wwPDB EM Validation Summary Report

Mar 5, 2024 – 12:26 PM EST

PDB ID	:	6MUV
EMDB ID	:	EMD-9257
Title	:	The structure of the Plasmodium falciparum 20S proteasome in complex with two PA28 activators
Authors	:	Metcalfe, R.D.; Xie, S.C.; Hanssen, E.; Gillett, D.L.; Leis, A.P.; Tilley, L.; Griffin, M.D.W.
Deposited on	:	2018-10-23
Resolution	:	3.80 Å(reported)
Based on initial model	:	6DFK

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:

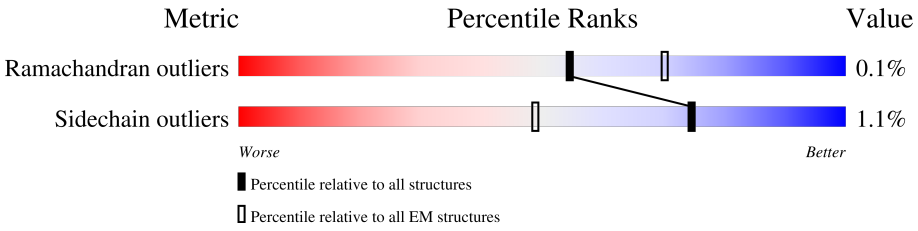
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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 <=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	260	10% 93% • 5%
1	O	260	11% 93% • 5%
2	B	235	9% 94% • 5%
2	P	235	8% 94% • 5%
3	C	246	6% 96% • •
3	Q	246	7% 96% • •
4	D	241	11% 93% • 6%
4	R	241	13% 93% • 6%
5	E	256	12% 88% 11%

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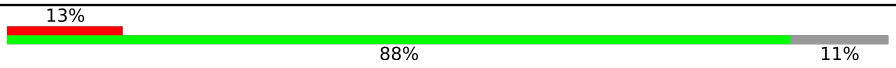
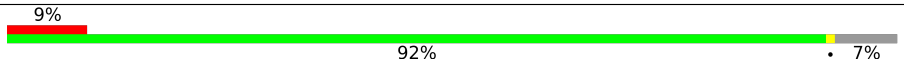
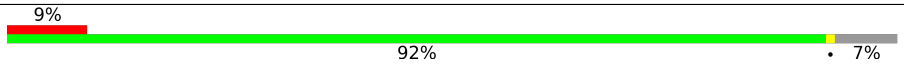
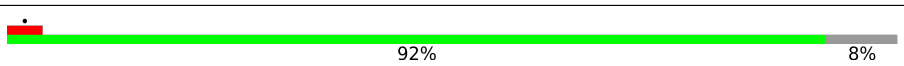
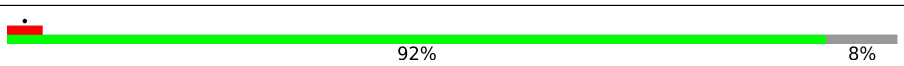
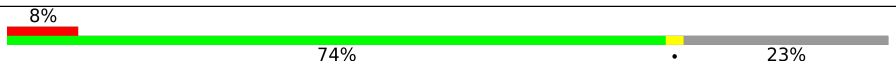
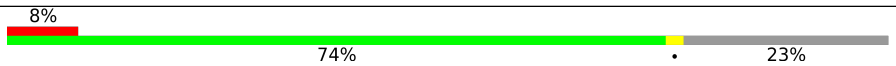
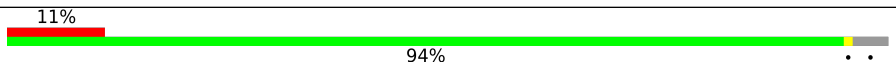
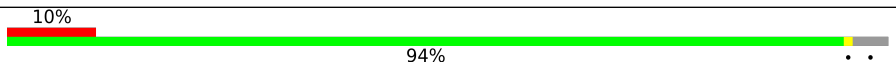
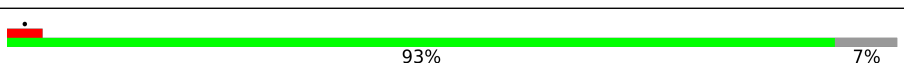
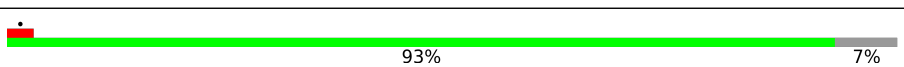
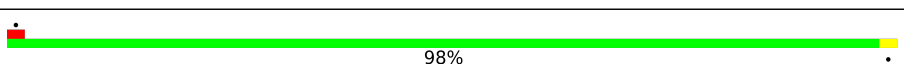
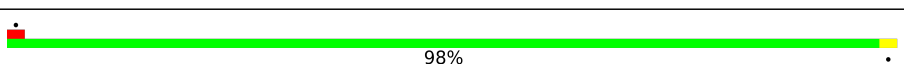
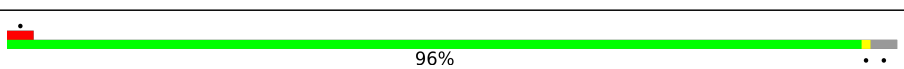
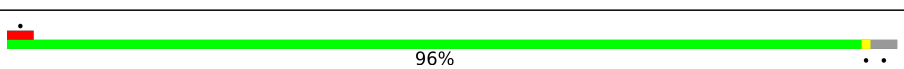
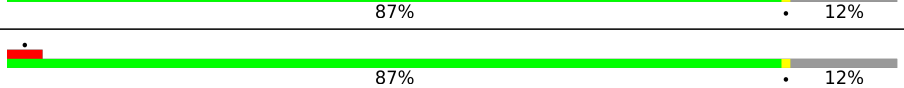
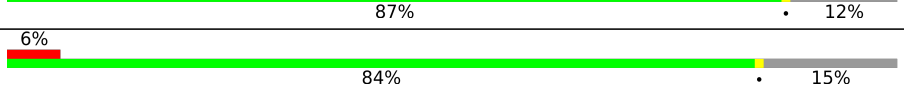
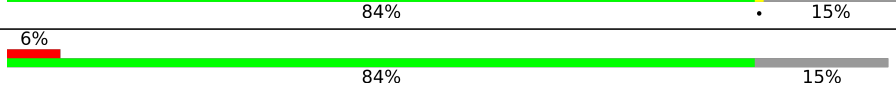
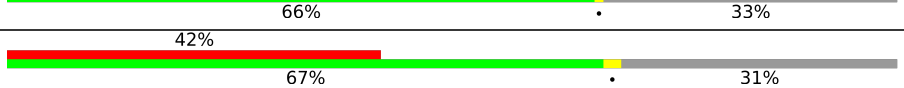
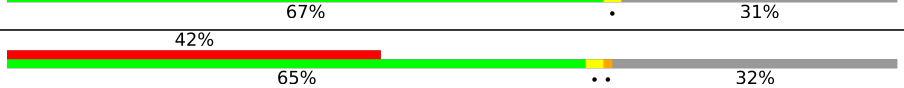
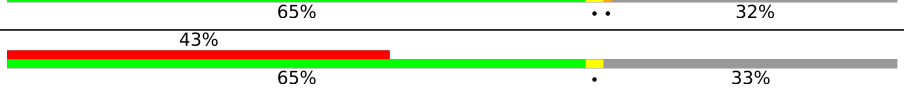
Mol	Chain	Length	Quality of chain
5	S	256	
6	F	254	
6	T	254	
7	G	252	
7	U	252	
8	H	252	
8	V	252	
9	I	229	
9	W	229	
10	J	218	
10	X	218	
11	K	195	
11	Y	195	
12	L	211	
12	Z	211	
13	M	240	
13	a	240	
14	N	265	
14	b	265	
15	c	279	
15	d	279	
15	e	279	
15	f	279	
15	g	279	
15	h	279	

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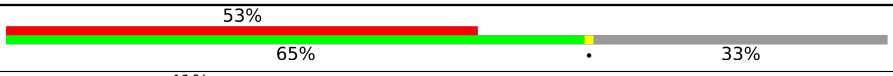
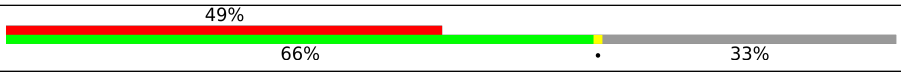
Mol	Chain	Length	Quality of chain
15	i	279	
15	j	279	
15	k	279	
15	l	279	
15	m	279	
15	n	279	
15	o	279	
15	p	279	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 71112 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 20S proteasome alpha-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	246	Total	C	N	O	S	0	0
			1943	1221	326	381	15		
1	O	246	Total	C	N	O	S	0	0
			1943	1221	326	381	15		

- Molecule 2 is a protein called 20S proteasome alpha-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1782	1146	293	337	6		
2	P	224	Total	C	N	O	S	0	0
			1782	1146	293	337	6		

- Molecule 3 is a protein called 20S proteasome alpha-3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	240	Total	C	N	O	S	0	0
			1917	1230	308	376	3		
3	Q	240	Total	C	N	O	S	0	0
			1917	1230	308	376	3		

- Molecule 4 is a protein called 20S proteasome alpha-4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	227	Total	C	N	O	S	0	0
			1795	1147	303	337	8		
4	R	227	Total	C	N	O	S	0	0
			1795	1147	303	337	8		

- Molecule 5 is a protein called 20S proteasome alpha-5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	227	Total	C	N	O	S	0	0
			1760	1109	291	350	10		
5	S	227	Total	C	N	O	S	0	0
			1760	1109	291	350	10		

- Molecule 6 is a protein called 20S proteasome alpha-6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	236	Total	C	N	O	S	0	0
			1878	1196	309	362	11		
6	T	236	Total	C	N	O	S	0	0
			1878	1196	309	362	11		

- Molecule 7 is a protein called 20S proteasome alpha-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1906	1215	319	360	12		
7	U	233	Total	C	N	O	S	0	0
			1906	1215	319	360	12		

- Molecule 8 is a protein called 20S proteasome beta-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	193	Total	C	N	O	S	0	0
			1536	969	264	291	12		
8	V	193	Total	C	N	O	S	0	0
			1536	969	264	291	12		

- Molecule 9 is a protein called 20S proteasome beta-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1676	1058	291	313	14		
9	W	219	Total	C	N	O	S	0	0
			1676	1058	291	313	14		

- Molecule 10 is a protein called 20S proteasome beta-3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	203	Total	C	N	O	S	0	0
			1595	1017	258	306	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	203	Total	C	N	O	S	0	0
			1595	1017	258	306	14		

- Molecule 11 is a protein called 20S proteasome beta-4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	195	Total	C	N	O	S	0	0
			1614	1042	266	298	8		
11	Y	195	Total	C	N	O	S	0	0
			1614	1042	266	298	8		

- Molecule 12 is a protein called 20S proteasome beta-5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	204	Total	C	N	O	S	0	0
			1600	1021	265	307	7		
12	Z	204	Total	C	N	O	S	0	0
			1600	1021	265	307	7		

- Molecule 13 is a protein called 20S proteasome beta-6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	211	Total	C	N	O	S	0	0
			1676	1073	277	319	7		
13	a	211	Total	C	N	O	S	0	0
			1676	1073	277	319	7		

- Molecule 14 is a protein called 20S proteasome beta-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	224	Total	C	N	O	S	0	0
			1845	1177	313	348	7		
14	b	224	Total	C	N	O	S	0	0
			1845	1177	313	348	7		

- Molecule 15 is a protein called Proteasome activator PA28.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	187	Total	C	N	O	S	0	0
			1568	1015	259	291	3		
15	d	187	Total	C	N	O	S	0	0
			1568	1015	259	291	3		

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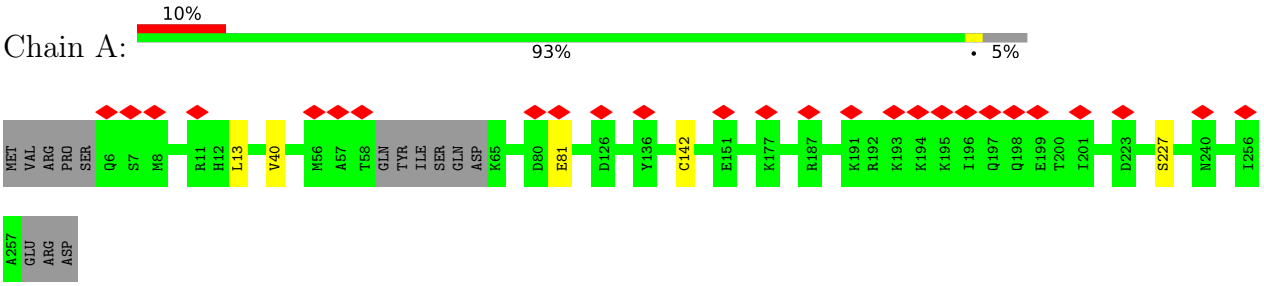
Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	188	Total	C	N	O	S	0	0
			1576	1019	261	293	3		
15	f	193	Total	C	N	O	S	0	0
			1618	1043	270	302	3		
15	g	189	Total	C	N	O	S	0	0
			1585	1024	262	296	3		
15	h	186	Total	C	N	O	S	0	0
			1559	1009	257	290	3		
15	i	186	Total	C	N	O	S	0	0
			1559	1009	257	290	3		
15	j	193	Total	C	N	O	S	0	0
			1618	1043	270	302	3		
15	k	189	Total	C	N	O	S	0	0
			1585	1024	262	296	3		
15	l	186	Total	C	N	O	S	0	0
			1559	1009	257	290	3		
15	m	187	Total	C	N	O	S	0	0
			1568	1015	259	291	3		
15	n	186	Total	C	N	O	S	0	0
			1559	1009	257	290	3		
15	o	187	Total	C	N	O	S	0	0
			1568	1015	259	291	3		
15	p	188	Total	C	N	O	S	0	0
			1576	1019	261	293	3		

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.

