



wwPDB EM Validation Summary Report ⓘ

Jul 25, 2026 – 12:58 PM EDT

PDB ID : 9PMQ / pdb_00009pmq
EMDB ID : EMD-71741
Title : Human 26S proteasome bound to TXNL1 with closed gate of core particle
Authors : Chen, X.; Negi, H.; Walters, K.J.
Deposited on : 2025-07-18
Resolution : 4.00 Å(reported)
Based on initial models : 7WSI, 1WWY

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:

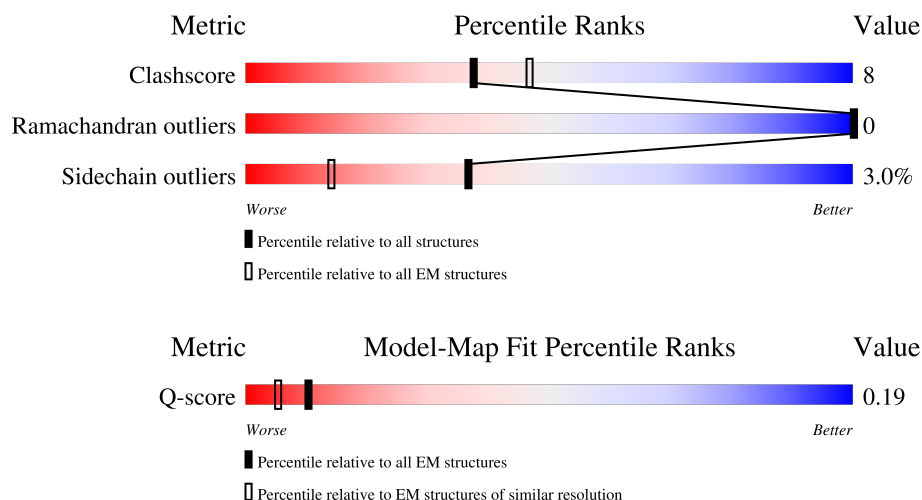
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 4.00 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.



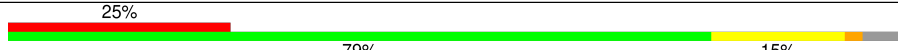
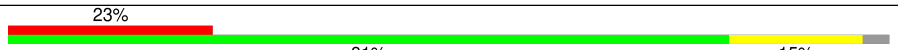
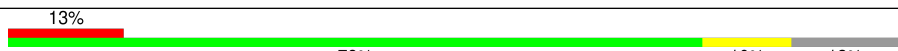
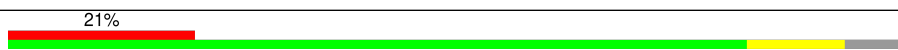
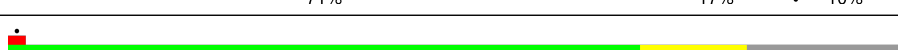
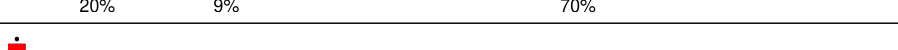
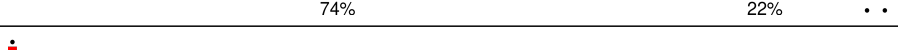
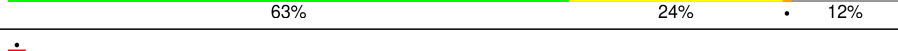
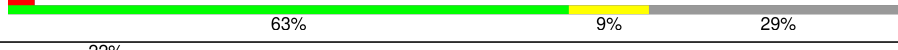
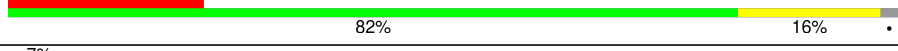
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	398	
4	D	418	

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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
8	H	234	
9	I	261	
10	J	248	
11	K	241	
12	L	269	
13	M	255	
14	U	953	
15	V	534	
16	W	456	
17	X	422	
18	Y	389	
19	Z	324	
20	a	376	
21	b	377	
22	c	310	
23	d	350	
24	e	70	
25	f	908	
26	g	289	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 69506 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total	C	N	O	S	0	0
			3237	2038	569	612	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	375	Total	C	N	O	S	0	0
			2960	1861	504	580	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	381	Total	C	N	O	S	0	0
			2988	1876	536	559	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	397	Total	C	N	O	S	0	0
			3112	1960	535	599	18		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1903	1206	320	364	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1971	1245	339	377	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	233	Total	C	N	O	S	0	0
			1778	1116	294	357	11		

- Molecule 12 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	853	Total	C	N	O	S	0	0
			6671	4235	1133	1259	44		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	442	Total	C	N	O	S	0	0
			3594	2287	643	651	13		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	446	Total	C	N	O	S	0	0
			3635	2302	622	687	24		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	125	Total	C	N	O	S	0	0
			1007	643	167	195	2		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	372	Total	C	N	O	S	0	0
			2987	1907	509	556	15		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 24 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	50	Total	C	N	O	S	0	0
			425	260	65	100			

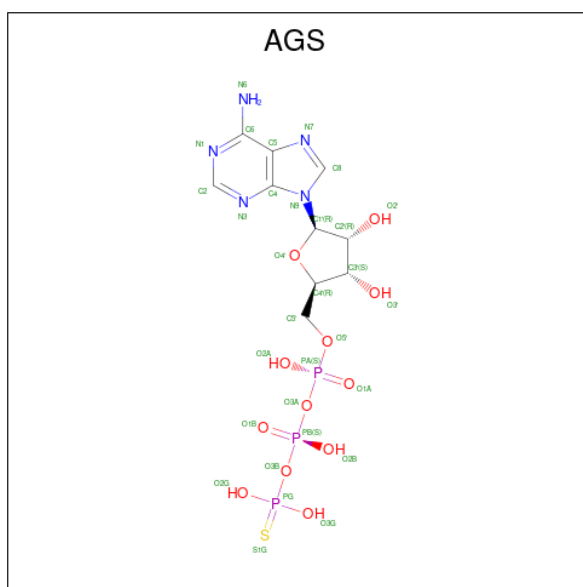
- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

- Molecule 26 is a protein called Thioredoxin-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	172	Total	C	N	O	S	0	0
			1376	865	226	276	9		

- Molecule 27 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

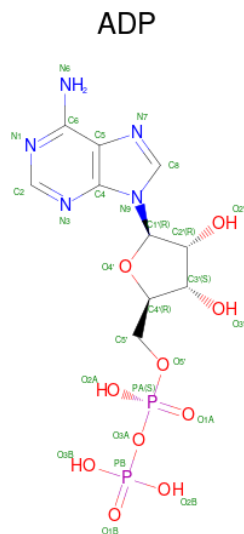


Mol	Chain	Residues	Atoms						AltConf
27	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
27	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
27	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
27	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Mg	0
			1	1	
28	D	1	Total	Mg	0
			1	1	
28	E	1	Total	Mg	0
			1	1	
28	F	1	Total	Mg	0
			1	1	

- Molecule 29 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 27	C 10	N 5	O 10	P 2	0
29	C	1	Total 27	C 10	N 5	O 10	P 2	0

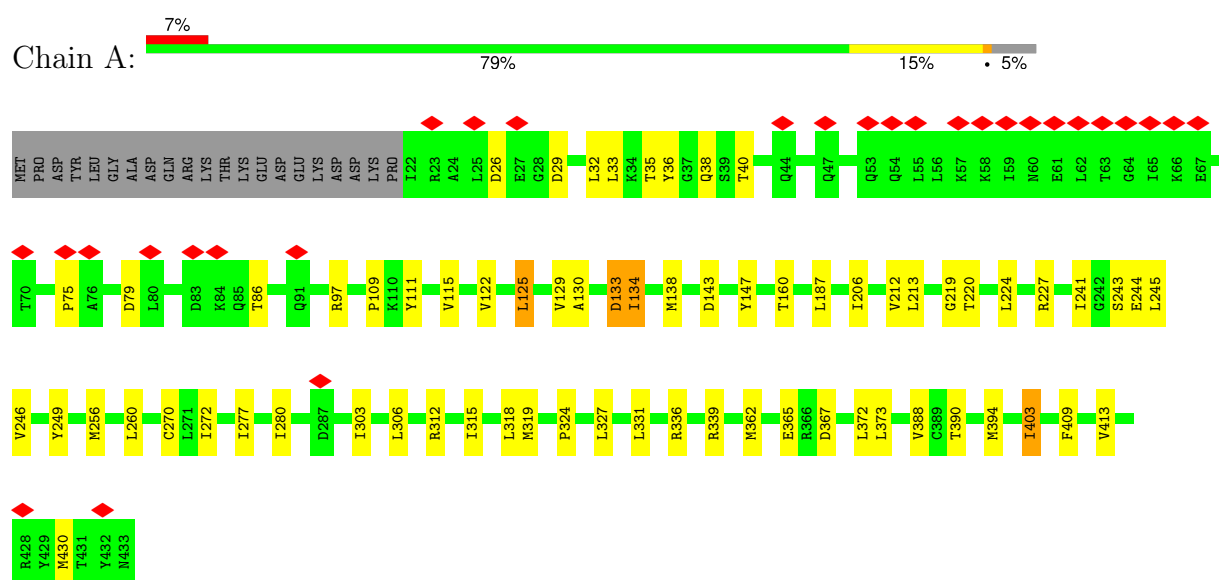
- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

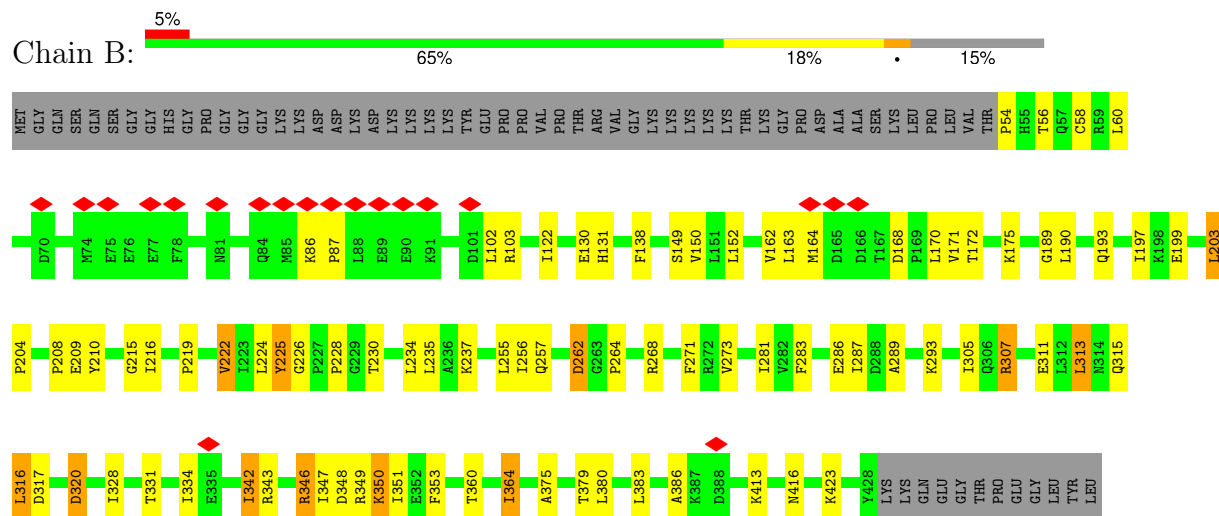
3 Residue-property plots

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

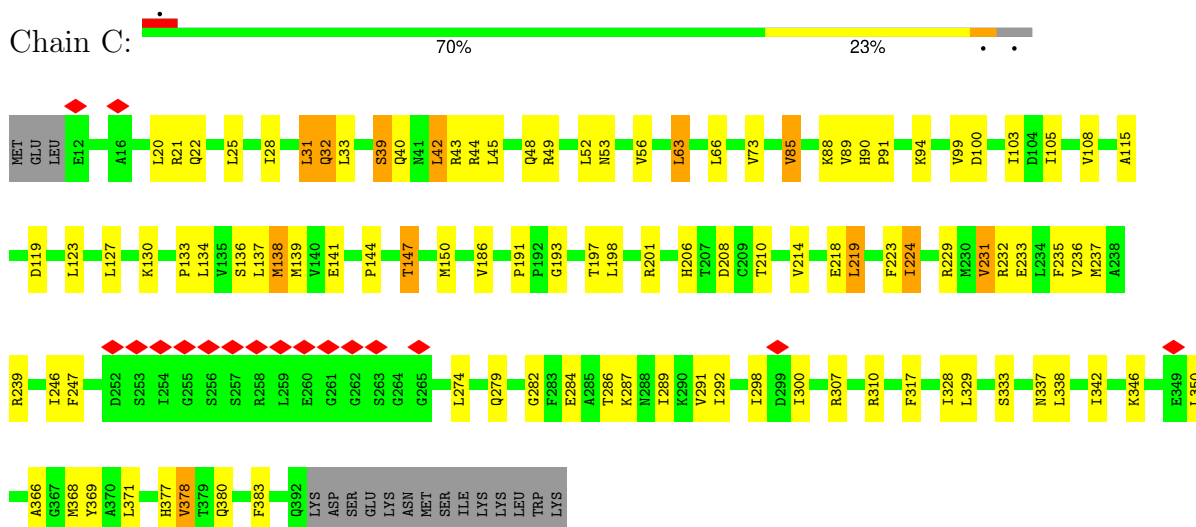
- Molecule 1: 26S proteasome regulatory subunit 7



- Molecule 2: 26S proteasome regulatory subunit 4



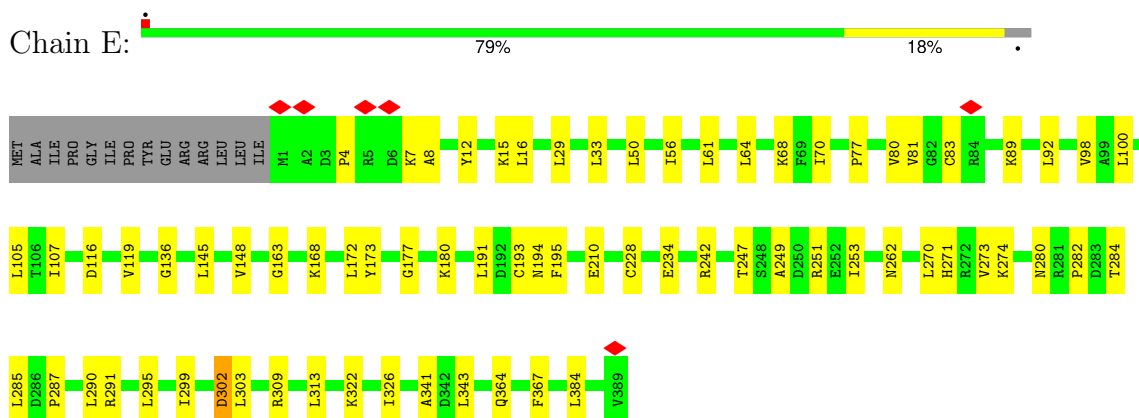
- Molecule 3: 26S proteasome regulatory subunit 8



