



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2025 – 03:53 PM EDT

PDB ID : 9BUI / pdb_00009bui
EMDB ID : EMD-44910
Title : M1A Midnolin-Proteasome (with Ubl)
Authors : Gao, J.; Yip, M.C.J.; Shao, S.
Deposited on : 2024-05-17
Resolution : 3.90 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.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
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)	:	2.43.1

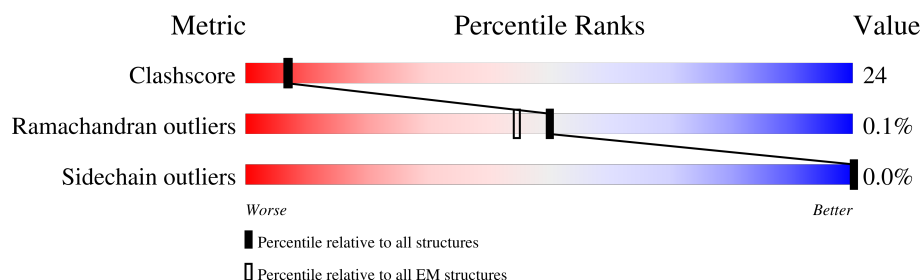
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	U	953	
2	V	534	
3	W	456	
4	X	422	
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	






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Mol	Chain	Length	Quality of chain
9	c	310	
10	d	350	
11	e	70	
12	f	908	
13	y	505	
14	A	433	
15	B	440	
16	C	406	
17	D	418	
18	E	389	
19	F	439	
20	G	246	
21	H	234	
22	I	261	
23	J	248	
24	L	263	
25	M	255	
26	N	239	
26	n	239	
27	O	277	
27	o	277	
28	P	205	
28	p	205	
29	Q	201	
29	q	201	

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Mol	Chain	Length	Quality of chain
30	R	263	
30	r	263	
31	S	241	
31	s	241	
32	T	264	
32	t	264	
33	K	241	
34	z	213	

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
35	ATP	D	501	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 90266 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 non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	812	Total	C	N	O	S	0	0
			6334	4021	1078	1190	45		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	444	Total	C	N	O	S	0	0
			3610	2300	644	653	13		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	436	Total	C	N	O	S	0	0
			3552	2249	608	672	23		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	413	Total	C	N	O	S	0	0
			3259	2073	556	618	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	379	Total	C	N	O	S	0	0
			3123	1993	534	579	17		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	375	Total	C	N	O	S	0	0
			3012	1921	513	563	15		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	191	Total	C	N	O	S	0	0
			1459	910	261	281	7		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	262	Total	C	N	O	S	0	0
			2131	1381	349	392	9		

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	36	Total	C	N	O	0	0
			314	193	50	71		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	829	Total	C	N	O	S	0	0
			6420	4063	1086	1226	45		

- Molecule 13 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	y	111	Total	C	N	O	S	0	0
			879	543	176	158	2		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-36	MET	-	initiating methionine	UNP Q504T8
y	-35	ASP	-	expression tag	UNP Q504T8
y	-34	TYR	-	expression tag	UNP Q504T8
y	-33	LYS	-	expression tag	UNP Q504T8
y	-32	ASP	-	expression tag	UNP Q504T8
y	-31	ASP	-	expression tag	UNP Q504T8
y	-30	ASP	-	expression tag	UNP Q504T8
y	-29	ASP	-	expression tag	UNP Q504T8
y	-28	LYS	-	expression tag	UNP Q504T8
y	-27	ASP	-	expression tag	UNP Q504T8
y	-26	TYR	-	expression tag	UNP Q504T8
y	-25	LYS	-	expression tag	UNP Q504T8
y	-24	ASP	-	expression tag	UNP Q504T8
y	-23	ASP	-	expression tag	UNP Q504T8
y	-22	ASP	-	expression tag	UNP Q504T8
y	-21	ASP	-	expression tag	UNP Q504T8
y	-20	LYS	-	expression tag	UNP Q504T8
y	-19	GLY	-	expression tag	UNP Q504T8
y	-18	GLY	-	expression tag	UNP Q504T8
y	-17	GLY	-	expression tag	UNP Q504T8
y	-16	GLY	-	expression tag	UNP Q504T8
y	-15	SER	-	expression tag	UNP Q504T8
y	-14	GLY	-	expression tag	UNP Q504T8
y	-13	GLY	-	expression tag	UNP Q504T8
y	-12	GLY	-	expression tag	UNP Q504T8
y	-11	GLY	-	expression tag	UNP Q504T8
y	-10	PHE	-	expression tag	UNP Q504T8
y	-9	GLU	-	expression tag	UNP Q504T8
y	-8	THR	-	expression tag	UNP Q504T8
y	-7	SER	-	expression tag	UNP Q504T8
y	-6	LEU	-	expression tag	UNP Q504T8
y	-5	TYR	-	expression tag	UNP Q504T8
y	-4	LYS	-	expression tag	UNP Q504T8
y	-3	LYS	-	expression tag	UNP Q504T8
y	-2	ALA	-	expression tag	UNP Q504T8
y	-1	GLY	-	expression tag	UNP Q504T8
y	0	THR	-	expression tag	UNP Q504T8
y	457	ALA	VAL	conflict	UNP Q504T8

- Molecule 14 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	373	Total	C	N	O	S	0	0
			2930	1846	519	548	17		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	371	Total	C	N	O	S	0	0
			2933	1846	499	574	14		

- Molecule 16 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	348	Total	C	N	O	S	0	0
			2729	1715	499	502	13		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	376	Total	C	N	O	S	0	0
			3009	1903	519	574	13		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	339	Total	C	N	O	S	0	0
			2678	1683	474	505	16		

- Molecule 19 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	339	Total	C	N	O	S	0	0
			2646	1672	454	505	15		

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	234	Total	C	N	O	S	0	0
			1836	1170	304	349	13		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	226	Total	C	N	O	S	0	0
			1760	1124	298	332	6		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	252	Total	C	N	O	S	0	0
			1990	1258	340	382	10		

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 24 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	237	Total	C	N	O	S	0	0
			1868	1168	338	351	11		

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	M	242	Total	C	N	O	S	0	0
			1905	1206	323	365	11		

- Molecule 26 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	198	Total	C	N	O	S	0	0
			1487	931	254	290	12		
26	n	179	Total	C	N	O	S	0	0
			1336	836	230	258	12		

- Molecule 27 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
27	o	176	Total	C	N	O	S	0	0
			1315	823	228	253	11		

- Molecule 28 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
28	p	164	Total	C	N	O	S	0	0
			1264	802	210	235	17		

- Molecule 29 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
29	q	173	Total	C	N	O	S	0	0
			1380	890	234	248	8		

- Molecule 30 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R	199	Total	C	N	O	S	0	0
			1549	977	272	291	9		
30	r	187	Total	C	N	O	S	0	0
			1432	904	248	271	9		

- Molecule 31 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
31	s	206	Total	C	N	O	S	0	0
			1597	1015	269	303	10		

- Molecule 32 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	T	213	Total	C	N	O	S	0	0
			1665	1050	288	316	11		
32	t	206	Total	C	N	O	S	0	0
			1609	1016	279	302	12		

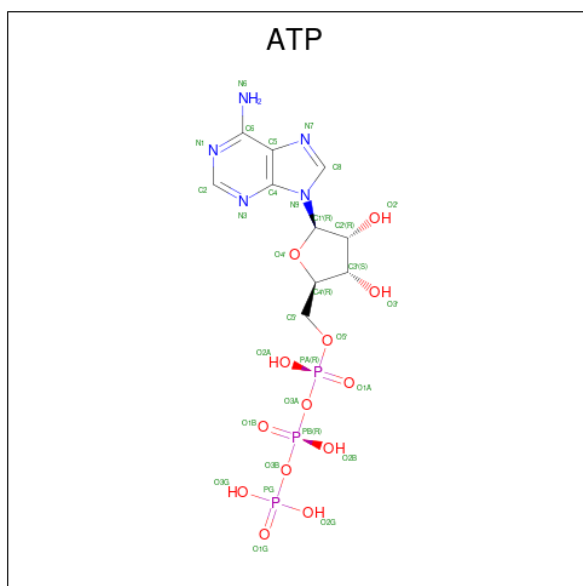
- Molecule 33 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	224	Total	C	N	O	S	0	0
			1715	1080	285	339	11		

- Molecule 34 is a protein called AN1-type zinc finger protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	z	59	Total	C	N	O	S	0	0
			471	295	89	80	7		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

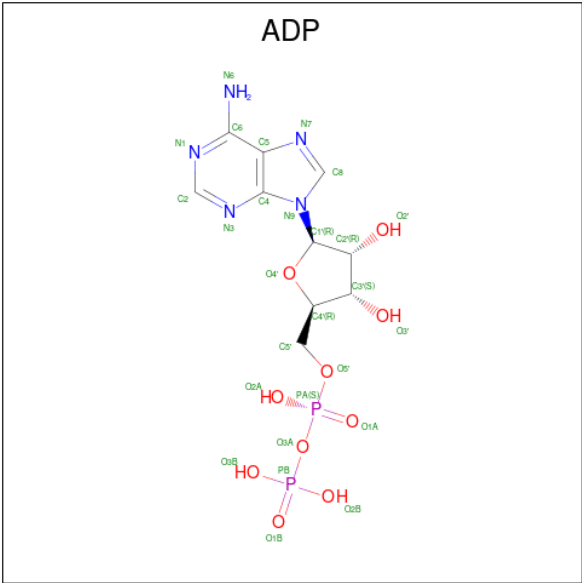
Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	B	1	1	1	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

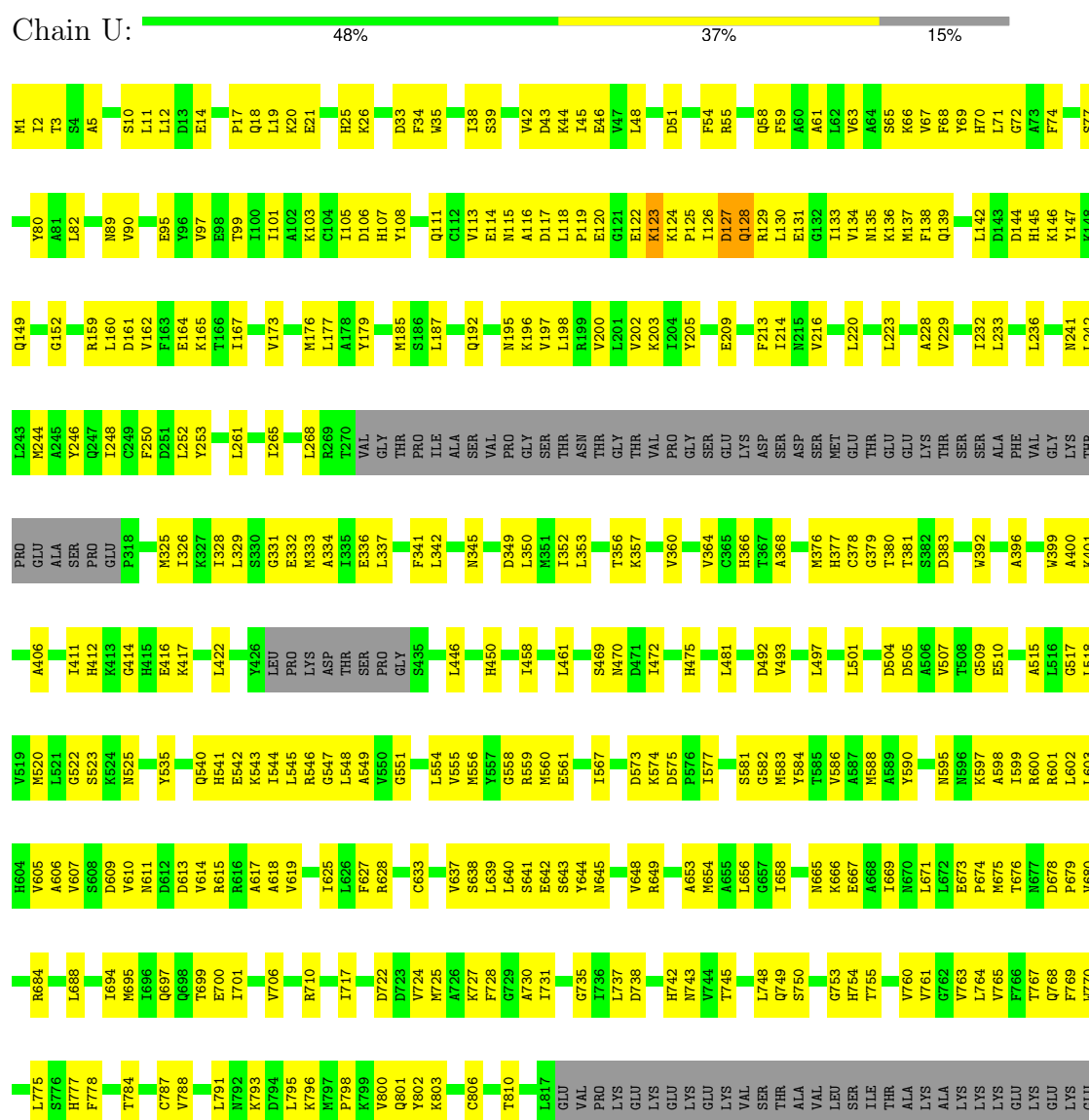


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
37	B	1	27	10	5	10	2	0

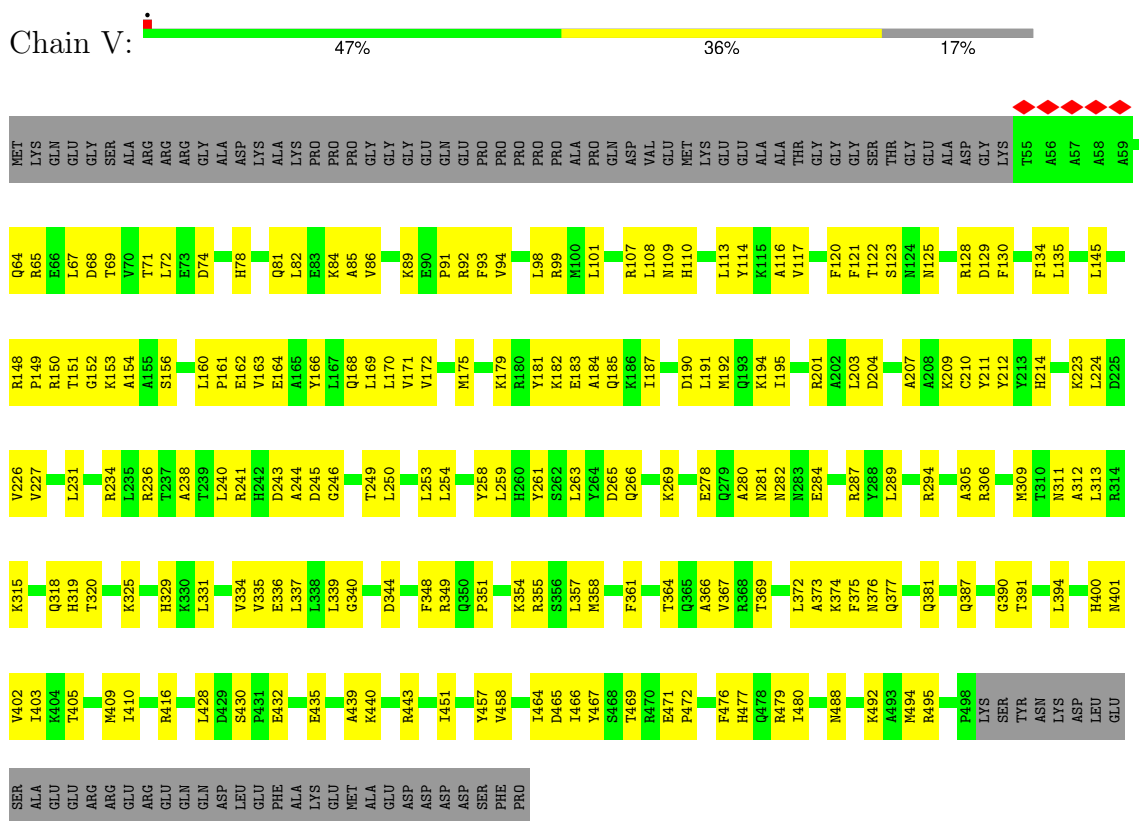
3 Residue-property plots

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.

