



wwPDB EM Validation Summary Report ⓘ

Sep 4, 2025 – 06:30 PM JST

PDB ID : 9UF8 / pdb_00009uf8
EMDB ID : EMD-64103
Title : The cryo-EM structure of 26S proteasome-Midnolin complex in the MA state
Authors : Wang, H.Y.; Xu, W.Q.; Wei, C.C.
Deposited on : 2025-04-10
Resolution : 4.32 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.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.45.1

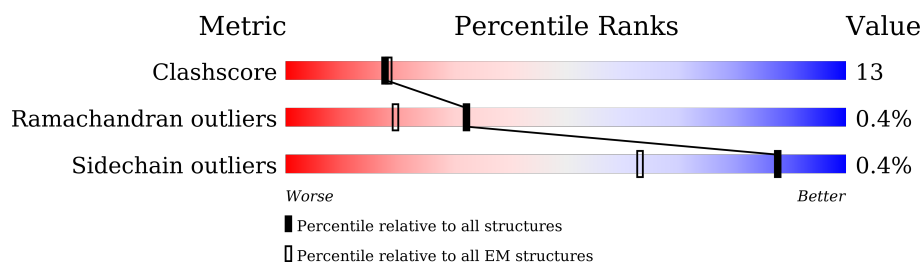
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.32 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.
















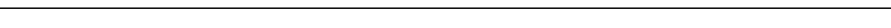











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	N	239	
1	n	239	
2	F	439	
3	O	277	
3	o	277	
4	G	246	
4	g	246	
5	P	205	

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Mol	Chain	Length	Quality of chain
5	p	205	
6	H	234	
6	h	234	
7	Q	201	
7	q	201	
8	I	261	
8	i	261	
9	R	263	
9	r	263	
10	J	248	
10	j	248	
11	S	241	
11	s	241	
12	K	241	
12	k	241	
13	T	264	
13	t	264	
14	L	263	
14	l	263	
15	M	255	
15	m	255	
16	U	953	
17	V	534	
18	W	456	
19	X	422	

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Mol	Chain	Length	Quality of chain
20	Y	389	
21	Z	324	
22	a	376	
23	b	377	
24	c	310	
25	d	350	
26	e	70	
27	f	908	
28	A	433	
29	u	491	
30	B	440	
31	C	406	
32	D	418	
33	E	389	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	ADP	F	501	-	-	X	-
35	ATP	D	501	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 103364 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	N	201	Total	C	N	O	S	0	0
			1506	943	257	294	12		
1	n	201	Total	C	N	O	S	0	0
			1506	943	257	294	12		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	375	Total	C	N	O	S	0	0
			2826	1780	492	540	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
3	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	238	Total	C	N	O	S	0	0
			1785	1135	303	335	12		
4	g	239	Total	C	N	O	S	0	0
			1865	1186	309	357	13		

- Molecule 5 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 6 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	226	Total	C	N	O	S	0	0
			1660	1057	285	314	4		
6	h	230	Total	C	N	O	S	0	0
			1793	1147	302	338	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
7	q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	249	Total	C	N	O	S	0	0
			1872	1179	321	364	8		
8	i	247	Total	C	N	O	S	0	0
			1945	1230	332	373	10		

- Molecule 9 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		
9	r	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	241	Total	C	N	O	S	0	0
			1703	1066	309	323	5		
10	j	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
11	s	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	228	Total	C	N	O	S	0	0
			1681	1060	276	337	8		
12	k	237	Total	C	N	O	S	0	0
			1816	1139	301	365	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	215	Total	C	N	O	S	0	0
			1681	1061	290	318	12		
13	t	215	Total	C	N	O	S	0	0
			1681	1061	290	318	12		

- Molecule 14 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	240	Total	C	N	O	S	0	0
			1853	1164	337	342	10		
14	l	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	242	Total	C	N	O	S	0	0
			1851	1174	313	354	10		
15	m	241	Total	C	N	O	S	0	0
			1885	1195	322	357	11		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	812	Total	C	N	O	S	0	0
			6237	3948	1066	1181	42		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	508	Total	C	N	O	S	0	0
			3905	2462	705	728	10		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	456	Total	C	N	O	S	0	0
			3598	2264	613	697	24		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	380	Total	C	N	O	S	0	0
			2938	1865	502	562	9		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	378	Total	C	N	O	S	0	0
			3062	1952	524	572	14		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	286	Total	C	N	O	S	0	0
			2246	1429	390	422	5		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	373	Total	C	N	O	S	0	0
			2974	1898	503	558	15		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	191	Total	C	N	O	S	0	0
			1432	892	257	276	7		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	c	279	Total	C	N	O	S	0	0
			2139	1346	374	400	19		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	252	Total	C	N	O	S	0	0
			1990	1276	332	375	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	39	Total	C	N	O	S	0	0
			313	188	52	71	2		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	889	Total	C	N	O	S	0	0
			6670	4171	1146	1311	42		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	393	Total	C	N	O	S	0	0
			3016	1896	526	577	17		

- Molecule 29 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	u	37	Total	C	N	O	S	0	0
			320	189	78	52	1		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	0	MET	-	initiating methionine	UNP Q504T8
u	469	GLY	-	expression tag	UNP Q504T8
u	470	SER	-	expression tag	UNP Q504T8
u	471	ASP	-	expression tag	UNP Q504T8
u	472	TYR	-	expression tag	UNP Q504T8
u	473	LYS	-	expression tag	UNP Q504T8
u	474	ASP	-	expression tag	UNP Q504T8
u	475	ASP	-	expression tag	UNP Q504T8
u	476	ASP	-	expression tag	UNP Q504T8
u	477	ASP	-	expression tag	UNP Q504T8
u	478	LYS	-	expression tag	UNP Q504T8
u	479	GLY	-	expression tag	UNP Q504T8
u	480	SER	-	expression tag	UNP Q504T8
u	481	HIS	-	expression tag	UNP Q504T8
u	482	HIS	-	expression tag	UNP Q504T8
u	483	HIS	-	expression tag	UNP Q504T8
u	484	HIS	-	expression tag	UNP Q504T8
u	485	HIS	-	expression tag	UNP Q504T8
u	486	HIS	-	expression tag	UNP Q504T8
u	487	HIS	-	expression tag	UNP Q504T8
u	488	HIS	-	expression tag	UNP Q504T8
u	489	HIS	-	expression tag	UNP Q504T8
u	490	HIS	-	expression tag	UNP Q504T8

- Molecule 30 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	384	Total	C	N	O	S	0	0
			2975	1870	510	581	14		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	C	363	Total	C	N	O	S	0	0
			2831	1784	507	525	15		

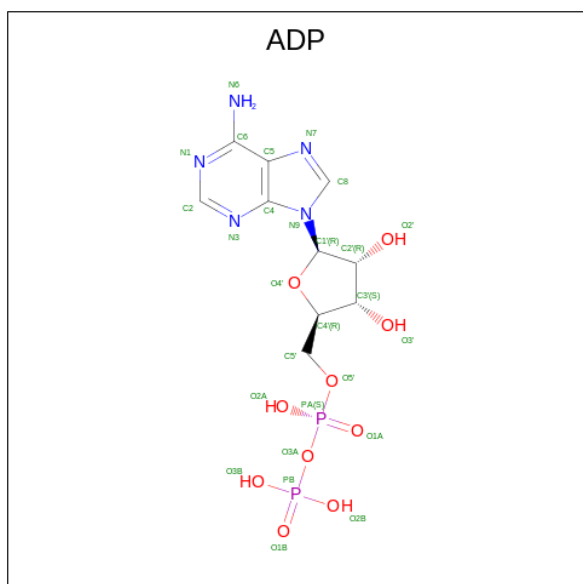
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	D	380	Total	C	N	O	S	0	0
			2991	1889	515	576	11		

- Molecule 33 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	E	375	Total	C	N	O	S	0	0
			2828	1777	507	528	16		

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





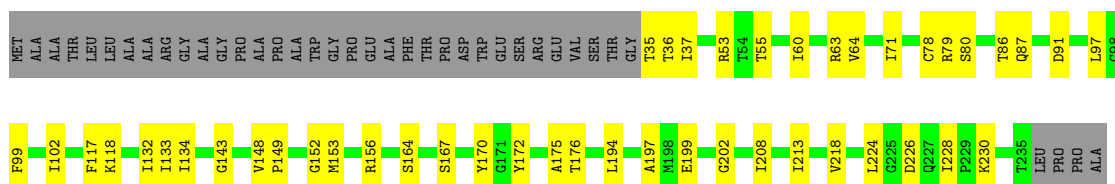
Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

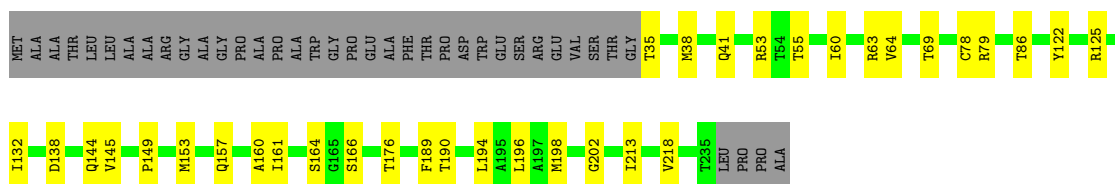
• Molecule 1: Proteasome subunit beta type-6

Chain N: 



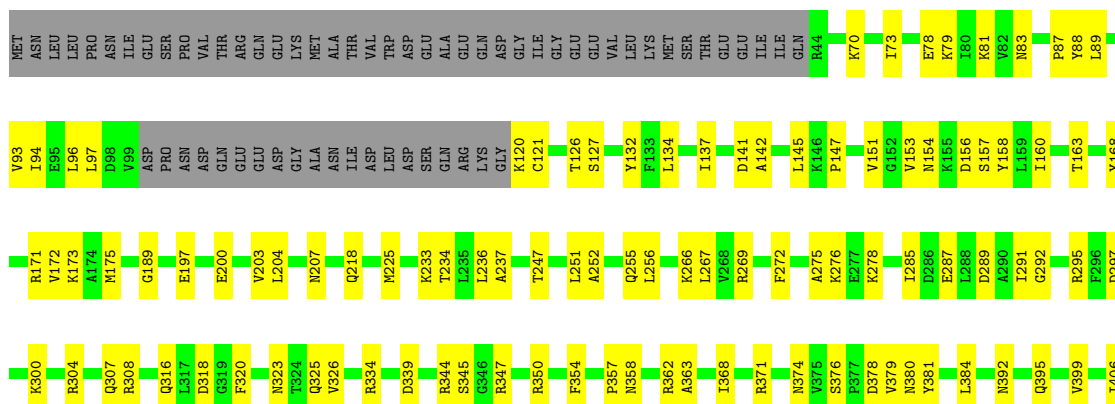
• Molecule 1: Proteasome subunit beta type-6

Chain n: 



• Molecule 2: 26S proteasome regulatory subunit 6A

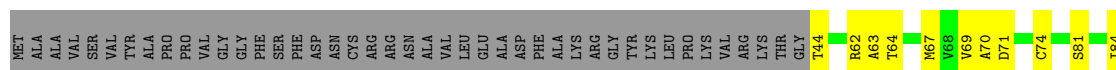
Chain F: 





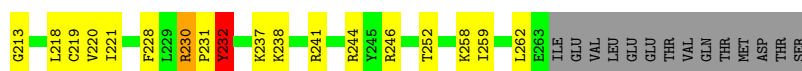
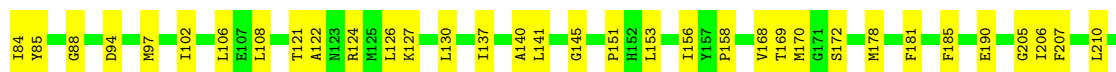
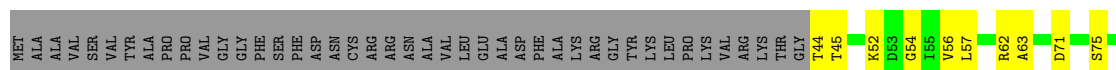
• Molecule 3: Proteasome subunit beta type-7

Chain O: 59% 19% 21%



• Molecule 3: Proteasome subunit beta type-7

Chain o: 57% 22% 21%



• Molecule 4: Proteasome subunit alpha type-6

Chain G: 70% 26% 4%



• Molecule 4: Proteasome subunit alpha type-6

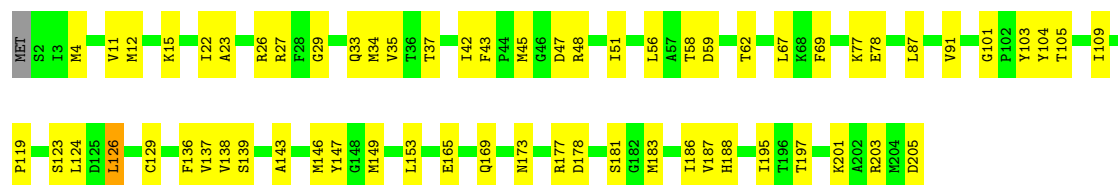
Chain g: 5% 75% 22% 4%





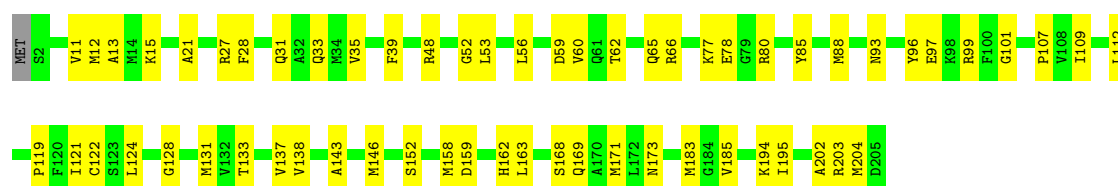
• Molecule 5: Proteasome subunit beta type-3

Chain P: 69% 30%



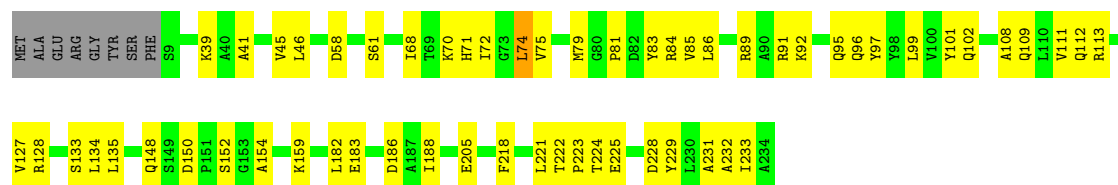
• Molecule 5: Proteasome subunit beta type-3

Chain p: 70% 29%



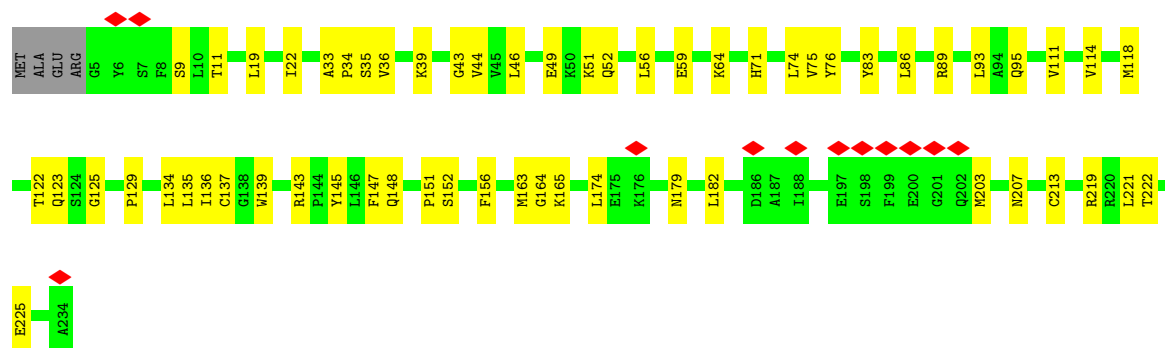
• Molecule 6: Proteasome subunit alpha type-2

Chain H: 72% 24%




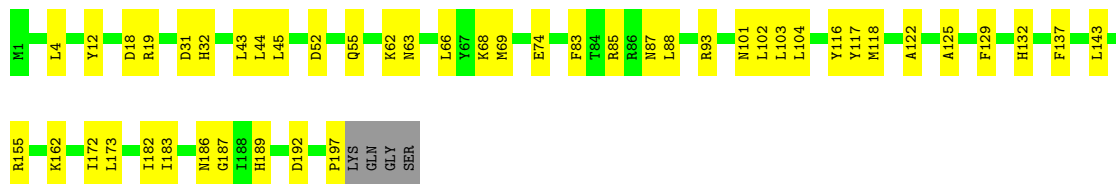
• Molecule 6: Proteasome subunit alpha type-2

Chain h: 5% 73% 25%



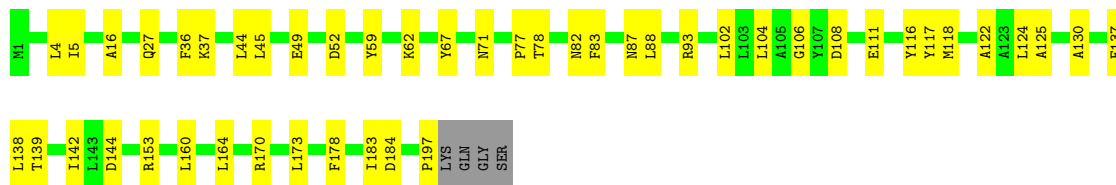
• Molecule 7: Proteasome subunit beta type-2

Chain Q:  75% 23% .




