wwPDB EM Validation Summary Report

Sep 16, 2024 – 05:33 pm BST

PDB ID	:	8RVO
EMDB ID	:	EMD-19527
Title	:	Proteasomal late precursor complex from pre1-1, state 1
Authors	:	Mark, E.; Ramos, P.C.; Kayser, F.; Hoeckendorff, J.; Dohmen, R.J.; Wendler, P.
Deposited on	:	2024-02-01
Resolution	:	2.69 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:

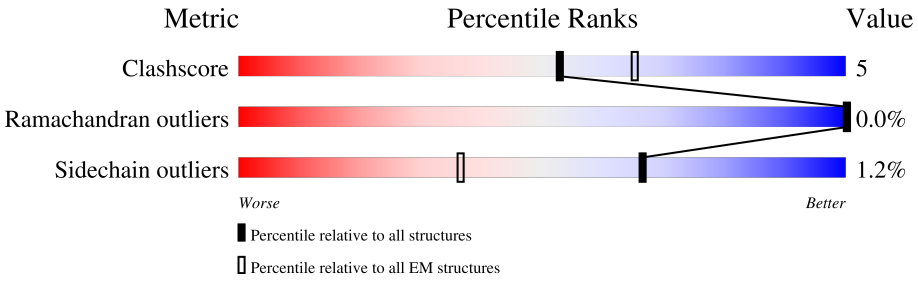
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.69 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	241	21% 75% 11% • 13%
1	M	241	• 74% 12% • 13%
2	2	266	8% 72% 12% 16%
2	N	266	• 71% 13% 16%
3	3	148	• 84% 11% •
3	6	148	• 79% 18% •
4	4	276	6% 77% 9% 13%
4	7	276	40% 73% 14% 13%

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Mol	Chain	Length	Quality of chain
5	5	267	81% 11% 9%
5	8	267	25% 67% 26% 7%
6	A	252	8% 80% 15%
6	O	252	13% 83% 12%
7	B	250	92% 8%
7	P	250	5% 87% 12%
8	C	258	5% 80% 11% 9%
8	Q	258	14% 78% 15% 6%
9	D	254	7% 82% 15%
9	R	254	12% 78% 17% 5%
10	E	260	83% 13%
10	S	260	17% 81% 14%
11	F	234	88% 12%
11	T	234	10% 89% 11%
12	G	288	8% 75% 9% 15%
12	U	288	12% 75% 10% 15%
13	H	215	80% 15% 5%
13	V	215	83% 12% 5%
14	I	261	8% 75% 8% 16%
14	W	261	74% 8% 19%
15	J	205	8% 79% 11% 9%
15	X	205	7% 82% 10% 8%
16	K	212	10% 78% 12% 10%
16	Y	212	11% 73% 17% 10%
17	L	287	8% 77% 11% 11%

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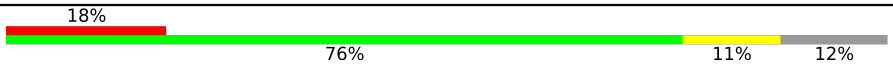
Mol	Chain	Length	Quality of chain
17	Z	287	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 60650 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 Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	210	Total	C	N	O	S	0	0
			1663	1058	286	315	4		
1	M	210	Total	C	N	O	S	0	0
			1663	1058	286	315	4		

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	224	Total	C	N	O	S	0	0
			1753	1108	300	338	7		
2	N	223	Total	C	N	O	S	0	0
			1745	1104	299	335	7		

- Molecule 3 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	142	Total	C	N	O	S	0	0
			1133	698	200	228	7		
3	6	143	Total	C	N	O	S	0	0
			1139	701	201	230	7		

- Molecule 4 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	239	Total	C	N	O	S	0	0
			1861	1211	288	349	13		
4	7	241	Total	C	N	O	S	0	0
			1879	1222	292	352	13		

- Molecule 5 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	244	Total	C	N	O	S	0	0
			1980	1285	320	367	8		
5	8	249	Total	C	N	O	S	0	0
			2025	1315	323	380	7		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	241	Total	C	N	O	S	0	0
			1900	1210	319	363	8		
6	O	241	Total	C	N	O	S	0	0
			1900	1210	319	363	8		

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	249	Total	C	N	O	S	0	0
			1906	1213	314	375	4		
7	P	250	Total	C	N	O	S	0	0
			1914	1219	315	376	4		

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	236	Total	C	N	O	S	0	0
			1856	1176	312	365	3		
8	Q	243	Total	C	N	O	S	0	0
			1900	1199	320	378	3		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	245	Total	C	N	O	S	0	0
			1923	1199	337	383	4		
9	R	242	Total	C	N	O	S	0	0
			1899	1186	333	376	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	250	Total	C	N	O	S	0	0
			1933	1209	325	391	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	249	Total	C	N	O	S	0	0
			1924	1204	324	388	8		

- Molecule 11 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		
11	T	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		

- Molecule 12 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	245	Total	C	N	O	S	0	0
			1900	1208	329	359	4		
12	U	244	Total	C	N	O	S	0	0
			1892	1205	328	355	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	207	LYS	ASN	conflict	UNP P21242
U	208	LYS	ASN	conflict	UNP P21242

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	205	Total	C	N	O	S	0	0
			1575	996	261	311	7		
13	V	205	Total	C	N	O	S	0	0
			1575	996	261	311	7		

- Molecule 14 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	218	Total	C	N	O	S	0	0
			1649	1035	288	320	6		
14	W	212	Total	C	N	O	S	0	0
			1604	1008	280	310	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	191	THR	LEU	conflict	UNP P25043
I	192	PRO	THR	conflict	UNP P25043
I	193	THR	-	insertion	UNP P25043
W	191	THR	LEU	conflict	UNP P25043
W	192	PRO	THR	conflict	UNP P25043
W	193	THR	-	insertion	UNP P25043

- Molecule 15 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	186	Total	C	N	O	S	0	0
			1452	937	234	273	8		
15	X	188	Total	C	N	O	S	0	0
			1458	939	236	275	8		

- Molecule 16 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	191	Total	C	N	O	S	0	0
			1532	973	260	294	5		
16	Y	190	Total	C	N	O	S	0	0
			1529	975	259	290	5		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	engineered mutation	UNP P22141
K	199	ASP	-	expression tag	UNP P22141
K	200	TYR	-	expression tag	UNP P22141
K	201	LYS	-	expression tag	UNP P22141
K	202	ASP	-	expression tag	UNP P22141
K	203	ASP	-	expression tag	UNP P22141
K	204	ASP	-	expression tag	UNP P22141
K	205	ASP	-	expression tag	UNP P22141
K	206	LYS	-	expression tag	UNP P22141
K	207	HIS	-	expression tag	UNP P22141
K	208	HIS	-	expression tag	UNP P22141
K	209	HIS	-	expression tag	UNP P22141
K	210	HIS	-	expression tag	UNP P22141
K	211	HIS	-	expression tag	UNP P22141
K	212	HIS	-	expression tag	UNP P22141
Y	142	PHE	SER	engineered mutation	UNP P22141
Y	199	ASP	-	expression tag	UNP P22141

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	200	TYR	-	expression tag	UNP P22141
Y	201	LYS	-	expression tag	UNP P22141
Y	202	ASP	-	expression tag	UNP P22141
Y	203	ASP	-	expression tag	UNP P22141
Y	204	ASP	-	expression tag	UNP P22141
Y	205	ASP	-	expression tag	UNP P22141
Y	206	LYS	-	expression tag	UNP P22141
Y	207	HIS	-	expression tag	UNP P22141
Y	208	HIS	-	expression tag	UNP P22141
Y	209	HIS	-	expression tag	UNP P22141
Y	210	HIS	-	expression tag	UNP P22141
Y	211	HIS	-	expression tag	UNP P22141
Y	212	HIS	-	expression tag	UNP P22141

- Molecule 17 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	254	Total	C	N	O	S	0	0
			1969	1248	338	374	9		
17	Z	252	Total	C	N	O	S	0	0
			1958	1241	337	371	9		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	1	43	Total	O	0
			43	43	
18	2	26	Total	O	0
			26	26	
18	3	12	Total	O	0
			12	12	
18	4	27	Total	O	0
			27	27	
18	5	25	Total	O	0
			25	25	
18	6	19	Total	O	0
			19	19	
18	7	43	Total	O	0
			43	43	
18	8	45	Total	O	0
			45	45	
18	A	36	Total	O	0
			36	36	

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Mol	Chain	Residues	Atoms	AltConf
18	B	28	Total O 28 28	0
18	C	26	Total O 26 26	0
18	D	40	Total O 40 40	0
18	E	28	Total O 28 28	0
18	F	29	Total O 29 29	0
18	G	34	Total O 34 34	0
18	H	21	Total O 21 21	0
18	I	29	Total O 29 29	0
18	J	17	Total O 17 17	0
18	K	24	Total O 24 24	0
18	L	31	Total O 31 31	0
18	M	24	Total O 24 24	0
18	N	29	Total O 29 29	0
18	O	40	Total O 40 40	0
18	P	30	Total O 30 30	0
18	Q	28	Total O 28 28	0
18	R	36	Total O 36 36	0
18	S	43	Total O 43 43	0
18	T	44	Total O 44 44	0
18	U	56	Total O 56 56	0
18	V	23	Total O 23 23	0

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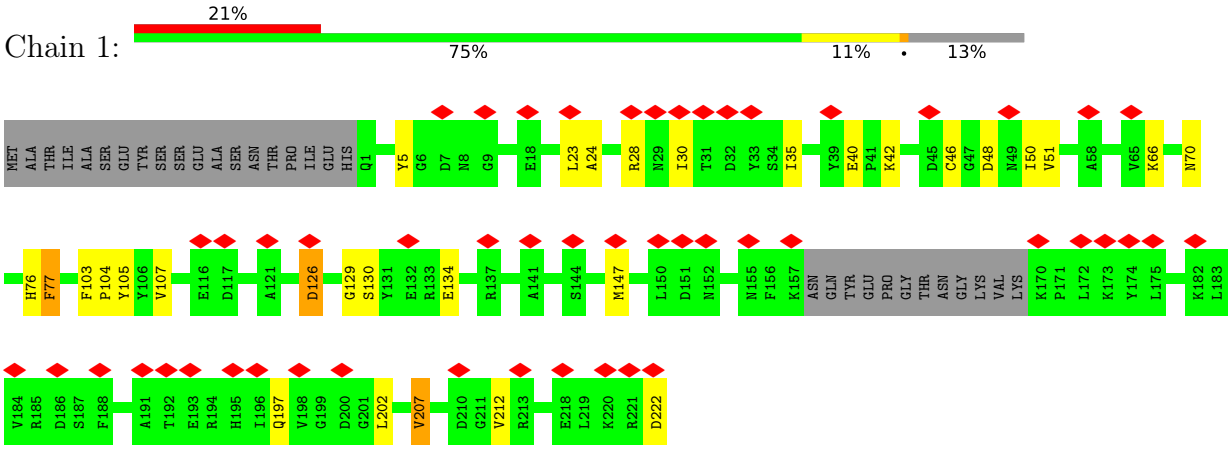
Mol	Chain	Residues	Atoms	AltConf
18	W	28	Total O 28 28	0
18	X	24	Total O 24 24	0
18	Y	33	Total O 33 33	0
18	Z	36	Total O 36 36	0

3 Residue-property plots (i)

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

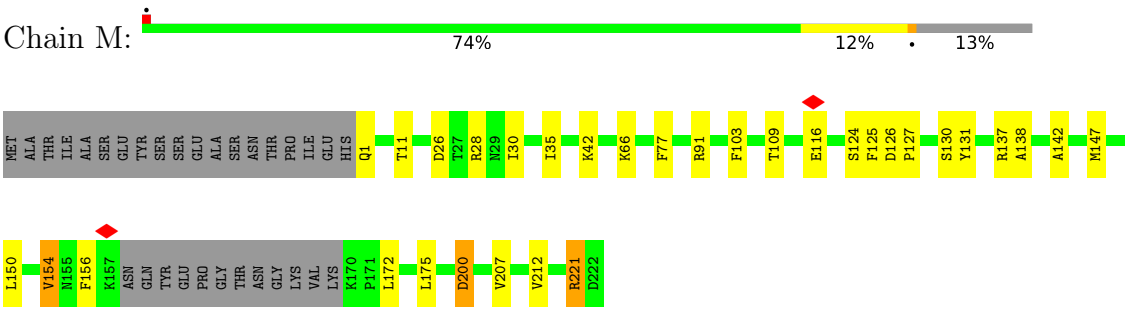
• Molecule 1: Proteasome subunit beta type-6

Chain 1:



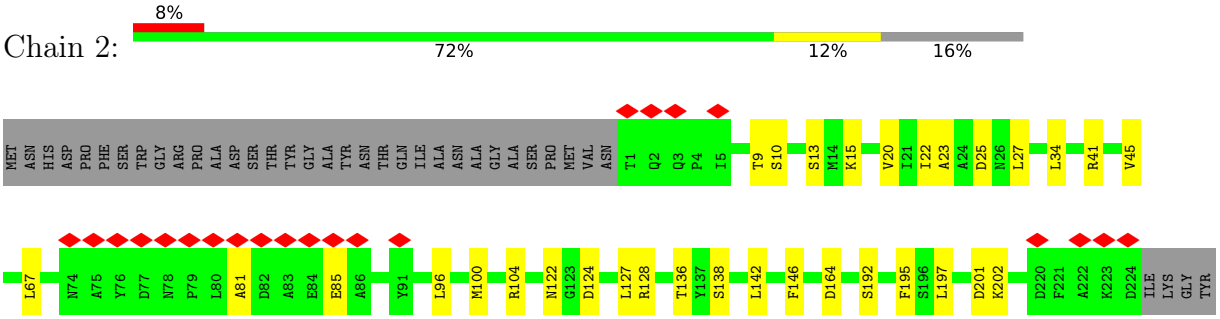
• Molecule 1: Proteasome subunit beta type-6

Chain M:



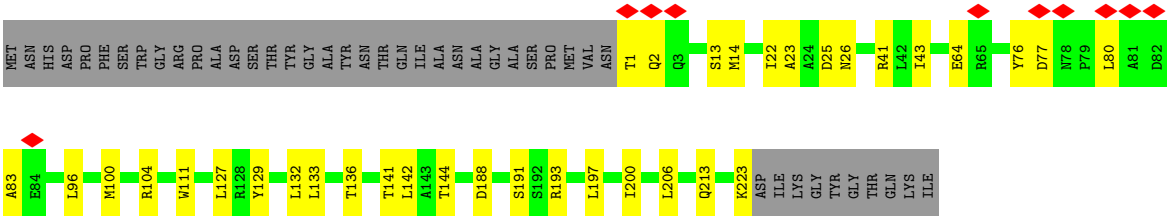
• Molecule 2: Proteasome subunit beta type-7

Chain 2:



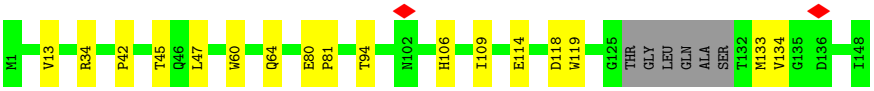
• Molecule 2: Proteasome subunit beta type-7

Chain N:



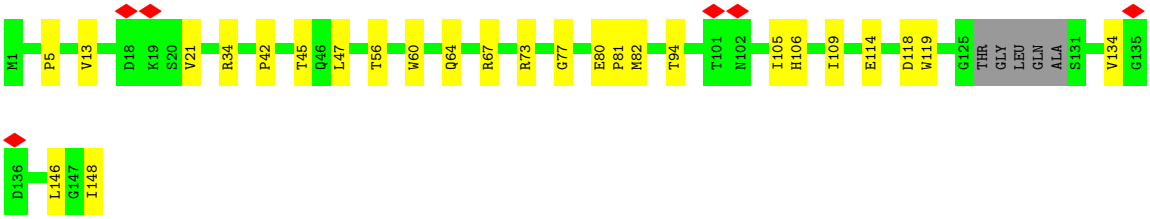
• Molecule 3: Proteasome maturation factor UMP1

Chain 3:



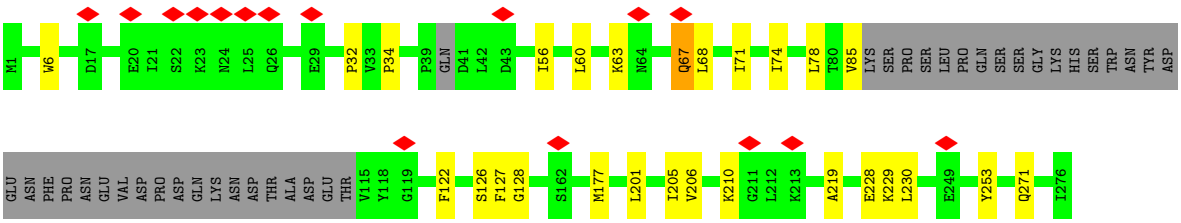
• Molecule 3: Proteasome maturation factor UMP1

Chain 6:



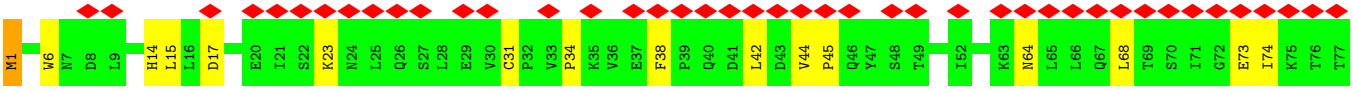
• Molecule 4: Proteasome chaperone 1

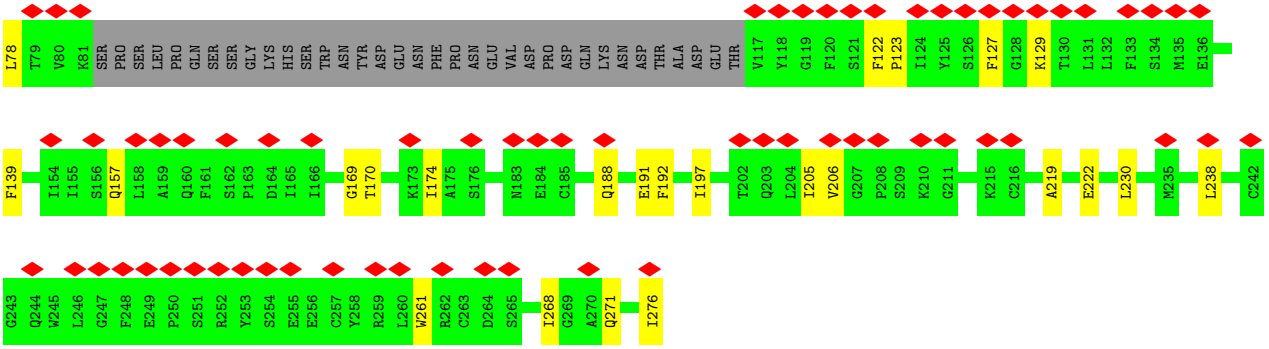
Chain 4:



• Molecule 4: Proteasome chaperone 1

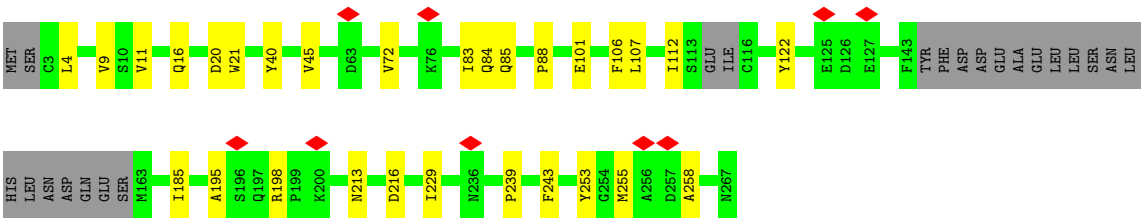
Chain 7:





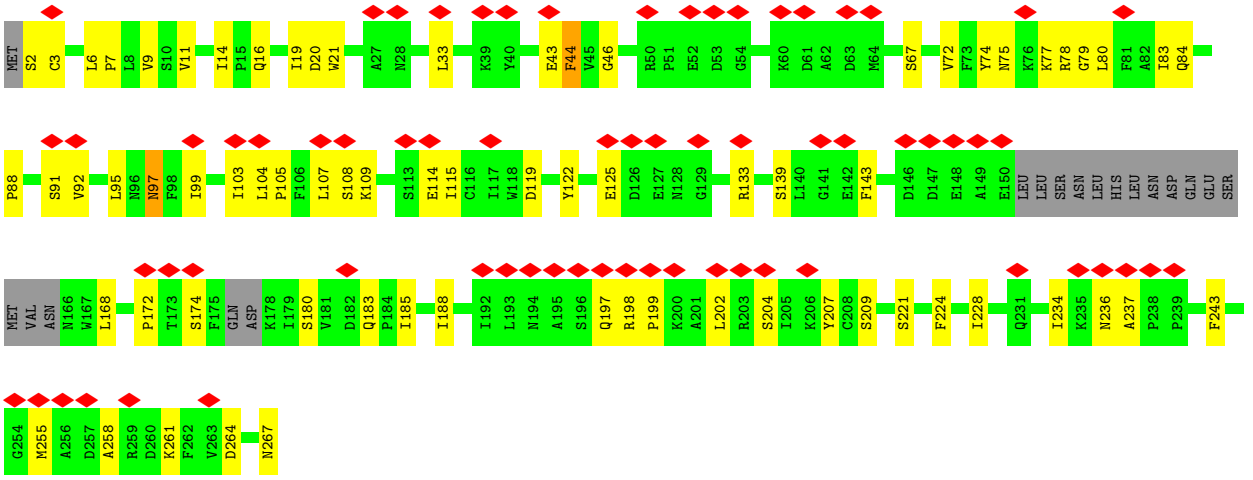
• Molecule 5: Proteasome assembly chaperone 2

Chain 5:



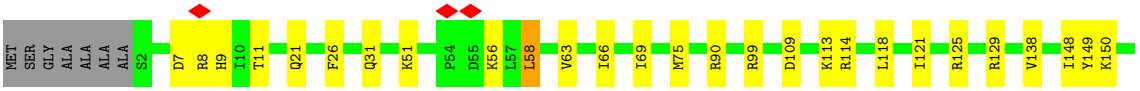
• Molecule 5: Proteasome assembly chaperone 2

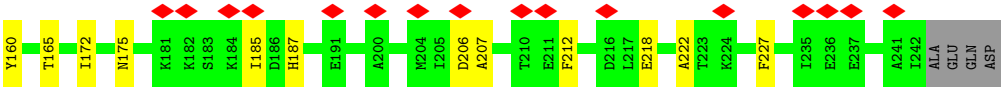
Chain 8:



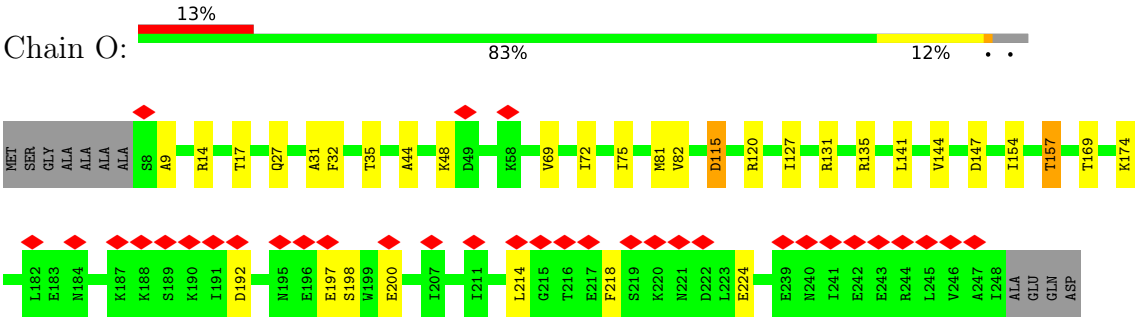
• Molecule 6: Proteasome subunit alpha type-1

Chain A:

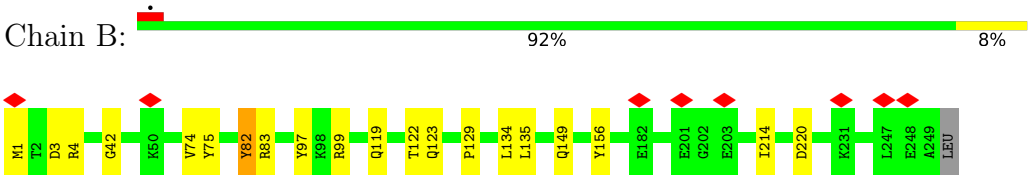




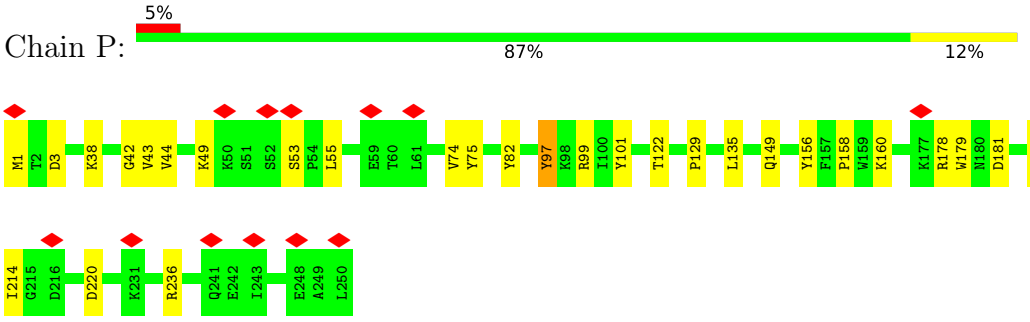
• Molecule 6: Proteasome subunit alpha type-1