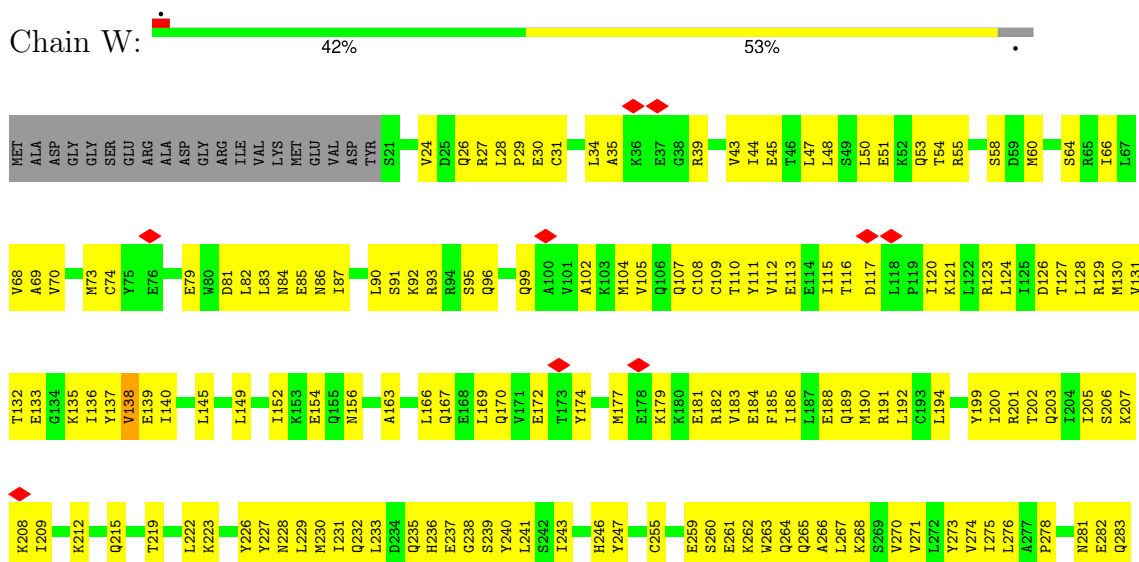
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1

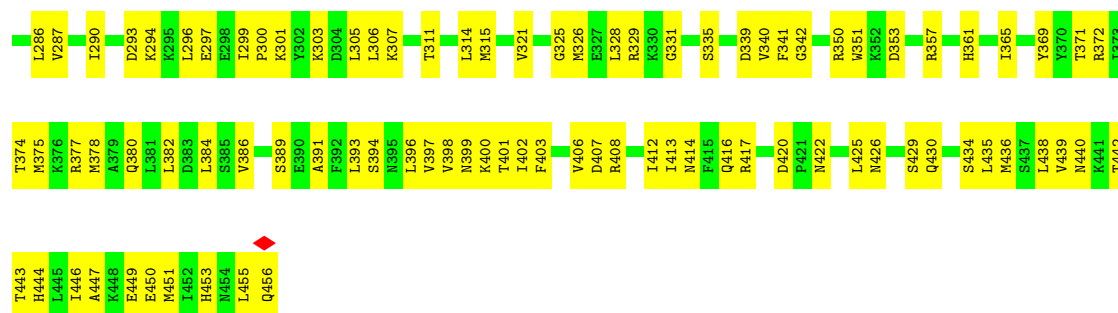


- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

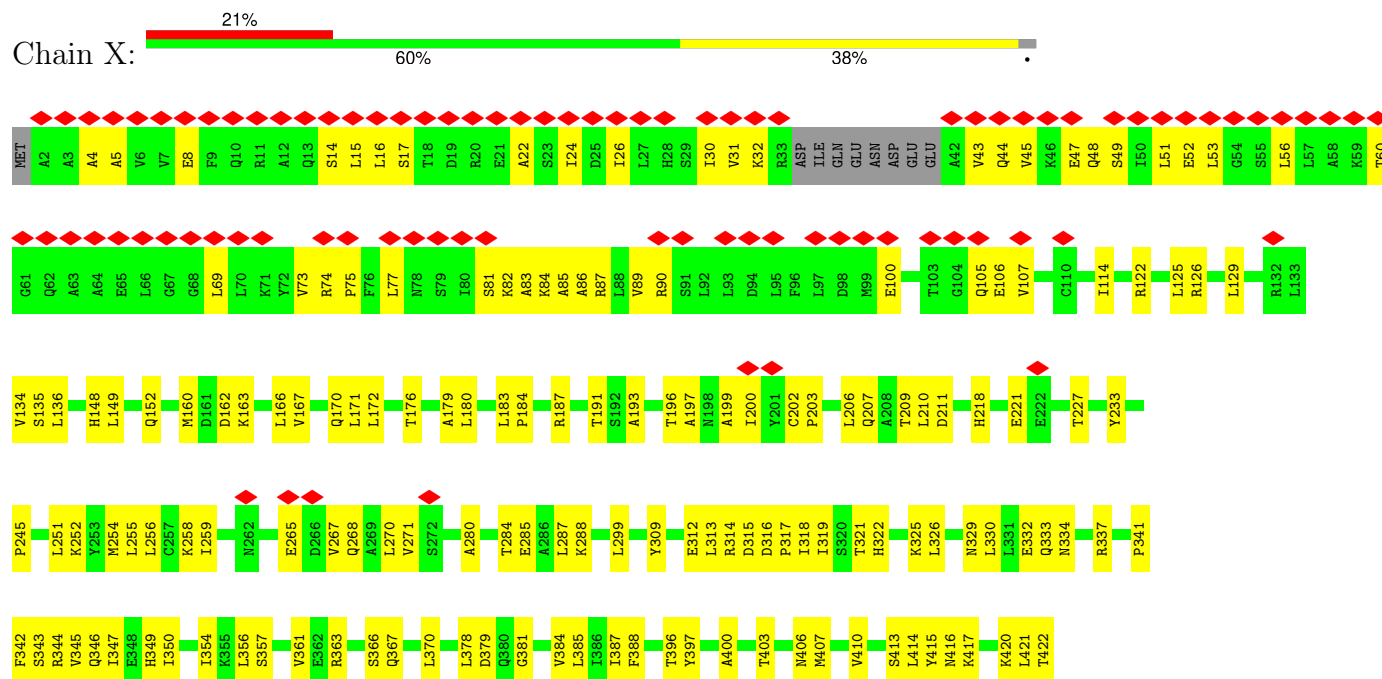


- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

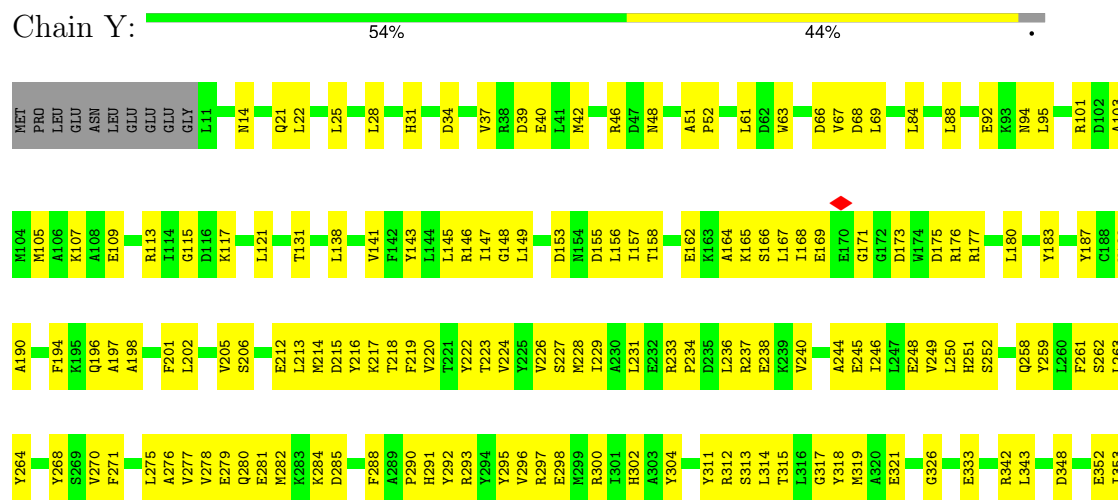




- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

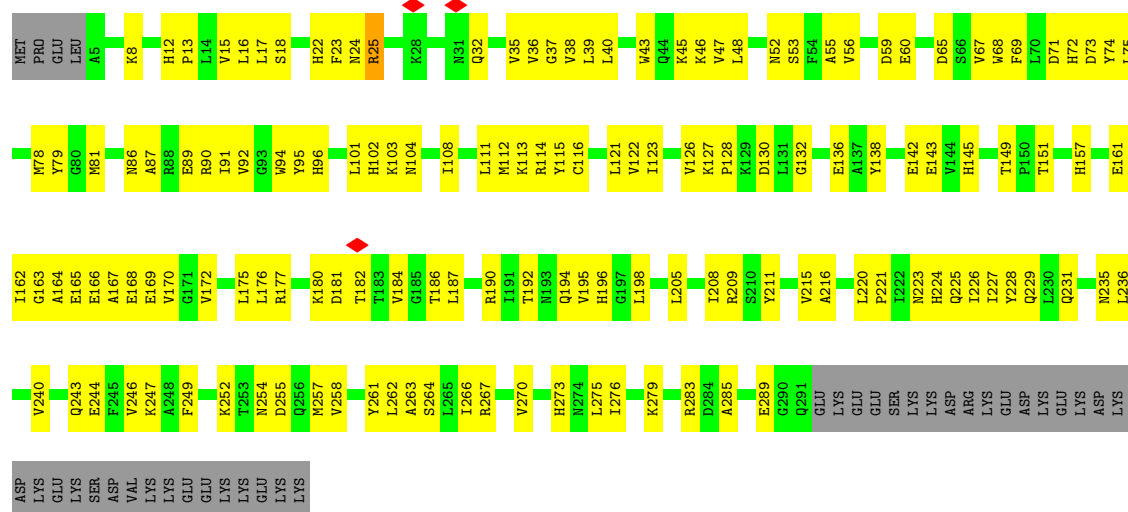


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

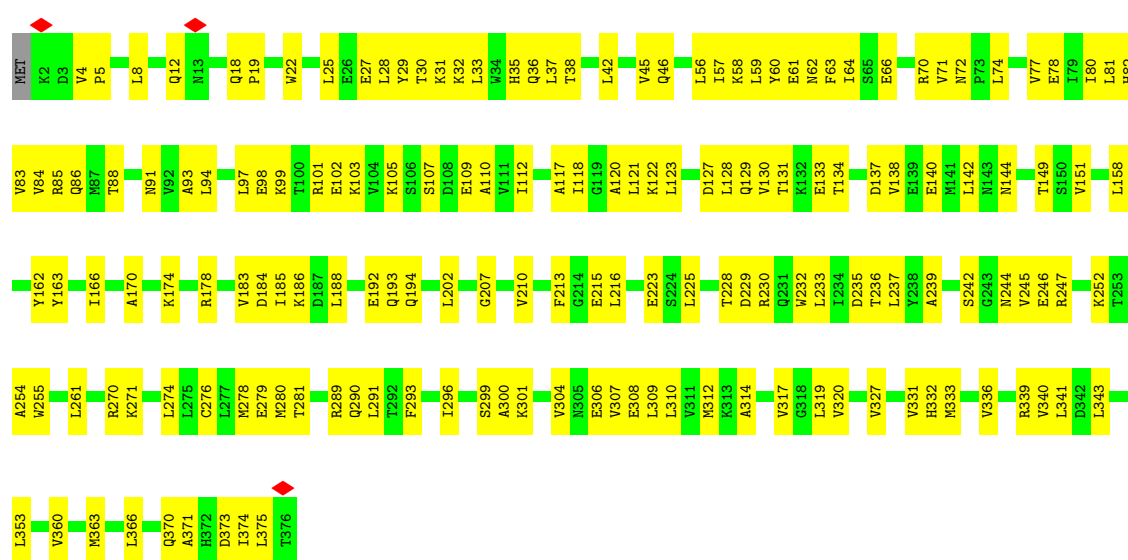




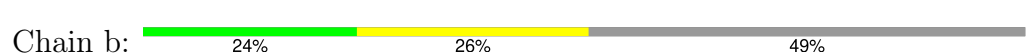
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7



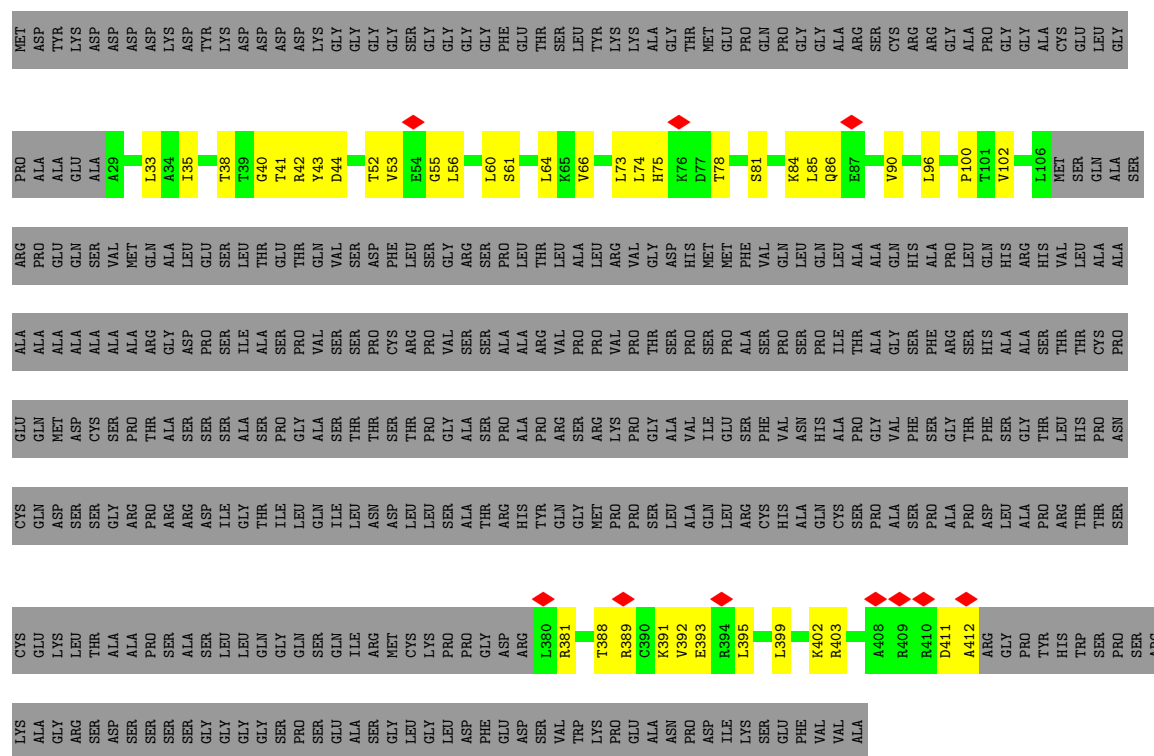
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13



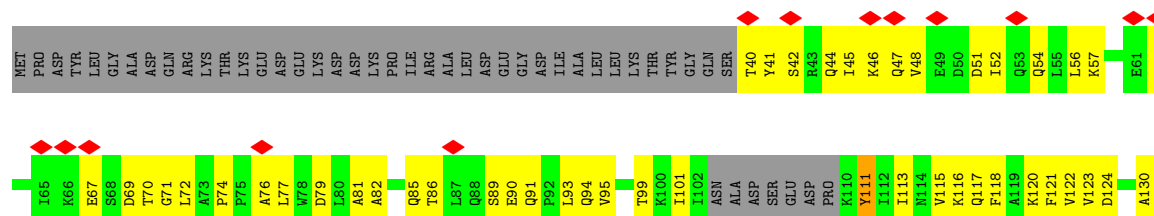
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

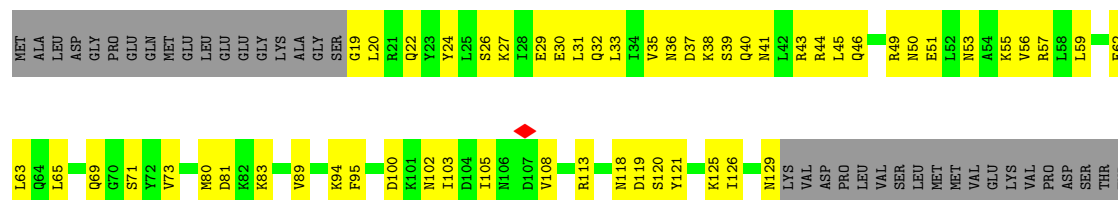


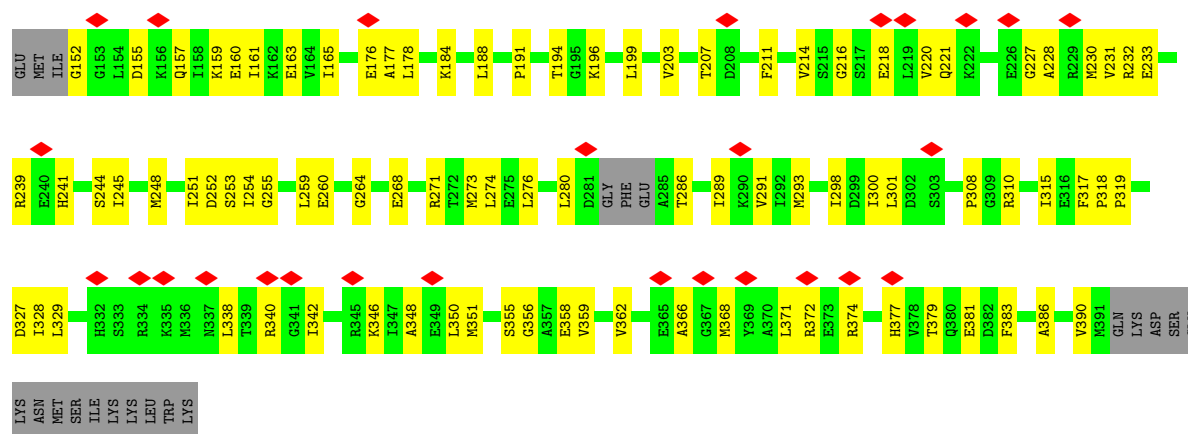
- Molecule 13: Midnolin



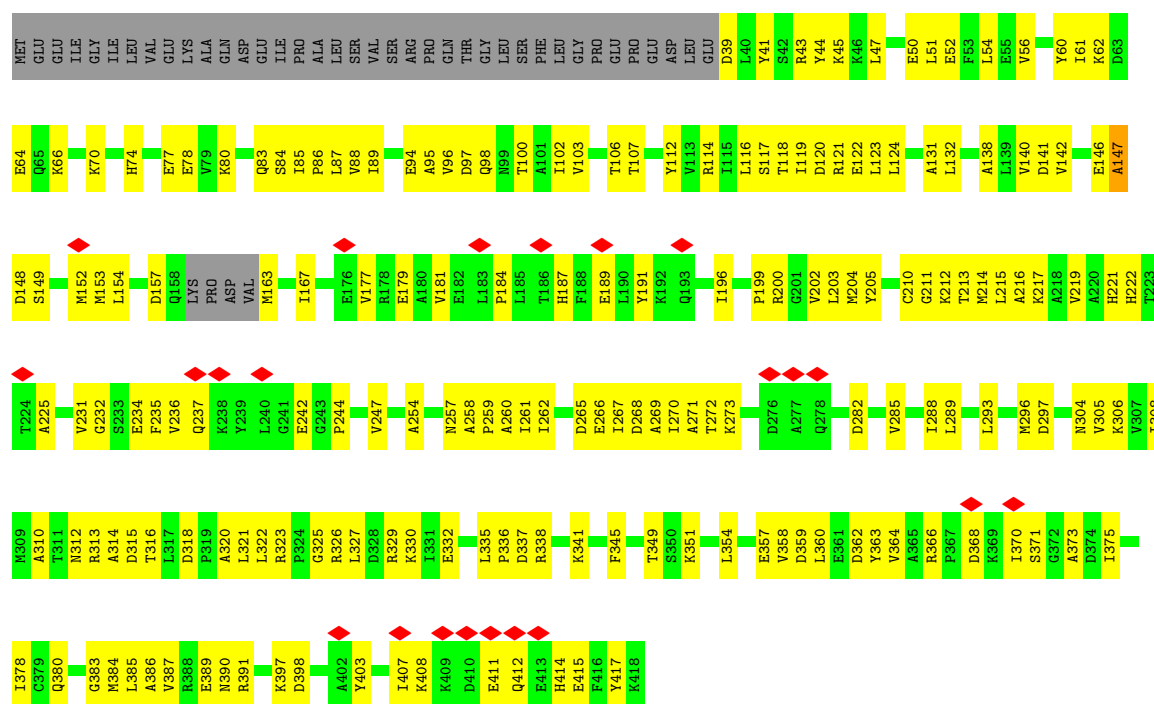
- Molecule 14: 26S proteasome regulatory subunit 7