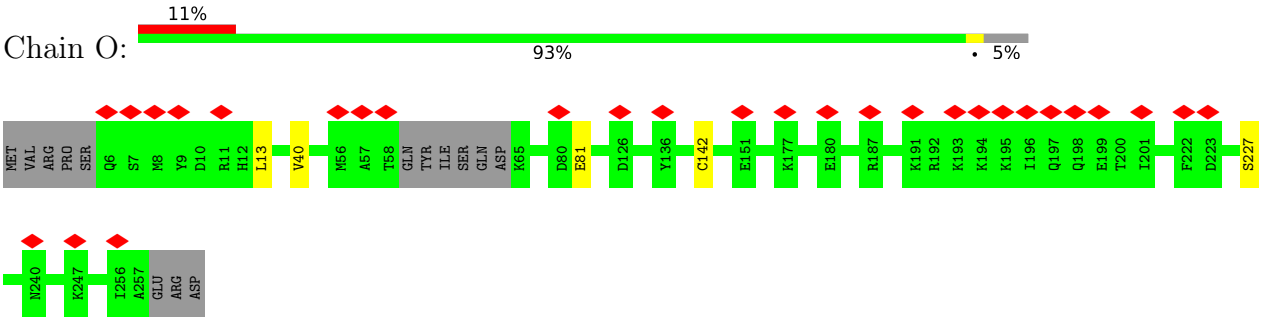
• Molecule 1: 20S proteasome alpha-1 subunit

Chain A:



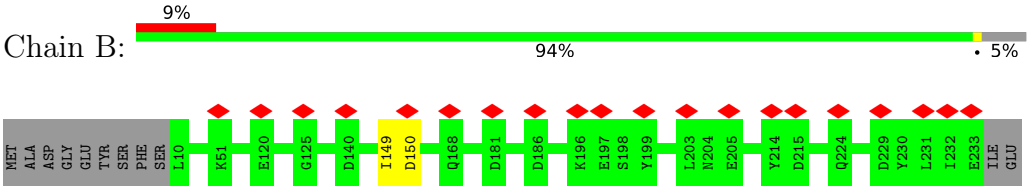
• Molecule 1: 20S proteasome alpha-1 subunit

Chain O:



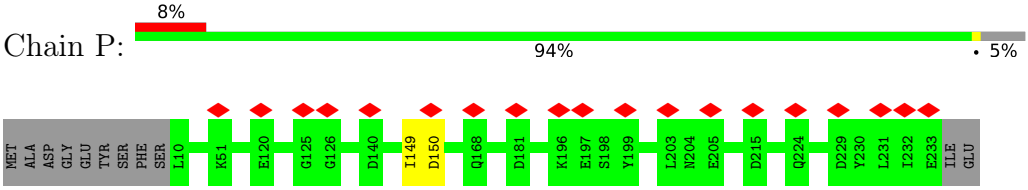
• Molecule 2: 20S proteasome alpha-2 subunit

Chain B:



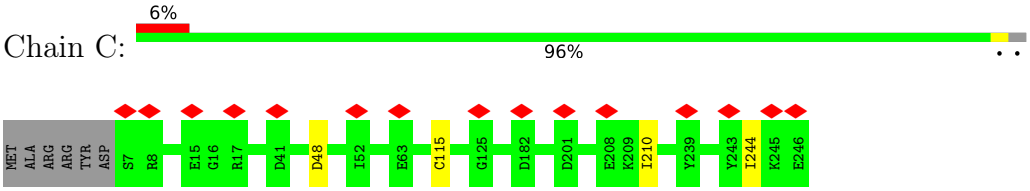
• Molecule 2: 20S proteasome alpha-2 subunit

Chain P:



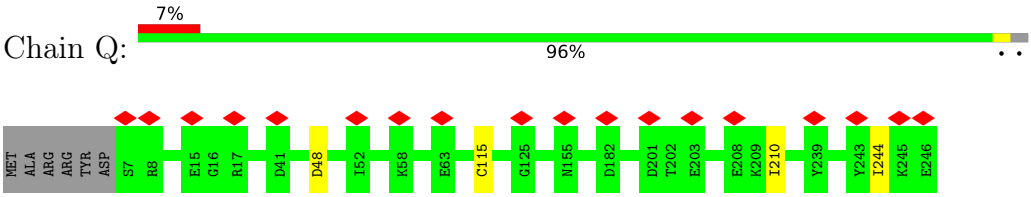
• Molecule 3: 20S proteasome alpha-3 subunit

Chain C:



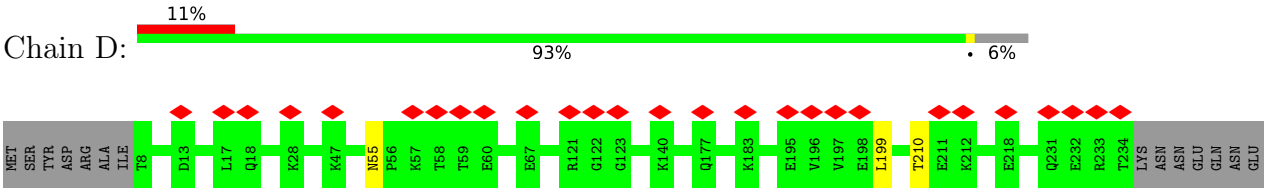
• Molecule 3: 20S proteasome alpha-3 subunit

Chain Q:



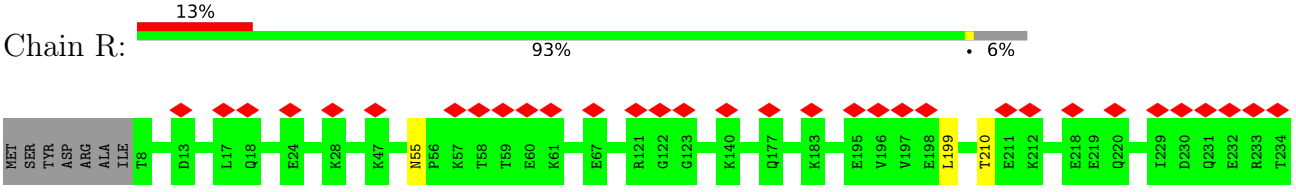
• Molecule 4: 20S proteasome alpha-4 subunit

Chain D:



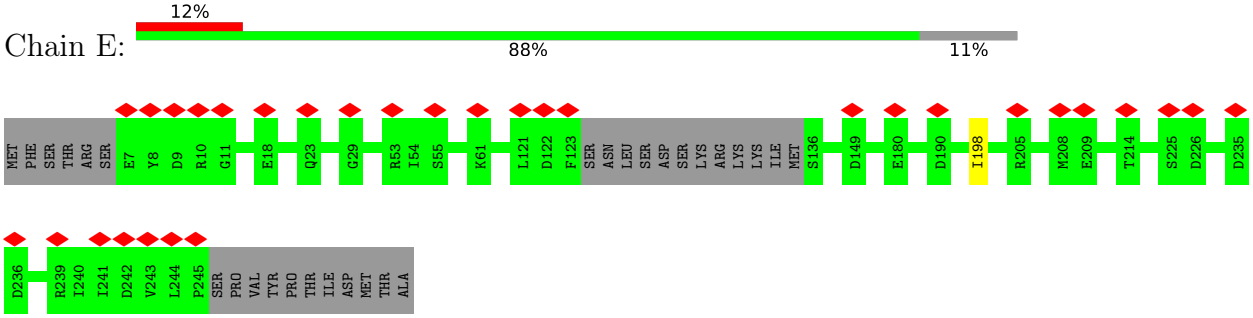
• Molecule 4: 20S proteasome alpha-4 subunit

Chain R:



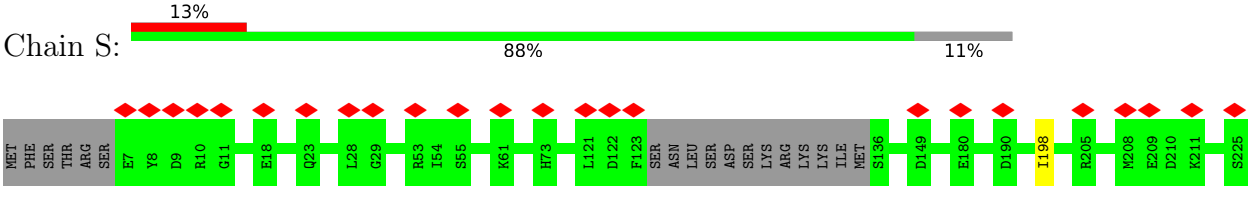
• Molecule 5: 20S proteasome alpha-5 subunit

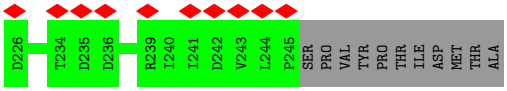
Chain E:



• Molecule 5: 20S proteasome alpha-5 subunit

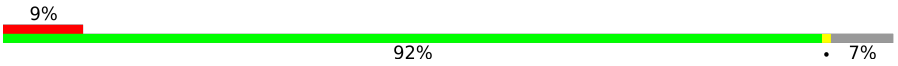
Chain S:

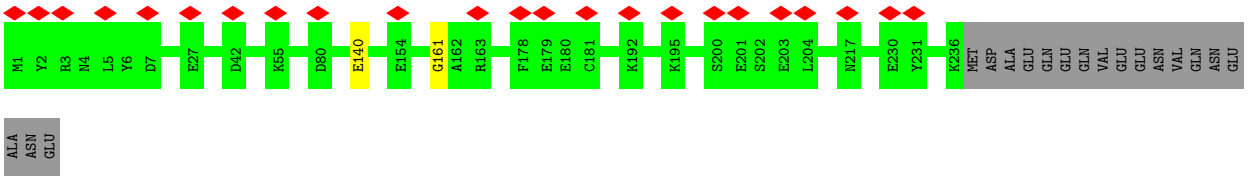




• Molecule 6: 20S proteasome alpha-6 subunit

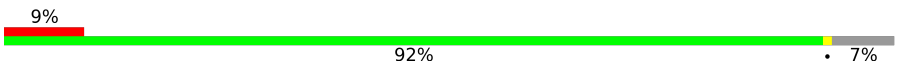
Chain F:

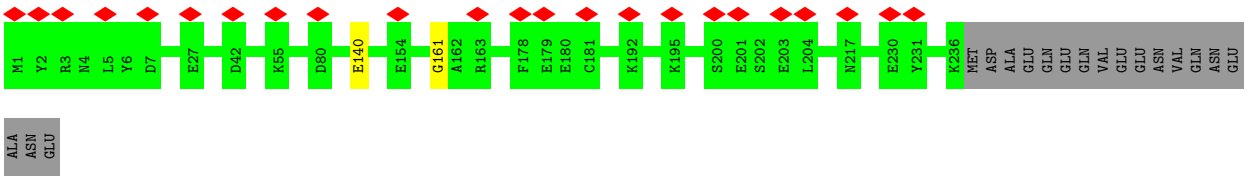




• Molecule 6: 20S proteasome alpha-6 subunit

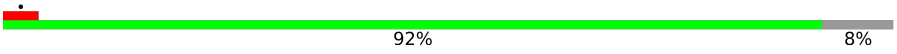
Chain T:

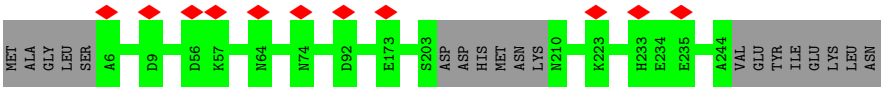




• Molecule 7: 20S proteasome alpha-7 subunit

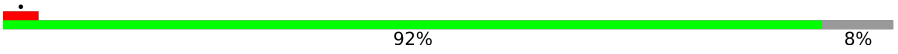
Chain G:

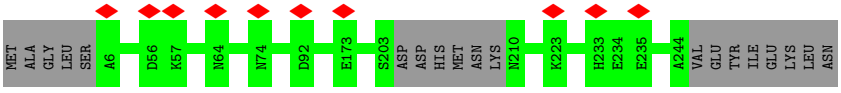




• Molecule 7: 20S proteasome alpha-7 subunit

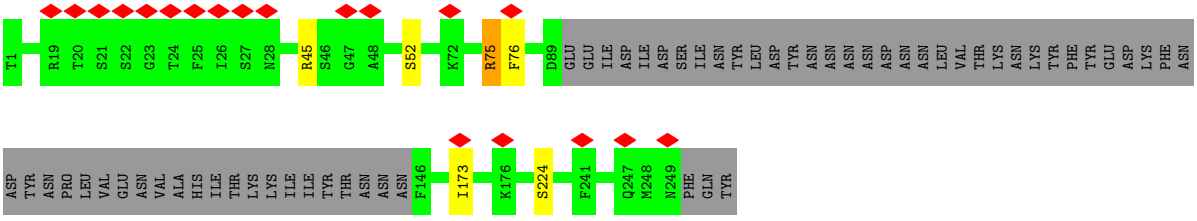
Chain U:





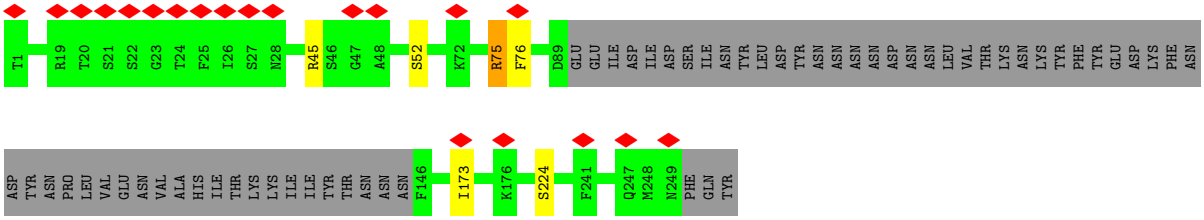
• Molecule 8: 20S proteasome beta-1 subunit

Chain H:



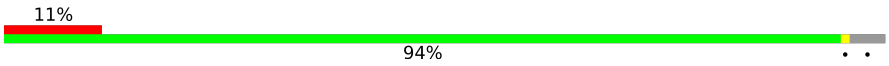
• Molecule 8: 20S proteasome beta-1 subunit

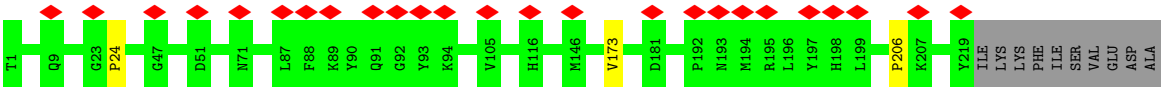
Chain V:



• Molecule 9: 20S proteasome beta-2 subunit

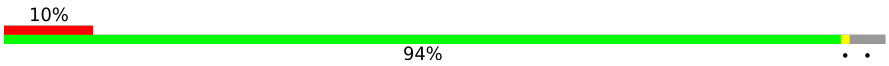
Chain I:





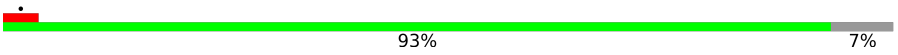
• Molecule 9: 20S proteasome beta-2 subunit

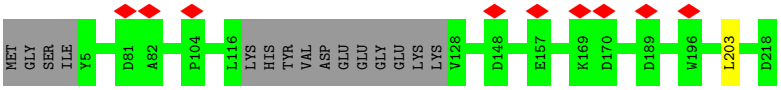
Chain W:



• Molecule 10: 20S proteasome beta-3 subunit

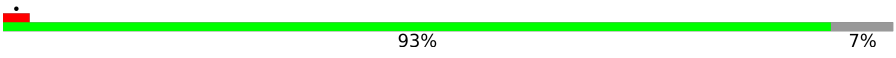
Chain J:

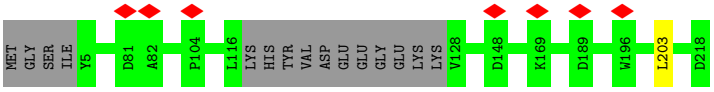




• Molecule 10: 20S proteasome beta-3 subunit

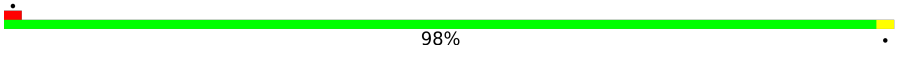
Chain X:

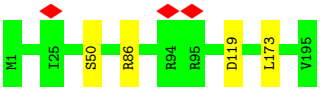




• Molecule 11: 20S proteasome beta-4 subunit

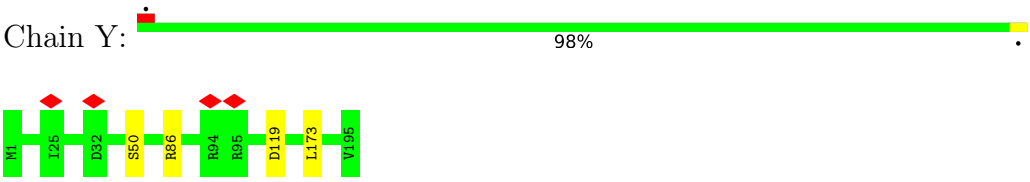
Chain K:





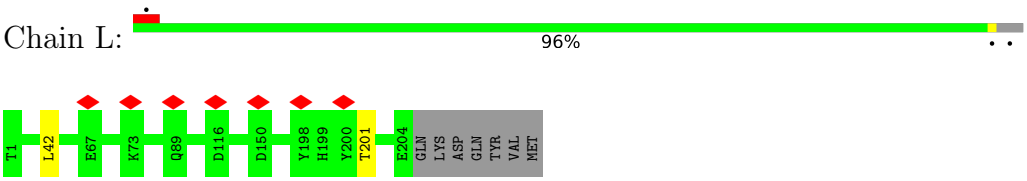
• Molecule 11: 20S proteasome beta-4 subunit

Chain Y:



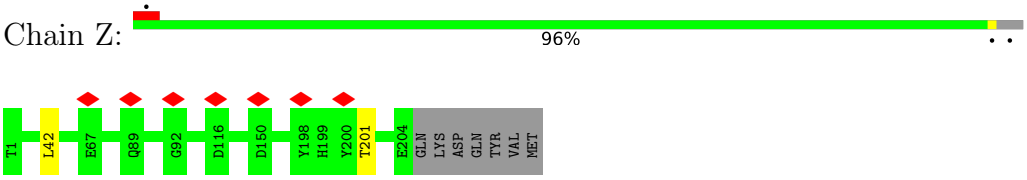
• Molecule 12: 20S proteasome beta-5 subunit

Chain L:



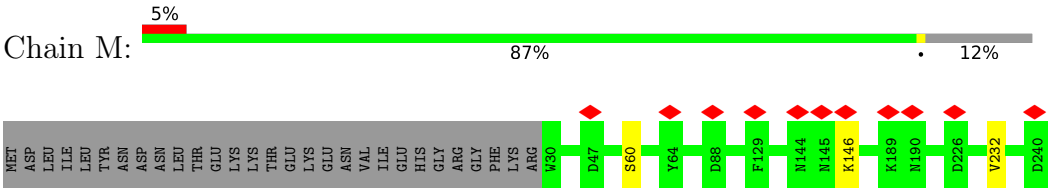
• Molecule 12: 20S proteasome beta-5 subunit

Chain Z:



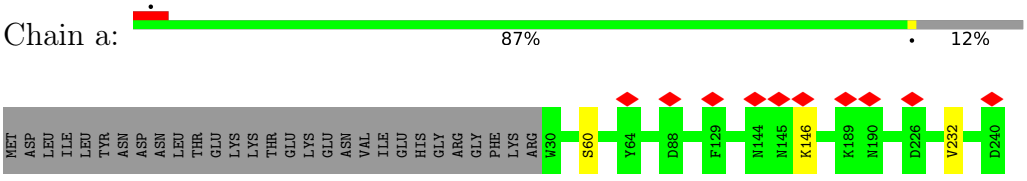
• Molecule 13: 20S proteasome beta-6 subunit

Chain M:



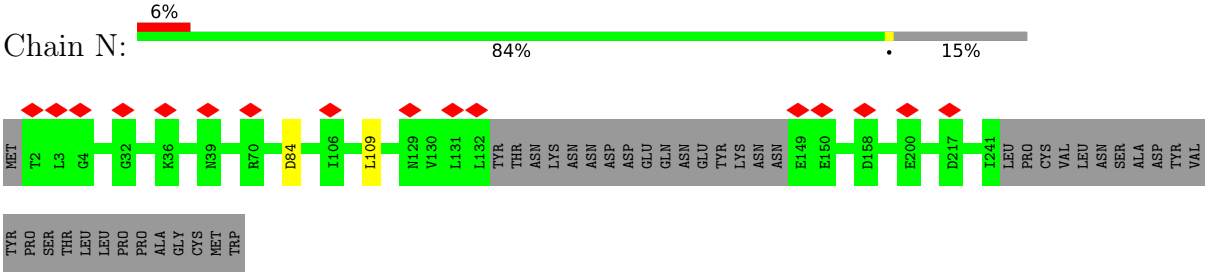
• Molecule 13: 20S proteasome beta-6 subunit

Chain a:



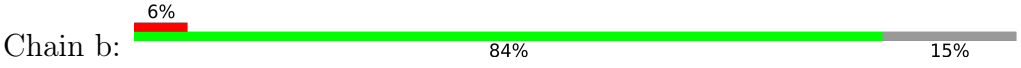
• Molecule 14: 20S proteasome beta-7 subunit

Chain N:



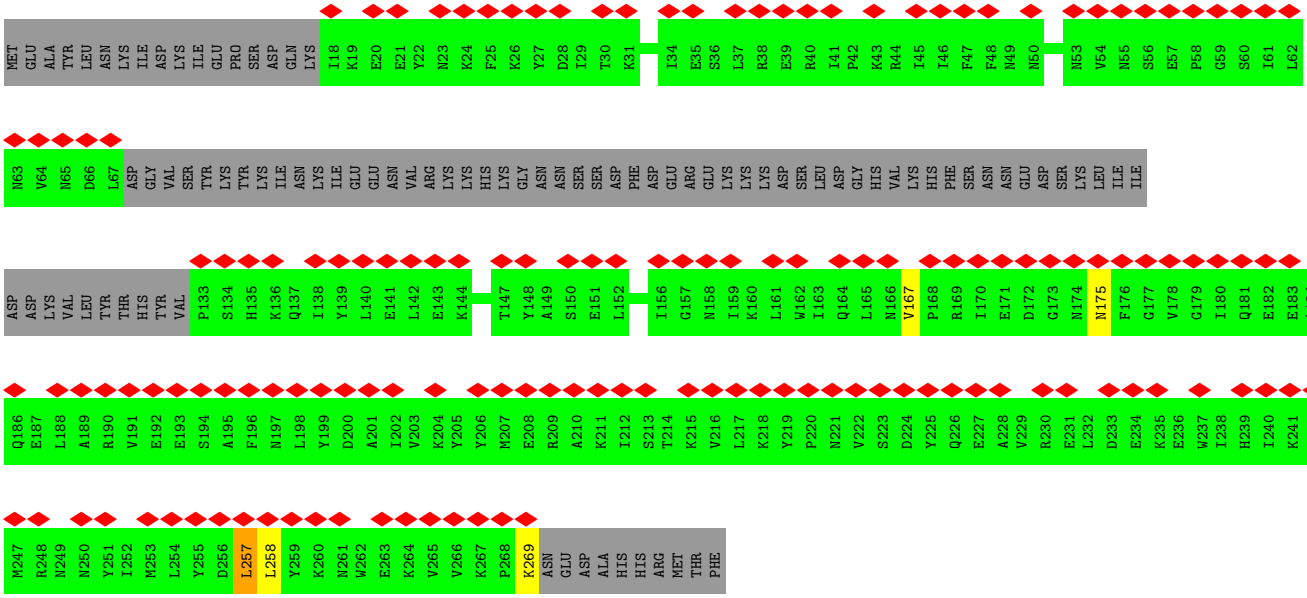
• Molecule 14: 20S proteasome beta-7 subunit

Chain b:



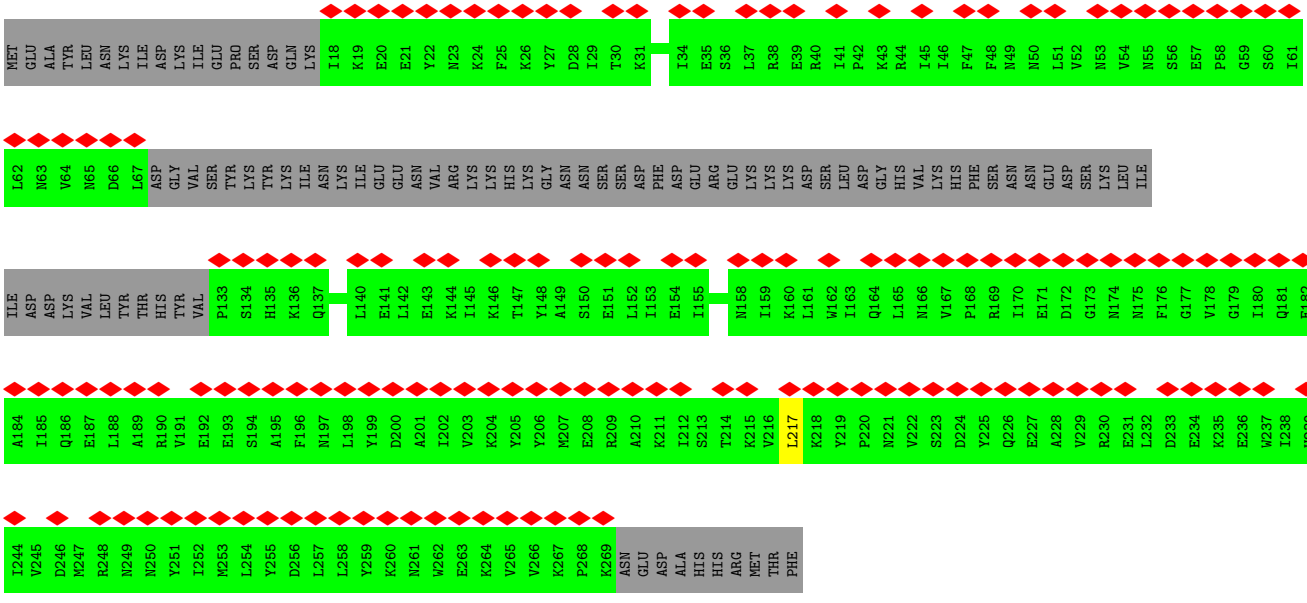
• Molecule 15: Proteasome activator PA28

Chain c:



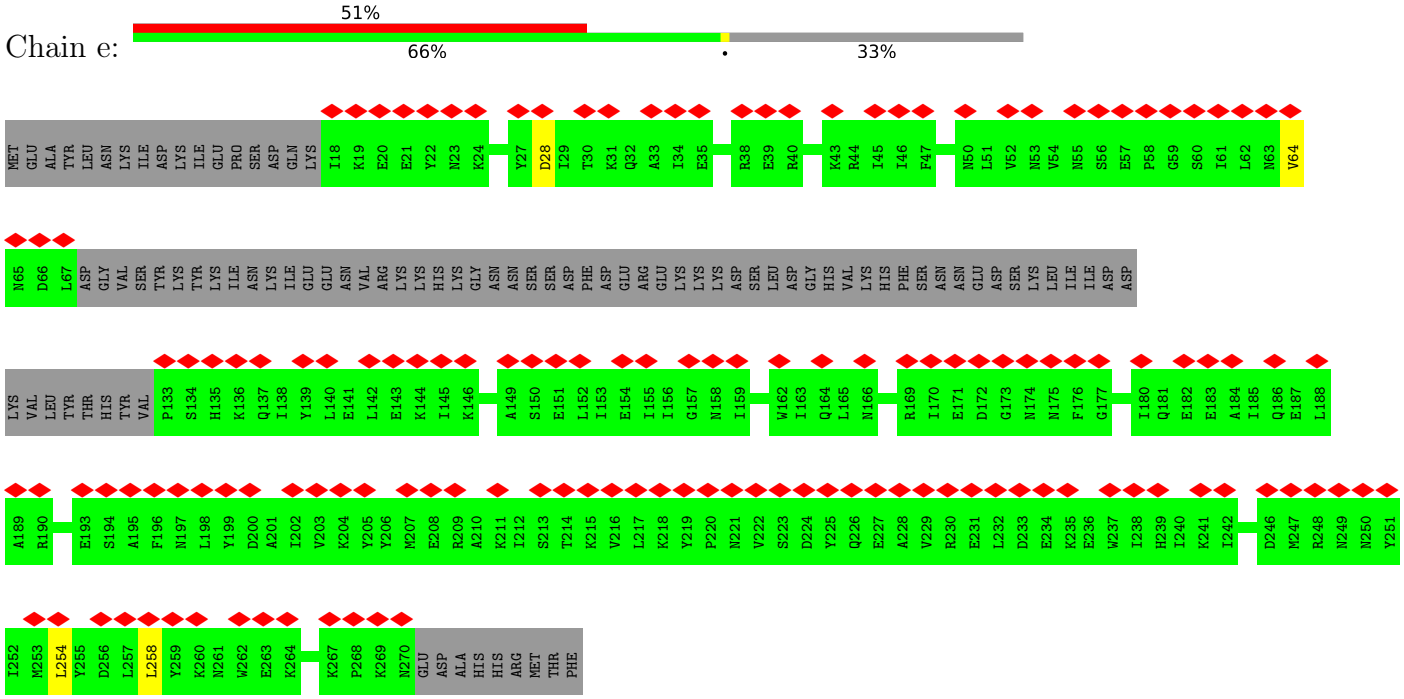
• Molecule 15: Proteasome activator PA28

Chain d:



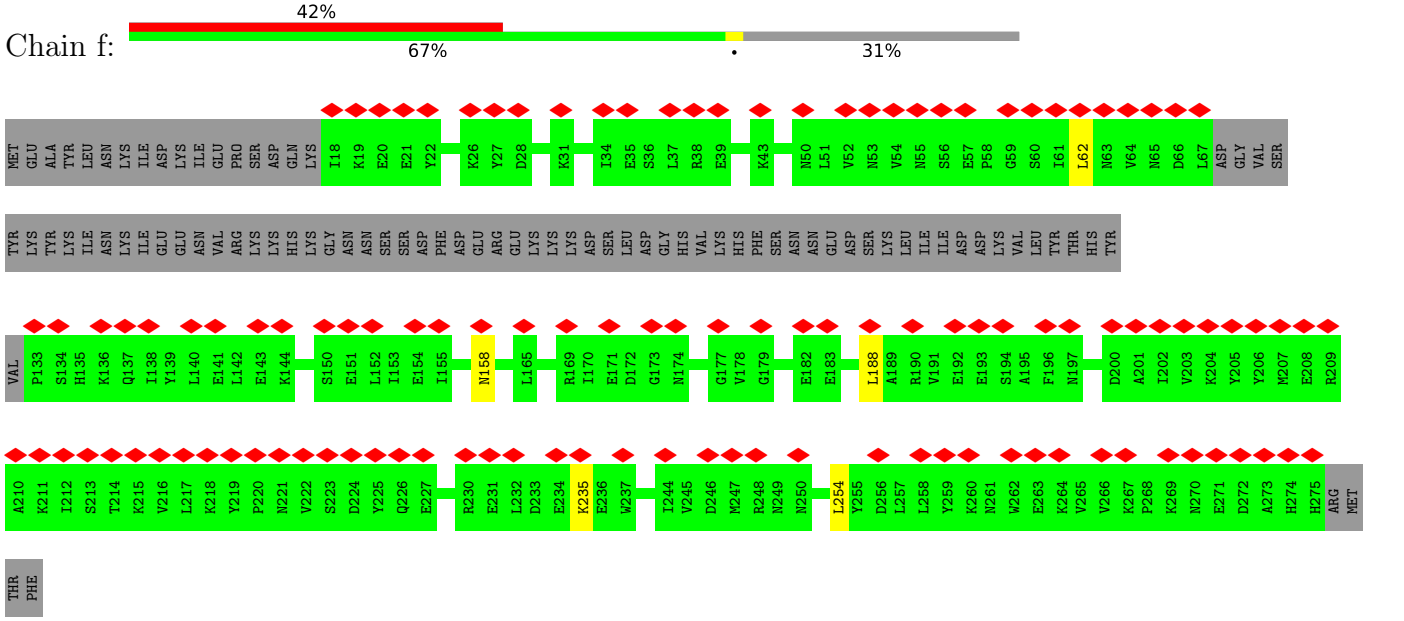
• Molecule 15: Proteasome activator PA28

Chain e:



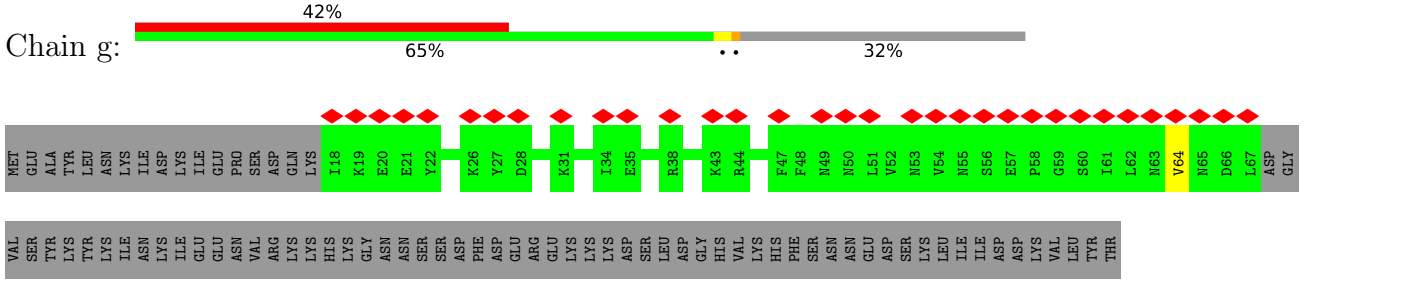
• Molecule 15: Proteasome activator PA28

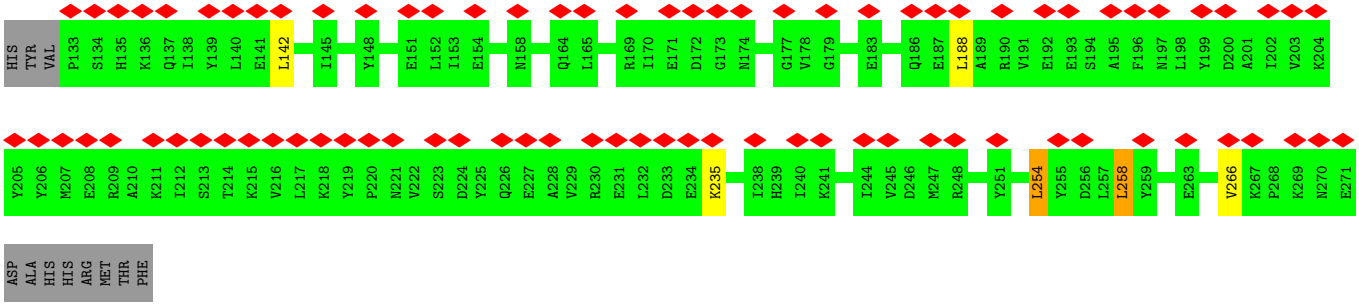
Chain f:



• Molecule 15: Proteasome activator PA28

Chain g:



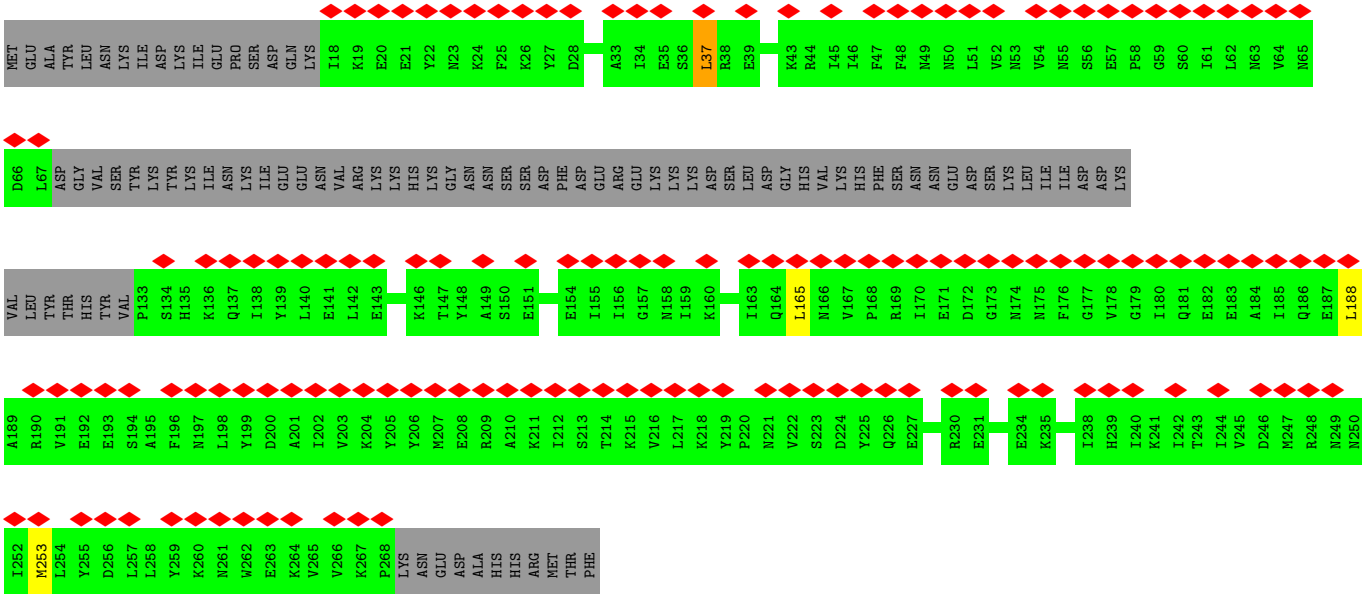


• Molecule 15: Proteasome activator PA28

Chain h:

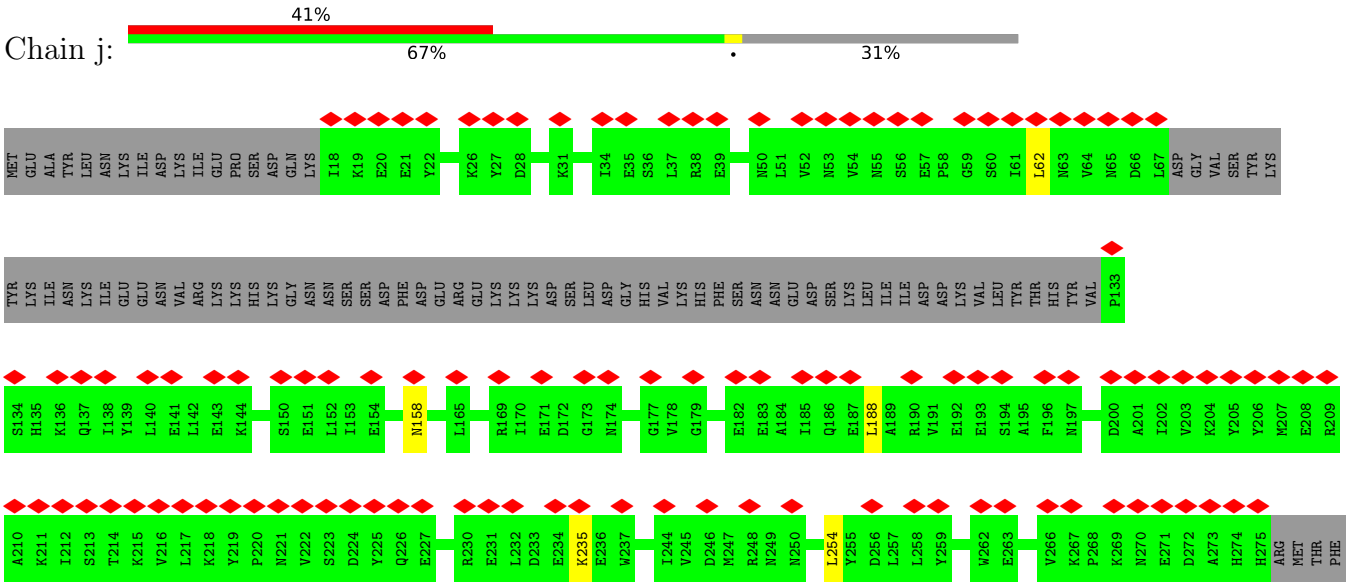
• Molecule 15: Proteasome activator PA28

Chain i:



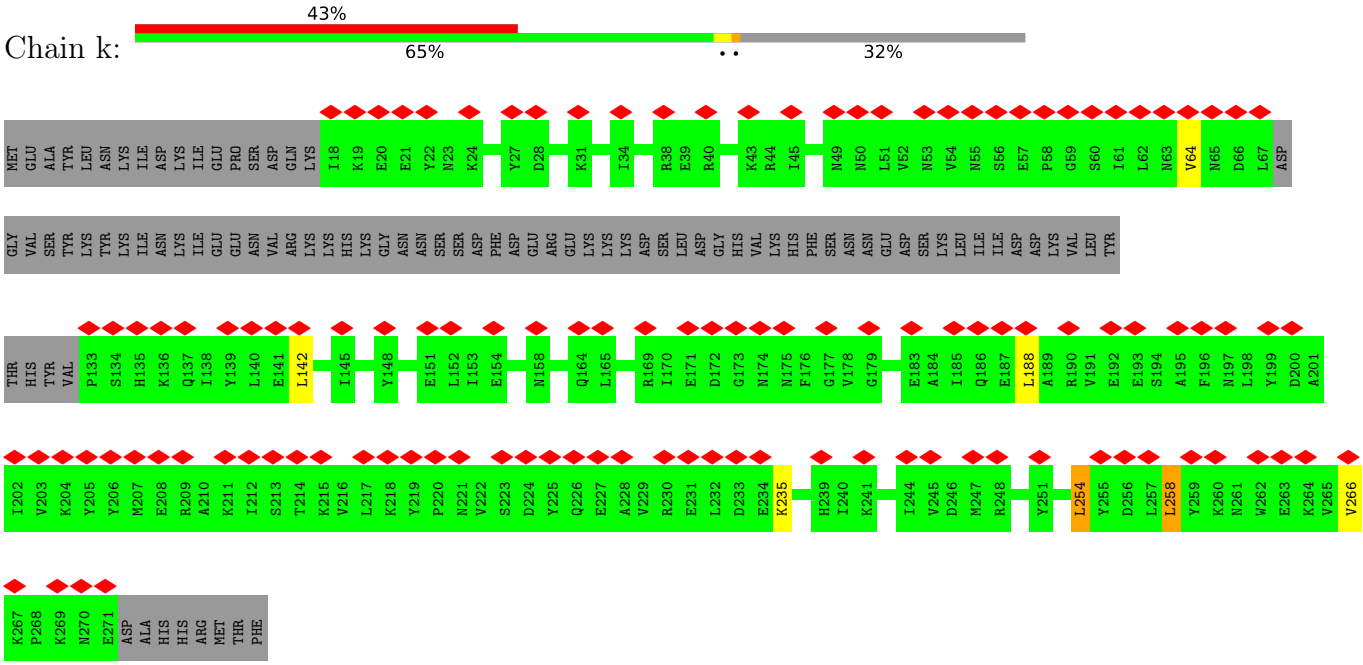
• Molecule 15: Proteasome activator PA28

Chain j:



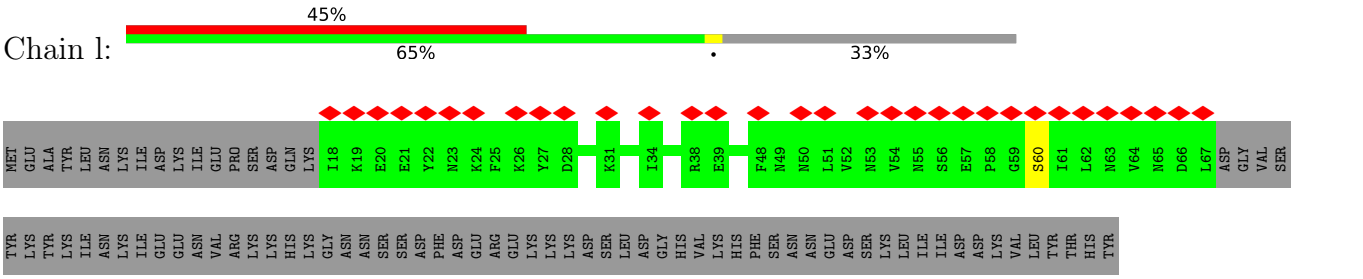
• Molecule 15: Proteasome activator PA28