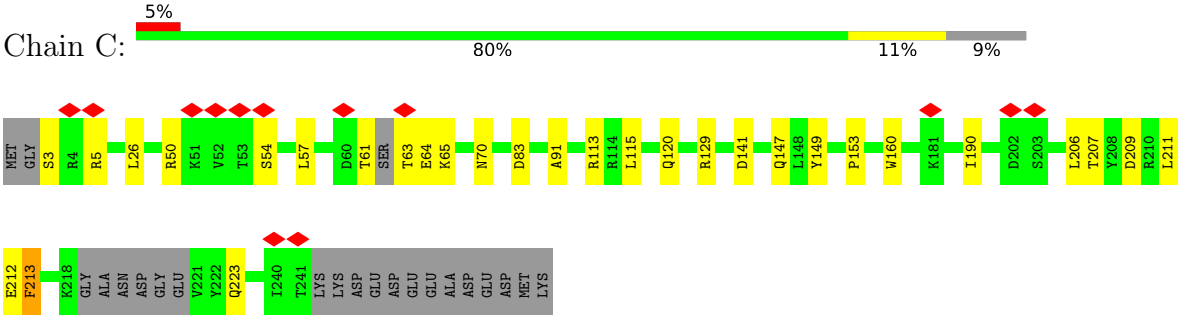
• Molecule 7: Proteasome subunit alpha type-2



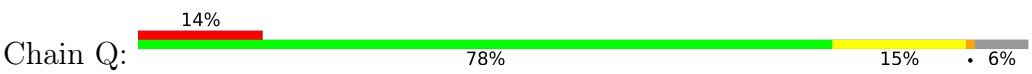
• Molecule 7: Proteasome subunit alpha type-2

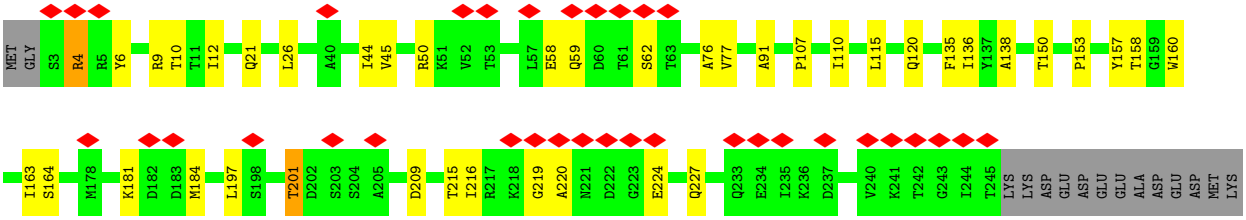


• Molecule 8: Proteasome subunit alpha type-3

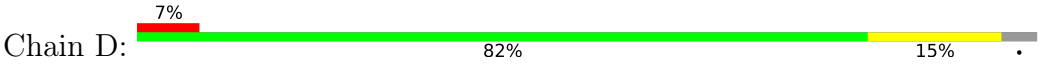


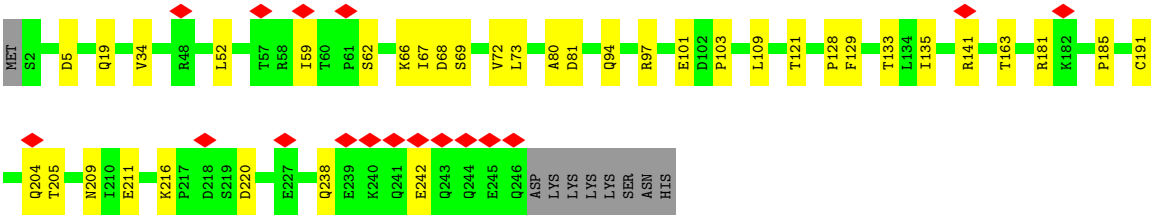
• Molecule 8: Proteasome subunit alpha type-3



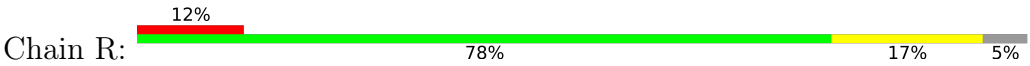


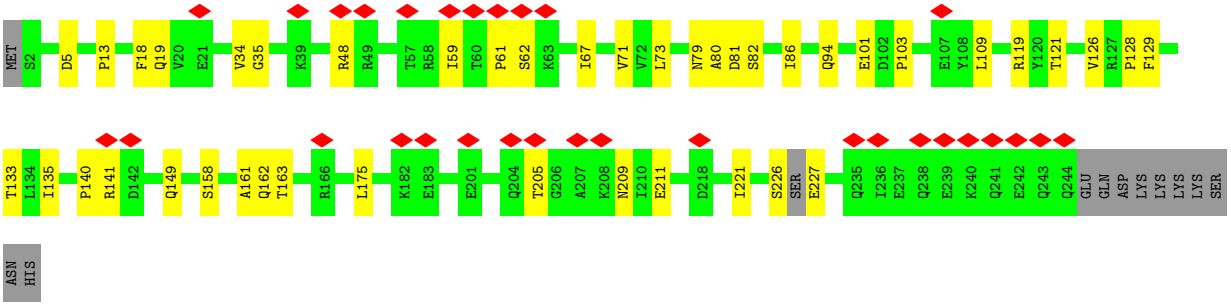
• Molecule 9: Proteasome subunit alpha type-4



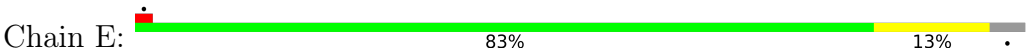


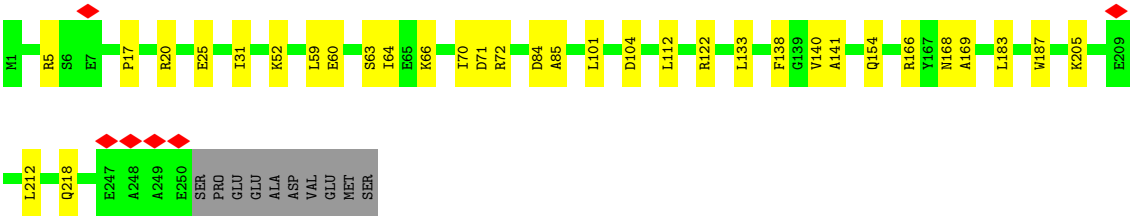
• Molecule 9: Proteasome subunit alpha type-4



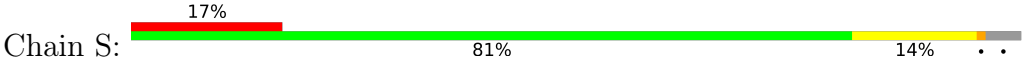


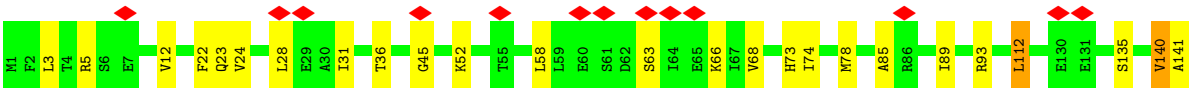
• Molecule 10: Proteasome subunit alpha type-5

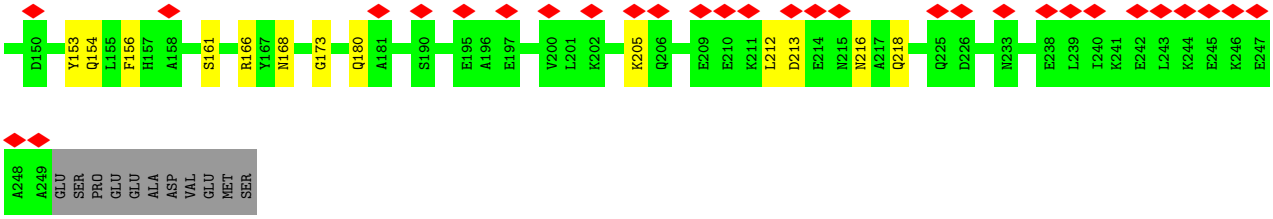




• Molecule 10: Proteasome subunit alpha type-5

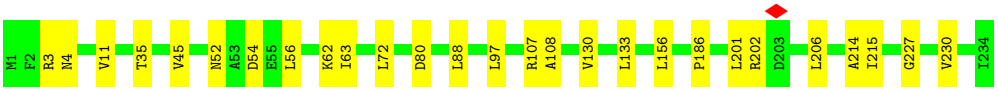






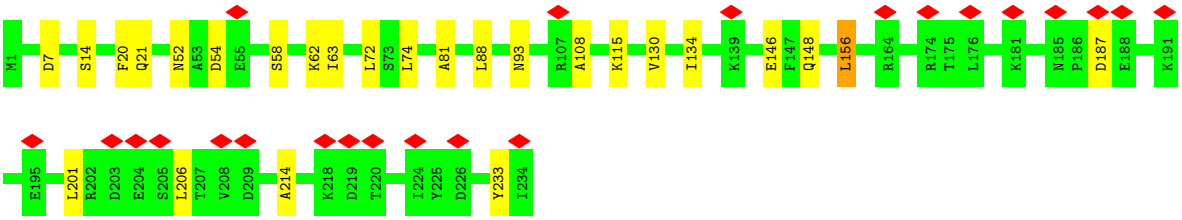
• Molecule 11: Proteasome subunit alpha type-6

Chain F:



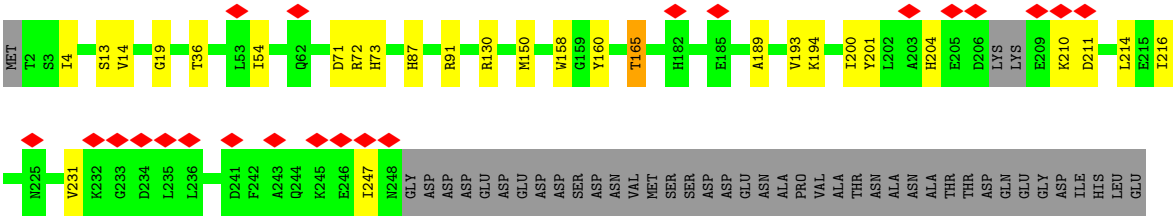
• Molecule 11: Proteasome subunit alpha type-6

Chain T:



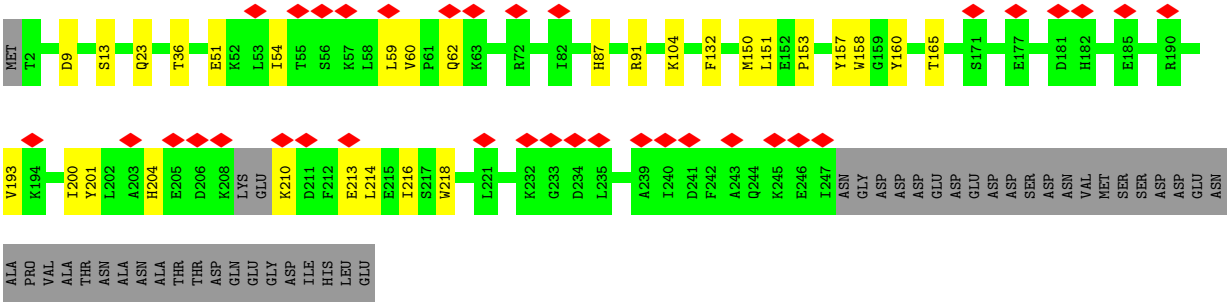
• Molecule 12: Probable proteasome subunit alpha type-7

Chain G:



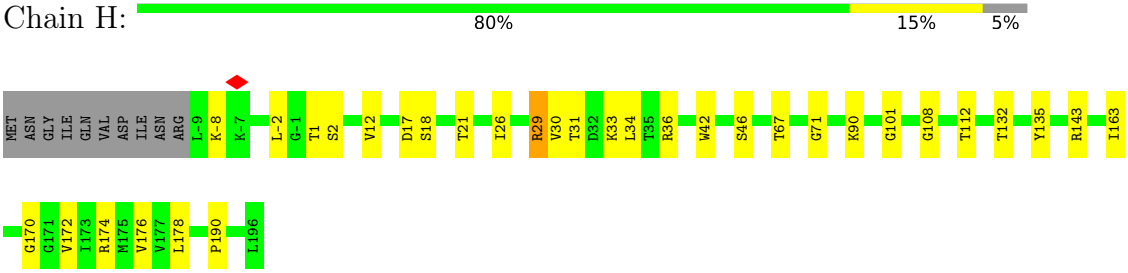
• Molecule 12: Probable proteasome subunit alpha type-7

Chain U:



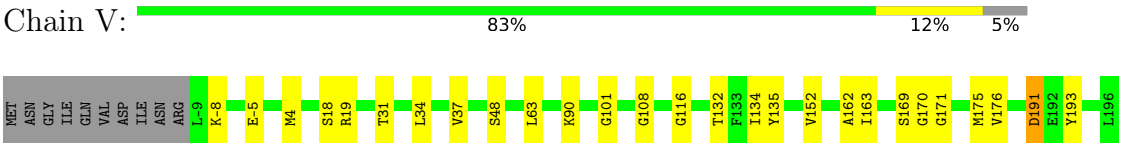
• Molecule 13: Proteasome subunit beta type-1

