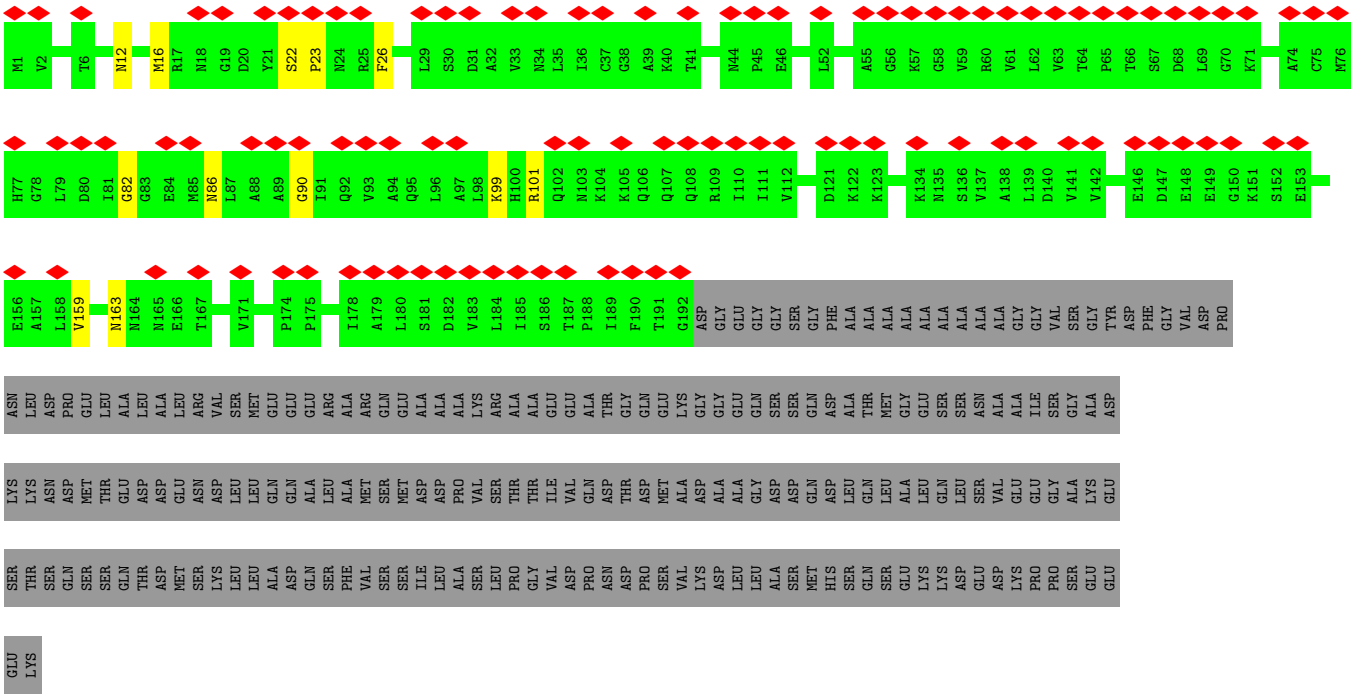
• Molecule 9: PCI domain-containing protein





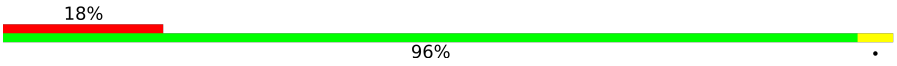
• Molecule 10: VWFA domain-containing protein

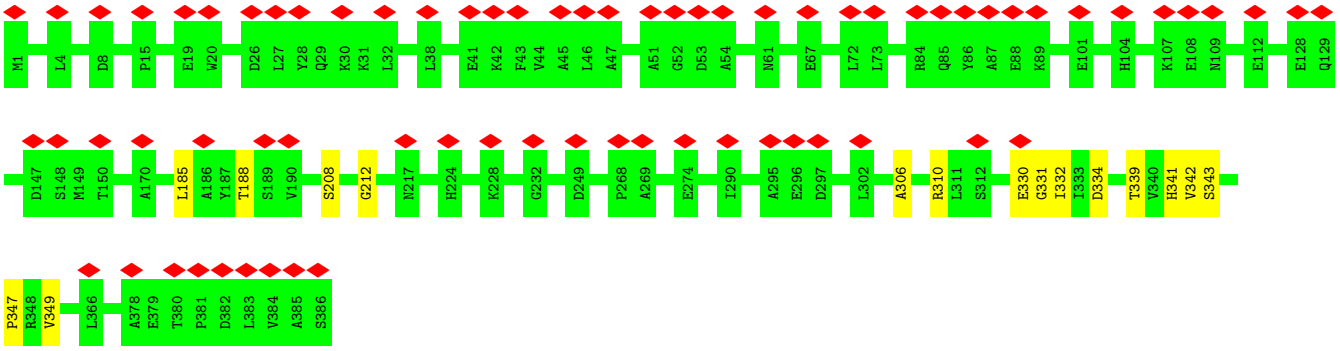
Chain W:



• Molecule 11: PCI domain-containing protein

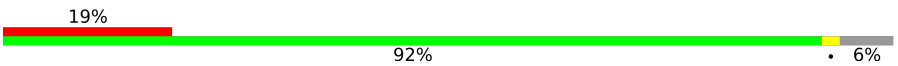
Chain O:

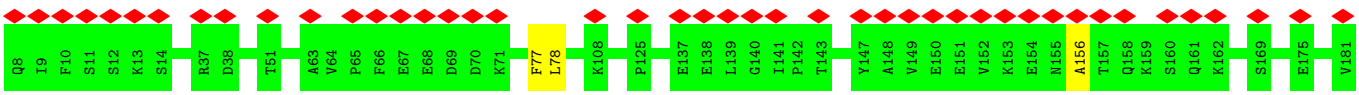


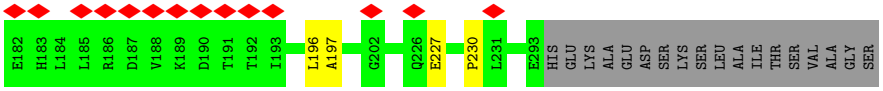


• Molecule 12: MPN domain-containing protein

Chain U:

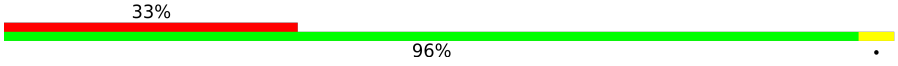


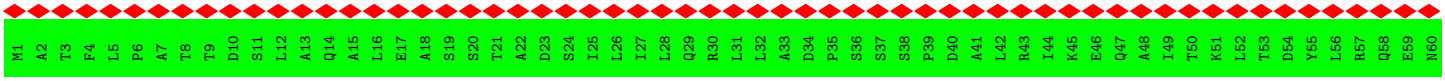


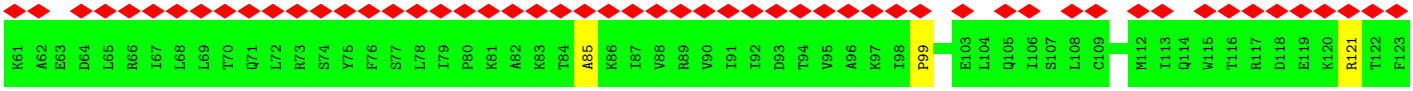


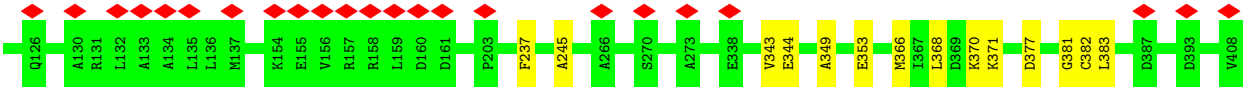
• Molecule 13: PCI domain-containing protein

Chain Q:



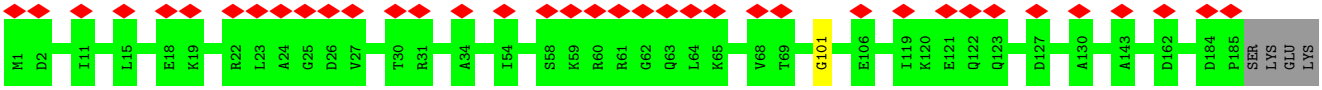


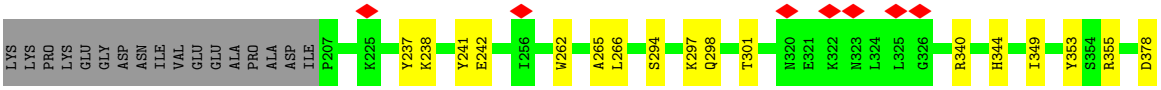


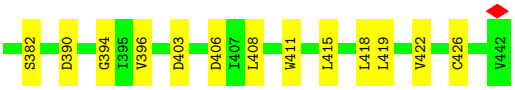


• Molecule 14: PCI domain-containing protein

Chain P:

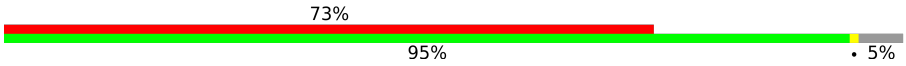


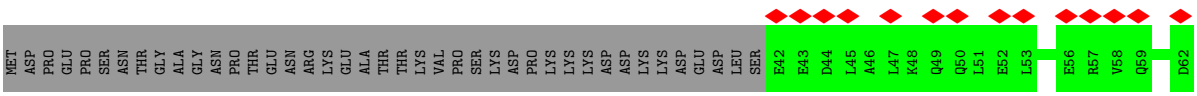


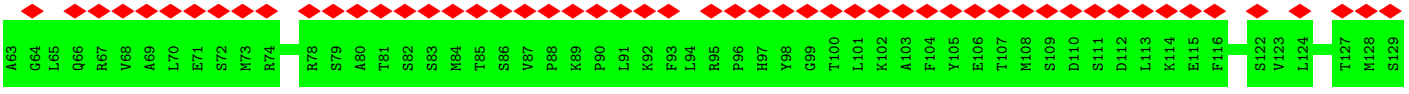


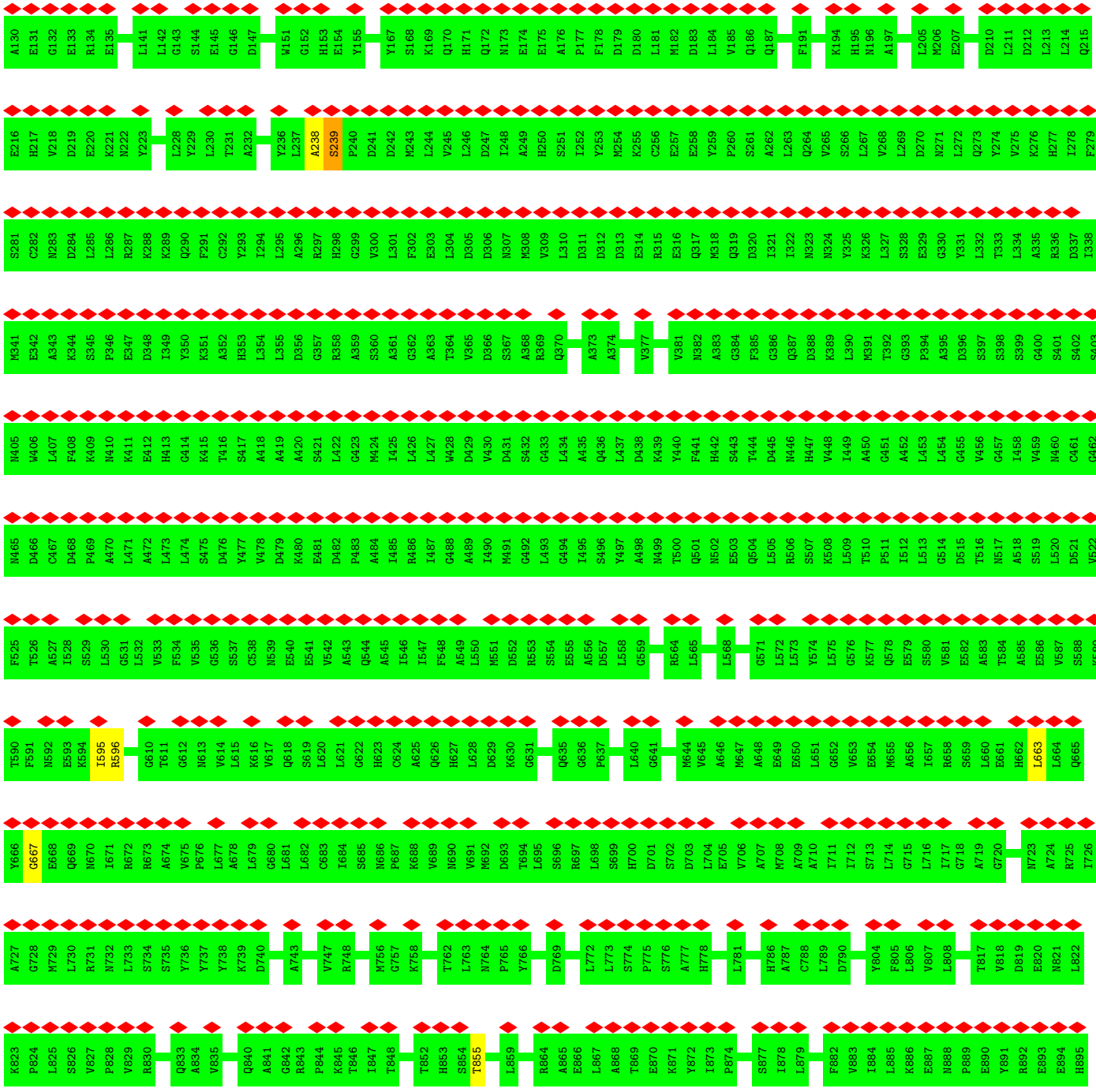
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 2 homolog

