



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 04:36 AM UTC

PDB ID : 9E8Q / pdb_00009e8q
EMDB ID : EMD-47727
Title : Nub1/Fat10-processing human 26S proteasome with Rpt2 at top of spiral staircase
Authors : Arkinson, C.; Gee, C.L.; Martin, A.
Deposited on : 2024-11-05
Resolution : 3.16 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:

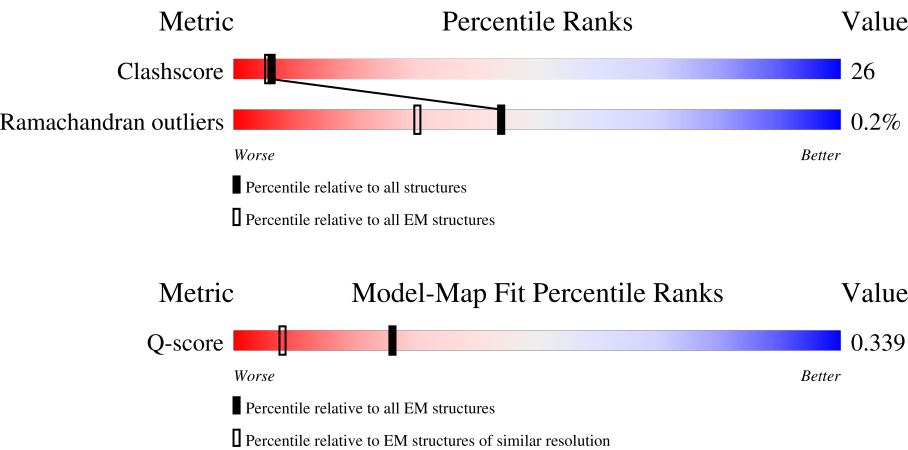
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	14474 (2.66 - 3.66)

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

Mol	Chain	Length	Quality of chain
1	A	433	23% 46% 44% 10%
2	B	440	8% 54% 36% 10%
3	C	406	63% 32% 5%
4	D	418	54% 36% 9%
5	E	389	9% 50% 43% 6%

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Mol	Chain	Length	Quality of chain
6	F	439	
7	G	246	
8	H	234	
9	I	261	
10	J	248	
11	K	241	
12	L	263	
13	M	255	
14	N	239	
15	O	277	
16	P	205	
17	Q	201	
18	R	263	
19	S	241	
20	T	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	424	
30	d	350	

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Mol	Chain	Length	Quality of chain
31	e	70	
32	f	908	
33	v	26	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 80403 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	391	Total	C	N	O	S	0	0
			3074	1936	541	580	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	397	Total	C	N	O	S	0	0
			3124	1968	530	611	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	386	Total	C	N	O	S	0	0
			3053	1921	547	567	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	364	Total	C	N	O	S	0	0
			2887	1814	515	542	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	359	Total	C	N	O	S	0	0
			2803	1774	483	529	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1801	1149	304	342	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1933	1222	330	371	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1860	1166	327	362	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	238	Total	C	N	O	S	0	0
			1817	1142	303	361	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	83	LYS	ALA	conflict	UNP P28066

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	240	Total	C	N	O	S	0	0
			1876	1175	338	352	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	0	0
			1890	1200	323	356	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	195	Total	C	N	O	S	0	0
			1462	913	250	287	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1645	1035	278	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	829	Total	C	N	O	S	0	0
			6459	4098	1098	1218	45		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	320	ASN	ASP	conflict	UNP Q99460

