



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 11:53 PM JST

PDB ID : 7DR6
EMDB ID : EMD-30824
Title : PA28alpha-beta in complex with immunoproteasome
Authors : Cong, Y.; Xu, C.
Deposited on : 2020-12-26
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

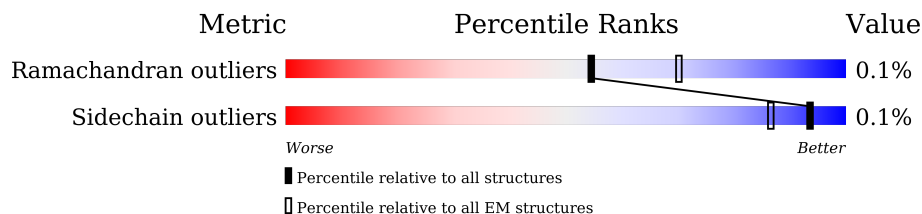
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	246	<div> <div>21%</div> <div>96%</div> <div>.</div> </div>
1	e	246	<div> <div>34%</div> <div>97%</div> <div>.</div> </div>
2	M	234	<div> <div>22%</div> <div>97%</div> <div>.</div> </div>
2	f	234	<div> <div>26%</div> <div>98%</div> <div>.</div> </div>
3	N	261	<div> <div>26%</div> <div>94%</div> <div>6%</div> </div>
3	g	261	<div> <div>30%</div> <div>94%</div> <div>6%</div> </div>
4	O	248	<div> <div>31%</div> <div>94%</div> <div>6%</div> </div>
4	a	248	<div> <div>30%</div> <div>94%</div> <div>6%</div> </div>
5	P	241	<div> <div>40%</div> <div>97%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	b	241	43% 97%
6	Q	263	32% 89% 11%
6	c	263	34% 89% 11%
7	R	255	24% 94% 6%
7	d	255	40% 94% 6%
8	A	239	50% 87% 13%
8	D	239	55% 85% 13%
8	F	239	64% 88% 12%
9	B	249	55% 85% 14%
9	C	249	54% 83% 17%
9	E	249	57% 83% 16%
9	G	249	55% 81% 18%
10	H	205	27% 100%
10	S	205	23% 99%
11	I	201	26% 99%
11	T	201	22% 98%
12	J	241	23% 88% 12%
12	U	241	24% 88% 12%
13	K	264	23% 81% 18%
13	V	264	24% 82% 18%
14	W	219	20% 91% 9%
14	Z	219	21% 91% 9%
15	1	273	20% 80% 20%
15	X	273	20% 79% 20%
16	2	276	18% 73% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	Y	276	<div><div></div><div></div><div></div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 59957 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 alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	236	Total	C	N	O	S	0	0
			1850	1178	306	353	13		
1	e	238	Total	C	N	O	S	0	0
			1856	1181	308	354	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	226	Total	C	N	O	S	0	0
			1763	1127	298	332	6		
2	f	230	Total	C	N	O	S	0	0
			1793	1147	302	338	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	246	Total	C	N	O	S	0	0
			1936	1225	331	369	11		
3	g	246	Total	C	N	O	S	0	0
			1936	1225	331	369	11		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	232	Total	C	N	O	S	0	0
			1824	1149	322	348	5		
4	a	232	Total	C	N	O	S	0	0
			1824	1149	322	348	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		
5	b	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	235	Total	C	N	O	S	0	0
			1846	1156	330	349	11		
6	c	235	Total	C	N	O	S	0	0
			1846	1156	330	349	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	240	Total	C	N	O	S	0	0
			1879	1191	321	356	11		
7	d	240	Total	C	N	O	S	0	0
			1879	1191	321	356	11		

- Molecule 8 is a protein called Proteasome activator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	209	Total	C	N	O	S	0	0
			1684	1084	286	310	4		
8	D	207	Total	C	N	O	S	0	0
			1678	1080	283	311	4		
8	F	210	Total	C	N	O	S	0	0
			1695	1091	287	313	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PRO	HIS	variant	UNP Q9UL46
D	89	PRO	HIS	variant	UNP Q9UL46
F	89	PRO	HIS	variant	UNP Q9UL46

- Molecule 9 is a protein called Proteasome activator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	213	Total	C	N	O	S	0	0
			1720	1102	292	320	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	206	Total	C	N	O	S	0	0
			1663	1063	284	310	6		
9	E	208	Total	C	N	O	S	0	0
			1685	1078	287	314	6		
9	G	205	Total	C	N	O	S	0	0
			1654	1057	283	306	8		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		
10	S	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	198	Total	C	N	O	S	0	0
			1593	1023	270	292	8		
11	T	197	Total	C	N	O	S	0	0
			1584	1017	268	291	8		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		
12	U	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	216	Total	C	N	O	S	0	0
			1685	1065	289	319	12		
13	V	216	Total	C	N	O	S	0	0
			1682	1063	289	318	12		

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	199	Total	C	N	O	S	0	0
			1500	942	257	291	10		
14	Z	199	Total	C	N	O	S	0	0
			1500	942	257	291	10		

- Molecule 15 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	219	Total	C	N	O	S	0	0
			1611	1010	281	309	11		
15	1	219	Total	C	N	O	S	0	0
			1611	1010	281	309	11		

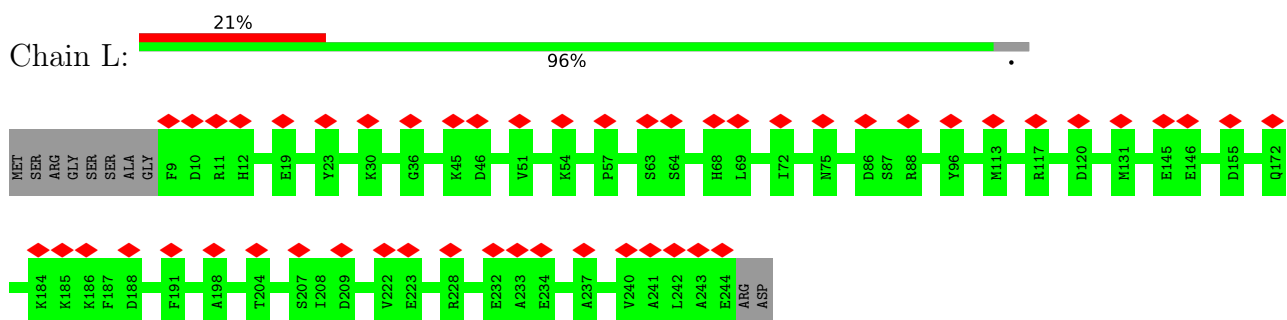
- Molecule 16 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	201	Total	C	N	O	S	0	0
			1561	975	273	297	16		
16	2	201	Total	C	N	O	S	0	0
			1561	975	273	297	16		

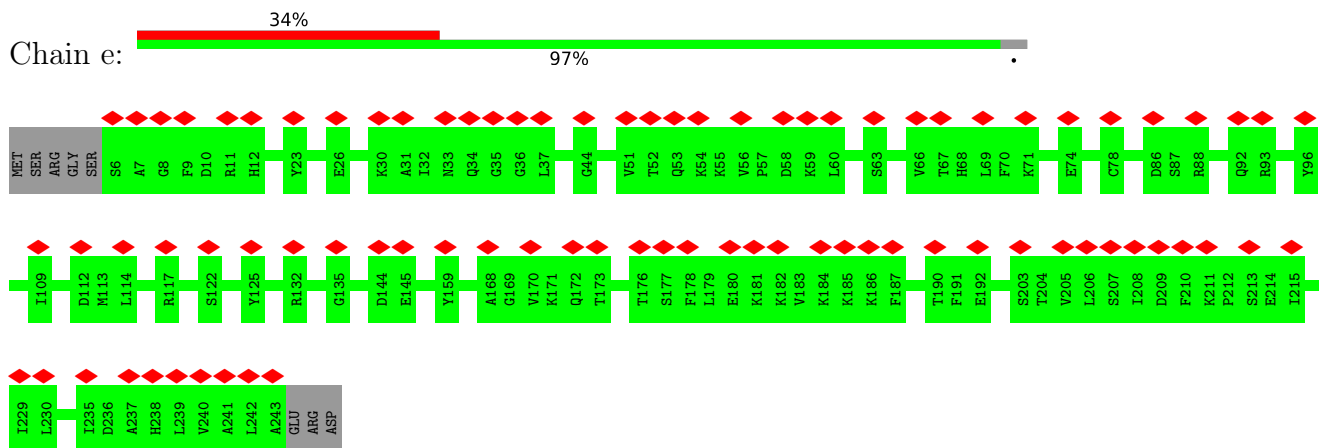
3 Residue-property plots [i](#)

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

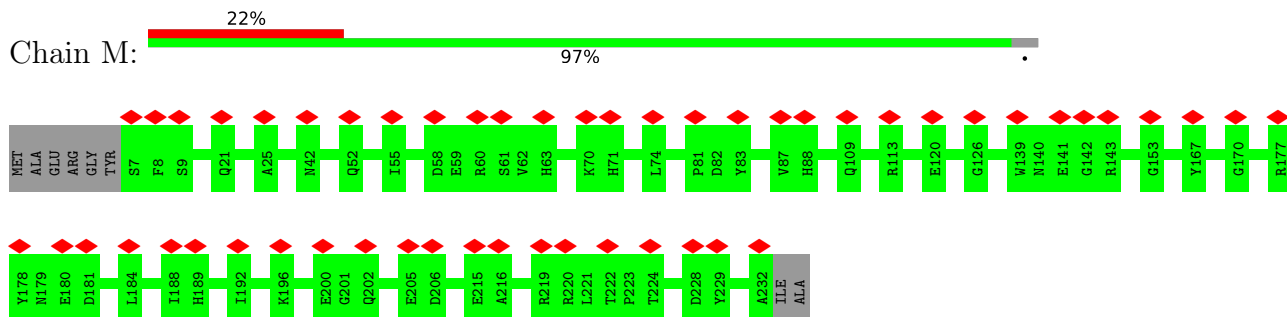
- Molecule 1: Proteasome subunit alpha type-6



