wwPDB EM Validation Summary Report

Nov 20, 2022 – 09:37 am GMT

PDB ID	:	5L4K
EMDB ID	:	EMD-4002
Title	:	The human 26S proteasome lid
Authors	:	Schweitzer, A.; Aufderheide, A.; Rudack, T.; Beck, F.
Deposited on	:	2016-05-25
Resolution	:	4.50 Å(reported)

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

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

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

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

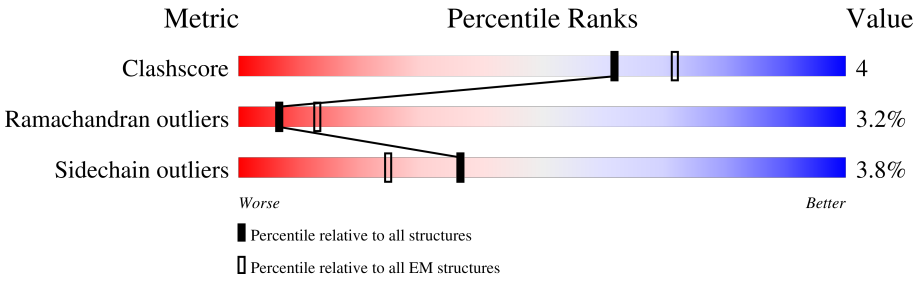
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 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
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	W	377	21% 49% · 48%
2	V	310	16% 72% 17% · · 5%
3	T	350	33% 65% 10% · 22%
4	Y	70	47% 70% 10% 20%
5	Z	908	91% 83% 13% · ·
6	N	953	56% 77% 14% · 8%
7	S	534	34% 79% 11% · 8%
8	P	456	11% 86% 14%

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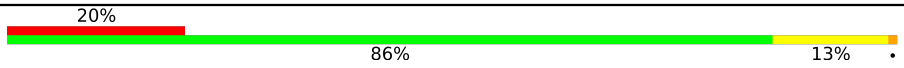
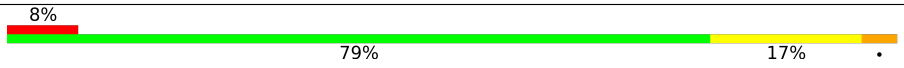
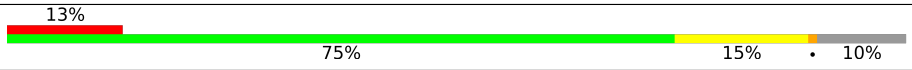
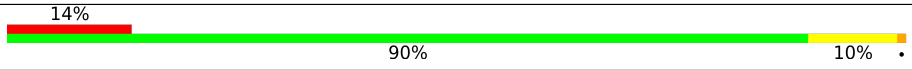
Mol	Chain	Length	Quality of chain
9	Q	422	
10	R	389	
11	U	324	
12	O	376	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 79649 atoms, of which 39990 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 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	W	196	3019	927	1531	266	286	9	0	0

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	V	293	4612	1456	2311	395	431	19	0	0

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	T	272	4435	1424	2231	362	409	9	0	0

- Molecule 4 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	Y	56	848	288	374	72	113	1	0	0

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	Z	881	13583	4270	6791	1159	1318	45	0	0

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	N	876	13720	4332	6890	1158	1295	45	0	0

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	S	491	Total	C	H	N	O	S	0	0
			7977	2516	3998	707	742	14		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	456	Total	C	H	N	O	S	0	0
			7525	2339	3822	635	704	25		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Q	422	Total	C	H	N	O	S	0	0
			6770	2116	3435	567	639	13		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	R	389	Total	C	H	N	O	S	0	0
			6406	2041	3204	545	598	18		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	U	292	Total	C	H	N	O	S	0	0
			4693	1488	2362	399	438	6		

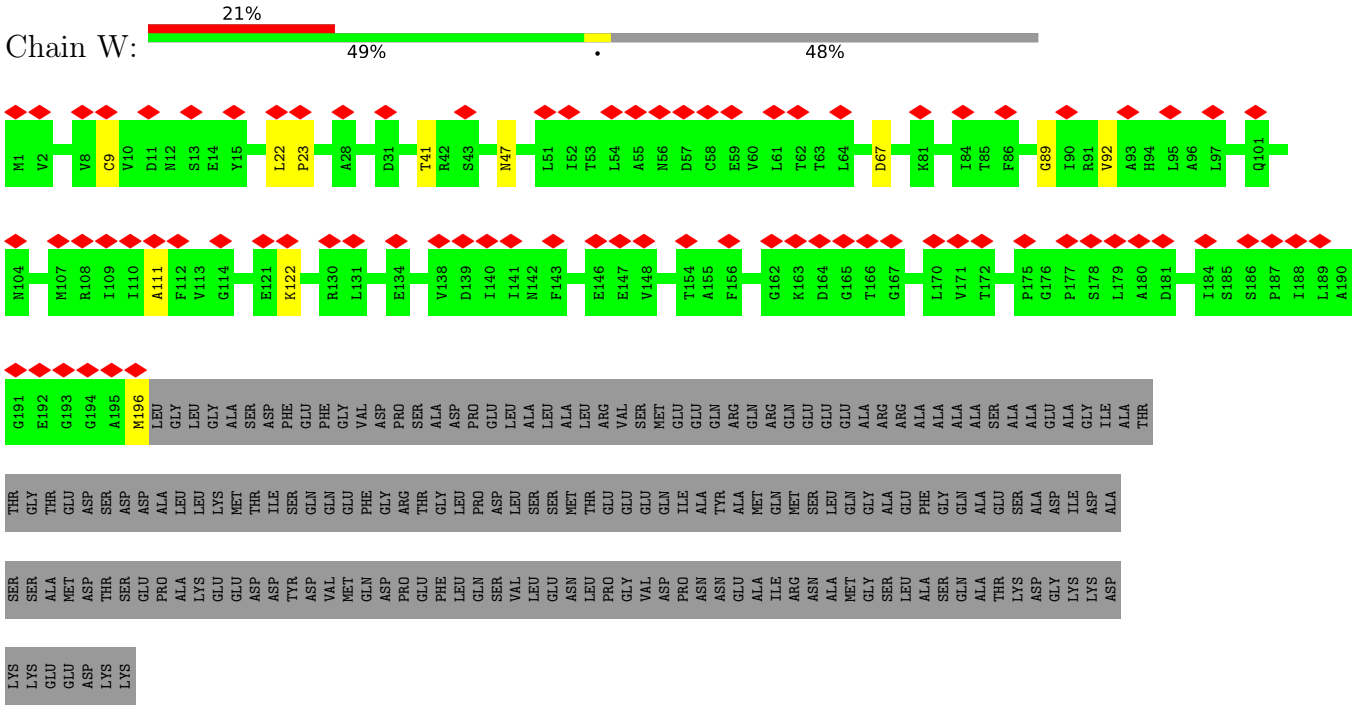
- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	O	376	Total	C	H	N	O	S	0	0
			6061	1926	3041	514	564	16		

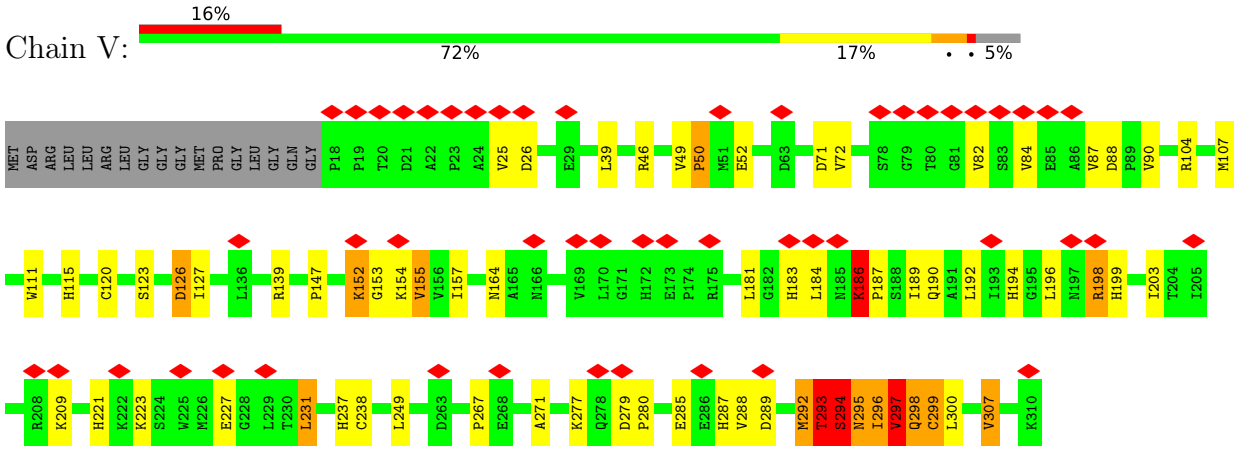
3 Residue-property plots (i)