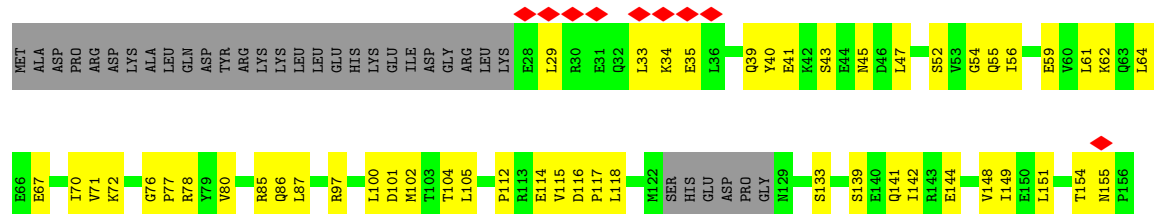


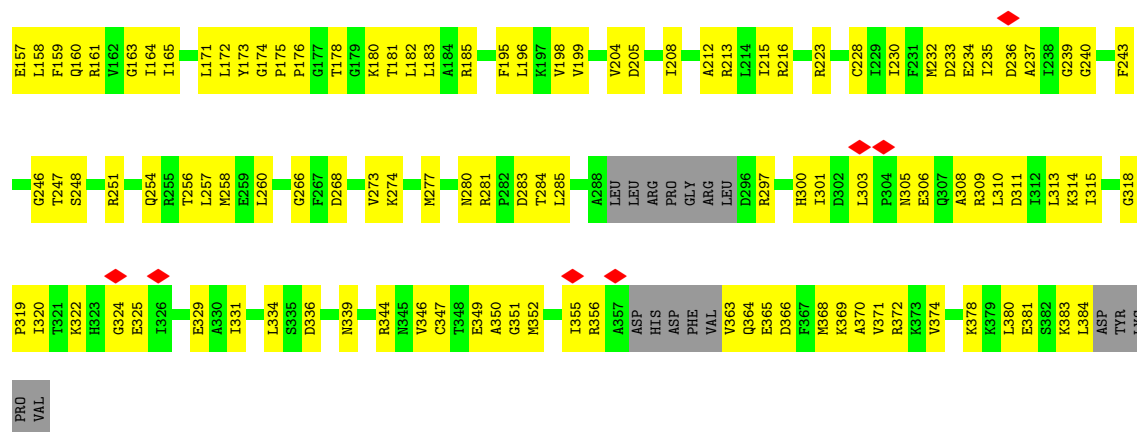


• Molecule 17: 26S proteasome regulatory subunit 6B

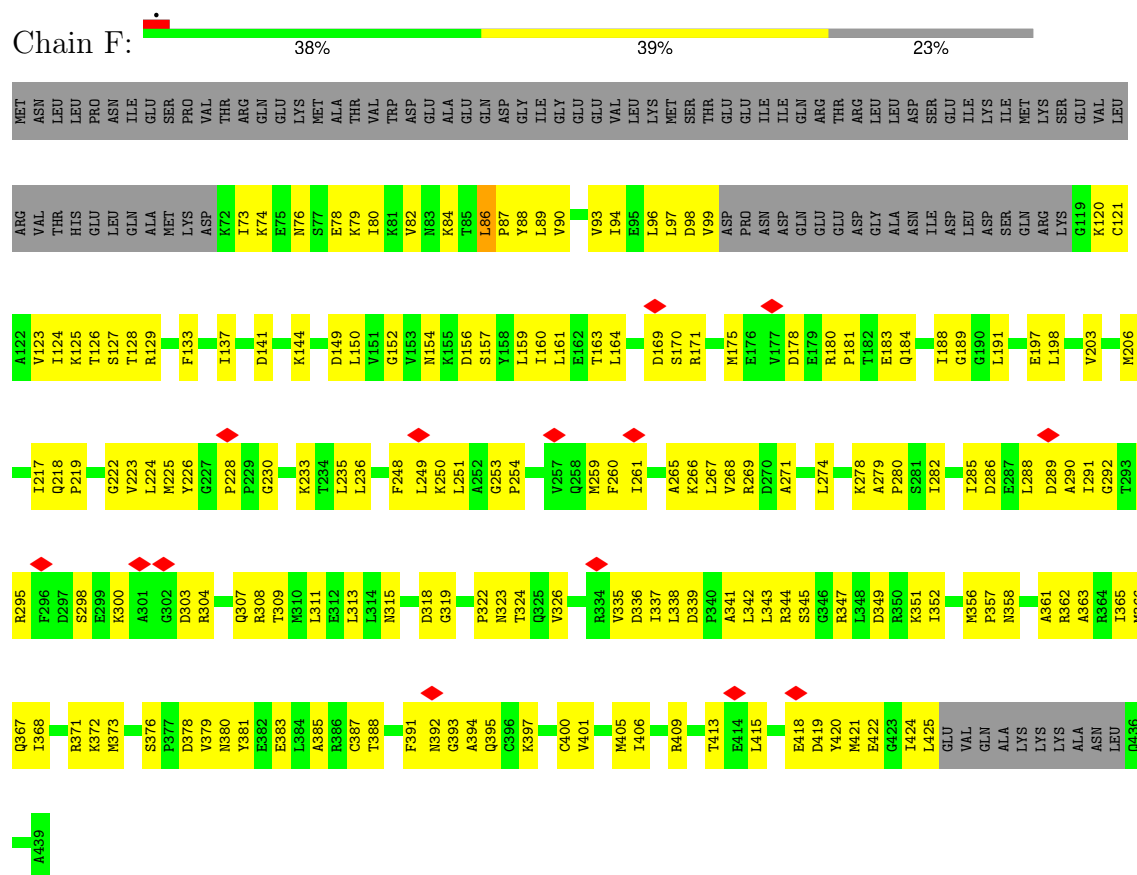


• Molecule 18: 26S protease regulatory subunit 10B

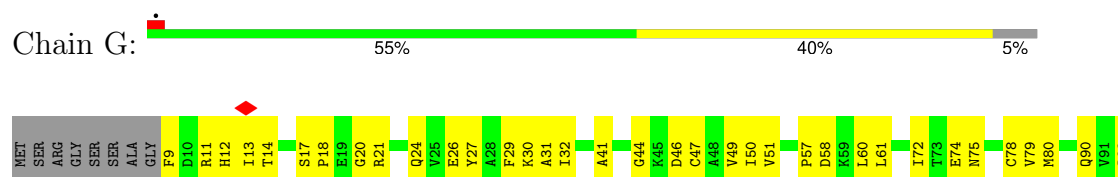


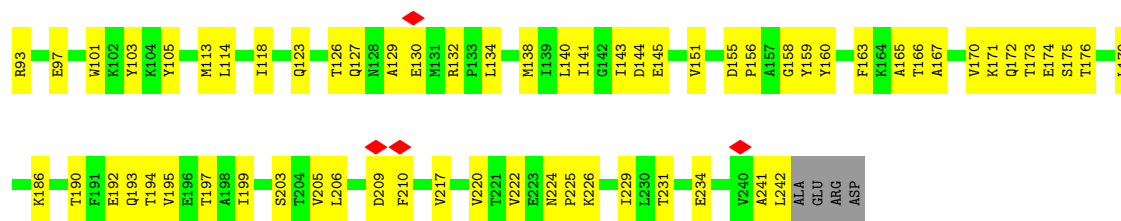


• Molecule 19: 26S proteasome regulatory subunit 6A

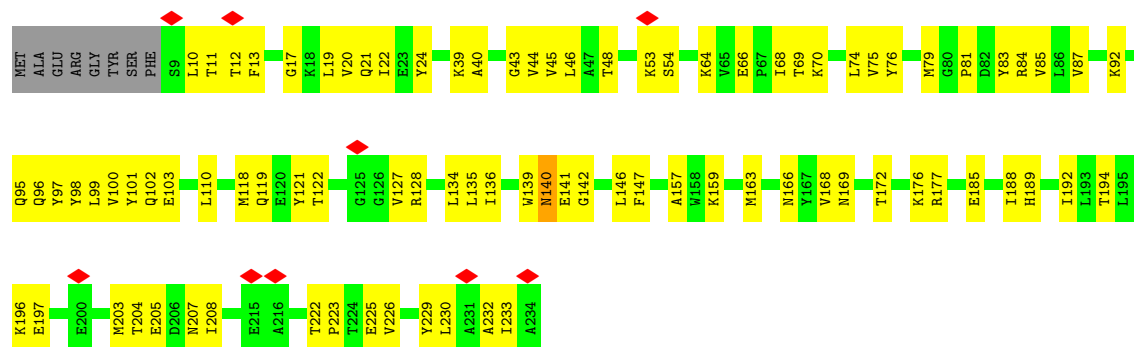


• Molecule 20: Proteasome subunit alpha type-6

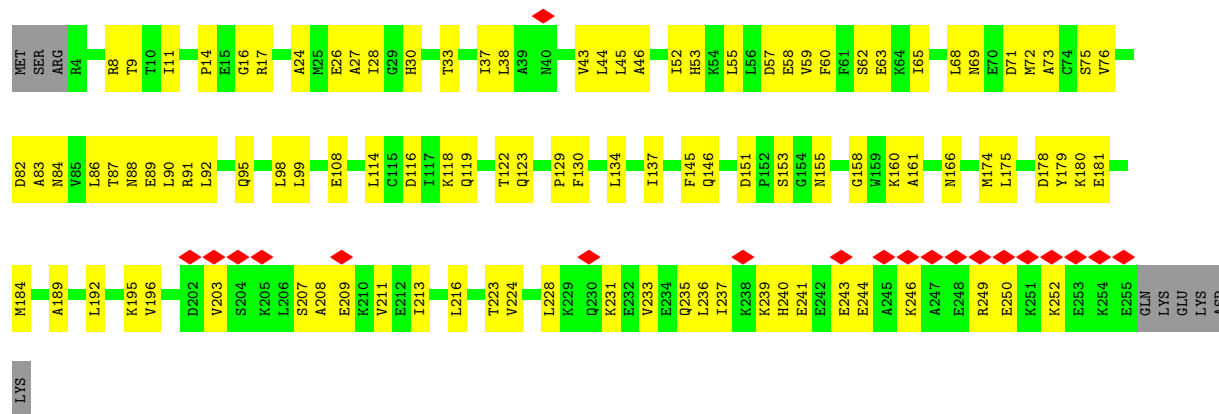




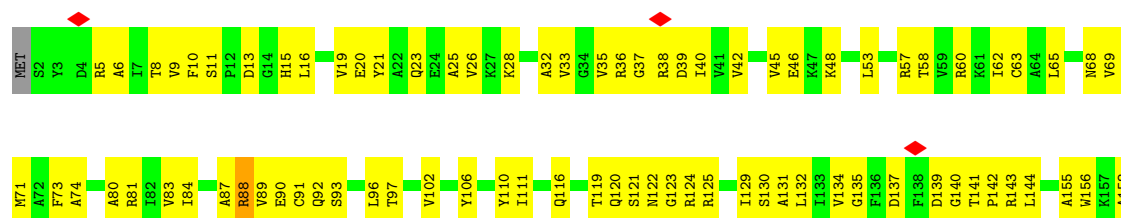
• Molecule 21: Proteasome subunit alpha type-2

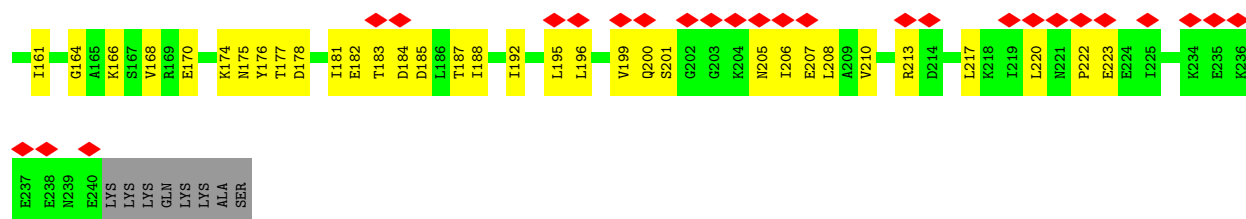


• Molecule 22: Proteasome subunit alpha type-4



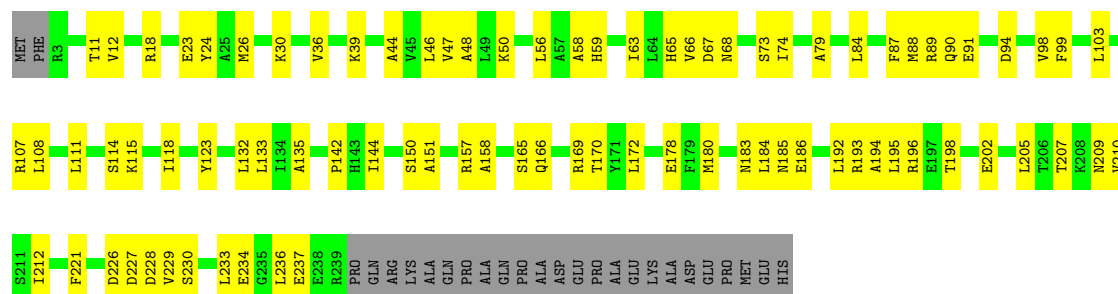
• Molecule 23: Proteasome subunit alpha type-7





• Molecule 24: Proteasome subunit alpha type-1

Chain L: 58% 32% 10%



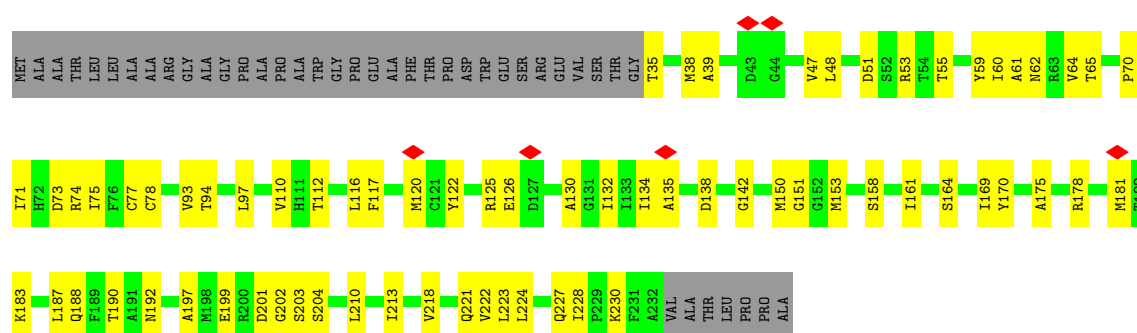
• Molecule 25: Proteasome subunit alpha type-3