Chain H:



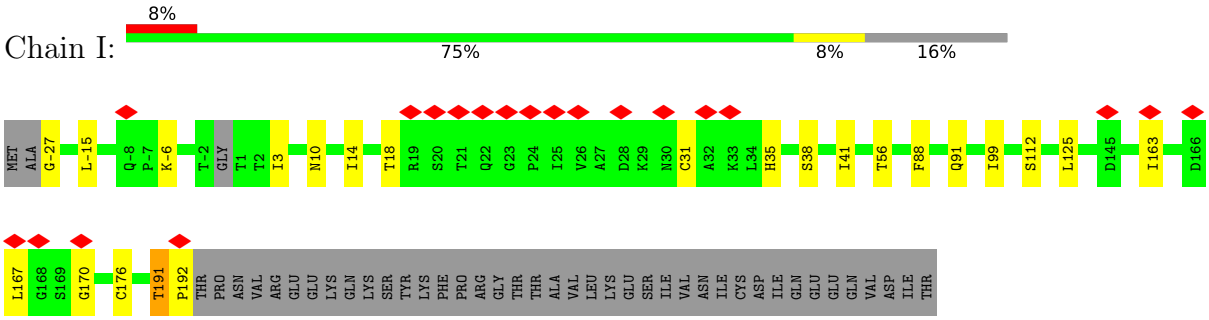
• Molecule 13: Proteasome subunit beta type-1

Chain V:



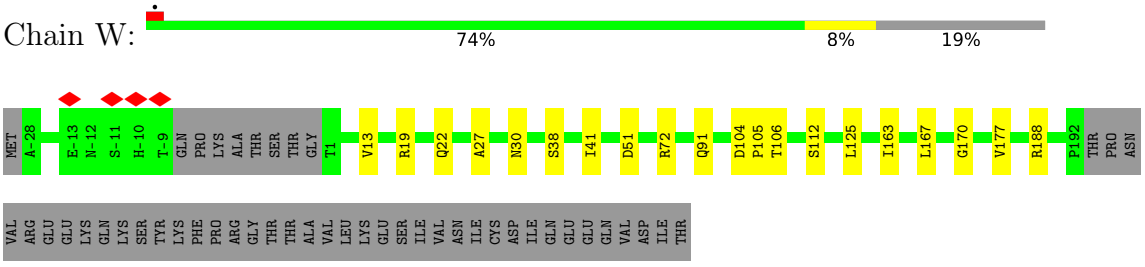
• Molecule 14: Proteasome subunit beta type-2

Chain I:



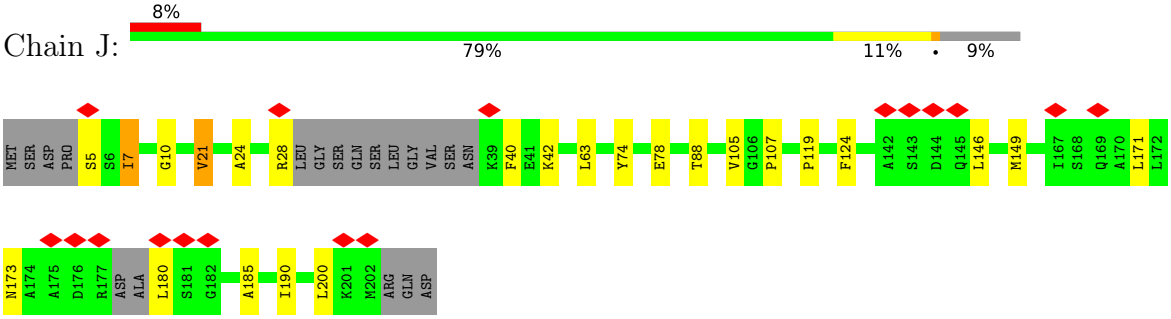
• Molecule 14: Proteasome subunit beta type-2

Chain W:



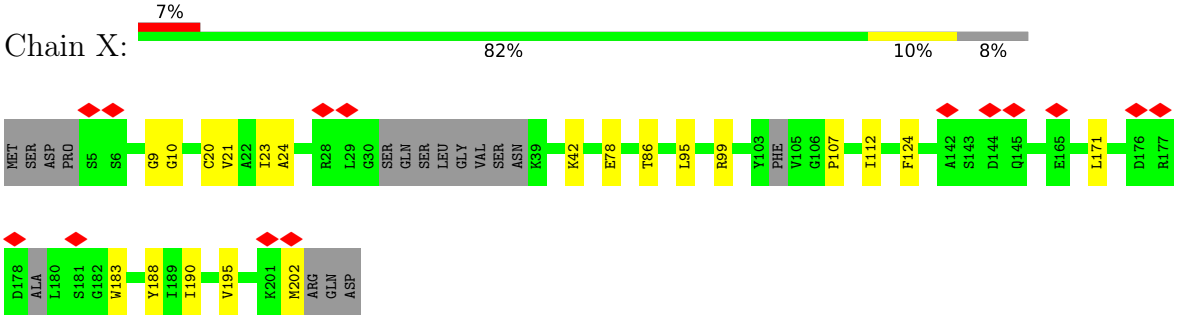
• Molecule 15: Proteasome subunit beta type-3

Chain J:



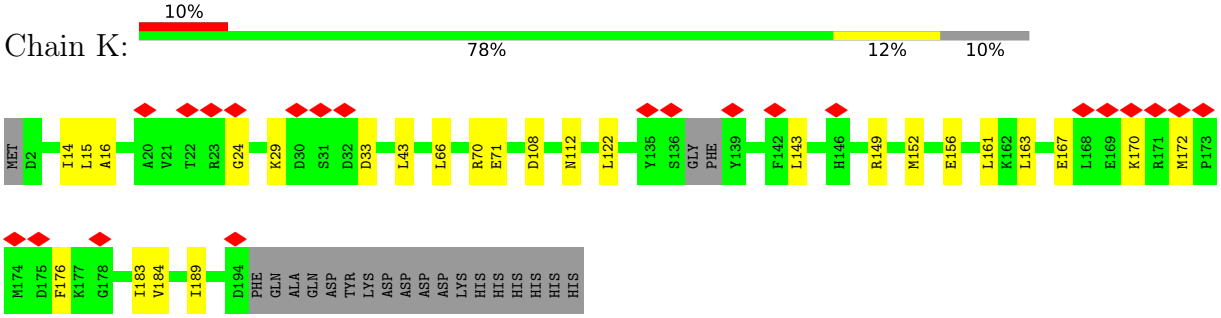
• Molecule 15: Proteasome subunit beta type-3

Chain X:



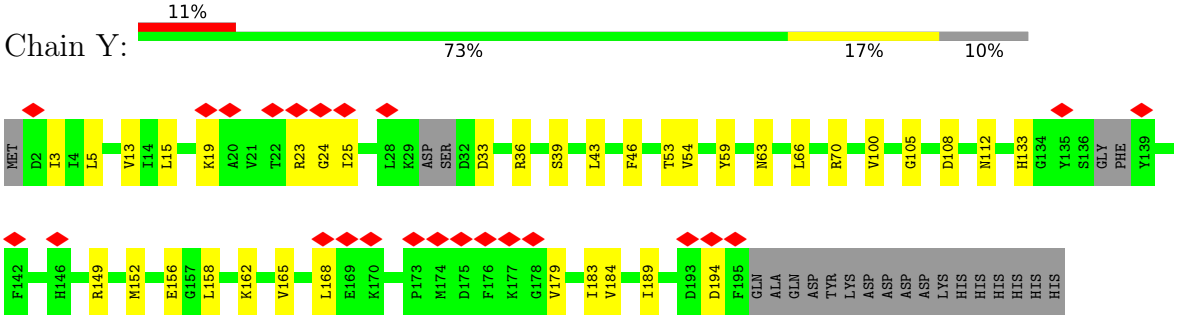
• Molecule 16: Proteasome subunit beta type-4

Chain K:



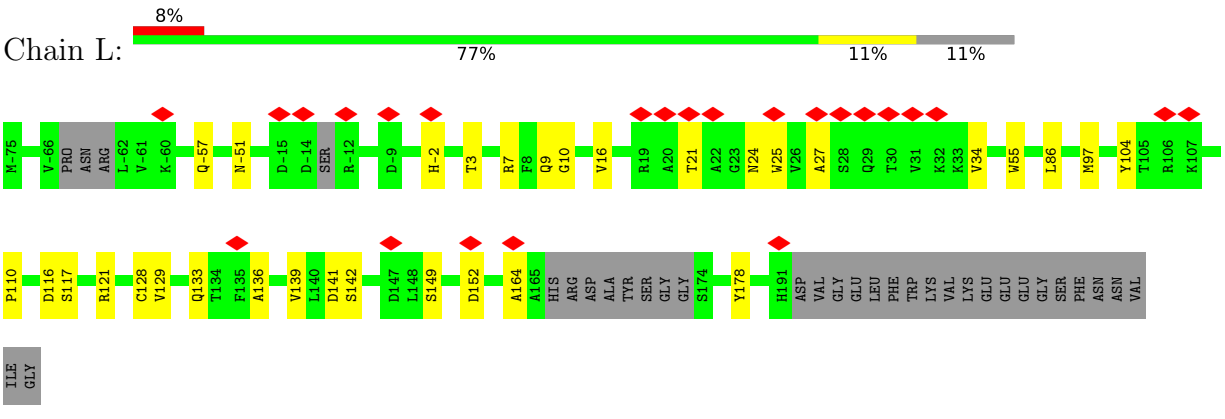
• Molecule 16: Proteasome subunit beta type-4

Chain Y:



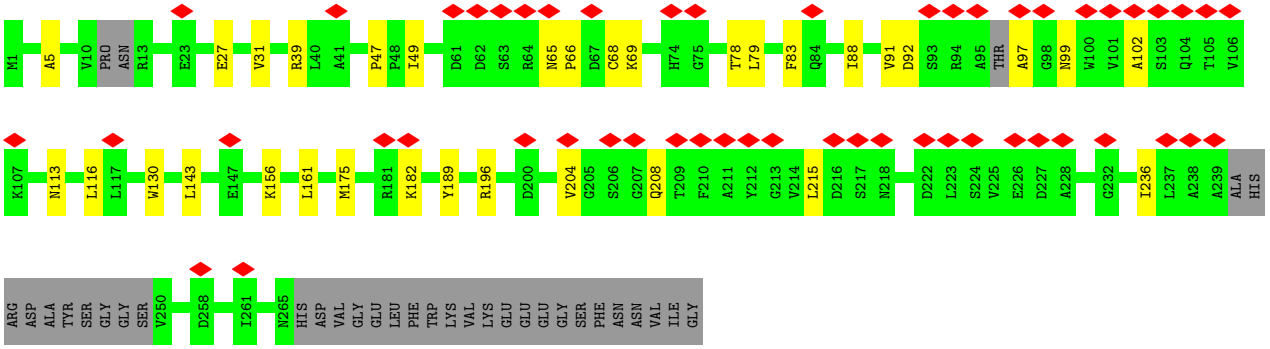
• Molecule 17: Proteasome subunit beta type-5

Chain L:



• Molecule 17: Proteasome subunit beta type-5

Chain Z:


M1 A5 V10 PRO ASN R13 E23 E27 V31 R39 L40 A41 P47 P48 I49 D61 D62 S63 R64 N65 P66 D67 C68 K69 H74 G75 T78 L79 F83 Q84 I88 V91 D92 S93 R94 A95 THR A97 G98 N99 W100 V101 A102 S103 Q104 T105 V106
K107 N113 L116 L117 W130 L143 E147 K156 L161 M175 R181 K182 Y189 R196 D200 V204 G205 S206 G207 Q208 T209 F210 A211 Y212 C213 V214 L215 D216 S217 N218 D222 L223 S224 V225 E226 D227 A228 G232 I236 L237 A238 A239 ALA HIS
ARG ASP ALA TYR SER GLY GLY SER V250 D258 I261 N265 HIS ASP VAL GLY GLU LEU PHE TRP LYS VAL LYS GLU GLU GLU GLY SER PHE ASN ASN VAL ILE GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.229	Depositor
Minimum map value	-0.712	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.206	Depositor
Map size (Å)	500.4, 500.4, 500.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	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	1	0.24	0/1698	0.46	0/2289
1	M	0.25	0/1698	0.47	0/2289
2	2	0.25	0/1783	0.48	0/2420
2	N	0.25	0/1775	0.49	0/2409
3	3	0.23	0/1151	0.46	0/1556
3	6	0.23	0/1157	0.46	0/1564
4	4	0.25	0/1904	0.43	0/2582
4	7	0.24	0/1923	0.43	0/2608
5	5	0.25	0/2028	0.42	0/2754
5	8	0.24	0/2075	0.42	0/2818
6	A	0.26	0/1938	0.46	0/2625
6	O	0.25	0/1938	0.46	0/2625
7	B	0.25	0/1943	0.46	0/2631
7	P	0.25	0/1951	0.45	0/2642
8	C	0.25	0/1884	0.48	0/2548
8	Q	0.24	0/1930	0.47	0/2613
9	D	0.25	0/1952	0.47	0/2642
9	R	0.24	0/1927	0.47	0/2607
10	E	0.25	0/1960	0.46	0/2640
10	S	0.24	0/1951	0.45	0/2628
11	F	0.25	0/1830	0.48	0/2473
11	T	0.24	0/1830	0.48	0/2473
12	G	0.25	0/1939	0.44	0/2618
12	U	0.25	0/1931	0.44	0/2606
13	H	0.25	0/1604	0.47	0/2171
13	V	0.25	0/1604	0.46	0/2171
14	I	0.24	0/1681	0.46	0/2282
14	W	0.25	0/1635	0.46	0/2219
15	J	0.25	0/1479	0.47	0/1993
15	X	0.25	0/1483	0.46	0/1997
16	K	0.24	0/1558	0.46	0/2100
16	Y	0.24	0/1555	0.45	0/2094
17	L	0.24	0/2009	0.45	0/2720
17	Z	0.24	0/1997	0.45	0/2702