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 4

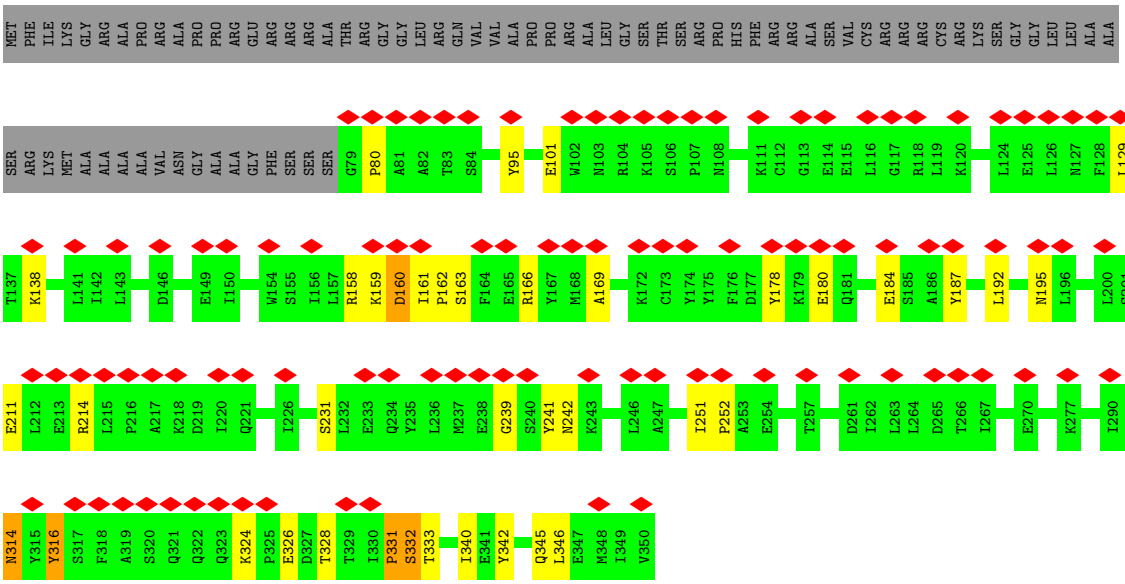


• Molecule 2: 26S proteasome non-ATPase regulatory subunit 14



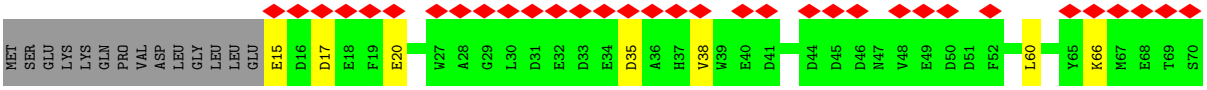
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 8

Chain T:



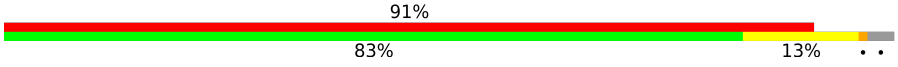
• Molecule 4: 26S proteasome complex subunit DSS1

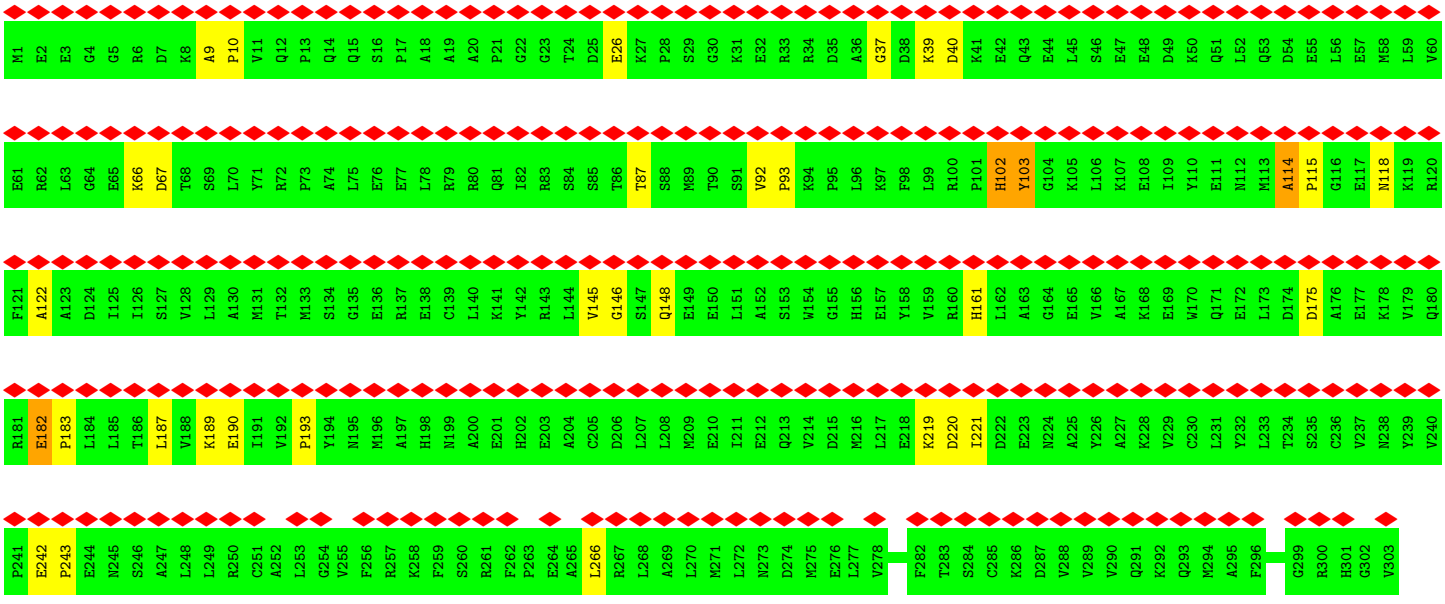
Chain Y:

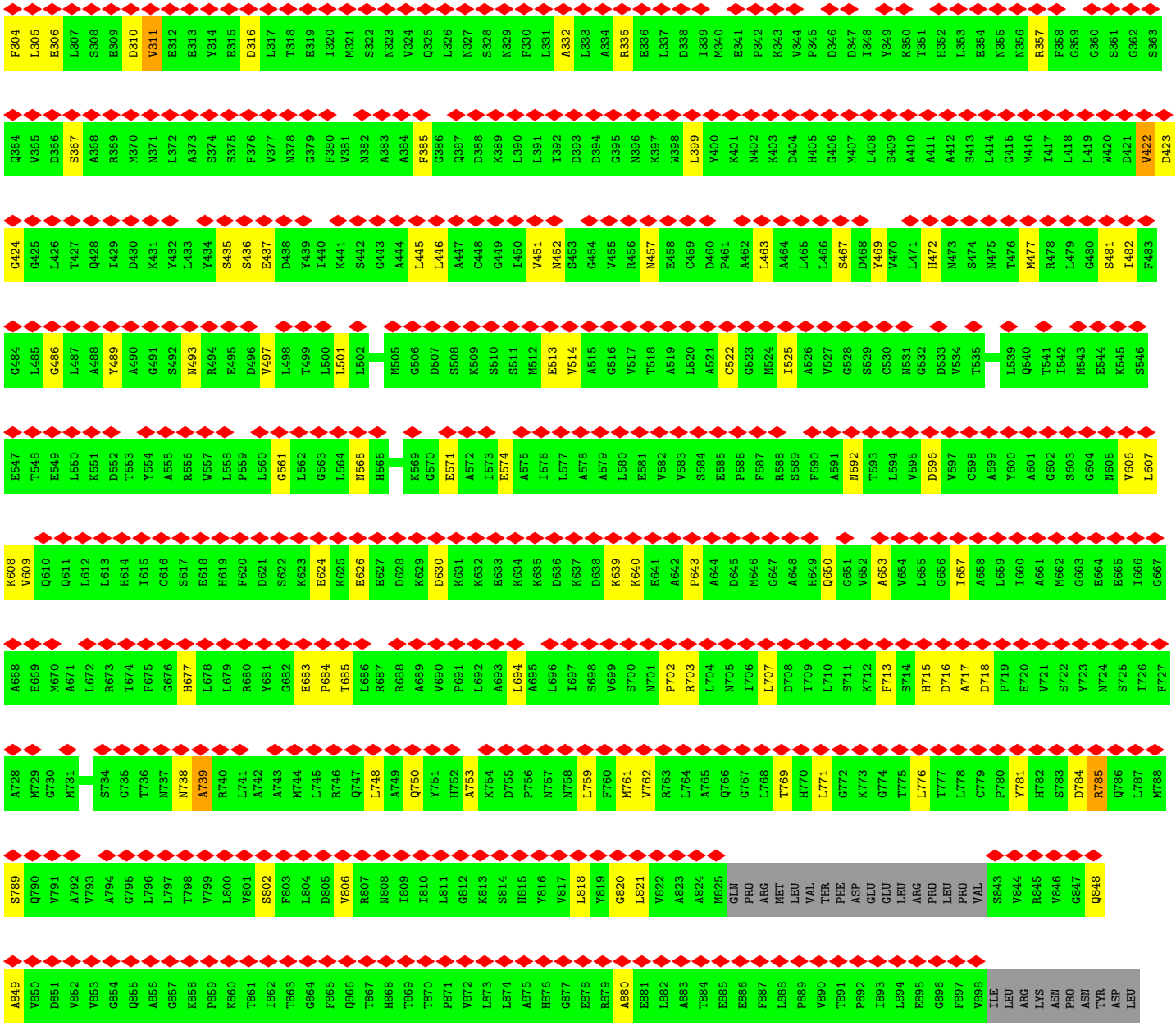


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 2

Chain Z:

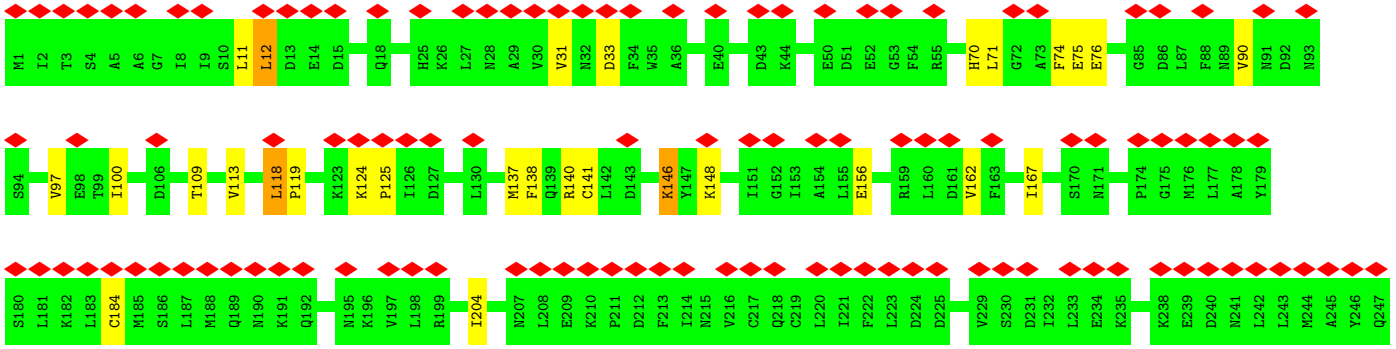


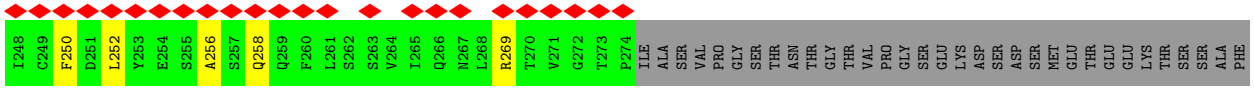


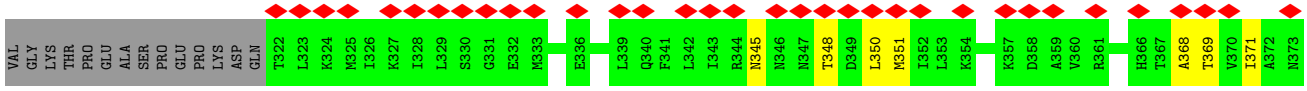


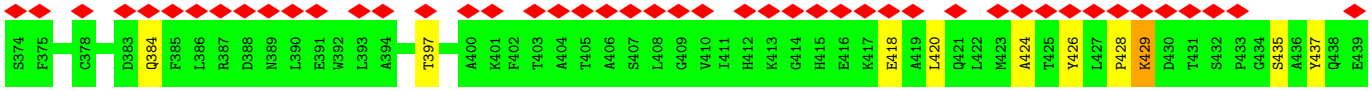
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 1

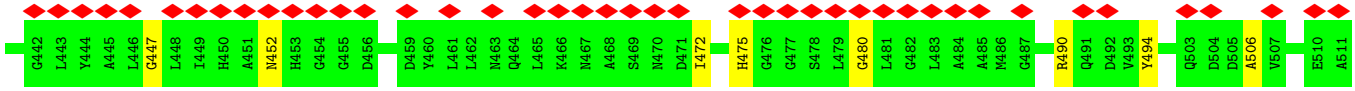
Chain N:

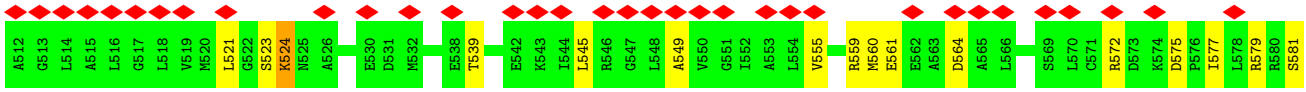


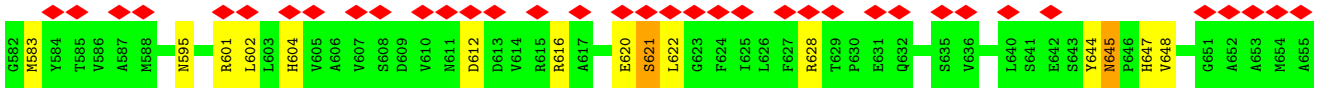


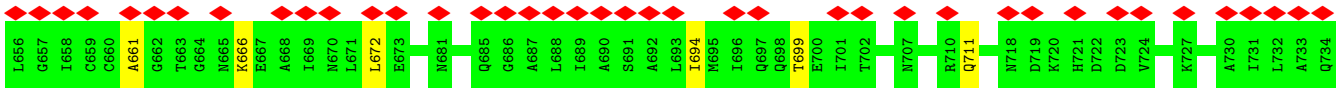


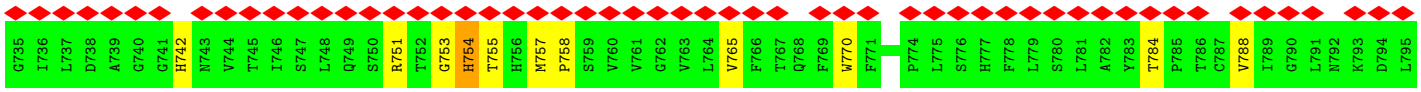


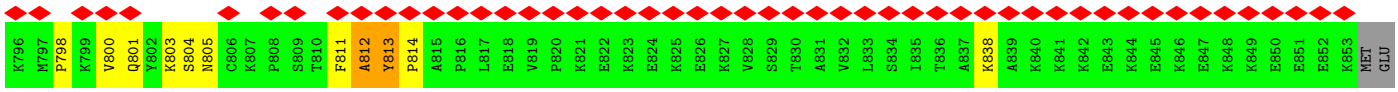


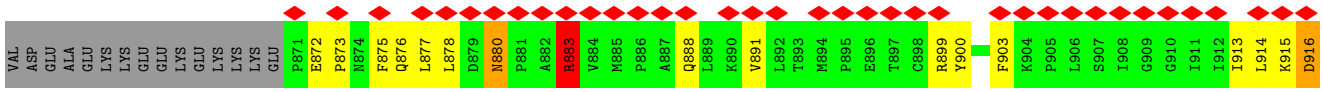


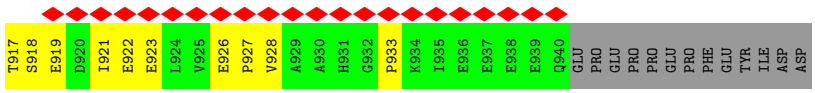




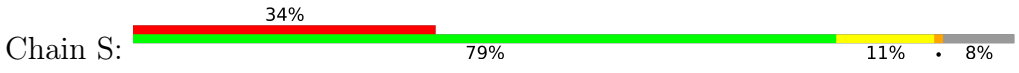


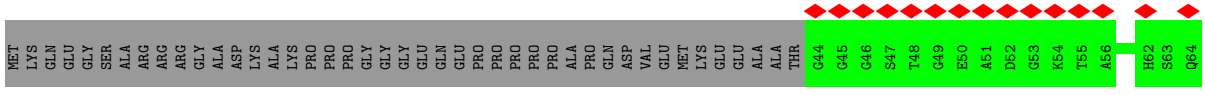


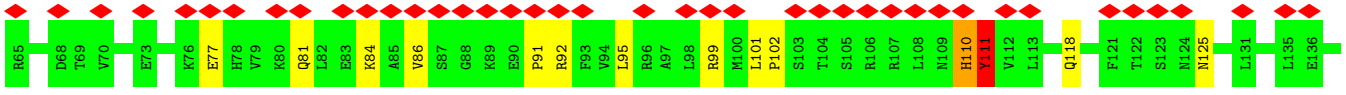


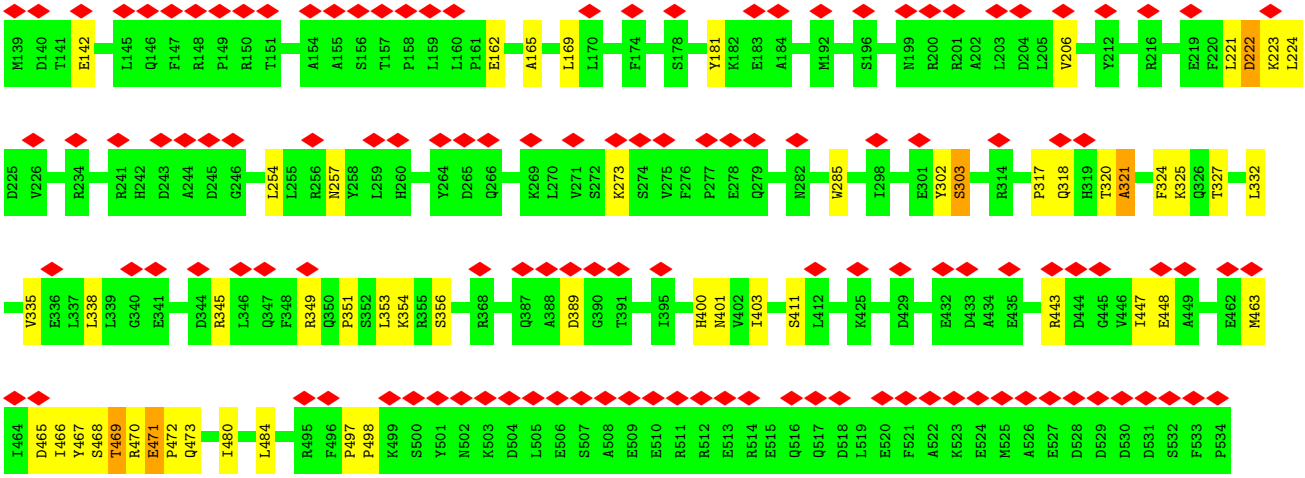


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 3



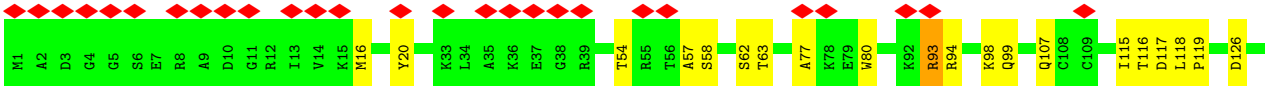


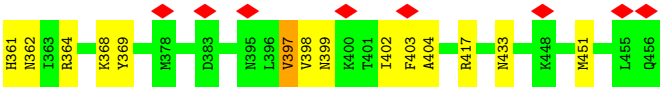




• Molecule 8: 26S proteasome non-ATPase regulatory subunit 12

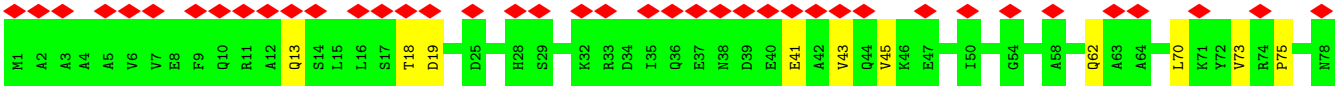
Chain P:

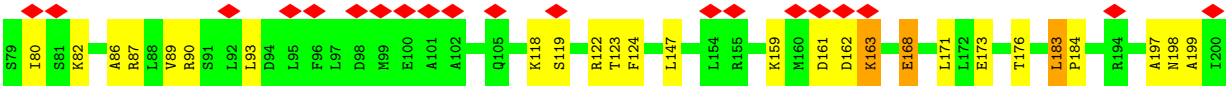


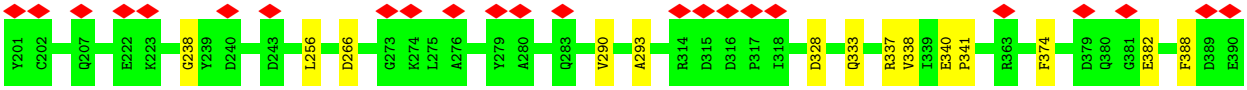


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 11

Chain Q:

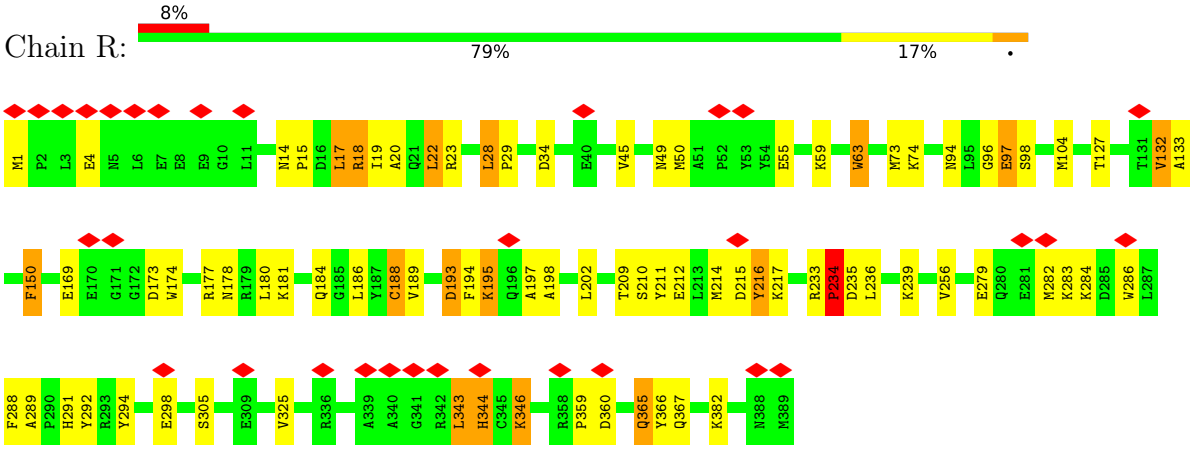






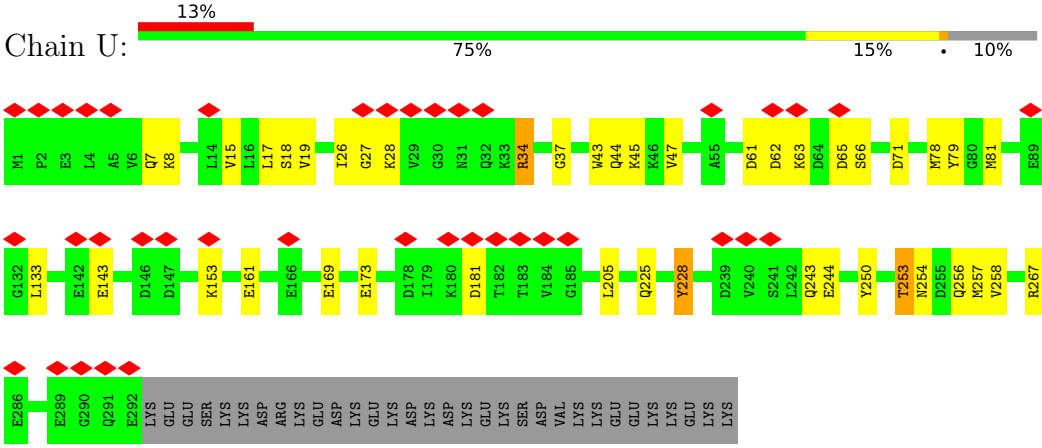
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 6