Chain k:



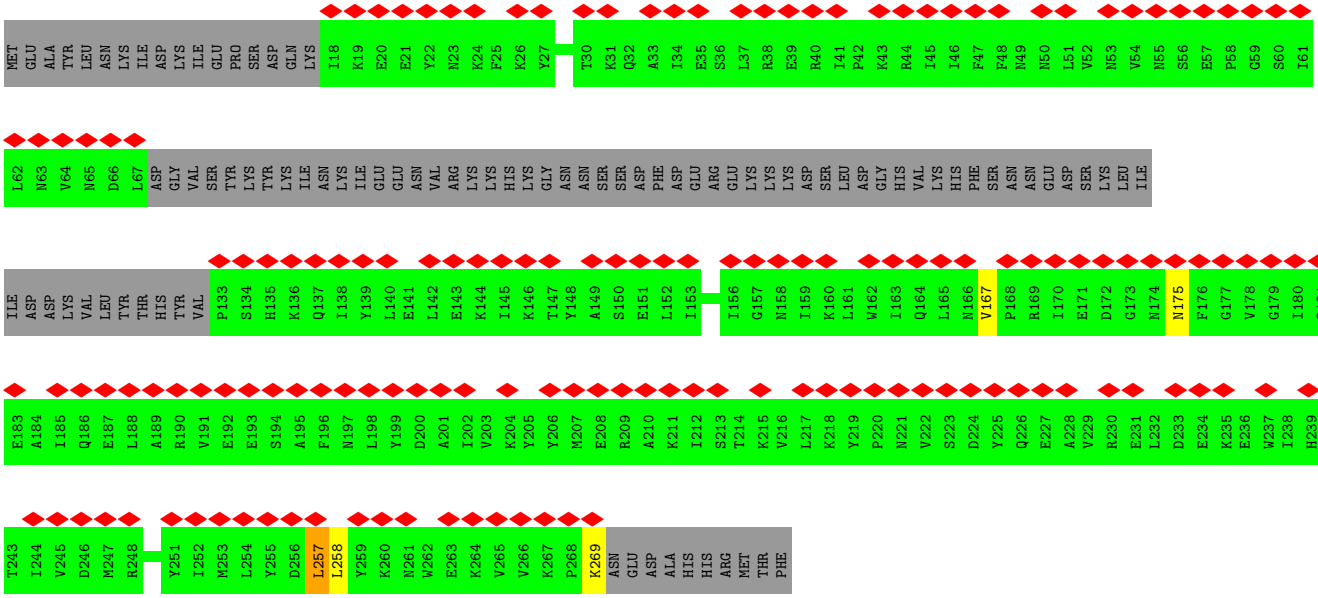
• Molecule 15: Proteasome activator PA28

Chain l:



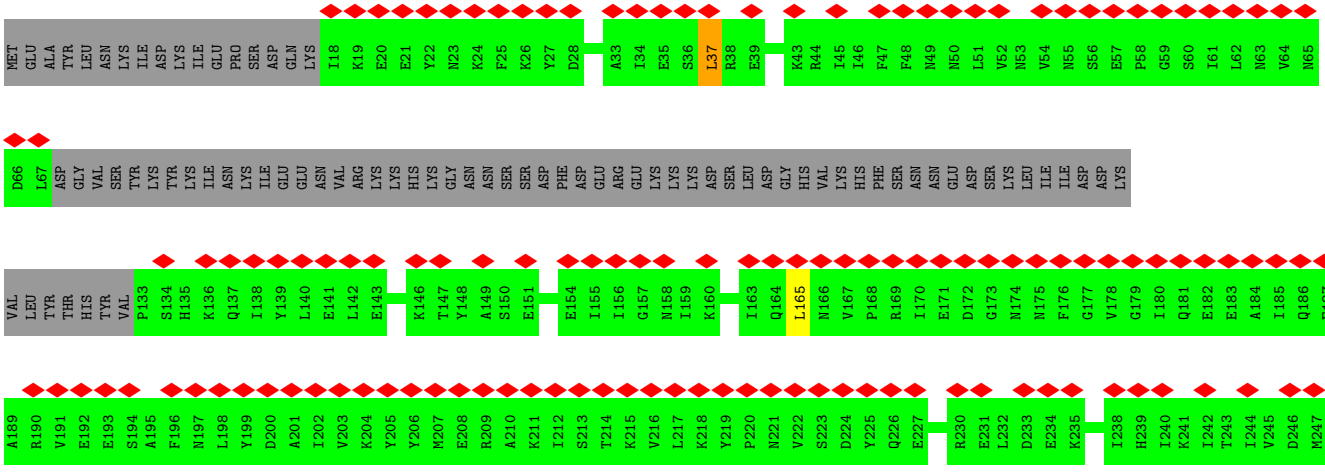
• Molecule 15: Proteasome activator PA28

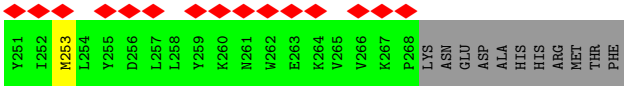
Chain m:



• Molecule 15: Proteasome activator PA28

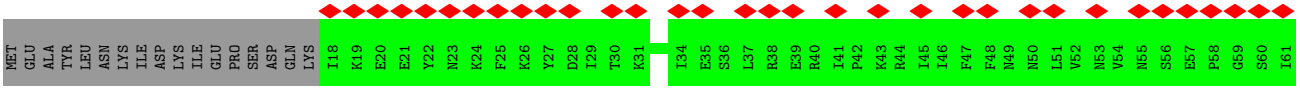
Chain n:

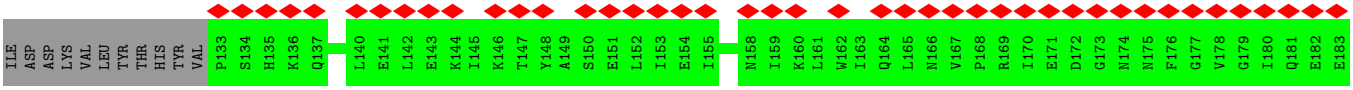


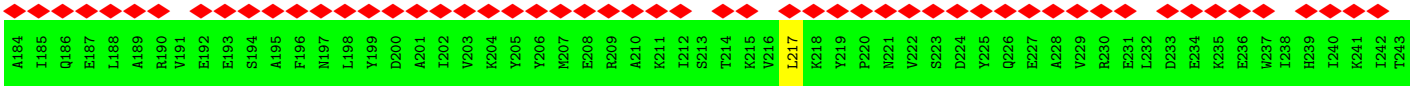


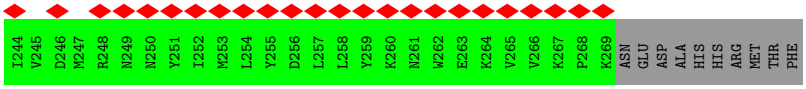
• Molecule 15: Proteasome activator PA28

Chain o:



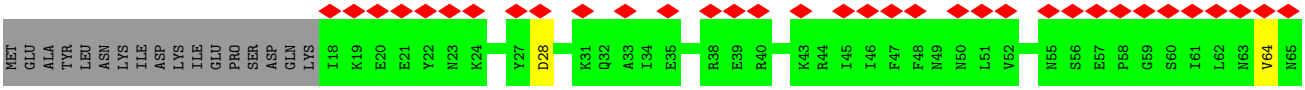


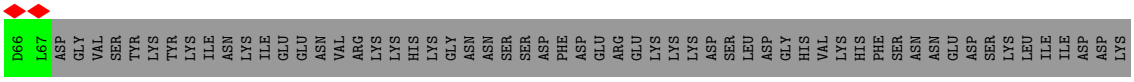


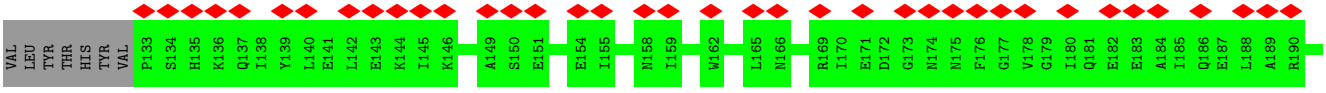


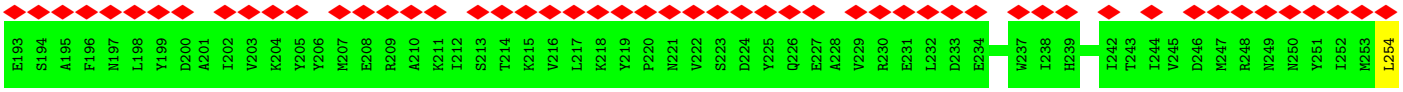
• Molecule 15: Proteasome activator PA28

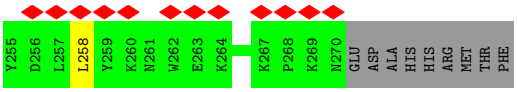
Chain p:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	27516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	29.237	Depositor
Minimum map value	-16.919	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	450.63998, 450.63998, 450.63998	wwPDB
Map dimensions	344, 344, 344	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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	0.44	0/1968	0.65	1/2652 (0.0%)
1	O	0.44	0/1968	0.65	1/2652 (0.0%)
2	B	0.44	0/1814	0.65	2/2450 (0.1%)
2	P	0.44	0/1814	0.65	2/2450 (0.1%)
3	C	0.49	0/1952	0.65	0/2643
3	Q	0.49	0/1952	0.65	0/2643
4	D	0.42	0/1824	0.66	1/2461 (0.0%)
4	R	0.42	0/1824	0.66	1/2461 (0.0%)
5	E	0.40	0/1784	0.60	0/2410
5	S	0.40	0/1784	0.60	0/2410
6	F	0.47	0/1913	0.63	2/2576 (0.1%)
6	T	0.47	0/1913	0.63	2/2576 (0.1%)
7	G	0.48	0/1947	0.67	0/2631
7	U	0.48	0/1947	0.67	0/2631
8	H	0.50	0/1559	0.66	1/2089 (0.0%)
8	V	0.50	0/1559	0.66	1/2089 (0.0%)
9	I	0.40	0/1712	0.62	0/2328
9	W	0.40	0/1712	0.62	0/2328
10	J	0.54	0/1621	0.68	1/2189 (0.0%)
10	X	0.55	0/1621	0.68	1/2189 (0.0%)
11	K	0.58	0/1649	0.64	1/2223 (0.0%)
11	Y	0.58	0/1649	0.64	1/2223 (0.0%)
12	L	0.54	0/1633	0.68	1/2202 (0.0%)
12	Z	0.54	0/1633	0.68	1/2202 (0.0%)
13	M	0.49	0/1708	0.69	2/2314 (0.1%)
13	a	0.49	0/1708	0.69	2/2314 (0.1%)
14	N	0.45	0/1882	0.65	1/2538 (0.0%)
14	b	0.45	0/1882	0.65	1/2538 (0.0%)
15	c	0.34	0/1597	0.67	1/2154 (0.0%)
15	d	0.36	0/1597	0.63	1/2154 (0.0%)
15	e	0.36	0/1605	0.68	2/2165 (0.1%)
15	f	0.35	0/1649	0.65	1/2225 (0.0%)
15	g	0.35	0/1614	0.70	3/2177 (0.1%)
15	h	0.35	0/1588	0.68	2/2143 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	i	0.34	0/1588	0.66	2/2143 (0.1%)
15	j	0.35	0/1649	0.65	1/2225 (0.0%)
15	k	0.35	0/1614	0.70	3/2177 (0.1%)
15	l	0.36	0/1588	0.68	2/2143 (0.1%)
15	m	0.34	0/1597	0.67	1/2154 (0.0%)
15	n	0.34	0/1588	0.66	2/2143 (0.1%)
15	o	0.35	0/1597	0.63	1/2154 (0.0%)
15	p	0.36	0/1605	0.68	2/2165 (0.1%)
All	All	0.44	0/72408	0.66	50/97734 (0.1%)

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	109	LEU	CA-CB-CG	9.11	136.24	115.30
14	b	109	LEU	CA-CB-CG	9.08	136.19	115.30
15	c	257	LEU	CA-CB-CG	8.81	135.57	115.30
15	m	257	LEU	CA-CB-CG	8.80	135.55	115.30
10	J	203	LEU	C-N-CA	8.02	141.74	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	242/260 (93%)	211 (87%)	31 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	242/260 (93%)	211 (87%)	31 (13%)	0	100	100
2	B	222/235 (94%)	207 (93%)	15 (7%)	0	100	100
2	P	222/235 (94%)	207 (93%)	15 (7%)	0	100	100
3	C	238/246 (97%)	217 (91%)	19 (8%)	2 (1%)	19	57
3	Q	238/246 (97%)	217 (91%)	19 (8%)	2 (1%)	19	57
4	D	225/241 (93%)	207 (92%)	18 (8%)	0	100	100
4	R	225/241 (93%)	207 (92%)	18 (8%)	0	100	100
5	E	223/256 (87%)	206 (92%)	17 (8%)	0	100	100
5	S	223/256 (87%)	206 (92%)	17 (8%)	0	100	100
6	F	234/254 (92%)	205 (88%)	29 (12%)	0	100	100
6	T	234/254 (92%)	205 (88%)	29 (12%)	0	100	100
7	G	229/252 (91%)	200 (87%)	29 (13%)	0	100	100
7	U	229/252 (91%)	200 (87%)	29 (13%)	0	100	100
8	H	189/252 (75%)	158 (84%)	30 (16%)	1 (0%)	29	66
8	V	189/252 (75%)	158 (84%)	30 (16%)	1 (0%)	29	66
9	I	217/229 (95%)	188 (87%)	27 (12%)	2 (1%)	17	54
9	W	217/229 (95%)	188 (87%)	27 (12%)	2 (1%)	17	54
10	J	199/218 (91%)	177 (89%)	22 (11%)	0	100	100
10	X	199/218 (91%)	176 (88%)	23 (12%)	0	100	100
11	K	193/195 (99%)	170 (88%)	23 (12%)	0	100	100
11	Y	193/195 (99%)	170 (88%)	23 (12%)	0	100	100
12	L	202/211 (96%)	175 (87%)	27 (13%)	0	100	100
12	Z	202/211 (96%)	175 (87%)	27 (13%)	0	100	100
13	M	209/240 (87%)	179 (86%)	29 (14%)	1 (0%)	29	66
13	a	209/240 (87%)	179 (86%)	29 (14%)	1 (0%)	29	66
14	N	220/265 (83%)	189 (86%)	31 (14%)	0	100	100
14	b	220/265 (83%)	189 (86%)	31 (14%)	0	100	100
15	c	183/279 (66%)	176 (96%)	7 (4%)	0	100	100
15	d	183/279 (66%)	177 (97%)	6 (3%)	0	100	100
15	e	184/279 (66%)	178 (97%)	6 (3%)	0	100	100
15	f	189/279 (68%)	181 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	g	185/279 (66%)	176 (95%)	9 (5%)	0	100	100
15	h	182/279 (65%)	176 (97%)	6 (3%)	0	100	100
15	i	182/279 (65%)	176 (97%)	6 (3%)	0	100	100
15	j	189/279 (68%)	181 (96%)	8 (4%)	0	100	100
15	k	185/279 (66%)	176 (95%)	9 (5%)	0	100	100
15	l	182/279 (65%)	176 (97%)	6 (3%)	0	100	100
15	m	183/279 (66%)	176 (96%)	7 (4%)	0	100	100
15	n	182/279 (65%)	176 (97%)	6 (3%)	0	100	100
15	o	183/279 (66%)	177 (97%)	6 (3%)	0	100	100
15	p	184/279 (66%)	178 (97%)	6 (3%)	0	100	100
All	All	8660/10614 (82%)	7857 (91%)	791 (9%)	12 (0%)	54	83