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	432	Total	C	N	O	S	0	0
			3527	2252	628	634	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	437	Total	C	N	O	S	0	0
			3564	2258	609	674	23		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	379	Total	C	N	O	S	0	0
			3001	1914	508	567	12		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	282	Total	C	N	O	S	0	0
			2220	1407	380	414	19		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	LEU	-	expression tag	UNP O00487
c	312	ILE	-	expression tag	UNP O00487
c	313	ASN	-	expression tag	UNP O00487
c	314	HIS	-	expression tag	UNP O00487
c	315	HIS	-	expression tag	UNP O00487
c	316	HIS	-	expression tag	UNP O00487
c	317	HIS	-	expression tag	UNP O00487
c	318	HIS	-	expression tag	UNP O00487
c	319	HIS	-	expression tag	UNP O00487
c	320	ASP	-	expression tag	UNP O00487
c	321	TYR	-	expression tag	UNP O00487
c	322	ASP	-	expression tag	UNP O00487
c	323	ILE	-	expression tag	UNP O00487
c	324	PRO	-	expression tag	UNP O00487
c	325	THR	-	expression tag	UNP O00487
c	326	THR	-	expression tag	UNP O00487
c	327	ALA	-	expression tag	UNP O00487
c	328	SER	-	expression tag	UNP O00487
c	329	GLU	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	330	ASN	-	expression tag	UNP O00487
c	331	LEU	-	expression tag	UNP O00487
c	332	TYR	-	expression tag	UNP O00487
c	333	PHE	-	expression tag	UNP O00487
c	334	GLN	-	expression tag	UNP O00487
c	335	GLY	-	expression tag	UNP O00487
c	336	GLU	-	expression tag	UNP O00487
c	337	LEU	-	expression tag	UNP O00487
c	338	GLY	-	expression tag	UNP O00487
c	339	MET	-	expression tag	UNP O00487
c	340	ARG	-	expression tag	UNP O00487
c	341	GLY	-	expression tag	UNP O00487
c	342	SER	-	expression tag	UNP O00487
c	343	ALA	-	expression tag	UNP O00487
c	344	GLY	-	expression tag	UNP O00487
c	345	LYS	-	expression tag	UNP O00487
c	346	ALA	-	expression tag	UNP O00487
c	347	GLY	-	expression tag	UNP O00487
c	348	GLU	-	expression tag	UNP O00487
c	349	GLY	-	expression tag	UNP O00487
c	350	GLU	-	expression tag	UNP O00487
c	351	ILE	-	expression tag	UNP O00487
c	352	PRO	-	expression tag	UNP O00487
c	353	ALA	-	expression tag	UNP O00487
c	354	PRO	-	expression tag	UNP O00487
c	355	LEU	-	expression tag	UNP O00487
c	356	ALA	-	expression tag	UNP O00487
c	357	GLY	-	expression tag	UNP O00487
c	358	THR	-	expression tag	UNP O00487
c	359	VAL	-	expression tag	UNP O00487
c	360	SER	-	expression tag	UNP O00487
c	361	LYS	-	expression tag	UNP O00487
c	362	ILE	-	expression tag	UNP O00487
c	363	LEU	-	expression tag	UNP O00487
c	364	VAL	-	expression tag	UNP O00487
c	365	LYS	-	expression tag	UNP O00487
c	366	GLU	-	expression tag	UNP O00487
c	367	GLY	-	expression tag	UNP O00487
c	368	ASP	-	expression tag	UNP O00487
c	369	THR	-	expression tag	UNP O00487
c	370	VAL	-	expression tag	UNP O00487
c	371	LYS	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	372	ALA	-	expression tag	UNP O00487
c	373	GLY	-	expression tag	UNP O00487
c	374	GLN	-	expression tag	UNP O00487
c	375	THR	-	expression tag	UNP O00487
c	376	VAL	-	expression tag	UNP O00487
c	377	LEU	-	expression tag	UNP O00487
c	378	VAL	-	expression tag	UNP O00487
c	379	LEU	-	expression tag	UNP O00487
c	380	GLU	-	expression tag	UNP O00487
c	381	ALA	-	expression tag	UNP O00487
c	382	MET	-	expression tag	UNP O00487
c	383	LYS	-	expression tag	UNP O00487
c	384	MET	-	expression tag	UNP O00487
c	385	GLU	-	expression tag	UNP O00487
c	386	THR	-	expression tag	UNP O00487
c	387	GLU	-	expression tag	UNP O00487
c	388	ILE	-	expression tag	UNP O00487
c	389	ASN	-	expression tag	UNP O00487
c	390	ALA	-	expression tag	UNP O00487
c	391	PRO	-	expression tag	UNP O00487
c	392	THR	-	expression tag	UNP O00487
c	393	ASP	-	expression tag	UNP O00487
c	394	GLY	-	expression tag	UNP O00487
c	395	LYS	-	expression tag	UNP O00487
c	396	VAL	-	expression tag	UNP O00487
c	397	GLU	-	expression tag	UNP O00487
c	398	LYS	-	expression tag	UNP O00487
c	399	VAL	-	expression tag	UNP O00487
c	400	LEU	-	expression tag	UNP O00487
c	401	VAL	-	expression tag	UNP O00487
c	402	LYS	-	expression tag	UNP O00487
c	403	GLU	-	expression tag	UNP O00487
c	404	ARG	-	expression tag	UNP O00487
c	405	ASP	-	expression tag	UNP O00487
c	406	ALA	-	expression tag	UNP O00487
c	407	VAL	-	expression tag	UNP O00487
c	408	GLN	-	expression tag	UNP O00487
c	409	GLY	-	expression tag	UNP O00487
c	410	GLY	-	expression tag	UNP O00487
c	411	GLN	-	expression tag	UNP O00487
c	412	GLY	-	expression tag	UNP O00487
c	413	LEU	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	414	ILE	-	expression tag	UNP O00487
c	415	LYS	-	expression tag	UNP O00487
c	416	ILE	-	expression tag	UNP O00487
c	417	GLY	-	expression tag	UNP O00487
c	418	VAL	-	expression tag	UNP O00487
c	419	HIS	-	expression tag	UNP O00487
c	420	HIS	-	expression tag	UNP O00487
c	421	HIS	-	expression tag	UNP O00487
c	422	HIS	-	expression tag	UNP O00487
c	423	HIS	-	expression tag	UNP O00487
c	424	HIS	-	expression tag	UNP O00487