- Molecule 4: 26S proteasome regulatory subunit 6B

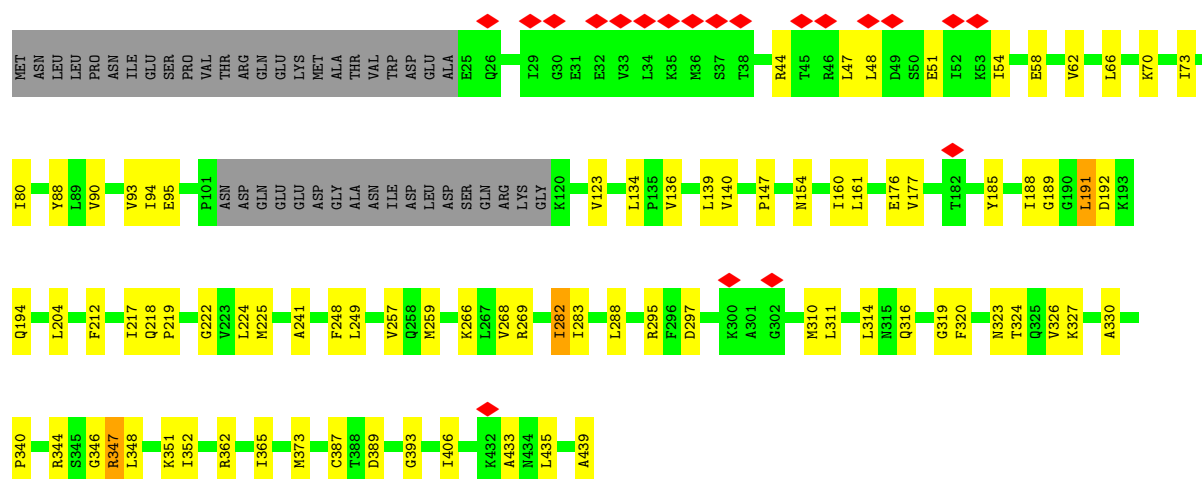


- Molecule 5: 26S proteasome regulatory subunit 10B



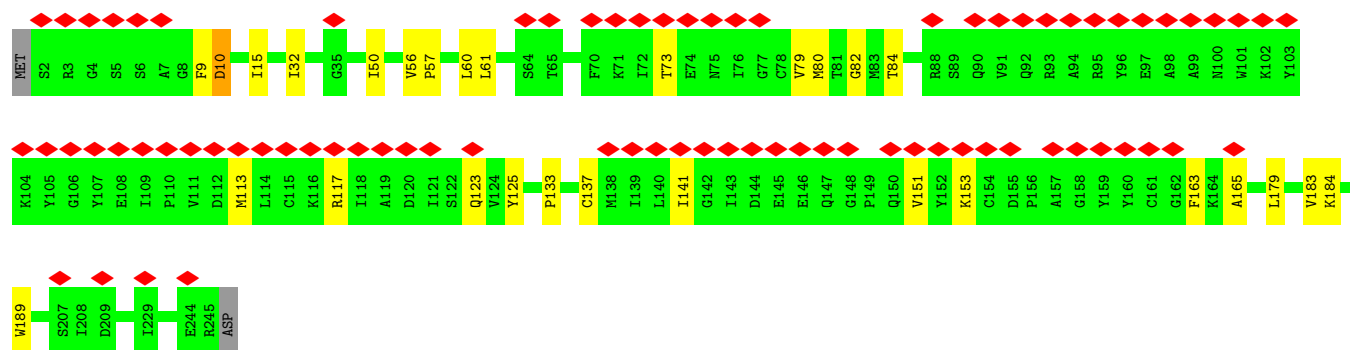
- Molecule 6: 26S proteasome regulatory subunit 6A

Chain F: 



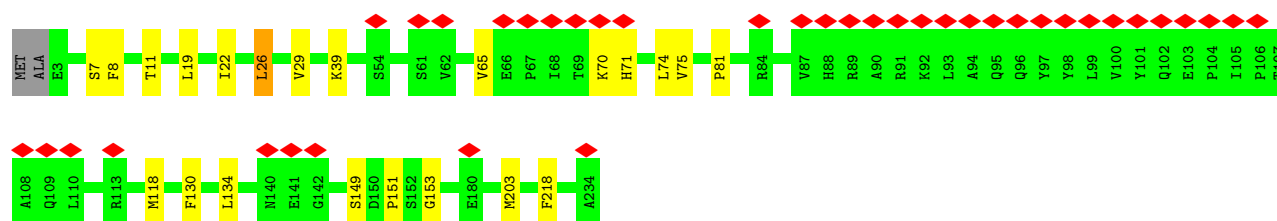
• Molecule 7: Proteasome subunit alpha type-6

Chain G: 



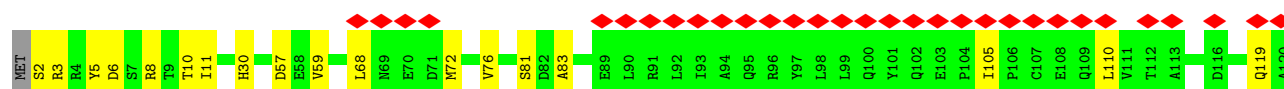
• Molecule 8: Proteasome subunit alpha type-2

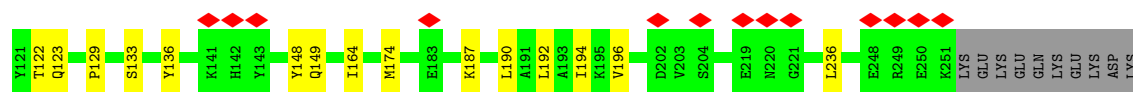
Chain H: 



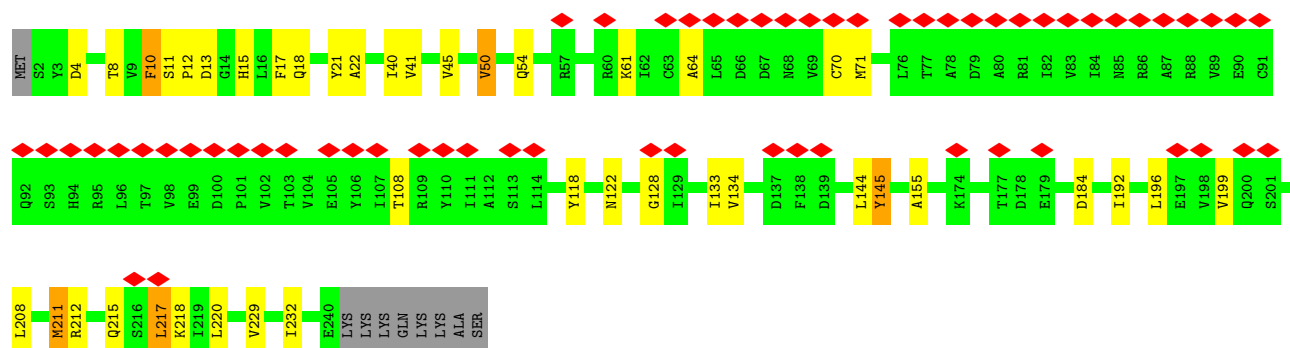
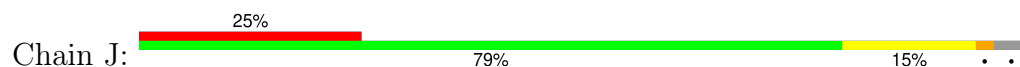
• Molecule 9: Proteasome subunit alpha type-4

Chain I: 

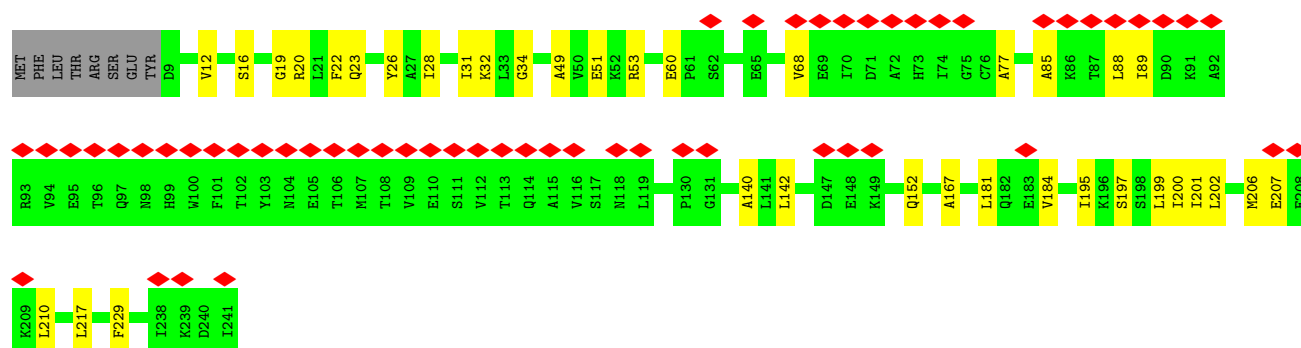
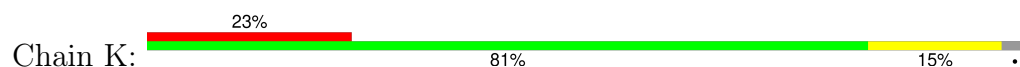




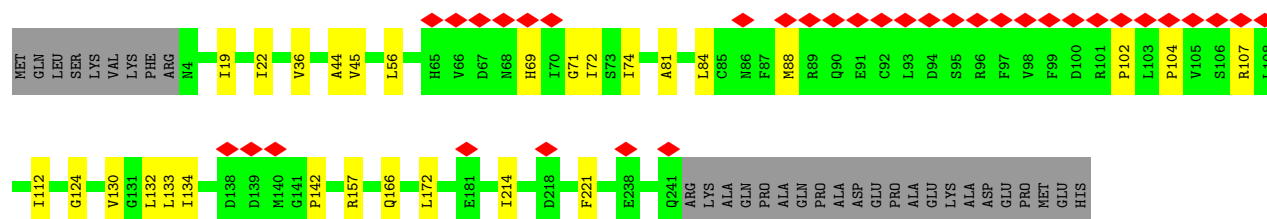
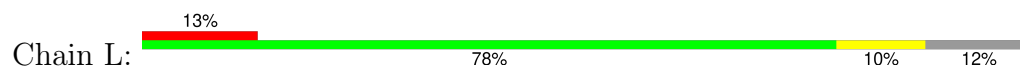
• Molecule 10: Proteasome subunit alpha type-7



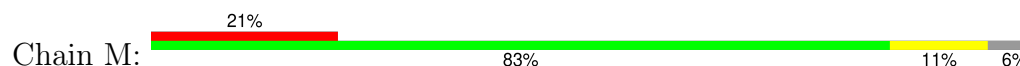
• Molecule 11: Proteasome subunit alpha type-5