• Molecule 7: Proteasome subunit beta type-2

Chain q:  75% 23% .



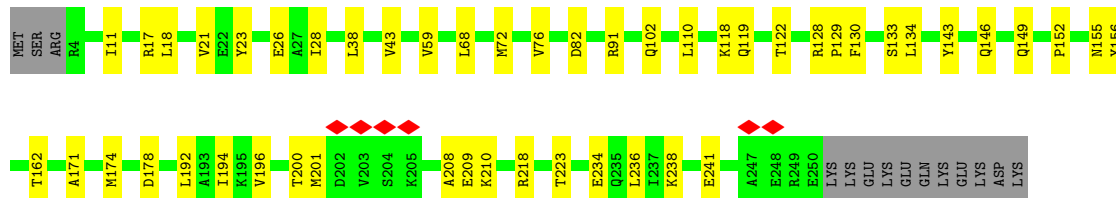
• Molecule 8: Proteasome subunit alpha type-4

Chain I:  81% 15% 5%



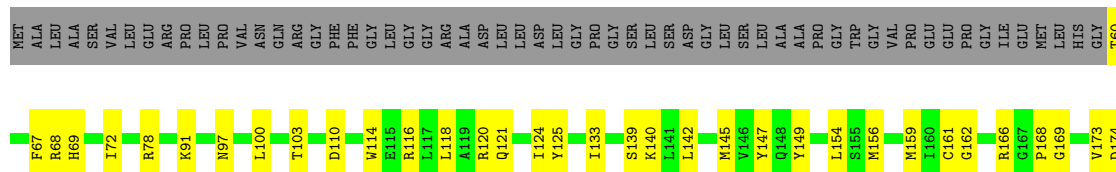
• Molecule 8: Proteasome subunit alpha type-4

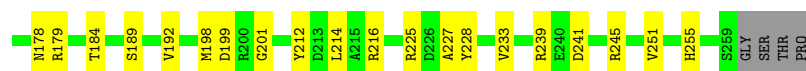
Chain i:  76% 19% 5%



• Molecule 9: Proteasome subunit beta type-5

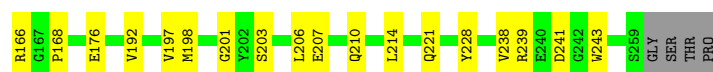
Chain R:  55% 21% 24%





• Molecule 9: Proteasome subunit beta type-5

Chain r: 56% 20% 24%



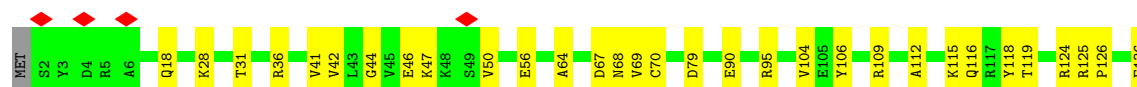
• Molecule 10: Proteasome subunit alpha type-7

Chain J: 77% 20% .



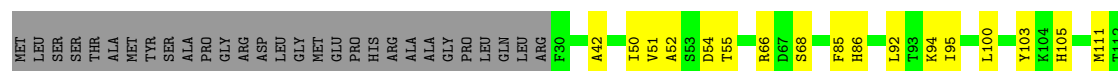
• Molecule 10: Proteasome subunit alpha type-7

Chain j: 72% 25% .



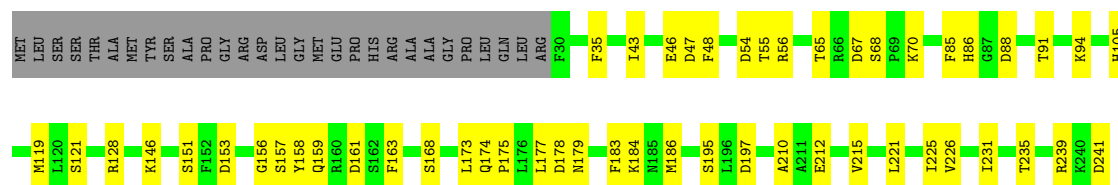
• Molecule 11: Proteasome subunit beta type-1

Chain S: 69% 18% 12%



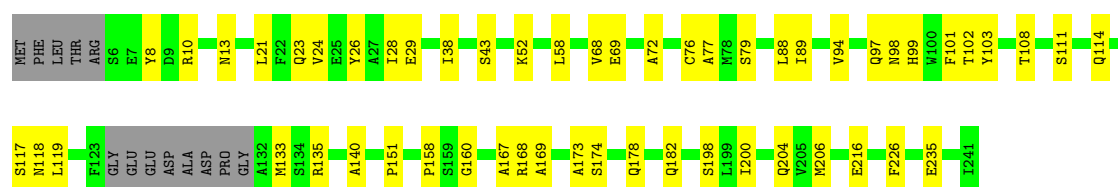
- Molecule 11: Proteasome subunit beta type-1

Chain s: 




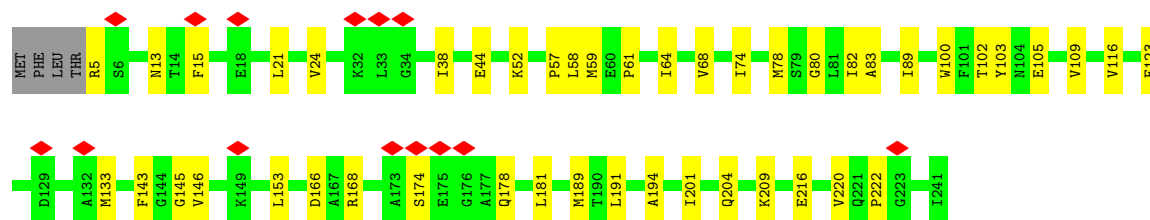
- Molecule 12: Proteasome subunit alpha type-5

Chain K: 



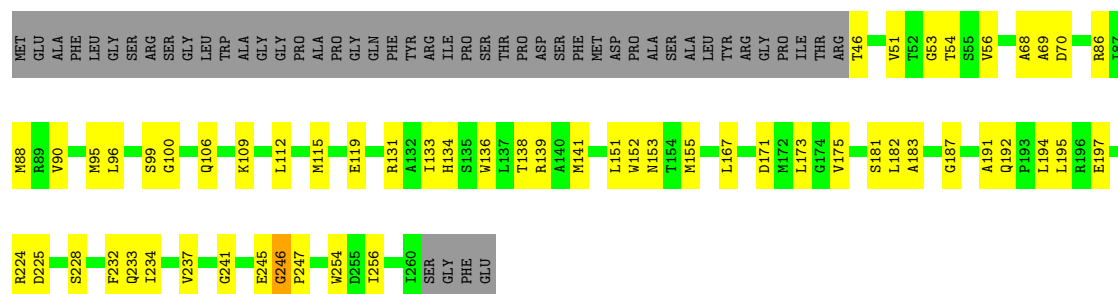
- Molecule 12: Proteasome subunit alpha type-5

Chain k: 



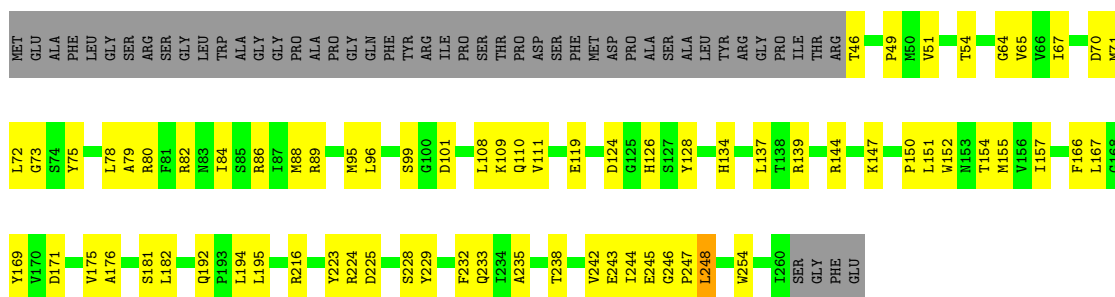
- Molecule 13: Proteasome subunit beta type-4

Chain T: 



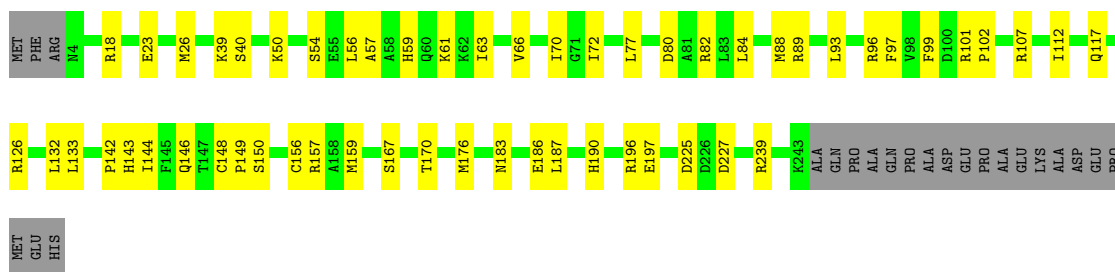
- Molecule 13: Proteasome subunit beta type-4

Chain t: 



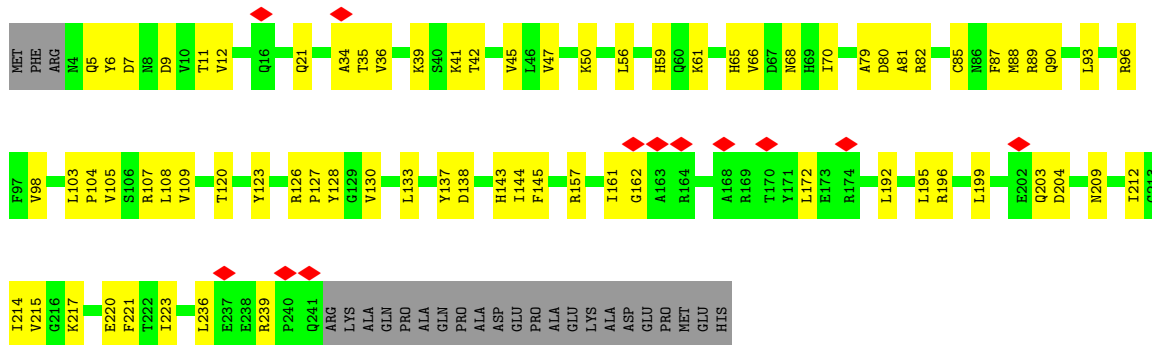
• Molecule 14: Proteasome subunit alpha type-1

Chain L: 70% 21% 9%



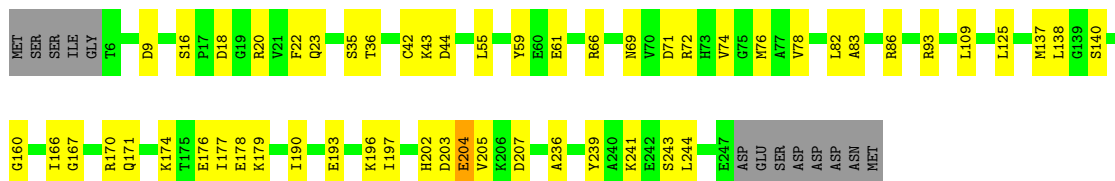
• Molecule 14: Proteasome subunit alpha type-1

Chain I: 5% 63% 28% 10%



• Molecule 15: Proteasome subunit alpha type-3

Chain M: 74% 21% 5%

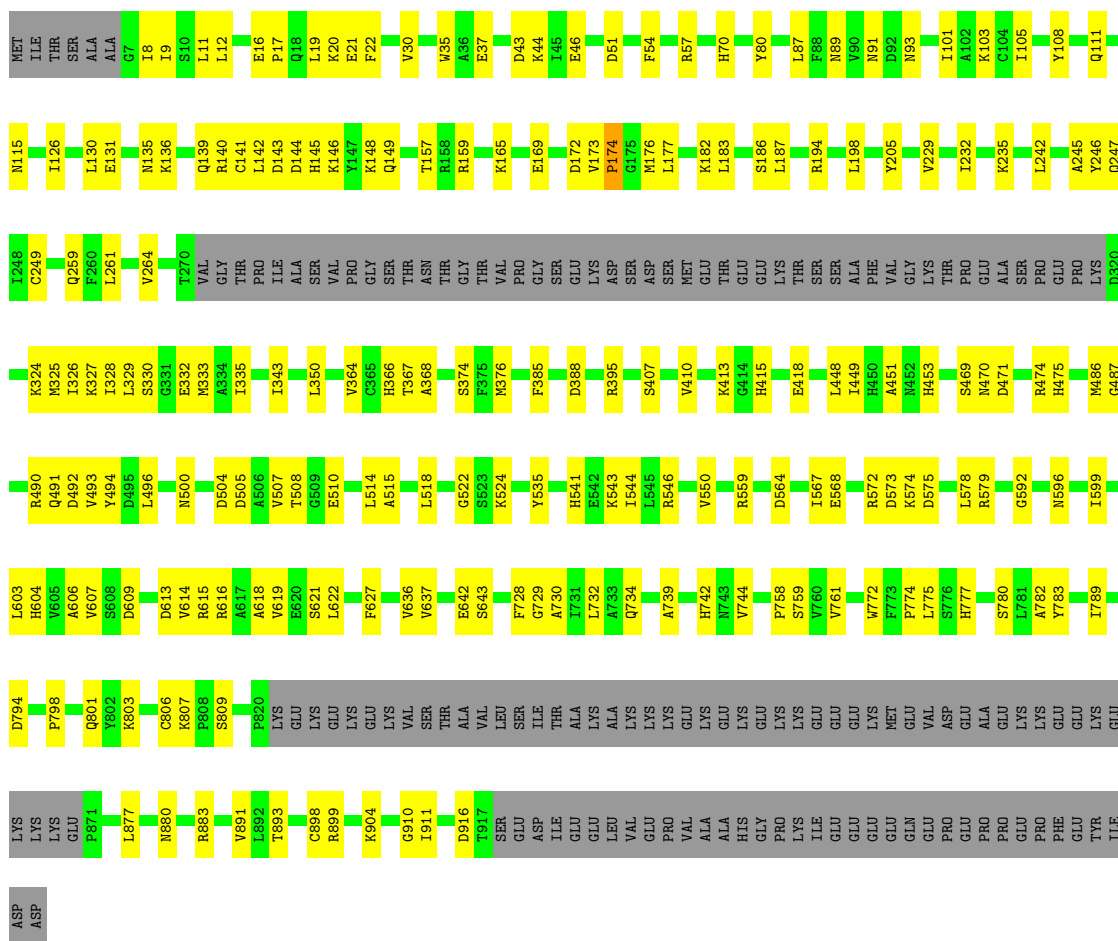


• Molecule 15: Proteasome subunit alpha type-3

Chain m: 74% 21% 5%

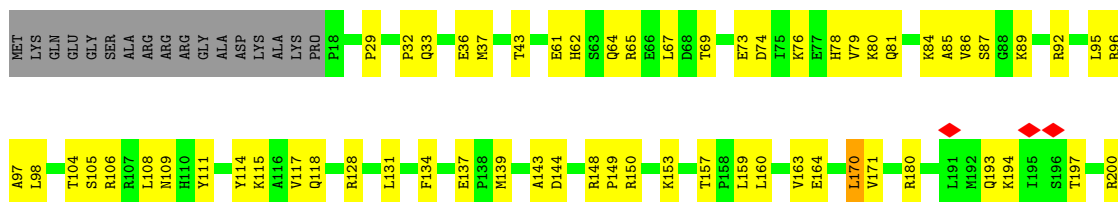
- Molecule 16: 26S proteasome non-ATPase regulatory subunit 1