Chain M: 56% 38% 5%

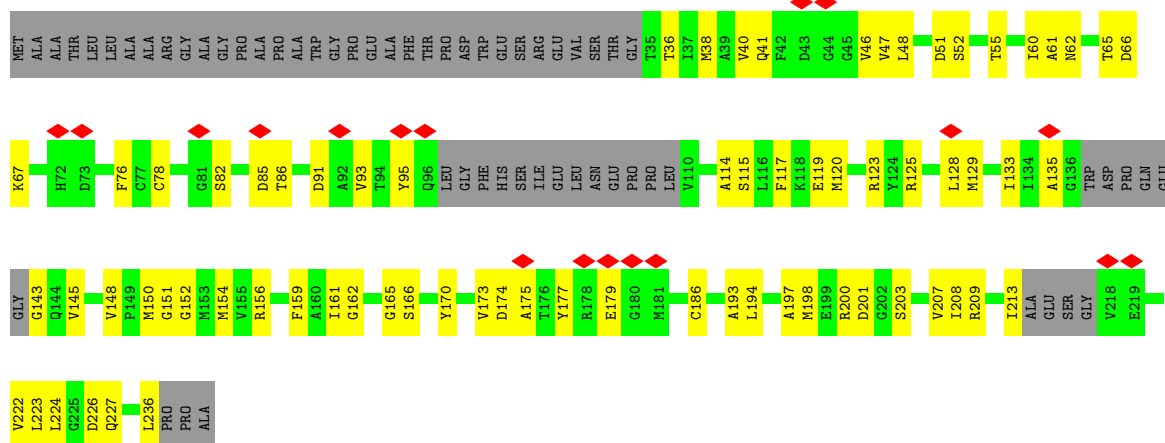
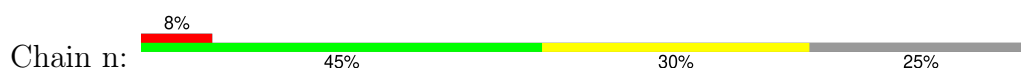


• Molecule 26: Proteasome subunit beta type-6

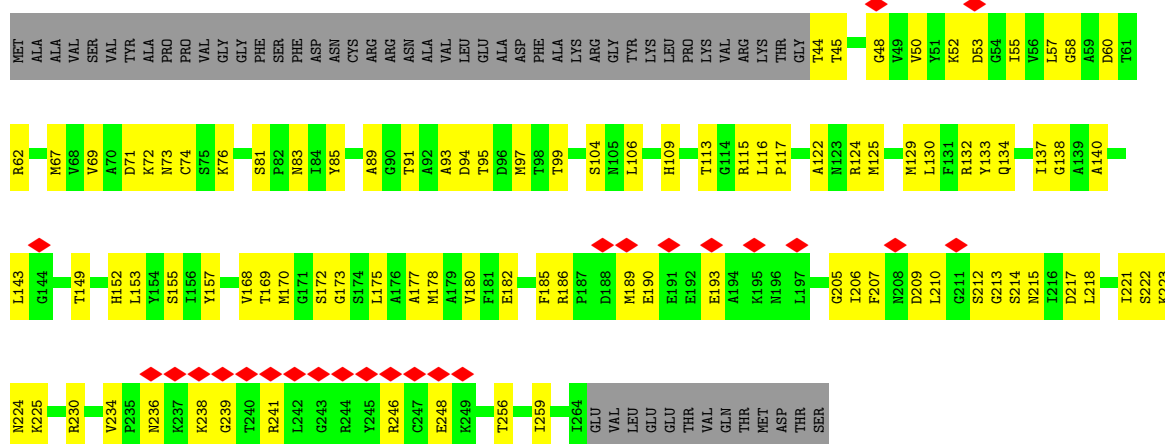
Chain N: 54% 29% 17%



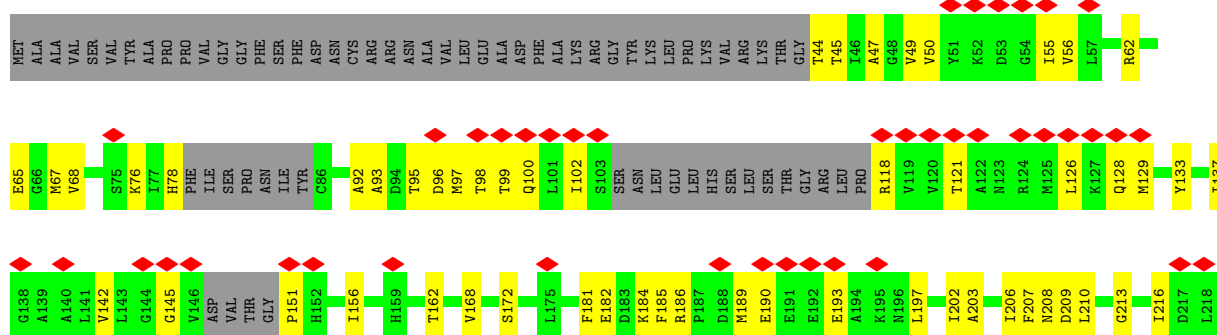
• Molecule 26: Proteasome subunit beta type-6

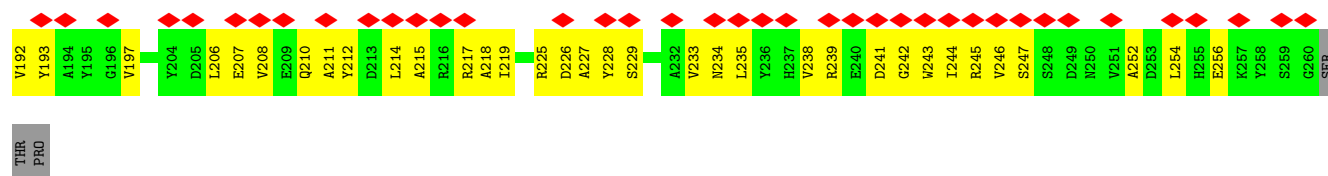


• Molecule 27: Proteasome subunit beta type-7

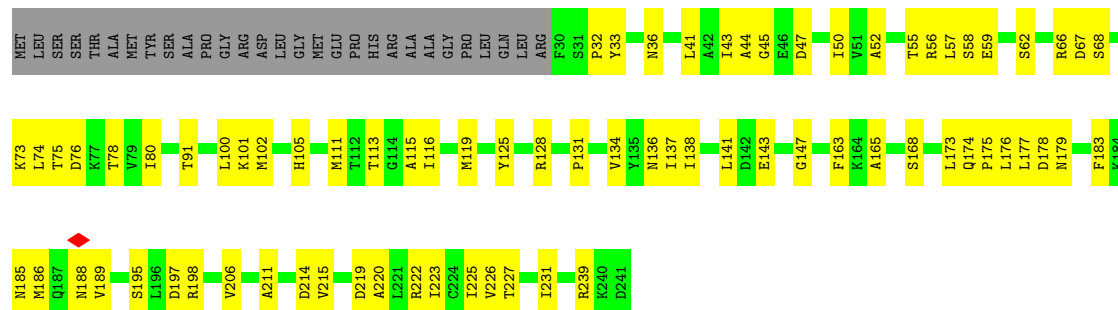


• Molecule 27: Proteasome subunit beta type-7

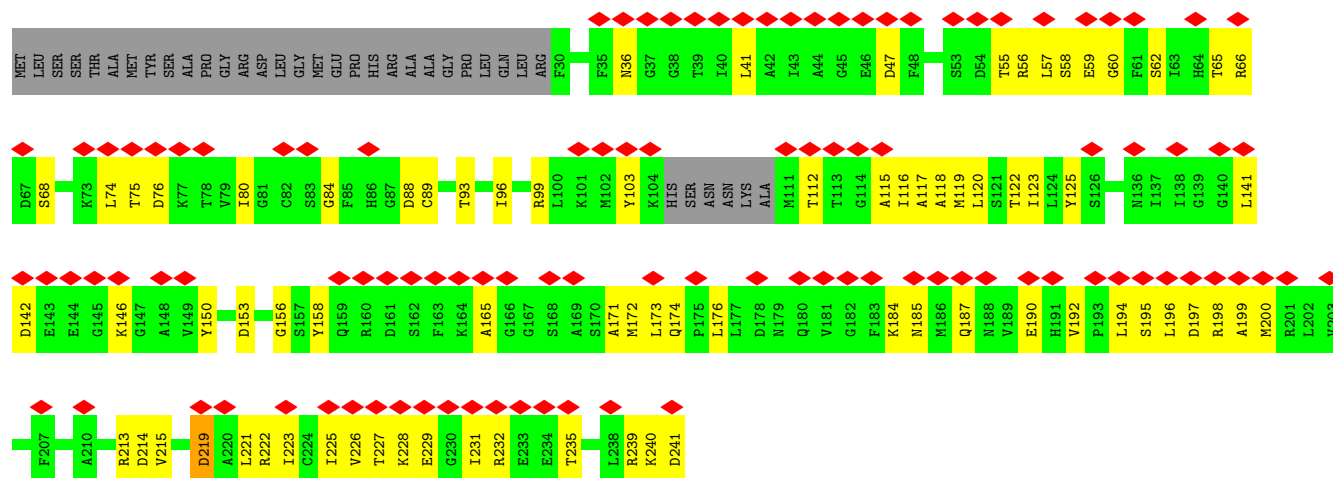
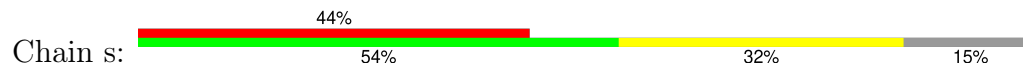




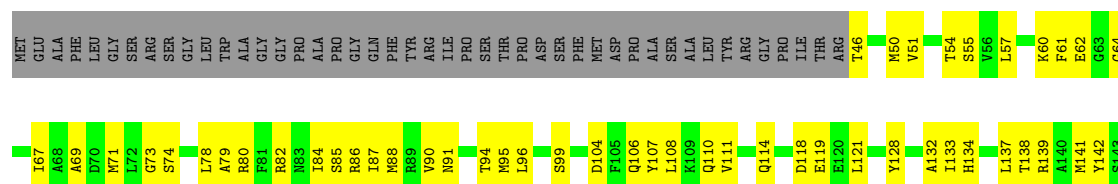
• Molecule 31: Proteasome subunit beta type-1

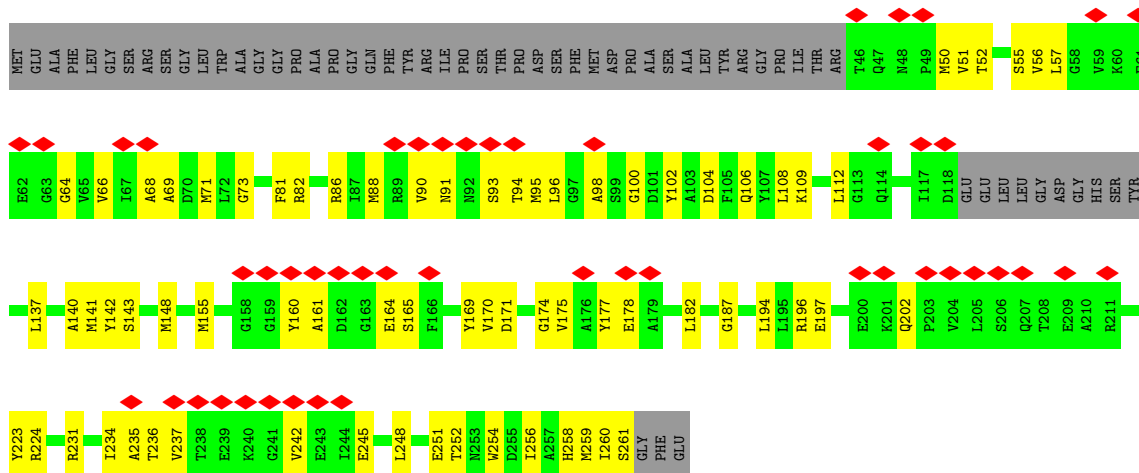


• Molecule 31: Proteasome subunit beta type-1

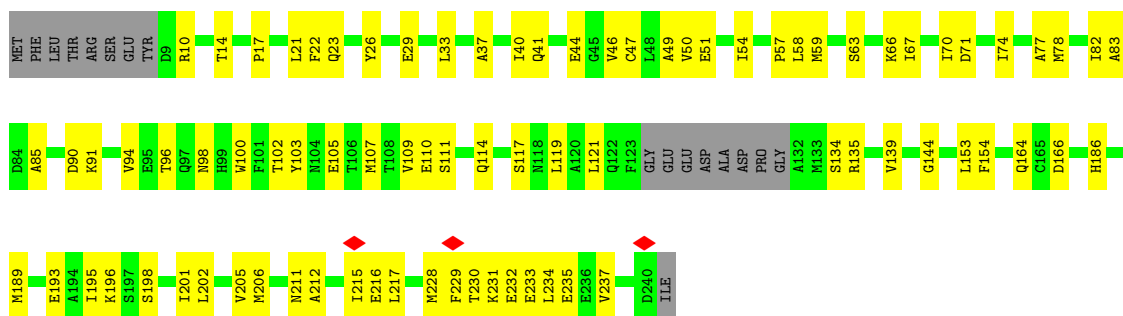


• Molecule 32: Proteasome subunit beta type-4

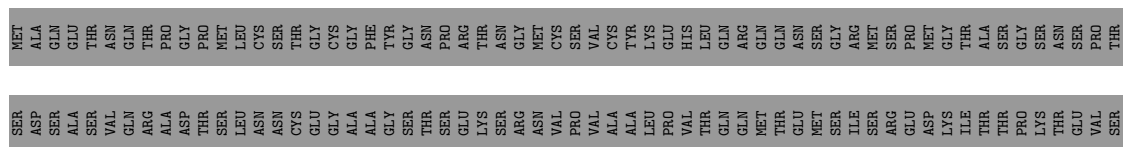


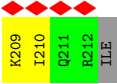
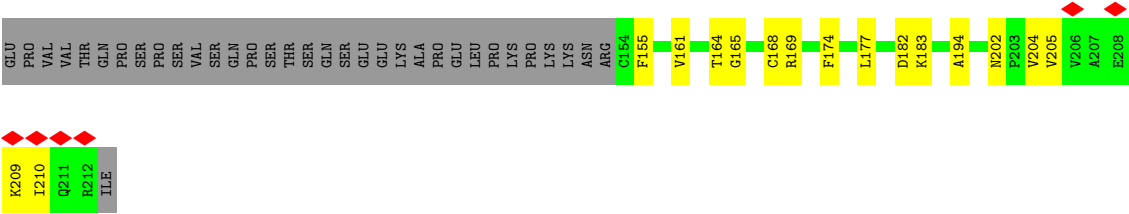


- Molecule 33: Proteasome subunit alpha type-5



- Molecule 34: AN1-type zinc finger protein 5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.719	Depositor
Minimum map value	-0.325	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	363.0, 363.0, 363.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	U	0.24	0/6446	0.40	0/8720
2	V	0.23	0/3680	0.38	0/4970
3	W	0.22	0/3599	0.43	1/4840 (0.0%)
4	X	0.18	0/3304	0.36	0/4453
5	Y	0.22	0/3181	0.38	0/4285
6	Z	0.28	0/2333	0.43	0/3162
7	a	0.23	0/3070	0.40	0/4155
8	b	0.18	0/1479	0.33	0/2003
9	c	0.27	0/2302	0.43	0/3110
10	d	0.20	0/2175	0.39	0/2938
11	e	0.22	0/322	0.42	0/436
12	f	0.14	0/6529	0.36	0/8839
13	y	0.15	0/886	0.30	0/1186
14	A	0.17	0/2975	0.39	0/4012
15	B	0.16	0/2974	0.37	0/4009
16	C	0.17	0/2762	0.33	0/3713
17	D	0.21	0/3057	0.42	0/4121
18	E	0.19	0/2713	0.39	0/3648
19	F	0.20	0/2683	0.45	0/3617
20	G	0.21	0/1870	0.34	0/2529
21	H	0.21	0/1797	0.35	0/2434
22	I	0.16	0/2020	0.31	0/2718
23	J	0.16	0/1913	0.35	0/2581
24	L	0.16	0/1902	0.33	0/2569
25	M	0.17	0/1940	0.37	0/2612
26	N	0.16	0/1513	0.31	0/2047
26	n	0.14	0/1352	0.31	0/1822
27	O	0.17	0/1694	0.32	0/2293
27	o	0.12	0/1331	0.30	0/1791
28	P	0.17	0/1620	0.38	0/2184
28	p	0.15	0/1282	0.37	0/1722
29	Q	0.16	0/1611	0.29	0/2180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	q	0.12	0/1405	0.26	0/1899
30	R	0.14	0/1580	0.29	0/2134
30	r	0.16	0/1460	0.40	2/1972 (0.1%)
31	S	0.14	0/1673	0.29	0/2254
31	s	0.14	0/1625	0.32	0/2188
32	T	0.16	0/1698	0.32	0/2299
32	t	0.13	0/1639	0.31	0/2217
33	K	0.16	0/1740	0.36	0/2348
34	z	0.16	0/480	0.39	0/640
All	All	0.19	0/91615	0.37	3/123650 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	Z	0	1
23	J	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	138	VAL	N-CA-C	-5.74	107.69	113.20
30	r	113	PHE	CA-C-N	-5.06	112.29	121.14
30	r	113	PHE	C-N-CA	-5.06	112.29	121.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	J	88	ARG	Sidechain
6	Z	25	ARG	Sidechain

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	U	6334	0	6368	343	0
2	V	3610	0	3676	177	0
3	W	3552	0	3676	226	0
4	X	3259	0	3371	160	0
5	Y	3123	0	3130	171	0
6	Z	2290	0	2320	180	0
7	a	3012	0	3029	162	0
8	b	1459	0	1499	91	0
9	c	2260	0	2276	201	0
10	d	2131	0	2164	117	0
11	e	314	0	247	17	0
12	f	6420	0	6442	331	0
13	y	879	0	944	33	0
14	A	2930	0	3003	169	0
15	B	2933	0	2994	166	0
16	C	2729	0	2835	137	0
17	D	3009	0	3042	212	0
18	E	2678	0	2743	171	0
19	F	2646	0	2711	168	0
20	G	1836	0	1848	99	0
21	H	1760	0	1761	96	0
22	I	1990	0	2012	83	0
23	J	1887	0	1905	112	0
24	L	1868	0	1858	69	0
25	M	1905	0	1880	88	0
26	N	1487	0	1452	65	0
26	n	1336	0	1324	57	0
27	O	1667	0	1689	96	0
27	o	1315	0	1321	45	0
28	P	1591	0	1609	105	0
28	p	1264	0	1255	73	0
29	Q	1578	0	1580	80	0
29	q	1380	0	1399	46	0
30	R	1549	0	1512	64	0
30	r	1432	0	1384	76	0
31	S	1643	0	1640	70	0
31	s	1597	0	1597	79	0
32	T	1665	0	1638	94	0
32	t	1609	0	1597	66	0
33	K	1715	0	1714	76	0
34	z	471	0	472	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	31	0	12	2	0
35	D	31	0	12	13	0
35	E	31	0	12	3	0
35	F	31	0	12	5	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
37	B	27	0	12	8	0
All	All	90266	0	90977	4332	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 24.