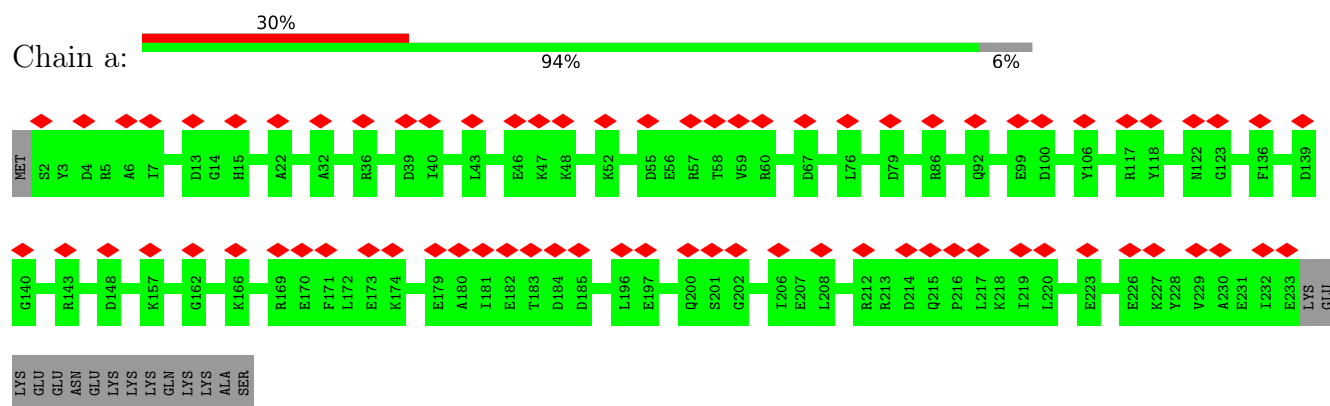
- Molecule 1: Proteasome subunit alpha type-6



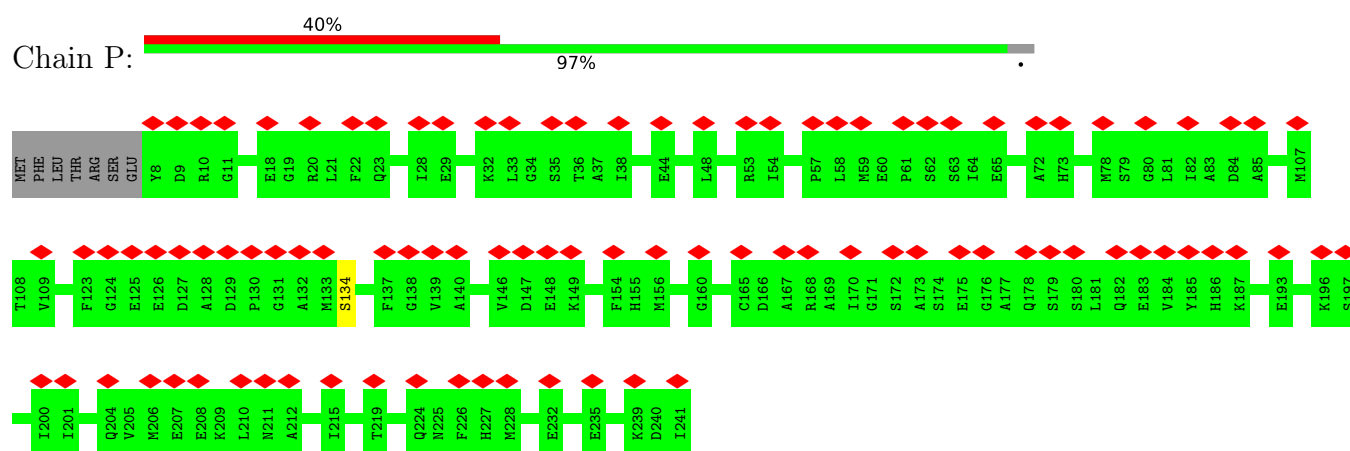
- Molecule 2: Proteasome subunit alpha type-2



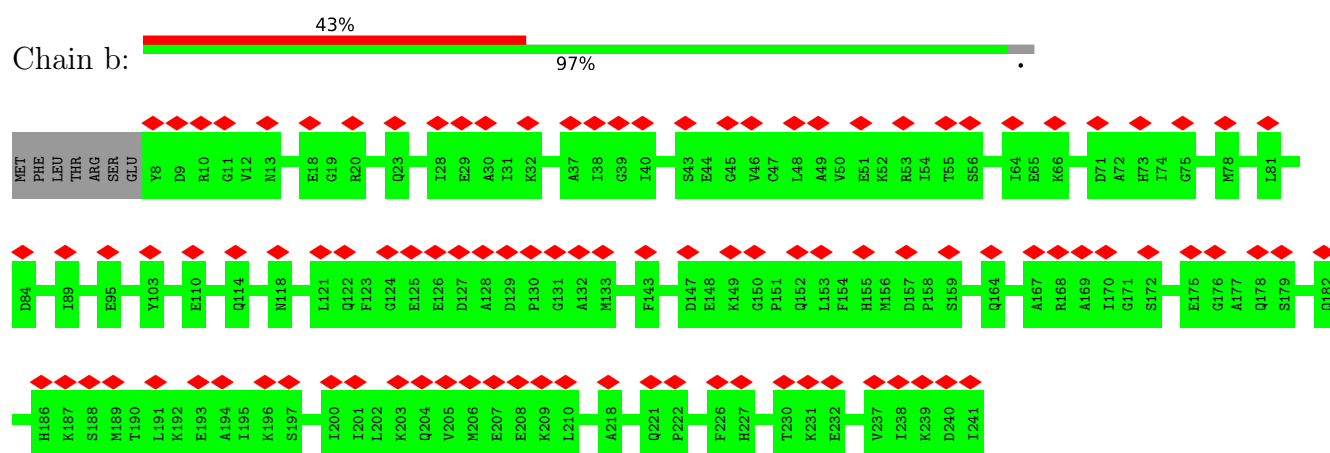
- Molecule 4: Proteasome subunit alpha type-7



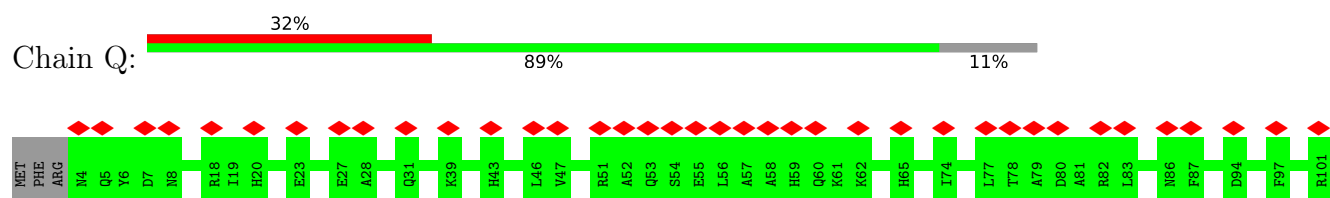
- Molecule 5: Proteasome subunit alpha type-5

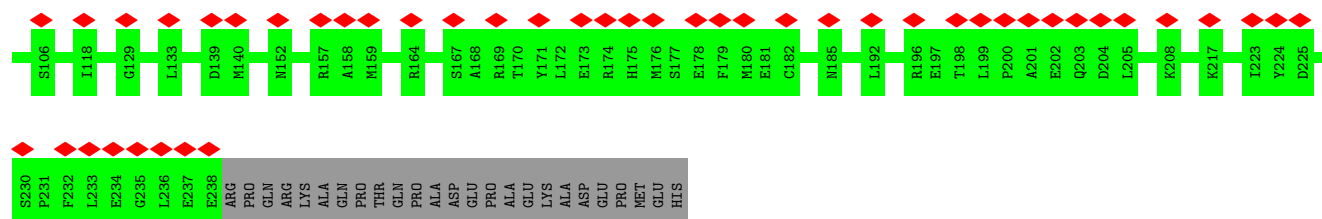


- Molecule 5: Proteasome subunit alpha type-5

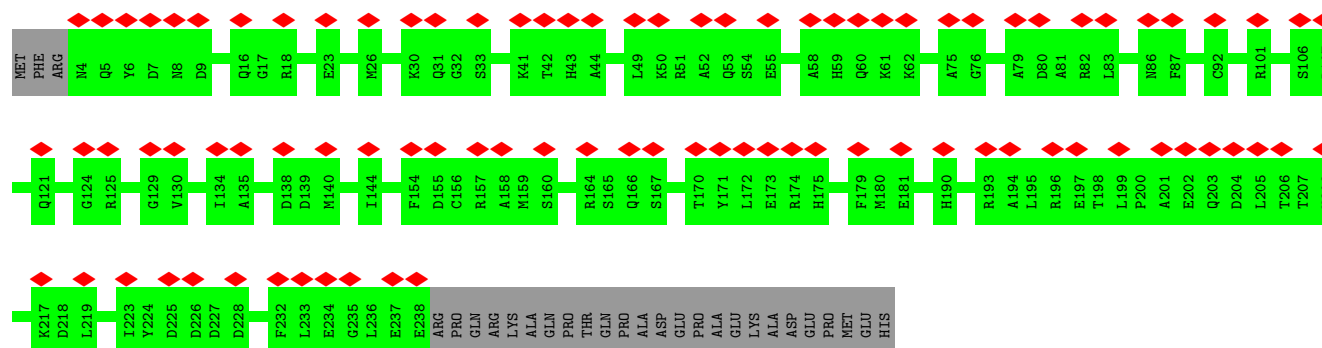
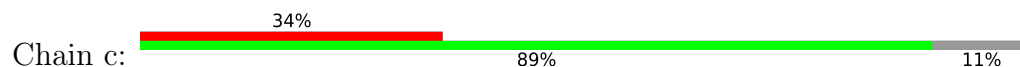