Chain R:



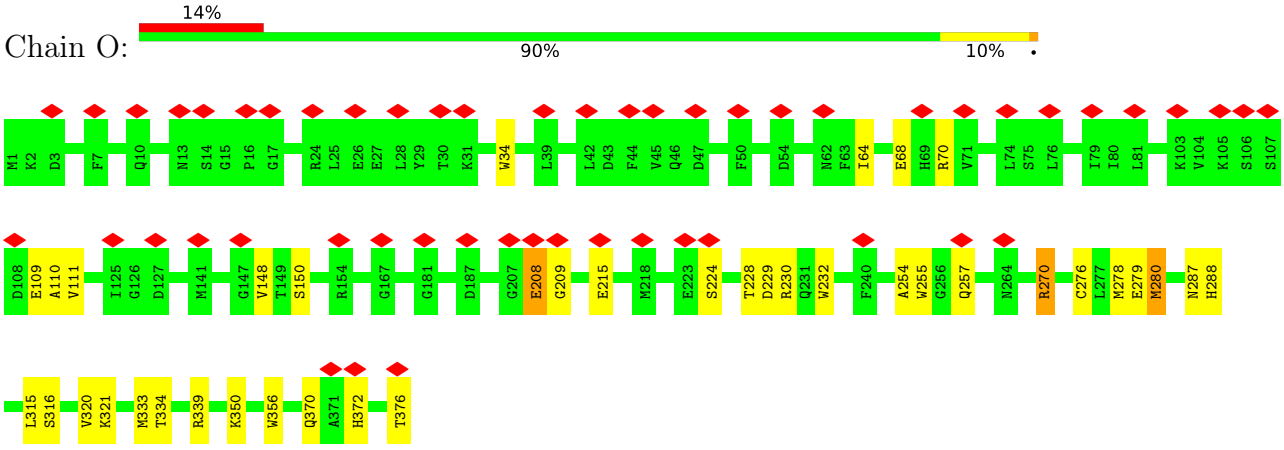
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 7

Chain U:



• Molecule 12: 26S proteasome non-ATPase regulatory subunit 13

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	461402	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	0.307	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	W	0.31	0/1508	0.51	0/2040
2	V	0.76	11/2346 (0.5%)	0.77	10/3173 (0.3%)
3	T	0.36	1/2251 (0.0%)	0.49	0/3042
4	Y	0.37	0/486	0.53	0/658
5	Z	0.29	0/6903	0.48	0/9327
6	N	0.33	1/6949 (0.0%)	0.49	0/9395
7	S	0.34	0/4053	0.52	1/5465 (0.0%)
8	P	0.35	0/3751	0.51	0/5042
9	Q	0.34	0/3381	0.49	0/4558
10	R	0.68	1/3261 (0.0%)	0.55	0/4393
11	U	0.37	0/2375	0.53	0/3219
12	O	0.32	0/3078	0.48	0/4165
All	All	0.41	14/40342 (0.0%)	0.52	11/54477 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	V	0	3
3	T	0	1
5	Z	0	1
8	P	0	1
10	R	0	1
12	O	0	1
All	All	0	8

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	R	28	LEU	C-N	31.06	1.93	1.34
2	V	295	ASN	N-CA	-12.65	1.21	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	294	SER	CA-C	-10.17	1.26	1.52
2	V	298	GLN	N-CA	-8.17	1.30	1.46
2	V	294	SER	N-CA	-7.93	1.30	1.46

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	294	SER	C-N-CA	-8.56	100.31	121.70
2	V	296	ILE	C-N-CA	-8.19	101.22	121.70
2	V	293	THR	O-C-N	-8.11	109.72	122.70
2	V	293	THR	CA-C-O	7.72	136.31	120.10
2	V	297	VAL	O-C-N	-7.66	110.44	122.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	241	TYR	Peptide
2	V	293	THR	Mainchain
2	V	294	SER	Mainchain
2	V	297	VAL	Mainchain
5	Z	102	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1488	1531	1531	2	0
2	V	2301	2311	2314	67	0
3	T	2204	2231	2231	18	0
4	Y	474	374	374	3	0
5	Z	6792	6791	6790	48	0
6	N	6830	6890	6890	76	0
7	S	3979	3998	3998	32	0
8	P	3703	3822	3822	26	0
9	Q	3335	3435	3435	19	0
10	R	3202	3204	3204	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	U	2331	2362	2362	29	0
12	O	3020	3041	3041	13	0
All	All	39659	39990	39992	357	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 4.

The worst 5 of 357 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)
2:V:289:ASP:O	2:V:293:THR:HG23	1.31	1.28
2:V:237:HIS:NE2	2:V:298:GLN:HG2	1.50	1.22
2:V:296:ILE:O	2:V:299:CYS:HB2	1.13	1.22
10:R:28:LEU:C	10:R:29:PRO:N	1.93	1.20
2:V:297:VAL:O	2:V:298:GLN:C	1.81	1.11

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	W	194/377 (52%)	171 (88%)	21 (11%)	2 (1%)	15 54
2	V	291/310 (94%)	236 (81%)	41 (14%)	14 (5%)	2 23
3	T	270/350 (77%)	242 (90%)	17 (6%)	11 (4%)	3 25
4	Y	54/70 (77%)	46 (85%)	6 (11%)	2 (4%)	3 28
5	Z	877/908 (97%)	737 (84%)	108 (12%)	32 (4%)	3 28
6	N	870/953 (91%)	741 (85%)	104 (12%)	25 (3%)	4 32
7	S	489/534 (92%)	425 (87%)	52 (11%)	12 (2%)	5 35
8	P	454/456 (100%)	384 (85%)	57 (13%)	13 (3%)	4 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Q	420/422 (100%)	349 (83%)	59 (14%)	12 (3%)	4	32
10	R	387/389 (100%)	321 (83%)	48 (12%)	18 (5%)	2	24
11	U	290/324 (90%)	245 (84%)	38 (13%)	7 (2%)	6	36
12	O	374/376 (100%)	329 (88%)	36 (10%)	9 (2%)	6	36
All	All	4970/5469 (91%)	4226 (85%)	587 (12%)	157 (3%)	7	30

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	23	PRO
3	T	180	GLU
3	T	332	SER
5	Z	311	VAL
5	Z	367	SER

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	W	169/312 (54%)	164 (97%)	5 (3%)	41	63
2	V	257/268 (96%)	247 (96%)	10 (4%)	32	57
3	T	238/294 (81%)	228 (96%)	10 (4%)	30	55
4	Y	50/63 (79%)	49 (98%)	1 (2%)	55	73
5	Z	736/763 (96%)	707 (96%)	29 (4%)	32	57
6	N	747/816 (92%)	723 (97%)	24 (3%)	39	62
7	S	428/460 (93%)	408 (95%)	20 (5%)	26	52
8	P	416/416 (100%)	404 (97%)	12 (3%)	42	64
9	Q	362/362 (100%)	345 (95%)	17 (5%)	26	52
10	R	344/344 (100%)	325 (94%)	19 (6%)	21	49
11	U	263/295 (89%)	253 (96%)	10 (4%)	33	58
12	O	336/336 (100%)	326 (97%)	10 (3%)	41	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4346/4729 (92%)	4179 (96%)	167 (4%)	36 58

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Q	87	ARG
10	R	305	SER
9	Q	256	LEU
10	R	63	TRP
11	U	100	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	V	237	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	28:LEU	C	29:PRO	N	1.93

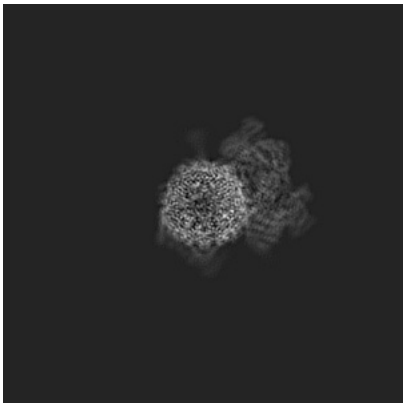
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4002. 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.