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	250	Total	C	N	O	S	0	0
			2048	1331	335	373	9		

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

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

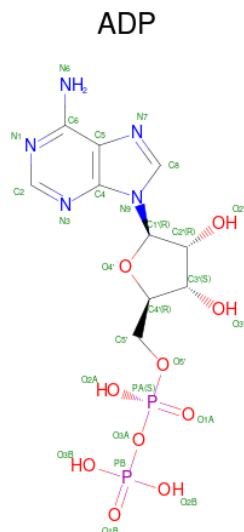
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	884	Total	C	N	O	S	0	0
			6836	4298	1169	1323	46		

- Molecule 33 is a protein called Substrate polypeptide.

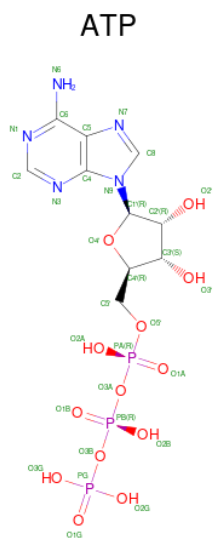
Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total 27	C 10	N 5	O 10	P 2	0
34	D	1	Total 27	C 10	N 5	O 10	P 2	0
34	E	1	Total 27	C 10	N 5	O 10	P 2	0
34	F	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

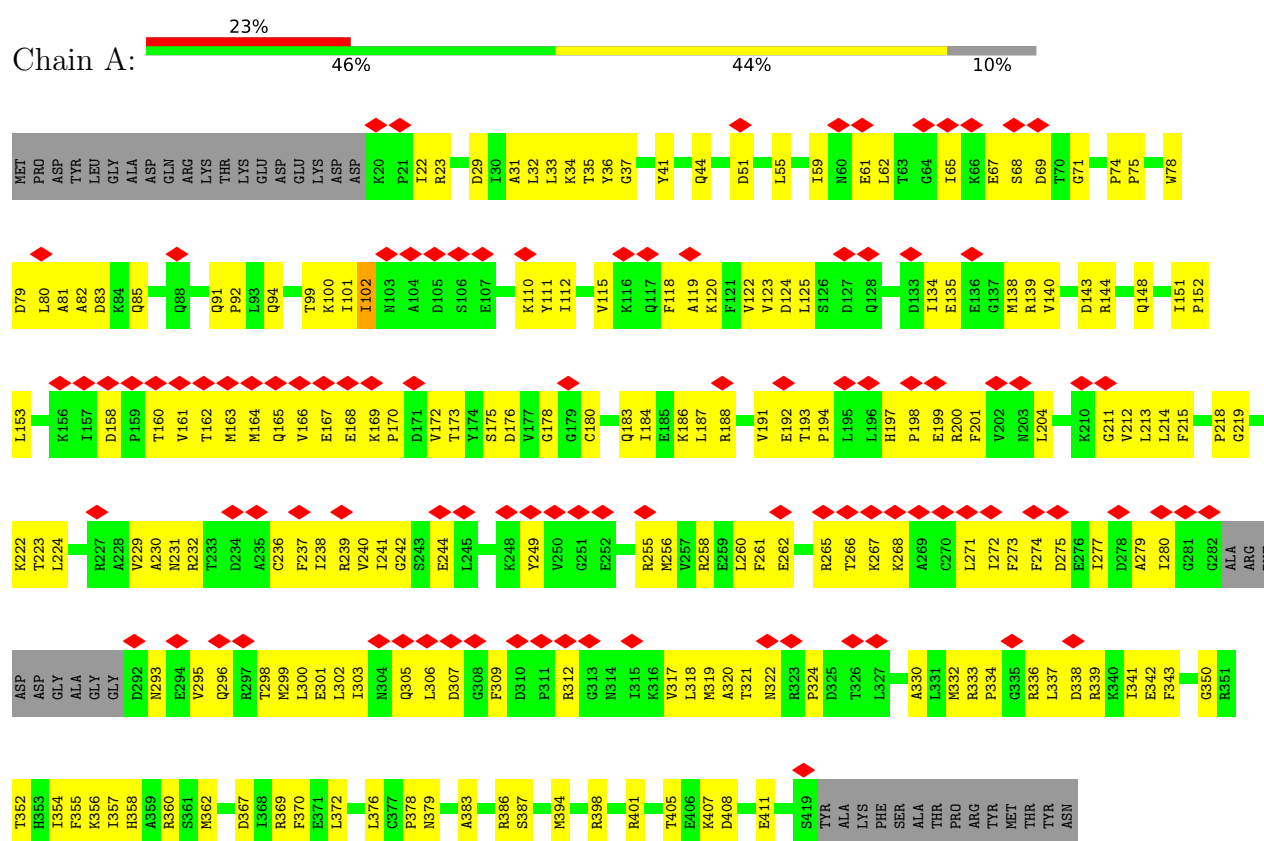
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