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.25	0/60701	0.46	0/82109

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	1	1663	0	1620	20	0
1	M	1663	0	1620	20	0
2	2	1753	0	1754	18	0
2	N	1745	0	1750	19	0
3	3	1133	0	1113	12	0
3	6	1139	0	1118	19	0
4	4	1861	0	1888	17	0
4	7	1879	0	1910	24	0
5	5	1980	0	1957	19	0
5	8	2025	0	1986	47	0
6	A	1900	0	1897	25	0
6	O	1900	0	1897	25	0
7	B	1906	0	1918	14	0
7	P	1914	0	1929	19	0
8	C	1856	0	1864	21	0
8	Q	1900	0	1898	30	0
9	D	1923	0	1927	25	0
9	R	1899	0	1907	30	0
10	E	1933	0	1908	21	0
10	S	1924	0	1902	26	0
11	F	1802	0	1809	22	0
11	T	1802	0	1809	18	0
12	G	1900	0	1889	20	0
12	U	1892	0	1890	17	0
13	H	1575	0	1555	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	V	1575	0	1555	17	0
14	I	1649	0	1625	14	0
14	W	1604	0	1578	13	0
15	J	1452	0	1453	13	0
15	X	1458	0	1459	13	0
16	K	1532	0	1539	15	0
16	Y	1529	0	1538	22	0
17	L	1969	0	1932	19	0
17	Z	1958	0	1920	23	0
18	1	43	0	0	1	0
18	2	26	0	0	0	0
18	3	12	0	0	0	0
18	4	27	0	0	0	0
18	5	25	0	0	0	0
18	6	19	0	0	0	0
18	7	43	0	0	1	0
18	8	45	0	0	2	0
18	A	36	0	0	0	0
18	B	28	0	0	0	0
18	C	26	0	0	0	0
18	D	40	0	0	2	0
18	E	28	0	0	0	0
18	F	29	0	0	2	0
18	G	34	0	0	1	0
18	H	21	0	0	2	0
18	I	29	0	0	2	0
18	J	17	0	0	0	0
18	K	24	0	0	0	0
18	L	31	0	0	0	0
18	M	24	0	0	0	0
18	N	29	0	0	1	0
18	O	40	0	0	1	0
18	P	30	0	0	1	0
18	Q	28	0	0	0	0
18	R	36	0	0	0	0
18	S	43	0	0	1	0
18	T	44	0	0	1	0
18	U	56	0	0	2	0
18	V	23	0	0	0	0
18	W	28	0	0	1	0
18	X	24	0	0	0	0
18	Y	33	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Z	36	0	0	1	0
All	All	60650	0	59314	609	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 5.

The worst 5 of 609 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)
4:4:74:ILE:HB	4:4:122:PHE:HB3	1.67	0.76
9:R:73:LEU:HD11	9:R:133:THR:HB	1.68	0.74
5:5:11:VAL:HG21	5:5:122:TYR:HB2	1.69	0.73
4:4:230:LEU:O	4:4:271:GLN:NE2	2.22	0.72
1:1:30:ILE:HG22	1:1:35:ILE:HA	1.73	0.70

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	1	206/241 (86%)	197 (96%)	9 (4%)	0	100	100
1	M	206/241 (86%)	193 (94%)	13 (6%)	0	100	100
2	2	222/266 (84%)	217 (98%)	5 (2%)	0	100	100
2	N	221/266 (83%)	212 (96%)	9 (4%)	0	100	100
3	3	138/148 (93%)	137 (99%)	1 (1%)	0	100	100
3	6	139/148 (94%)	138 (99%)	1 (1%)	0	100	100
4	4	233/276 (84%)	229 (98%)	4 (2%)	0	100	100
4	7	237/276 (86%)	235 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	238/267 (89%)	233 (98%)	5 (2%)	0	100	100
5	8	243/267 (91%)	232 (96%)	11 (4%)	0	100	100
6	A	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
6	O	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
7	B	247/250 (99%)	242 (98%)	5 (2%)	0	100	100
7	P	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
8	C	230/258 (89%)	226 (98%)	4 (2%)	0	100	100
8	Q	241/258 (93%)	232 (96%)	9 (4%)	0	100	100
9	D	243/254 (96%)	237 (98%)	6 (2%)	0	100	100
9	R	238/254 (94%)	229 (96%)	8 (3%)	1 (0%)	30	55
10	E	248/260 (95%)	247 (100%)	1 (0%)	0	100	100
10	S	247/260 (95%)	246 (100%)	1 (0%)	0	100	100
11	F	232/234 (99%)	224 (97%)	8 (3%)	0	100	100
11	T	232/234 (99%)	228 (98%)	4 (2%)	0	100	100
12	G	241/288 (84%)	240 (100%)	1 (0%)	0	100	100
12	U	240/288 (83%)	234 (98%)	6 (2%)	0	100	100
13	H	203/215 (94%)	200 (98%)	3 (2%)	0	100	100
13	V	203/215 (94%)	197 (97%)	6 (3%)	0	100	100
14	I	214/261 (82%)	210 (98%)	4 (2%)	0	100	100
14	W	208/261 (80%)	206 (99%)	2 (1%)	0	100	100
15	J	180/205 (88%)	164 (91%)	15 (8%)	1 (1%)	22	45
15	X	180/205 (88%)	171 (95%)	9 (5%)	0	100	100
16	K	187/212 (88%)	182 (97%)	5 (3%)	0	100	100
16	Y	184/212 (87%)	176 (96%)	8 (4%)	0	100	100
17	L	246/287 (86%)	235 (96%)	11 (4%)	0	100	100
17	Z	244/287 (85%)	240 (98%)	4 (2%)	0	100	100
All	All	7497/8348 (90%)	7297 (97%)	198 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	R	221	ILE
15	J	7	ILE

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	1	175/201 (87%)	171 (98%)	4 (2%)	45	74
1	M	175/201 (87%)	168 (96%)	7 (4%)	27	55
2	2	192/224 (86%)	189 (98%)	3 (2%)	58	82
2	N	191/224 (85%)	189 (99%)	2 (1%)	73	89
3	3	132/136 (97%)	132 (100%)	0	100	100
3	6	133/136 (98%)	132 (99%)	1 (1%)	79	91
4	4	216/251 (86%)	213 (99%)	3 (1%)	62	84
4	7	218/251 (87%)	213 (98%)	5 (2%)	45	74
5	5	222/244 (91%)	221 (100%)	1 (0%)	86	95
5	8	226/244 (93%)	219 (97%)	7 (3%)	35	64
6	A	205/210 (98%)	198 (97%)	7 (3%)	32	61
6	O	205/210 (98%)	202 (98%)	3 (2%)	60	83
7	B	208/209 (100%)	205 (99%)	3 (1%)	62	84
7	P	209/209 (100%)	206 (99%)	3 (1%)	62	84
8	C	199/216 (92%)	198 (100%)	1 (0%)	86	95
8	Q	203/216 (94%)	201 (99%)	2 (1%)	73	89
9	D	217/226 (96%)	217 (100%)	0	100	100
9	R	214/226 (95%)	213 (100%)	1 (0%)	86	95
10	E	206/215 (96%)	206 (100%)	0	100	100
10	S	205/215 (95%)	203 (99%)	2 (1%)	73	89
11	F	193/193 (100%)	192 (100%)	1 (0%)	86	95
11	T	193/193 (100%)	192 (100%)	1 (0%)	86	95
12	G	202/239 (84%)	200 (99%)	2 (1%)	73	89
12	U	201/239 (84%)	199 (99%)	2 (1%)	73	89
13	H	169/178 (95%)	167 (99%)	2 (1%)	67	86
13	V	169/178 (95%)	168 (99%)	1 (1%)	84	94

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	I	176/215 (82%)	174 (99%)	2 (1%)	70 87
14	W	170/215 (79%)	169 (99%)	1 (1%)	84 94
15	J	157/173 (91%)	154 (98%)	3 (2%)	52 79
15	X	157/173 (91%)	157 (100%)	0	100 100
16	K	170/189 (90%)	168 (99%)	2 (1%)	67 86
16	Y	169/189 (89%)	166 (98%)	3 (2%)	54 80
17	L	208/235 (88%)	206 (99%)	2 (1%)	73 89
17	Z	207/235 (88%)	207 (100%)	0	100 100
All	All	6492/7108 (91%)	6415 (99%)	77 (1%)	66 86

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	223	LYS
12	U	218	TRP
6	O	157	THR
8	Q	201	THR
16	Y	39	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	6	106	HIS
12	G	21	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 oligosaccharides 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)

There are no chain breaks in this entry.

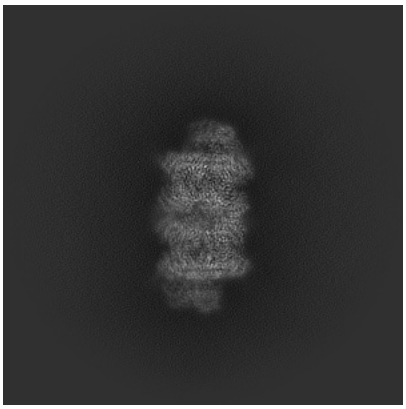
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19527. These allow visual inspection of the internal detail of the map and identification of artifacts.

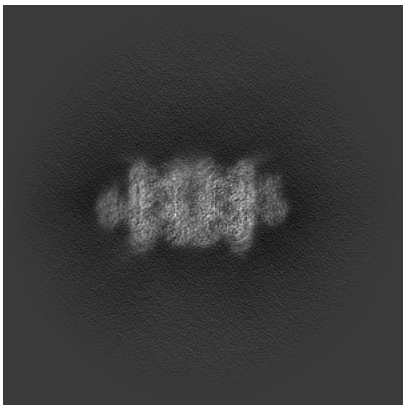
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

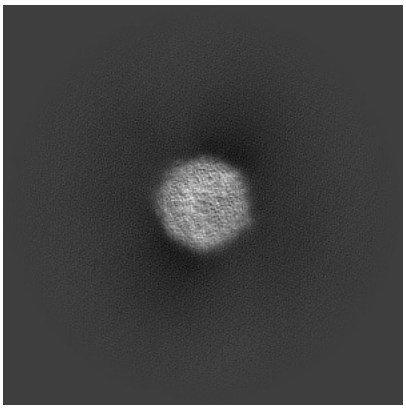
6.1.1 Primary map



X

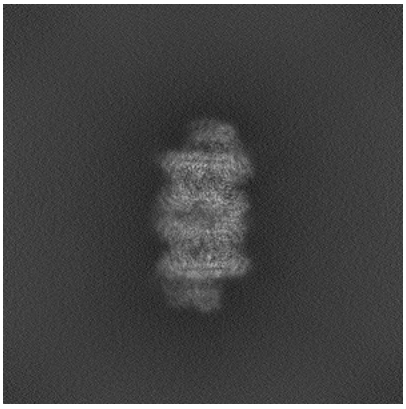


Y

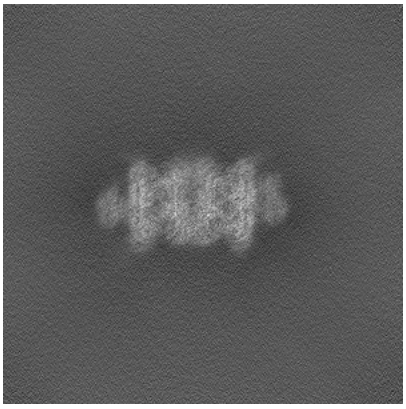


Z

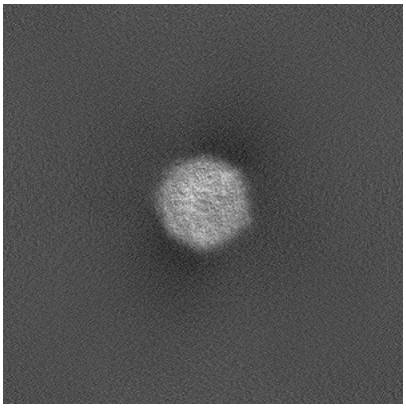
6.1.2 Raw map



X



Y

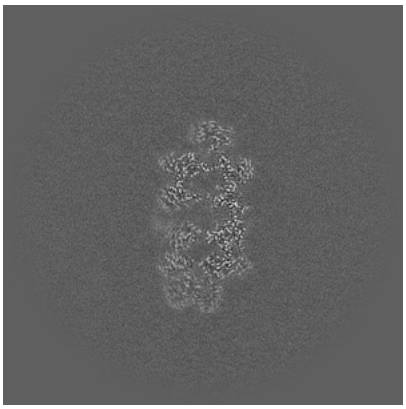


Z

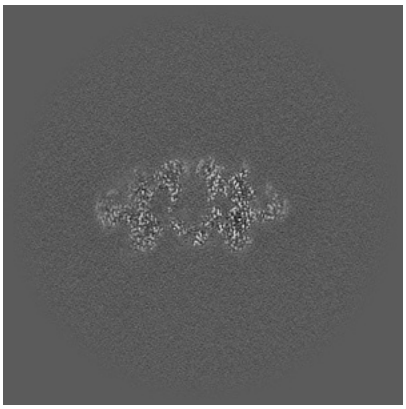
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