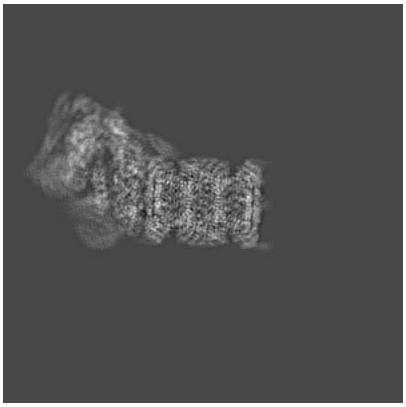
6.1 Orthogonal projections

6.1.1 Primary map



X

Y

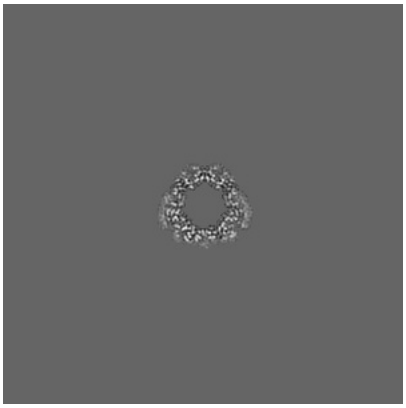


Z

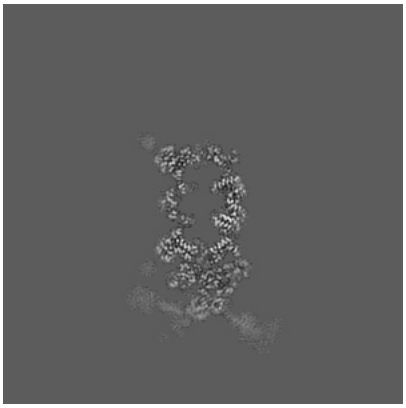
The images above show the map projected in three orthogonal directions.

6.2 Central slices

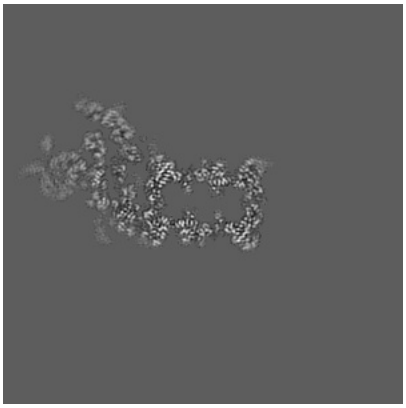
6.2.1 Primary map



X Index: 192



Y Index: 192

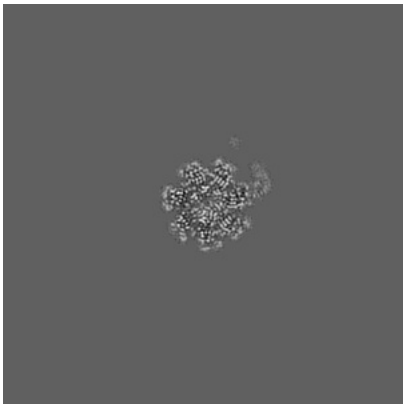


Z Index: 192

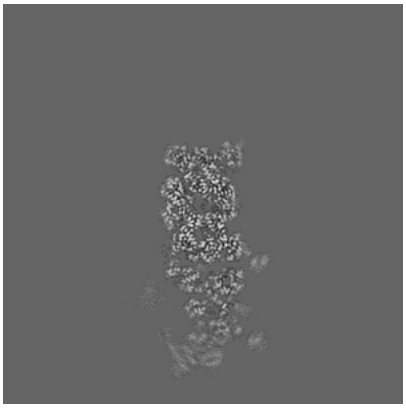
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

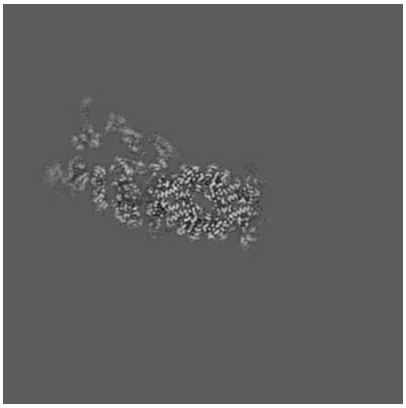
6.3.1 Primary map



X Index: 150



Y Index: 212

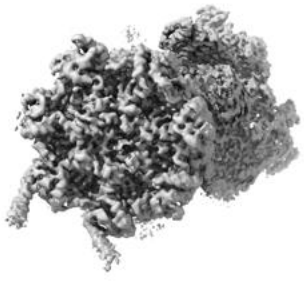


Z Index: 210

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

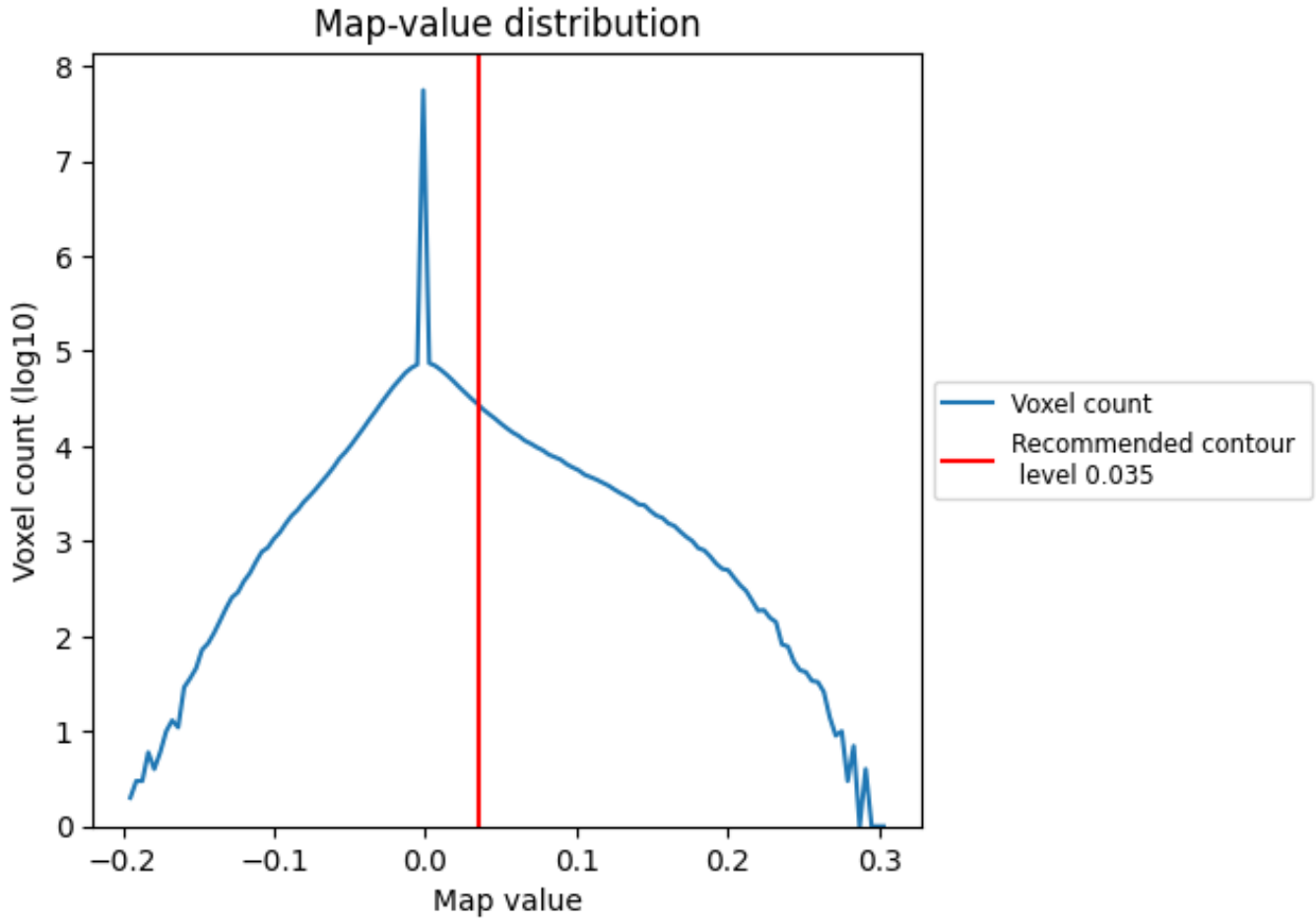
6.5 Mask visualisation (i)

