



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2022 – 10:33 AM EDT

PDB ID : 5VHS
EMDB ID : EMD-8684
Title : Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle
Authors : Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on : 2017-04-13
Resolution : 8.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

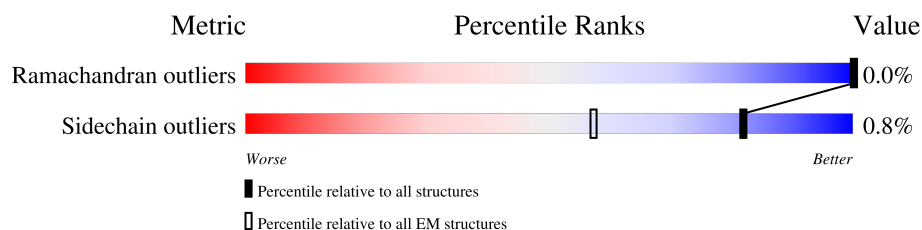
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 8.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	352	<div> <div>73%</div> <div>95%</div> <div>• •</div> </div>
2	B	341	<div> <div>74%</div> <div>92%</div> <div>• 7%</div> </div>
3	C	385	<div> <div>76%</div> <div>90%</div> <div>• 9%</div> </div>
4	D	368	<div> <div>73%</div> <div>89%</div> <div>• 10%</div> </div>
5	E	379	<div> <div>70%</div> <div>82%</div> <div>• 17%</div> </div>
6	F	380	<div> <div>71%</div> <div>88%</div> <div>• 11%</div> </div>
7	U	935	<div> <div>48%</div> <div>80%</div> <div>20%</div> </div>
8	V	488	<div> <div>32%</div> <div>54%</div> <div>46%</div> </div>
9	W	456	<div> <div>49%</div> <div>85%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
10	X	385	
11	Y	378	
12	Z	286	
13	a	374	
14	b	191	
15	c	287	
16	d	257	
17	e	33	
18	f	784	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 47840 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
1	A	338	Total	C	N	O	S	0	0
			2665	1682	470	496	17		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	317	Total	C	N	O	S	0	0
			2476	1557	421	487	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	349	Total	C	N	O	S	0	0
			2752	1724	502	512	14		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	332	Total	C	N	O	S	0	0
			2649	1677	466	497	9		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	313	Total	C	N	O	S	0	0
			2493	1566	448	464	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	339	Total	C	N	O	S	0	0
			2647	1673	460	498	16		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	751	Total	C	N	O	S	0	0
			5829	3696	1001	1088	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	262	Total	C	N	O	S	0	0
			2129	1360	377	385	7		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	391	Total	C	N	O	S	0	0
			3206	2040	545	600	21		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	280	Total	C	N	O	S	0	0
			2221	1414	373	425	9		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

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

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

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	176	Total	C	N	O	S	0	0
			1452	943	232	272	5		

- Molecule 17 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	33	Total	C	N	O	S	0	0
			283	172	46	64	1		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	636	Total	C	N	O	S	0	0
			4920	3110	830	945	35		

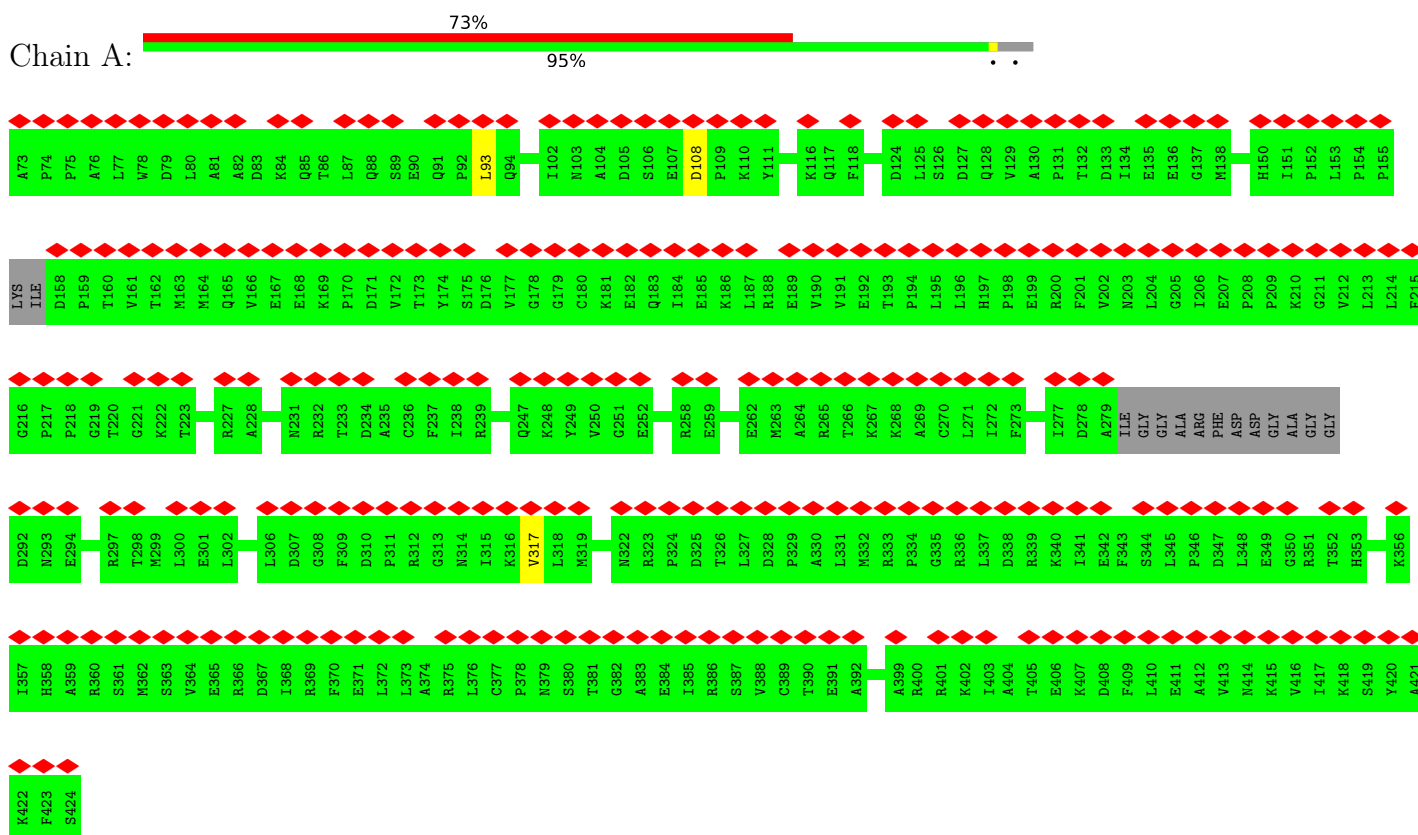
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	c	1	Total	Zn	0
			1	1	

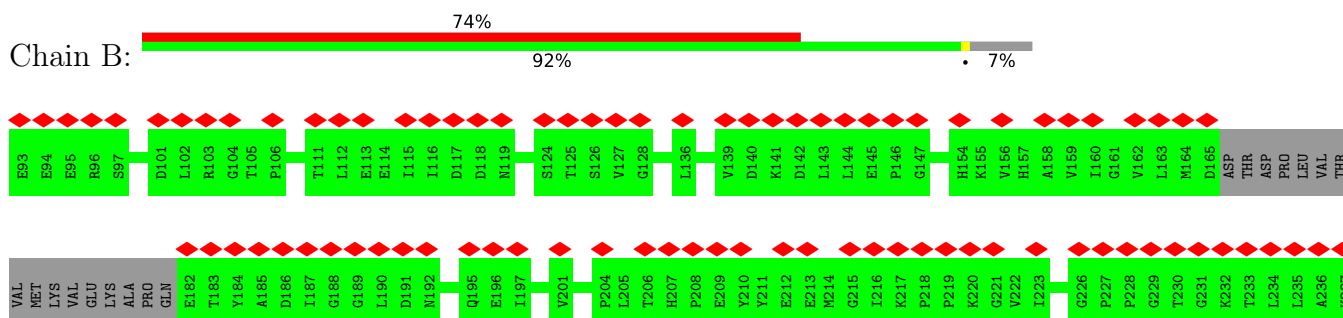
3 Residue-property plots

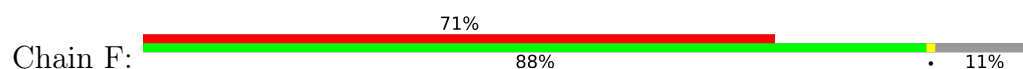
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