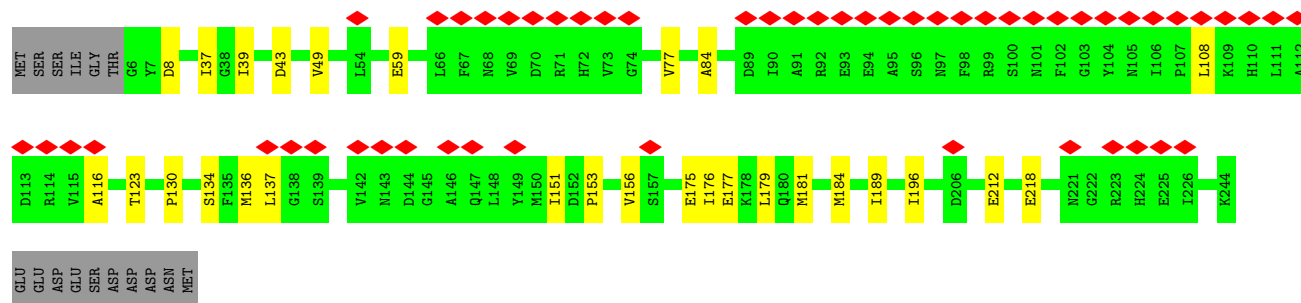


• Molecule 12: Isoform Long of Proteasome subunit alpha type-1

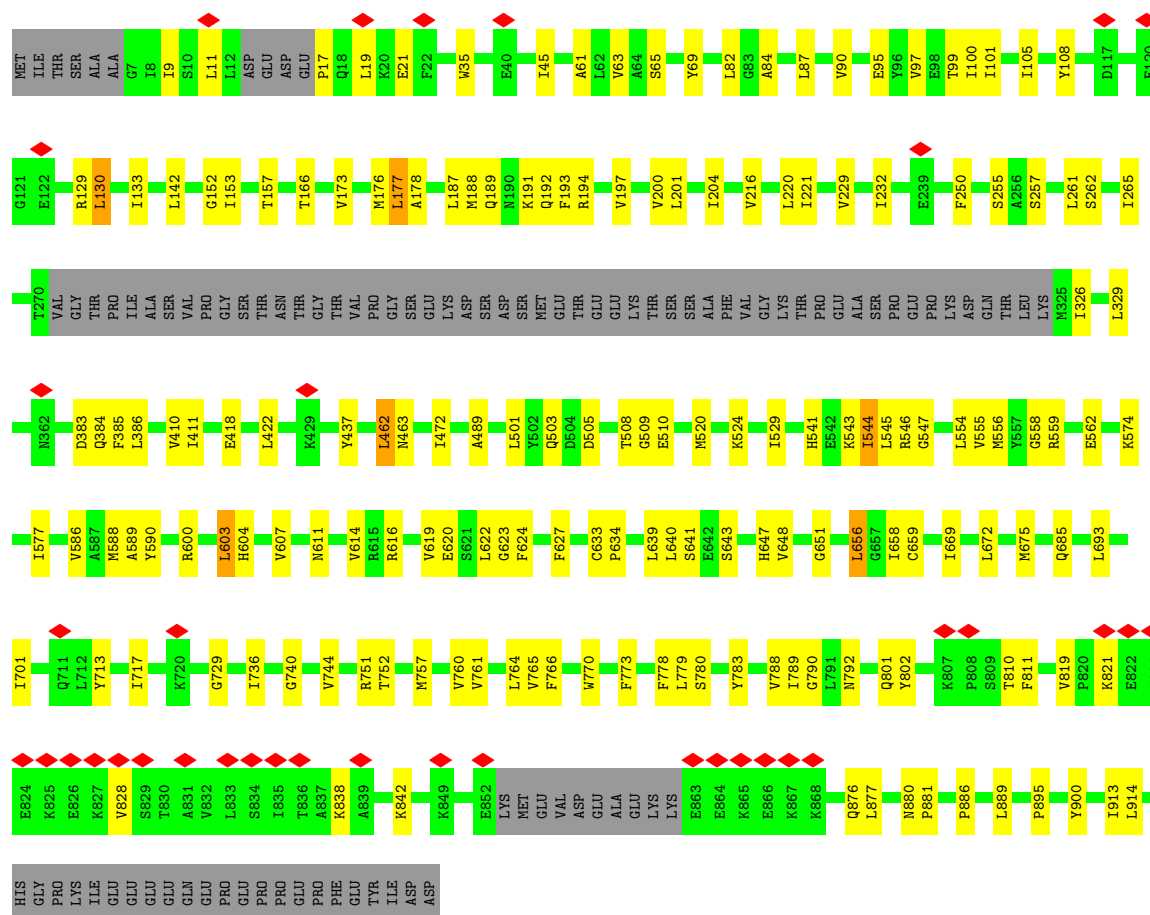


• Molecule 13: Proteasome subunit alpha type-3

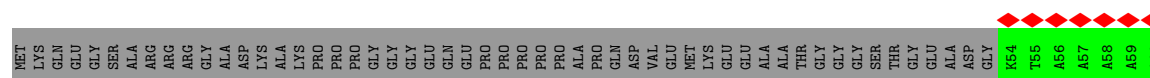


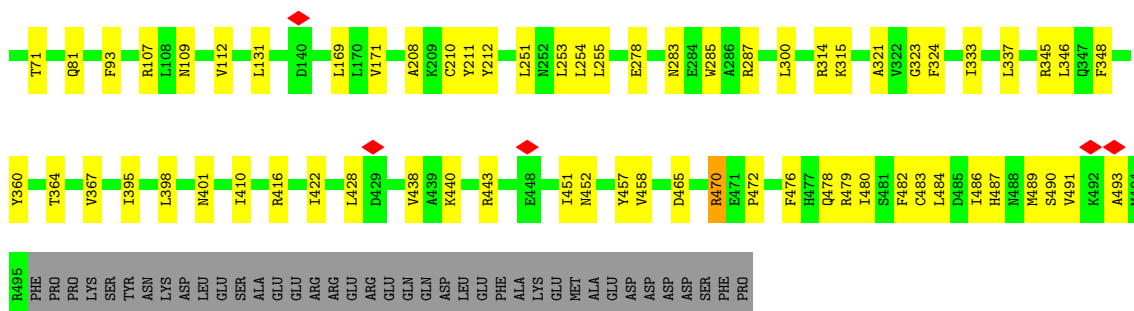


- Molecule 14: 26S proteasome non-ATPase regulatory subunit 1

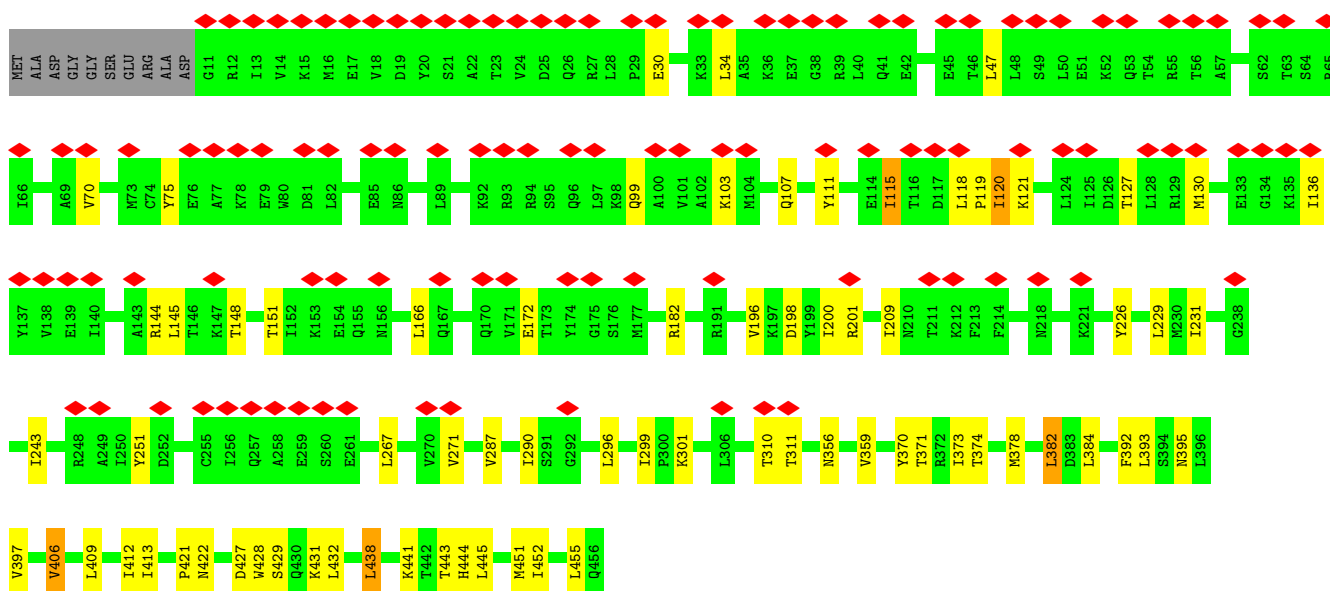
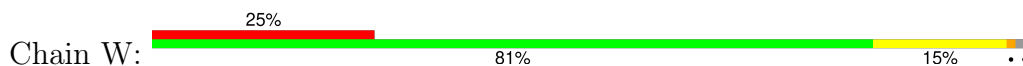


- Molecule 15: 26S proteasome non-ATPase regulatory subunit 3

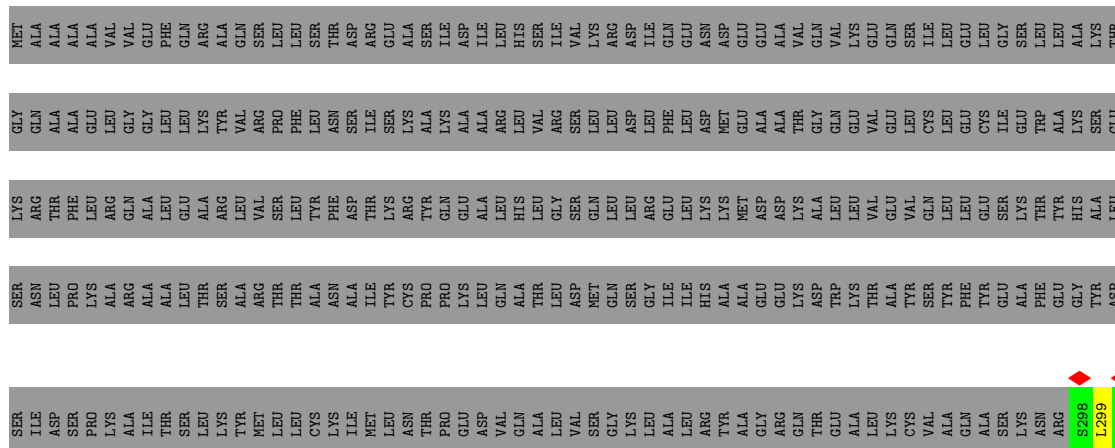




• Molecule 16: 26S proteasome non-ATPase regulatory subunit 12



• Molecule 17: 26S proteasome non-ATPase regulatory subunit 11

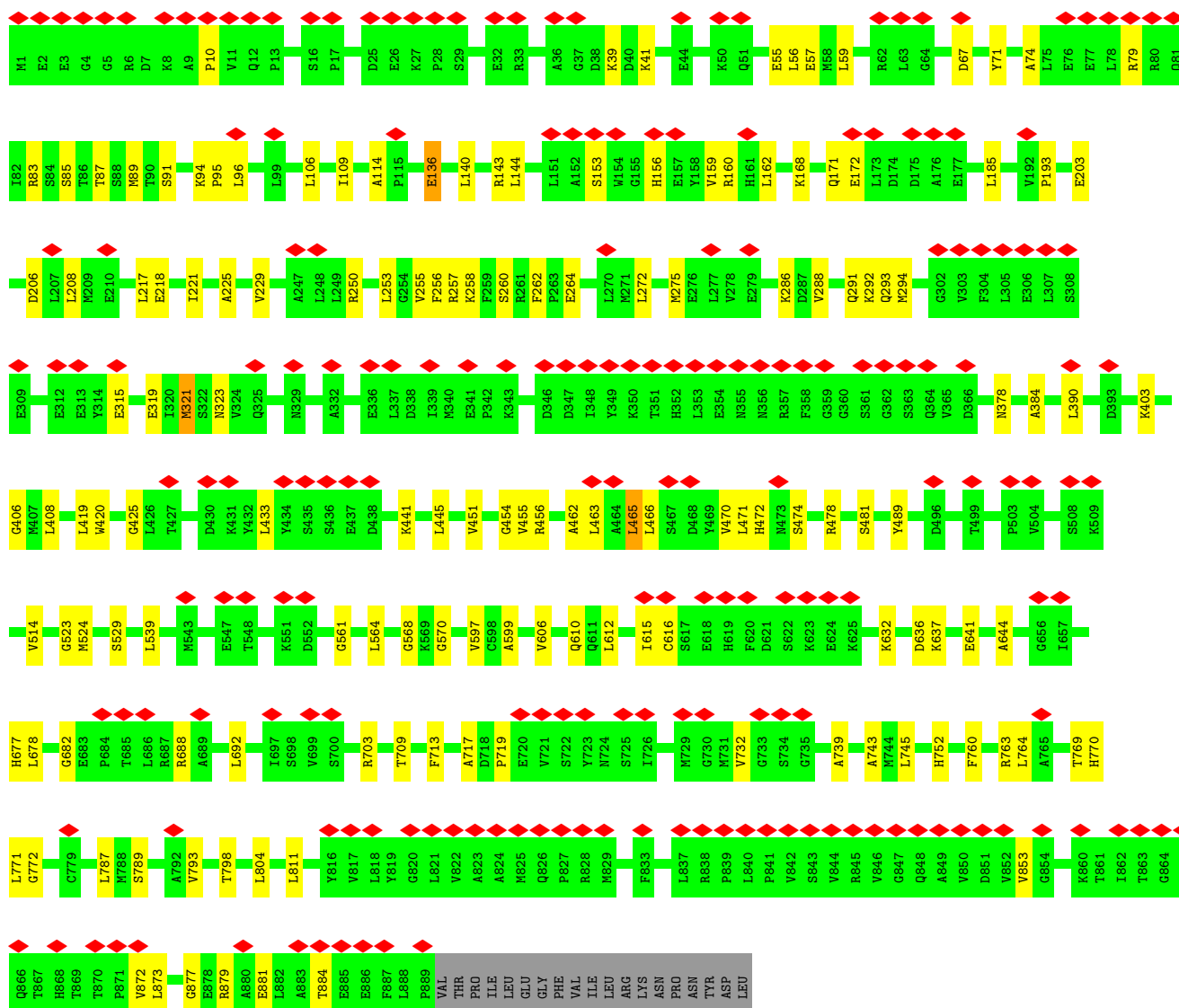
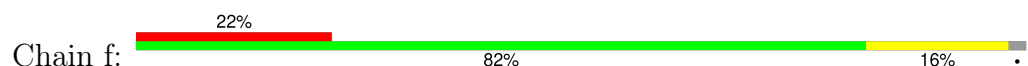




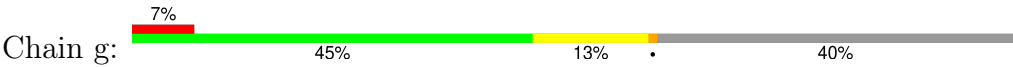
- Molecule 24: 26S proteasome complex subunit SEM1



- Molecule 25: 26S proteasome non-ATPase regulatory subunit 2



- Molecule 26: Thioredoxin-like protein 1



MET VAL VAL GLY VAL LYS PRO VAL GLY SER ASP PRO ASP PHE GLN PRO LEU SER GLY ALA GLY SER ARG LEU ALA VAL VAL LYS PHE THR MET ARG GLY CYS PRO CYS LEU ARG ILE ALA PRO ALA PHE SER MET SER ASN LYS TYR PRO GLN ALA VAL PHE LEU VAL ASP

VAL HIS GLN CYS GLY THR ALA THR ASN ASN ILE SER THR PRO THR PHE LEU PHE PHE ARG ASN LYS VAL ARG ILE ASP TVR GLN GLY ALA ASP ALA VAL GLY LEU GLU GLU LYS ILE LYS GLN HIS LEU GLU ASN ASP PRO GLY SER ASN ASP THR D118 I119 P120

K121 G122 L126 E136 C137 L138 H144 G145 F146 L160 D163 L167 E163 V175 K176 M180 K181 F182 P185 Q189 V194 I198 M199 S203 M204 E208 A209 E210 R211 S212 E213 P214 A217 L218 E219 E227 I230 Y235 V241

V244 N251 Q252 E256 T257 T258 T260 F263 T266 V270 Q271 A272 T273 N274 N275 F278 V281 V282 K285 Q286 E287 S288 H289

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100351	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.259	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	388.8, 388.8, 388.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/3290	0.79	0/4441
2	B	0.55	0/3002	0.89	0/4047
3	C	0.65	0/3027	0.92	0/4070
4	D	0.61	0/3089	0.89	0/4168
5	E	0.44	0/3145	0.75	0/4233
6	F	0.51	0/3152	0.80	0/4246
7	G	0.38	0/1937	0.67	0/2617
8	H	0.30	0/1852	0.56	0/2507
9	I	0.37	0/2001	0.69	0/2694
10	J	0.33	0/1913	0.64	0/2581
11	K	0.44	0/1805	0.71	0/2437
12	L	0.28	0/1908	0.53	0/2579
13	M	0.23	0/1909	0.58	0/2570
14	U	0.48	0/6786	0.79	0/9167
15	V	0.39	0/3661	0.66	0/4941
16	W	0.44	0/3683	0.79	0/4952
17	X	0.57	0/1021	0.94	0/1375
18	Y	0.47	0/3173	0.80	0/4273
19	Z	0.53	0/2324	0.84	0/3150
20	a	0.46	0/3045	0.84	0/4123
21	b	0.53	0/1478	0.89	0/2001
22	c	0.84	0/2302	1.08	0/3110
23	d	0.31	0/2162	0.75	0/2919
24	e	0.30	0/437	0.74	0/595
25	f	0.34	0/6980	0.70	0/9433
26	g	0.59	0/1403	0.93	0/1892
All	All	0.47	0/70485	0.78	0/95121

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

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	A	3237	0	3291	52	0
2	B	2960	0	3010	67	0
3	C	2988	0	3089	65	0
4	D	3039	0	3076	61	0
5	E	3097	0	3174	49	0
6	F	3112	0	3198	57	0
7	G	1903	0	1911	17	0
8	H	1813	0	1806	17	0
9	I	1971	0	1992	23	0
10	J	1887	0	1905	25	0
11	K	1778	0	1764	27	0
12	L	1873	0	1860	21	0
13	M	1874	0	1861	15	0
14	U	6671	0	6738	106	0
15	V	3594	0	3666	53	0
16	W	3635	0	3762	59	0
17	X	1007	0	1038	41	0
18	Y	3115	0	3120	64	0
19	Z	2281	0	2312	83	0
20	a	2987	0	3005	55	0
21	b	1458	0	1505	32	0
22	c	2260	0	2276	87	0
23	d	2116	0	2146	31	0
24	e	425	0	328	6	0
25	f	6866	0	6866	88	0
26	g	1376	0	1324	27	0
27	A	31	0	12	4	0
27	D	31	0	12	1	0
27	E	31	0	12	2	0
27	F	31	0	12	2	0
28	A	1	0	0	0	0
28	D	1	0	0	0	0
28	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	1	0	0	0	0
29	B	27	0	12	1	0
29	C	27	0	12	4	0
30	c	1	0	0	0	0
All	All	69506	0	70095	1053	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 8.