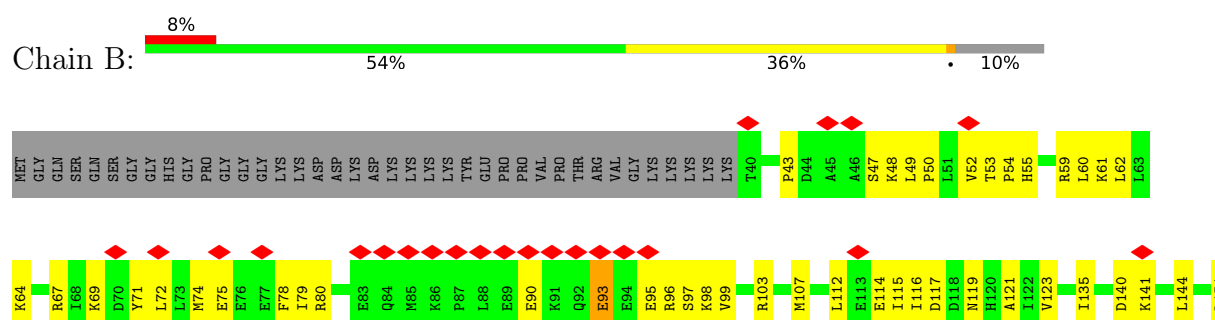
3 Residue-property plots

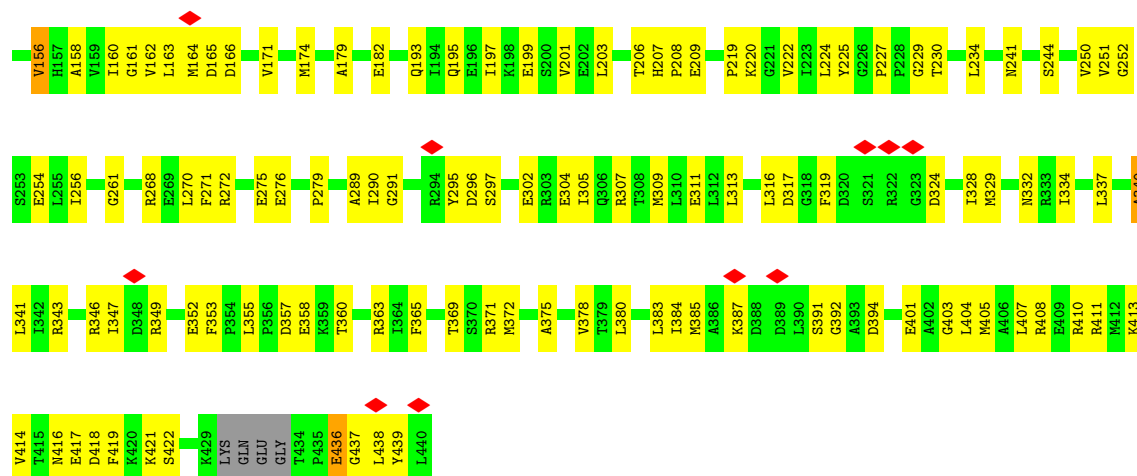
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 26S proteasome regulatory subunit 7