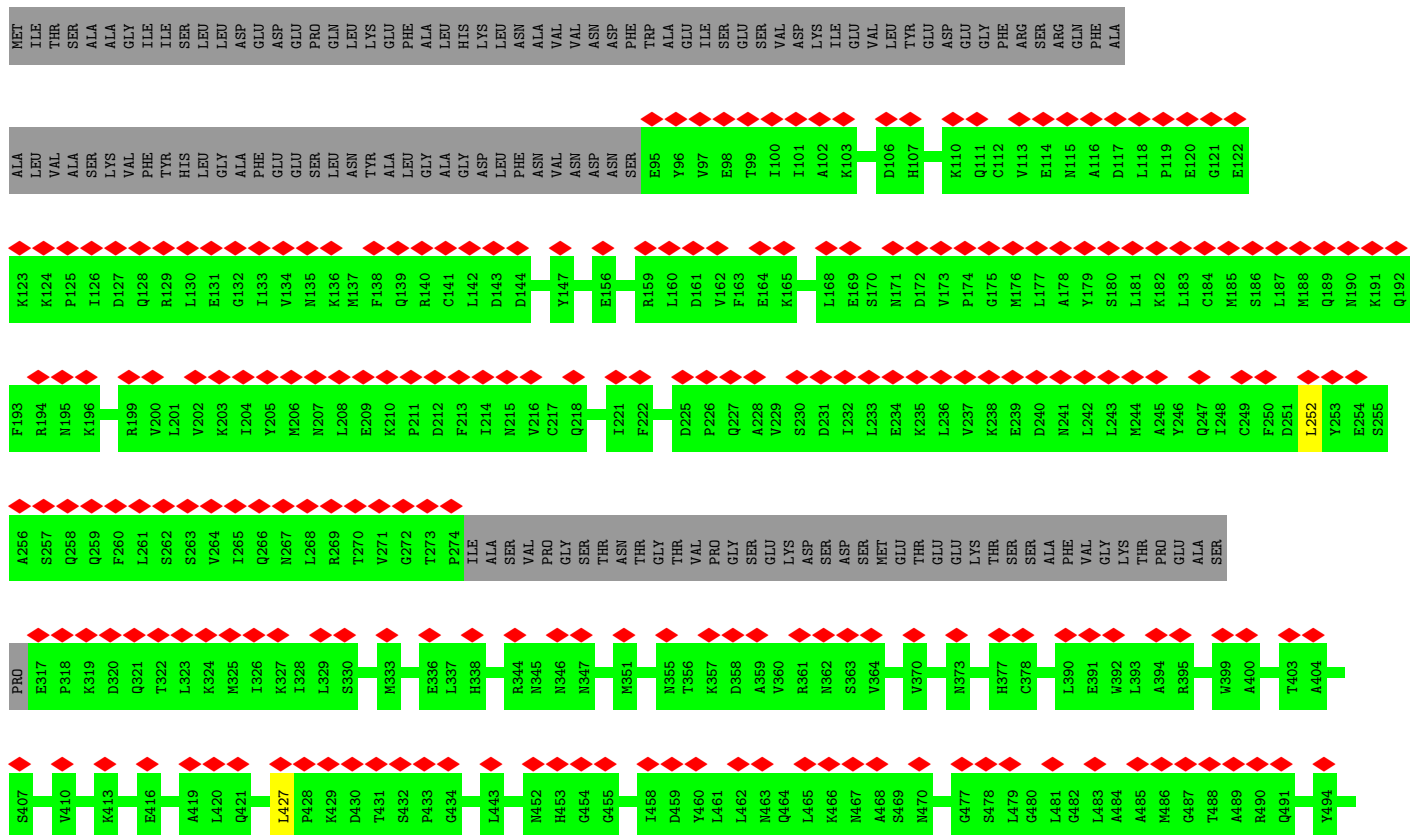
- Molecule 1: 26S proteasome regulatory subunit 7



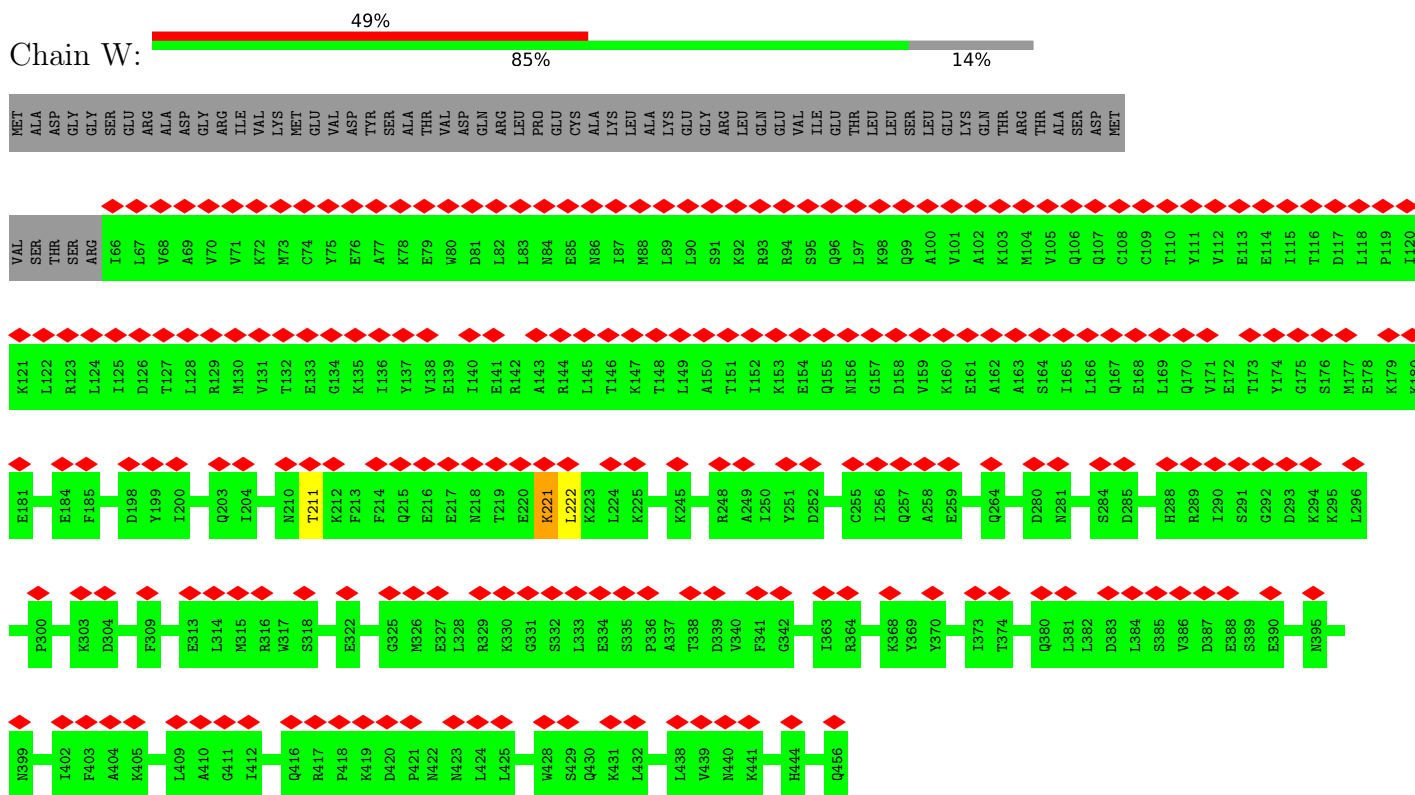
- Molecule 2: 26S proteasome regulatory subunit 4