The worst 5 of 4332 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:o:44:THR:N	27:o:172:SER:HG	1.56	1.03
31:S:41:LEU:HD11	31:S:177:LEU:HD11	1.39	1.03
27:o:118:ARG:N	27:o:121:THR:HG1	1.58	1.01
17:D:214:MET:HE3	35:D:501:ATP:H5'2	1.40	1.00
10:d:141:LEU:HD13	10:d:182:LEU:HD12	1.43	0.97

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	U	804/953 (84%)	716 (89%)	85 (11%)	3 (0%)	30	65
2	V	442/534 (83%)	397 (90%)	45 (10%)	0	100	100
3	W	434/456 (95%)	371 (86%)	63 (14%)	0	100	100
4	X	409/422 (97%)	361 (88%)	48 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Y	377/389 (97%)	354 (94%)	23 (6%)	0	100	100
6	Z	285/324 (88%)	258 (90%)	27 (10%)	0	100	100
7	a	373/376 (99%)	338 (91%)	35 (9%)	0	100	100
8	b	189/377 (50%)	166 (88%)	22 (12%)	1 (0%)	25	60
9	c	285/310 (92%)	238 (84%)	47 (16%)	0	100	100
10	d	258/350 (74%)	214 (83%)	44 (17%)	0	100	100
11	e	32/70 (46%)	22 (69%)	10 (31%)	0	100	100
12	f	823/908 (91%)	697 (85%)	124 (15%)	2 (0%)	44	75
13	y	107/505 (21%)	98 (92%)	9 (8%)	0	100	100
14	A	369/433 (85%)	315 (85%)	53 (14%)	1 (0%)	37	70
15	B	369/440 (84%)	322 (87%)	47 (13%)	0	100	100
16	C	342/406 (84%)	290 (85%)	52 (15%)	0	100	100
17	D	372/418 (89%)	316 (85%)	55 (15%)	1 (0%)	37	70
18	E	331/389 (85%)	265 (80%)	65 (20%)	1 (0%)	37	70
19	F	333/439 (76%)	264 (79%)	68 (20%)	1 (0%)	37	70
20	G	232/246 (94%)	209 (90%)	23 (10%)	0	100	100
21	H	224/234 (96%)	204 (91%)	20 (9%)	0	100	100
22	I	250/261 (96%)	235 (94%)	15 (6%)	0	100	100
23	J	237/248 (96%)	212 (90%)	25 (10%)	0	100	100
24	L	235/263 (89%)	218 (93%)	17 (7%)	0	100	100
25	M	240/255 (94%)	218 (91%)	22 (9%)	0	100	100
26	N	196/239 (82%)	175 (89%)	21 (11%)	0	100	100
26	n	171/239 (72%)	160 (94%)	11 (6%)	0	100	100
27	O	219/277 (79%)	199 (91%)	20 (9%)	0	100	100
27	o	166/277 (60%)	154 (93%)	12 (7%)	0	100	100
28	P	202/205 (98%)	175 (87%)	27 (13%)	0	100	100
28	p	152/205 (74%)	132 (87%)	20 (13%)	0	100	100
29	Q	195/201 (97%)	178 (91%)	17 (9%)	0	100	100
29	q	163/201 (81%)	150 (92%)	13 (8%)	0	100	100
30	R	197/263 (75%)	181 (92%)	16 (8%)	0	100	100
30	r	181/263 (69%)	163 (90%)	18 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	S	210/241 (87%)	191 (91%)	19 (9%)	0	100	100
31	s	202/241 (84%)	187 (93%)	14 (7%)	1 (0%)	25	60
32	T	211/264 (80%)	190 (90%)	21 (10%)	0	100	100
32	t	202/264 (76%)	184 (91%)	18 (9%)	0	100	100
33	K	220/241 (91%)	201 (91%)	19 (9%)	0	100	100
34	z	57/213 (27%)	51 (90%)	6 (10%)	0	100	100
All	All	11296/13840 (82%)	9969 (88%)	1316 (12%)	11 (0%)	50	80

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	b	87	CYS
17	D	147	ALA
19	F	86	LEU
1	U	127	ASP
1	U	128	GLN

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	U	691/816 (85%)	691 (100%)	0	100	100
2	V	390/460 (85%)	390 (100%)	0	100	100
3	W	401/416 (96%)	401 (100%)	0	100	100
4	X	353/362 (98%)	353 (100%)	0	100	100
5	Y	335/344 (97%)	335 (100%)	0	100	100
6	Z	258/295 (88%)	258 (100%)	0	100	100
7	a	335/336 (100%)	335 (100%)	0	100	100
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/268 (94%)	252 (100%)	0	100	100
10	d	231/294 (79%)	231 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	e	34/63 (54%)	34 (100%)	0	100	100
12	f	700/763 (92%)	700 (100%)	0	100	100
13	y	96/403 (24%)	96 (100%)	0	100	100
14	A	321/372 (86%)	321 (100%)	0	100	100
15	B	329/385 (86%)	329 (100%)	0	100	100
16	C	297/352 (84%)	297 (100%)	0	100	100
17	D	329/366 (90%)	329 (100%)	0	100	100
18	E	295/341 (86%)	295 (100%)	0	100	100
19	F	288/379 (76%)	288 (100%)	0	100	100
20	G	202/210 (96%)	202 (100%)	0	100	100
21	H	185/191 (97%)	184 (100%)	1 (0%)	86	90
22	I	212/221 (96%)	212 (100%)	0	100	100
23	J	203/211 (96%)	203 (100%)	0	100	100
24	L	203/224 (91%)	203 (100%)	0	100	100
25	M	201/212 (95%)	201 (100%)	0	100	100
26	N	154/181 (85%)	154 (100%)	0	100	100
26	n	138/181 (76%)	138 (100%)	0	100	100
27	O	182/228 (80%)	182 (100%)	0	100	100
27	o	139/228 (61%)	139 (100%)	0	100	100
28	P	173/174 (99%)	173 (100%)	0	100	100
28	p	136/174 (78%)	136 (100%)	0	100	100
29	Q	168/171 (98%)	168 (100%)	0	100	100
29	q	148/171 (86%)	148 (100%)	0	100	100
30	R	155/202 (77%)	155 (100%)	0	100	100
30	r	142/202 (70%)	142 (100%)	0	100	100
31	S	177/199 (89%)	177 (100%)	0	100	100
31	s	172/199 (86%)	172 (100%)	0	100	100
32	T	176/215 (82%)	176 (100%)	0	100	100
32	t	171/215 (80%)	171 (100%)	0	100	100
33	K	189/203 (93%)	189 (100%)	0	100	100
34	z	50/185 (27%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9778/11724 (83%)	9777 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	H	140	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
27	O	78	HIS
28	P	157	ASN
31	S	86	HIS
10	d	313	ASN
10	d	195	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 ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
35	ATP	A	501	36	28,33,33	0.71	0	34,52,52	0.96	1 (2%)
37	ADP	B	501	36	24,29,29	0.87	1 (4%)	29,45,45	1.33	2 (6%)
35	ATP	D	501	-	28,33,33	0.70	0	34,52,52	0.84	1 (2%)
35	ATP	F	501	-	28,33,33	0.63	0	34,52,52	0.92	1 (2%)
35	ATP	E	401	-	28,33,33	0.83	1 (3%)	34,52,52	0.95	1 (2%)

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
35	ATP	A	501	36	-	6/18/38/38	0/3/3/3
37	ADP	B	501	36	-	1/12/32/32	0/3/3/3
35	ATP	D	501	-	-	3/18/38/38	0/3/3/3
35	ATP	F	501	-	-	5/18/38/38	0/3/3/3
35	ATP	E	401	-	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	501	ADP	O4'-C1'	2.04	1.43	1.40
35	E	401	ATP	PA-O3A	-2.03	1.57	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	501	ADP	N3-C2-N1	-4.03	123.21	128.67
37	B	501	ADP	C4-C5-N7	-2.66	106.53	109.34
35	F	501	ATP	C5-C6-N6	2.30	123.81	120.31
35	E	401	ATP	C5-C6-N6	2.29	123.80	120.31
35	A	501	ATP	C5-C6-N6	2.23	123.71	120.31

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O2A
35	A	501	ATP	O4'-C4'-C5'-O5'

Continued on next page...

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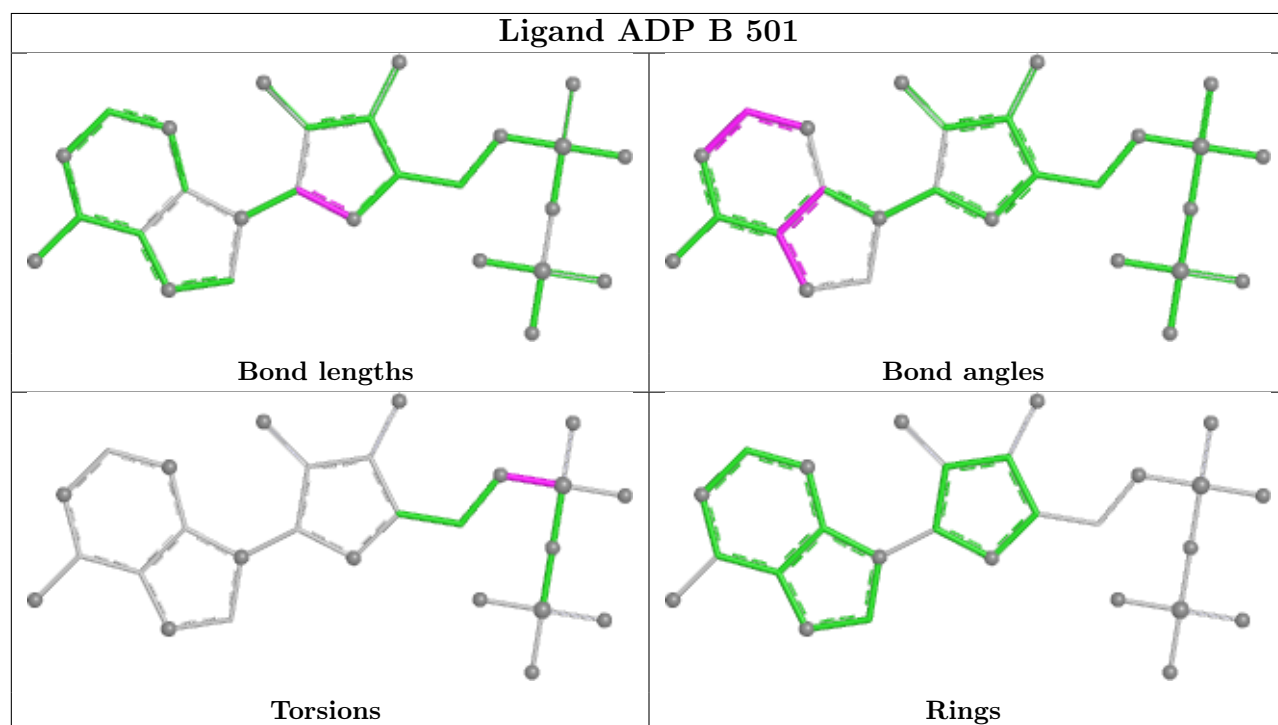
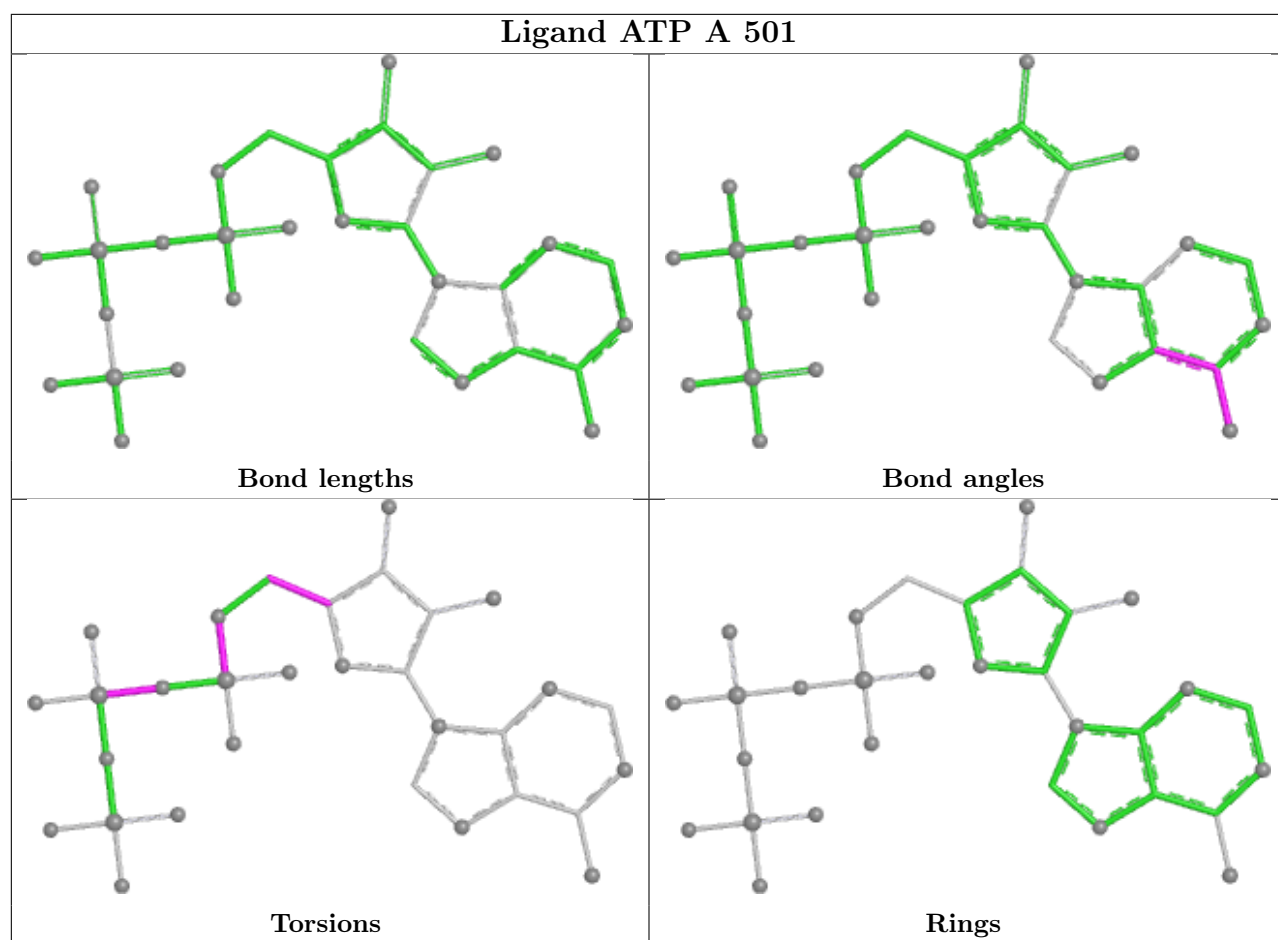
Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C3'-C4'-C5'-O5'
35	D	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	C5'-O5'-PA-O3A

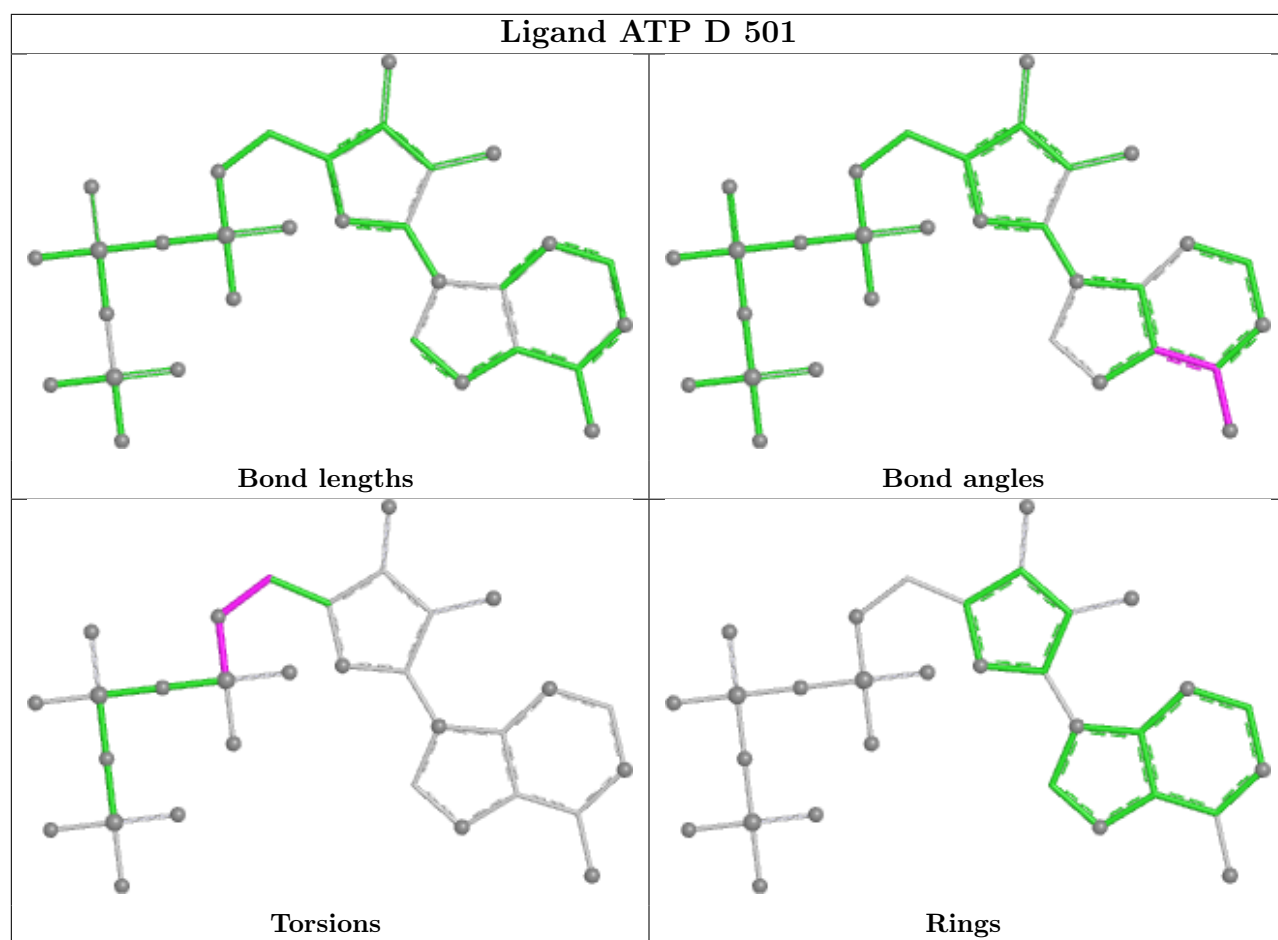
There are no ring outliers.