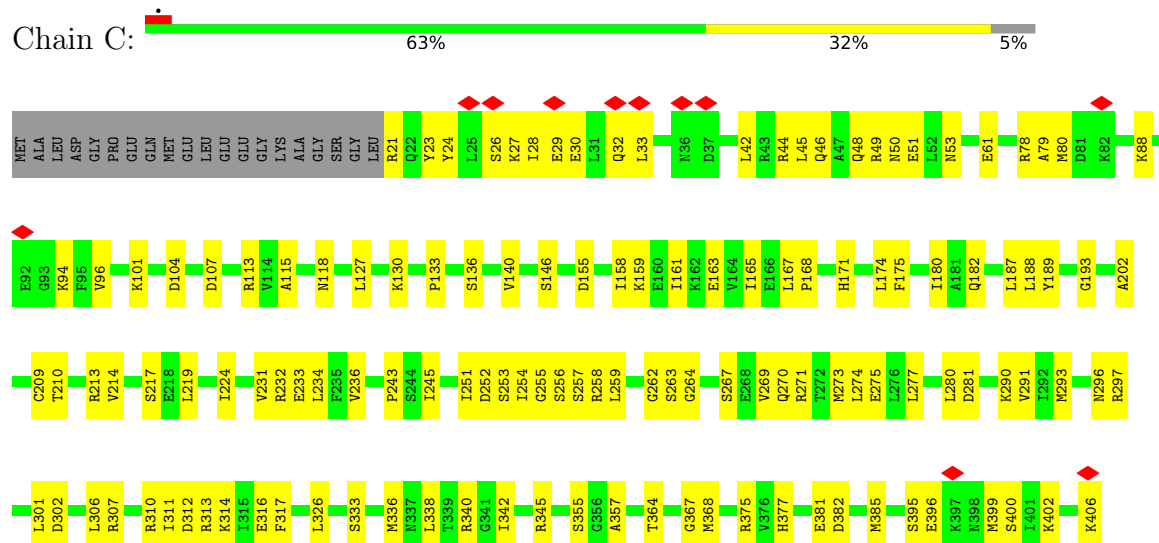


- Molecule 2: 26S proteasome regulatory subunit 4

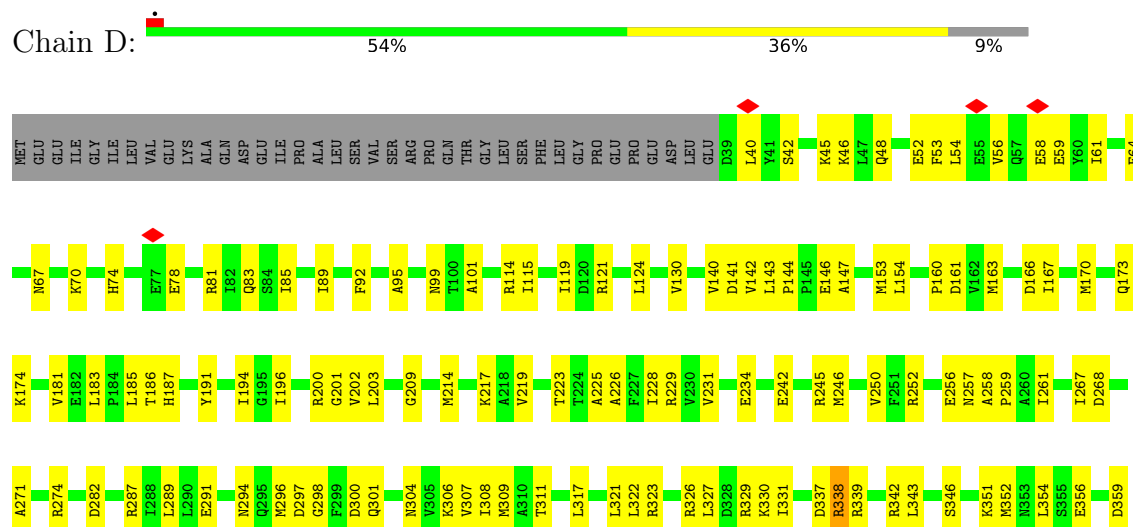


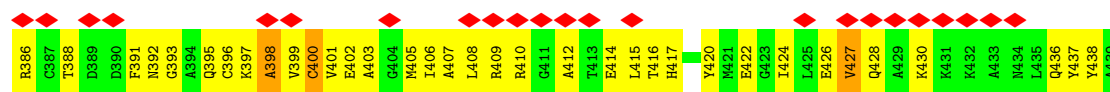


• Molecule 3: 26S protease regulatory subunit 8