- Molecule 6: Proteasome subunit alpha type-1

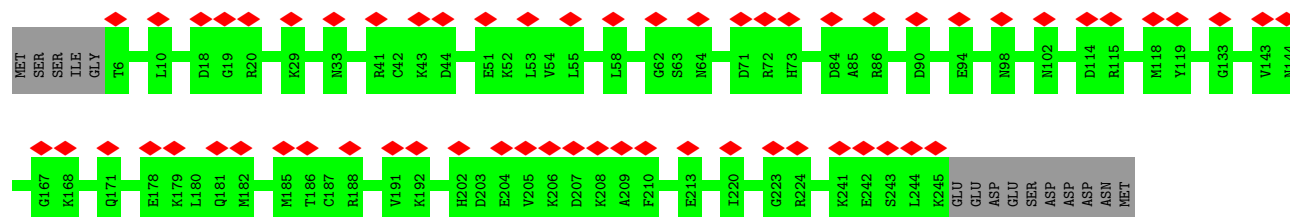




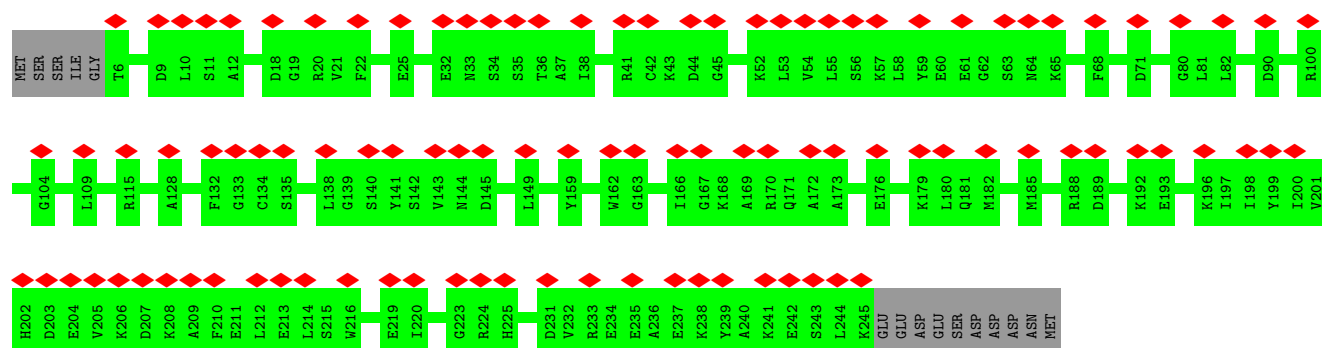
• Molecule 6: Proteasome subunit alpha type-1



• Molecule 7: Proteasome subunit alpha type-3



• Molecule 7: Proteasome subunit alpha type-3

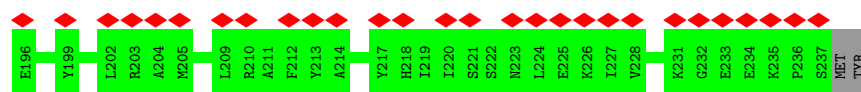


• Molecule 8: Proteasome activator complex subunit 2

[illegible]

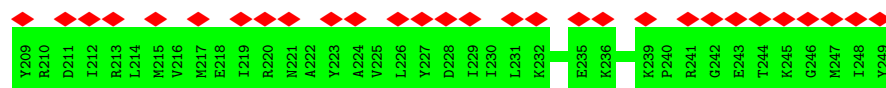
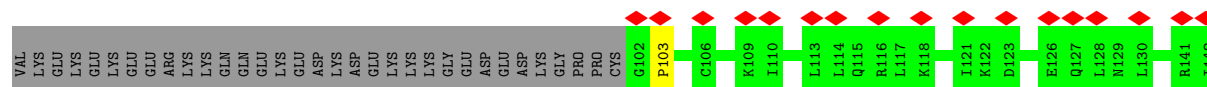
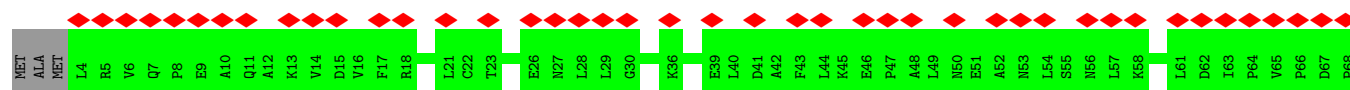
L216	Y217	H218	I219	S222	N223	L224	E225	K226	I227	V228	N229	P230	K231	G232	E233	E234	K235	P236	S237	M238	Y239	E144	L147	E148	M151	K154	E158	A159	F160	Q161	I164	F168	S169	E170	R171	G172	D173	A174	V175	A176	K177	A178	S179	K180	M185	D186	Y187	R188	A189	L190	V191	H192	E193	R194	D195	E196	A197	A198	Y199	C200	E201	L202	R203	A204	M205	D208	L209	R210	A211	F212	Y213	F215
ALA	ASP	PRO	PRO	LYS	ASP	GLU	GLU	THR	ASP	LYS	GLN	GLU	LYS	GLU	VAL	PRO	LYS	GLY	PHE	L94	E98	L101	S102	L103	L104	A105	L106	V107	W111	W112	L122	H127	L128	I129	P130	K131	I132	E133	D134	G135	M136	D137	F138	G139	V140	A141	I142	Q143	L43	N44	Q45	L46	L47	Q48	E49	D50	S51	L52	N53	V54	A55	D56	L57	T58	S59	L60	R61	A62	P63	L64	D65	L66
ALA	ASP	PRO	PRO	LYS	ASP	GLU	GLU	THR	ASP	LYS	GLN	GLU	LYS	GLU	VAL	PRO	LYS	GLY	PHE	L94	E98	L101	S102	L103	L104	A105	L106	V107	W111	W112	L122	H127	L128	I129	P130	K131	I132	E133	D134	G135	M136	D137	F138	G139	V140	A141	I142	Q143	L43	N44	Q45	L46	L47	Q48	E49	D50	S51	L52	N53	V54	A55	D56	L57	T58	S59	L60	R61	A62	P63	L64	D65	L66
ALA	ASP	PRO	PRO	LYS	ASP	GLU	GLU	THR	ASP	LYS	GLN	GLU	LYS	GLU	VAL	PRO	LYS	GLY	PHE	L94	E98	L101	S102	L103	L104	A105	L106	V107	W111	W112	L122	H127	L128	I129	P130	K131	I132	E133	D134	G135	M136	D137	F138	G139	V140	A141	I142	Q143	L43	N44	Q45	L46	L47	Q48	E49	D50	S51	L52	N53	V54	A55	D56	L57	T58	S59	L60	R61	A62	P63	L64	D65	L66

W124	W125	Q126	H127	L128	K131	I132	E133	D134	G135	M136	D137	F138	Q139	V140	Q143	E144	K145	V146	L147	E148	R149	V150	M151	K154	T155	K156	V157	E158	Q161	I164	S165	F168	R171	G172	D173	A174	V175	A176	K180	H183	V184	M185	D186	V187	R188	A189	L190	R194	D195								
A62	P63	L64	D65	T66	P67	I1E	PRO	ASP	PRO	PRO	PRO	LYS	ASP	ASP	GLU	GLU	THR	ASP	LYS	GLN	GLU	LYS	LYS	VAL	P89	C91	Q92	F93	L94	P95	Q96	N97	E98	X99	V100	L101	S102	L103	L104	A105	L106	V107	K108	P109	V110	V111	V112	T113	L114	K115	E116	K117	C118	I119	L120		
MET	ALA	LYS	PRO	CYS	GLY	V7	R8	L9	S10	G11	E12	A13	R14	K15	Q16	V17	E18	V19	F20	R21	Q22	N23	L24	F25	Q26	E27	A28	E29	E30	F31	L32	Y33	R34	F35	L36	P37	Q38	I41	Y42	L43	M44	Q45	L46	L47	Q48	E49	D50	S51	L52	N53	V54	A55	D56	L57	T58	S59	L60



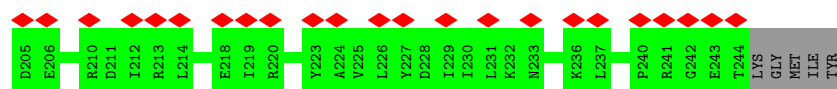
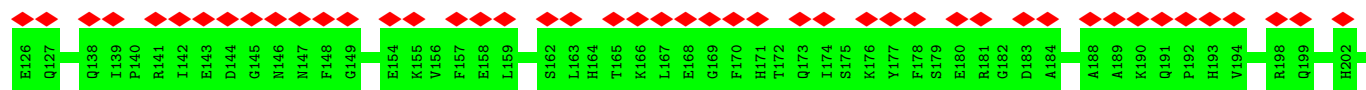
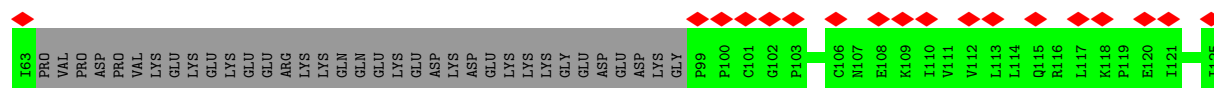
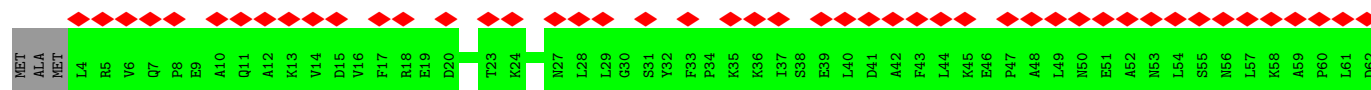
• Molecule 9: Proteasome activator complex subunit 1

Chain B: 55% 85% 14%



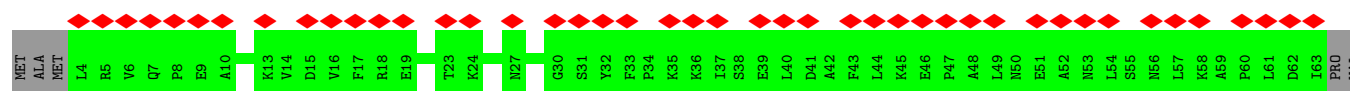
• Molecule 9: Proteasome activator complex subunit 1