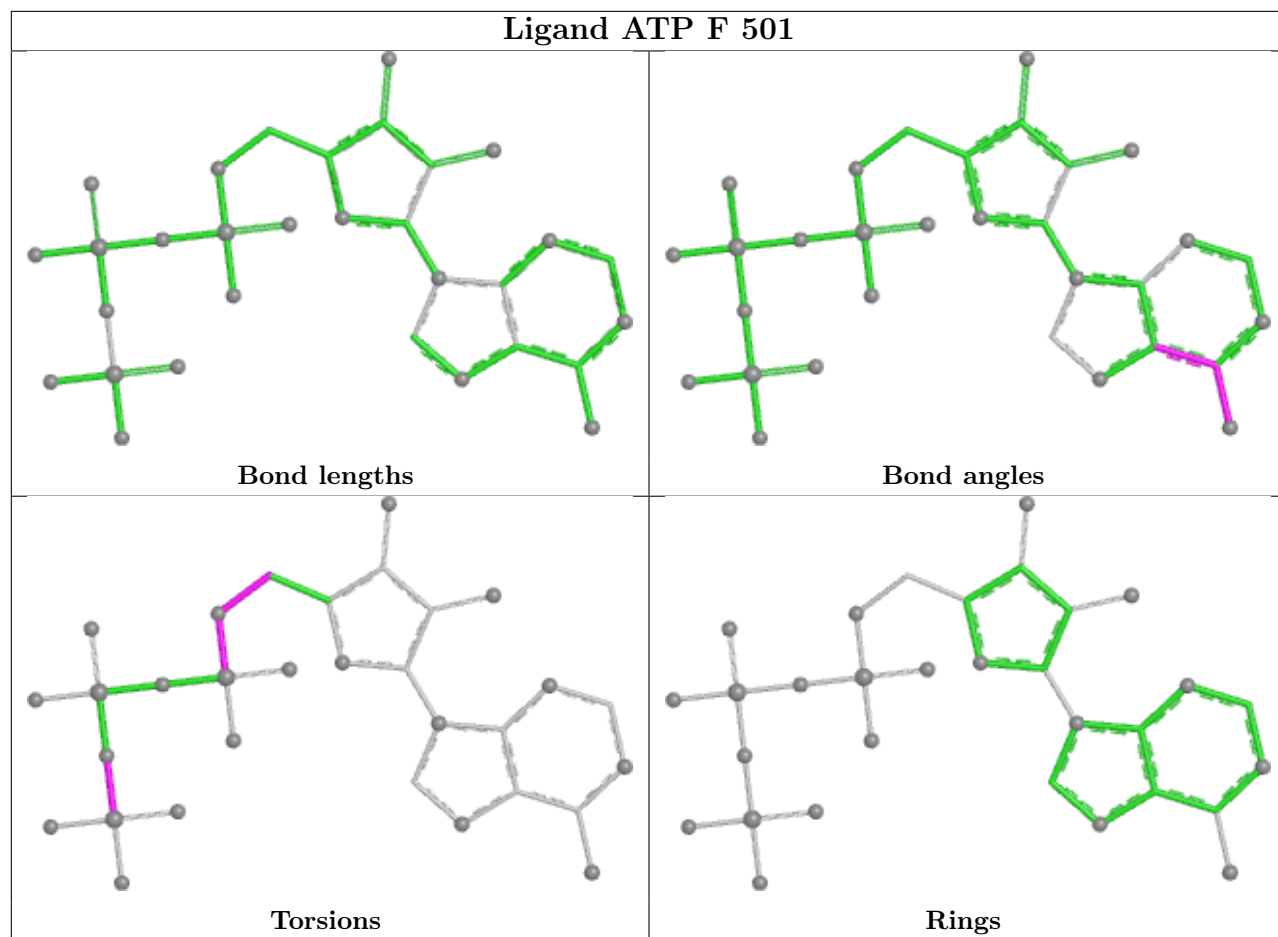
5 monomers are involved in 31 short contacts:

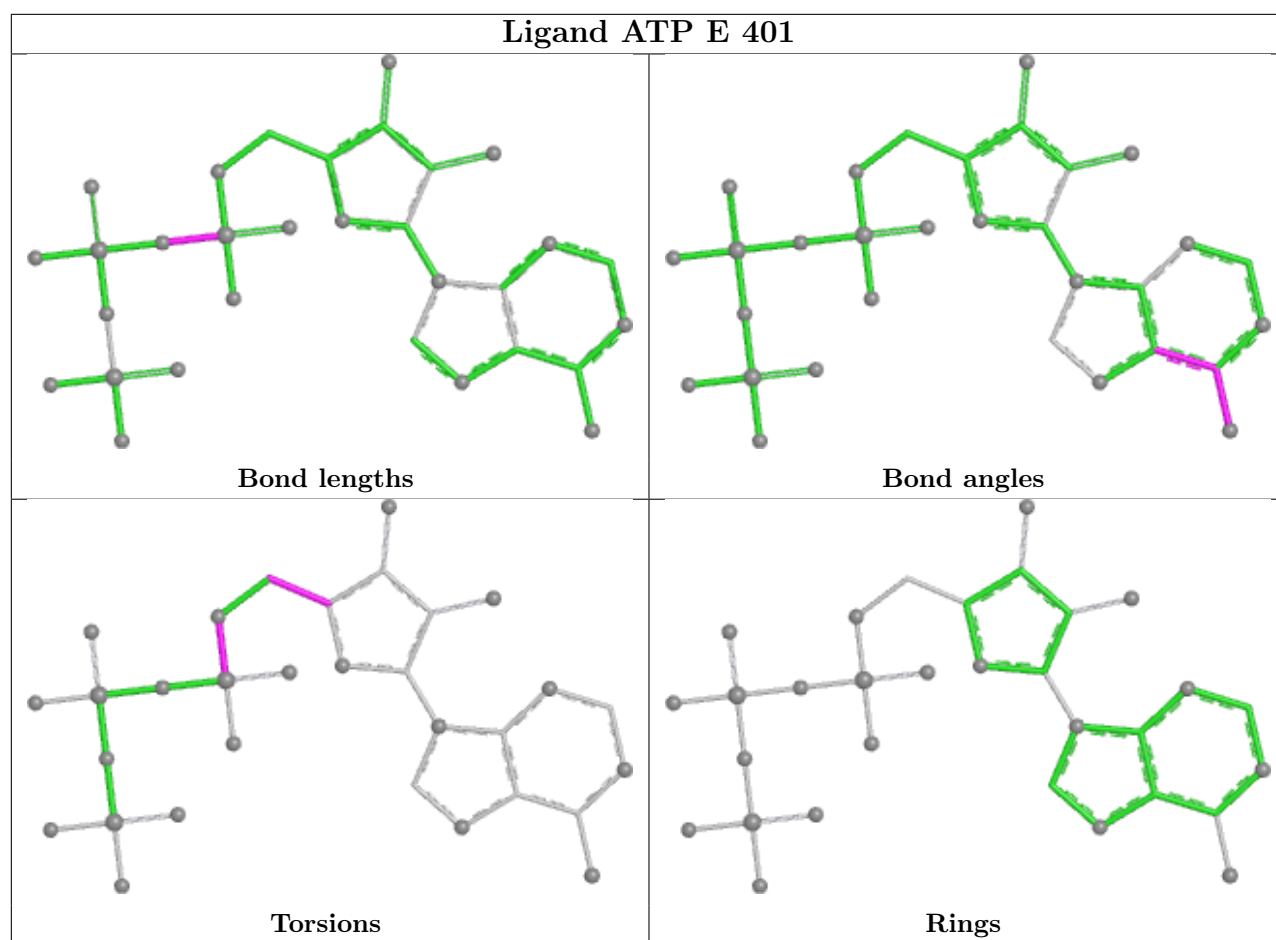
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ATP	2	0
37	B	501	ADP	8	0
35	D	501	ATP	13	0
35	F	501	ATP	5	0
35	E	401	ATP	3	0

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.

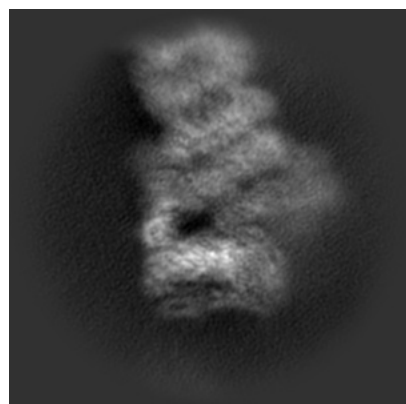
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44910. These allow visual inspection of the internal detail of the map and identification of artifacts.

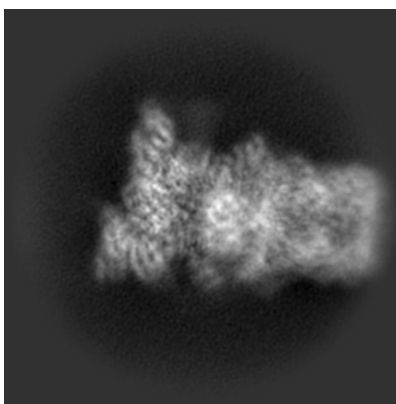
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

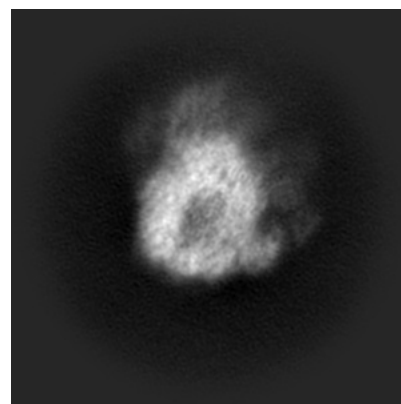
6.1.1 Primary map



X

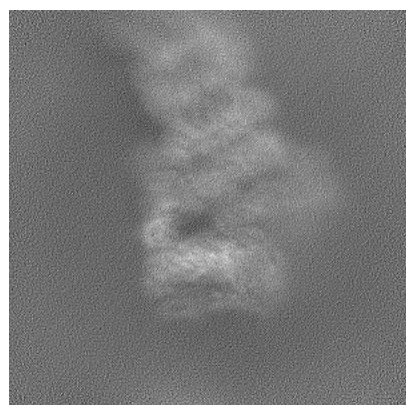


Y

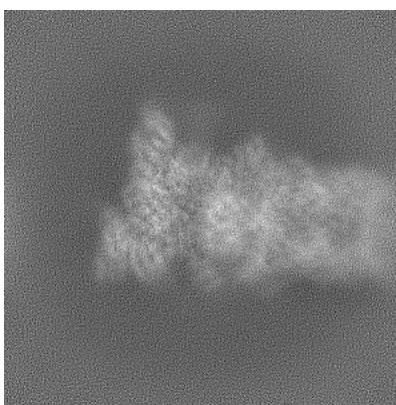


Z

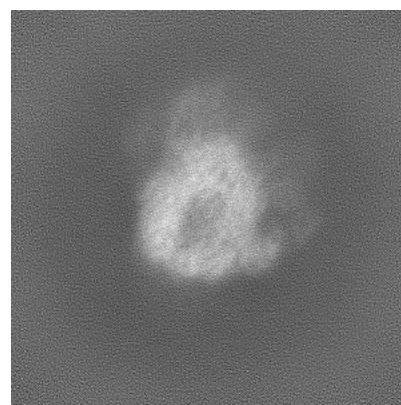
6.1.2 Raw map



X



Y

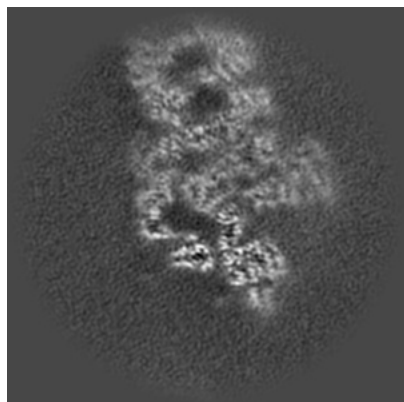


Z

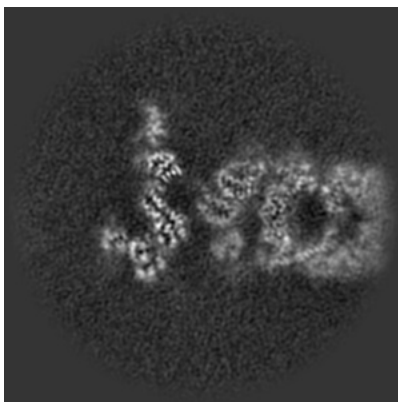
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

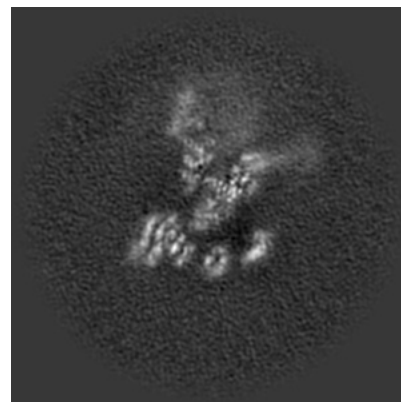
6.2.1 Primary map



X Index: 220

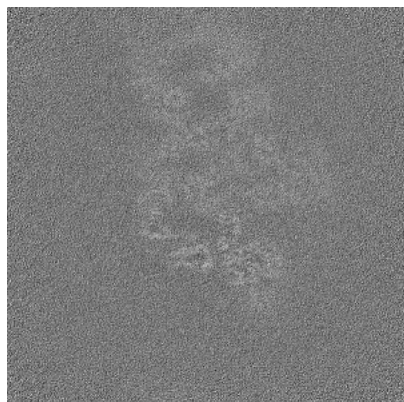


Y Index: 220

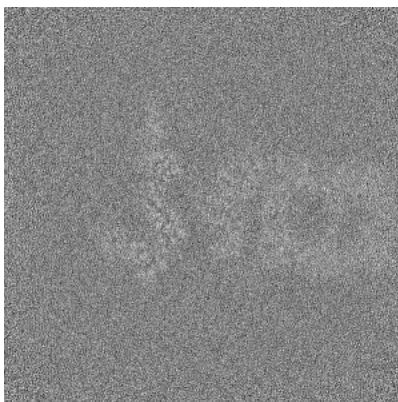


Z Index: 220

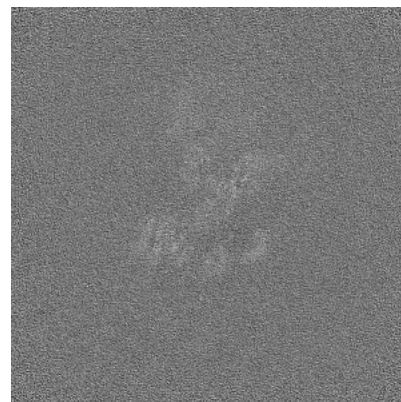
6.2.2 Raw map



X Index: 220



Y Index: 220

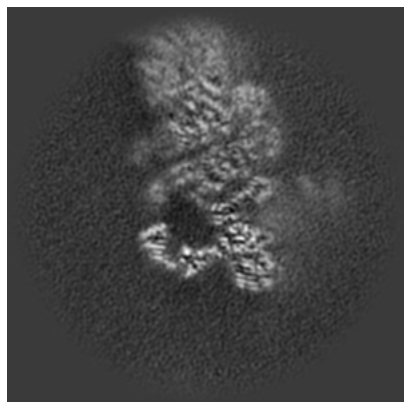


Z Index: 220

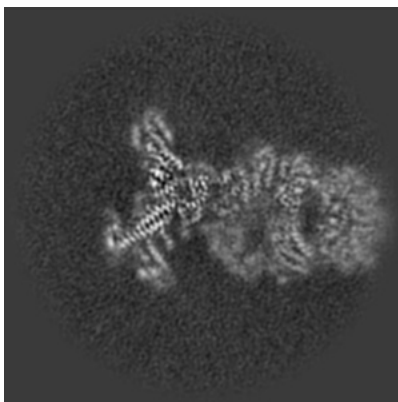
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