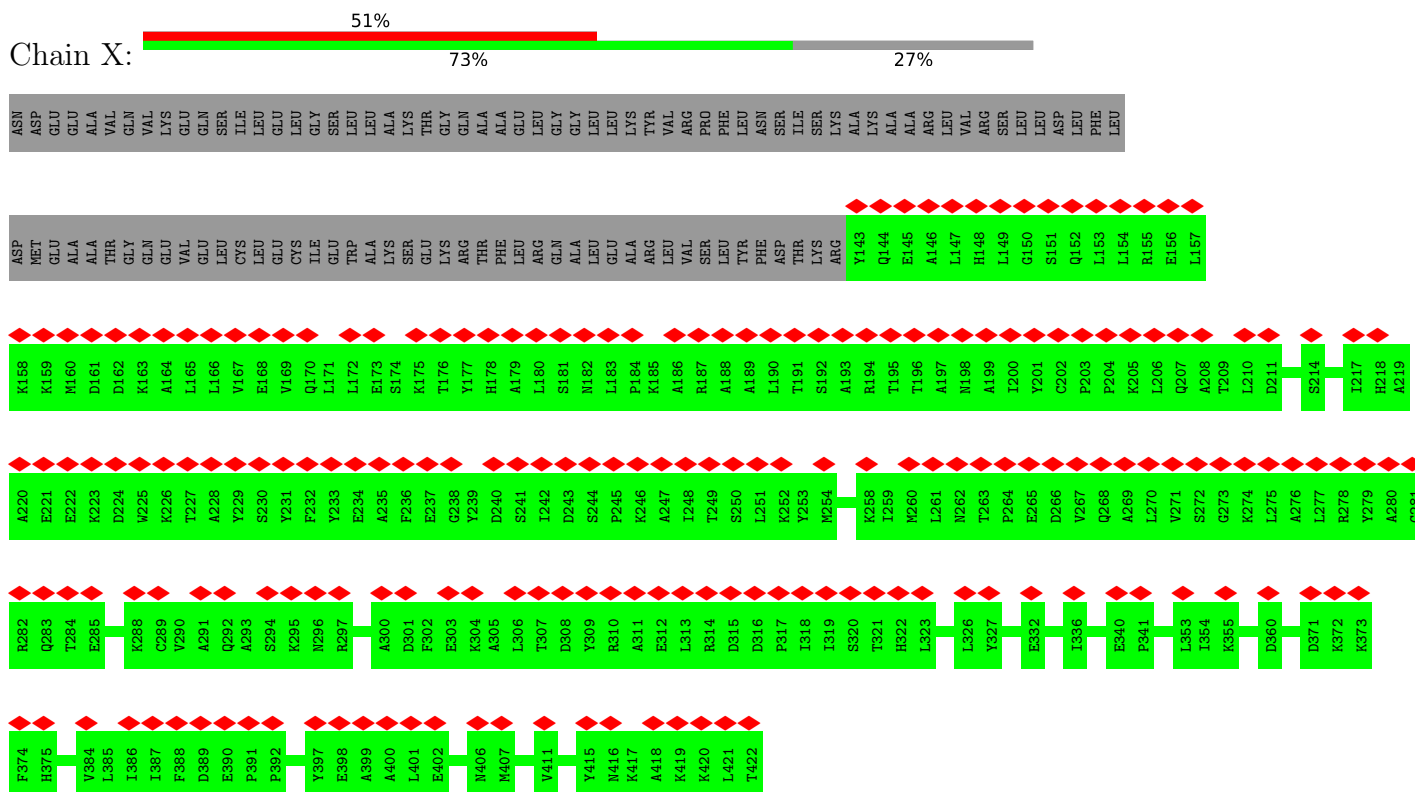




- Molecule 9: 26S proteasome non-ATPase regulatory subunit 12



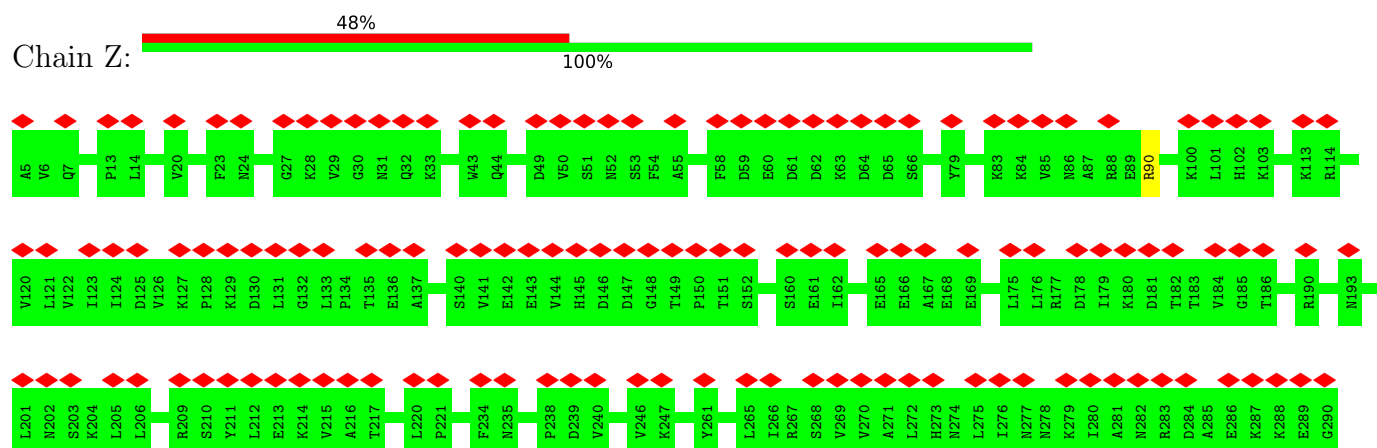
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 11



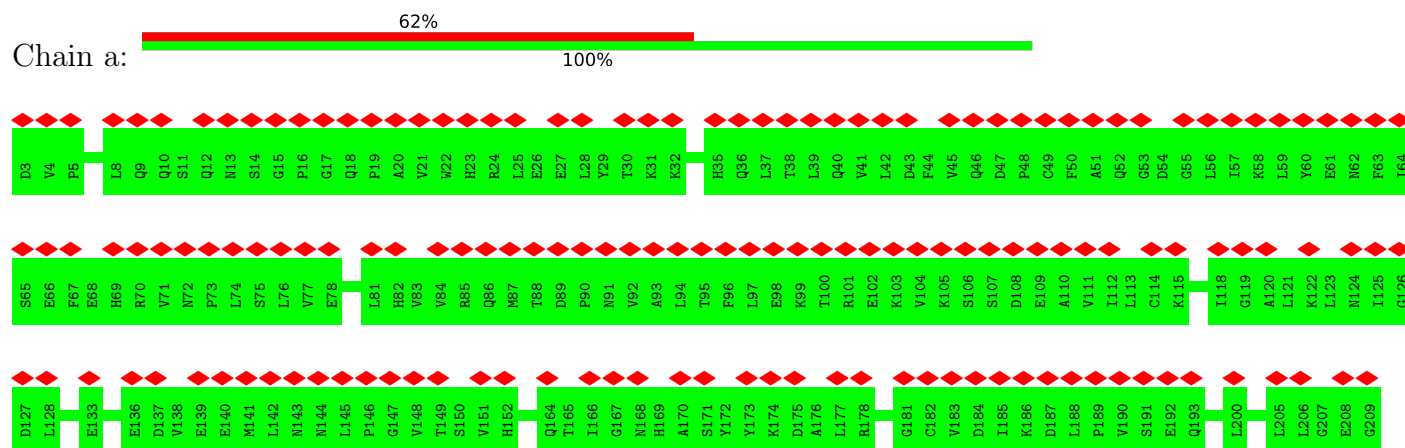
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