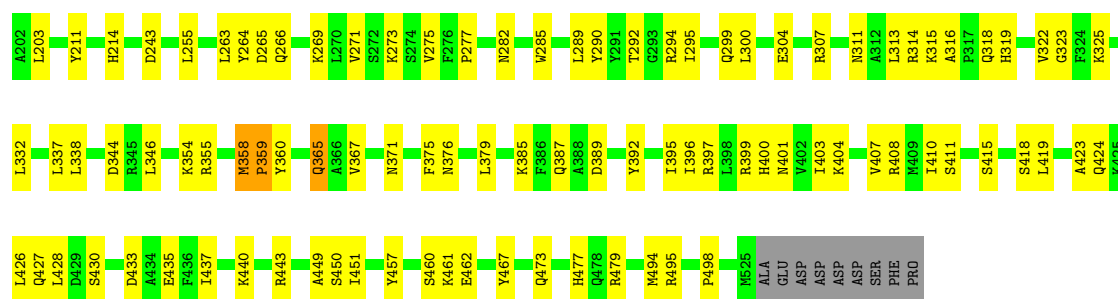
Chain U:  64% 21% 15%



- Molecule 17: 26S proteasome non-ATPase regulatory subunit 3

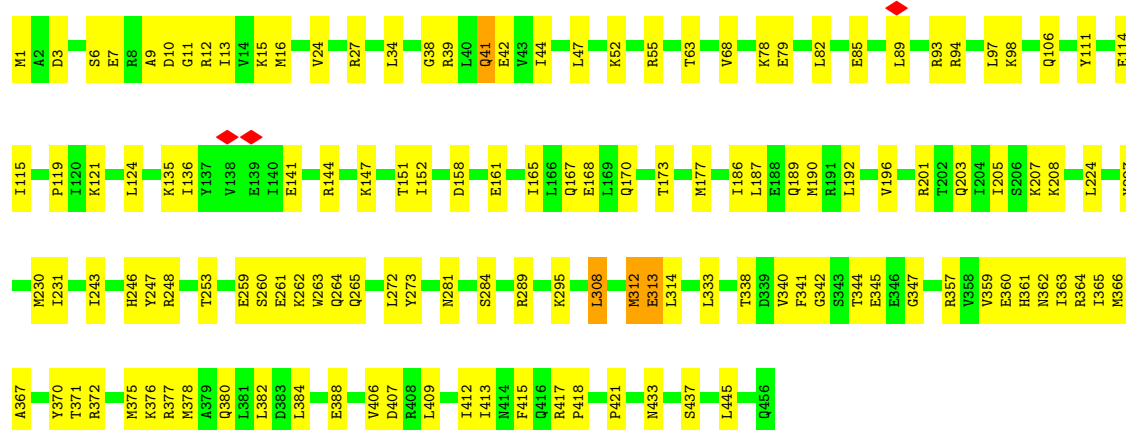
Chain V: 66% 29% 5%





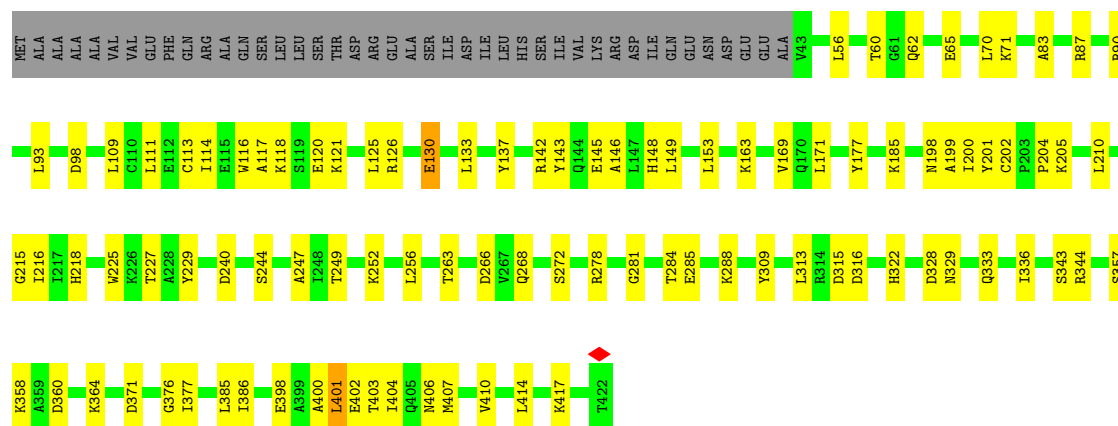
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 71% 28%



• Molecule 19: 26S proteasome non-ATPase regulatory subunit 11

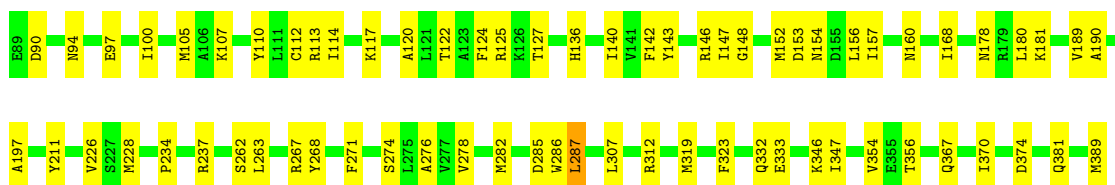
Chain X: 67% 23% 10%



• Molecule 20: 26S proteasome non-ATPase regulatory subunit 6

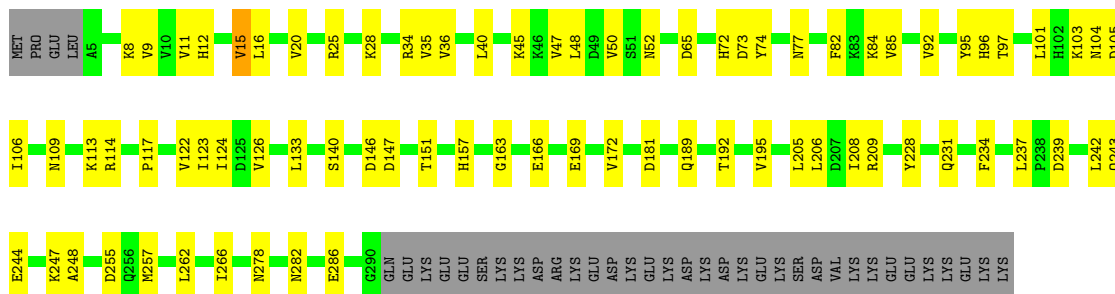
Chain Y: 72% 25%





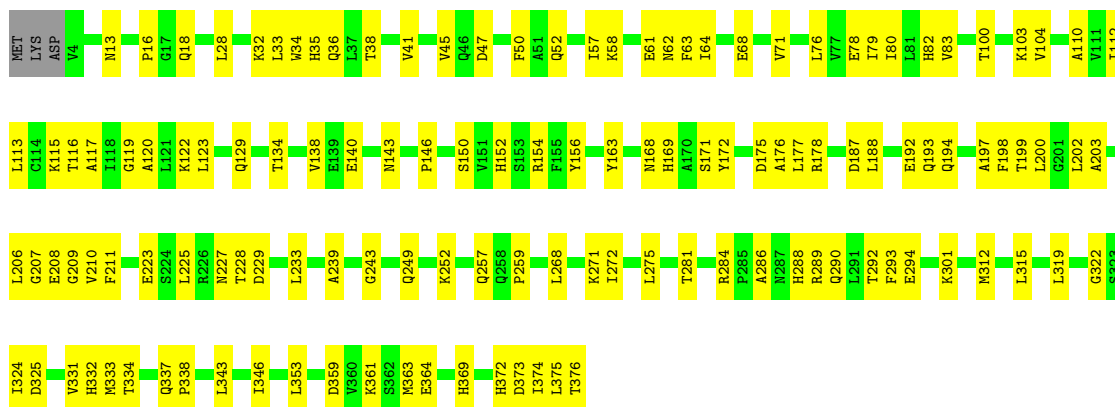
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 64% 24% 12%



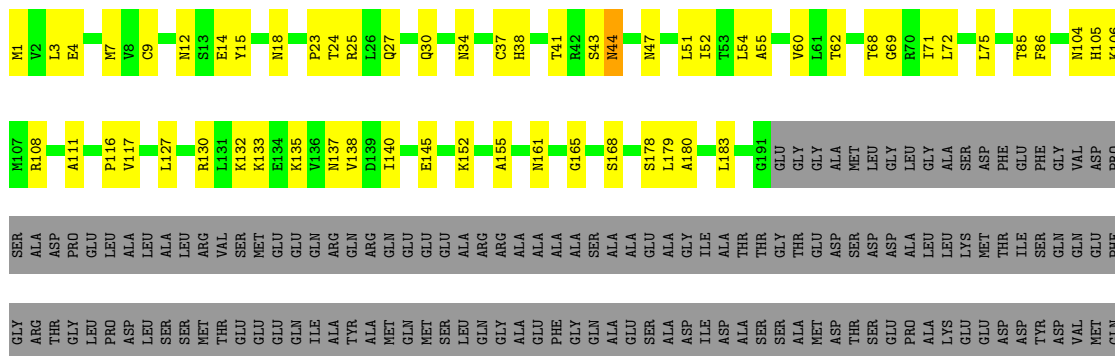
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 13

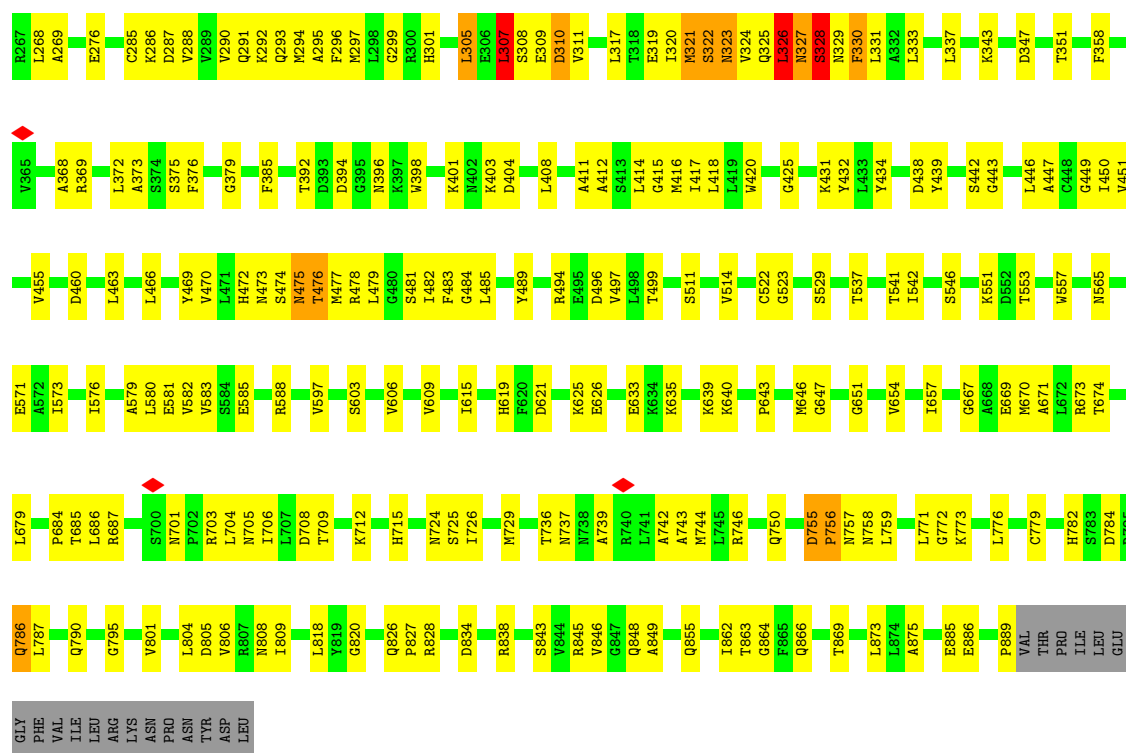
Chain a: 65% 34%



• Molecule 23: 26S proteasome non-ATPase regulatory subunit 4

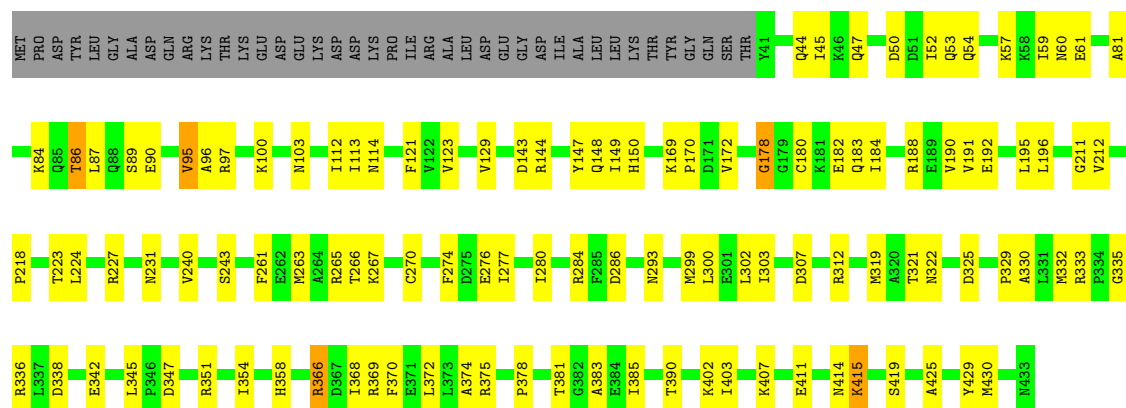
Chain b: 35% 15% 49%





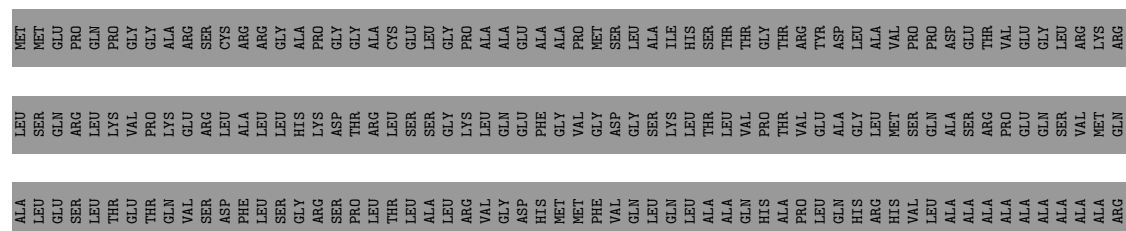
• Molecule 28: 26S proteasome regulatory subunit 7