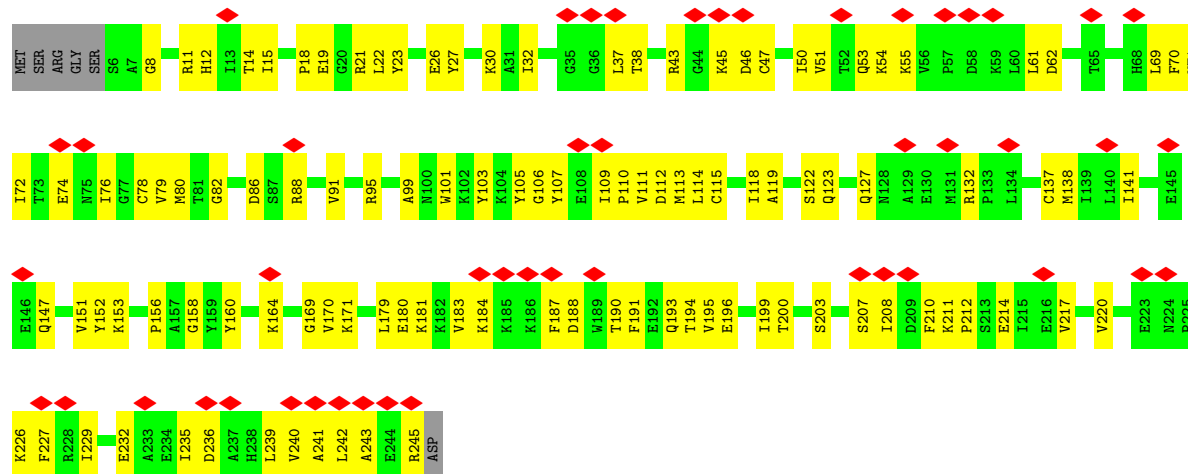


• Molecule 4: 26S proteasome regulatory subunit 6B

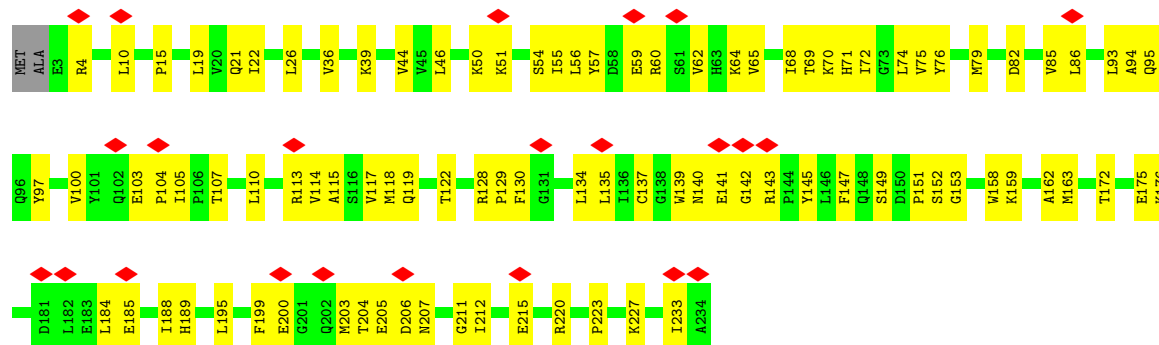




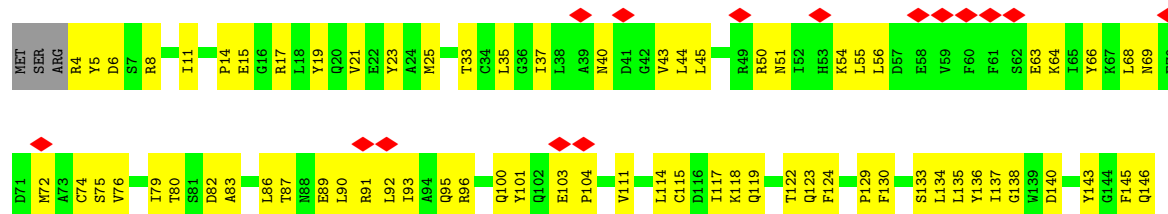
• Molecule 7: Proteasome subunit alpha type-6