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	76	PHE
8	V	76	PHE
3	C	210	ILE
3	Q	210	ILE
9	I	206	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/231 (94%)	213 (98%)	4 (2%)	59	77
1	O	217/231 (94%)	213 (98%)	4 (2%)	59	77
2	B	196/205 (96%)	196 (100%)	0	100	100
2	P	196/205 (96%)	196 (100%)	0	100	100
3	C	208/213 (98%)	206 (99%)	2 (1%)	76	86
3	Q	208/213 (98%)	206 (99%)	2 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	194/207 (94%)	192 (99%)	2 (1%)	76 86
4	R	194/207 (94%)	192 (99%)	2 (1%)	76 86
5	E	195/223 (87%)	194 (100%)	1 (0%)	88 94
5	S	195/223 (87%)	194 (100%)	1 (0%)	88 94
6	F	211/227 (93%)	211 (100%)	0	100 100
6	T	211/227 (93%)	211 (100%)	0	100 100
7	G	212/229 (93%)	212 (100%)	0	100 100
7	U	212/229 (93%)	212 (100%)	0	100 100
8	H	173/231 (75%)	168 (97%)	5 (3%)	42 67
8	V	173/231 (75%)	168 (97%)	5 (3%)	42 67
9	I	185/194 (95%)	184 (100%)	1 (0%)	88 94
9	W	185/194 (95%)	184 (100%)	1 (0%)	88 94
10	J	178/191 (93%)	178 (100%)	0	100 100
10	X	178/191 (93%)	178 (100%)	0	100 100
11	K	174/174 (100%)	171 (98%)	3 (2%)	60 78
11	Y	174/174 (100%)	171 (98%)	3 (2%)	60 78
12	L	169/176 (96%)	168 (99%)	1 (1%)	86 92
12	Z	169/176 (96%)	168 (99%)	1 (1%)	86 92
13	M	189/216 (88%)	188 (100%)	1 (0%)	88 94
13	a	189/216 (88%)	188 (100%)	1 (0%)	88 94
14	N	201/239 (84%)	200 (100%)	1 (0%)	88 94
14	b	201/239 (84%)	201 (100%)	0	100 100
15	c	174/261 (67%)	169 (97%)	5 (3%)	42 67
15	d	174/261 (67%)	174 (100%)	0	100 100
15	e	175/261 (67%)	173 (99%)	2 (1%)	73 85
15	f	179/261 (69%)	175 (98%)	4 (2%)	52 72
15	g	176/261 (67%)	170 (97%)	6 (3%)	37 64
15	h	173/261 (66%)	169 (98%)	4 (2%)	50 72
15	i	173/261 (66%)	170 (98%)	3 (2%)	60 78
15	j	179/261 (69%)	175 (98%)	4 (2%)	52 72
15	k	176/261 (67%)	170 (97%)	6 (3%)	37 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	l	173/261 (66%)	169 (98%)	4 (2%)	50 72
15	m	174/261 (67%)	169 (97%)	5 (3%)	42 67
15	n	173/261 (66%)	170 (98%)	3 (2%)	60 78
15	o	174/261 (67%)	174 (100%)	0	100 100
15	p	175/261 (67%)	173 (99%)	2 (1%)	73 85
All	All	7852/9566 (82%)	7763 (99%)	89 (1%)	74 85

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	i	253	MET
15	l	258	LEU
15	j	158	ASN
15	k	254	LEU
15	m	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
13	a	86	GLN
15	h	158	ASN
12	Z	40	ASN
13	a	200	ASN
15	d	250	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

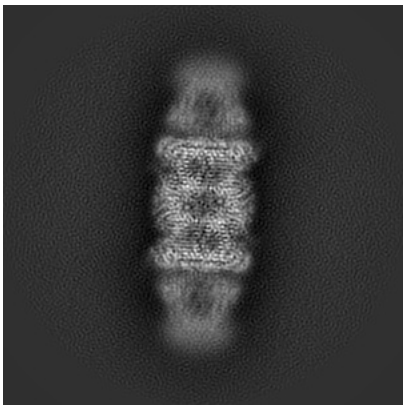
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9257. These allow visual inspection of the internal detail of the map and identification of artifacts.

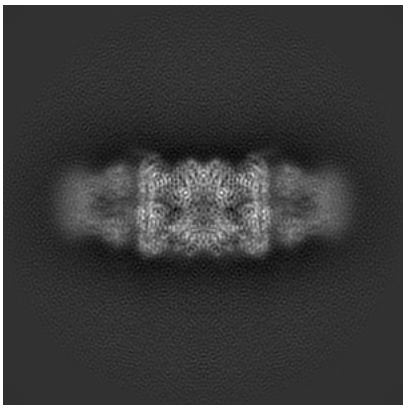
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

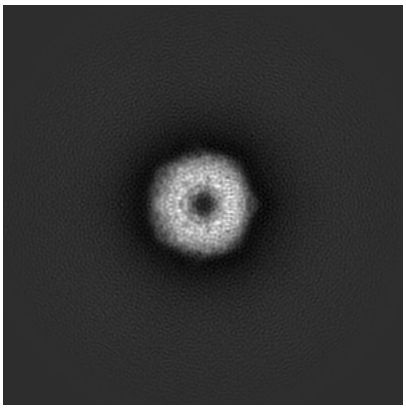
6.1.1 Primary map



X

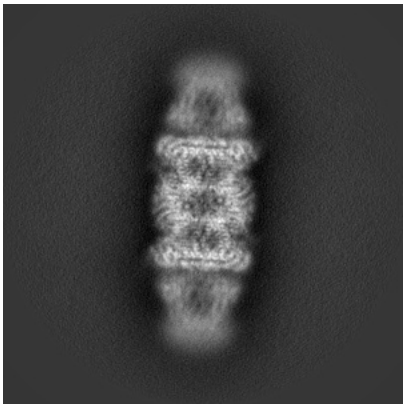


Y

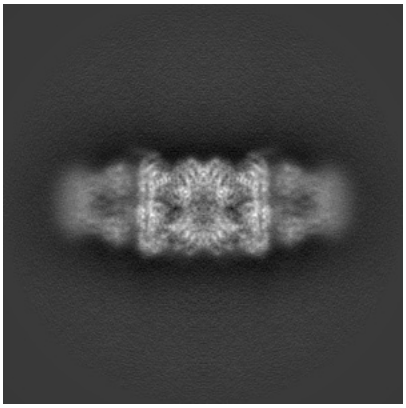


Z

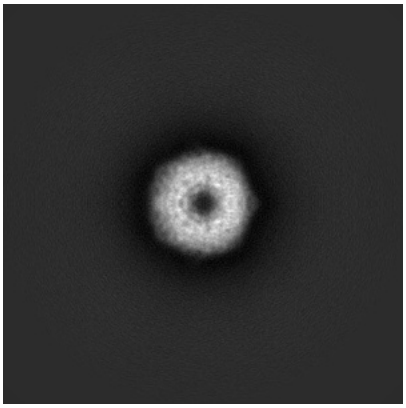
6.1.2 Raw map



X



Y

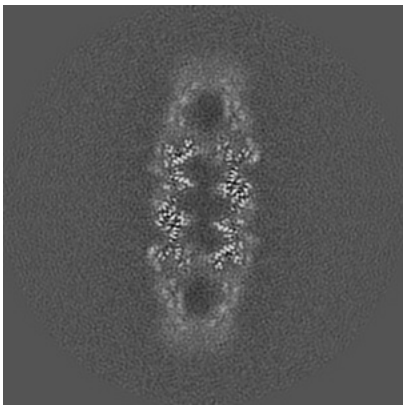


Z

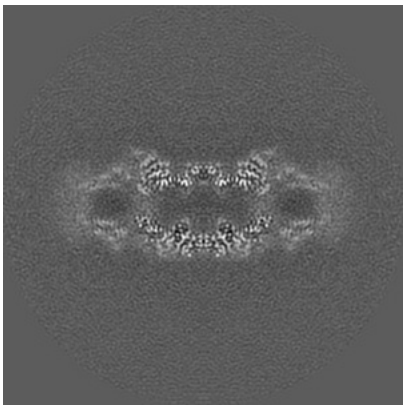
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

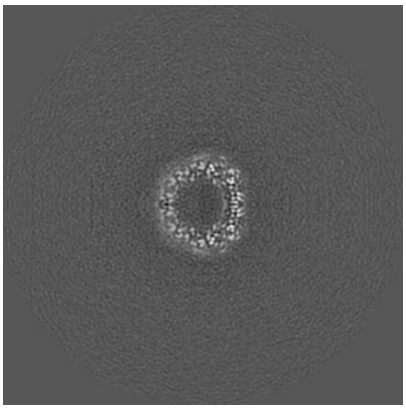
6.2.1 Primary map



X Index: 172

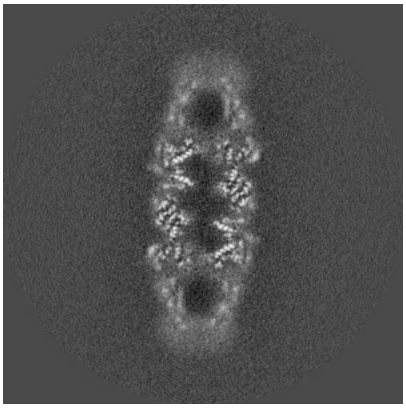


Y Index: 172

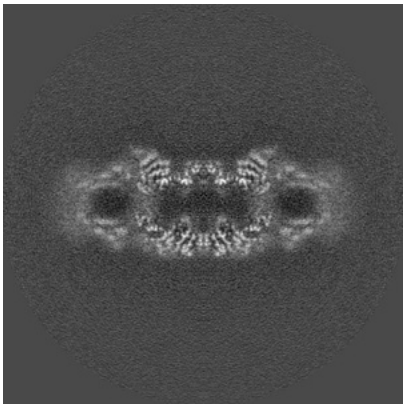


Z Index: 172

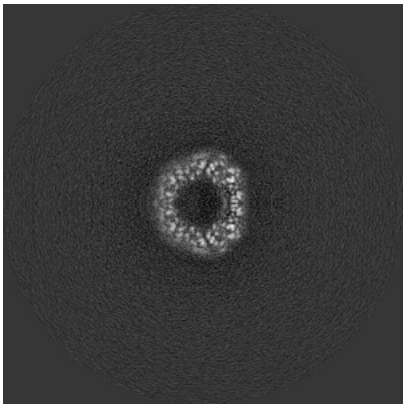
6.2.2 Raw map



X Index: 172



Y Index: 172

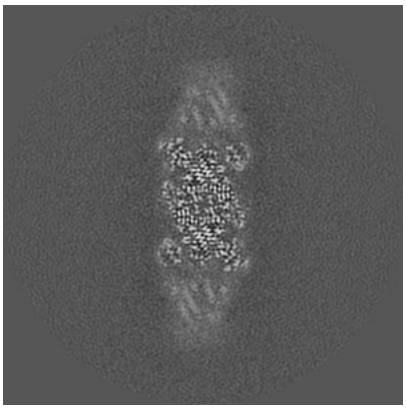


Z Index: 172

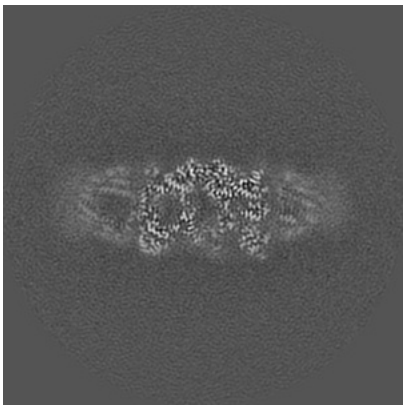
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

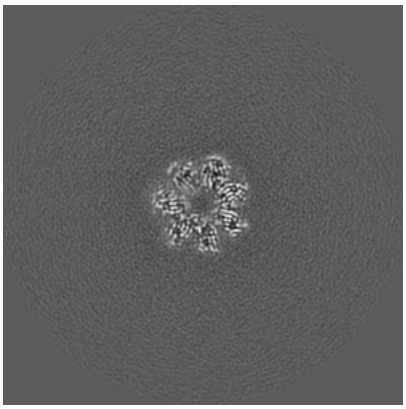
6.3.1 Primary map



X Index: 193

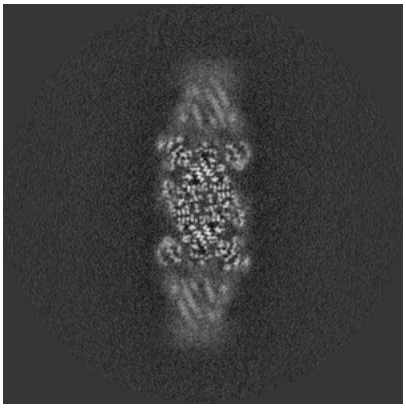


Y Index: 156

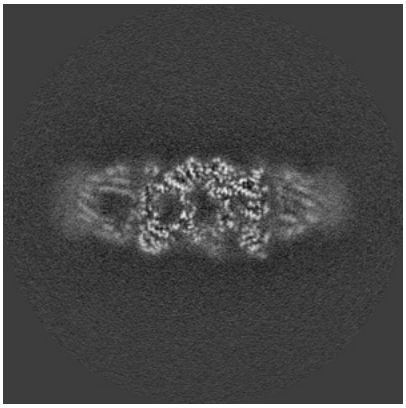


Z Index: 158

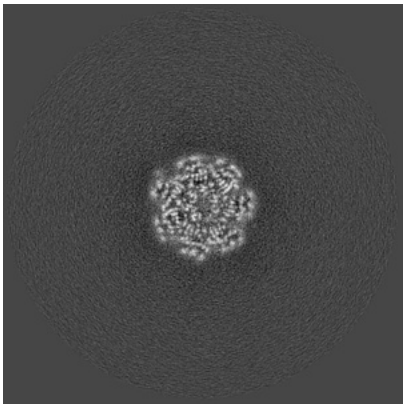
6.3.2 Raw map



X Index: 193



Y Index: 156

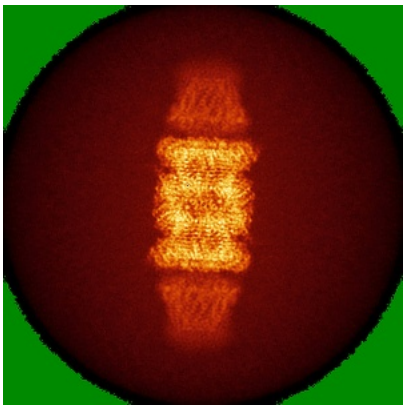


Z Index: 128

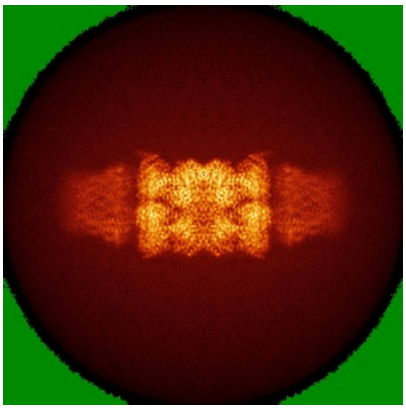
The images above show the largest variance slices of the map in three orthogonal directions.