Chain Z:

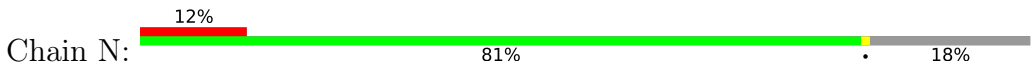


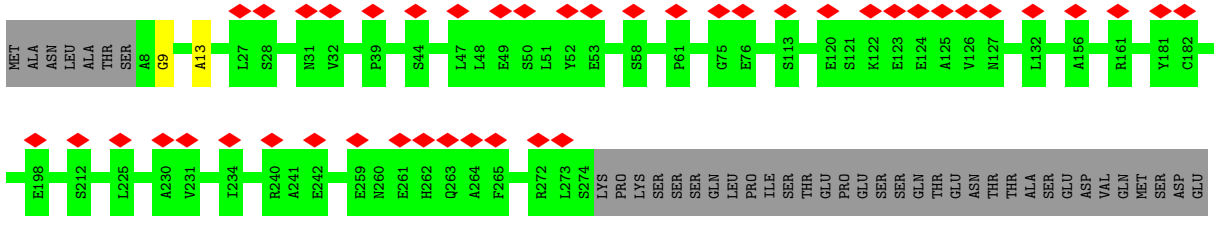


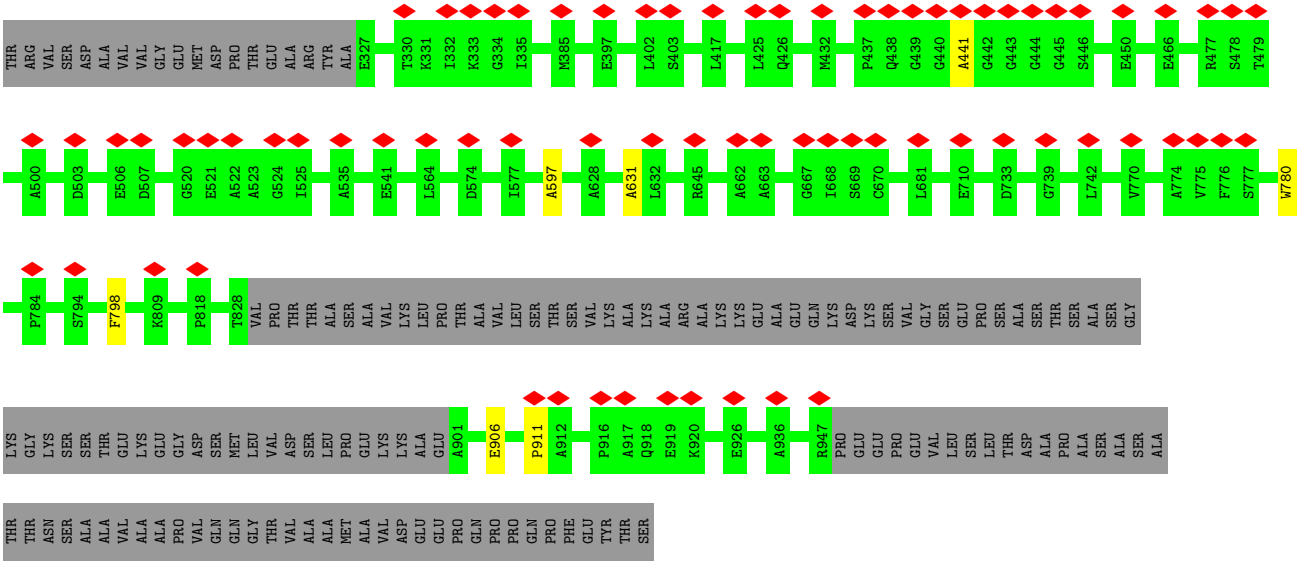




• Molecule 16: 26S proteasome non-ATPase regulatory subunit 1 homolog

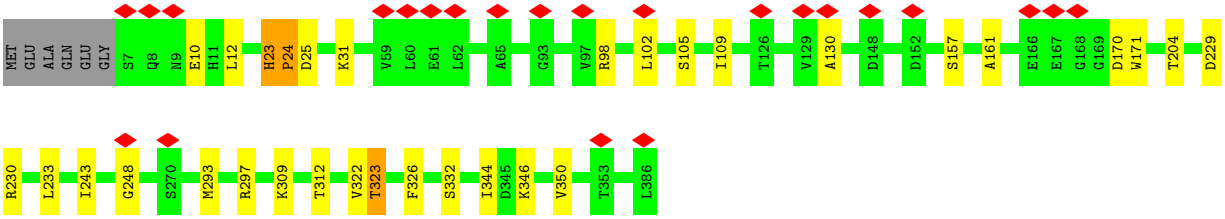






• Molecule 17: PCI domain-containing protein

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	951422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80, 50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.932	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.0168	Depositor
Map size (Å)	541.696, 541.696, 541.696	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2311273, 1.2311273, 1.2311273	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	H	0.24	0/1940	0.43	0/2697
2	I	0.27	0/1896	0.42	0/2639
3	J	0.24	0/1786	0.42	0/2484
4	K	0.43	0/1878	0.50	0/2615
5	L	0.24	0/1848	0.42	0/2570
6	M	0.24	0/1857	0.41	0/2584
7	V	0.33	0/1415	0.49	0/1968
8	S	0.26	0/2005	0.39	0/2793
9	T	0.41	0/1329	0.49	0/1856
10	W	0.30	0/941	0.46	0/1305
11	O	0.27	0/1915	0.44	0/2671
12	U	0.34	0/1419	0.51	0/1979
13	Q	0.32	0/2094	0.43	0/2924
14	P	0.23	0/2089	0.40	0/2913
15	Z	0.25	0/4211	0.40	0/5859
16	N	0.40	0/4021	0.68	0/5591
17	R	0.52	0/1884	0.68	0/2627
All	All	0.32	0/34528	0.49	0/48075

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1941	0	870	29	0
2	I	1897	0	833	32	0
3	J	1788	0	782	41	0
4	K	1879	0	845	43	0
5	L	1849	0	839	44	0
6	M	1859	0	841	34	0
7	V	1416	0	624	2	0
8	S	2007	0	934	58	0
9	T	1330	0	590	18	0
10	W	942	0	443	6	0
11	O	1916	0	874	8	0
12	U	1420	0	613	5	0
13	Q	2095	0	981	11	0
14	P	2091	0	927	17	0
15	Z	4212	0	1987	3	0
16	N	4024	0	1902	9	0
17	R	1885	0	841	25	0
18	H	31	0	12	0	0
19	I	27	0	12	1	0
All	All	34609	0	15750	350	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 350 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:87:GLN:CB	16:N:13:ALA:HB2	1.13	1.56