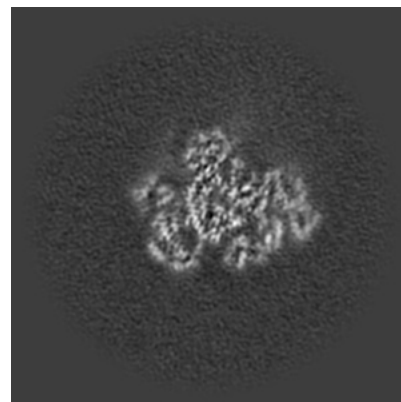
6.3.1 Primary map



X Index: 240

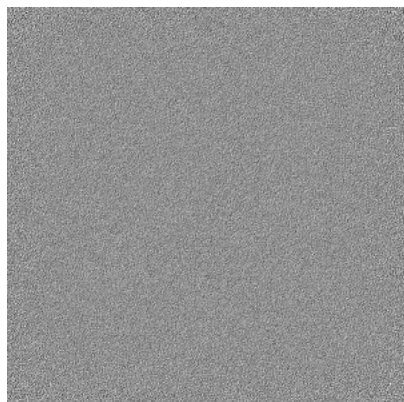


Y Index: 239

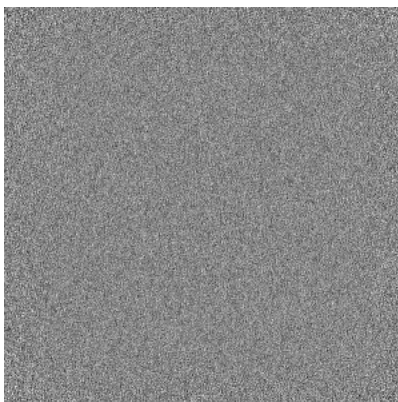


Z Index: 167

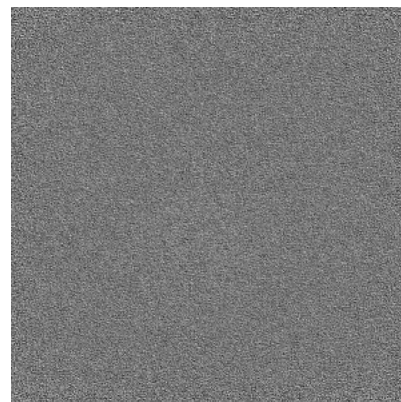
6.3.2 Raw map



X Index: 0



Y Index: 0

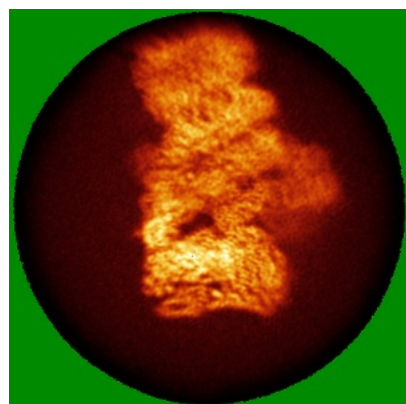


Z Index: 0

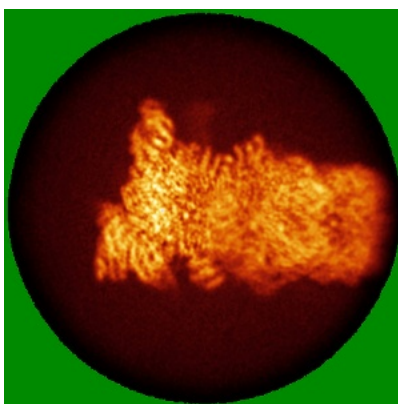
The images above show the largest variance slices of the map in three orthogonal directions.

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

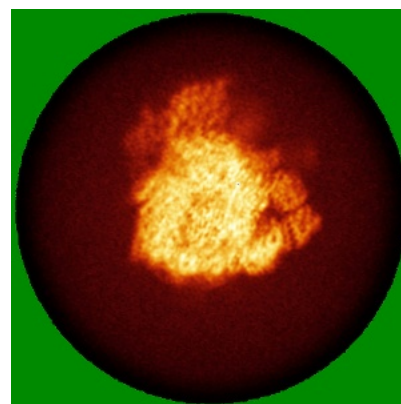
6.4.1 Primary map



X

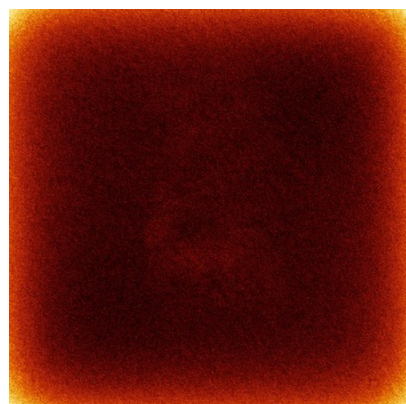


Y

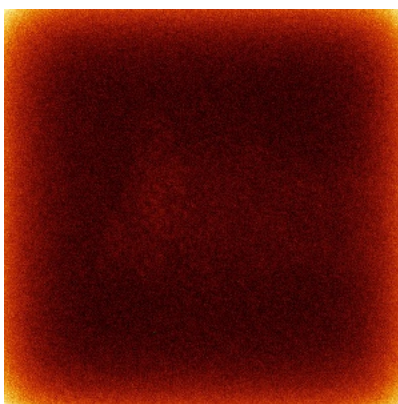


Z

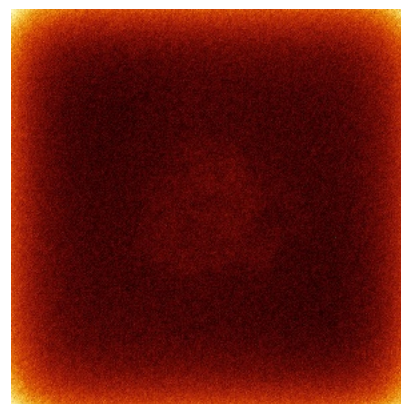
6.4.2 Raw map



X



Y

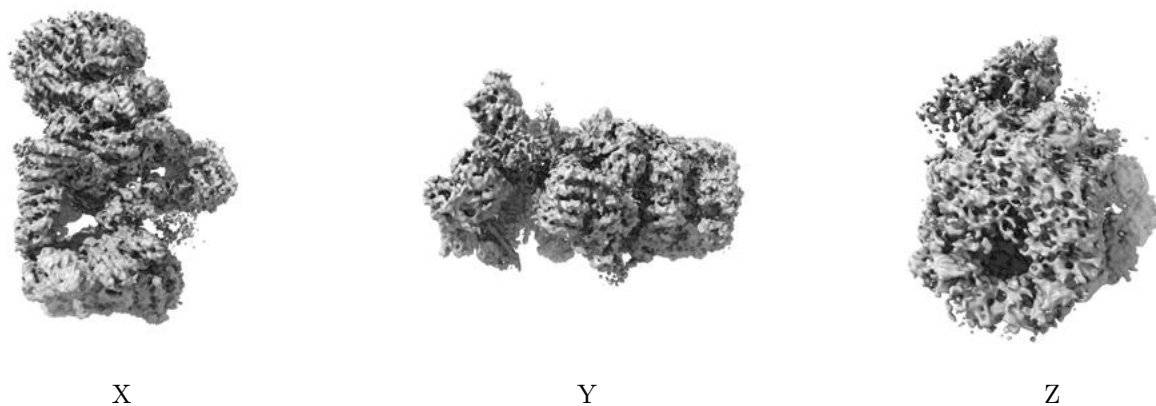


Z

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.

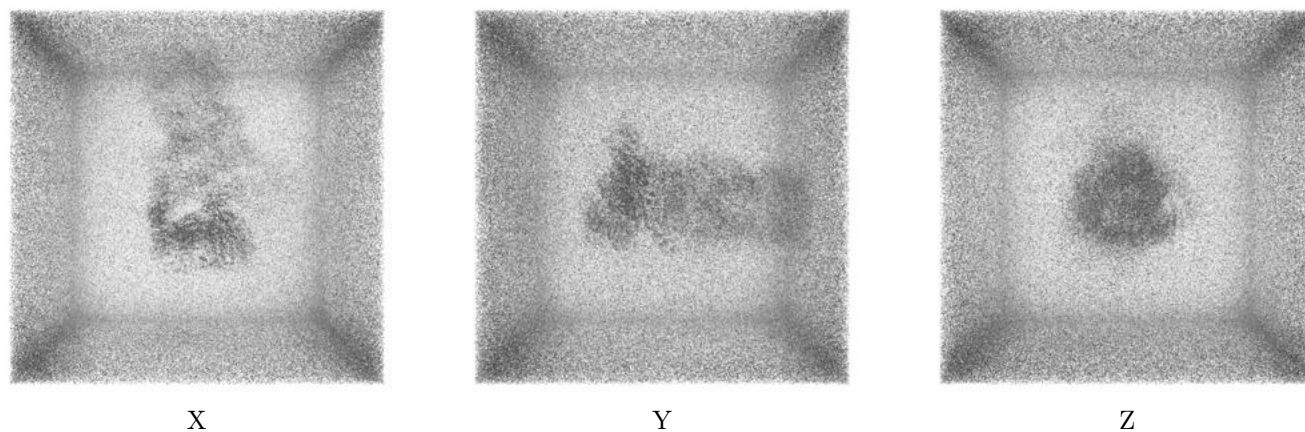
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

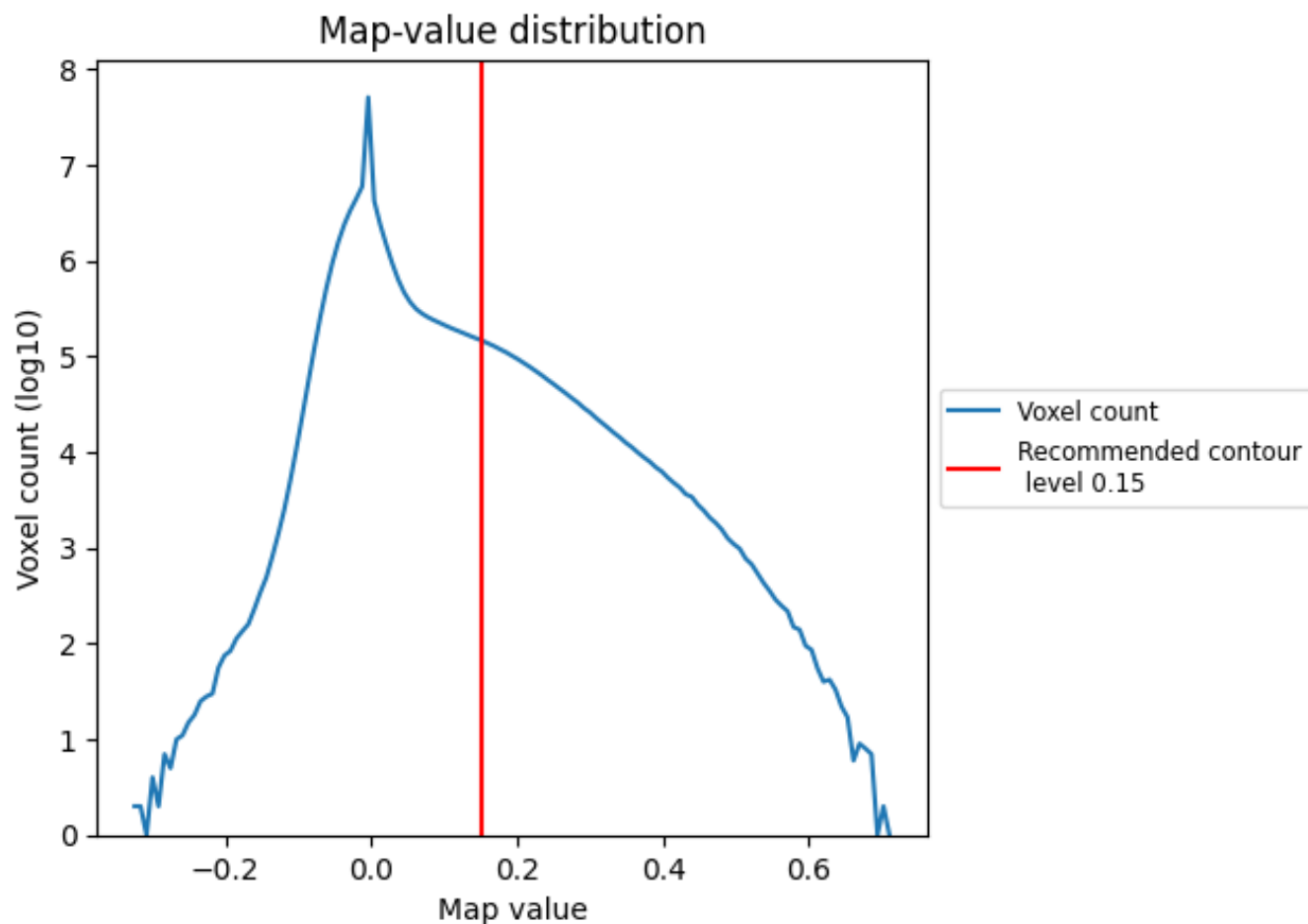
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

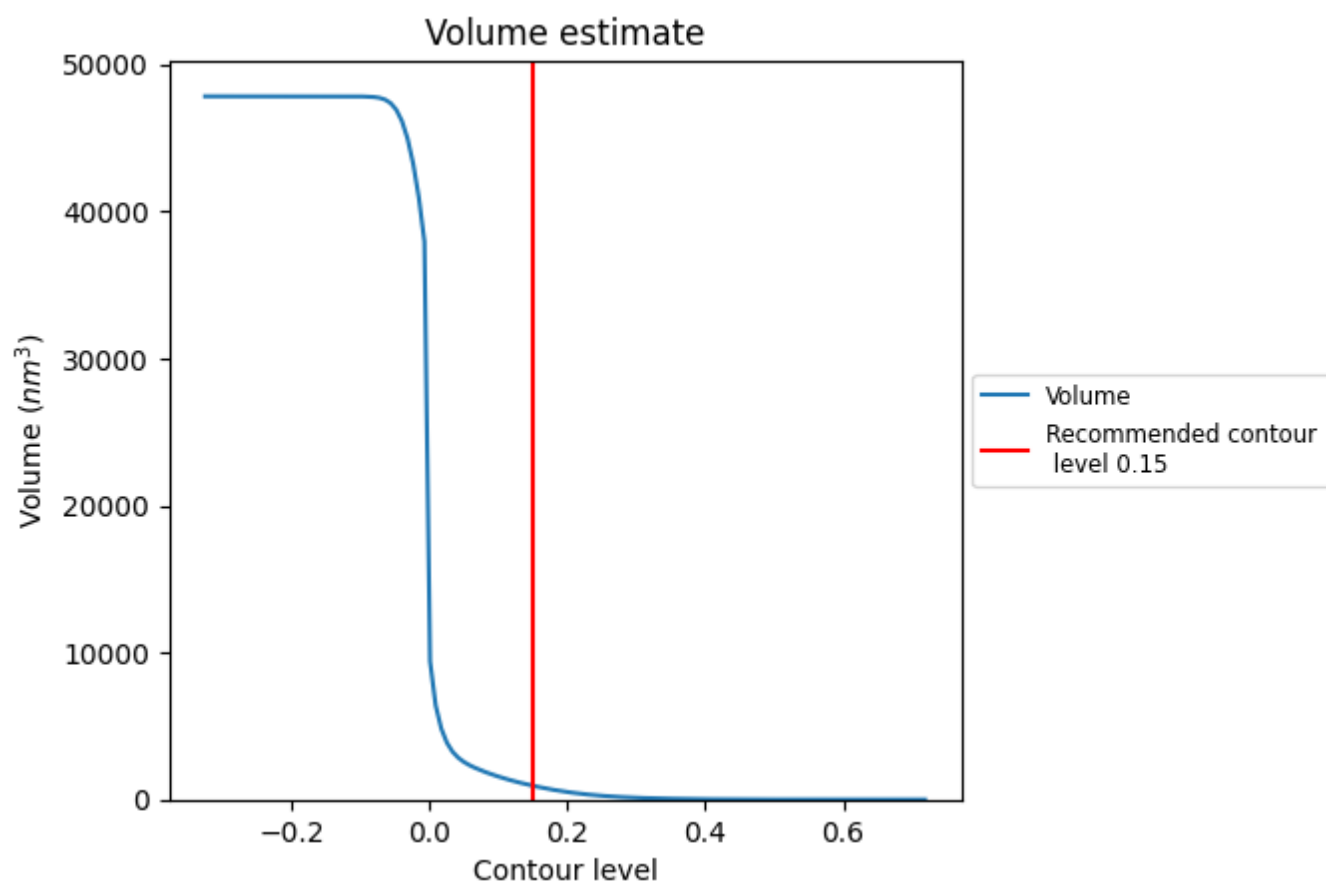
This section contains the results of statistical analysis of the map.

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.