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

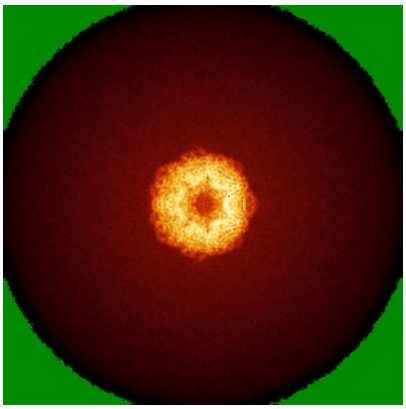
6.4.1 Primary map



X

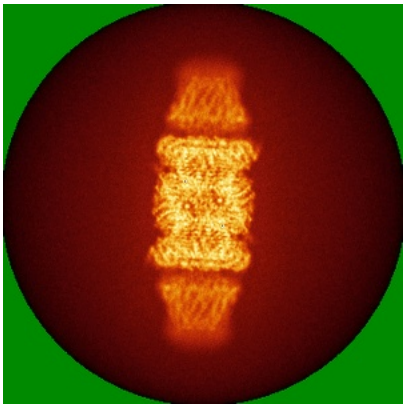


Y

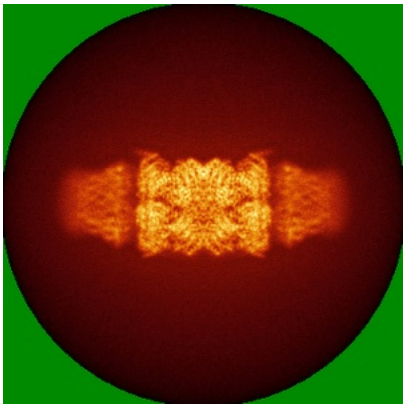


Z

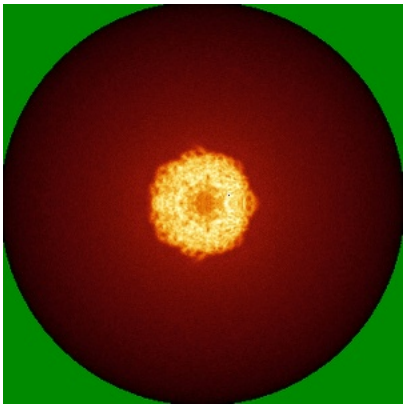
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

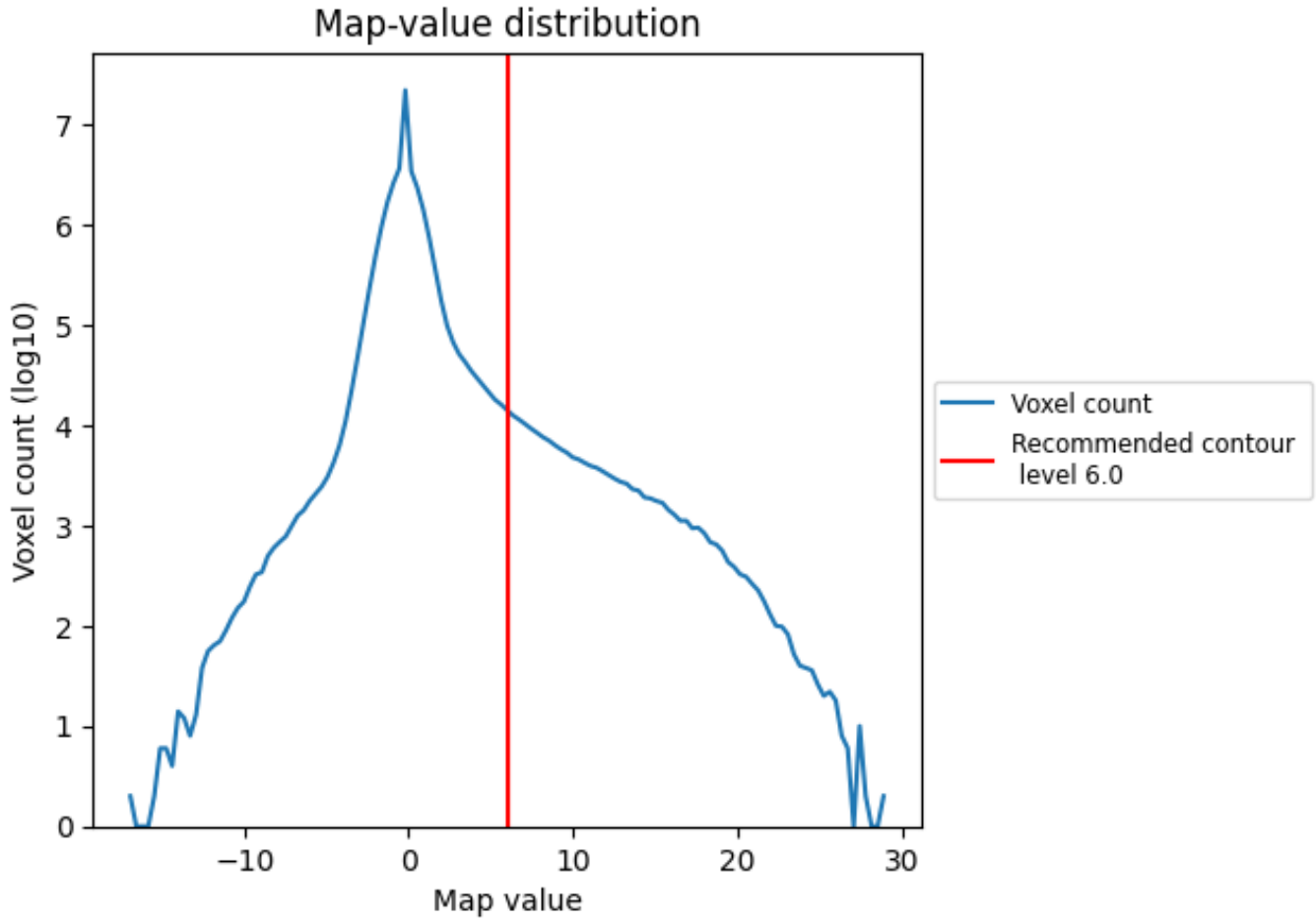
6.6 Mask visualisation (i)

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

7 Map analysis

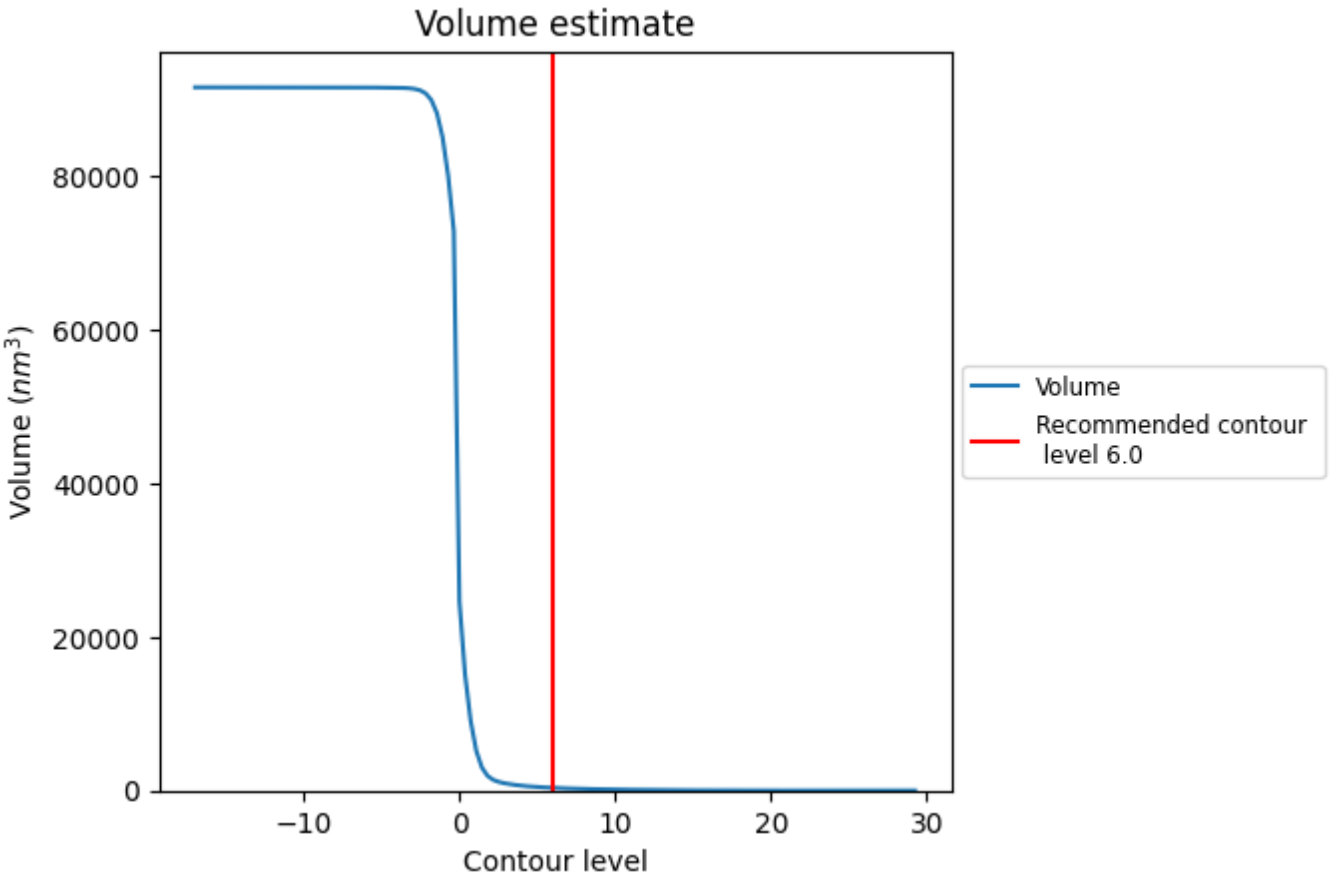
This section contains the results of statistical analysis of the map.

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.

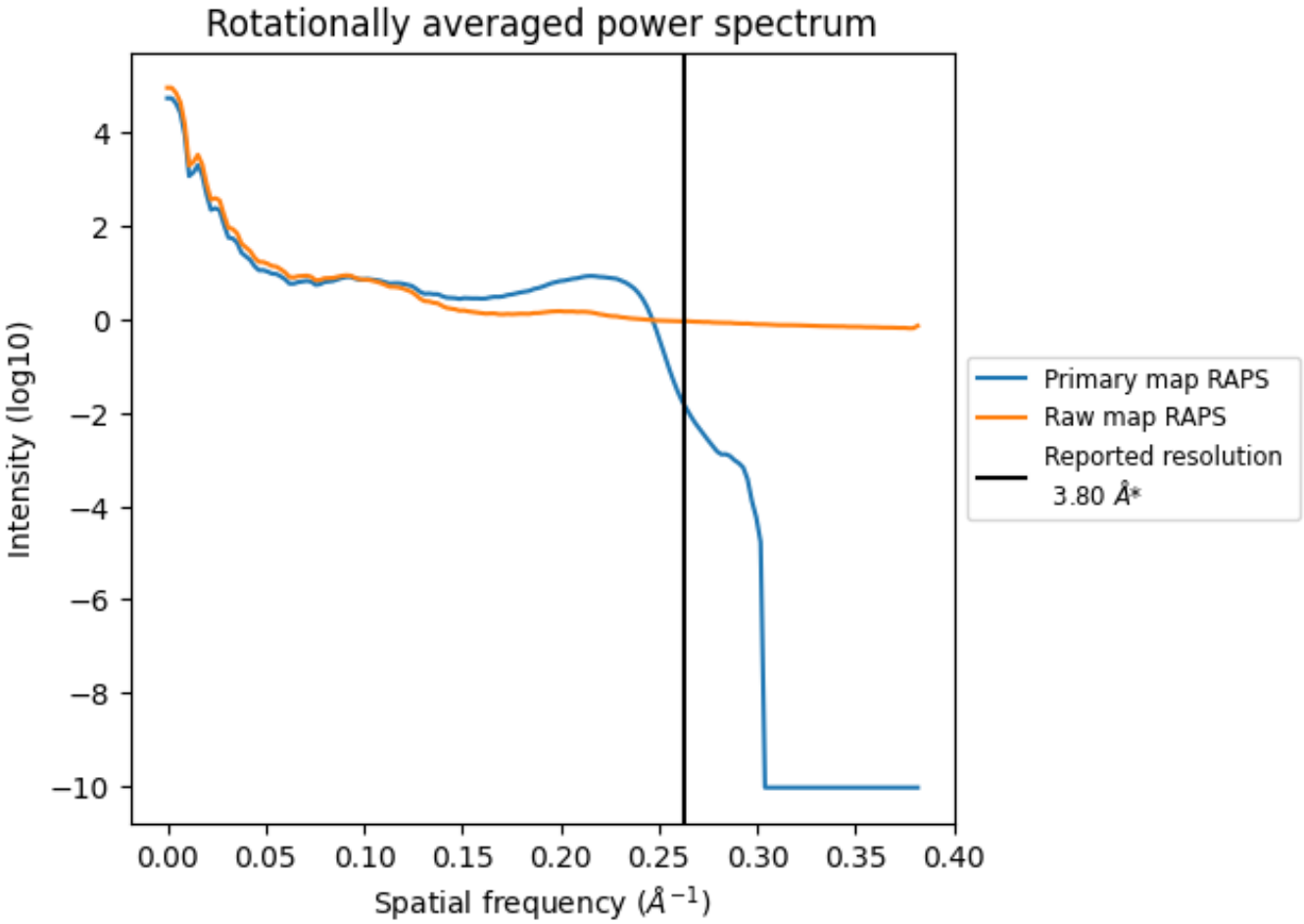
7.2 Volume estimate (i)