9:T:87:GLN:CB	16:N:13:ALA:CB	1.85	1.54
3:J:144:THR:CB	17:R:130:ALA:CB	2.16	1.24
9:T:43:SER:CB	9:T:61:ALA:CB	2.17	1.22
9:T:43:SER:CB	9:T:61:ALA:HB3	1.78	1.14

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	392/426 (92%)	348 (89%)	44 (11%)	0	100	100
2	I	382/444 (86%)	352 (92%)	28 (7%)	2 (0%)	29	61
3	J	358/404 (89%)	332 (93%)	26 (7%)	0	100	100
4	K	378/420 (90%)	336 (89%)	39 (10%)	3 (1%)	19	51
5	L	373/397 (94%)	343 (92%)	30 (8%)	0	100	100
6	M	372/427 (87%)	345 (93%)	27 (7%)	0	100	100
7	V	285/309 (92%)	265 (93%)	20 (7%)	0	100	100
8	S	401/487 (82%)	390 (97%)	7 (2%)	4 (1%)	15	46
9	T	265/267 (99%)	247 (93%)	17 (6%)	1 (0%)	34	66
10	W	190/403 (47%)	183 (96%)	5 (3%)	2 (1%)	14	45
11	O	384/386 (100%)	376 (98%)	6 (2%)	2 (0%)	29	61
12	U	284/304 (93%)	277 (98%)	5 (2%)	2 (1%)	22	54
13	Q	419/421 (100%)	404 (96%)	13 (3%)	2 (0%)	29	61
14	P	417/442 (94%)	407 (98%)	10 (2%)	0	100	100
15	Z	852/895 (95%)	828 (97%)	22 (3%)	2 (0%)	47	77
16	N	810/1000 (81%)	782 (96%)	26 (3%)	2 (0%)	47	77
17	R	378/386 (98%)	336 (89%)	37 (10%)	5 (1%)	12	40
All	All	6940/7818 (89%)	6551 (94%)	362 (5%)	27 (0%)	38	66

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	S	426	GLU
10	W	22	SER
11	O	347	PRO
12	U	227	GLU
15	Z	239	SER

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	ATP	H	501	-	26,33,33	0.72	0	31,52,52	0.91	2 (6%)
19	ADP	I	501	-	24,29,29	0.70	0	29,45,45	0.92	2 (6%)

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
18	ATP	H	501	-	-	5/18/38/38	0/3/3/3
19	ADP	I	501	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	I	501	ADP	O4'-C1'-C2'	-2.40	103.41	106.93
19	I	501	ADP	C5-C6-N6	2.18	123.67	120.35
18	H	501	ATP	C5-C6-N6	2.09	123.52	120.35
18	H	501	ATP	PB-O3B-PG	-2.04	125.82	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