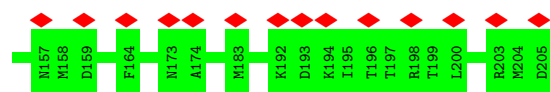
Chain C: 54% 83% 17%



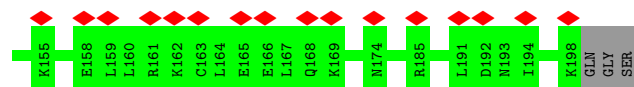
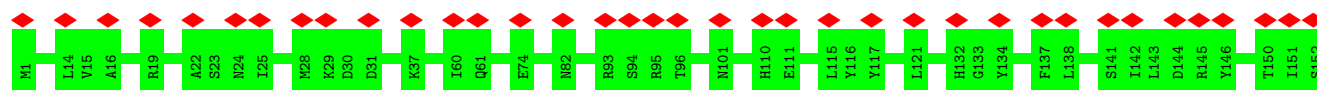
• Molecule 9: Proteasome activator complex subunit 1

Chain E: 57% 83% 16%

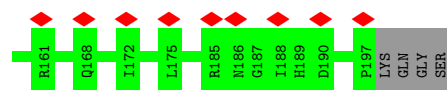
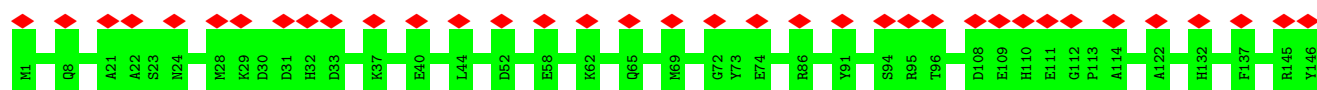




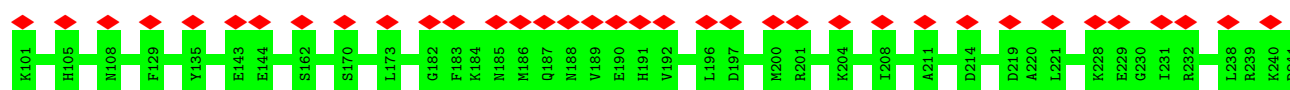
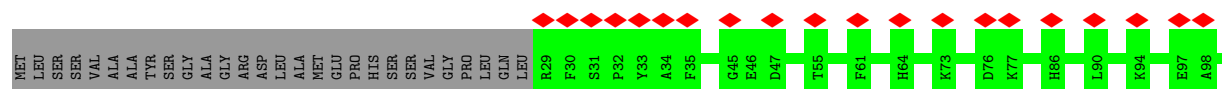
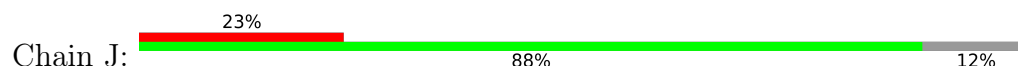
- Molecule 11: Proteasome subunit beta type-2



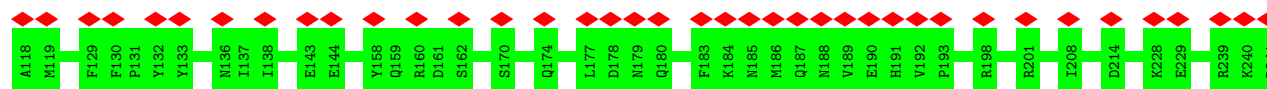
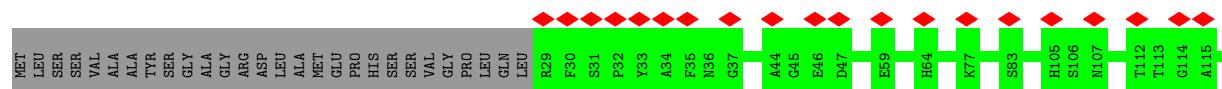
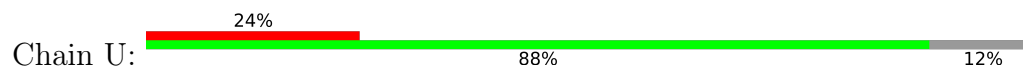
- Molecule 11: Proteasome subunit beta type-2



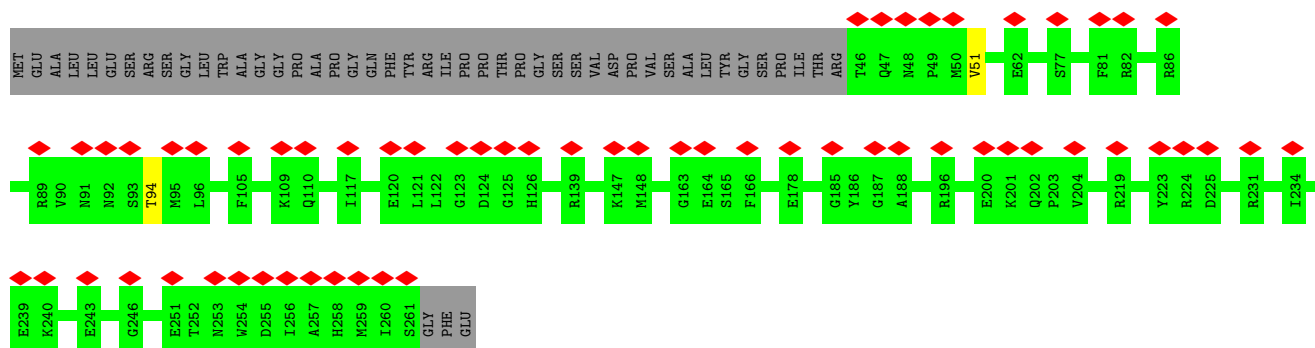
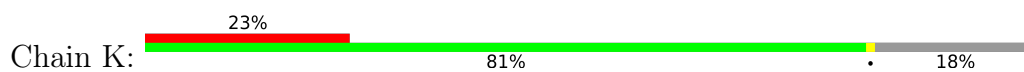
- Molecule 12: Proteasome subunit beta type-1



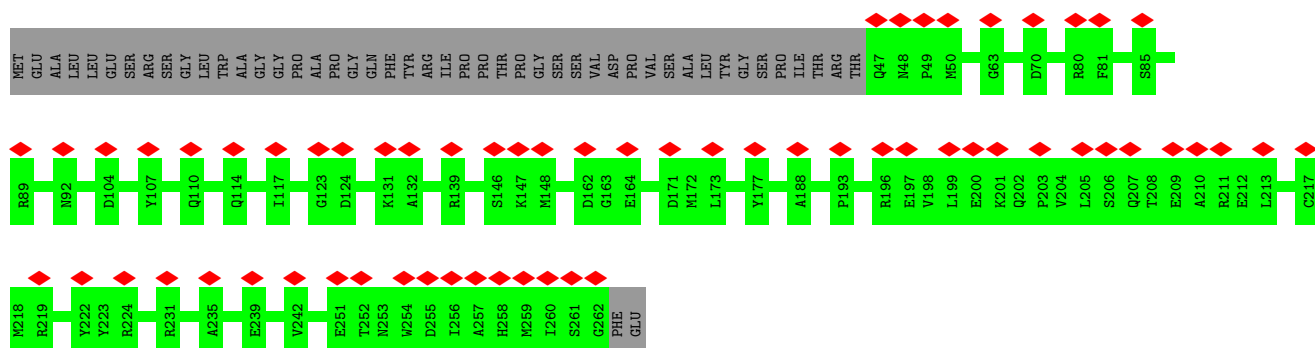
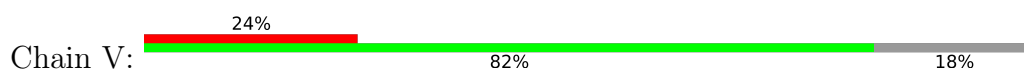
- Molecule 12: Proteasome subunit beta type-1



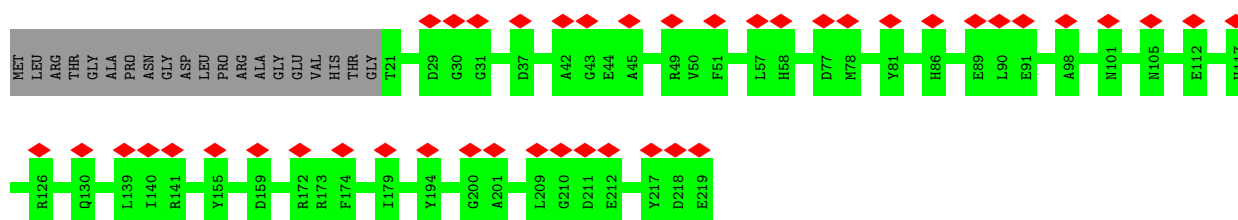
- Molecule 13: Proteasome subunit beta type-4



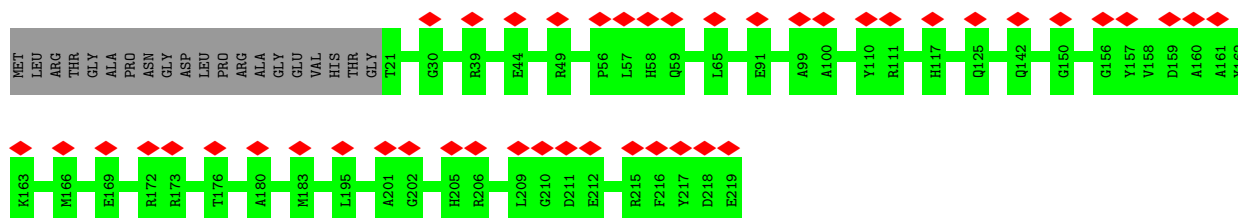
• Molecule 13: Proteasome subunit beta type-4