The worst 5 of 1053 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:D:73:LEU:HB3	19:Z:184:VAL:HG12	1.61	0.83
23:d:41:THR:HG22	23:d:44:THR:HB	1.61	0.81
1:A:125:LEU:HG	1:A:134:ILE:HD11	1.63	0.80
2:B:197:ILE:HD13	2:B:235:LEU:HD13	1.65	0.79
22:c:122:LEU:H	22:c:196:LEU:HD11	1.47	0.79

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	A	410/433 (95%)	365 (89%)	45 (11%)	0	100	100
2	B	373/440 (85%)	330 (88%)	43 (12%)	0	100	100
3	C	379/398 (95%)	341 (90%)	38 (10%)	0	100	100
4	D	378/418 (90%)	344 (91%)	34 (9%)	0	100	100
5	E	387/403 (96%)	357 (92%)	30 (8%)	0	100	100
6	F	393/439 (90%)	348 (88%)	45 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
8	H	230/234 (98%)	221 (96%)	9 (4%)	0	100	100
9	I	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
11	K	231/241 (96%)	214 (93%)	17 (7%)	0	100	100
12	L	236/269 (88%)	231 (98%)	5 (2%)	0	100	100
13	M	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
14	U	845/953 (89%)	791 (94%)	54 (6%)	0	100	100
15	V	440/534 (82%)	423 (96%)	17 (4%)	0	100	100
16	W	444/456 (97%)	419 (94%)	25 (6%)	0	100	100
17	X	123/422 (29%)	116 (94%)	7 (6%)	0	100	100
18	Y	376/389 (97%)	346 (92%)	30 (8%)	0	100	100
19	Z	284/324 (88%)	248 (87%)	36 (13%)	0	100	100
20	a	370/376 (98%)	342 (92%)	28 (8%)	0	100	100
21	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100
22	c	285/310 (92%)	245 (86%)	40 (14%)	0	100	100
23	d	255/350 (73%)	220 (86%)	35 (14%)	0	100	100
24	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
25	f	887/908 (98%)	796 (90%)	91 (10%)	0	100	100
26	g	170/289 (59%)	157 (92%)	13 (8%)	0	100	100
All	All	8697/10043 (87%)	7991 (92%)	706 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/372 (95%)	344 (98%)	9 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	333/385 (86%)	314 (94%)	19 (6%)	18	43
3	C	329/346 (95%)	299 (91%)	30 (9%)	9	30
4	D	333/366 (91%)	310 (93%)	23 (7%)	14	39
5	E	341/353 (97%)	334 (98%)	7 (2%)	47	65
6	F	342/379 (90%)	332 (97%)	10 (3%)	37	58
7	G	208/210 (99%)	205 (99%)	3 (1%)	59	71
8	H	190/191 (100%)	186 (98%)	4 (2%)	47	65
9	I	210/221 (95%)	207 (99%)	3 (1%)	59	71
10	J	203/211 (96%)	197 (97%)	6 (3%)	36	57
11	K	195/203 (96%)	192 (98%)	3 (2%)	57	70
12	L	204/230 (89%)	204 (100%)	0	100	100
13	M	197/212 (93%)	194 (98%)	3 (2%)	57	70
14	U	730/816 (90%)	713 (98%)	17 (2%)	44	64
15	V	388/460 (84%)	381 (98%)	7 (2%)	51	68
16	W	410/416 (99%)	403 (98%)	7 (2%)	53	68
17	X	114/362 (32%)	112 (98%)	2 (2%)	51	68
18	Y	334/344 (97%)	328 (98%)	6 (2%)	51	68
19	Z	257/295 (87%)	251 (98%)	6 (2%)	44	64
20	a	332/336 (99%)	324 (98%)	8 (2%)	43	63
21	b	167/312 (54%)	157 (94%)	10 (6%)	17	42
22	c	252/268 (94%)	229 (91%)	23 (9%)	9	30
23	d	231/294 (79%)	227 (98%)	4 (2%)	53	68
24	e	44/63 (70%)	44 (100%)	0	100	100
25	f	745/763 (98%)	736 (99%)	9 (1%)	63	73
26	g	156/253 (62%)	148 (95%)	8 (5%)	21	45
All	All	7598/8661 (88%)	7371 (97%)	227 (3%)	37	57

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	152	GLN
26	g	175	VAL
15	V	470	ARG

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Mol	Chain	Res	Type
26	g	126	LEU
22	c	203	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
18	Y	388	ASN
21	b	142	ASN
19	Z	72	HIS
20	a	12	GLN
22	c	219	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](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	AGS	F	501	28	32,33,33	0.66	1 (3%)	45,52,52	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	AGS	E	501	28	32,33,33	0.67	1 (3%)	45,52,52	0.48	0
27	AGS	D	501	28	32,33,33	0.66	1 (3%)	45,52,52	0.52	0
29	ADP	C	501	-	28,29,29	0.45	0	43,45,45	0.55	0
29	ADP	B	501	-	28,29,29	0.46	0	43,45,45	0.51	0
27	AGS	A	501	28	32,33,33	0.66	1 (3%)	45,52,52	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	AGS	F	501	28	-	5/21/38/38	0/3/3/3
27	AGS	E	501	28	-	0/21/38/38	0/3/3/3
27	AGS	D	501	28	-	3/21/38/38	0/3/3/3
29	ADP	C	501	-	-	3/16/32/32	0/3/3/3
29	ADP	B	501	-	-	3/16/32/32	0/3/3/3
27	AGS	A	501	28	-	2/21/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	501	AGS	PG-S1G	2.12	1.95	1.90
27	A	501	AGS	PG-S1G	2.12	1.95	1.90
27	D	501	AGS	PG-S1G	2.11	1.95	1.90
27	F	501	AGS	PG-S1G	2.09	1.95	1.90

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	D	501	AGS	C5'-O5'-PA-O3A
27	F	501	AGS	C5'-O5'-PA-O3A
29	C	501	ADP	C5'-O5'-PA-O3A
27	D	501	AGS	C4'-C5'-O5'-PA
29	B	501	ADP	PB-O3A-PA-O5'

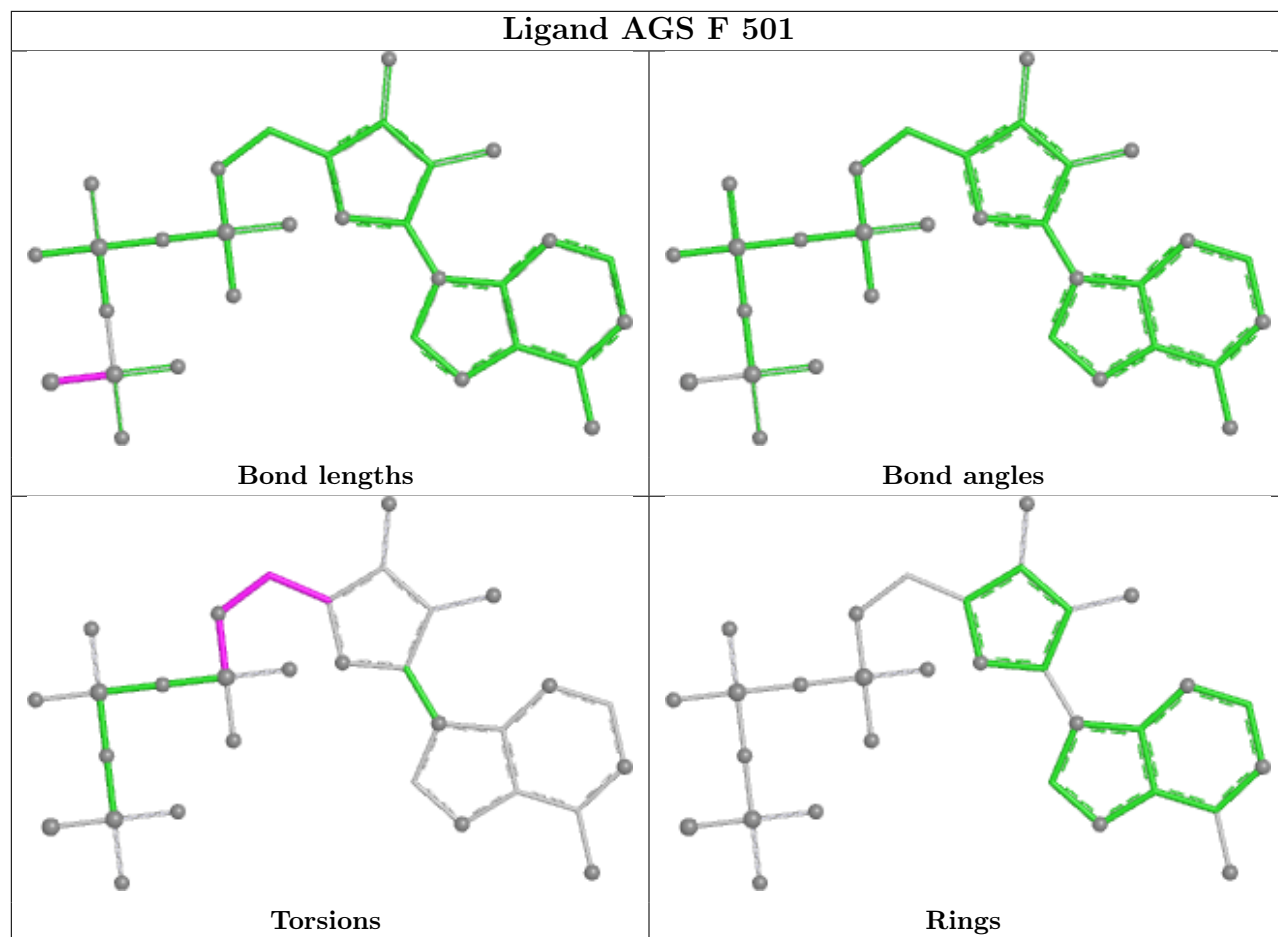
There are no ring outliers.

6 monomers are involved in 14 short contacts:

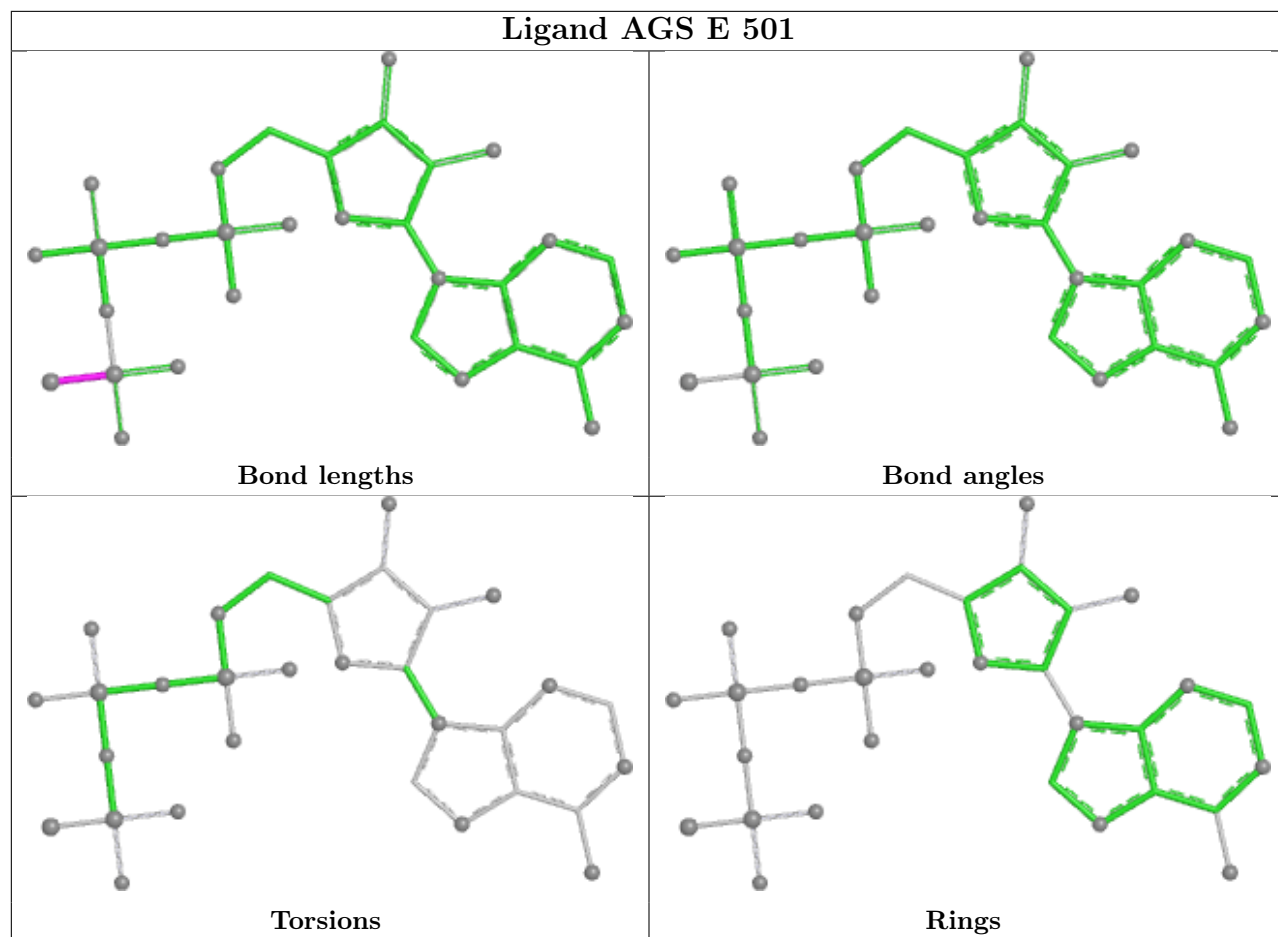
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	F	501	AGS	2	0
27	E	501	AGS	2	0
27	D	501	AGS	1	0
29	C	501	ADP	4	0
29	B	501	ADP	1	0
27	A	501	AGS	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