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

7 Map analysis

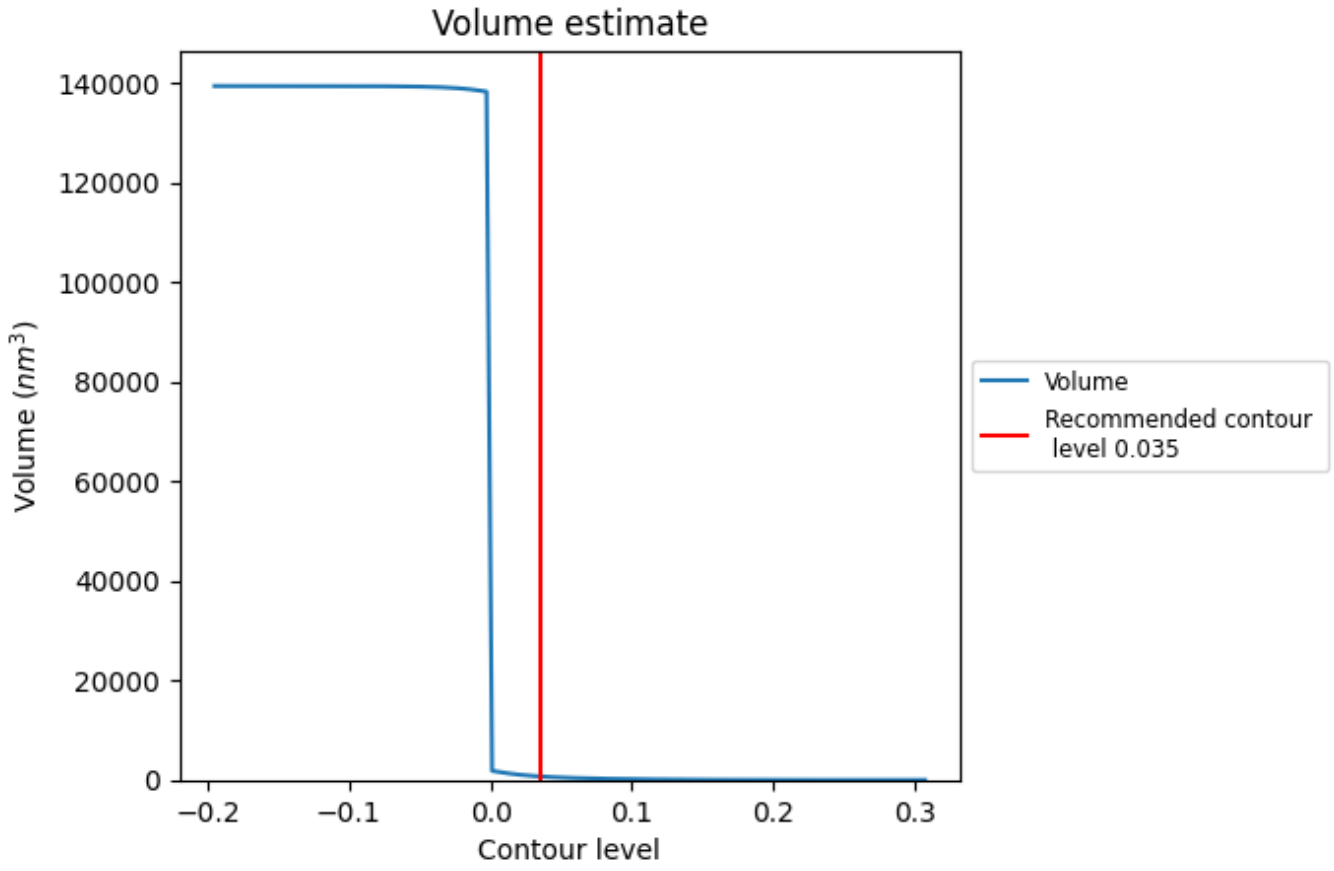
This section contains the results of statistical analysis of the map.

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.

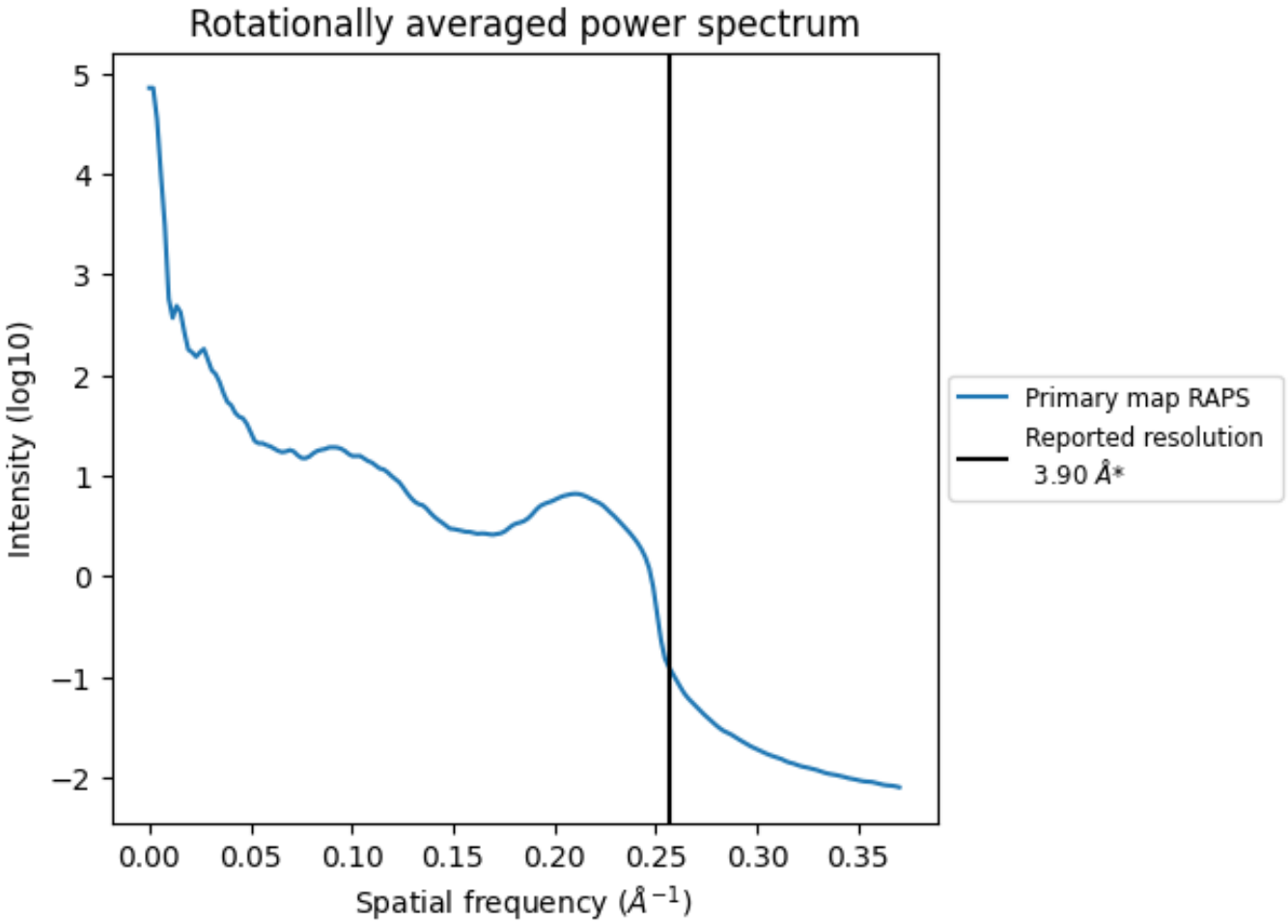
7.2 Volume estimate (i)



The volume at the recommended contour level is 708 nm^3; this corresponds to an approximate mass of 639 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 0.256 Å^{-1}

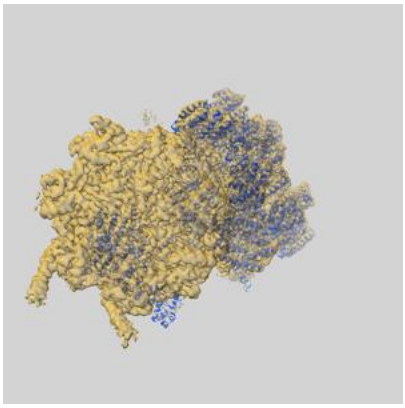
8 Fourier-Shell correlation (i)

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

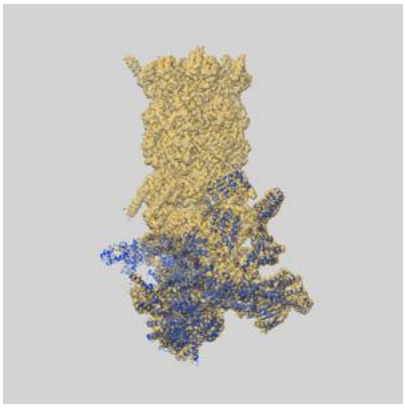
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4002 and PDB model 5L4K. Per-residue inclusion information can be found in section 3 on page 6.