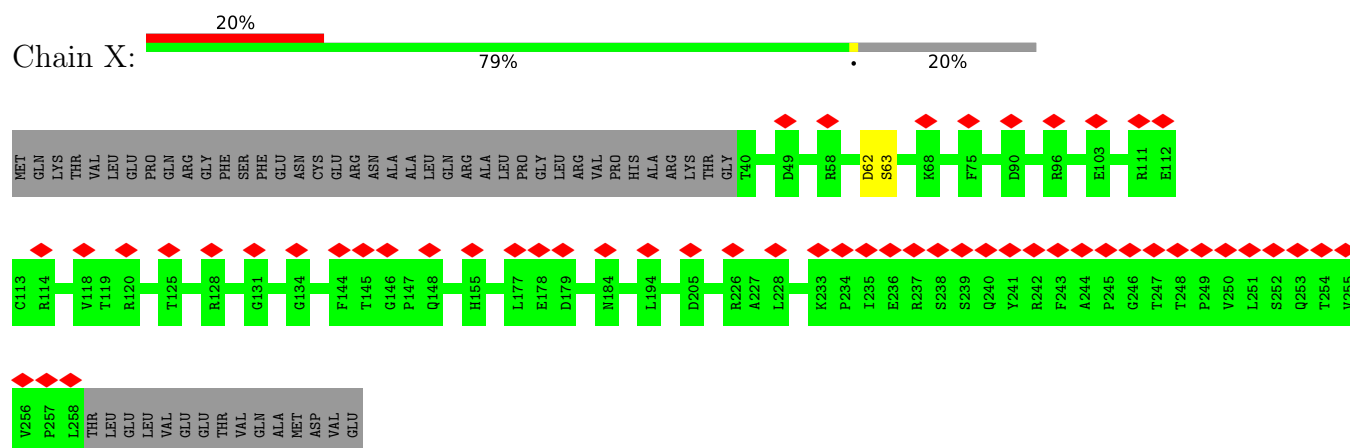
• Molecule 14: Proteasome subunit beta type-9



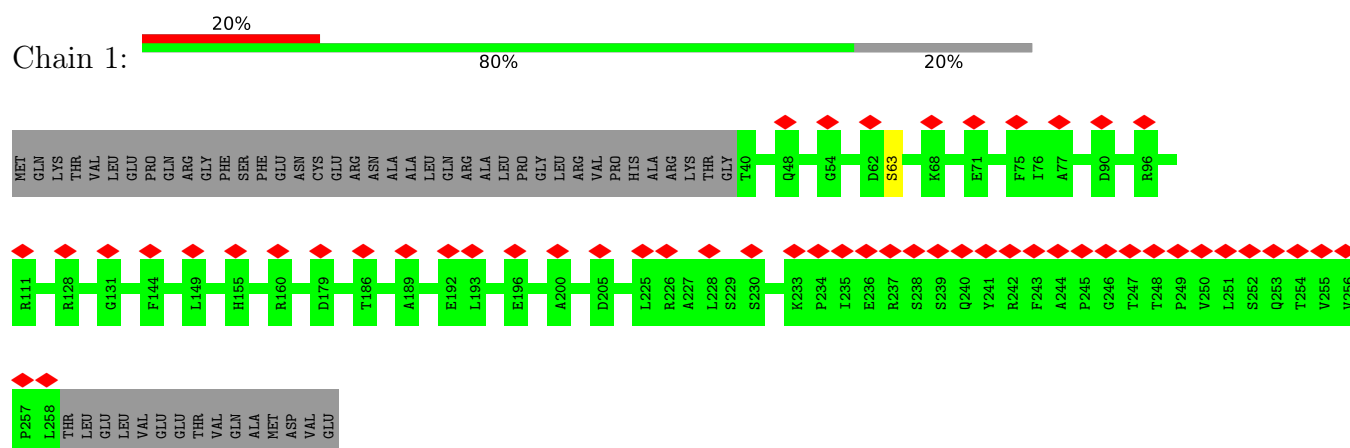
• Molecule 14: Proteasome subunit beta type-9



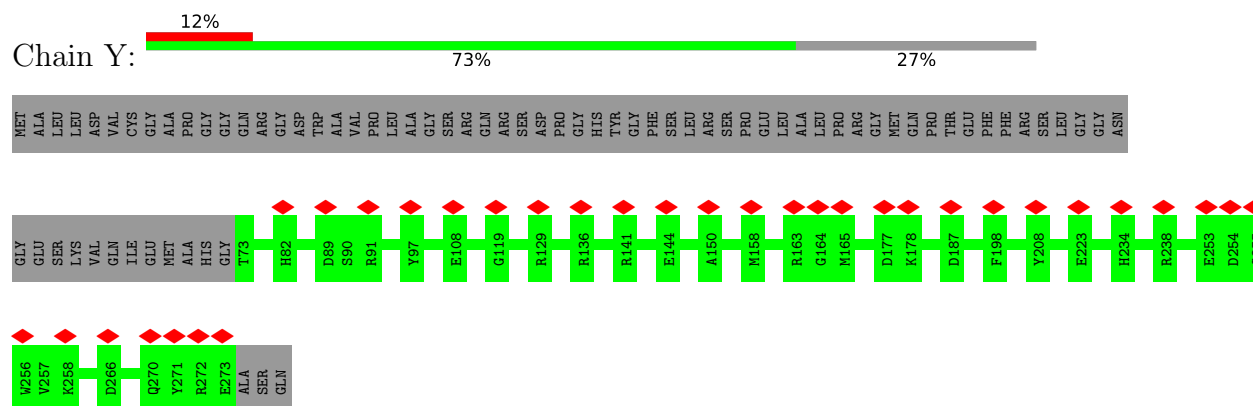
● Molecule 15: Proteasome subunit beta type-10



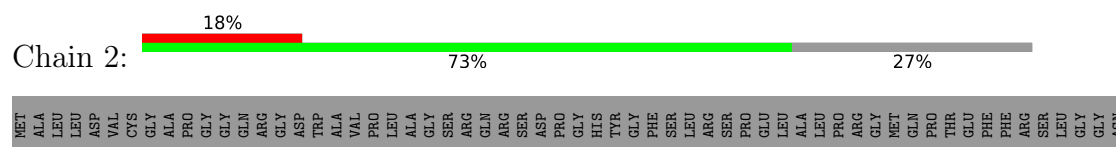
● Molecule 15: Proteasome subunit beta type-10

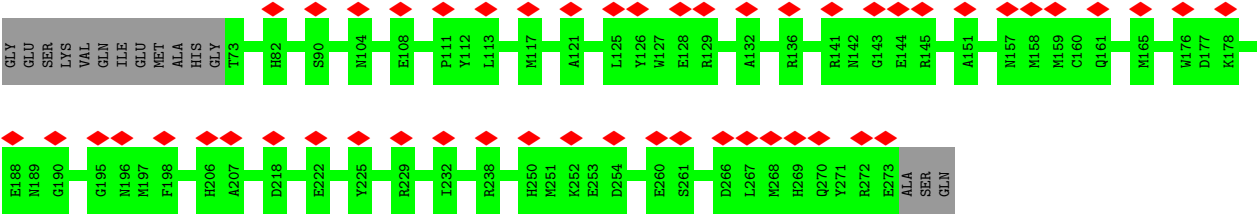


● Molecule 16: Proteasome subunit beta type-8



● Molecule 16: Proteasome subunit beta type-8





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.322	Depositor
Minimum map value	-1.426	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.619	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	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	L	0.24	0/1884	0.41	0/2548
1	e	0.23	0/1890	0.41	0/2556
2	M	0.24	0/1801	0.40	0/2440
2	f	0.24	0/1832	0.41	0/2481
3	N	0.24	0/1966	0.40	0/2648
3	g	0.24	0/1966	0.42	0/2648
4	O	0.23	0/1851	0.43	0/2501
4	a	0.23	0/1851	0.42	0/2501
5	P	0.24	0/1818	0.42	0/2455
5	b	0.23	0/1818	0.40	0/2455
6	Q	0.23	0/1880	0.41	0/2541
6	c	0.23	0/1880	0.43	0/2541
7	R	0.24	0/1914	0.39	0/2578
7	d	0.24	0/1914	0.41	0/2578
8	A	0.24	0/1714	0.36	0/2315
8	D	0.23	0/1708	0.35	0/2308
8	F	0.23	0/1726	0.37	0/2331
9	B	0.25	0/1751	0.36	0/2366
9	C	0.23	0/1692	0.36	0/2285
9	E	0.24	0/1713	0.37	0/2309
9	G	0.23	0/1681	0.37	0/2267
10	H	0.24	0/1623	0.45	0/2188
10	S	0.25	0/1623	0.44	0/2188
11	I	0.24	0/1627	0.42	0/2201
11	T	0.24	0/1618	0.42	0/2190
12	J	0.24	0/1676	0.43	0/2258
12	U	0.24	0/1676	0.43	0/2258
13	K	0.23	0/1718	0.43	0/2324
13	V	0.24	0/1715	0.45	0/2319
14	W	0.24	0/1529	0.41	0/2071
14	Z	0.24	0/1529	0.42	0/2071
15	1	0.25	0/1637	0.45	0/2225
15	X	0.25	0/1637	0.44	0/2225
16	2	0.24	0/1592	0.43	0/2145

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	Y	0.25	0/1592	0.41	0/2145
All	All	0.24	0/61042	0.41	0/82460

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](#)

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

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	L	234/246 (95%)	220 (94%)	14 (6%)	0	100	100
1	e	236/246 (96%)	217 (92%)	19 (8%)	0	100	100
2	M	224/234 (96%)	217 (97%)	7 (3%)	0	100	100
2	f	228/234 (97%)	220 (96%)	8 (4%)	0	100	100
3	N	244/261 (94%)	234 (96%)	10 (4%)	0	100	100
3	g	244/261 (94%)	226 (93%)	17 (7%)	1 (0%)	34	71
4	O	230/248 (93%)	220 (96%)	10 (4%)	0	100	100
4	a	230/248 (93%)	218 (95%)	12 (5%)	0	100	100
5	P	232/241 (96%)	218 (94%)	14 (6%)	0	100	100
5	b	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
6	Q	233/263 (89%)	217 (93%)	16 (7%)	0	100	100
6	c	233/263 (89%)	224 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	R	238/255 (93%)	230 (97%)	8 (3%)	0	100	100
7	d	238/255 (93%)	227 (95%)	11 (5%)	0	100	100
8	A	205/239 (86%)	204 (100%)	1 (0%)	0	100	100
8	D	203/239 (85%)	193 (95%)	9 (4%)	1 (0%)	29	67
8	F	206/239 (86%)	202 (98%)	4 (2%)	0	100	100
9	B	209/249 (84%)	202 (97%)	6 (3%)	1 (0%)	29	67
9	C	202/249 (81%)	198 (98%)	4 (2%)	0	100	100
9	E	204/249 (82%)	194 (95%)	9 (4%)	1 (0%)	29	67
9	G	201/249 (81%)	194 (96%)	4 (2%)	3 (2%)	10	44
10	H	202/205 (98%)	188 (93%)	14 (7%)	0	100	100
10	S	202/205 (98%)	185 (92%)	16 (8%)	1 (0%)	29	67
11	I	196/201 (98%)	186 (95%)	10 (5%)	0	100	100
11	T	195/201 (97%)	183 (94%)	12 (6%)	0	100	100
12	J	211/241 (88%)	198 (94%)	13 (6%)	0	100	100
12	U	211/241 (88%)	197 (93%)	14 (7%)	0	100	100
13	K	214/264 (81%)	206 (96%)	7 (3%)	1 (0%)	29	67
13	V	214/264 (81%)	203 (95%)	11 (5%)	0	100	100
14	W	197/219 (90%)	185 (94%)	12 (6%)	0	100	100
14	Z	197/219 (90%)	191 (97%)	6 (3%)	0	100	100
15	1	217/273 (80%)	203 (94%)	13 (6%)	1 (0%)	29	67
15	X	217/273 (80%)	199 (92%)	17 (8%)	1 (0%)	29	67
16	2	199/276 (72%)	186 (94%)	13 (6%)	0	100	100
16	Y	199/276 (72%)	185 (93%)	14 (7%)	0	100	100
All	All	7577/8567 (88%)	7194 (95%)	372 (5%)	11 (0%)	54	84