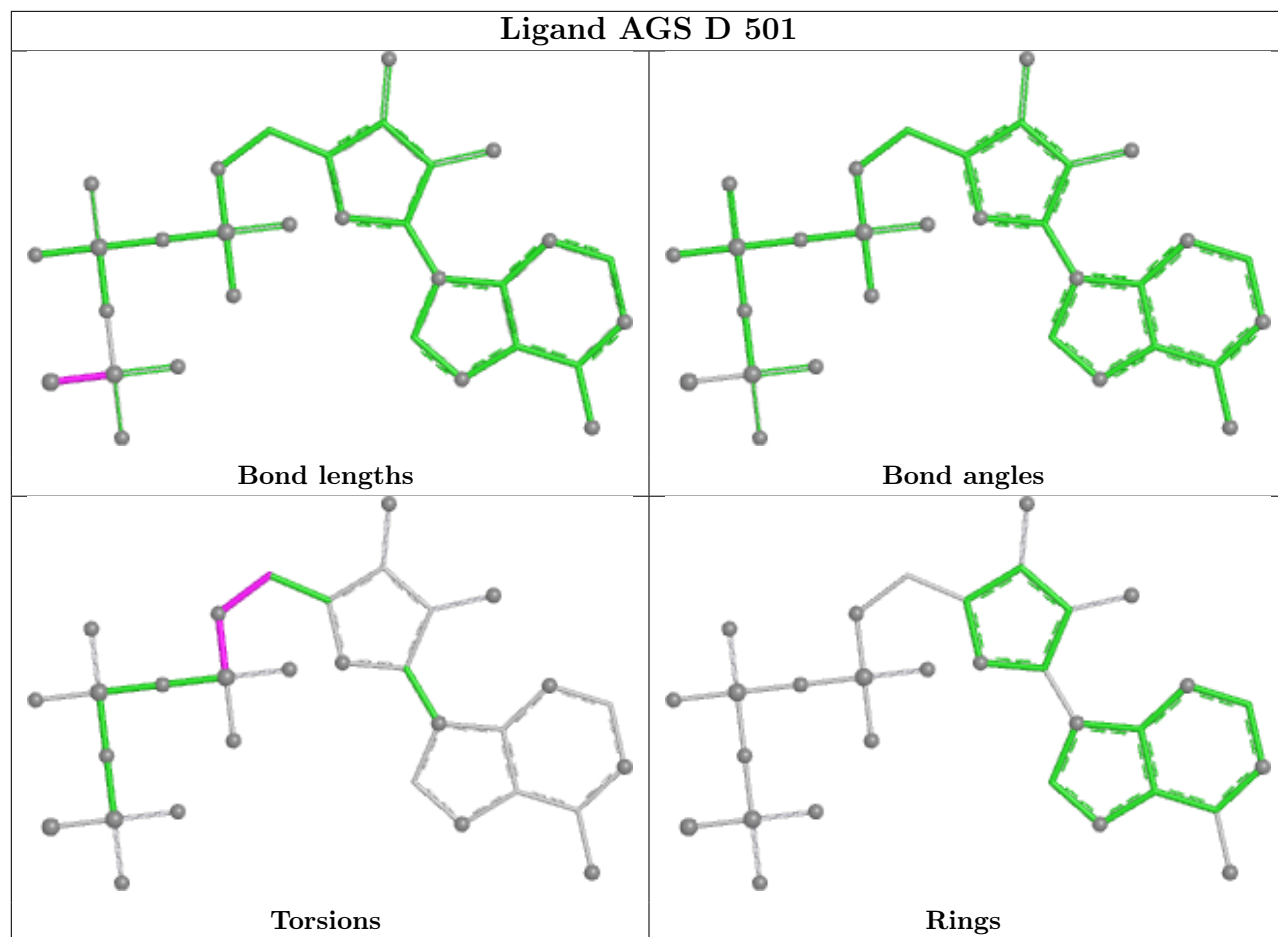
Ligand AGS F 501



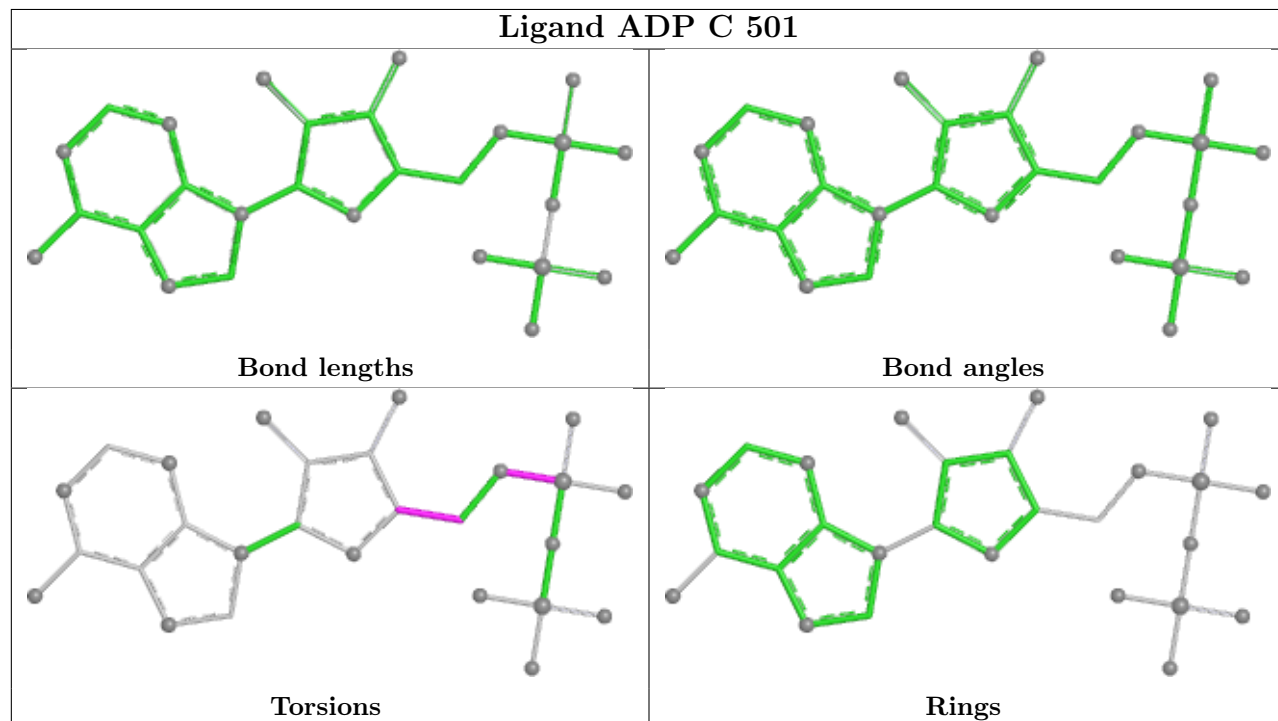
Ligand AGS E 501

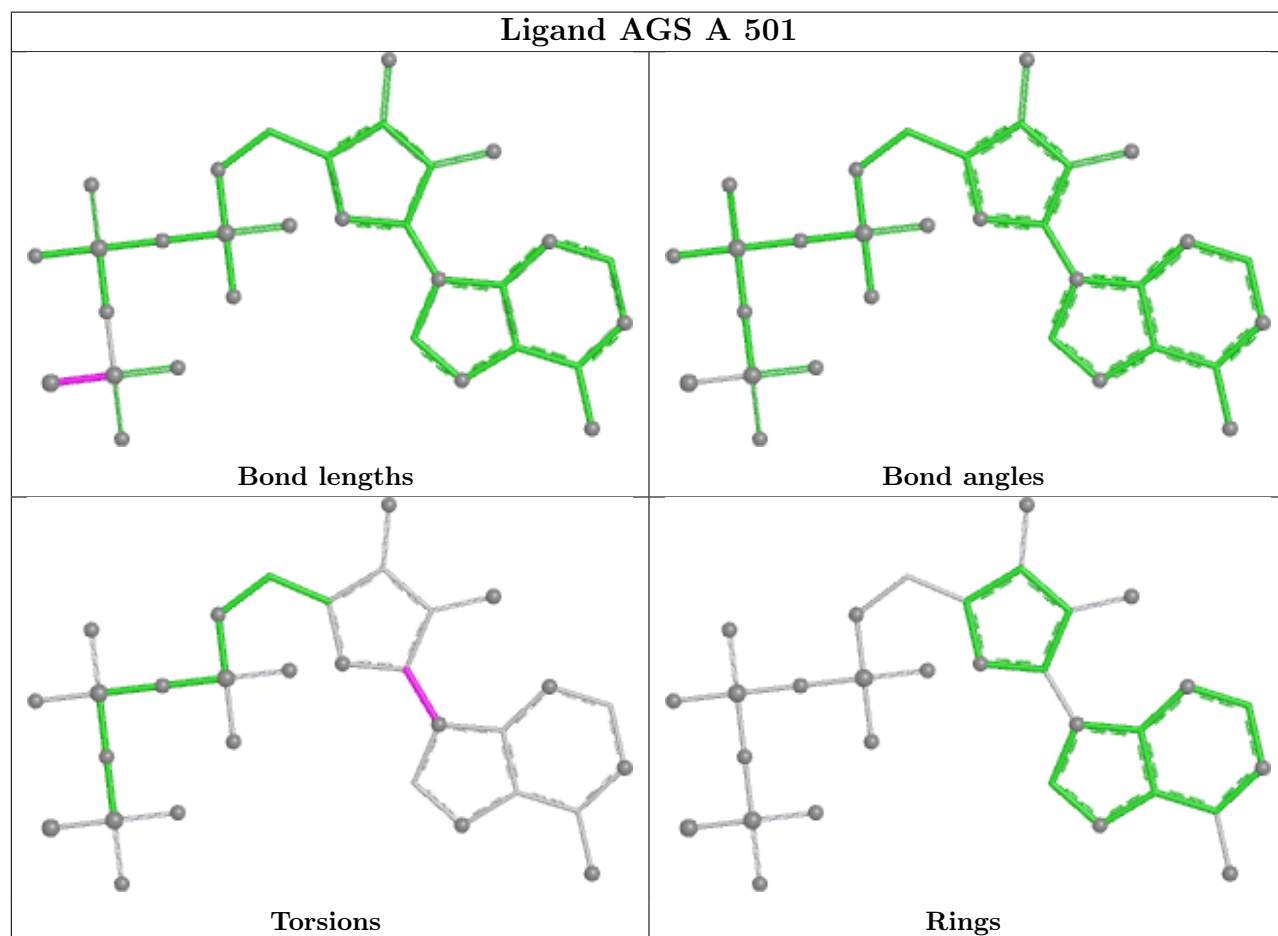
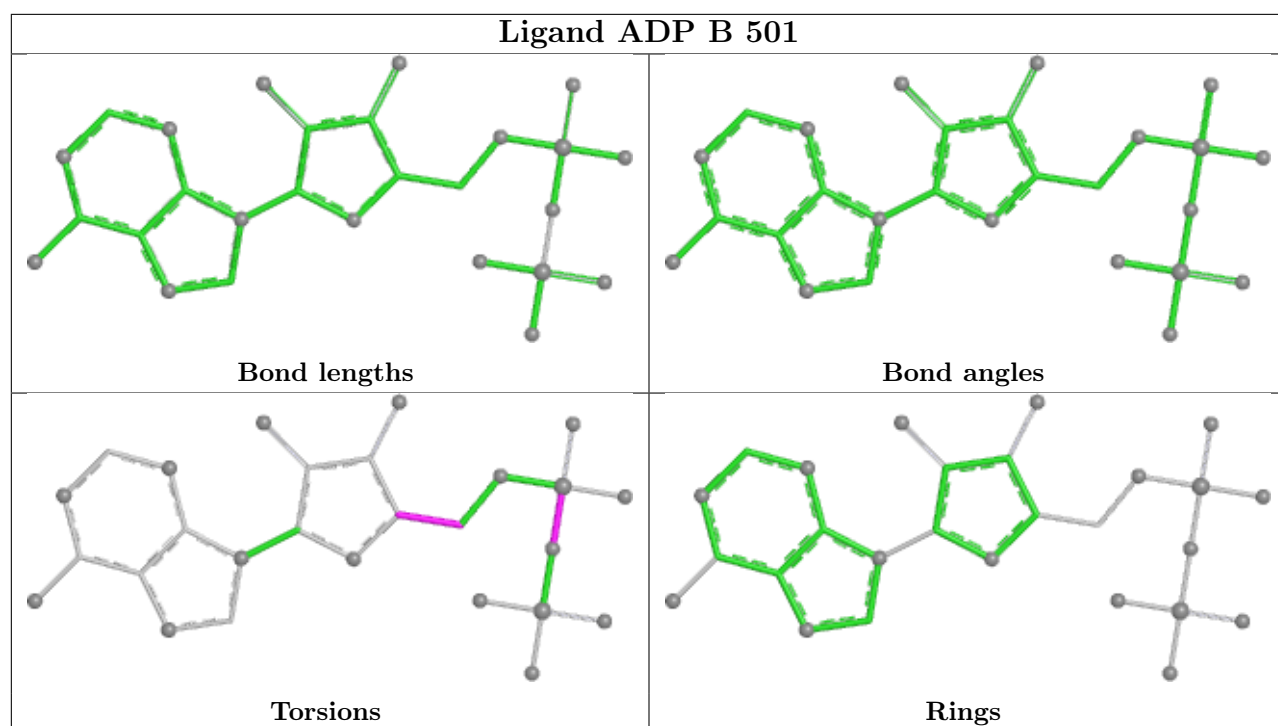


Ligand AGS D 501



Ligand ADP C 501





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.