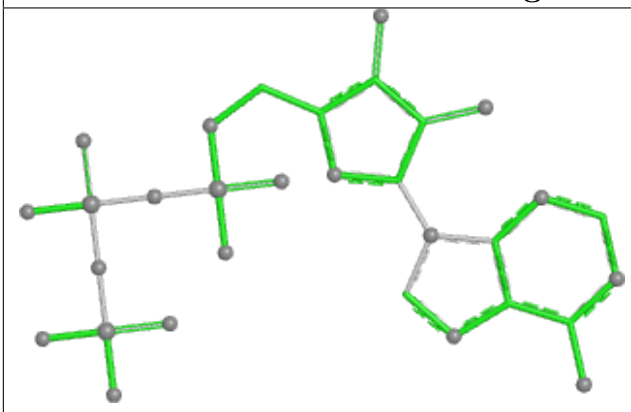
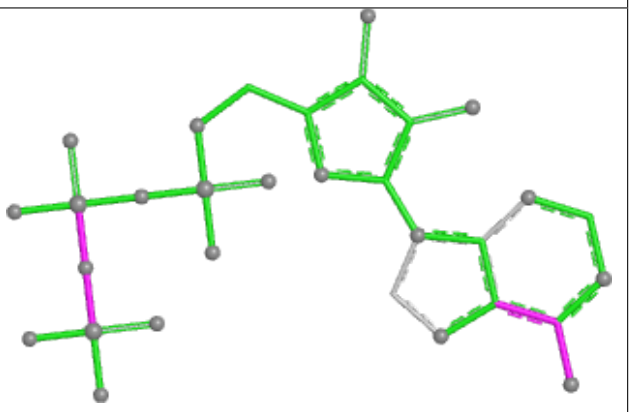
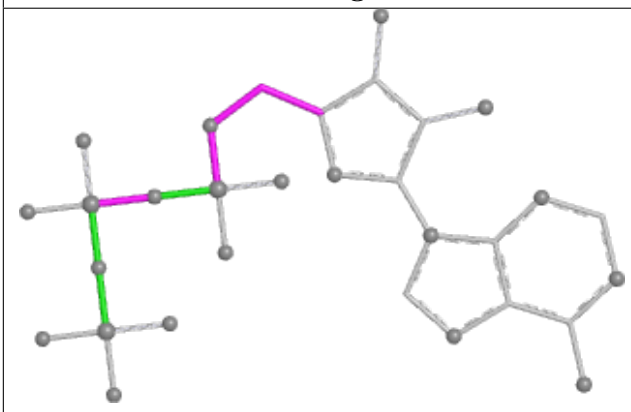
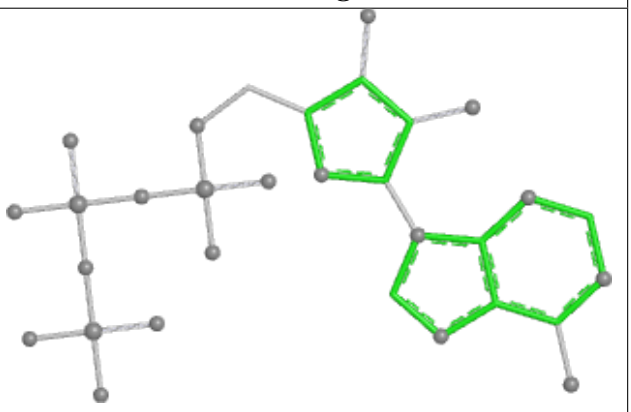
Mol	Chain	Res	Type	Atoms
18	H	501	ATP	C5'-O5'-PA-O1A
19	I	501	ADP	C5'-O5'-PA-O3A
18	H	501	ATP	C3'-C4'-C5'-O5'
19	I	501	ADP	O4'-C4'-C5'-O5'
19	I	501	ADP	C3'-C4'-C5'-O5'

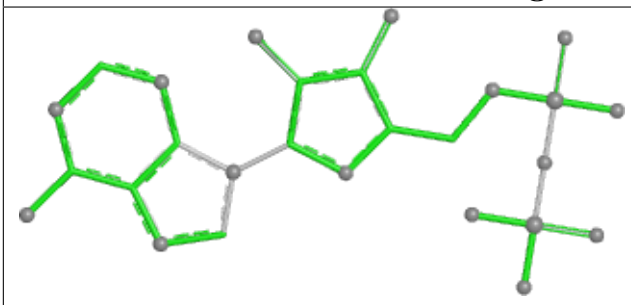
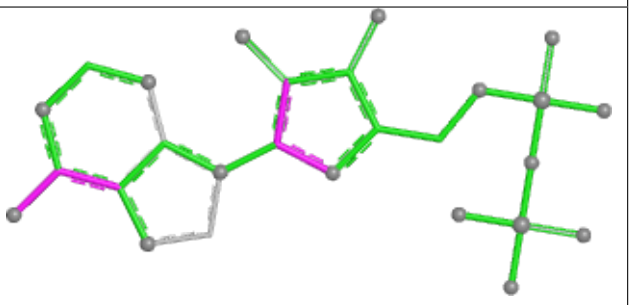
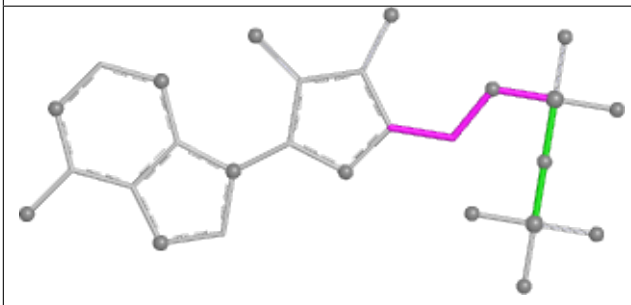
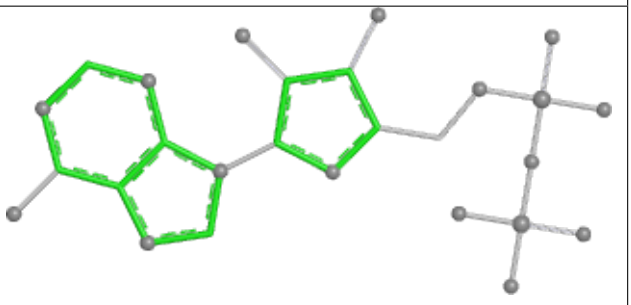
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	I	501	ADP	1	0

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 ATP H 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

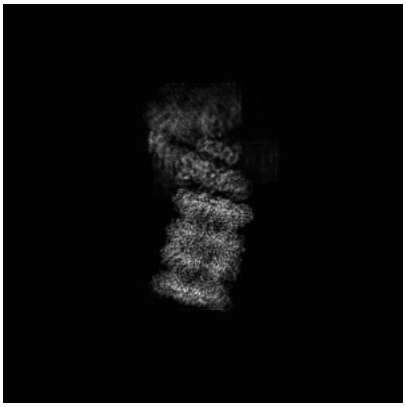
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14175. These allow visual inspection of the internal detail of the map and identification of artifacts.