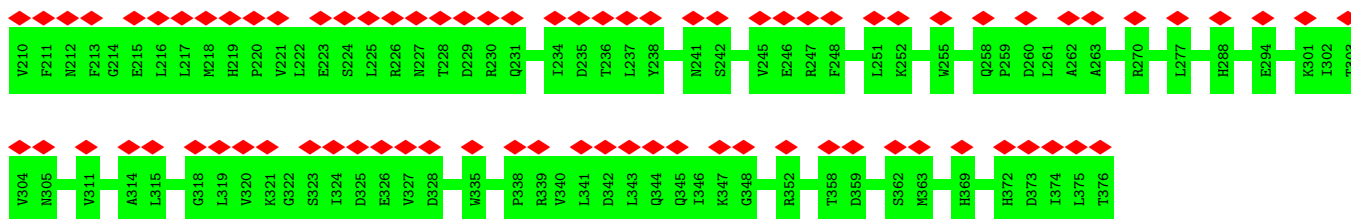


• Molecule 12: 26S proteasome non-ATPase regulatory subunit 7

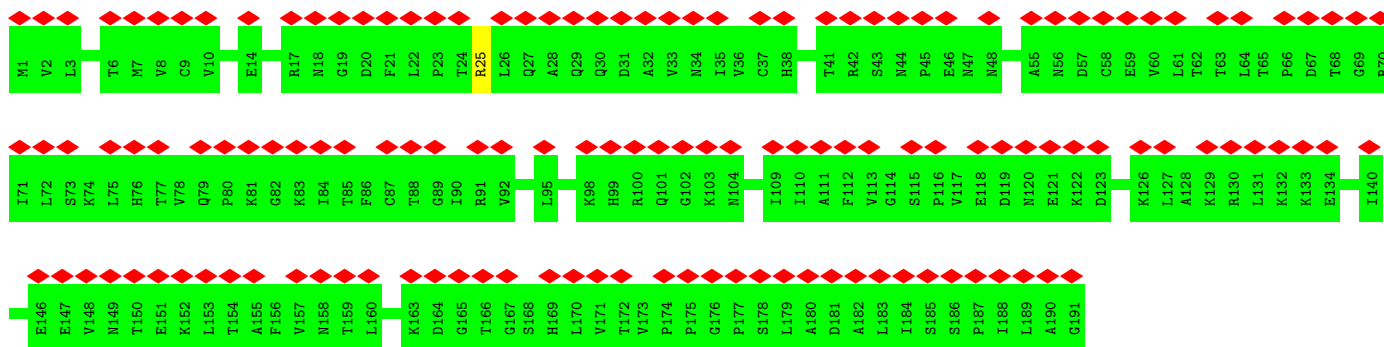


• Molecule 13: 26S proteasome non-ATPase regulatory subunit 13

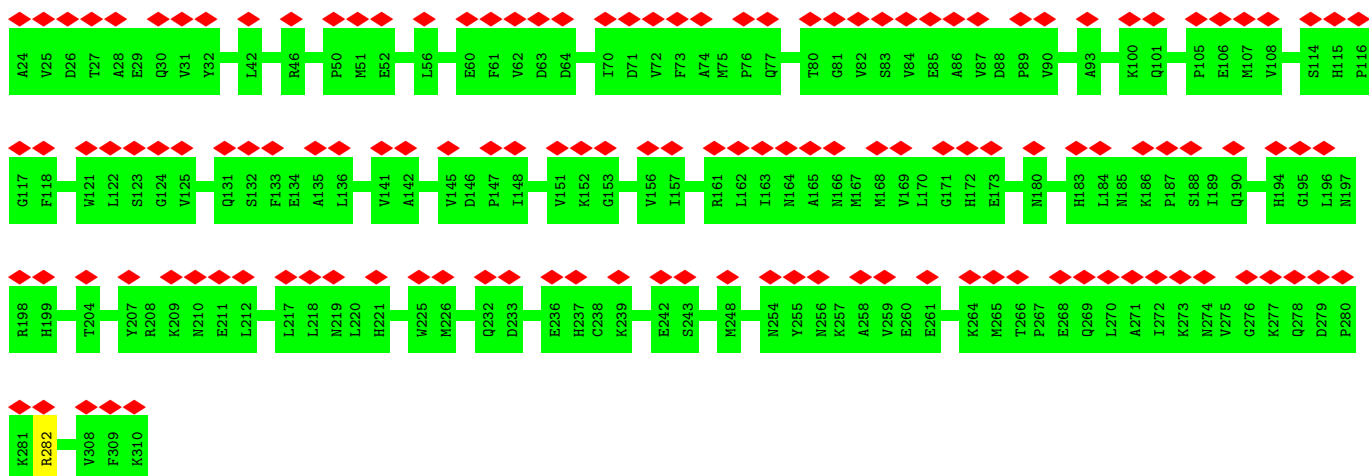




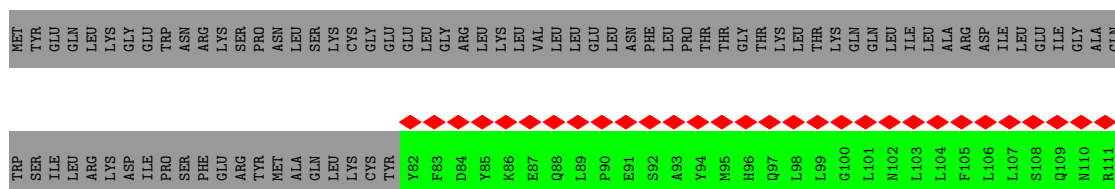
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 4



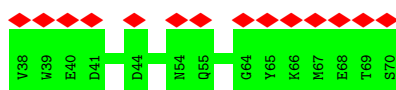
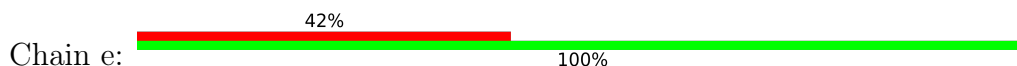
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 14



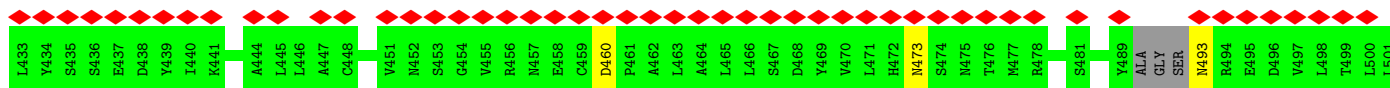
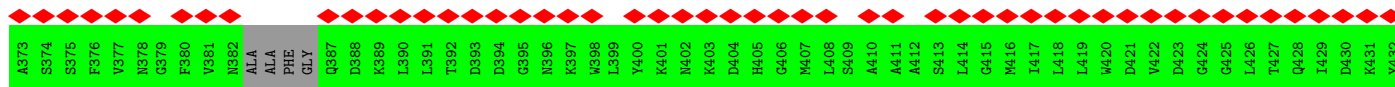
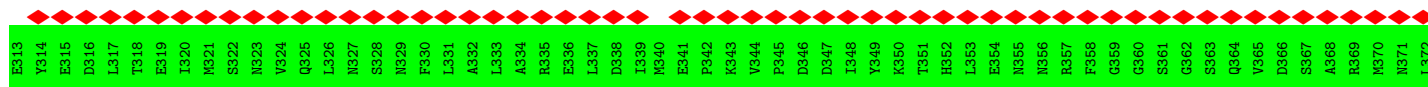
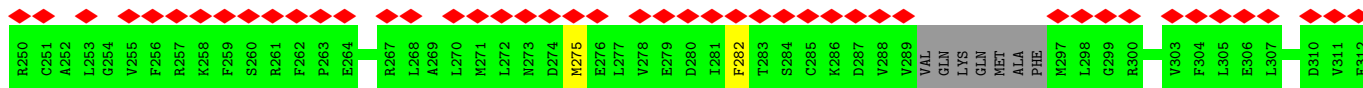
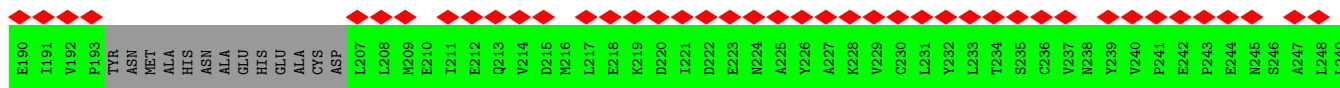
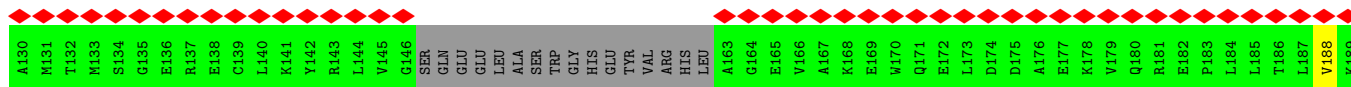
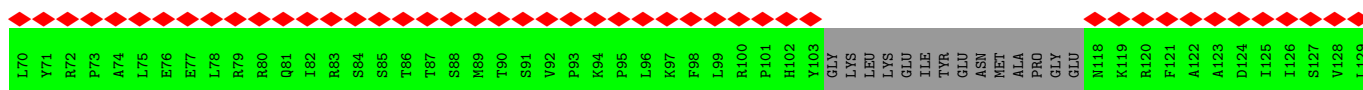
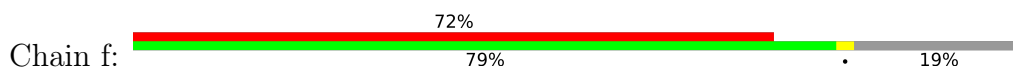
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 17: 26S proteasome complex subunit SEM1