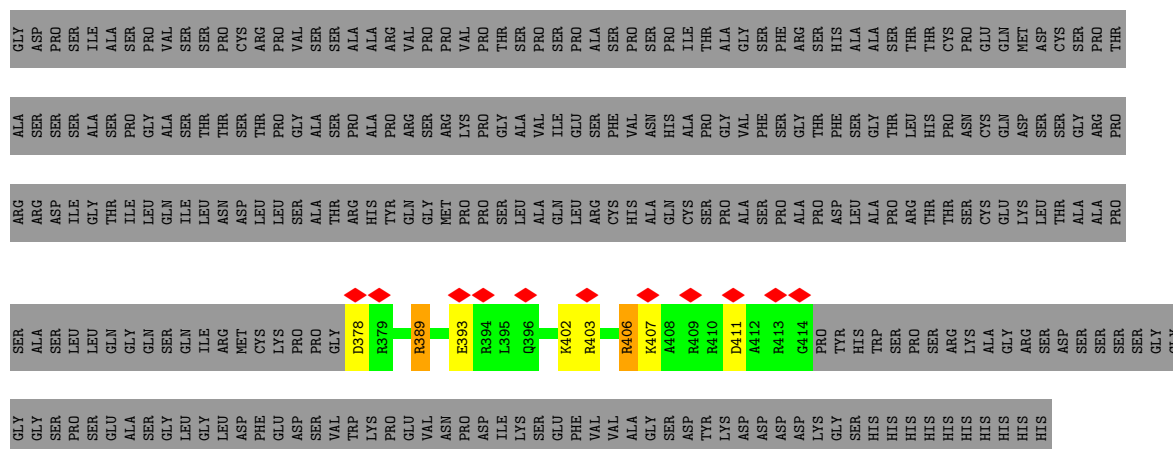
Chain A: 64% 25% 9%



• Molecule 29: Midnolin

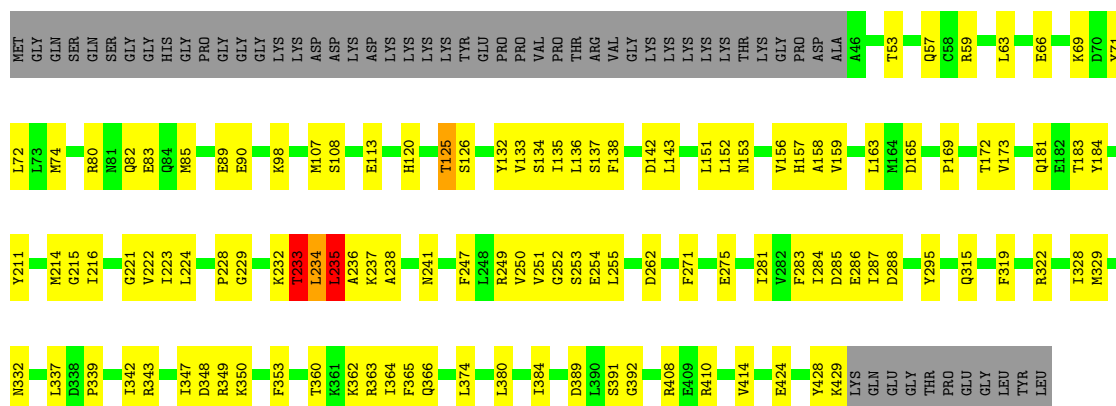
Chain u: 6% 92%





• Molecule 30: 26S proteasome regulatory subunit 4

Chain B: 61% 25% 13%



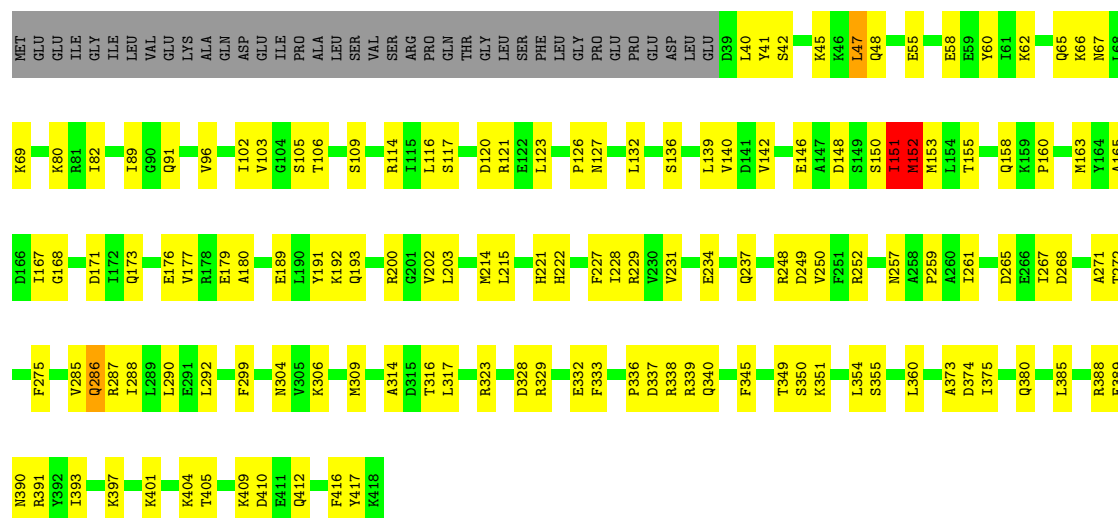
• Molecule 31: 26S proteasome regulatory subunit 8

Chain C: 63% 27% 11%



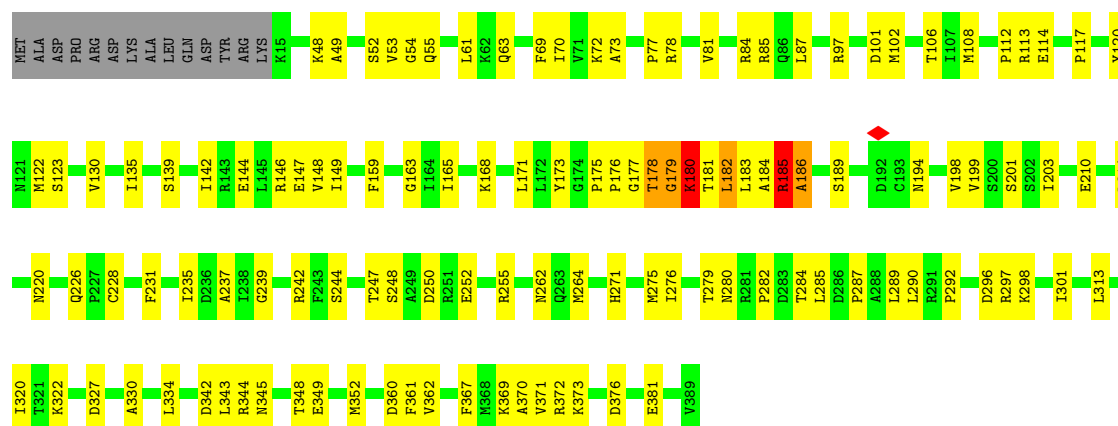
• Molecule 32: 26S proteasome regulatory subunit 6B

Chain D: 59% 31% 9%



• Molecule 33: 26S proteasome regulatory subunit 10B

Chain E: 65% 30%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22328	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.397	Depositor
Minimum map value	-0.171	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	N	0.19	0/1532	0.47	0/2074
1	n	0.17	0/1532	0.42	0/2074
2	F	0.27	0/2864	0.59	0/3873
3	O	0.25	0/1686	0.52	1/2282 (0.0%)
3	o	0.19	0/1686	0.47	2/2282 (0.1%)
4	G	0.22	0/1818	0.55	0/2470
4	g	0.17	0/1899	0.42	0/2568
5	P	0.22	0/1620	0.49	0/2184
5	p	0.20	0/1620	0.48	0/2184
6	H	0.25	0/1695	0.57	1/2308 (0.0%)
6	h	0.16	0/1832	0.40	0/2481
7	Q	0.19	0/1611	0.50	0/2180
7	q	0.18	0/1611	0.49	0/2180
8	I	0.20	0/1900	0.53	0/2572
8	i	0.16	0/1975	0.43	0/2661
9	R	0.17	0/1586	0.41	0/2142
9	r	0.16	0/1586	0.40	0/2142
10	J	0.21	0/1727	0.55	1/2355 (0.0%)
10	j	0.14	0/1913	0.37	0/2581
11	S	0.19	0/1673	0.43	0/2254
11	s	0.17	0/1673	0.44	0/2254
12	K	0.19	0/1706	0.48	0/2314
12	k	0.16	0/1844	0.44	1/2489 (0.0%)
13	T	0.23	0/1714	0.55	0/2320
13	t	0.25	0/1714	0.58	1/2320 (0.0%)
14	L	0.20	0/1888	0.52	0/2555
14	l	0.18	0/1908	0.44	0/2579
15	M	0.19	0/1886	0.48	0/2550
15	m	0.17	0/1920	0.45	0/2585
16	U	0.22	0/6348	0.53	0/8603
17	V	0.30	0/3980	0.71	0/5394
18	W	0.26	0/3646	0.63	0/4916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	X	0.25	0/2979	0.62	3/4023 (0.1%)
20	Y	0.26	0/3120	0.63	2/4208 (0.0%)
21	Z	0.26	0/2287	0.63	3/3102 (0.1%)
22	a	0.25	0/3032	0.62	0/4107
23	b	0.31	0/1452	0.70	0/1968
24	c	0.27	0/2176	0.66	0/2939
25	d	0.31	0/2031	0.71	0/2751
26	e	0.26	0/317	0.69	0/425
27	f	0.36	0/6779	0.75	3/9183 (0.0%)
28	A	0.28	0/3065	0.68	3/4146 (0.1%)
29	u	0.84	0/319	1.44	0/419
30	B	0.26	0/3017	0.63	6/4076 (0.1%)
31	C	0.29	0/2868	0.66	2/3861 (0.1%)
32	D	0.31	0/3041	0.75	3/4111 (0.1%)
33	E	0.28	0/2871	0.70	4/3882 (0.1%)
All	All	0.25	0/104947	0.59	36/141927 (0.0%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	E	185	ARG	N-CA-C	-10.46	100.00	113.17
33	E	182	LEU	N-CA-C	-9.74	100.62	111.14
33	E	186	ALA	N-CA-C	-9.05	101.81	113.12
30	B	235	LEU	N-CA-C	-7.98	101.54	111.75
27	f	330	PHE	N-CA-C	-6.98	103.60	111.07

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	N	1506	0	1473	37	0
1	n	1506	0	1473	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2826	0	2786	100	0
3	O	1659	0	1678	64	0
3	o	1659	0	1678	59	0
4	G	1785	0	1736	46	0
4	g	1865	0	1872	41	0
5	P	1591	0	1609	57	0
5	p	1591	0	1609	41	0
6	H	1660	0	1577	53	0
6	h	1793	0	1787	39	0
7	Q	1578	0	1580	41	0
7	q	1578	0	1580	33	0
8	I	1872	0	1798	25	0
8	i	1945	0	1961	32	0
9	R	1555	0	1517	37	0
9	r	1555	0	1517	34	0
10	J	1703	0	1549	41	0
10	j	1887	0	1905	38	0
11	S	1643	0	1640	31	0
11	s	1643	0	1640	41	0
12	K	1681	0	1609	38	0
12	k	1816	0	1797	34	0
13	T	1681	0	1658	40	0
13	t	1681	0	1658	51	0
14	L	1853	0	1826	41	0
14	l	1873	0	1860	55	0
15	M	1851	0	1785	40	0
15	m	1885	0	1871	36	0
16	U	6237	0	6165	139	0
17	V	3905	0	3779	123	0
18	W	3598	0	3576	100	0
19	X	2938	0	2979	76	0
20	Y	3062	0	3008	74	0
21	Z	2246	0	2244	69	0
22	a	2974	0	2968	91	0
23	b	1432	0	1447	49	0
24	c	2139	0	2095	59	0
25	d	1990	0	1939	51	0
26	e	313	0	261	12	0
27	f	6670	0	6464	310	0
28	A	3016	0	2992	103	0
29	u	320	0	351	17	0
30	B	2975	0	2998	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	C	2831	0	2896	118	0
32	D	2991	0	2965	144	0
33	E	2828	0	2780	120	0
34	C	27	0	12	0	0
34	F	27	0	12	9	0
35	A	31	0	12	5	0
35	B	31	0	12	7	0
35	D	31	0	12	34	0
35	E	31	0	12	8	0
All	All	103364	0	102008	2715	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 13.

The worst 5 of 2715 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)
27:f:404:ASP:HB3	27:f:439:TYR:CZ	1.50	1.44
27:f:414:LEU:HD12	27:f:417:ILE:CD1	1.49	1.40
19:X:256:LEU:HD21	19:X:322:HIS:NE2	1.42	1.31
27:f:404:ASP:HB3	27:f:439:TYR:CE2	1.69	1.28
30:B:233:THR:HG21	30:B:285:ASP:OD2	1.32	1.28

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	N	199/239 (83%)	194 (98%)	5 (2%)	0	100	100
1	n	199/239 (83%)	194 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	371/439 (84%)	334 (90%)	37 (10%)	0	100	100
3	O	218/277 (79%)	209 (96%)	8 (4%)	1 (0%)	25	63
3	o	218/277 (79%)	211 (97%)	6 (3%)	1 (0%)	25	63
4	G	236/246 (96%)	224 (95%)	12 (5%)	0	100	100
4	g	237/246 (96%)	230 (97%)	7 (3%)	0	100	100
5	P	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
5	p	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
6	H	224/234 (96%)	212 (95%)	11 (5%)	1 (0%)	30	67
6	h	228/234 (97%)	224 (98%)	4 (2%)	0	100	100
7	Q	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
7	q	195/201 (97%)	188 (96%)	7 (4%)	0	100	100
8	I	247/261 (95%)	226 (92%)	19 (8%)	2 (1%)	16	53
8	i	245/261 (94%)	244 (100%)	1 (0%)	0	100	100
9	R	198/263 (75%)	193 (98%)	5 (2%)	0	100	100
9	r	198/263 (75%)	194 (98%)	4 (2%)	0	100	100
10	J	239/248 (96%)	219 (92%)	18 (8%)	2 (1%)	16	53
10	j	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
11	S	210/241 (87%)	201 (96%)	8 (4%)	1 (0%)	25	63
11	s	210/241 (87%)	201 (96%)	9 (4%)	0	100	100
12	K	224/241 (93%)	209 (93%)	15 (7%)	0	100	100
12	k	235/241 (98%)	229 (97%)	6 (3%)	0	100	100
13	T	213/264 (81%)	205 (96%)	6 (3%)	2 (1%)	14	50
13	t	213/264 (81%)	203 (95%)	9 (4%)	1 (0%)	25	63
14	L	238/263 (90%)	229 (96%)	9 (4%)	0	100	100
14	l	236/263 (90%)	231 (98%)	5 (2%)	0	100	100
15	M	240/255 (94%)	228 (95%)	10 (4%)	2 (1%)	16	53
15	m	239/255 (94%)	233 (98%)	6 (2%)	0	100	100
16	U	806/953 (85%)	742 (92%)	63 (8%)	1 (0%)	48	82
17	V	506/534 (95%)	438 (87%)	65 (13%)	3 (1%)	22	59
18	W	454/456 (100%)	414 (91%)	37 (8%)	3 (1%)	19	55
19	X	378/422 (90%)	338 (89%)	38 (10%)	2 (0%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Y	376/389 (97%)	348 (93%)	28 (7%)	0	100	100
21	Z	284/324 (88%)	253 (89%)	31 (11%)	0	100	100
22	a	371/376 (99%)	328 (88%)	41 (11%)	2 (0%)	25	63
23	b	189/377 (50%)	156 (82%)	30 (16%)	3 (2%)	8	37
24	c	275/310 (89%)	242 (88%)	30 (11%)	3 (1%)	12	46
25	d	250/350 (71%)	200 (80%)	48 (19%)	2 (1%)	16	53
26	e	35/70 (50%)	25 (71%)	9 (26%)	1 (3%)	3	24
27	f	887/908 (98%)	741 (84%)	137 (15%)	9 (1%)	13	48
28	A	391/433 (90%)	328 (84%)	59 (15%)	4 (1%)	13	48
29	u	35/491 (7%)	35 (100%)	0	0	100	100
30	B	382/440 (87%)	349 (91%)	33 (9%)	0	100	100
31	C	359/406 (88%)	323 (90%)	36 (10%)	0	100	100
32	D	378/418 (90%)	330 (87%)	43 (11%)	5 (1%)	10	41
33	E	373/389 (96%)	341 (91%)	31 (8%)	1 (0%)	37	72
All	All	13275/15361 (86%)	12206 (92%)	1017 (8%)	52 (0%)	32	67

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	X	200	ILE
23	b	117	VAL
24	c	284	LEU
25	d	201	ASN
26	e	8	VAL

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	N	156/181 (86%)	156 (100%)	0	100	100
1	n	156/181 (86%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	288/379 (76%)	287 (100%)	1 (0%)	91	92
3	O	181/228 (79%)	178 (98%)	3 (2%)	56	72
3	o	181/228 (79%)	180 (99%)	1 (1%)	84	88
4	G	183/210 (87%)	183 (100%)	0	100	100
4	g	204/210 (97%)	204 (100%)	0	100	100
5	P	173/174 (99%)	172 (99%)	1 (1%)	84	88
5	p	173/174 (99%)	173 (100%)	0	100	100
6	H	159/191 (83%)	158 (99%)	1 (1%)	84	88
6	h	188/191 (98%)	188 (100%)	0	100	100
7	Q	168/171 (98%)	168 (100%)	0	100	100
7	q	168/171 (98%)	168 (100%)	0	100	100
8	I	185/221 (84%)	185 (100%)	0	100	100
8	i	207/221 (94%)	207 (100%)	0	100	100
9	R	156/202 (77%)	156 (100%)	0	100	100
9	r	156/202 (77%)	156 (100%)	0	100	100
10	J	150/211 (71%)	150 (100%)	0	100	100
10	j	203/211 (96%)	203 (100%)	0	100	100
11	S	177/199 (89%)	177 (100%)	0	100	100
11	s	177/199 (89%)	177 (100%)	0	100	100
12	K	174/203 (86%)	174 (100%)	0	100	100
12	k	199/203 (98%)	199 (100%)	0	100	100
13	T	178/215 (83%)	178 (100%)	0	100	100
13	t	178/215 (83%)	177 (99%)	1 (1%)	84	88
14	L	195/224 (87%)	195 (100%)	0	100	100
14	l	204/224 (91%)	204 (100%)	0	100	100
15	M	188/212 (89%)	188 (100%)	0	100	100
15	m	198/212 (93%)	198 (100%)	0	100	100
16	U	667/816 (82%)	667 (100%)	0	100	100
17	V	391/460 (85%)	388 (99%)	3 (1%)	79	85
18	W	388/416 (93%)	386 (100%)	2 (0%)	86	90
19	X	309/362 (85%)	308 (100%)	1 (0%)	91	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Y	319/344 (93%)	318 (100%)	1 (0%)	91	92
21	Z	248/295 (84%)	248 (100%)	0	100	100
22	a	328/336 (98%)	327 (100%)	1 (0%)	91	92
23	b	159/312 (51%)	158 (99%)	1 (1%)	84	88
24	c	228/268 (85%)	228 (100%)	0	100	100
25	d	206/294 (70%)	205 (100%)	1 (0%)	86	90
26	e	33/63 (52%)	33 (100%)	0	100	100
27	f	694/763 (91%)	683 (98%)	11 (2%)	58	74
28	A	319/372 (86%)	318 (100%)	1 (0%)	91	92
29	u	33/398 (8%)	30 (91%)	3 (9%)	7	25
30	B	328/385 (85%)	325 (99%)	3 (1%)	75	83
31	C	305/352 (87%)	304 (100%)	1 (0%)	91	92
32	D	320/366 (87%)	317 (99%)	3 (1%)	75	83
33	E	290/341 (85%)	287 (99%)	3 (1%)	73	81
All	All	10868/13006 (84%)	10825 (100%)	43 (0%)	88	91