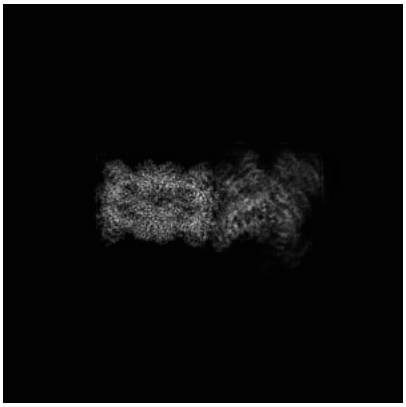
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

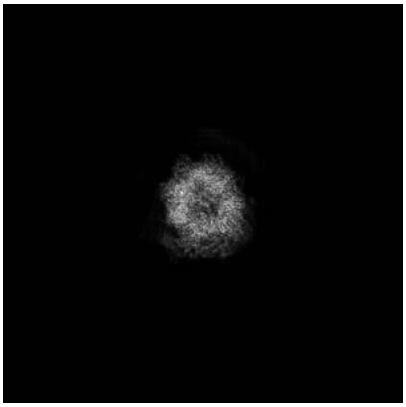
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 220

Y Index: 220

Z Index: 220

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: 199

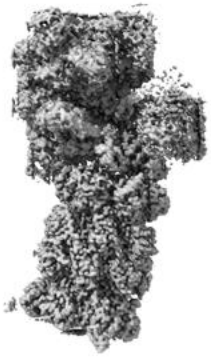
Y Index: 200

Z Index: 210

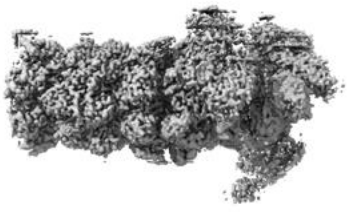
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

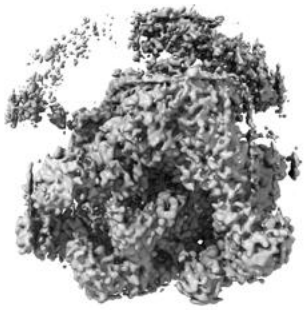
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0168. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

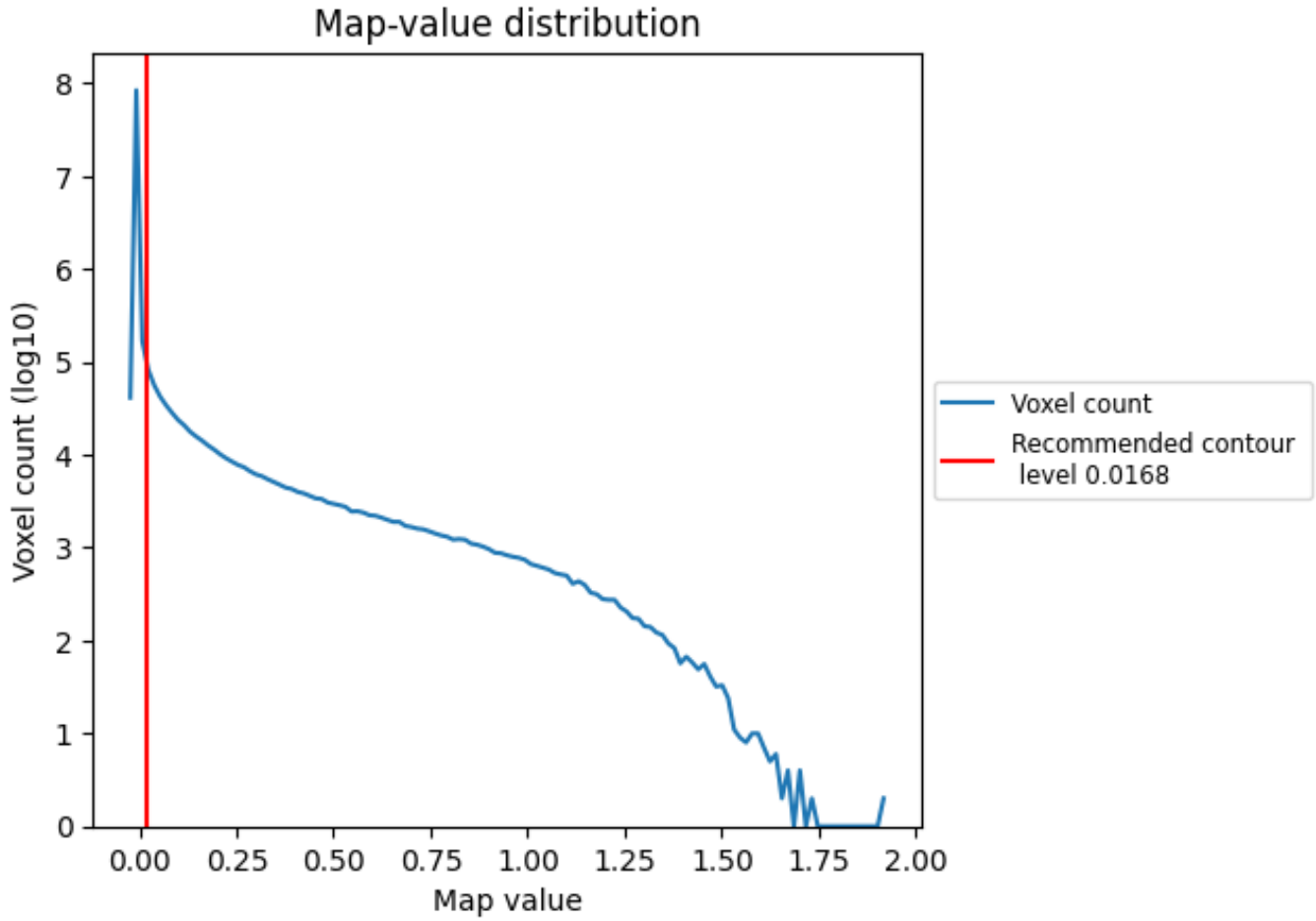
6.5 Mask visualisation (i)