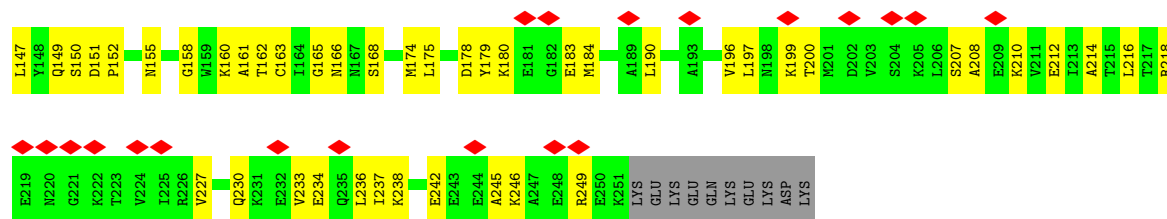


• Molecule 8: Proteasome subunit alpha type-2

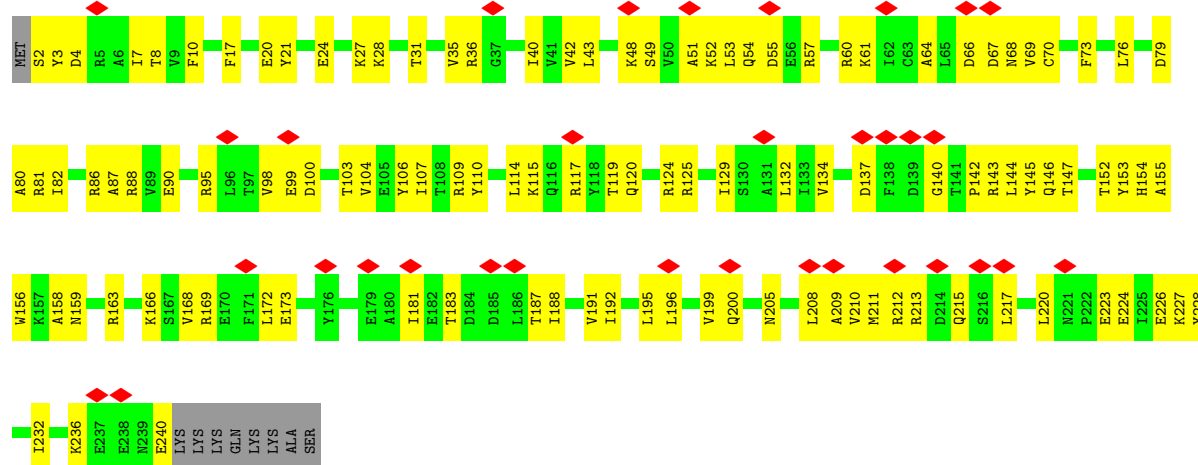


• Molecule 9: Proteasome subunit alpha type-4

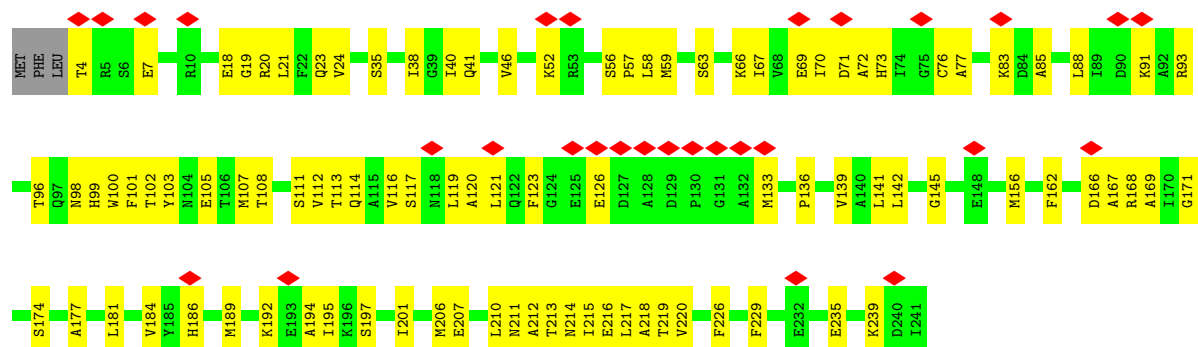




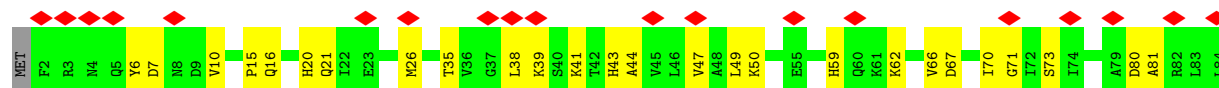