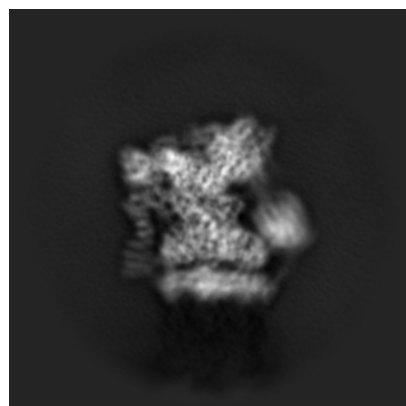
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71741. These allow visual inspection of the internal detail of the map and identification of artifacts.

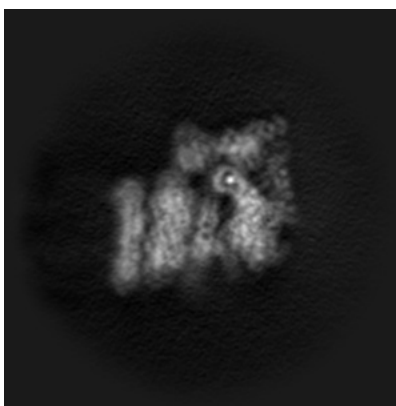
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

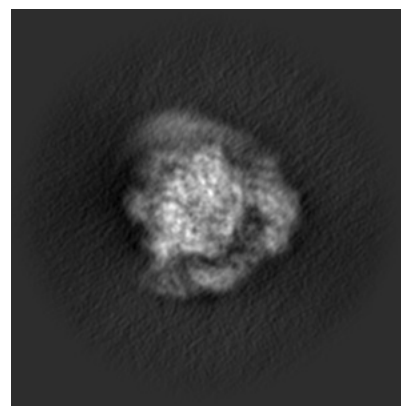
6.1.1 Primary map



X

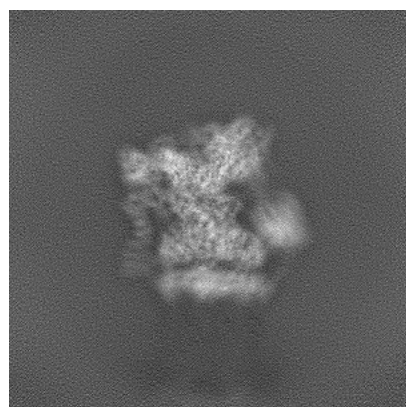


Y

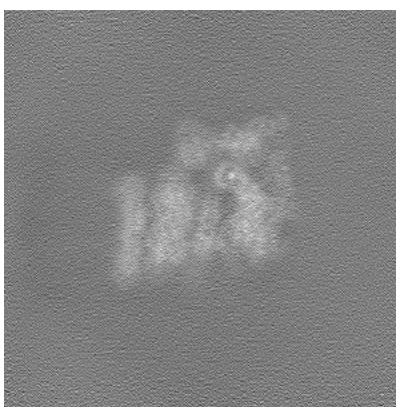


Z

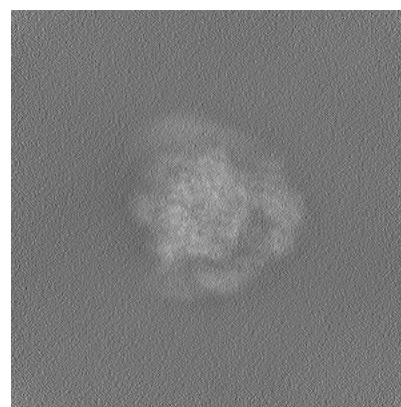
6.1.2 Raw map



X



Y

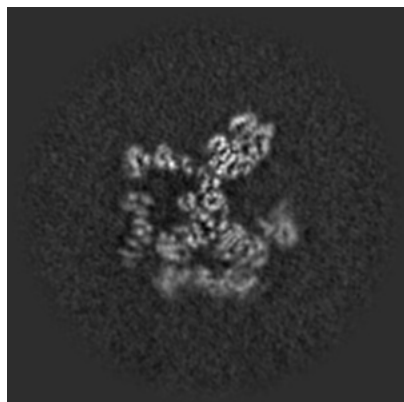


Z

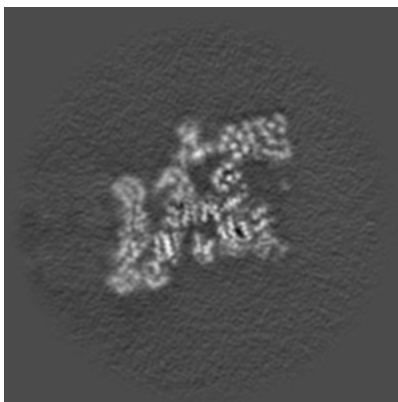
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

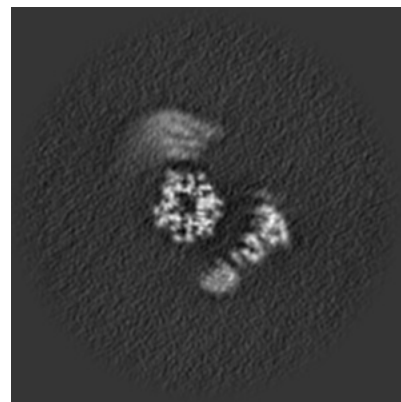
6.2.1 Primary map



X Index: 240

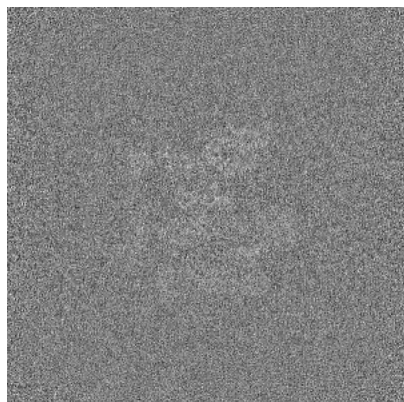


Y Index: 240

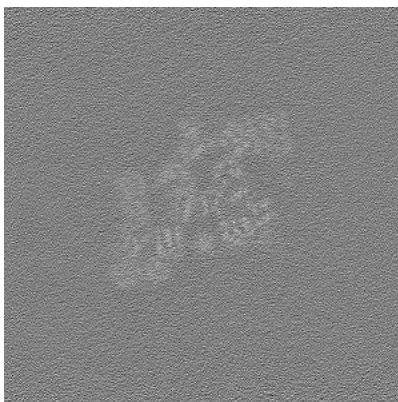


Z Index: 240

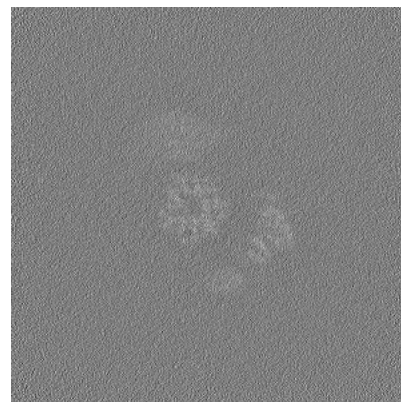
6.2.2 Raw map



X Index: 240



Y Index: 240

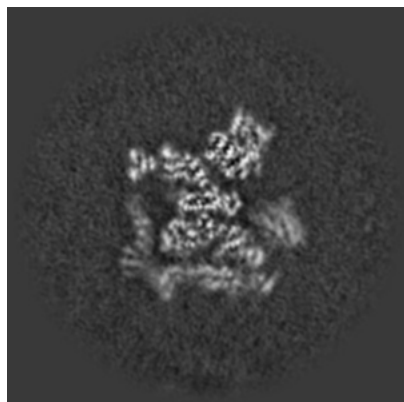


Z Index: 240

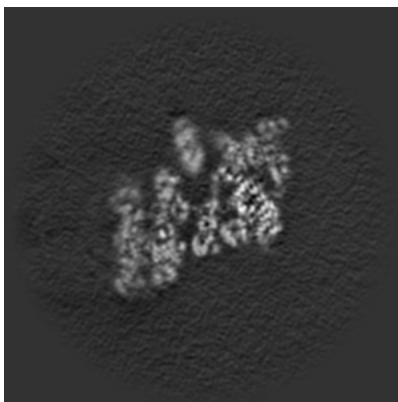
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

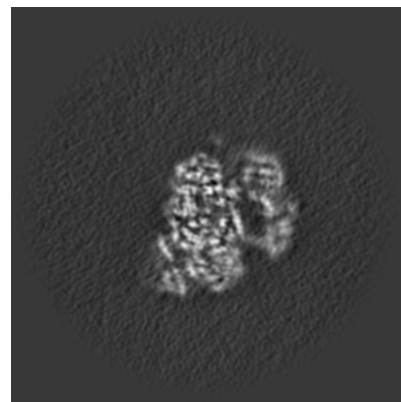
6.3.1 Primary map



X Index: 228

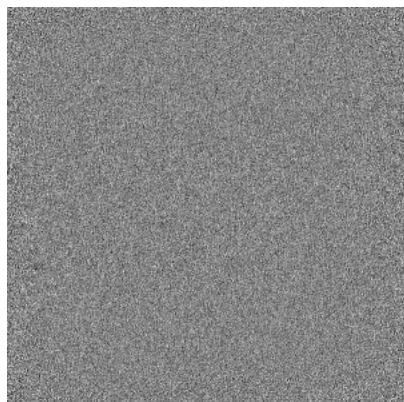


Y Index: 257

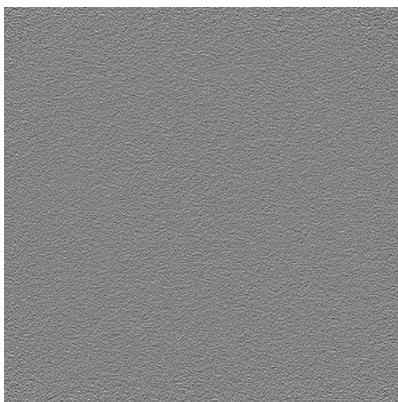


Z Index: 288

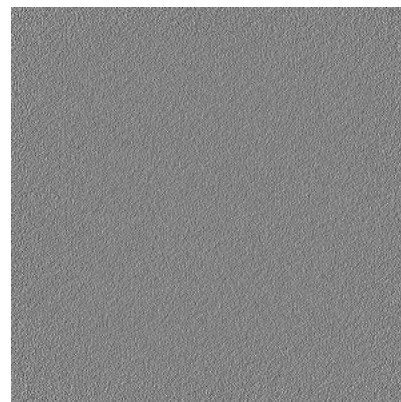
6.3.2 Raw map



X Index: 0



Y Index: 0

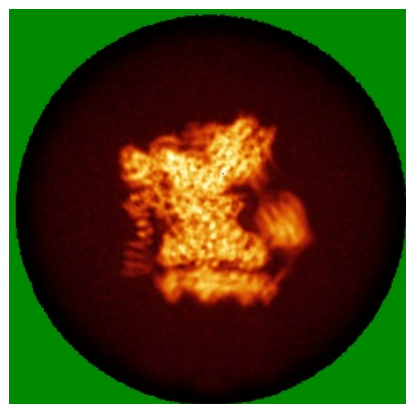


Z Index: 0

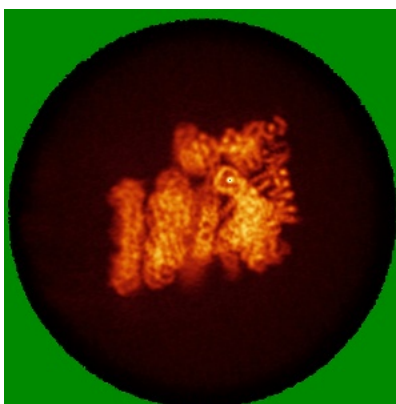
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

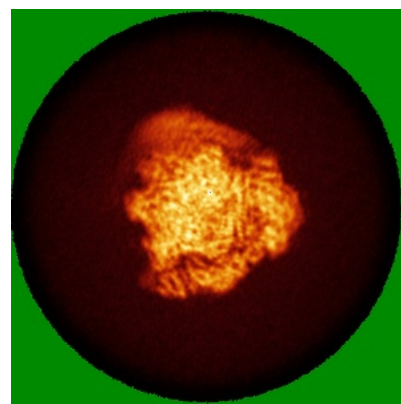
6.4.1 Primary map



X

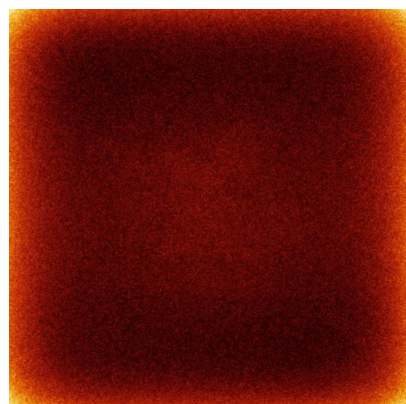


Y

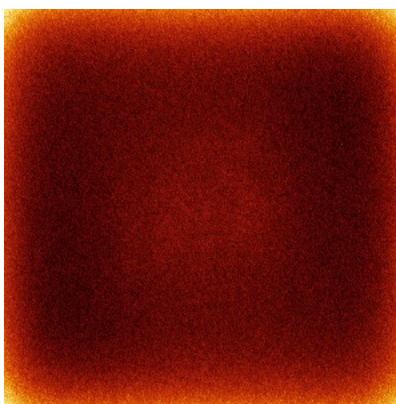


Z

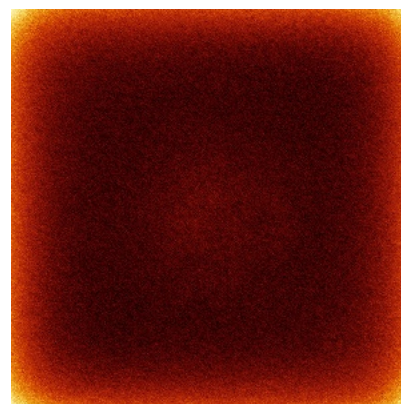
6.4.2 Raw map



X



Y

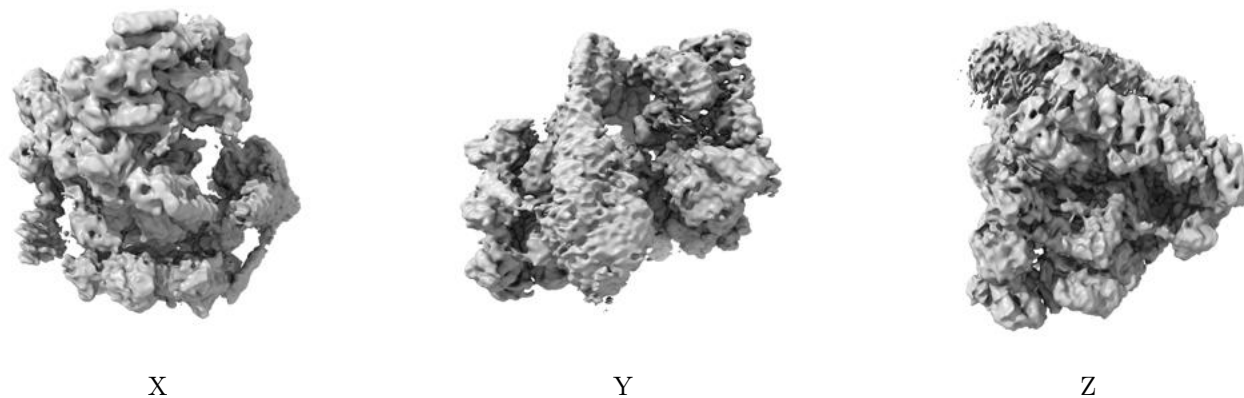


Z

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.