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

7 Map analysis

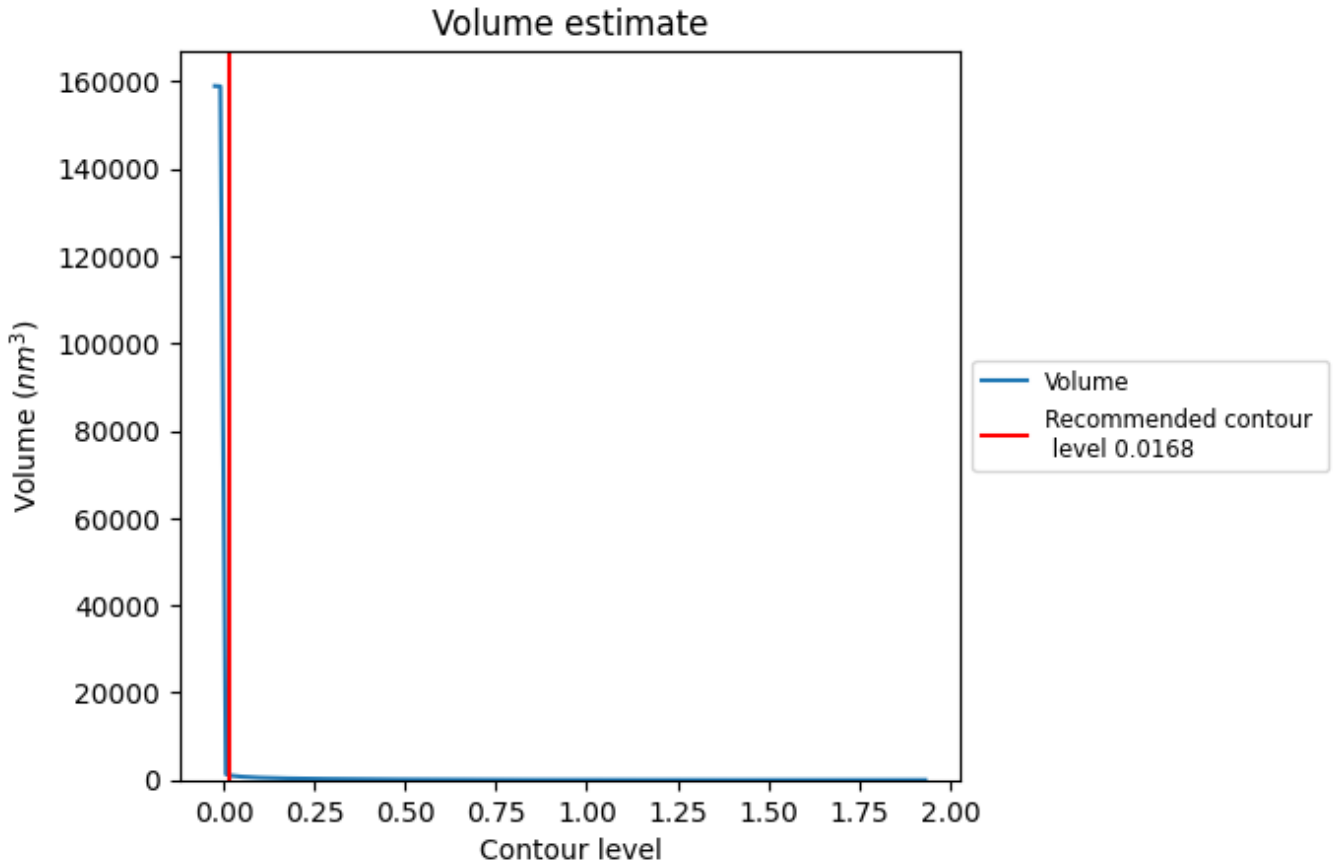
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

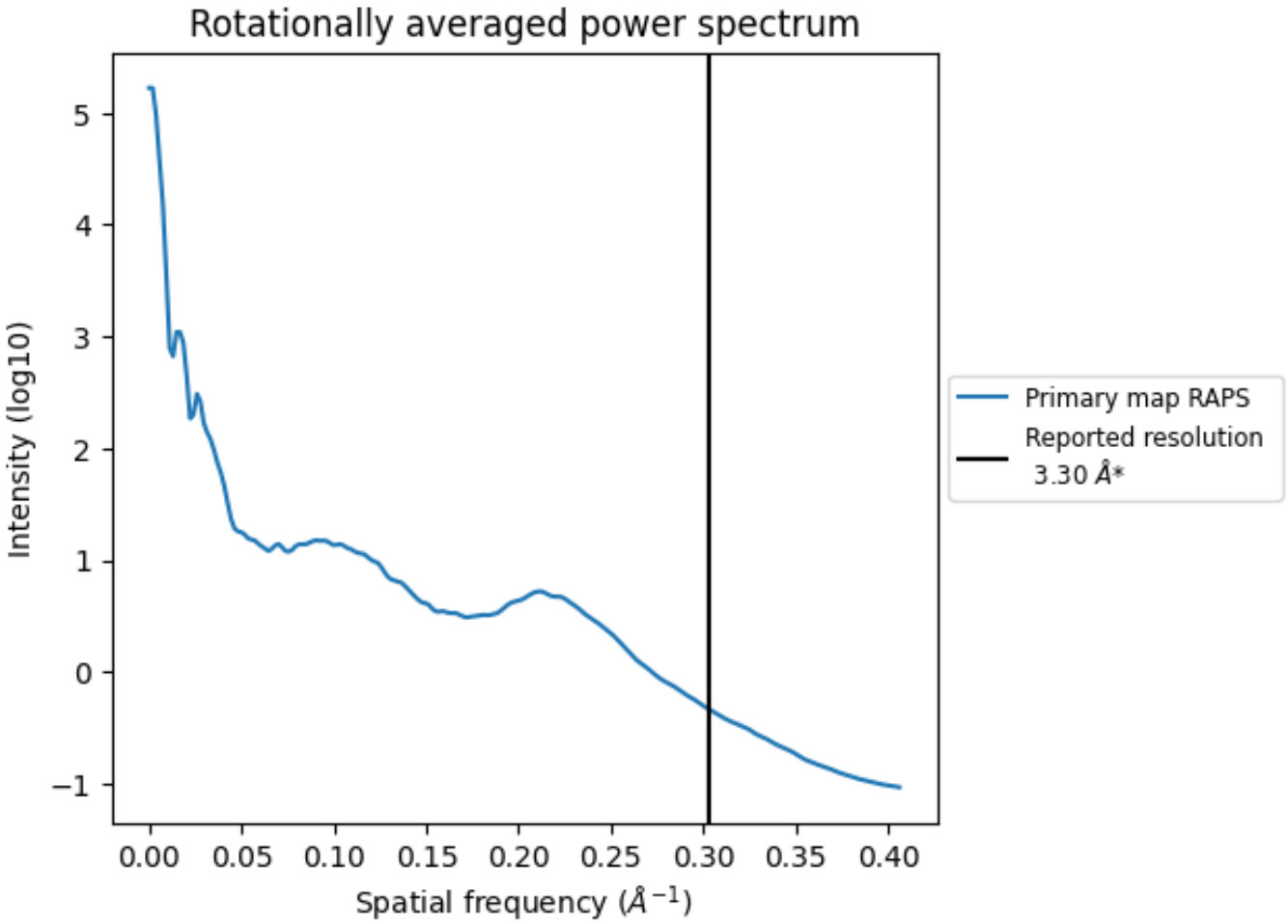
7.2 Volume estimate (i)