- Molecule 18: 26S proteasome non-ATPase regulatory subunit 2



ASN	ILE	ILE	LEU	GLY	LYS	SER	HIS	TYR	VAL	LEU	TYR	GLY	LEU	VAL	ALA	ALA	MET	GLN	PRO	ARG	LEU	ALA	MET	GLN	GLY	LEU	THR	PHE	ASP	GLU	LEU	GLY	K773	G774	T775	L776	T777	L778	C779	P780	Y781	H782	S783	D784	R785	Q786	L787	M788	S789	Q790	V791	A792	V793	L796	L797	T798	V799	L800	V801	S802	F803	L804	ASP	VAL	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21885	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.009	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/2710	0.42	0/3659
2	B	0.23	0/2509	0.42	0/3383
3	C	0.23	0/2784	0.41	0/3737
4	D	0.24	0/2690	0.41	1/3630 (0.0%)
5	E	0.23	0/2525	0.40	0/3387
6	F	0.23	0/2681	0.41	0/3611
7	U	0.23	0/5930	0.40	0/8021
8	V	0.23	0/2170	0.39	0/2929
9	W	0.24	0/3251	0.41	1/4370 (0.0%)
10	X	0.23	0/2255	0.36	0/3041
11	Y	0.23	0/3173	0.37	0/4273
12	Z	0.23	0/2324	0.39	0/3150
13	a	0.23	0/3061	0.37	0/4144
14	b	0.23	0/1478	0.40	0/2001
15	c	0.23	0/2302	0.39	0/3110
16	d	0.24	0/1486	0.37	0/2010
17	e	0.21	0/289	0.41	0/389
18	f	0.24	0/4989	0.42	0/6729
All	All	0.23	0/48607	0.40	2/65574 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	221	LYS	C-N-CA	5.92	136.51	121.70
4	D	332	GLU	C-N-CA	5.16	134.59	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	332/352 (94%)	299 (90%)	33 (10%)	0	100	100
2	B	311/341 (91%)	271 (87%)	40 (13%)	0	100	100
3	C	343/385 (89%)	323 (94%)	20 (6%)	0	100	100
4	D	326/368 (89%)	315 (97%)	11 (3%)	0	100	100
5	E	307/379 (81%)	290 (94%)	17 (6%)	0	100	100
6	F	333/380 (88%)	311 (93%)	22 (7%)	0	100	100
7	U	743/935 (80%)	716 (96%)	27 (4%)	0	100	100
8	V	260/488 (53%)	237 (91%)	23 (9%)	0	100	100
9	W	387/456 (85%)	359 (93%)	26 (7%)	2 (0%)	29	69
10	X	276/385 (72%)	269 (98%)	7 (2%)	0	100	100
11	Y	376/378 (100%)	359 (96%)	17 (4%)	0	100	100
12	Z	284/286 (99%)	272 (96%)	12 (4%)	0	100	100
13	a	372/374 (100%)	351 (94%)	21 (6%)	0	100	100
14	b	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
15	c	285/287 (99%)	277 (97%)	8 (3%)	0	100	100
16	d	174/257 (68%)	160 (92%)	14 (8%)	0	100	100
17	e	31/33 (94%)	28 (90%)	3 (10%)	0	100	100
18	f	616/784 (79%)	556 (90%)	60 (10%)	0	100	100
All	All	5945/7059 (84%)	5568 (94%)	375 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	W	221	LYS
9	W	222	LEU

5.3.2 Protein sidechains ⓘ

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	A	293/300 (98%)	290 (99%)	3 (1%)	76	86
2	B	276/298 (93%)	273 (99%)	3 (1%)	73	84
3	C	302/333 (91%)	298 (99%)	4 (1%)	69	81
4	D	290/321 (90%)	288 (99%)	2 (1%)	84	90
5	E	273/333 (82%)	270 (99%)	3 (1%)	73	84
6	F	291/326 (89%)	288 (99%)	3 (1%)	76	86
7	U	639/798 (80%)	635 (99%)	4 (1%)	86	92
8	V	231/422 (55%)	231 (100%)	0	100	100
9	W	361/416 (87%)	360 (100%)	1 (0%)	92	95
10	X	243/331 (73%)	243 (100%)	0	100	100
11	Y	334/334 (100%)	334 (100%)	0	100	100
12	Z	257/257 (100%)	256 (100%)	1 (0%)	91	94
13	a	334/334 (100%)	334 (100%)	0	100	100
14	b	167/167 (100%)	166 (99%)	1 (1%)	86	92
15	c	252/252 (100%)	251 (100%)	1 (0%)	91	94
16	d	158/231 (68%)	157 (99%)	1 (1%)	86	92
17	e	31/31 (100%)	31 (100%)	0	100	100
18	f	538/660 (82%)	525 (98%)	13 (2%)	49	69
All	All	5270/6144 (86%)	5230 (99%)	40 (1%)	82	89

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	f	275	MET

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Mol	Chain	Res	Type
18	f	583	VAL
18	f	282	PHE
18	f	493	ASN
18	f	662	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
8	V	329	HIS
18	f	301	HIS
10	X	406	ASN
18	f	273	ASN
18	f	493	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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
9	W	1
10	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	205:ILE	C	206:SER	N	3.21
1	X	311:ALA	C	312:GLU	N	3.20

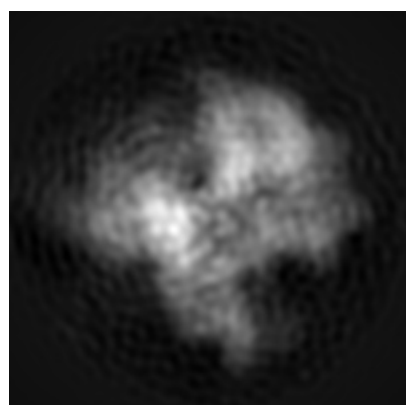
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8684. These allow visual inspection of the internal detail of the map and identification of artifacts.

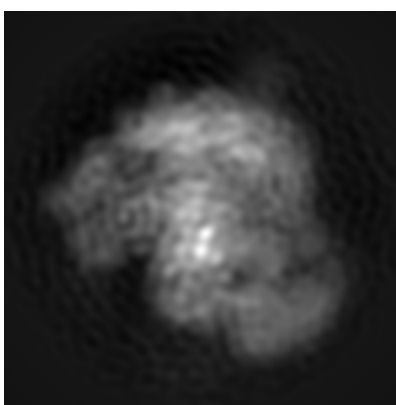
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

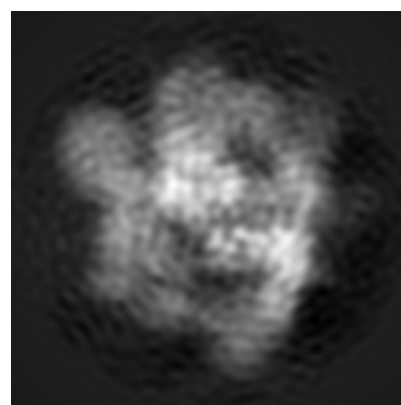
6.1.1 Primary map



X



Y

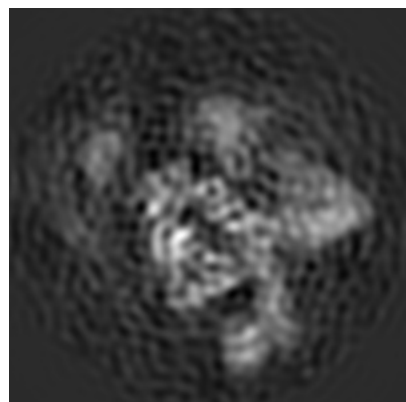


Z

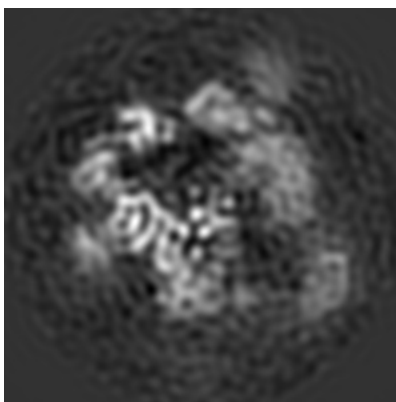
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