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	t	248	LEU
30	B	235	LEU
28	A	403	ILE
29	u	406	ARG
32	D	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
31	C	32	GLN
31	C	64	GLN
10	j	85	ASN
10	j	18	GLN
31	C	111	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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
34	ADP	F	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.34	4 (13%)
34	ADP	C	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)
35	ATP	E	401	-	26,33,33	0.57	0	31,52,52	0.82	2 (6%)
35	ATP	D	501	-	26,33,33	0.72	0	31,52,52	0.89	1 (3%)
35	ATP	A	501	-	26,33,33	0.63	0	31,52,52	0.85	2 (6%)
35	ATP	B	501	-	26,33,33	0.65	0	31,52,52	0.84	1 (3%)

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
34	ADP	F	501	-	-	4/12/32/32	0/3/3/3
34	ADP	C	501	-	-	3/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	E	401	-	-	1/18/38/38	0/3/3/3
35	ATP	D	501	-	-	10/18/38/38	0/3/3/3
35	ATP	A	501	-	-	6/18/38/38	0/3/3/3
35	ATP	B	501	-	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	501	ADP	C5-C4	2.39	1.47	1.40
34	F	501	ADP	C5-C4	2.34	1.47	1.40

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	501	ADP	C3'-C2'-C1'	3.75	106.62	100.98
34	F	501	ADP	C3'-C2'-C1'	3.42	106.13	100.98
34	C	501	ADP	PA-O3A-PB	-3.03	122.44	132.83
34	F	501	ADP	N3-C2-N1	-2.97	124.03	128.68
34	C	501	ADP	N3-C2-N1	-2.94	124.08	128.68

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

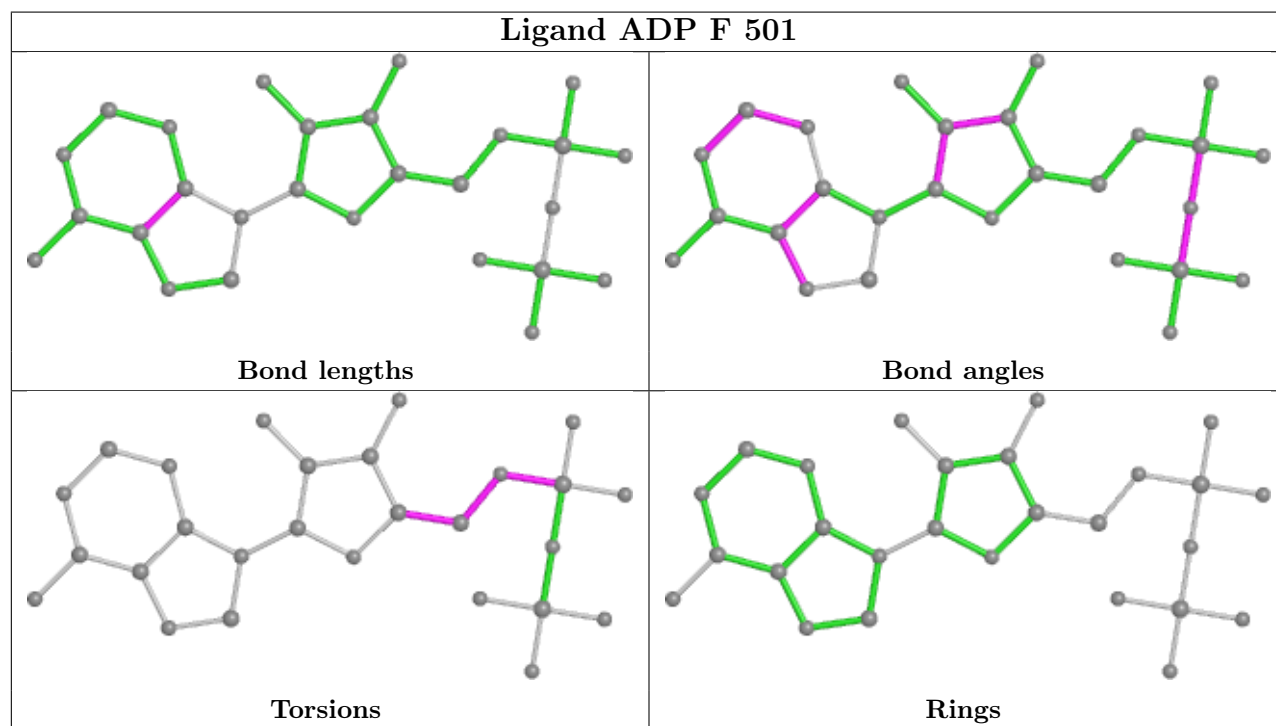
Mol	Chain	Res	Type	Atoms
34	F	501	ADP	C5'-O5'-PA-O1A
34	C	501	ADP	PB-O3A-PA-O5'
34	C	501	ADP	O4'-C4'-C5'-O5'
34	C	501	ADP	C3'-C4'-C5'-O5'
35	A	501	ATP	PB-O3B-PG-O2G

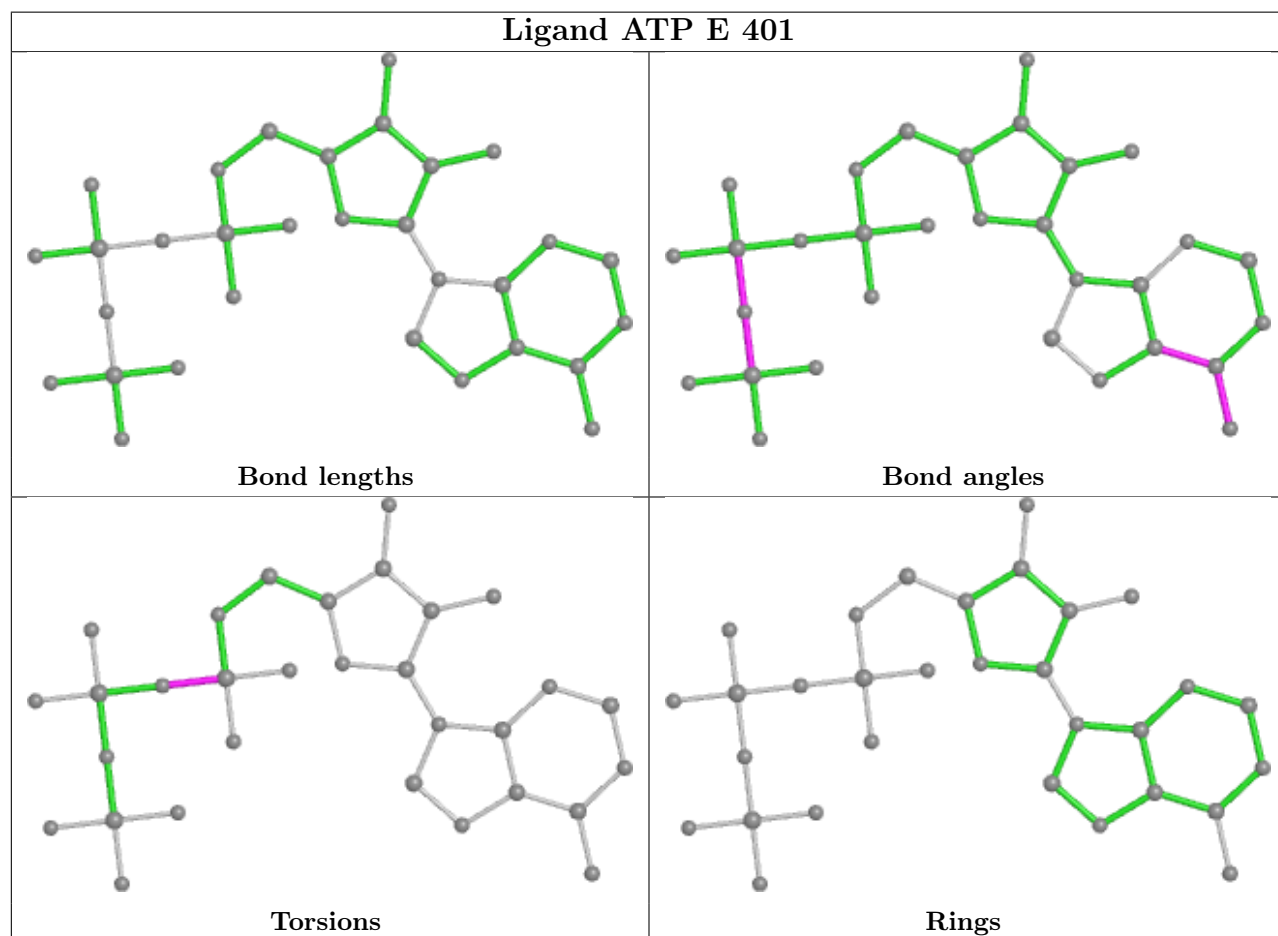
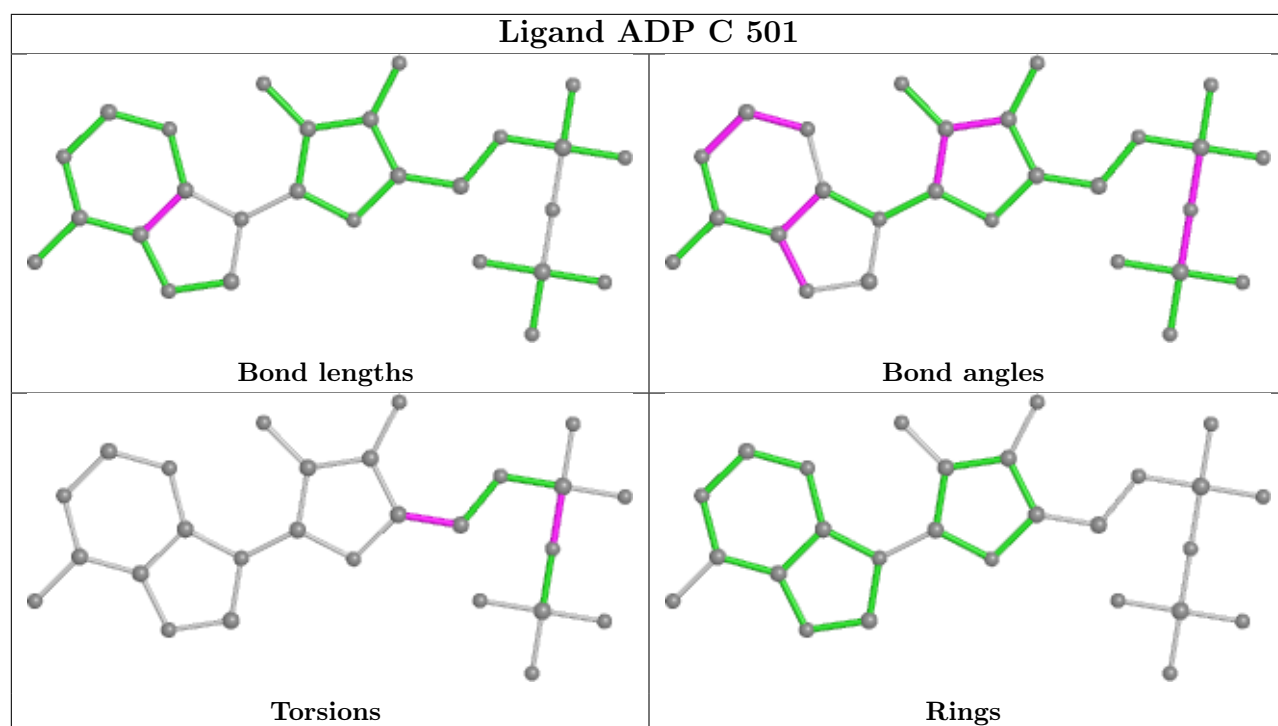
There are no ring outliers.

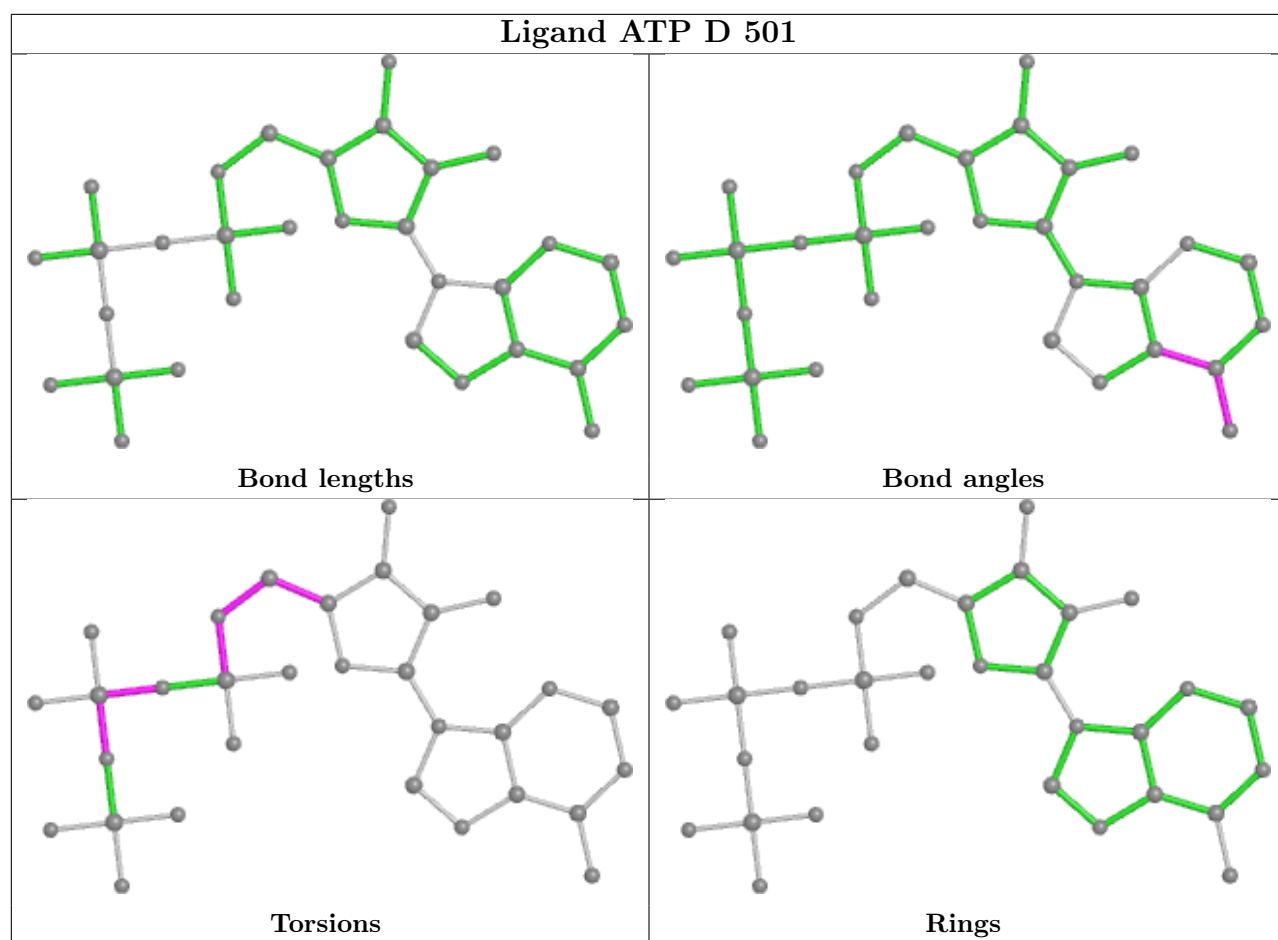
5 monomers are involved in 63 short contacts:

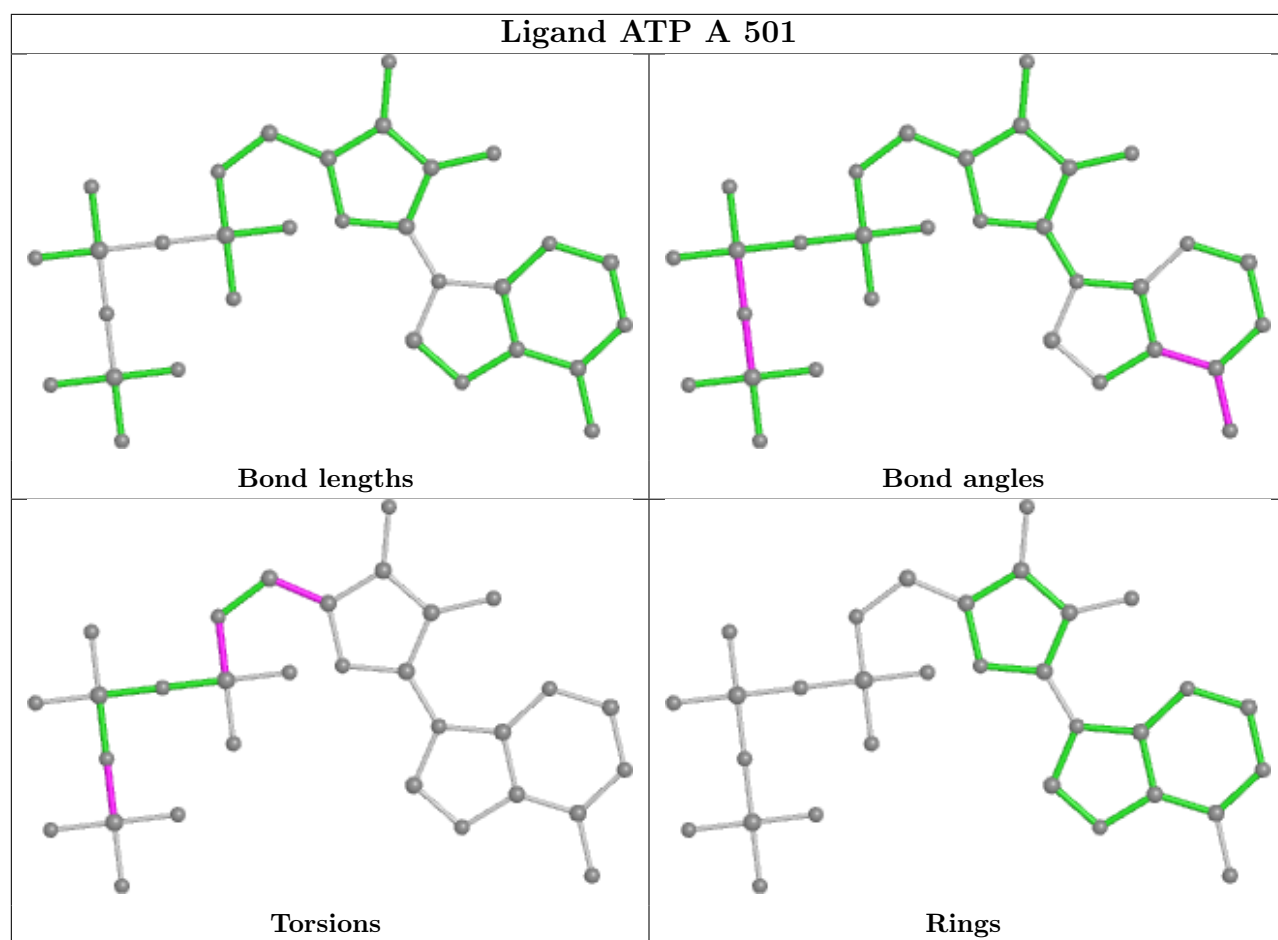
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	F	501	ADP	9	0
35	E	401	ATP	8	0
35	D	501	ATP	34	0
35	A	501	ATP	5	0
35	B	501	ATP	7	0

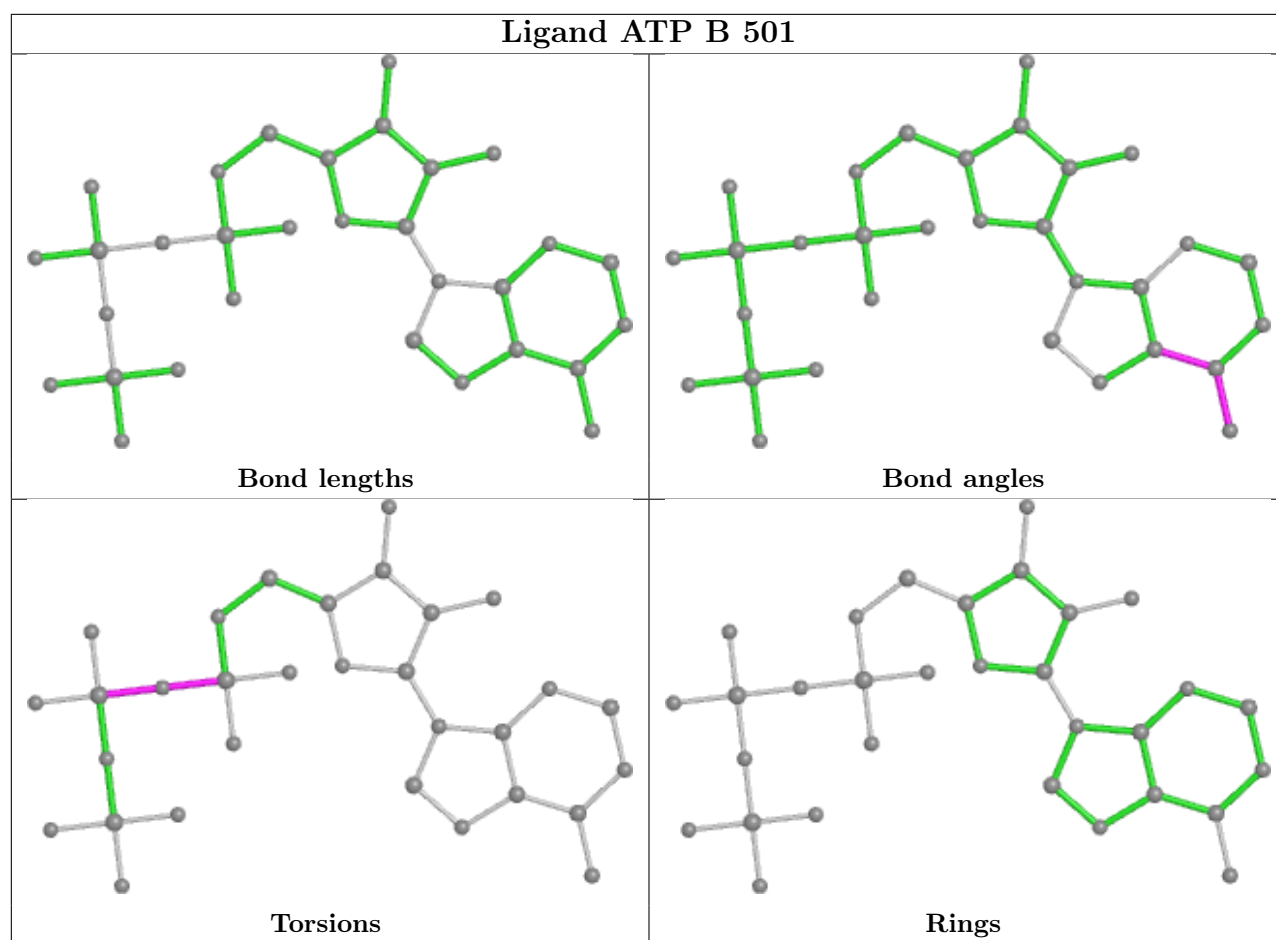
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











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.

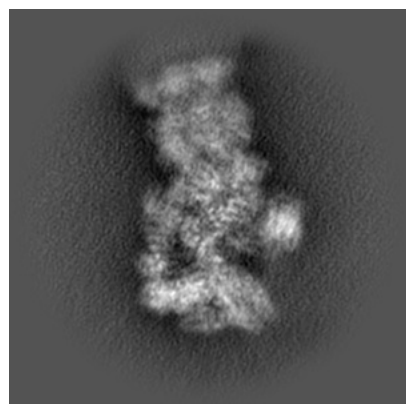
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64103. These allow visual inspection of the internal detail of the map and identification of artifacts.

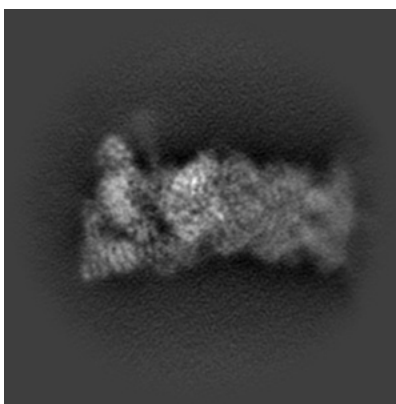
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

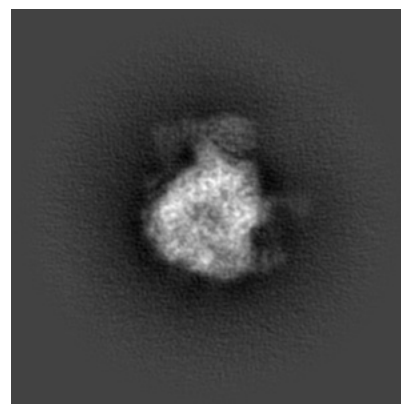
6.1.1 Primary map



X

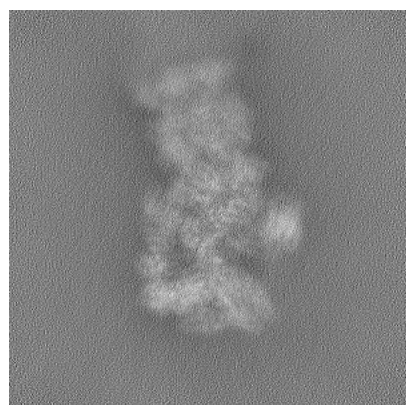


Y

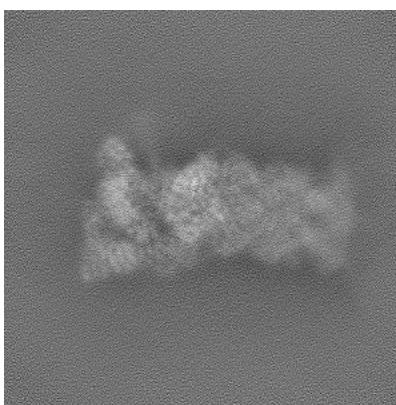


Z

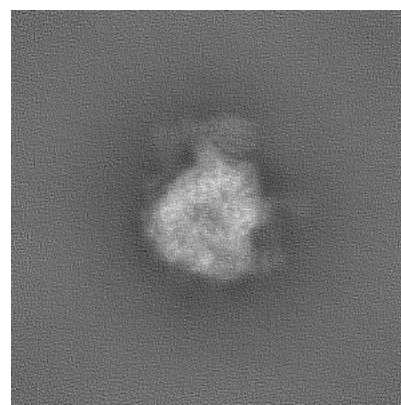
6.1.2 Raw map



X



Y

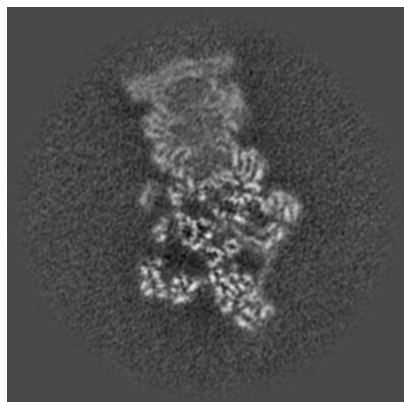


Z

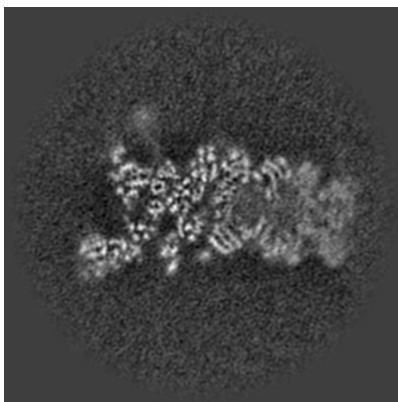
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

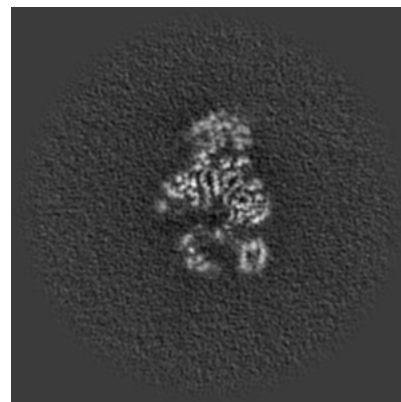
6.2.1 Primary map



X Index: 210

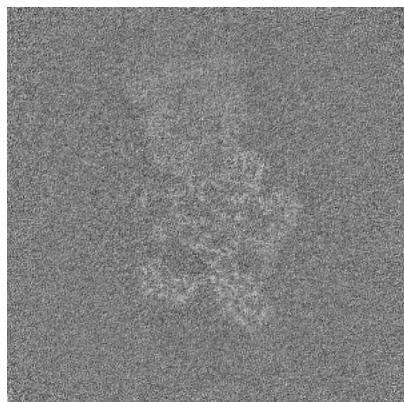


Y Index: 210

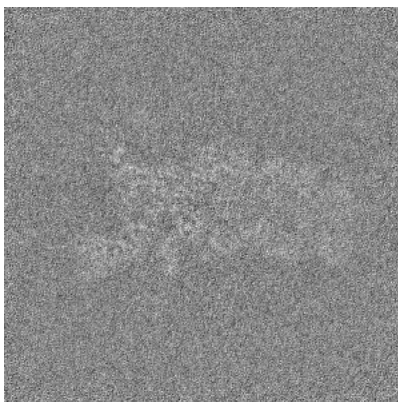


Z Index: 210

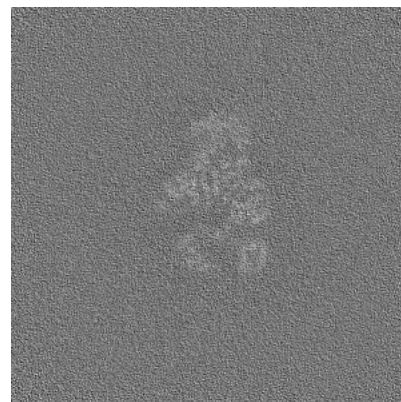
6.2.2 Raw map



X Index: 210



Y Index: 210

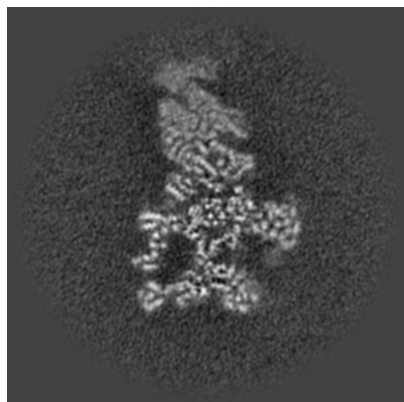


Z Index: 210

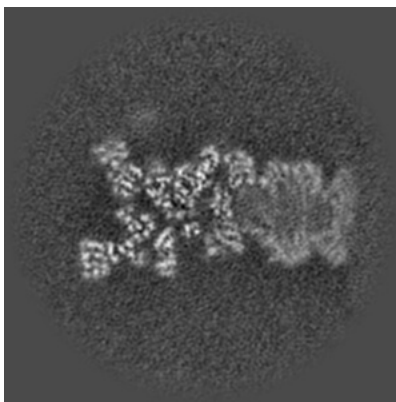
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

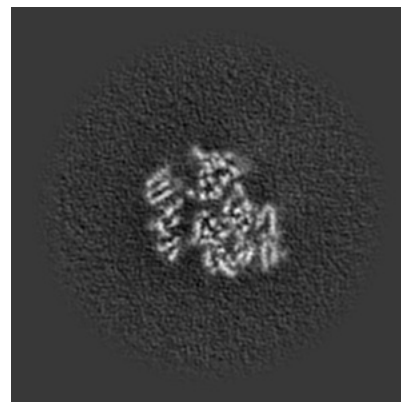
6.3.1 Primary map



X Index: 238

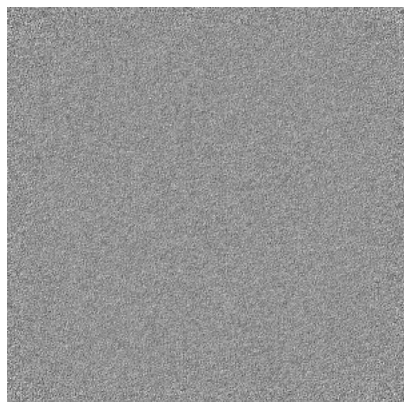


Y Index: 203

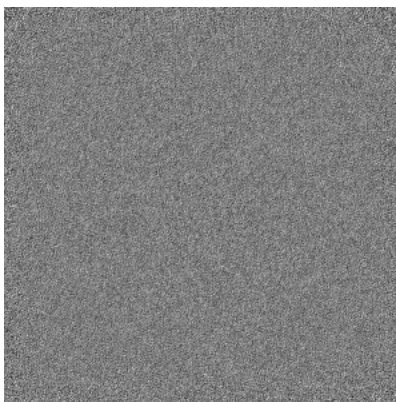


Z Index: 123

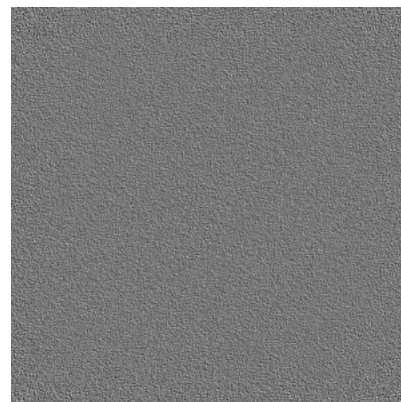
6.3.2 Raw map



X Index: 0



Y Index: 0

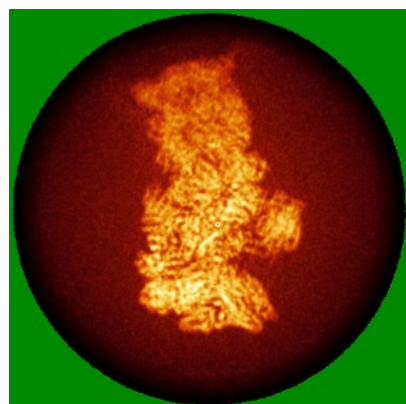


Z Index: 419

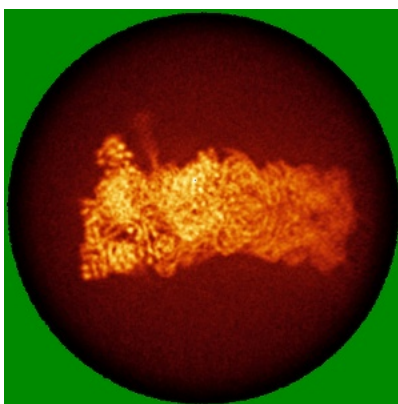
The images above show the largest variance slices of the map in three orthogonal directions.