The volume at the recommended contour level is 1112 nm^3; this corresponds to an approximate mass of 1004 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 0.303 Å^{-1}

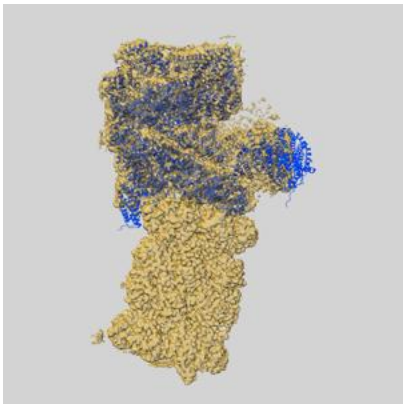
8 Fourier-Shell correlation (i)

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

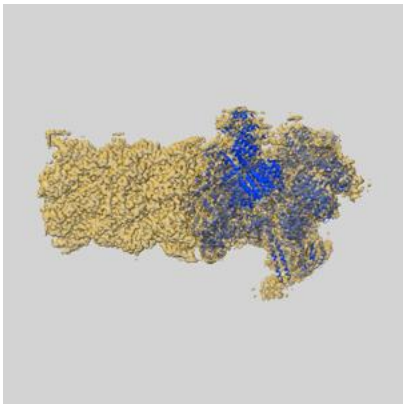
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14175 and PDB model 8AMZ. Per-residue inclusion information can be found in section 3 on page 8.

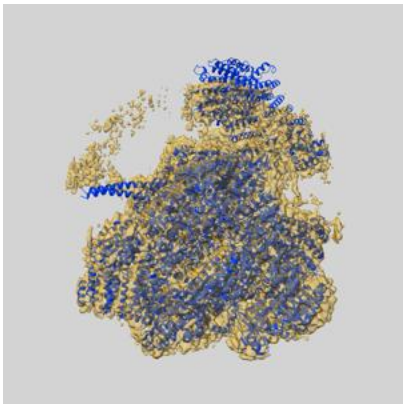
9.1 Map-model overlay



X



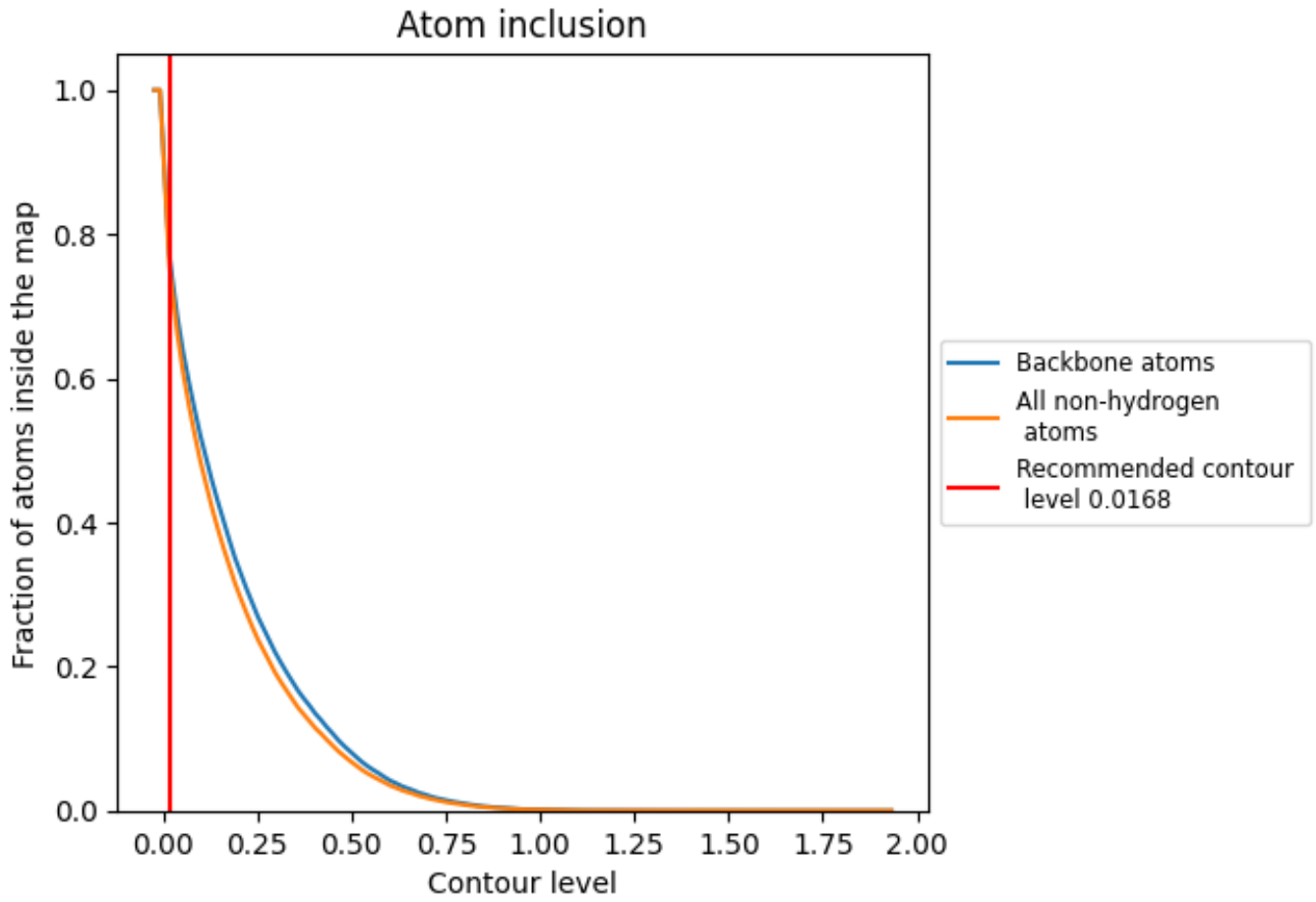
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0168 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 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.