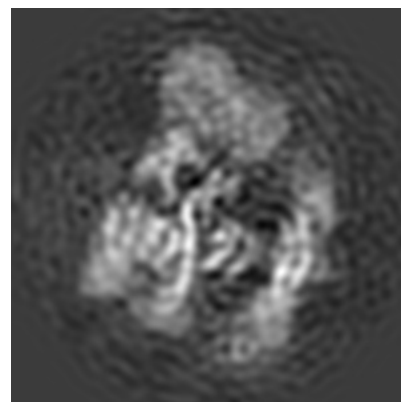
6.2.1 Primary map



X Index: 150



Y Index: 150

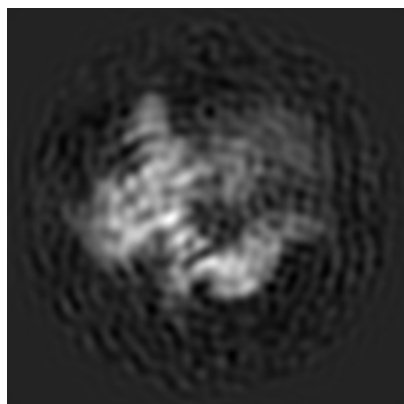


Z Index: 150

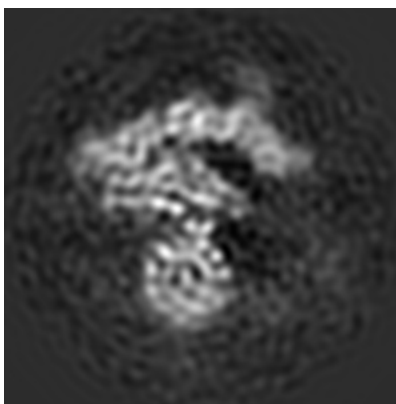
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

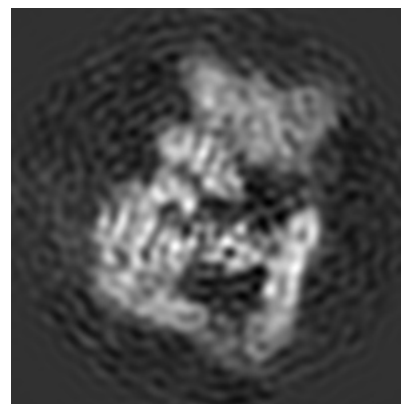
6.3.1 Primary map



X Index: 209



Y Index: 128

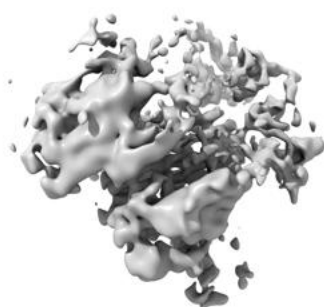


Z Index: 135

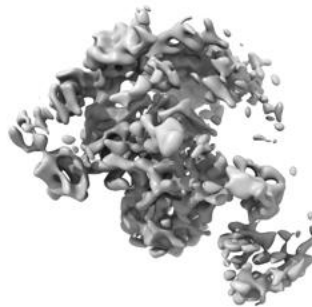
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

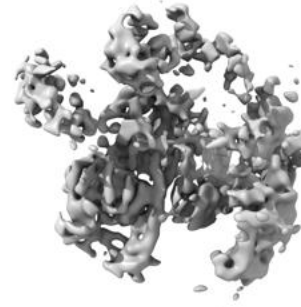
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