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	232	GLY
15	1	63	SER
15	X	63	SER
9	G	240	PRO
9	G	241	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	203/210 (97%)	203 (100%)	0	100	100
1	e	203/210 (97%)	203 (100%)	0	100	100
2	M	186/191 (97%)	186 (100%)	0	100	100
2	f	188/191 (98%)	188 (100%)	0	100	100
3	N	207/221 (94%)	207 (100%)	0	100	100
3	g	207/221 (94%)	207 (100%)	0	100	100
4	O	196/211 (93%)	196 (100%)	0	100	100
4	a	196/211 (93%)	196 (100%)	0	100	100
5	P	196/203 (97%)	195 (100%)	1 (0%)	88	93
5	b	196/203 (97%)	196 (100%)	0	100	100
6	Q	201/225 (89%)	201 (100%)	0	100	100
6	c	201/225 (89%)	201 (100%)	0	100	100
7	R	198/212 (93%)	198 (100%)	0	100	100
7	d	198/212 (93%)	198 (100%)	0	100	100
8	A	183/212 (86%)	183 (100%)	0	100	100
8	D	183/212 (86%)	180 (98%)	3 (2%)	62	78
8	F	185/212 (87%)	185 (100%)	0	100	100
9	B	191/224 (85%)	191 (100%)	0	100	100
9	C	185/224 (83%)	185 (100%)	0	100	100
9	E	186/224 (83%)	186 (100%)	0	100	100
9	G	183/224 (82%)	183 (100%)	0	100	100
10	H	174/175 (99%)	174 (100%)	0	100	100
10	S	174/175 (99%)	173 (99%)	1 (1%)	86	92
11	I	169/171 (99%)	169 (100%)	0	100	100
11	T	168/171 (98%)	168 (100%)	0	100	100
12	J	177/198 (89%)	177 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	U	177/198 (89%)	177 (100%)	0	100	100
13	K	178/215 (83%)	177 (99%)	1 (1%)	86	92
13	V	177/215 (82%)	177 (100%)	0	100	100
14	W	153/167 (92%)	153 (100%)	0	100	100
14	Z	153/167 (92%)	153 (100%)	0	100	100
15	1	170/216 (79%)	170 (100%)	0	100	100
15	X	170/216 (79%)	169 (99%)	1 (1%)	86	92
16	2	166/222 (75%)	166 (100%)	0	100	100
16	Y	166/222 (75%)	166 (100%)	0	100	100
All	All	6444/7206 (89%)	6437 (100%)	7 (0%)	93	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	D	238	MET
13	K	94	THR
15	X	62	ASP
10	S	116	THR
8	D	237	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
10	H	33	GLN
12	U	105	HIS
16	2	247	ASN
12	J	86	HIS
12	J	185	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

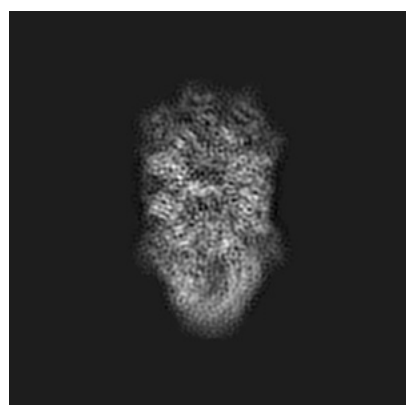
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30824. These allow visual inspection of the internal detail of the map and identification of artifacts.

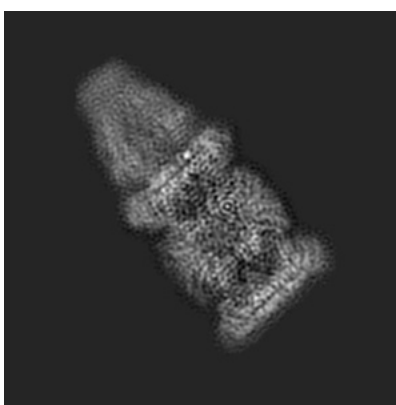
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

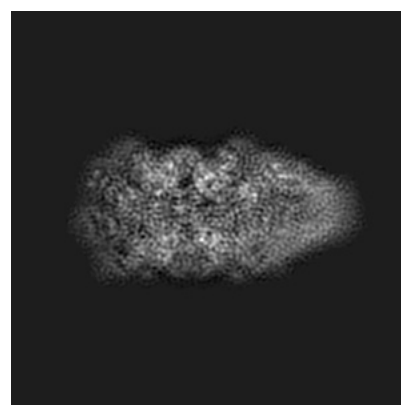
6.1.1 Primary map



X



Y



Z

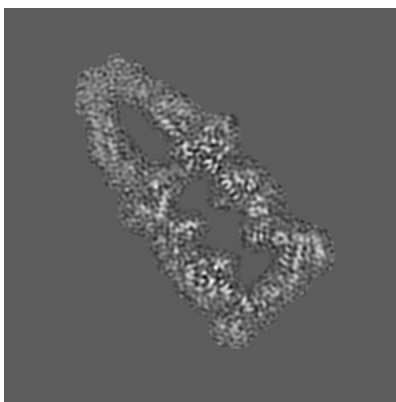
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

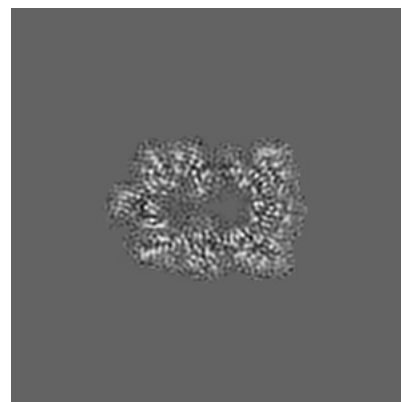
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

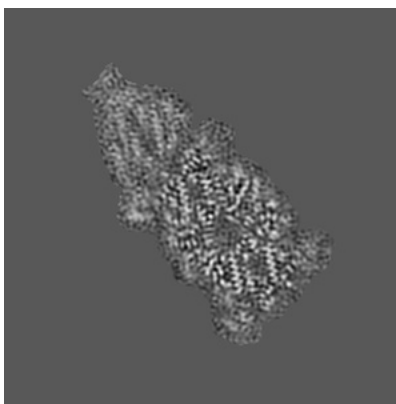
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

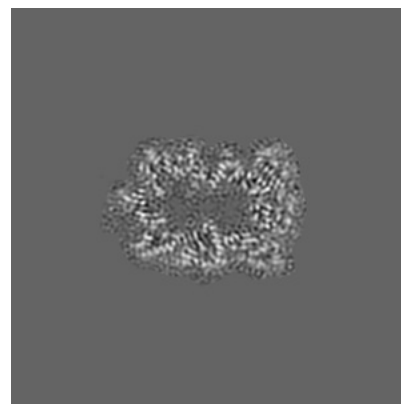
6.3.1 Primary map



X Index: 120



Y Index: 109



Z Index: 130

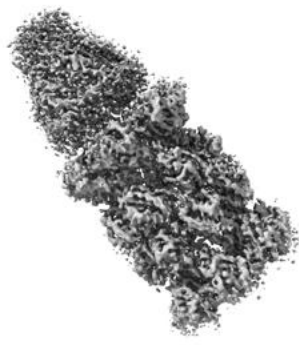
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

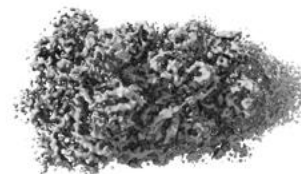
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.619. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