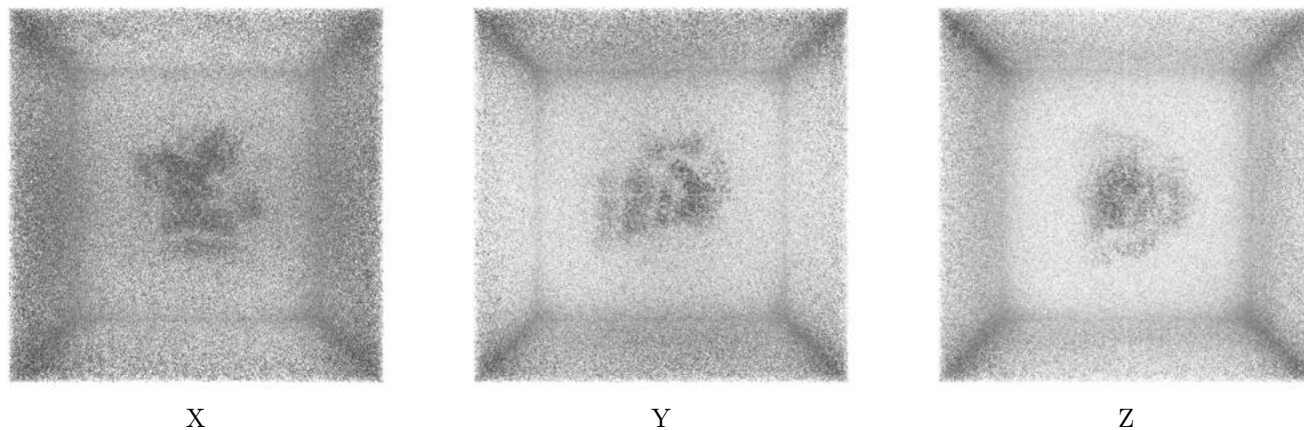
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



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.

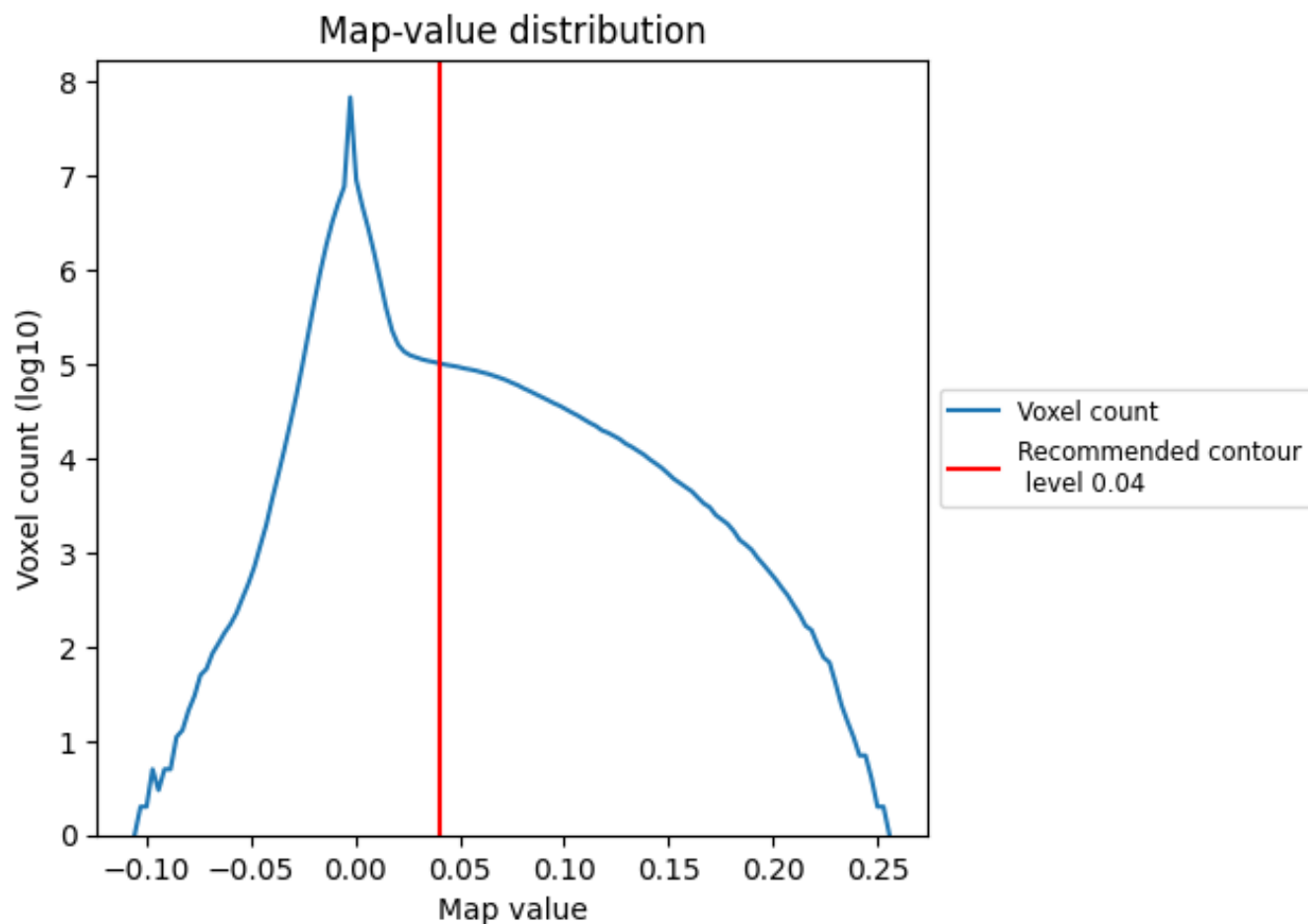
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

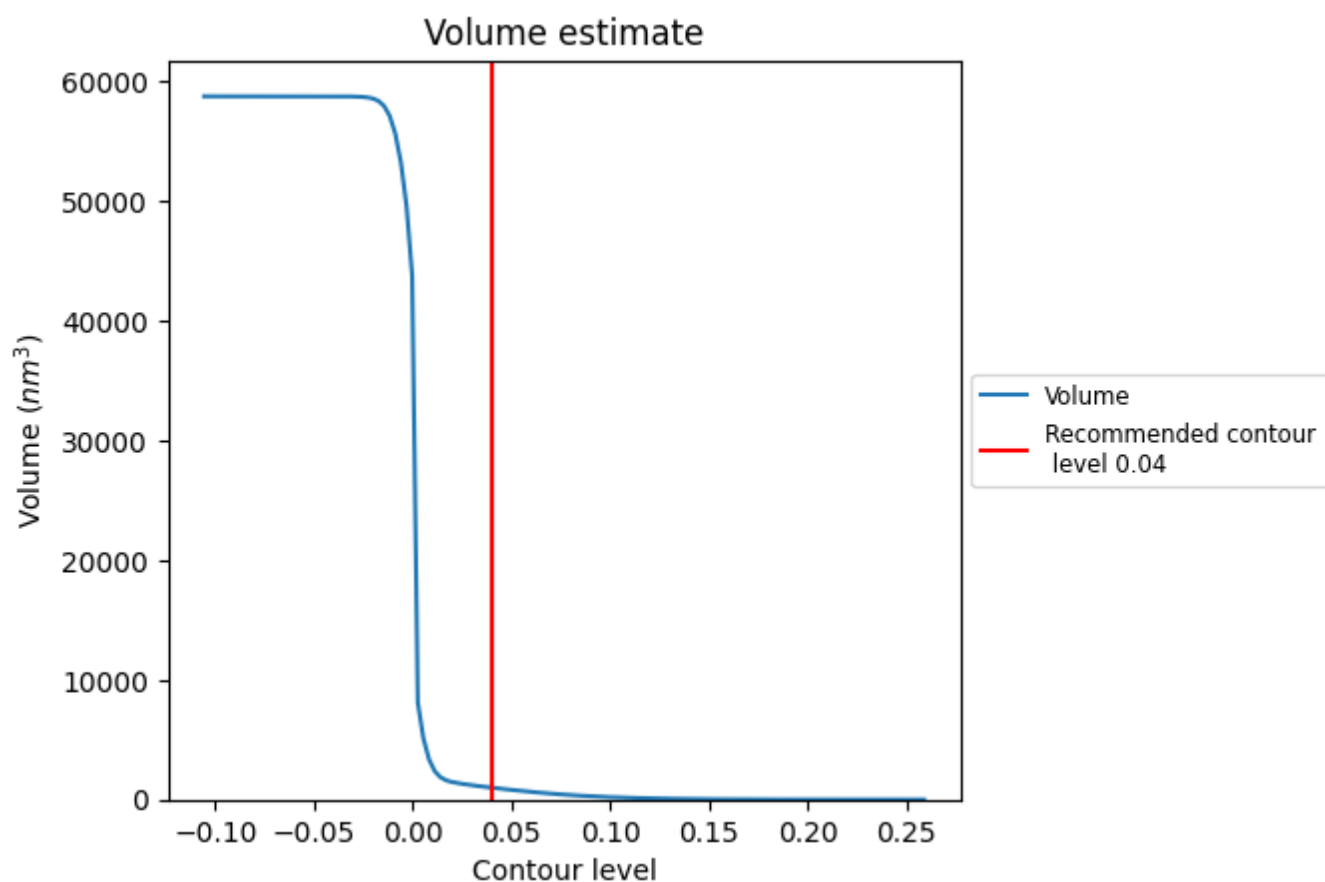
This section contains the results of statistical analysis of the map.

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.

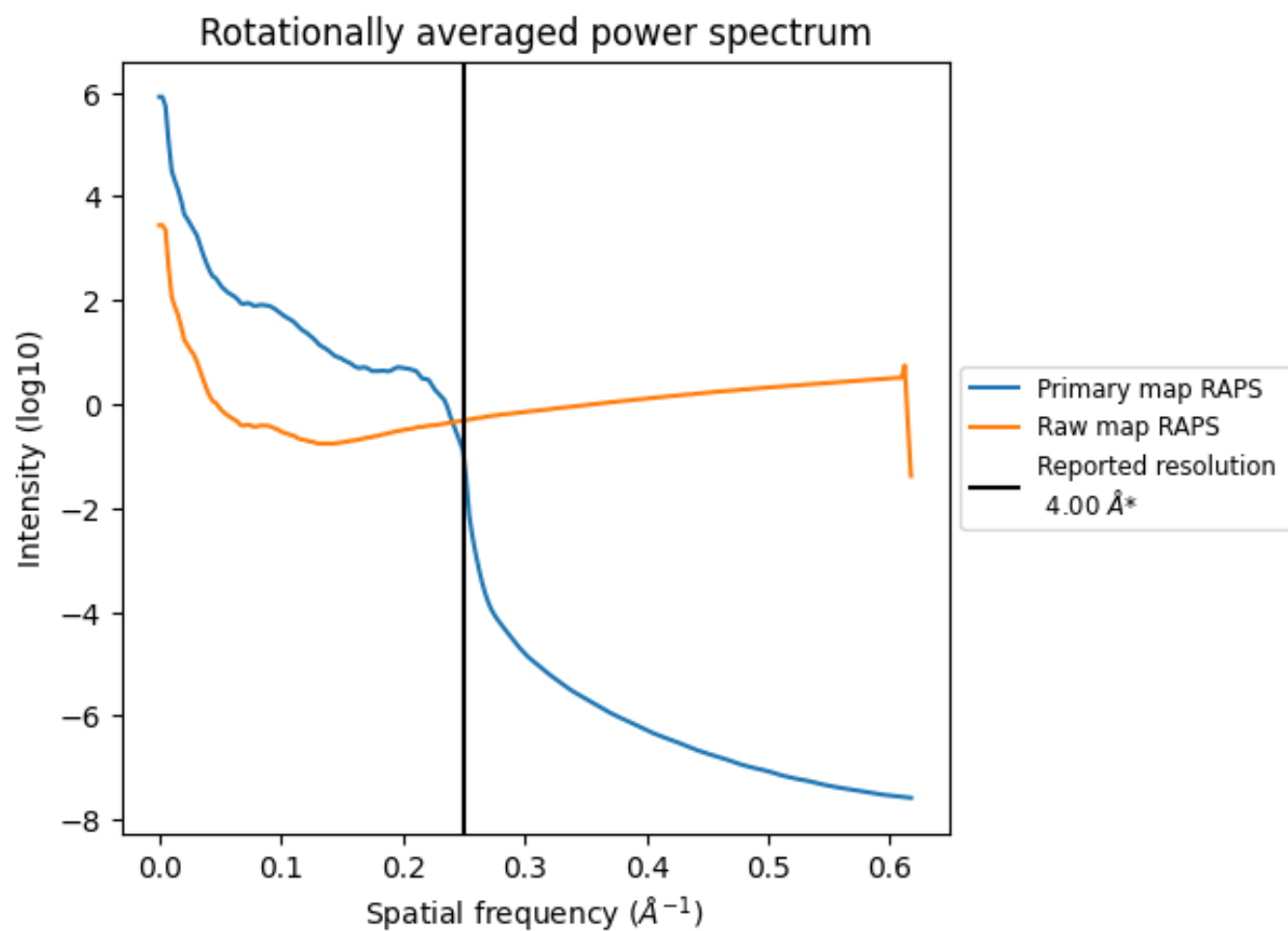
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 989 nm³; this corresponds to an approximate mass of 893 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](#)