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

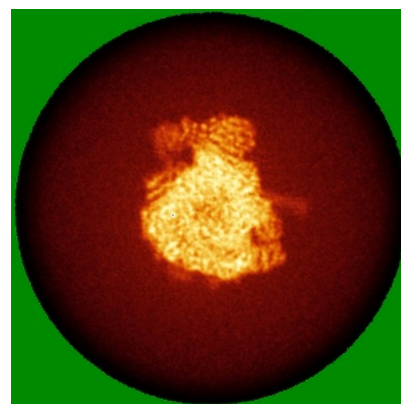
6.4.1 Primary map



X

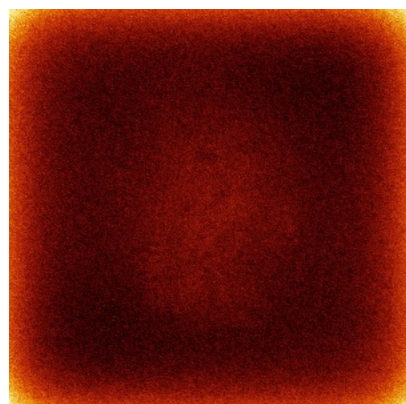


Y

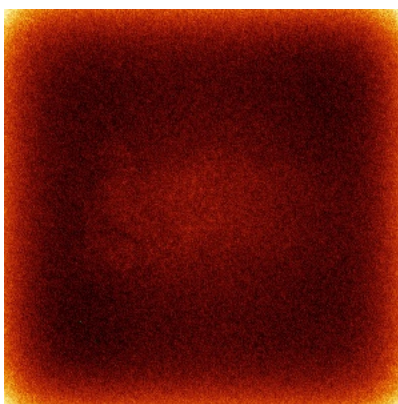


Z

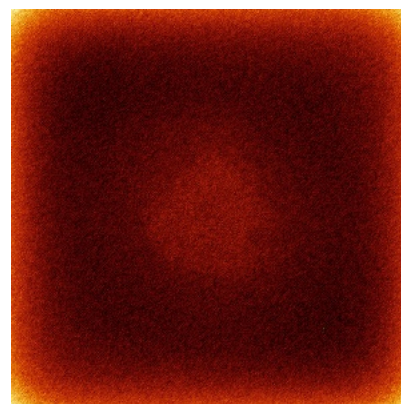
6.4.2 Raw map



X



Y

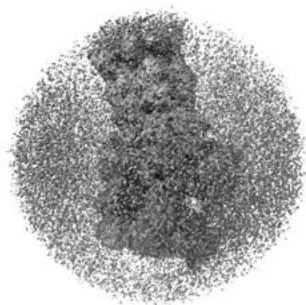


Z

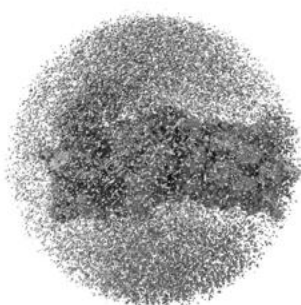
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

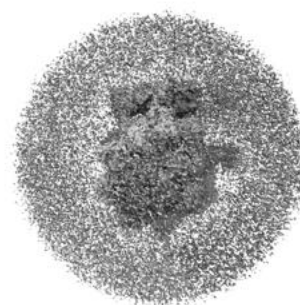
6.5.1 Primary map



X



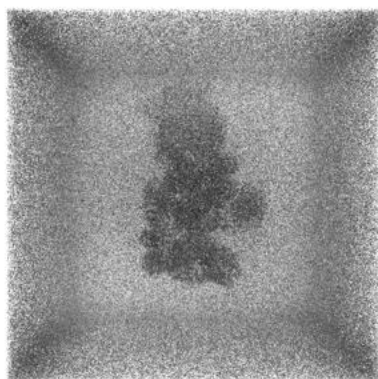
Y



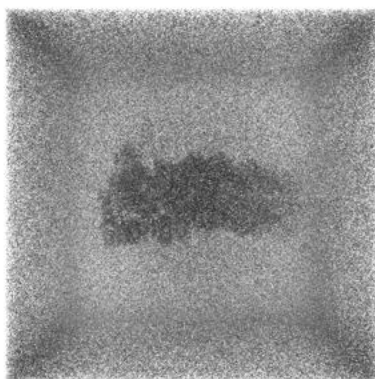
Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

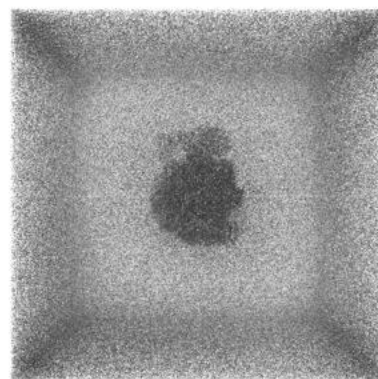
6.5.2 Raw map



X



Y



Z

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

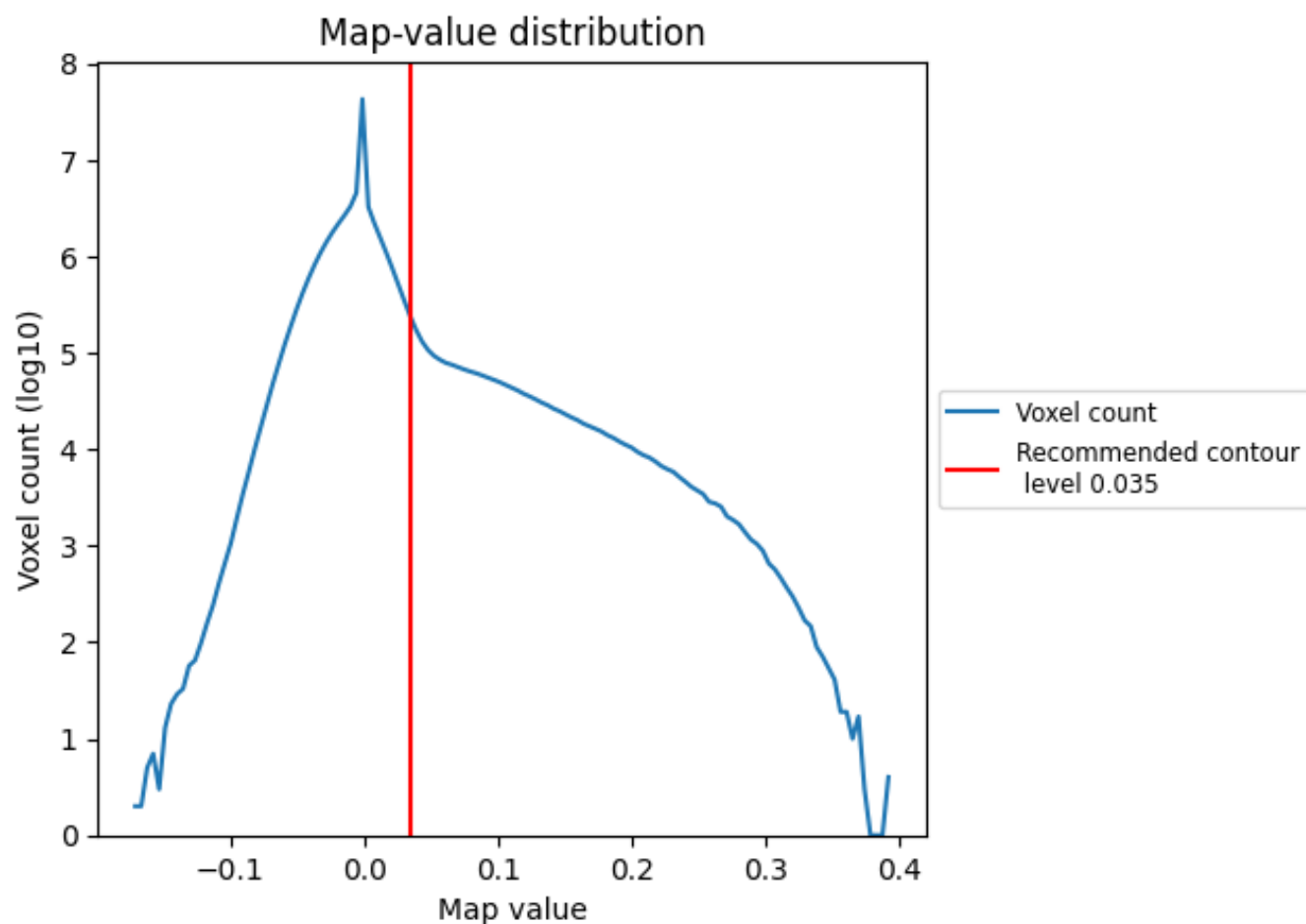
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

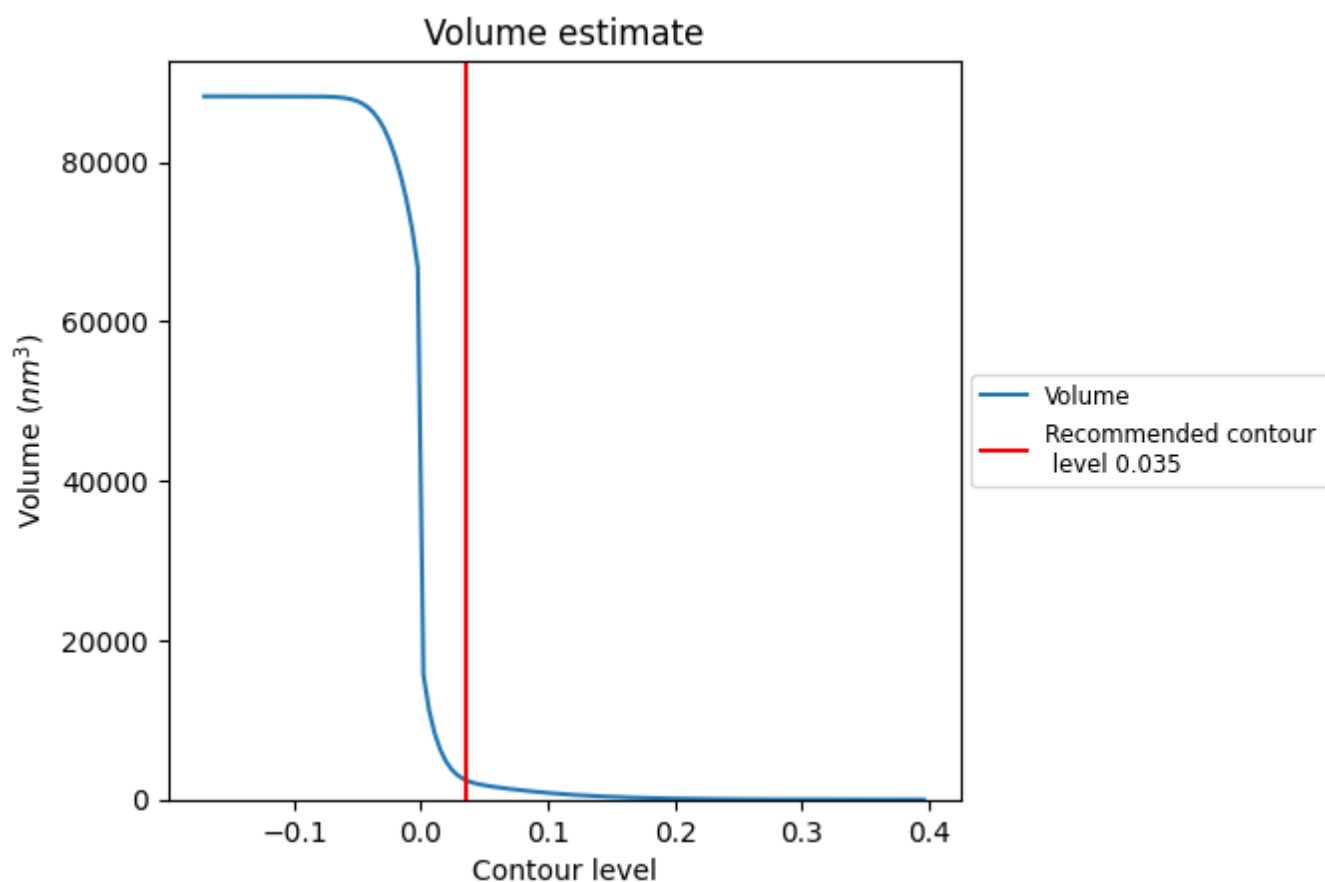
This section contains the results of statistical analysis of the map.

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.