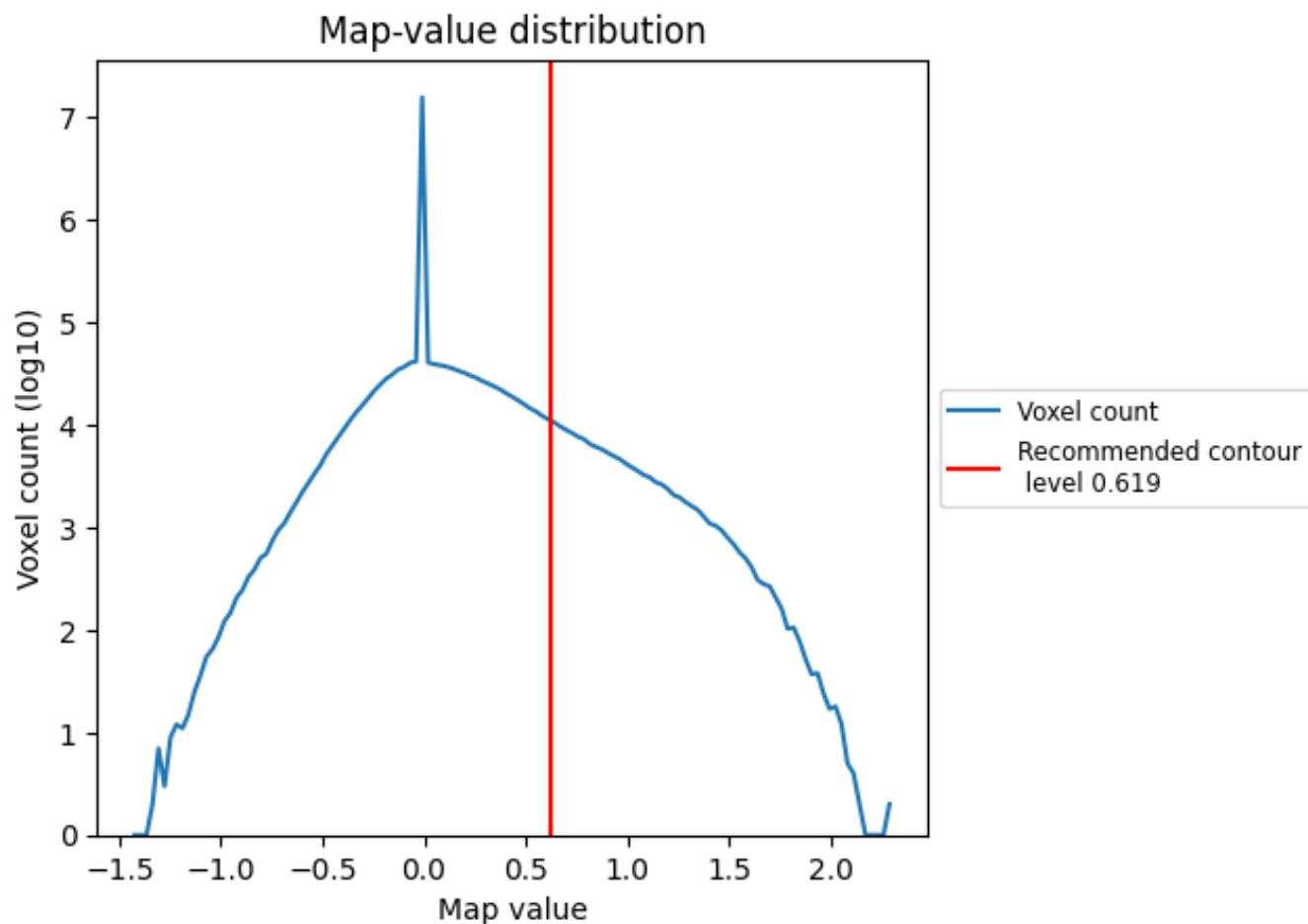
6.5 Mask visualisation

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

7 Map analysis [i](#)

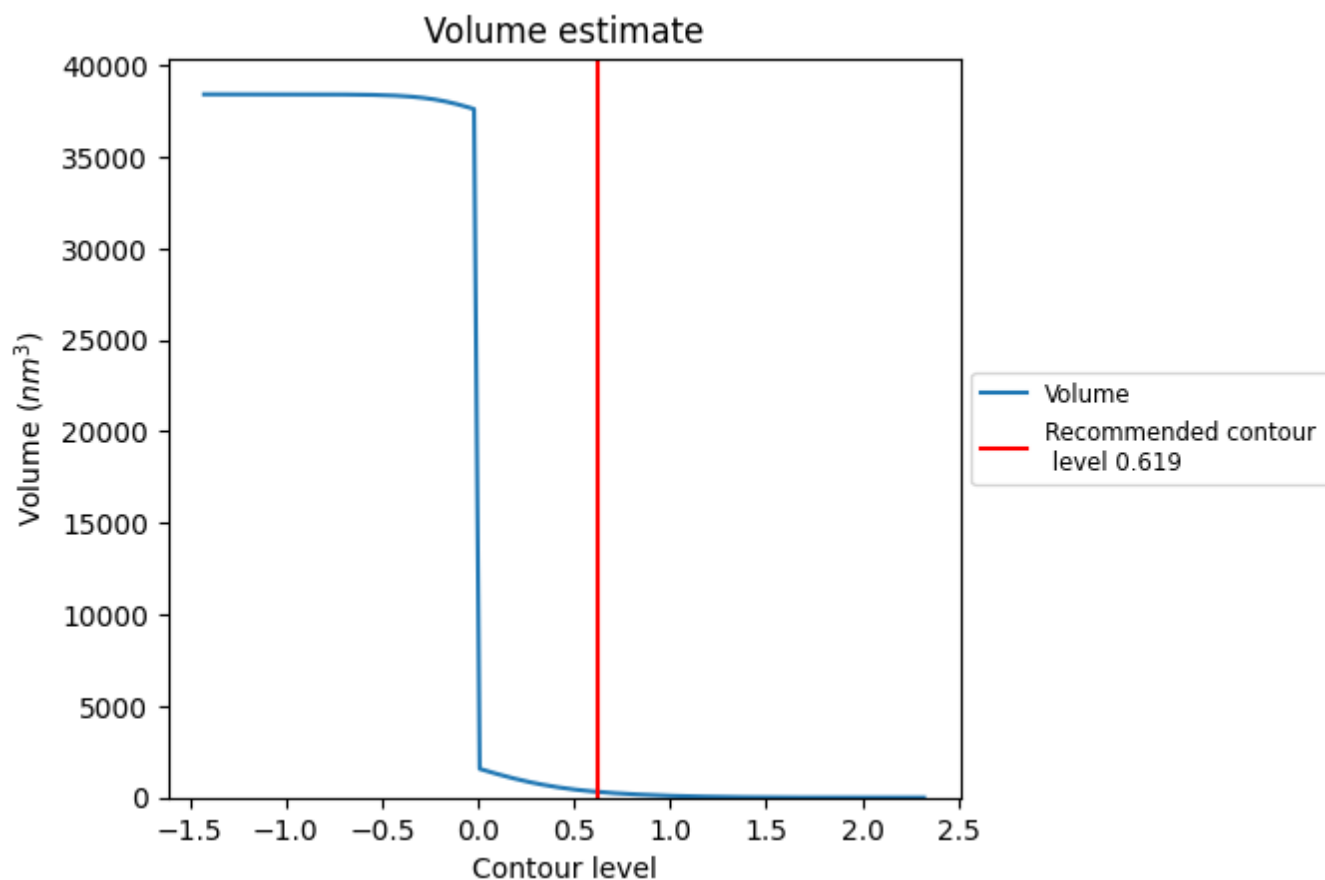
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

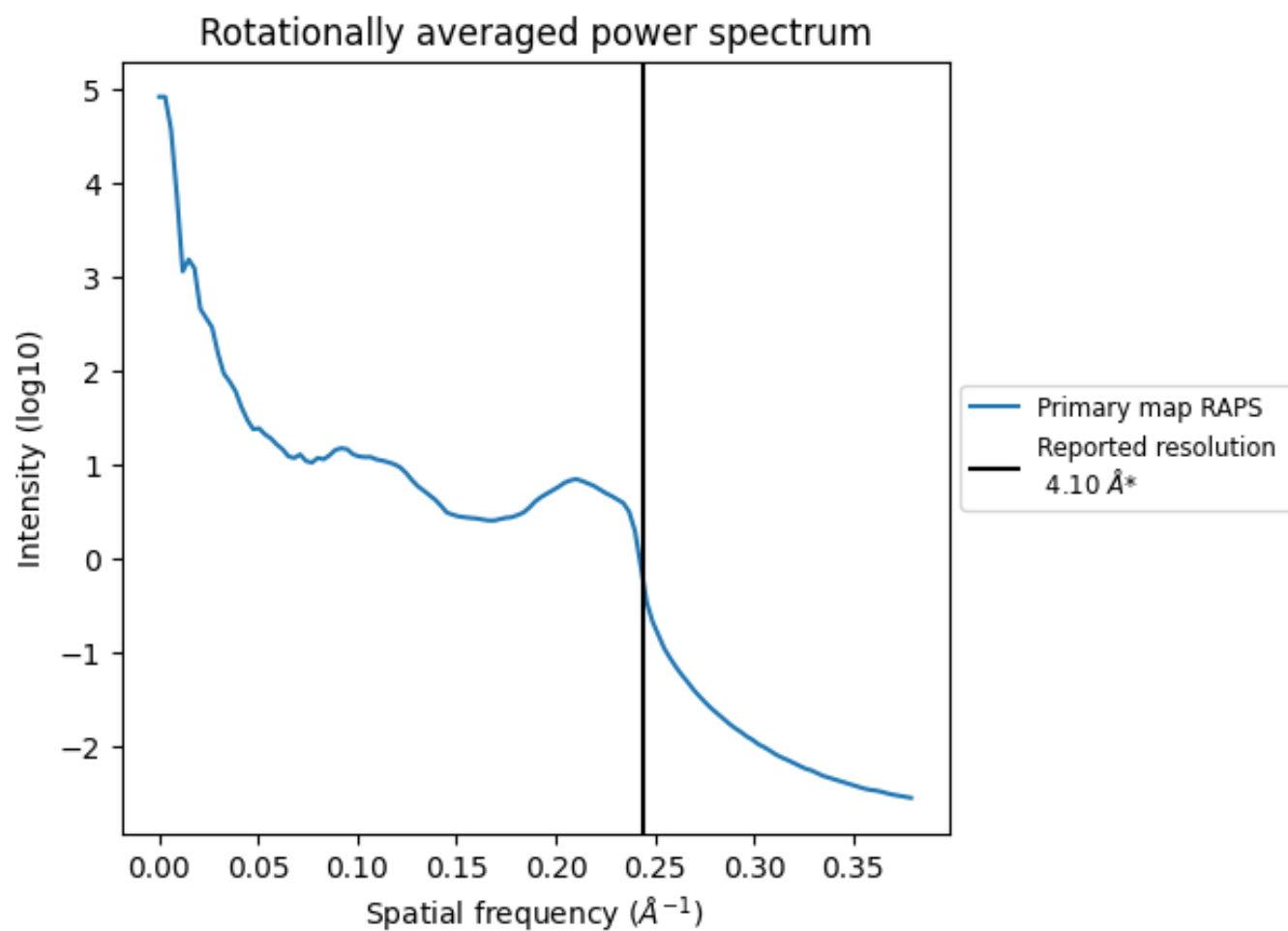
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm^3 ; this corresponds to an approximate mass of 285 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