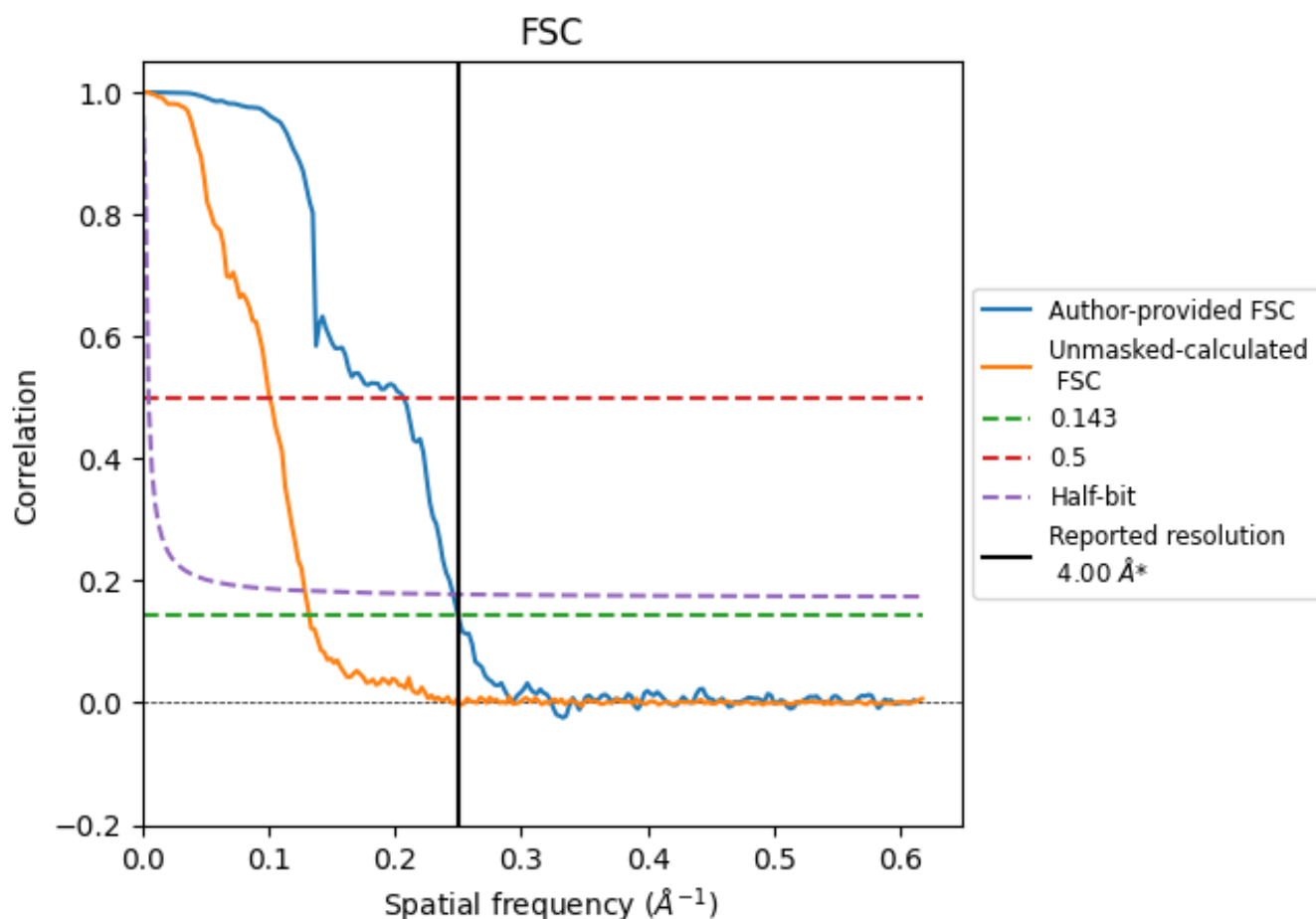


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

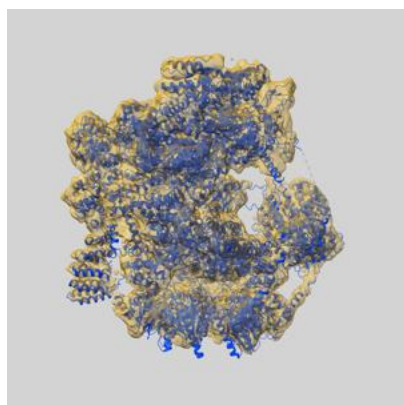
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	4.83	4.07
Unmasked-calculated*	7.57	9.92	7.78

*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 7.57 differs from the reported value 4.0 by more than 10 %

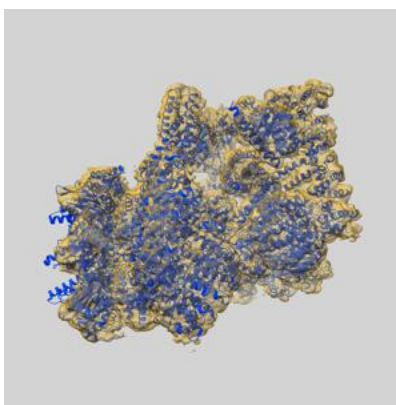
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71741 and PDB model 9PMQ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

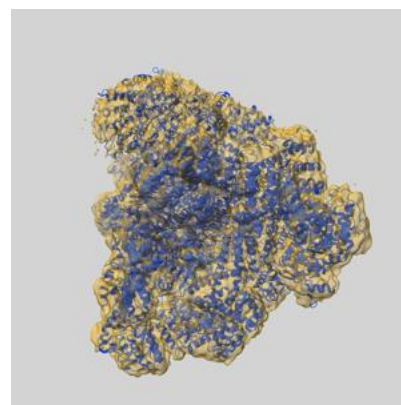
9.1 Map-model overlay [i](#)



X



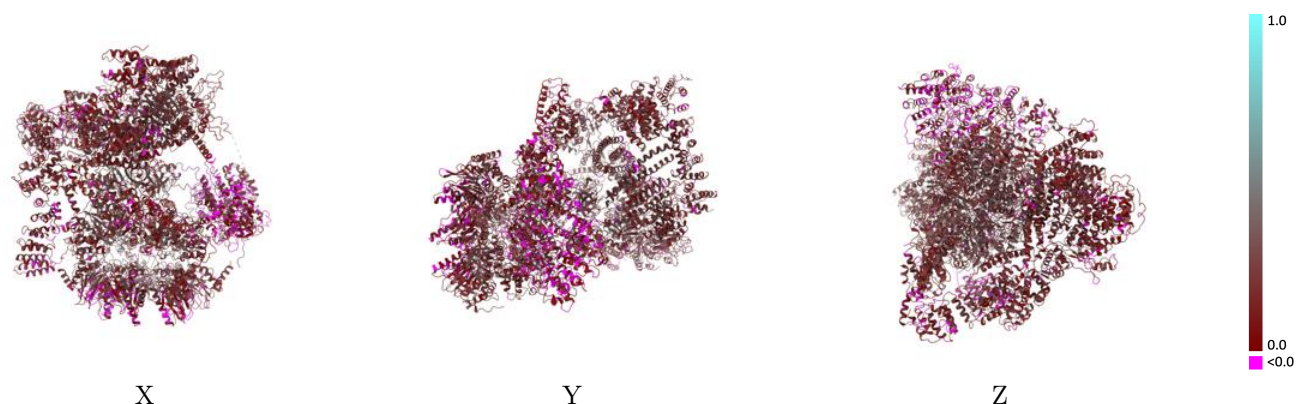
Y



Z

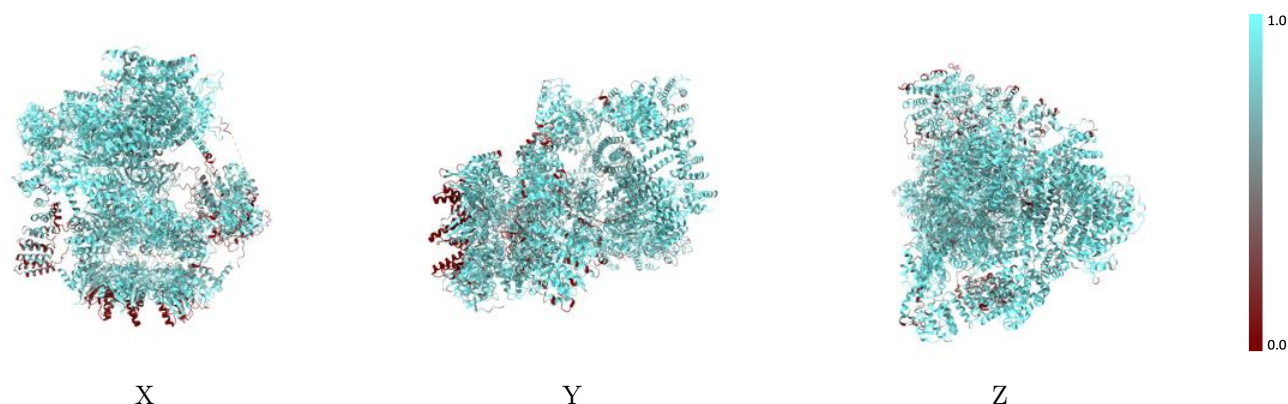
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



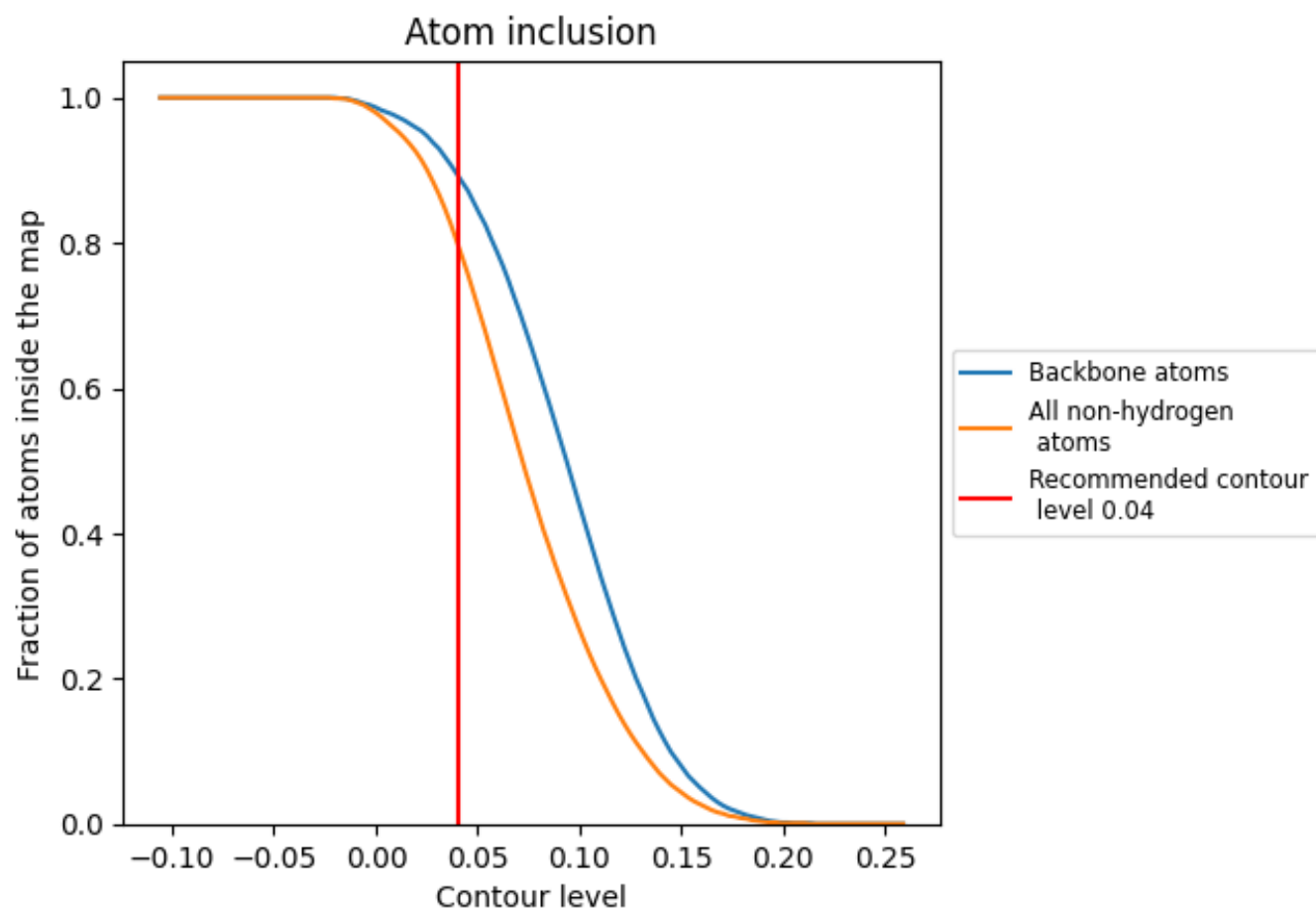
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.1900
A	 0.8160	 0.2190
B	 0.7970	 0.2040
C	 0.8340	 0.2240
D	 0.8650	 0.2430
E	 0.8740	 0.2340
F	 0.8580	 0.2380
G	 0.6280	 0.1520
H	 0.7700	 0.1740
I	 0.7410	 0.1810
J	 0.6490	 0.1500
K	 0.6710	 0.1710
L	 0.7890	 0.2120
M	 0.6860	 0.1750
U	 0.8580	 0.2250
V	 0.8870	 0.1990
W	 0.6490	 0.1560
X	 0.7350	 0.1730
Y	 0.8900	 0.1720
Z	 0.8980	 0.2510
a	 0.8920	 0.1790
b	 0.8950	 0.2200
c	 0.8610	 0.2610
d	 0.8440	 0.1460
e	 0.9070	 0.2020
f	 0.7150	 0.0620
g	 0.6660	 0.2490