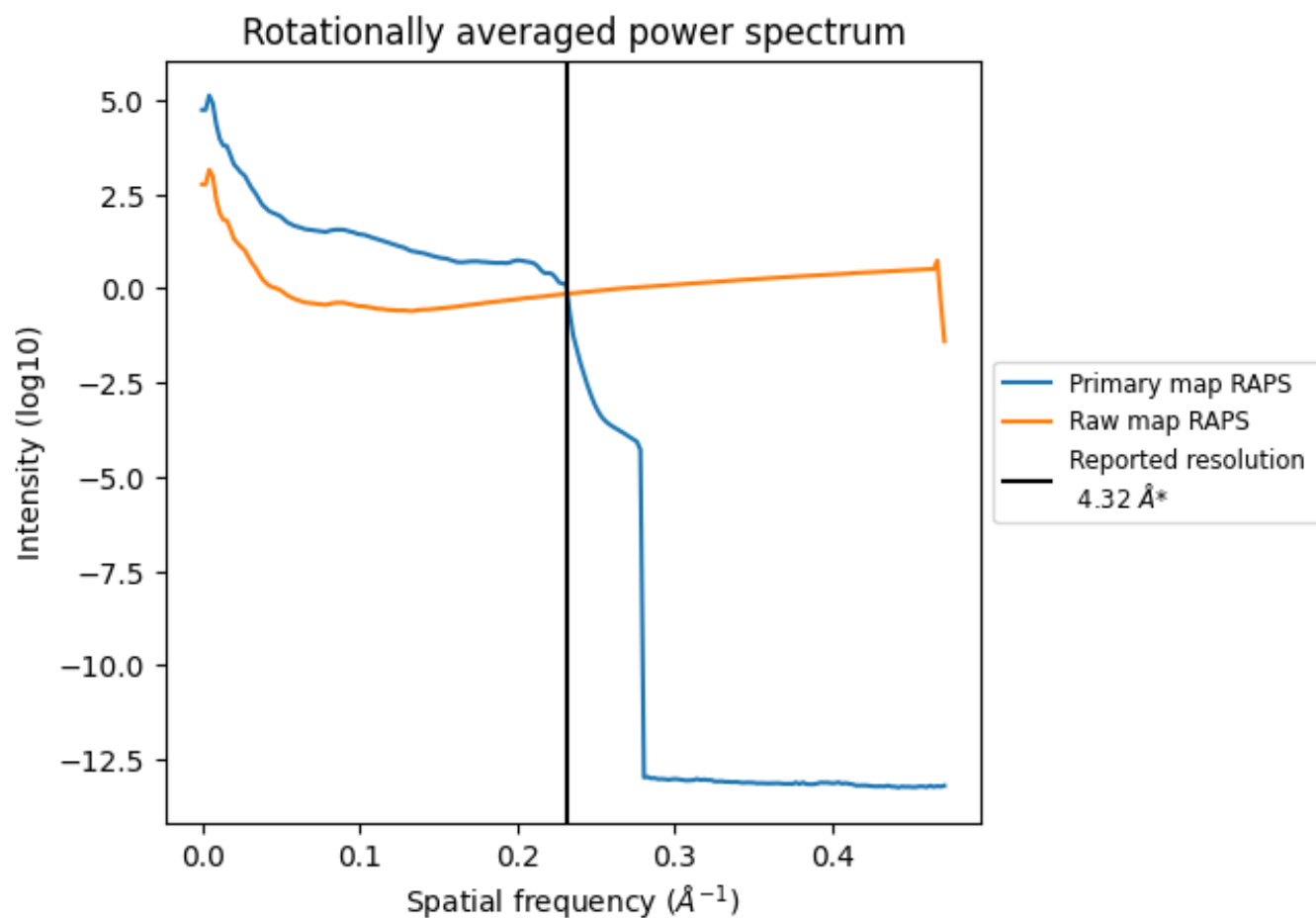
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2478 nm³; this corresponds to an approximate mass of 2238 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 ⓘ

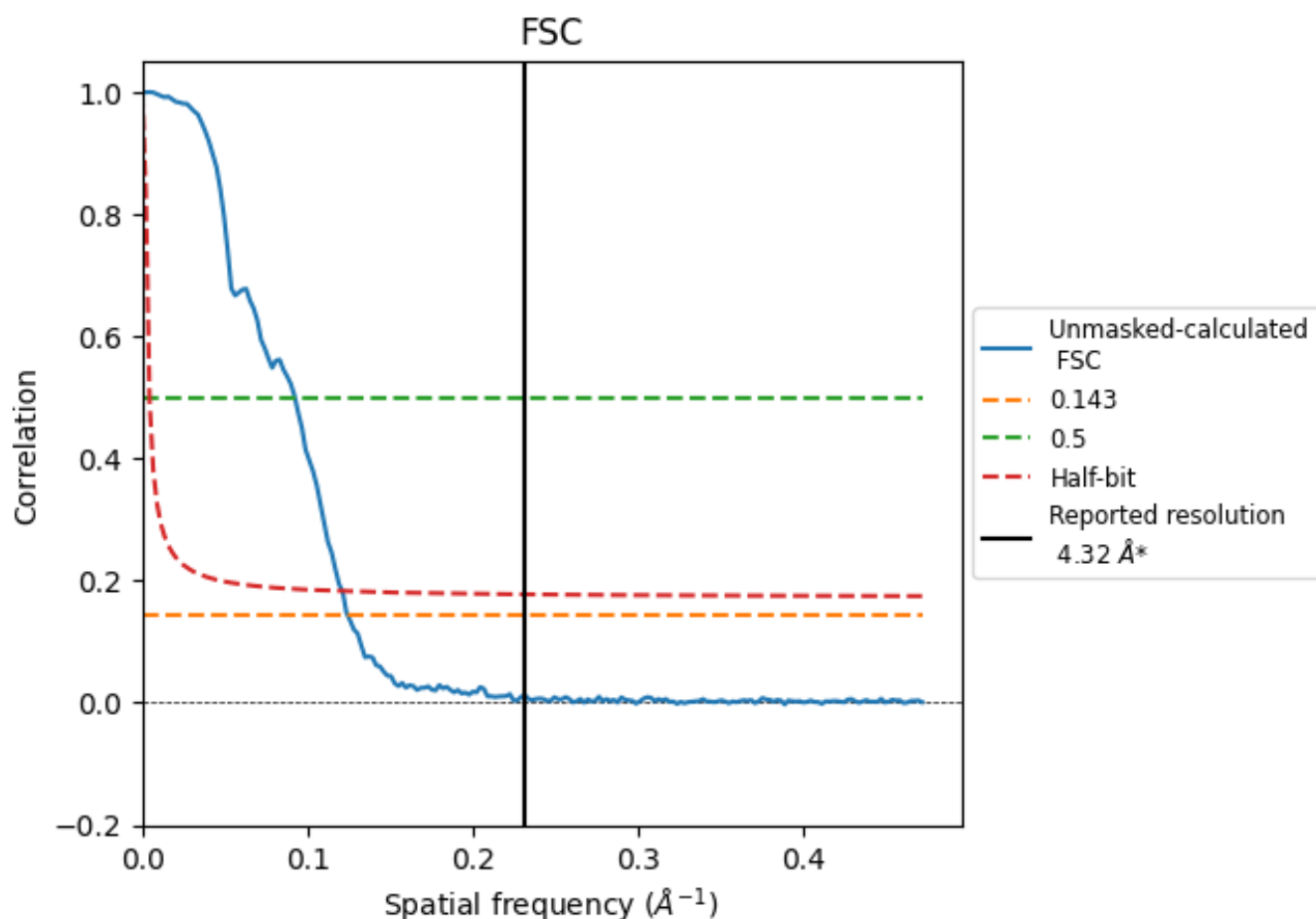


*Reported resolution corresponds to spatial frequency of 0.231 \AA^{-1}

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 0.231 Å⁻¹

8.2 Resolution estimates [i](#)

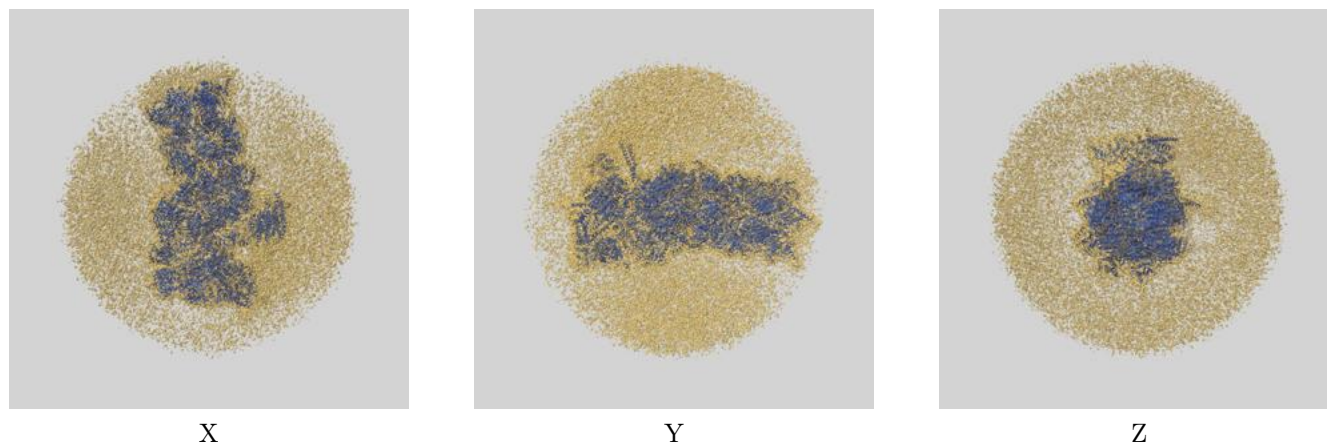
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.05	10.83	8.26

*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 8.05 differs from the reported value 4.32 by more than 10 %

9 Map-model fit [i](#)

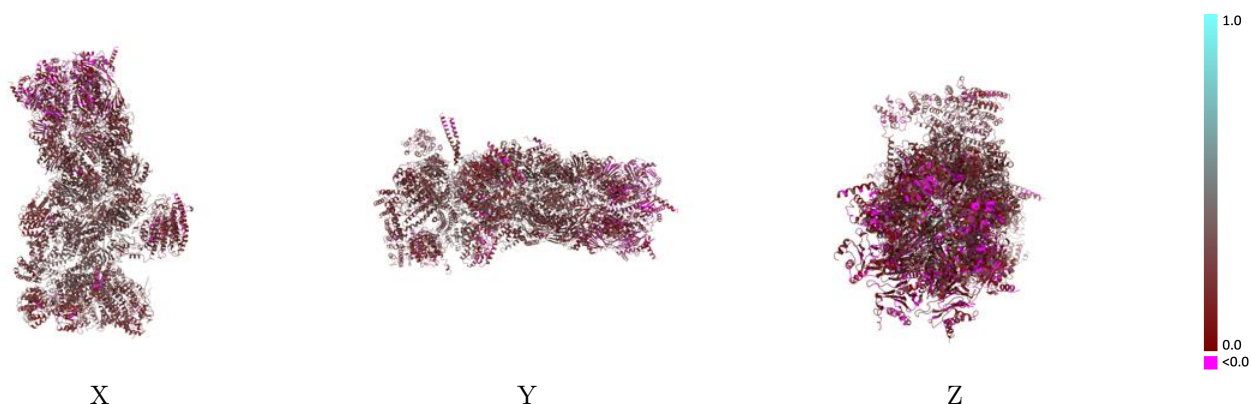
This section contains information regarding the fit between EMDB map EMD-64103 and PDB model 9UF8. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



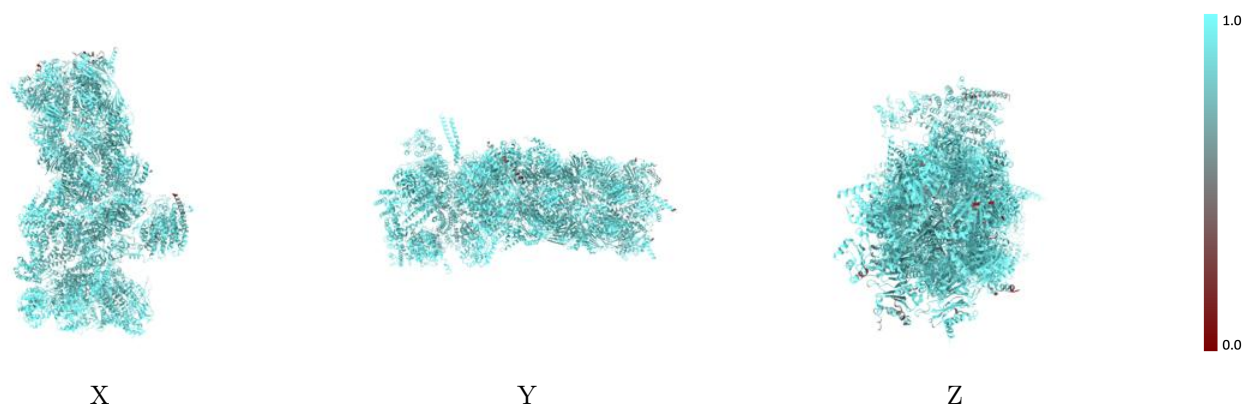
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



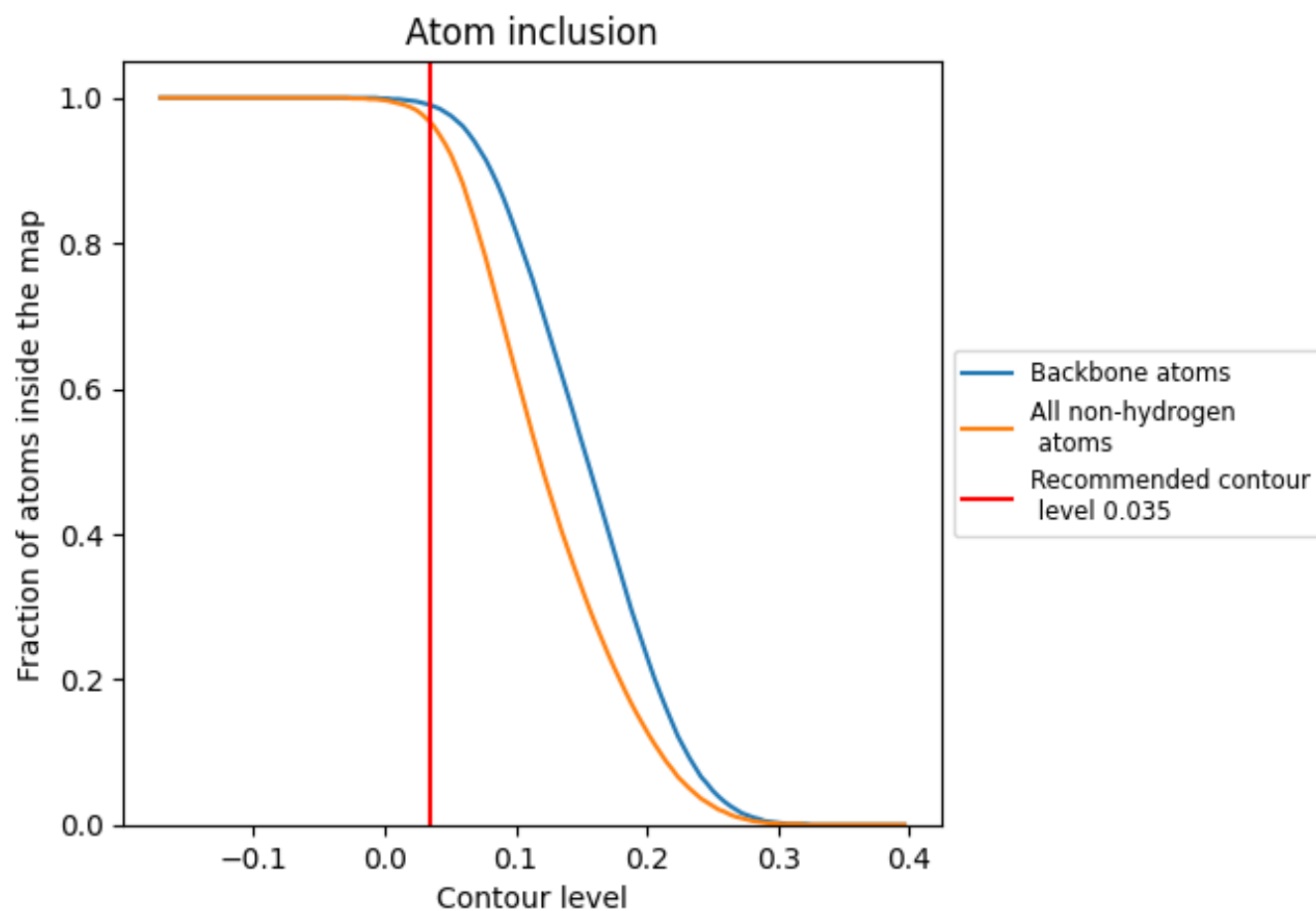
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.2340
A	 0.9640	 0.2960
B	 0.9700	 0.2910
C	 0.9570	 0.3180
D	 0.9580	 0.3130
E	 0.9730	 0.3070
F	 0.9670	 0.3010
G	 0.9810	 0.3110
H	 0.9720	 0.3100
I	 0.9830	 0.3010
J	 0.9890	 0.2860
K	 0.9770	 0.2990
L	 0.9810	 0.2950
M	 0.9850	 0.2870
N	 0.9870	 0.2390
O	 0.9820	 0.2330
P	 0.9850	 0.2130
Q	 0.9750	 0.2300
R	 0.9850	 0.2260
S	 0.9840	 0.2400
T	 0.9800	 0.2330
U	 0.9840	 0.2520
V	 0.9590	 0.2200
W	 0.9680	 0.2360
X	 0.9820	 0.2720
Y	 0.9750	 0.2810
Z	 0.9730	 0.2900
a	 0.9900	 0.2480
b	 0.9870	 0.2080
c	 0.9620	 0.2840
d	 0.9890	 0.2340
e	 0.9740	 0.2450
f	 0.9460	 0.1830
g	 0.9200	 0.1220
h	 0.8820	 0.1160



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.9420	 0.1310
j	 0.9330	 0.1150
k	 0.9060	 0.1290
l	 0.9030	 0.0970
m	 0.9430	 0.1330
n	 0.9910	 0.1700
o	 0.9850	 0.1680
p	 0.9840	 0.1610
q	 0.9810	 0.1730
r	 0.9790	 0.1510
s	 0.9860	 0.1820
t	 0.9880	 0.1790
u	 0.5340	 0.0840