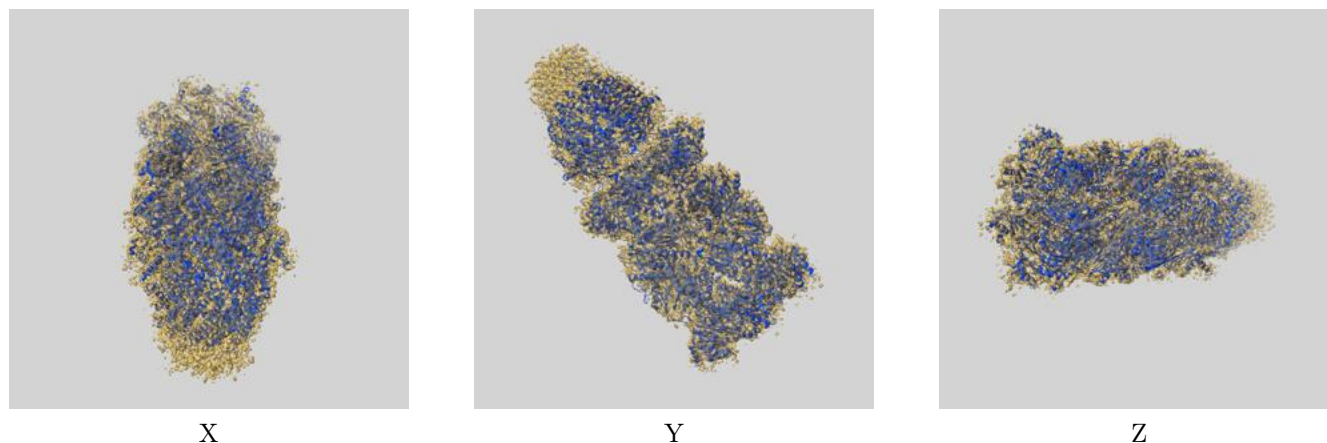
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

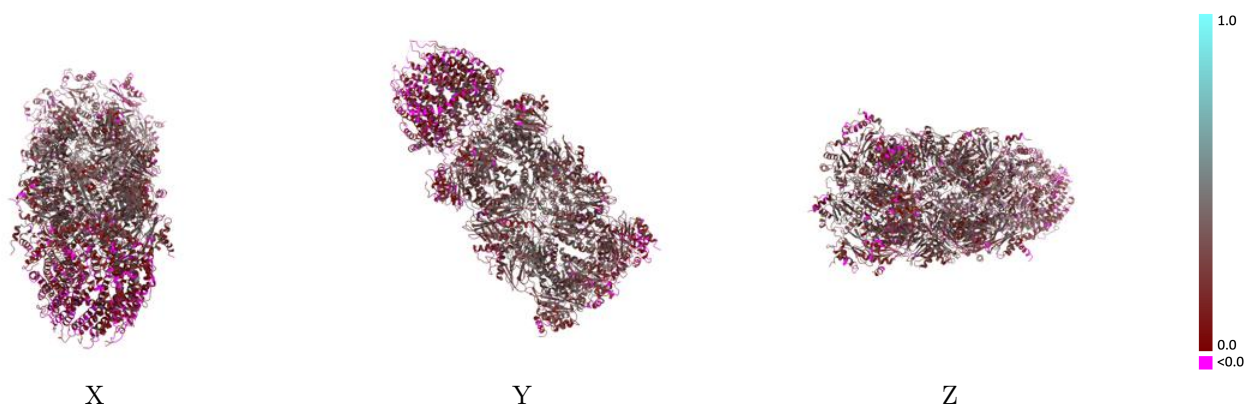
This section contains information regarding the fit between EMDB map EMD-30824 and PDB model 7DR6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



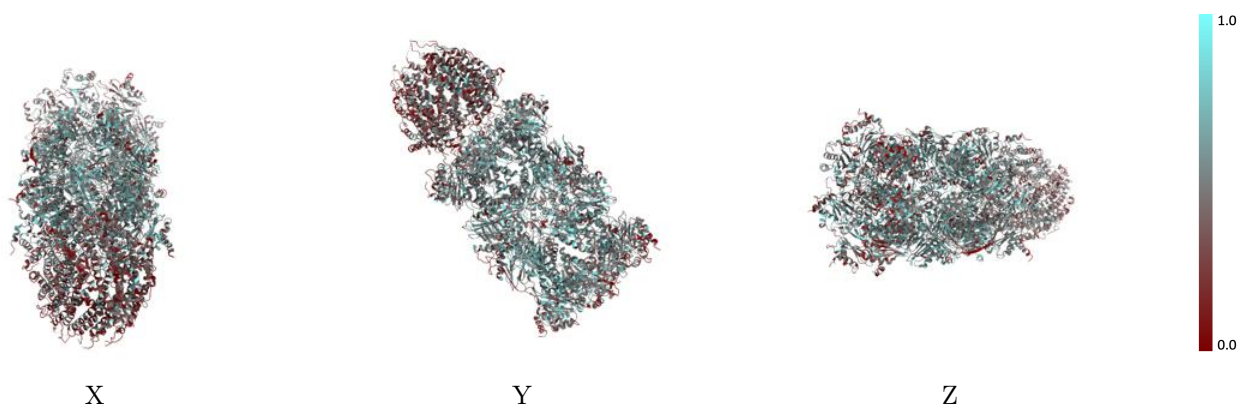
The images above show the 3D surface view of the map at the recommended contour level 0.619 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



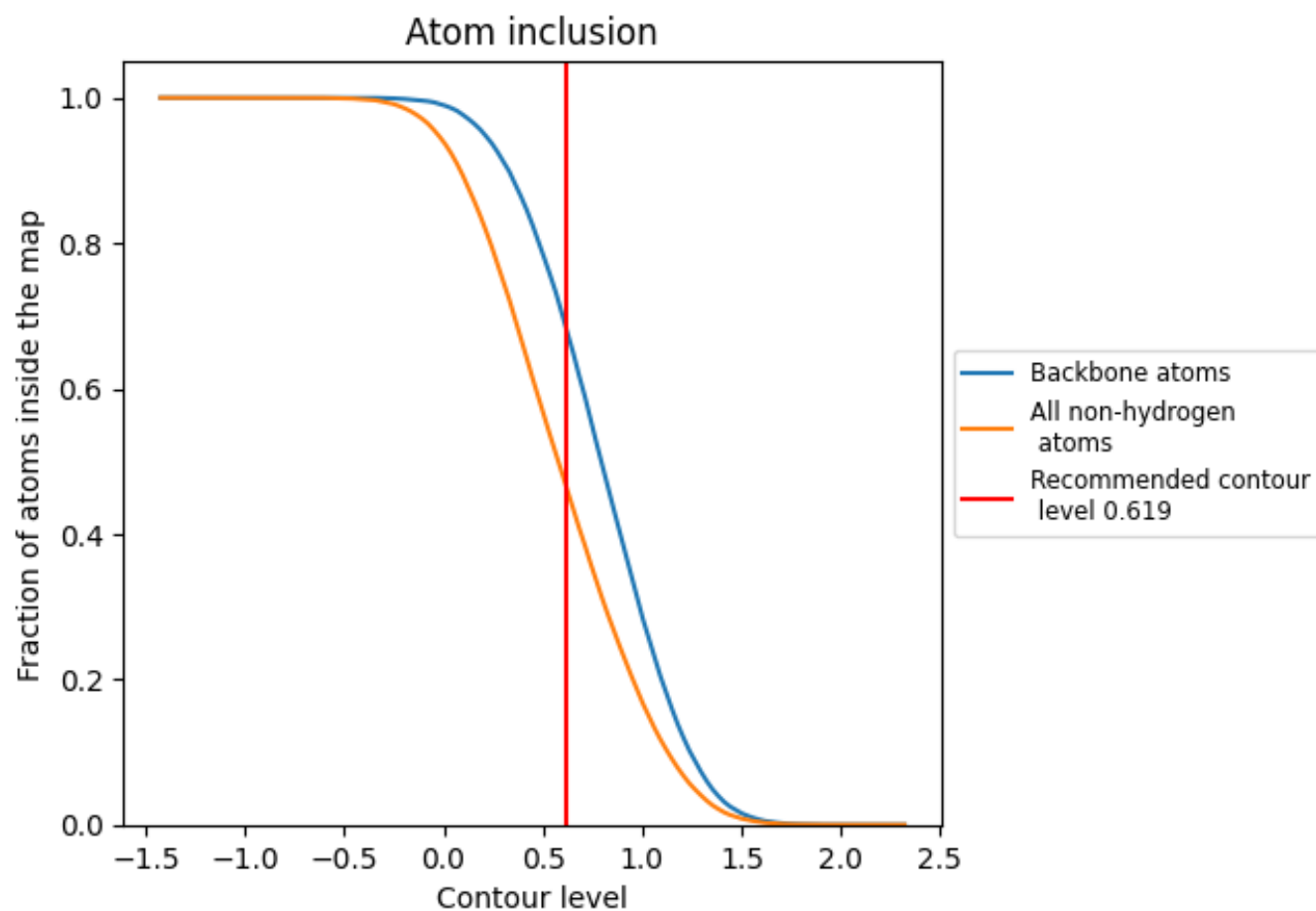
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.619).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 46% 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 (0.619) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4639	 0.2400
1	 0.5174	 0.2920
2	 0.5309	 0.2430
A	 0.3708	 0.1670
B	 0.3286	 0.1390
C	 0.3178	 0.1130
D	 0.3305	 0.1600
E	 0.2951	 0.1240
F	 0.2722	 0.0870
G	 0.3159	 0.1060
H	 0.5310	 0.3120
I	 0.5087	 0.2890
J	 0.5115	 0.2890
K	 0.4960	 0.2680
L	 0.5203	 0.2840
M	 0.5307	 0.2810
N	 0.4953	 0.2640
O	 0.4826	 0.2330
P	 0.4236	 0.1750
Q	 0.4842	 0.2320
R	 0.5152	 0.2770
S	 0.5297	 0.3110
T	 0.5304	 0.2860
U	 0.4910	 0.2600
V	 0.5055	 0.2960
W	 0.5491	 0.3100
X	 0.5136	 0.3000
Y	 0.5566	 0.3170
Z	 0.5512	 0.2920
a	 0.4882	 0.2780
b	 0.4298	 0.2190
c	 0.4609	 0.2200
d	 0.4304	 0.1920
e	 0.4496	 0.2300
f	 0.5122	 0.2870
g	 0.4916	 0.2890