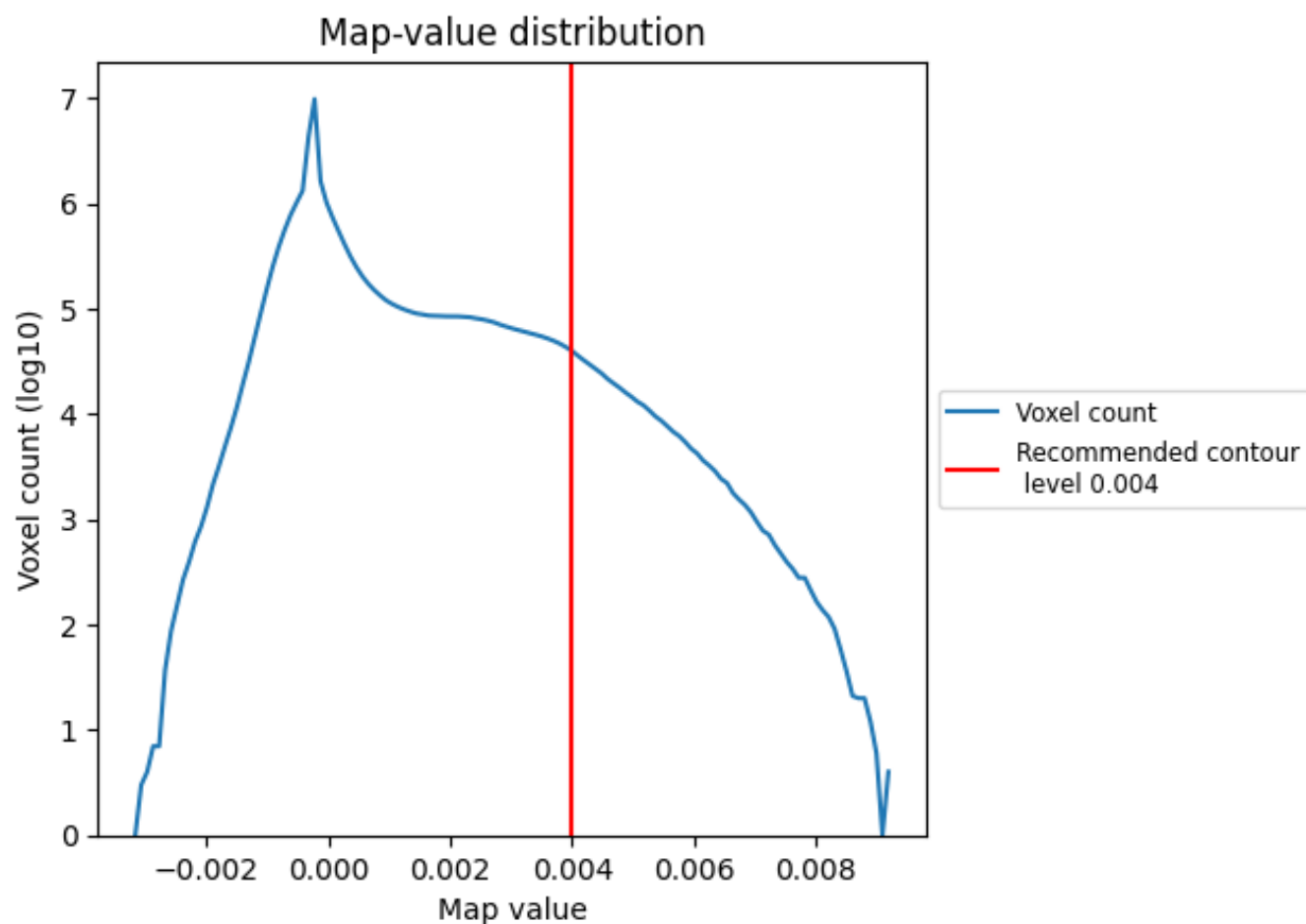
6.5 Mask visualisation

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

7 Map analysis [i](#)

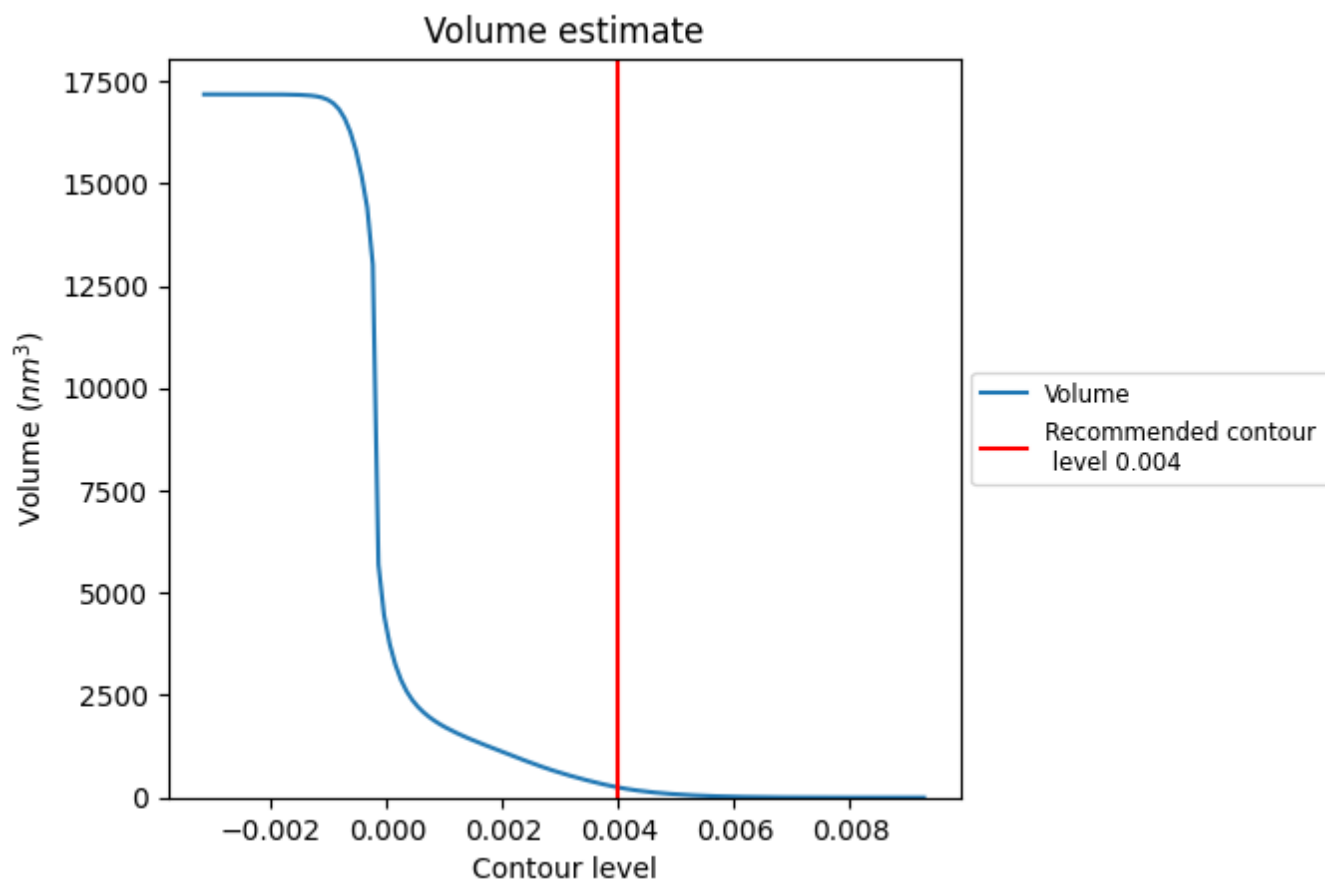
This section contains the results of statistical analysis of the map.

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.

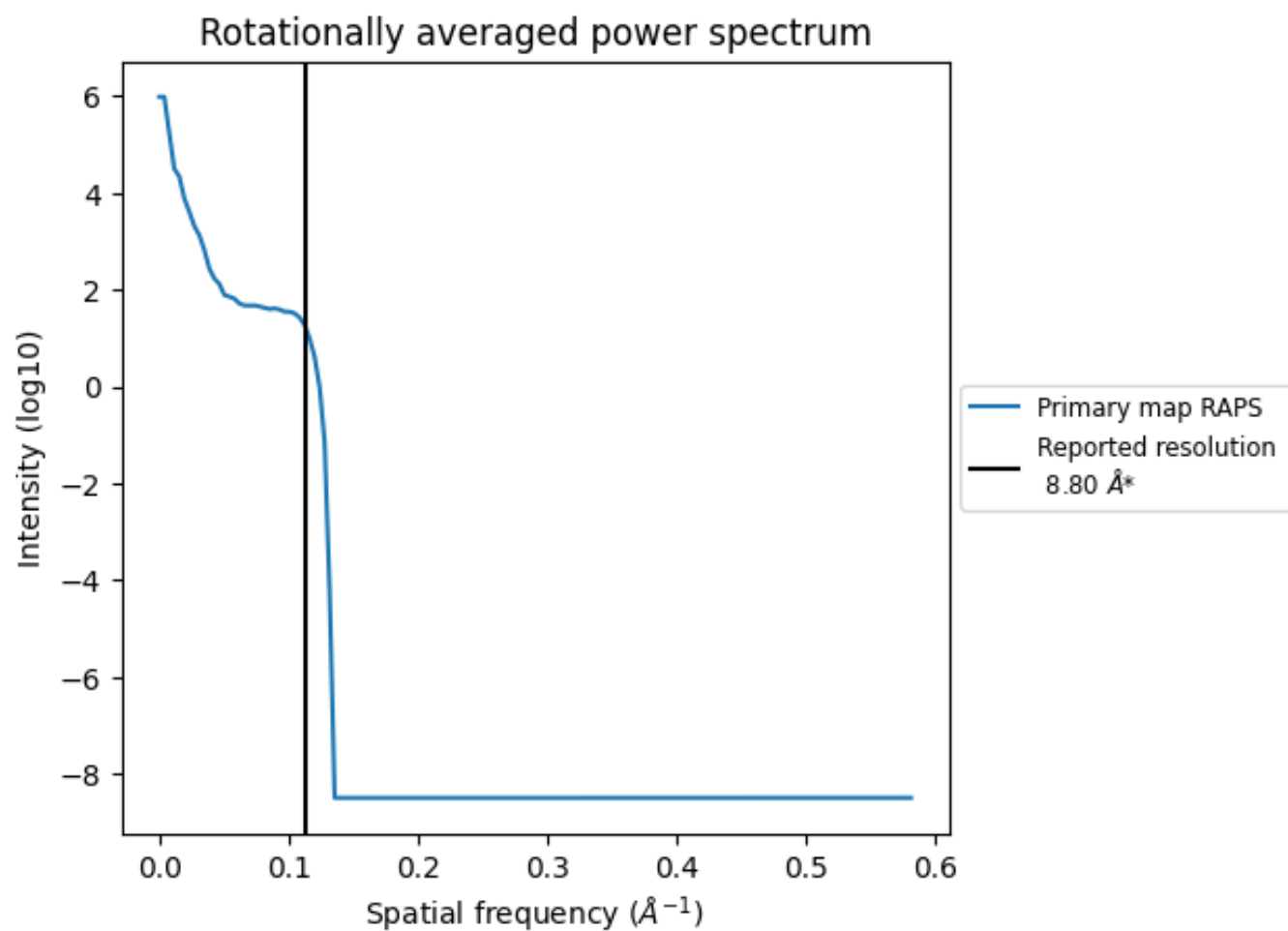
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 248 nm³; this corresponds to an approximate mass of 224 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.114 Å⁻¹

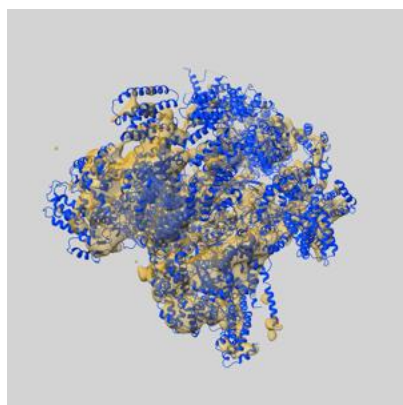
8 Fourier-Shell correlation

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

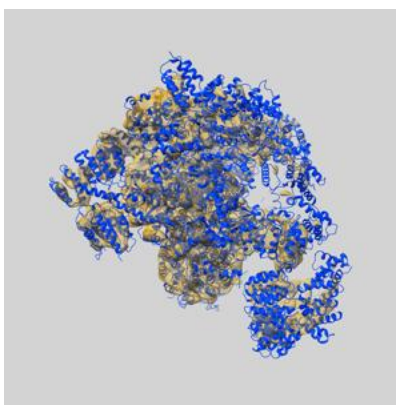
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8684 and PDB model 5VHS. Per-residue inclusion information can be found in section 3 on page 7.