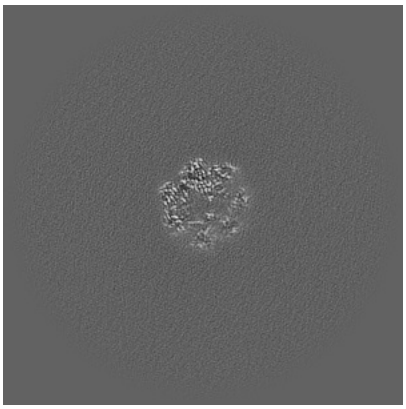
6.2.1 Primary map



X Index: 300

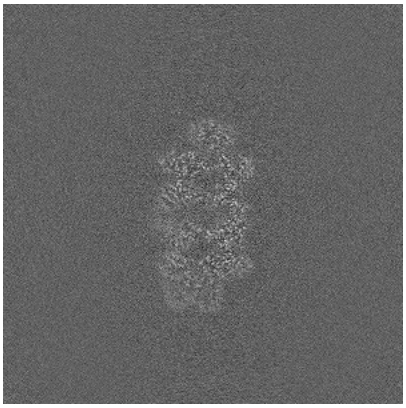


Y Index: 300

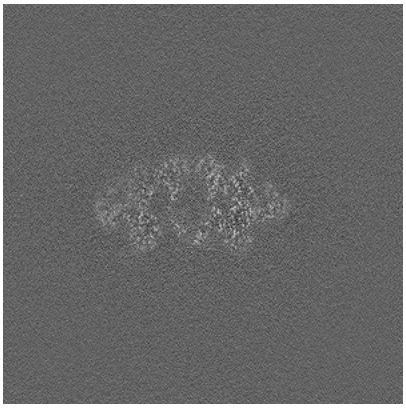


Z Index: 300

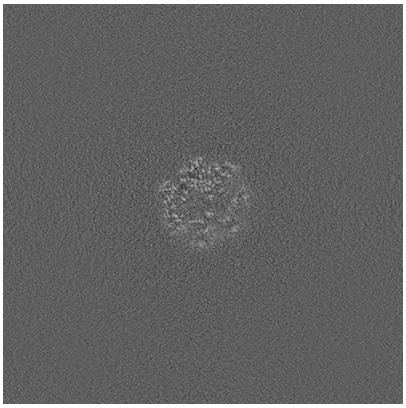
6.2.2 Raw map



X Index: 300



Y Index: 300

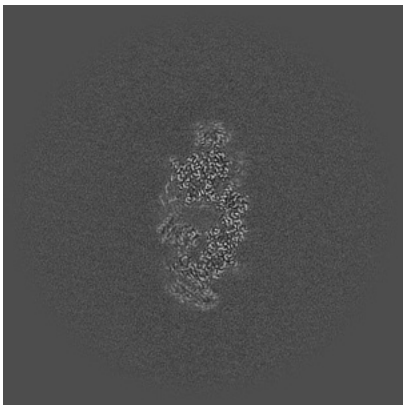


Z Index: 300

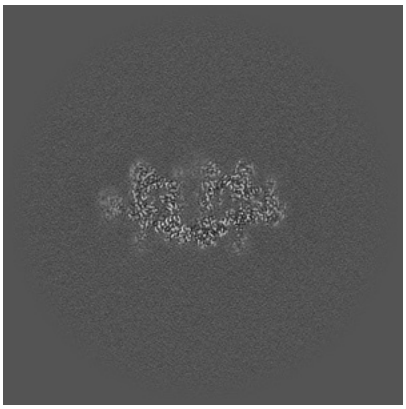
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

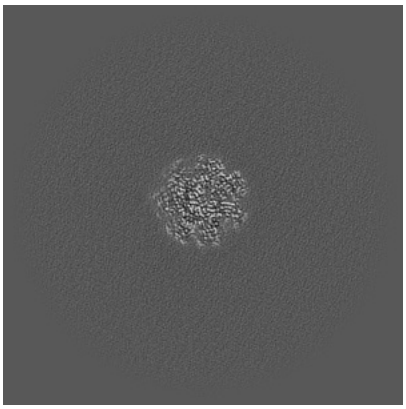
6.3.1 Primary map



X Index: 282

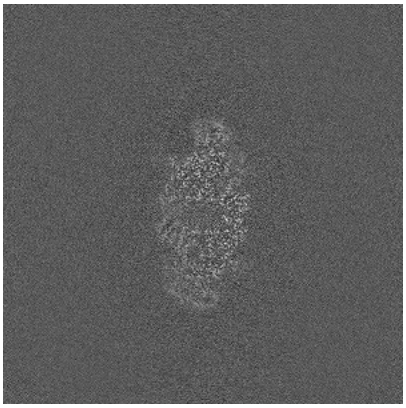


Y Index: 319



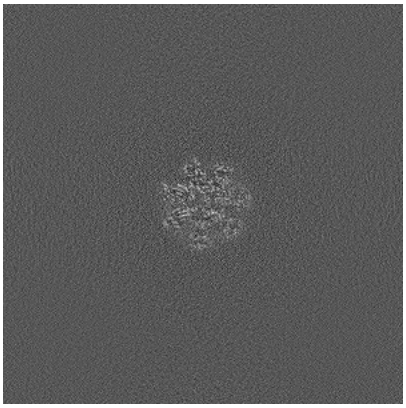
Z Index: 356

6.3.2 Raw map



X Index: 283

Y Index: 319

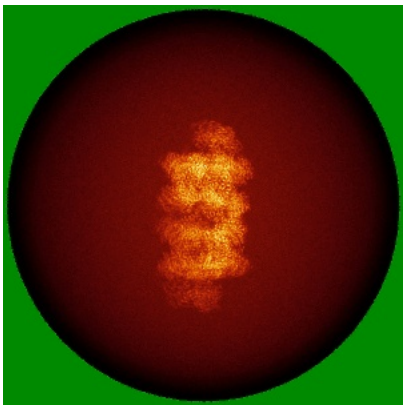


Z Index: 306

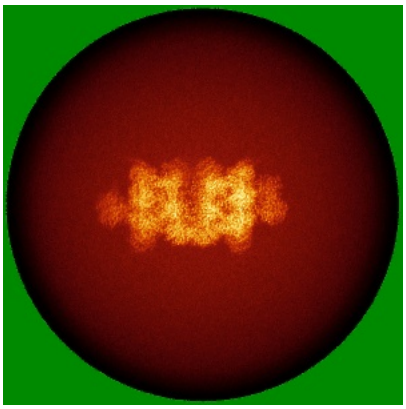
The images above show the largest variance slices of the map in three orthogonal directions.

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

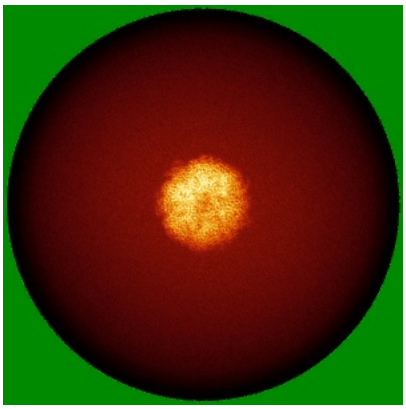
6.4.1 Primary map



X

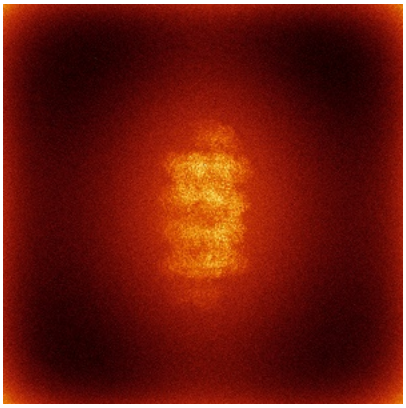


Y

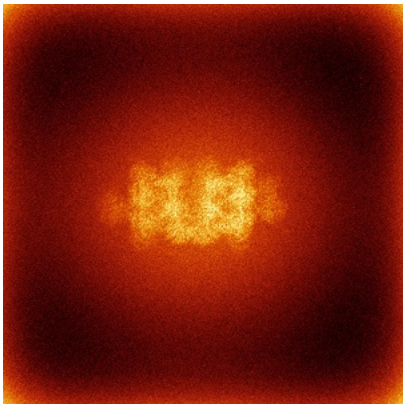


Z

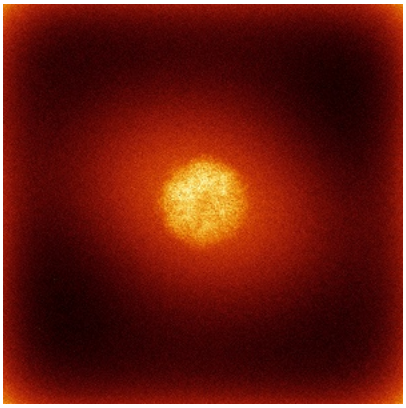
6.4.2 Raw map



X



Y

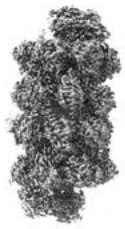


Z

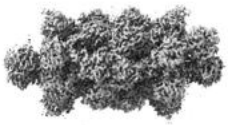
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

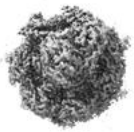
6.5.1 Primary map



X



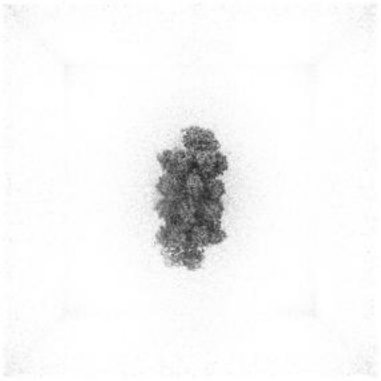
Y



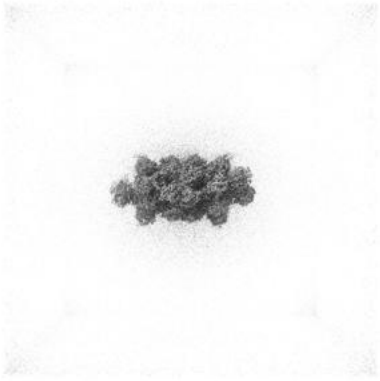
Z

The images above show the 3D surface view of the map at the recommended contour level 0.206. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

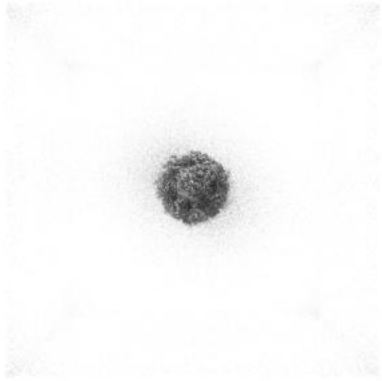
6.5.2 Raw map



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.