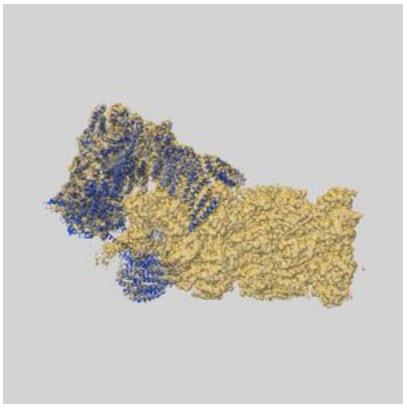
9.1 Map-model overlay



X



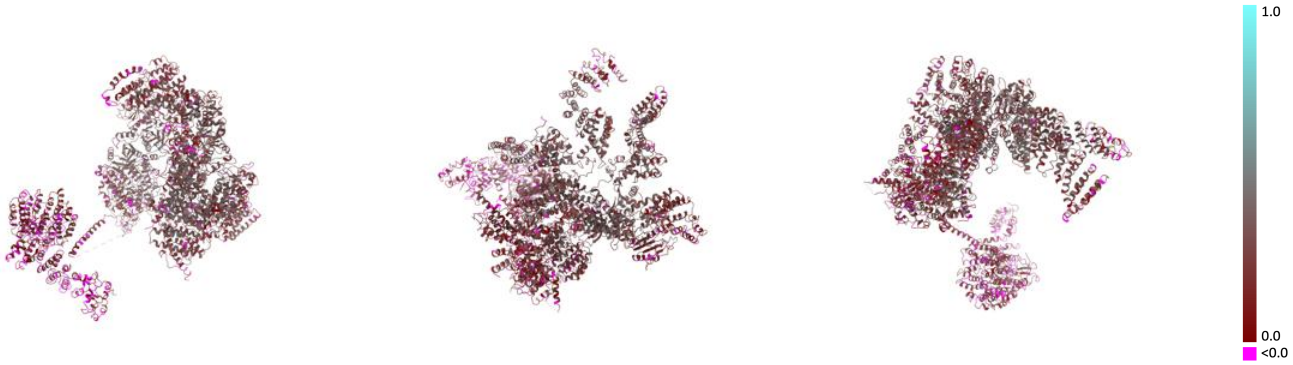
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

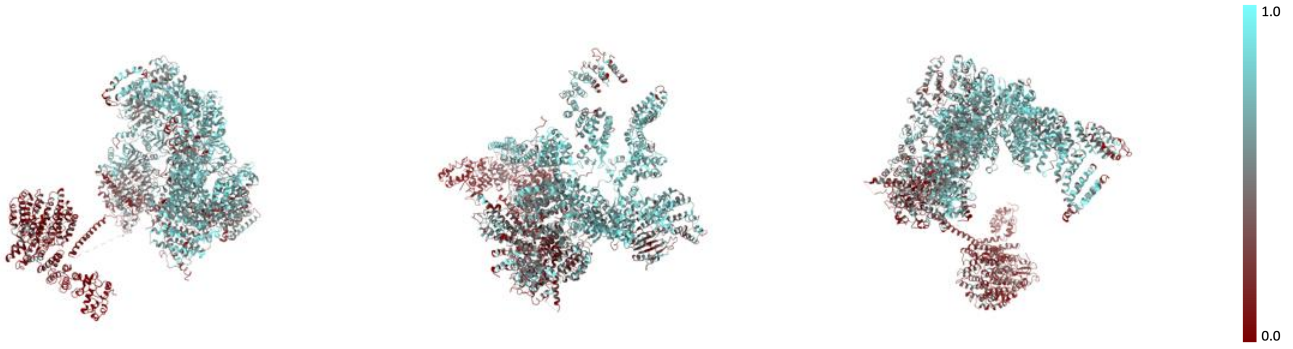
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

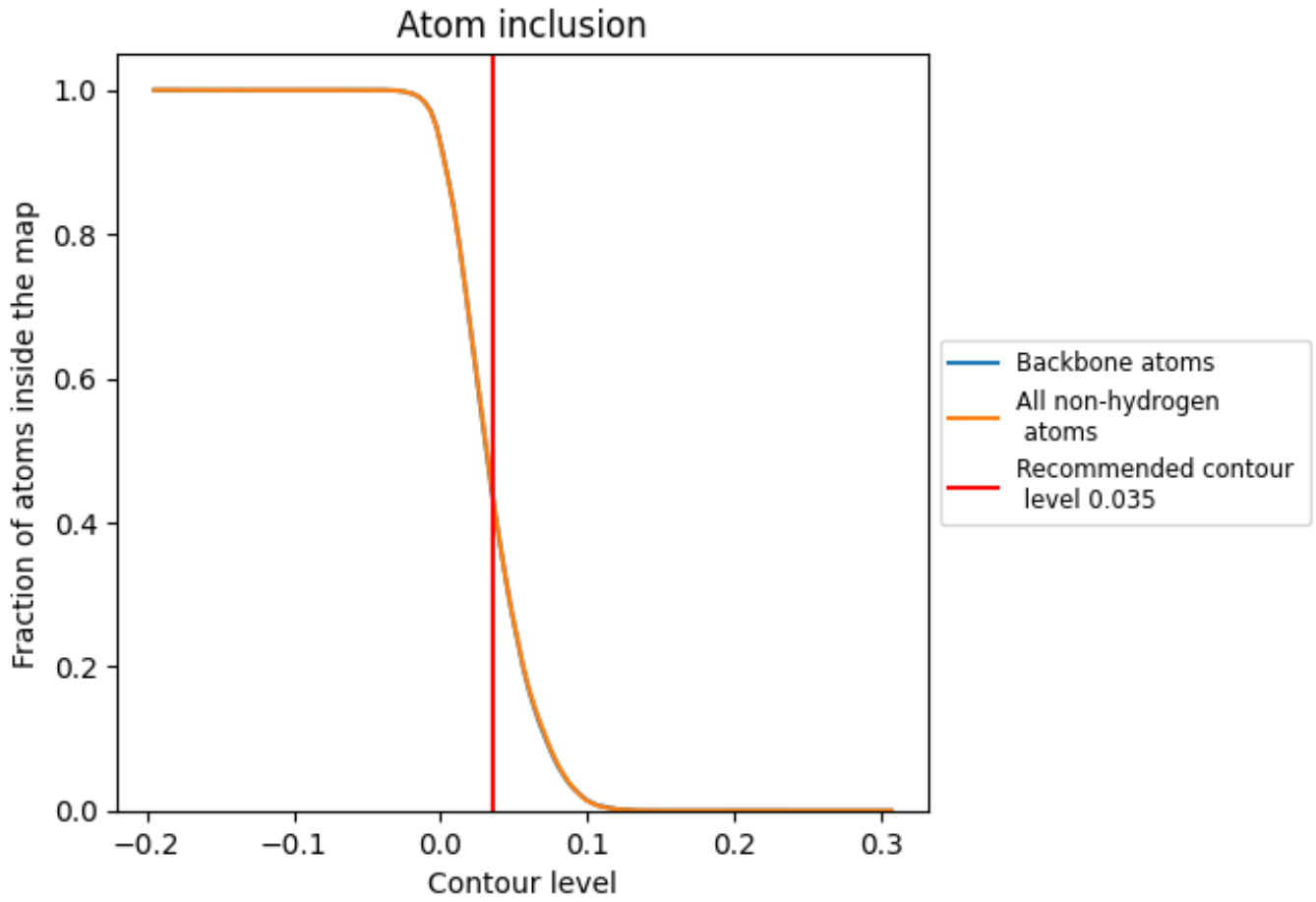
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4441	0.2300
N	0.3430	0.1980
O	0.6258	0.2510
P	0.6680	0.2840
Q	0.5678	0.2830
R	0.6883	0.3350
S	0.4733	0.2340
T	0.4409	0.2190
U	0.6281	0.3270
V	0.5995	0.3020
W	0.4460	0.2160
Y	0.3697	0.1830
Z	0.1071	0.1000