The volume at the recommended contour level is 355 nm^3; this corresponds to an approximate mass of 321 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)

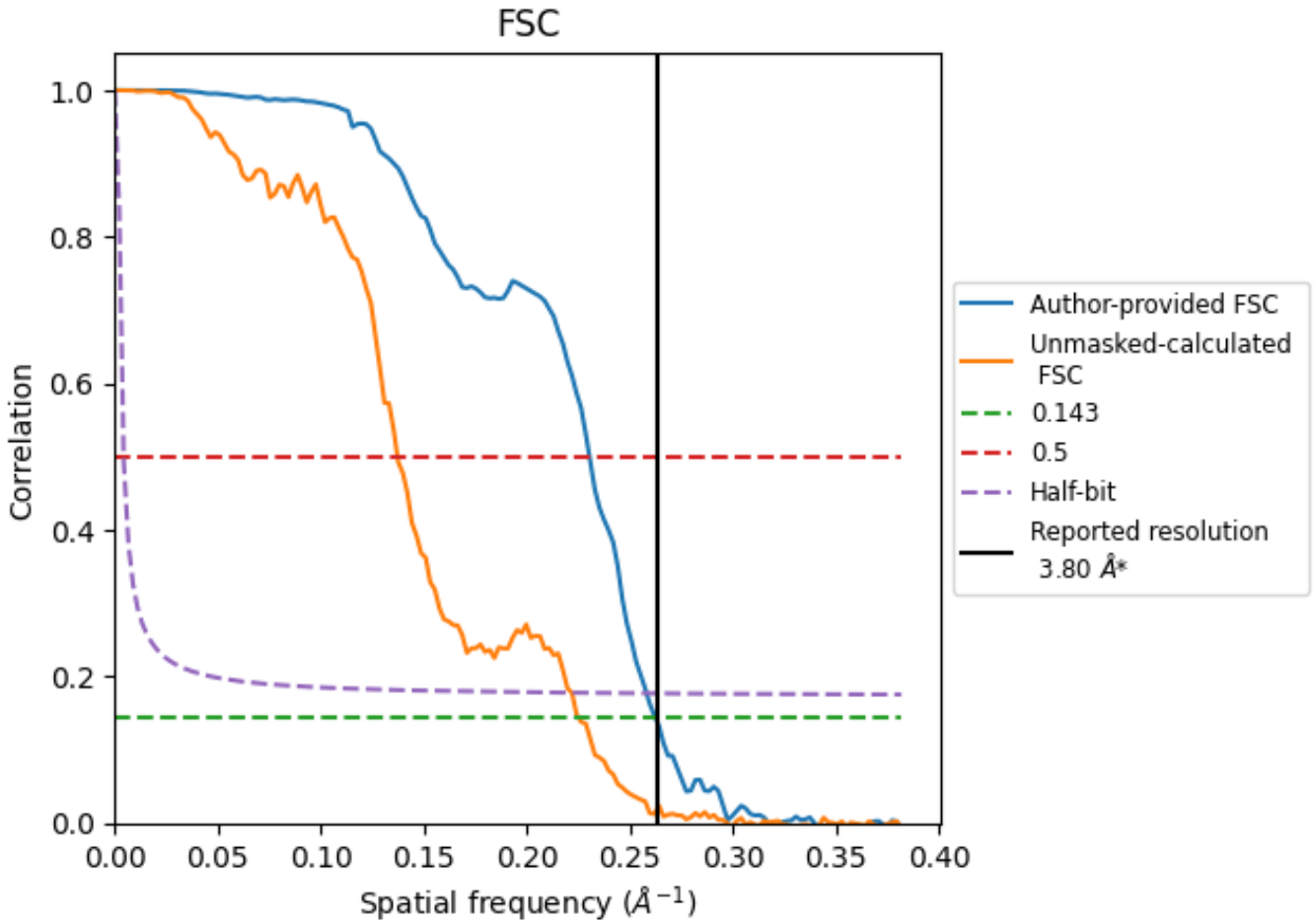


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

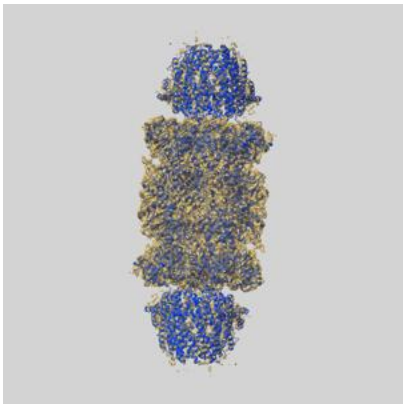
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.34	3.87
Unmasked-calculated*	4.44	7.29	4.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.8 by more than 10 %

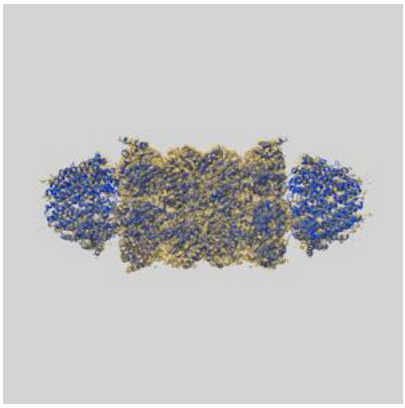
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9257 and PDB model 6MUV. Per-residue inclusion information can be found in section 3 on page 9.

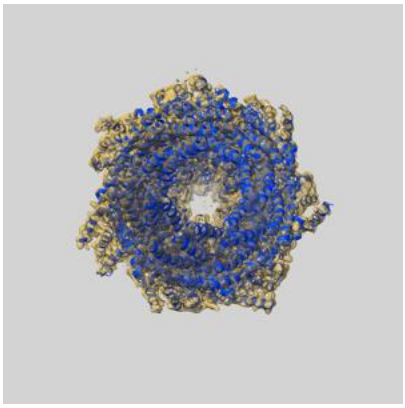
9.1 Map-model overlay



X



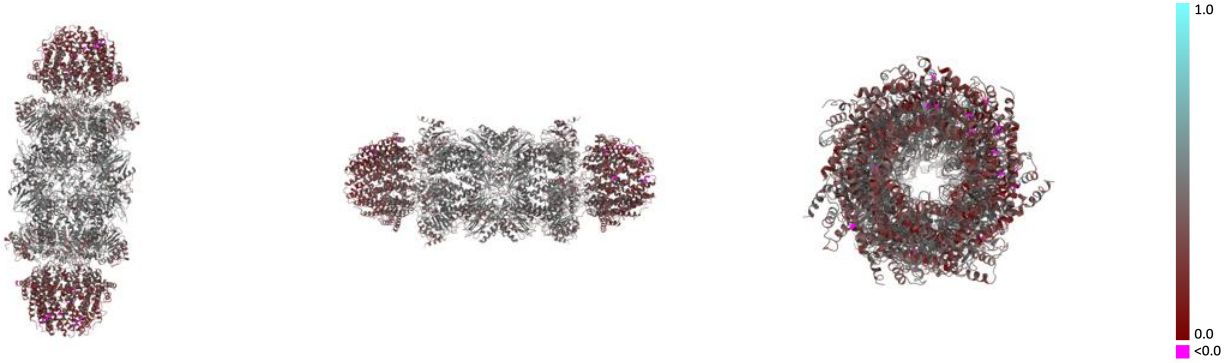
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

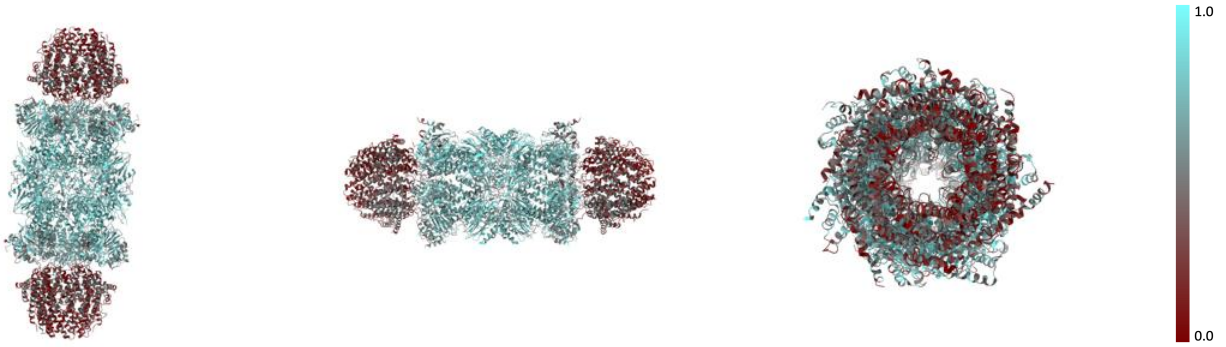
9.2 Q-score mapped to coordinate model



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.

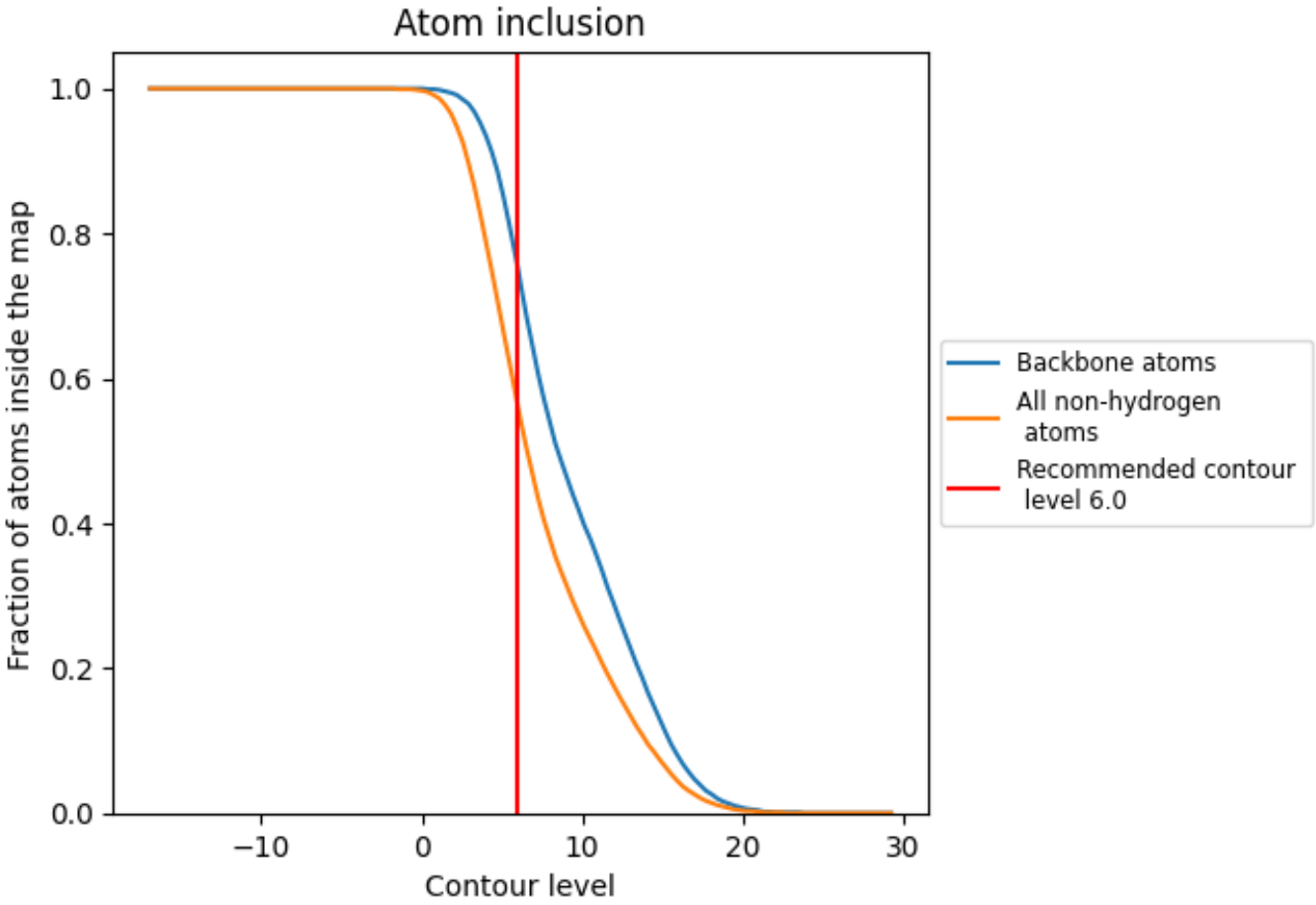
9.3 Atom inclusion mapped to coordinate model



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 (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 56% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.3970
A	0.6380	0.4320
B	0.6650	0.4380
C	0.6910	0.4350
D	0.6430	0.4280
E	0.6060	0.4220
F	0.6680	0.4400
G	0.6820	0.4430
H	0.6790	0.4250
I	0.6590	0.4200
J	0.7480	0.4560
K	0.7770	0.4560
L	0.7520	0.4530
M	0.7290	0.4620
N	0.6860	0.4520
O	0.6370	0.4320
P	0.6690	0.4380
Q	0.6900	0.4360
R	0.6420	0.4270
S	0.6040	0.4200
T	0.6690	0.4390
U	0.6810	0.4430
V	0.6750	0.4240
W	0.6580	0.4220
X	0.7490	0.4570
Y	0.7750	0.4560
Z	0.7550	0.4520
a	0.7260	0.4600
b	0.6890	0.4520
c	0.2330	0.2640
d	0.2060	0.2730
e	0.2870	0.2960
f	0.3380	0.3290
g	0.3350	0.3340
h	0.3200	0.3230

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Chain	Atom inclusion	Q-score
i	0.2470	0.2860
j	0.3380	0.3300
k	0.3420	0.3320
l	0.3200	0.3240
m	0.2320	0.2800
n	0.2410	0.2880
o	0.2140	0.2740
p	0.2800	0.2950