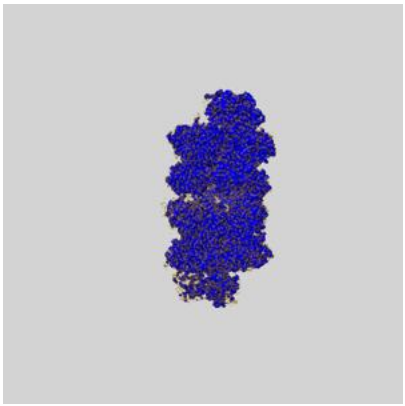
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

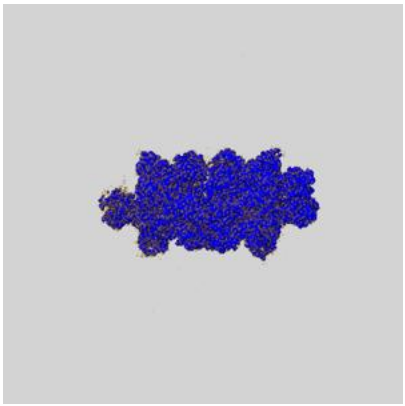
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

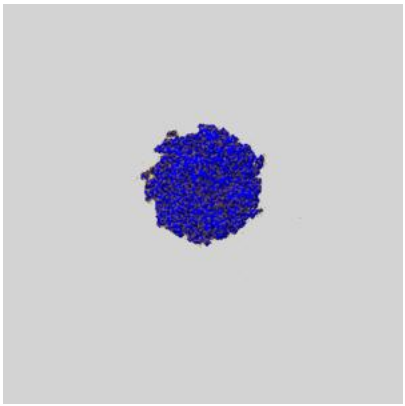
6.6.1 emd_19527_msk_1.map (i)



X



Y

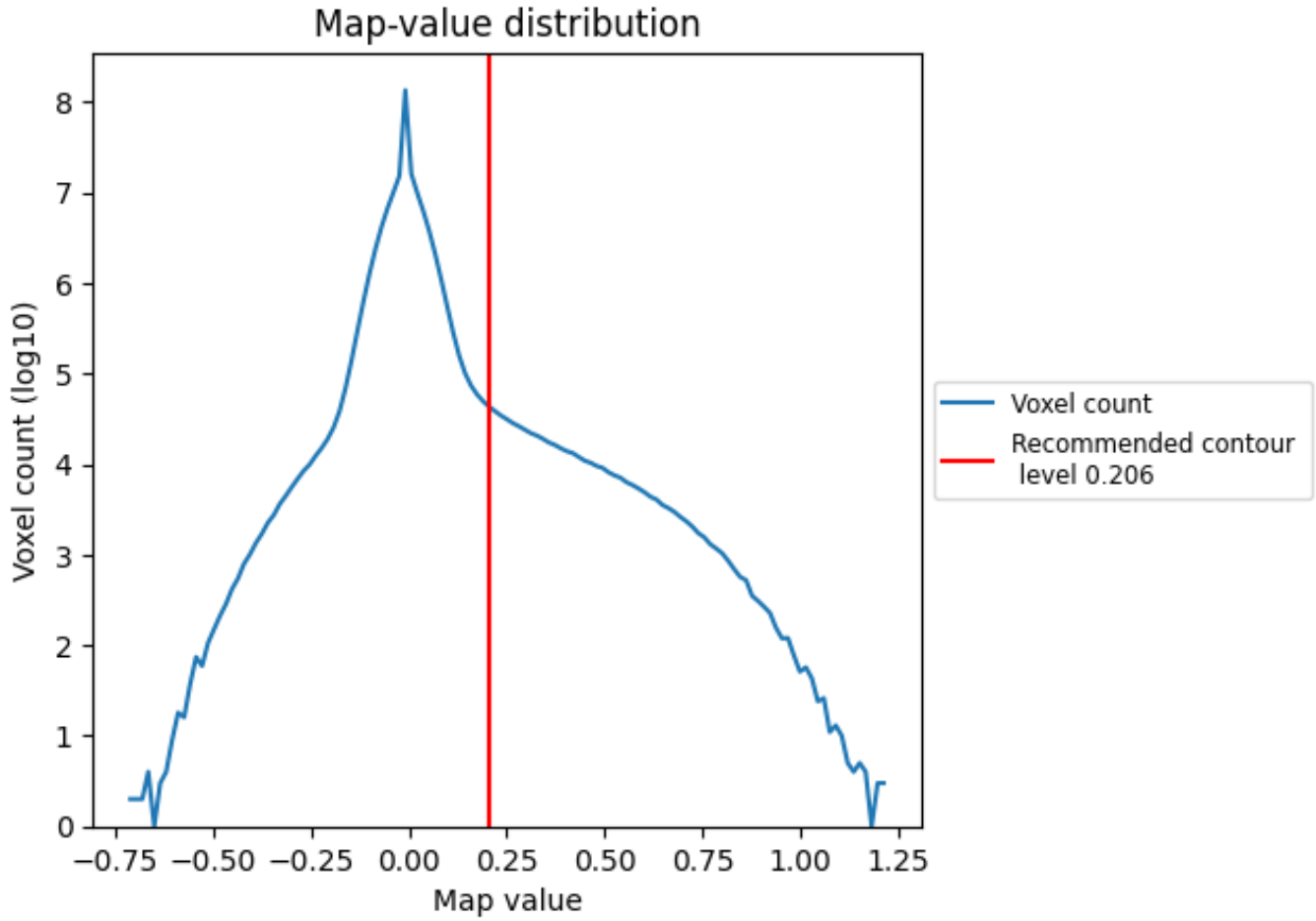


Z

7 Map analysis

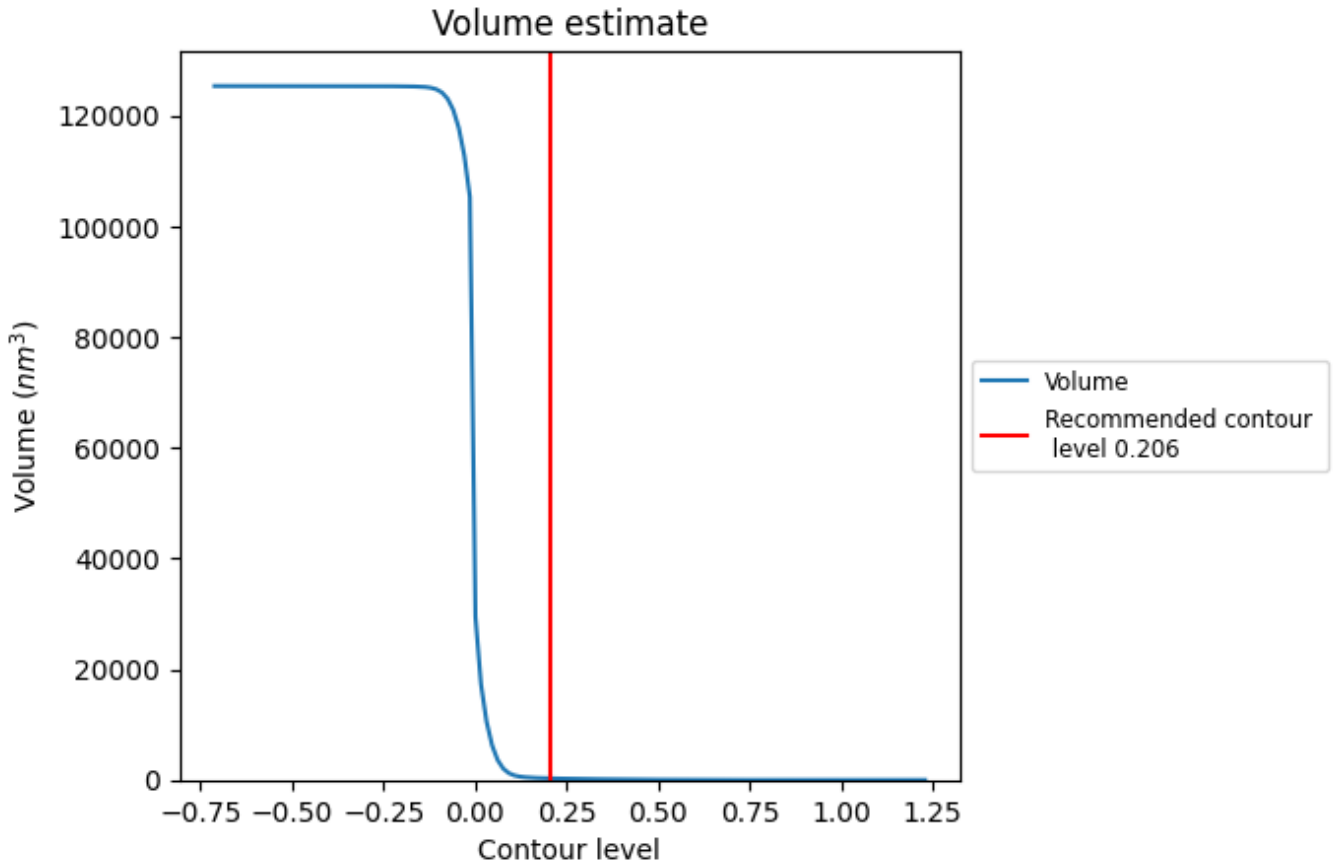
This section contains the results of statistical analysis of the map.

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.

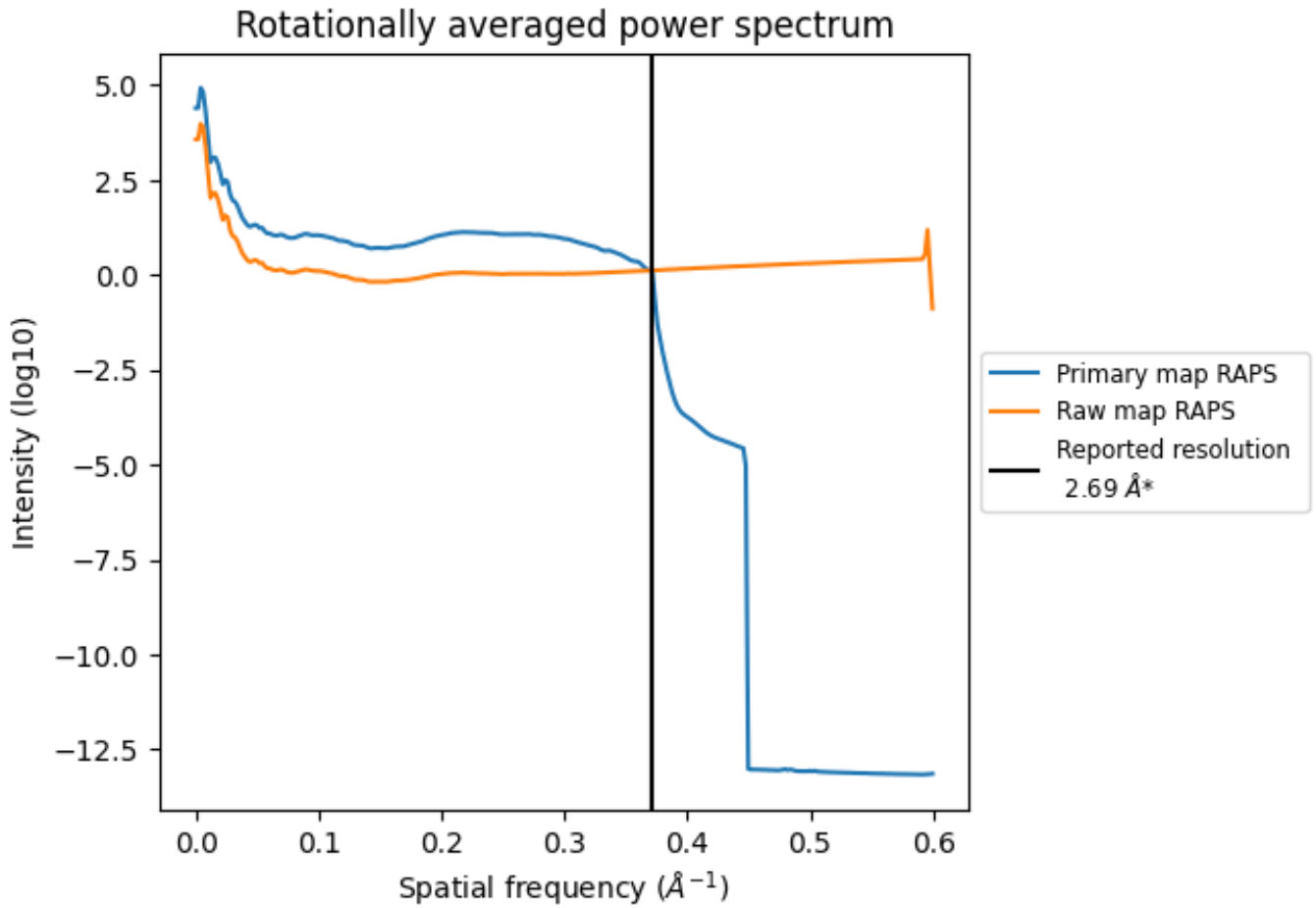
7.2 Volume estimate (i)



The volume at the recommended contour level is 286 nm^3; this corresponds to an approximate mass of 259 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)