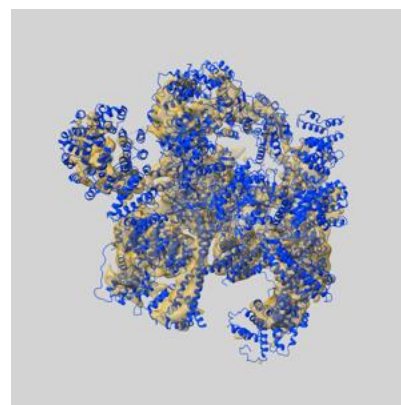
9.1 Map-model overlay [i](#)



X



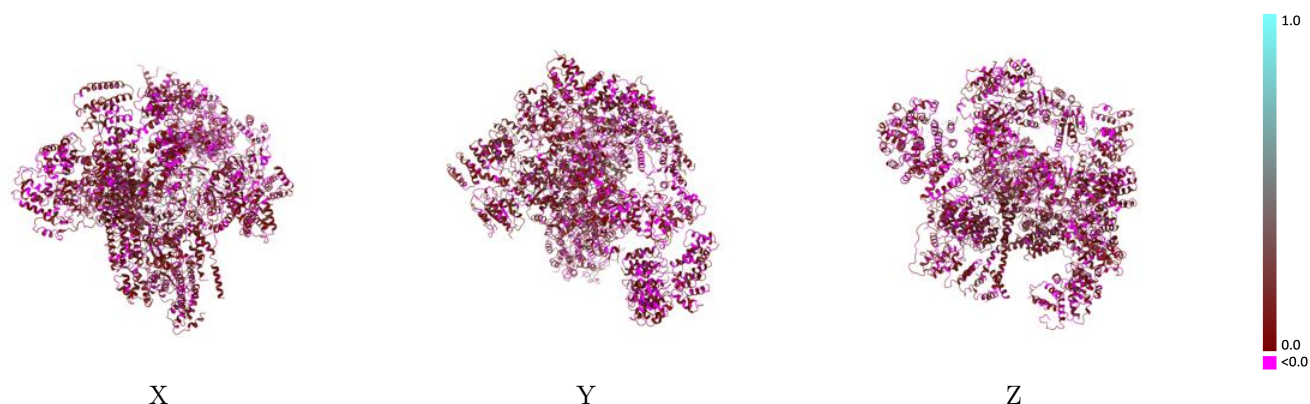
Y



Z

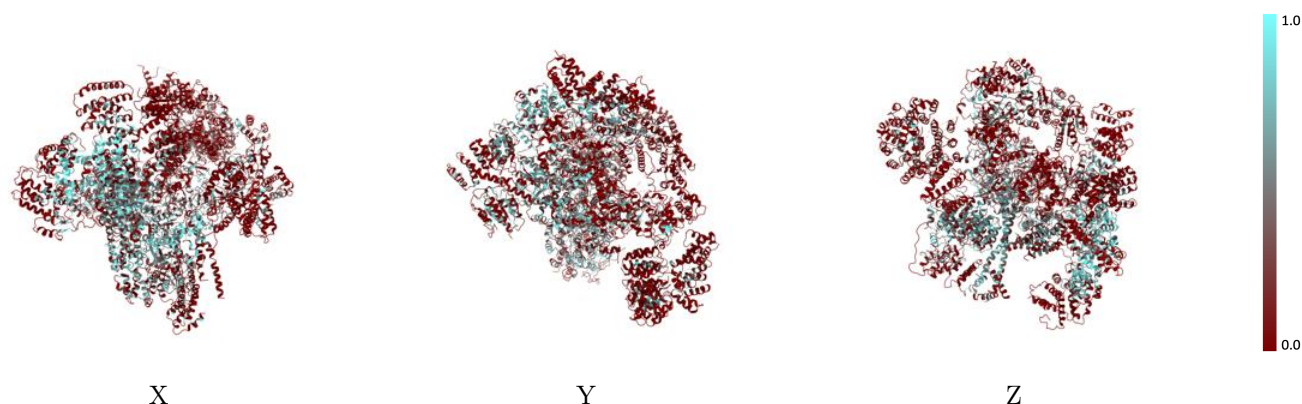
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



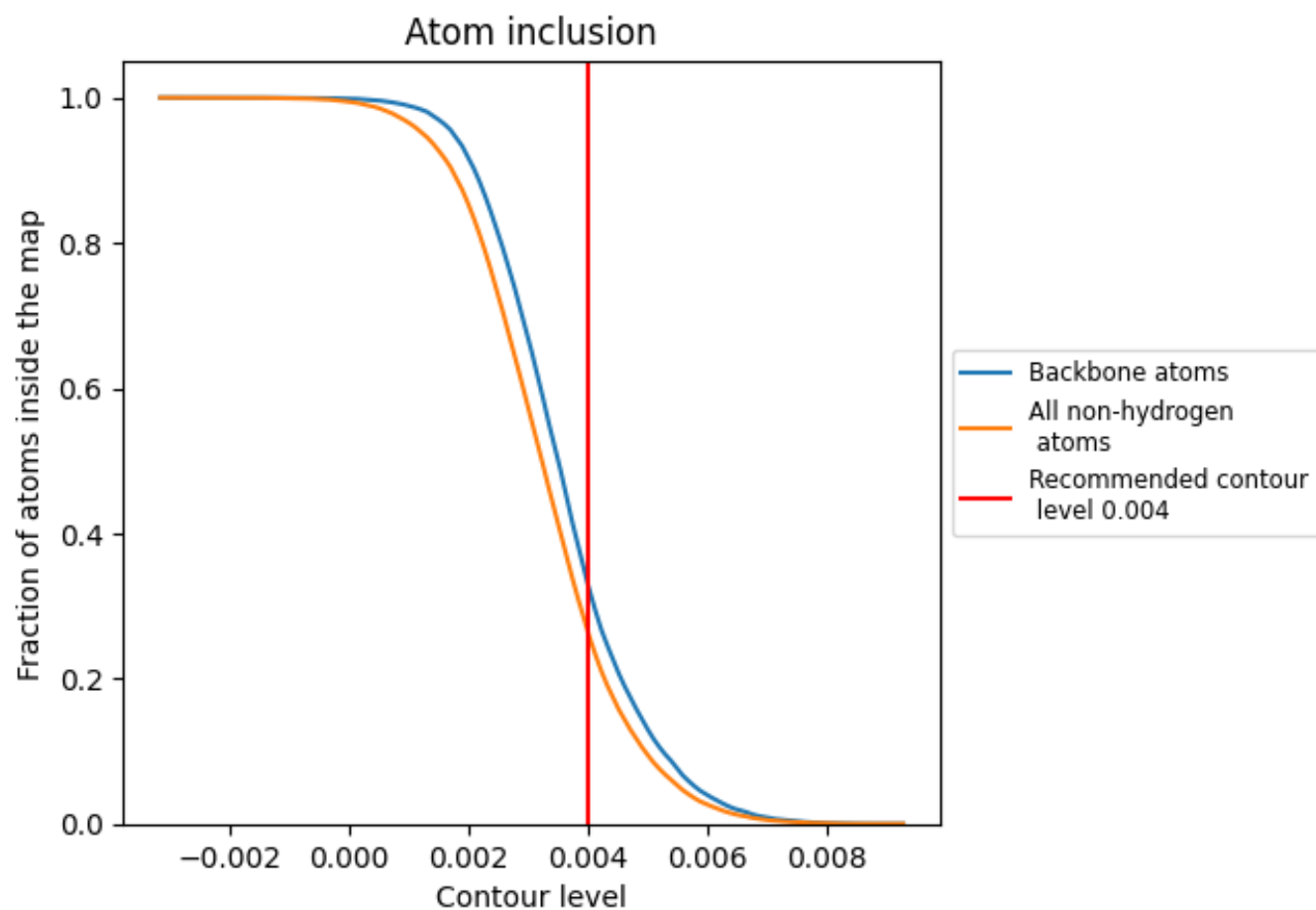
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 33% of all backbone atoms, 26% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2642	 0.0810
A	 0.2056	 0.0660
B	 0.1873	 0.0520
C	 0.1352	 0.0890
D	 0.1708	 0.0710
E	 0.1206	 0.0800
F	 0.1973	 0.0870
U	 0.3520	 0.0840
V	 0.3627	 0.0530
W	 0.3719	 0.1050
X	 0.2595	 0.0780
Y	 0.4018	 0.0940
Z	 0.4242	 0.1220
a	 0.3307	 0.1080
b	 0.2464	 0.0840
c	 0.4198	 0.1130
d	 0.1416	 0.0550
e	 0.5288	 0.1110
f	 0.1038	 0.0460