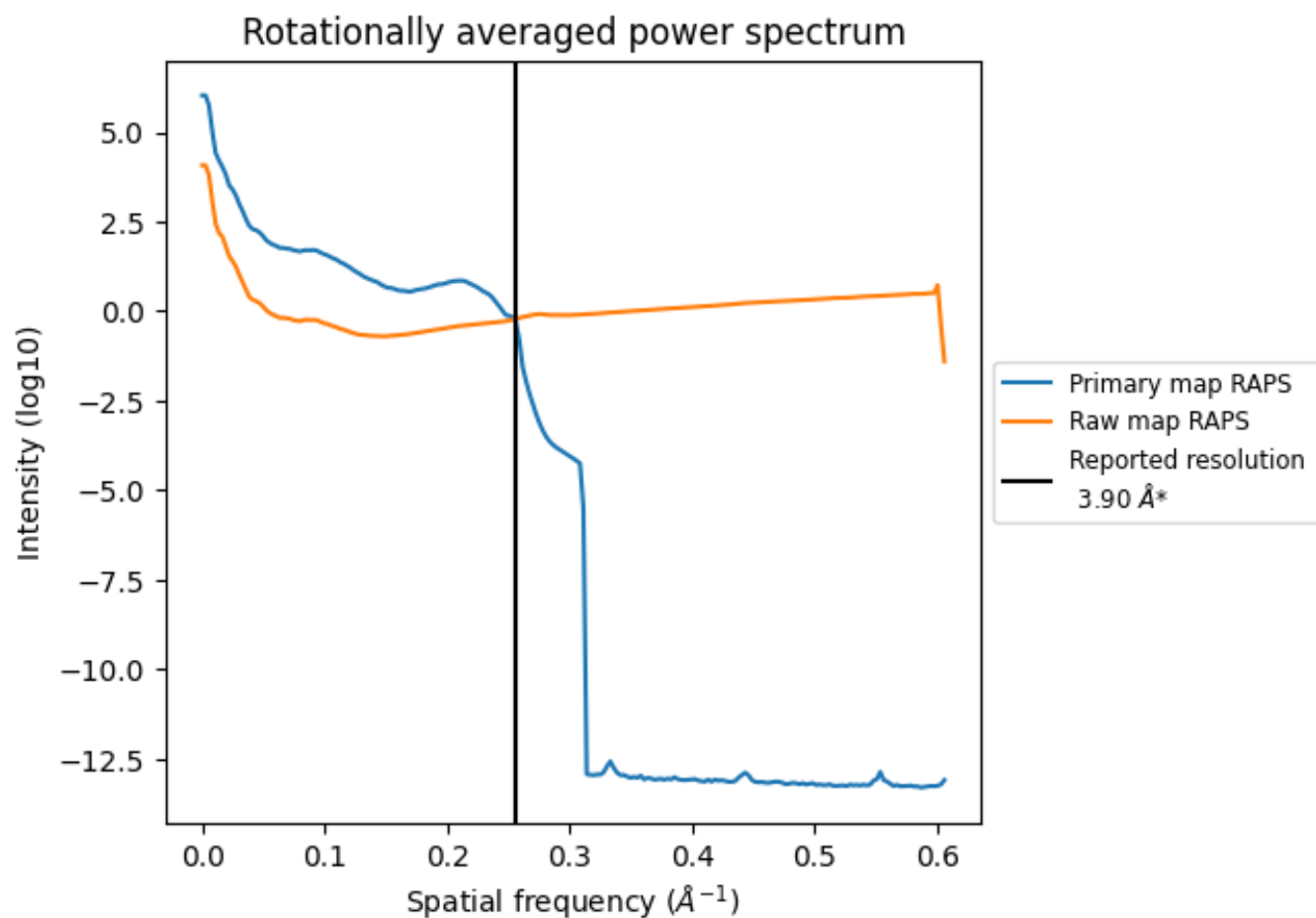
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 943 nm³; this corresponds to an approximate mass of 852 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 ⓘ

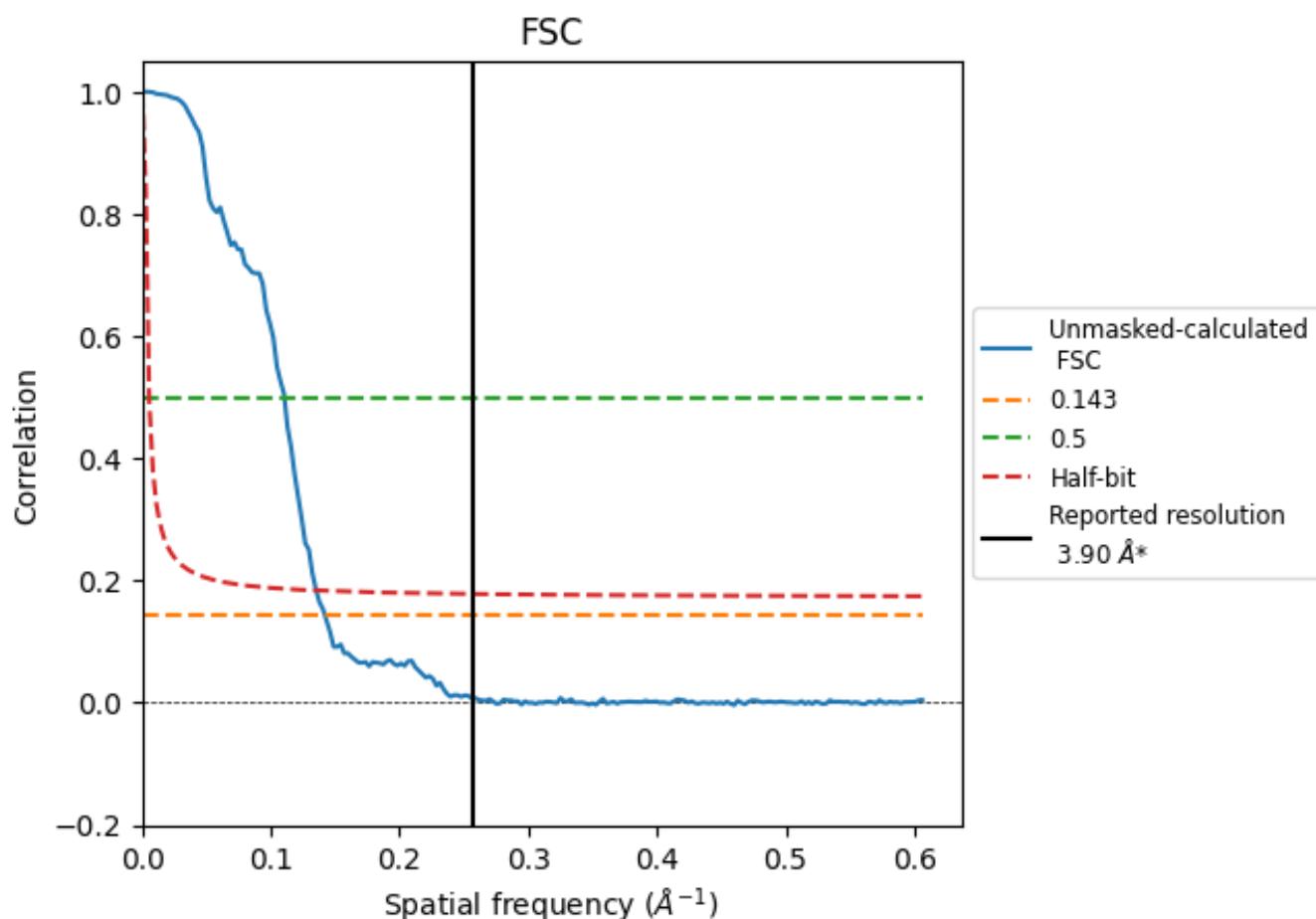


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

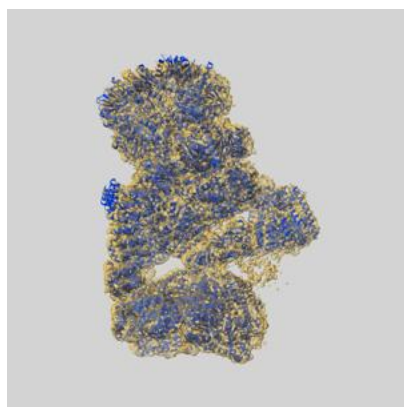
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.05	9.05	7.40

*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 7.05 differs from the reported value 3.9 by more than 10 %

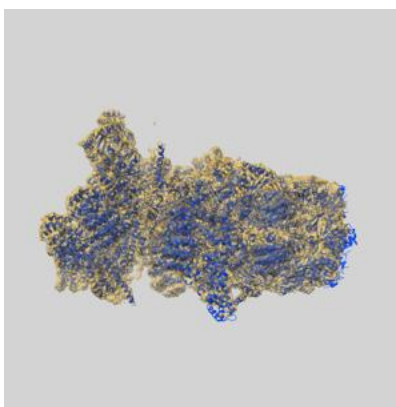
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44910 and PDB model 9BUI. Per-residue inclusion information can be found in section [3](#) on page [13](#).

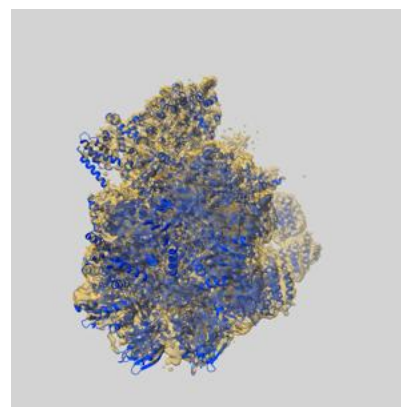
9.1 Map-model overlay [i](#)



X



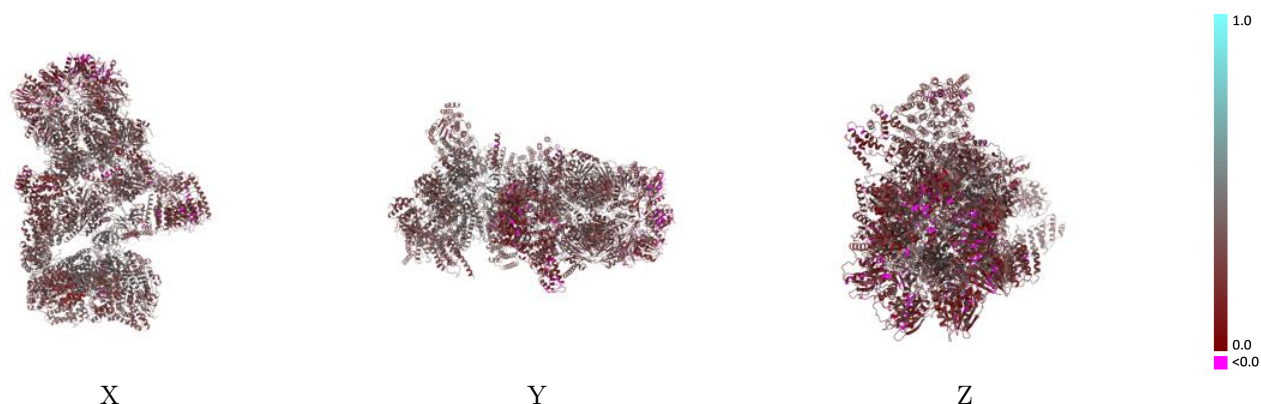
Y



Z

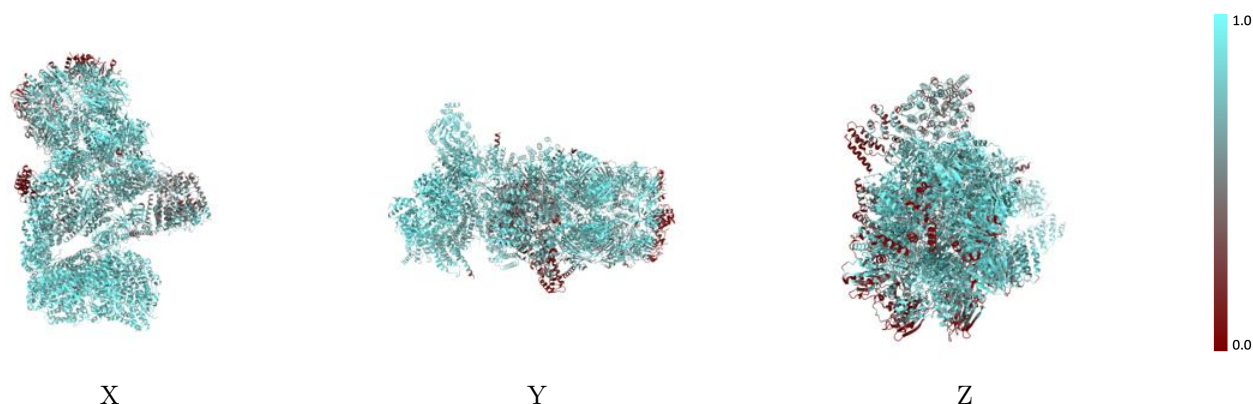
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



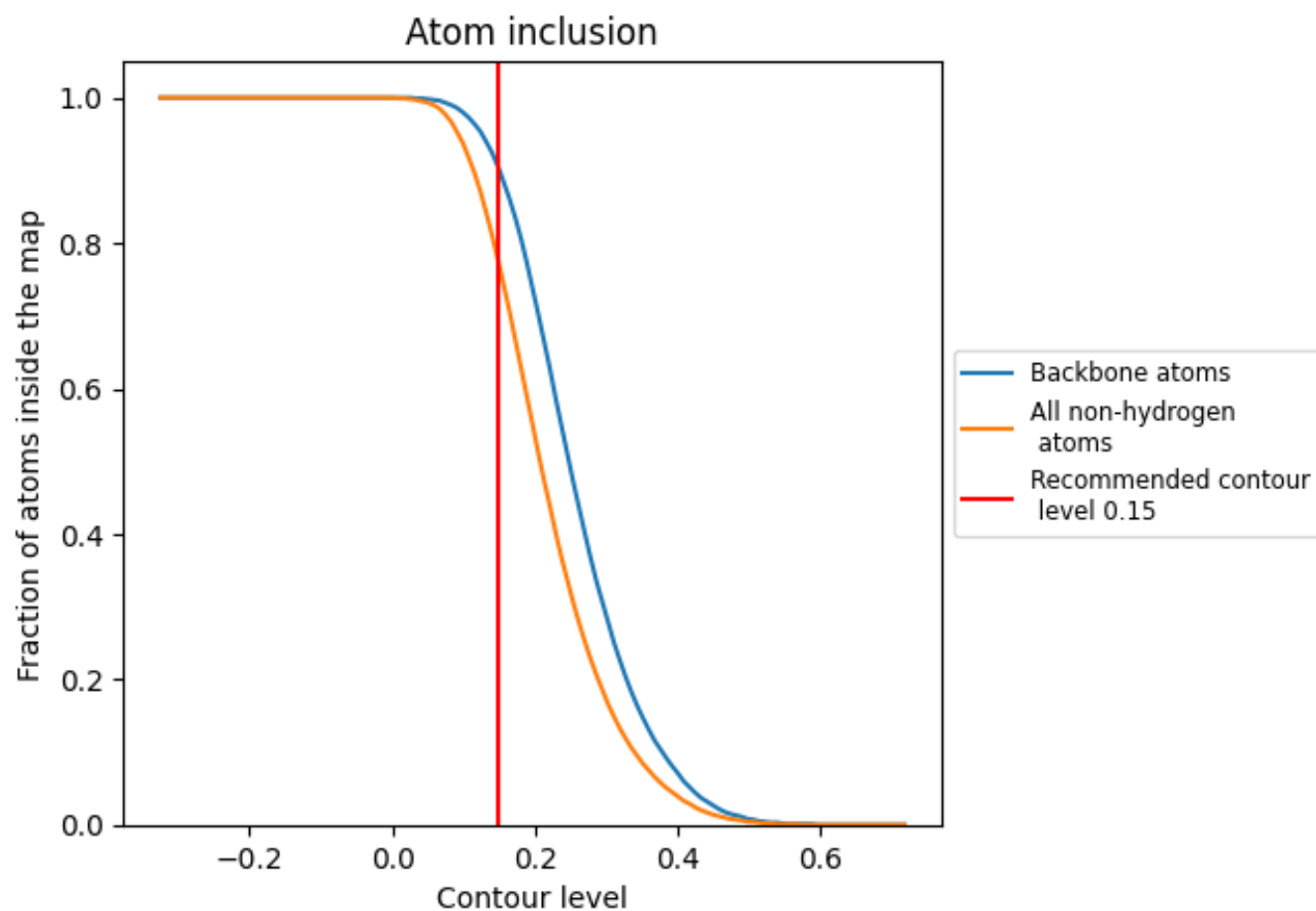
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 77% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.3010
A	 0.7720	 0.3100
B	 0.6670	 0.2880
C	 0.7580	 0.2930
D	 0.7780	 0.3470
E	 0.8130	 0.3460
F	 0.8000	 0.3330
G	 0.8390	 0.3610
H	 0.8450	 0.3510
I	 0.7600	 0.3150
J	 0.7610	 0.3020
K	 0.8450	 0.3050
L	 0.9130	 0.3330
M	 0.8760	 0.3500
N	 0.8330	 0.3080
O	 0.7680	 0.3160
P	 0.7350	 0.2900
Q	 0.8210	 0.2760
R	 0.8730	 0.2690
S	 0.8630	 0.2740
T	 0.9020	 0.2750
U	 0.9000	 0.3440
V	 0.8580	 0.3290
W	 0.8300	 0.3020
X	 0.6800	 0.2960
Y	 0.8660	 0.3200
Z	 0.8850	 0.3970
a	 0.8950	 0.3110
b	 0.8680	 0.3120
c	 0.8710	 0.3900
d	 0.8630	 0.2960
e	 0.9190	 0.3460
f	 0.5430	 0.2250
n	 0.7750	 0.2350
o	 0.6180	 0.1750



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Chain	Atom inclusion	Q-score
p	 0.3920	 0.1750
q	 0.4610	 0.2030
r	 0.4330	 0.2050
s	 0.4300	 0.2260
t	 0.6230	 0.2210
y	 0.6920	 0.3370
z	 0.7970	 0.2770