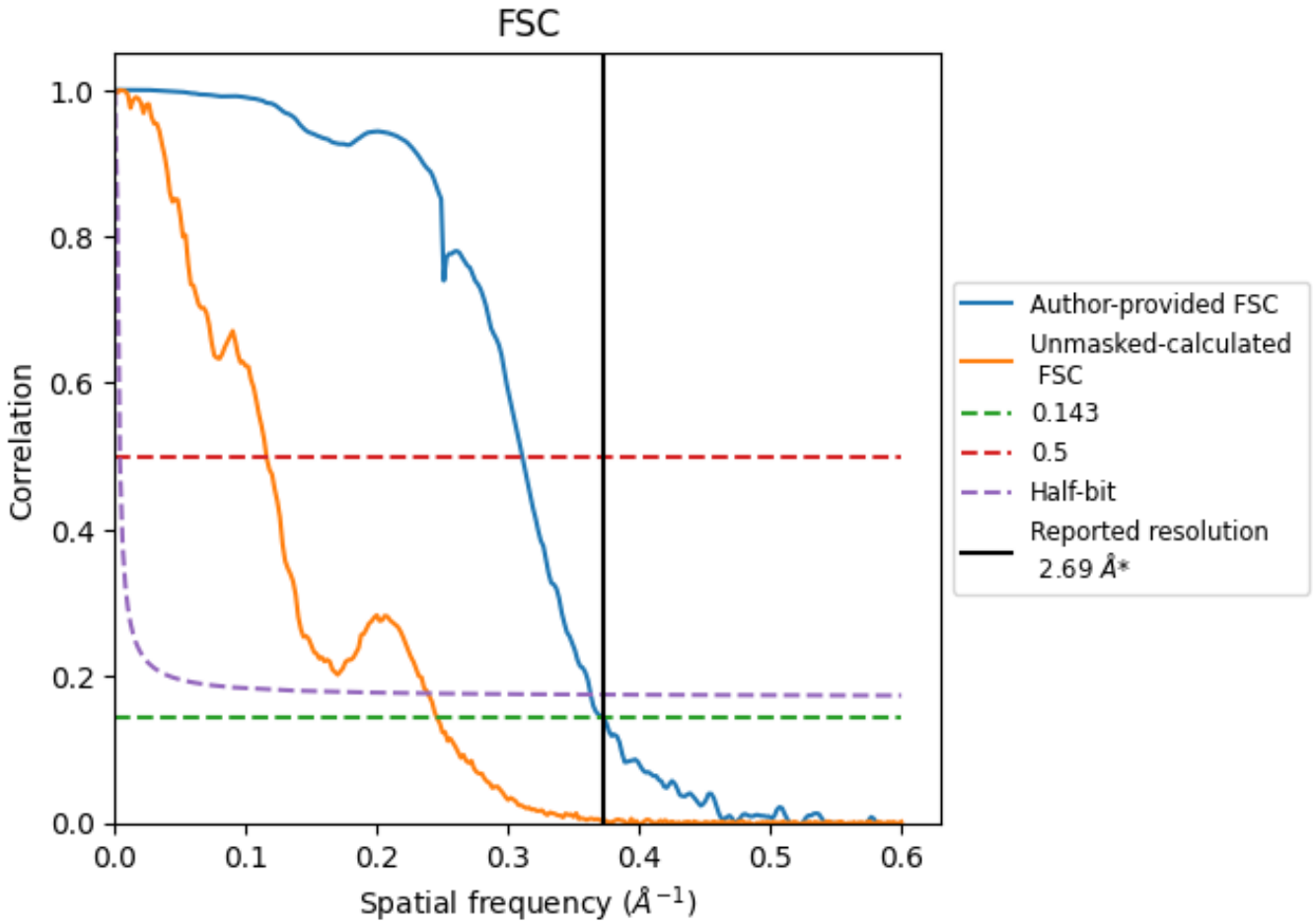


*Reported resolution corresponds to spatial frequency of 0.372 $Å^{-1}$

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 0.372 Å^{-1}

8.2 Resolution estimates (i)

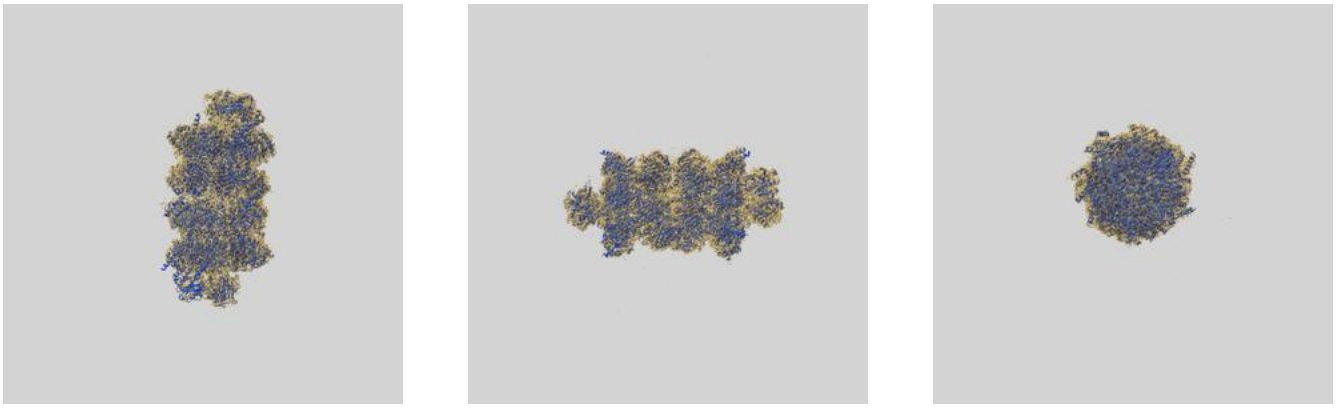
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	3.22	2.76
Unmasked-calculated*	4.07	8.64	4.19

*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 4.07 differs from the reported value 2.69 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19527 and PDB model 8RVO. Per-residue inclusion information can be found in section 3 on page 12.

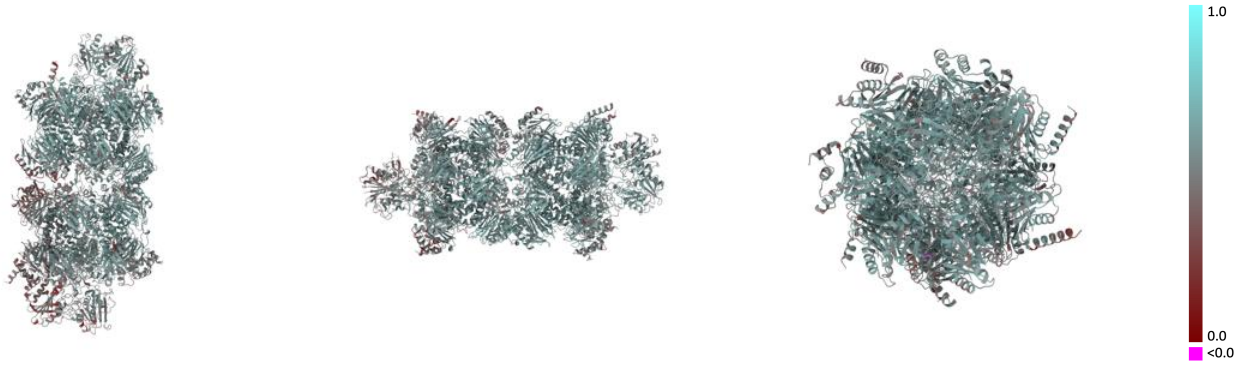
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.206 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.

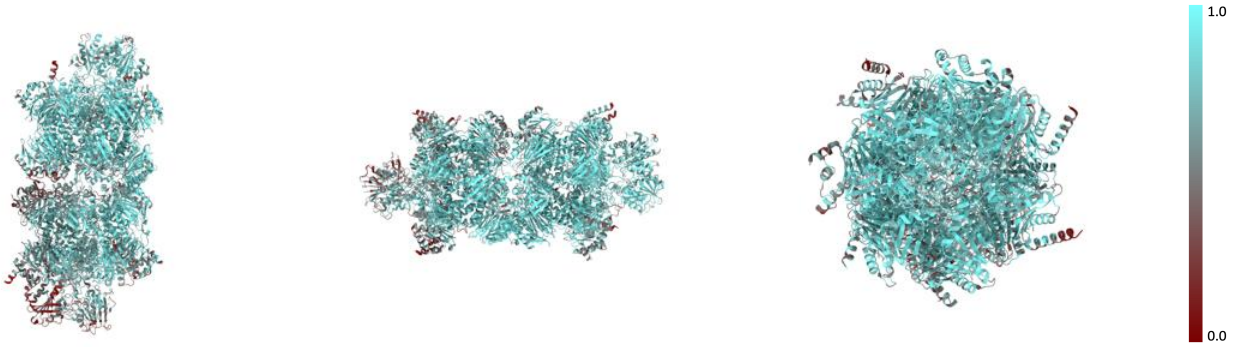
9.2 Q-score mapped to coordinate model



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.

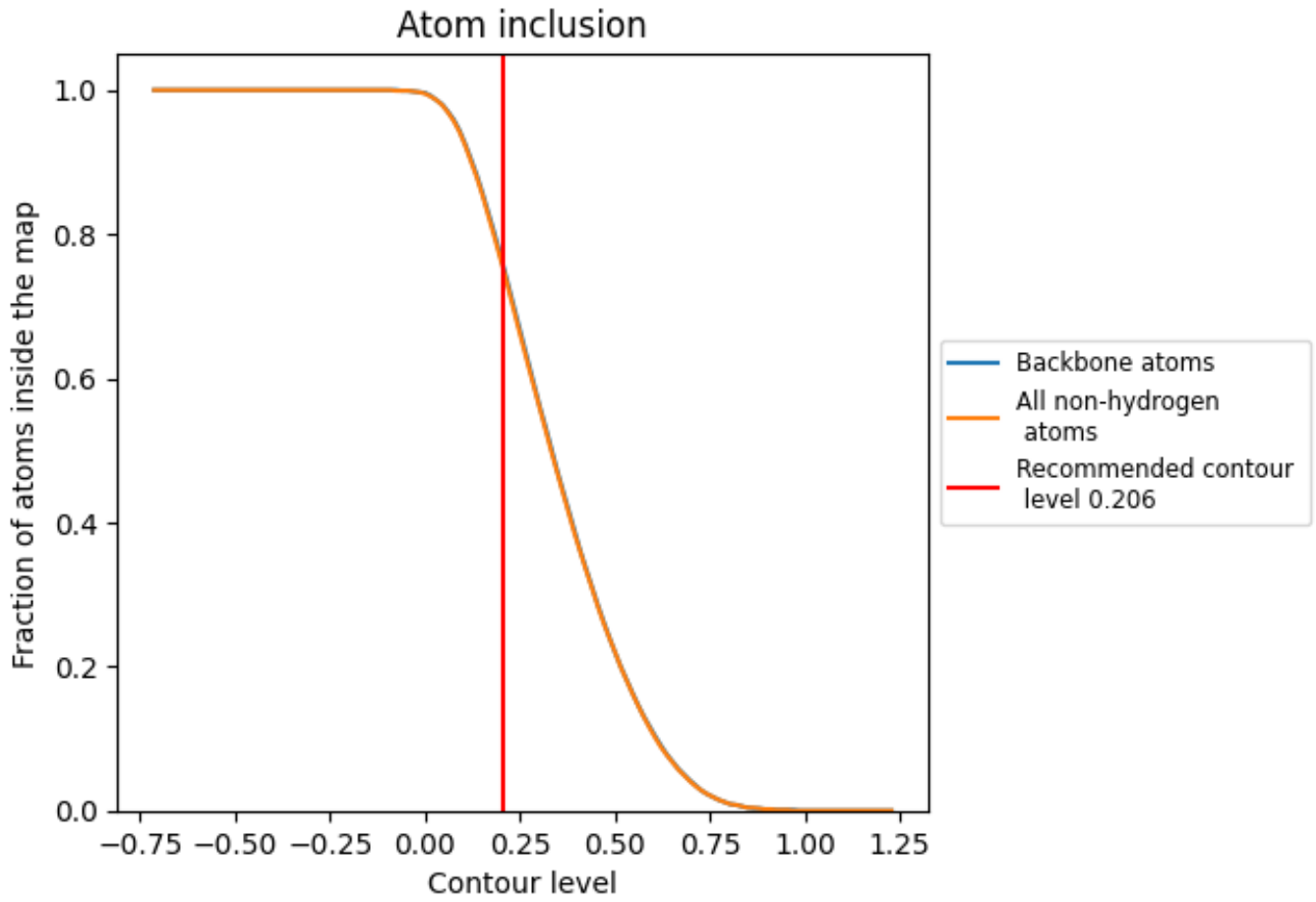
9.3 Atom inclusion mapped to coordinate model



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 (0.206).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 75% 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 (0.206) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7530	0.5470
1	0.5910	0.4440
2	0.7700	0.5520
3	0.8700	0.6040
4	0.7420	0.5360
5	0.7840	0.5530
6	0.8220	0.5870
7	0.4350	0.4290
8	0.5640	0.4790
A	0.8000	0.5670
B	0.8310	0.5770
C	0.8070	0.5670
D	0.7960	0.5660
E	0.8540	0.5920
F	0.8770	0.5970
G	0.7720	0.5600
H	0.8970	0.6080
I	0.8090	0.5710
J	0.7550	0.5230
K	0.7500	0.5440
L	0.7690	0.5580
M	0.8800	0.5960
N	0.8650	0.5890
O	0.7220	0.5440
P	0.7930	0.5610
Q	0.7200	0.5360
R	0.6830	0.5140
S	0.6300	0.4880
T	0.6940	0.5160
U	0.6950	0.5200
V	0.9010	0.6040
W	0.9060	0.6100
X	0.7990	0.5680
Y	0.6990	0.5260
Z	0.6330	0.4840