• Molecule 10: Proteasome subunit alpha type-7

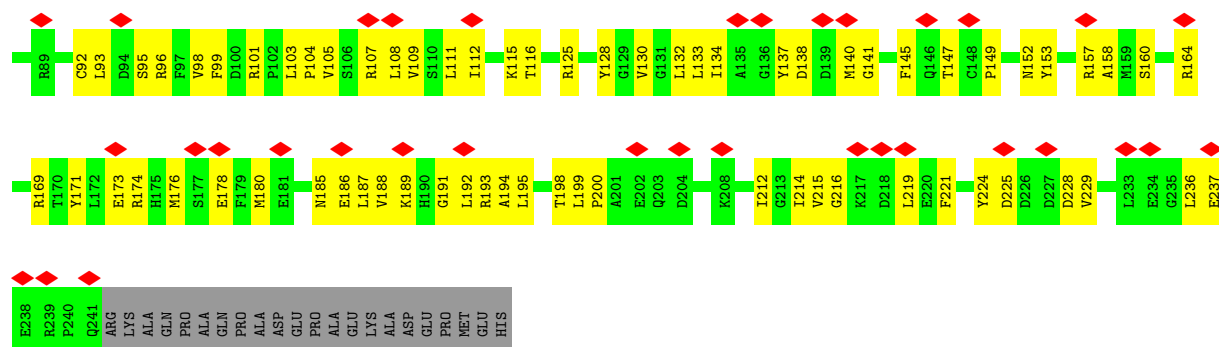


• Molecule 11: Proteasome subunit alpha type-5

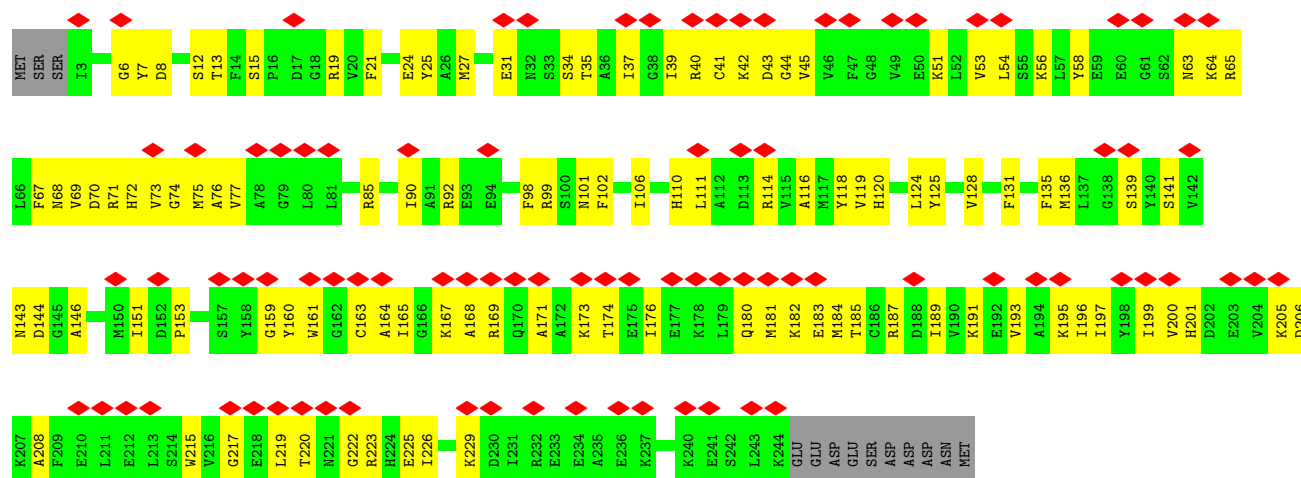


• Molecule 12: Proteasome subunit alpha type-1

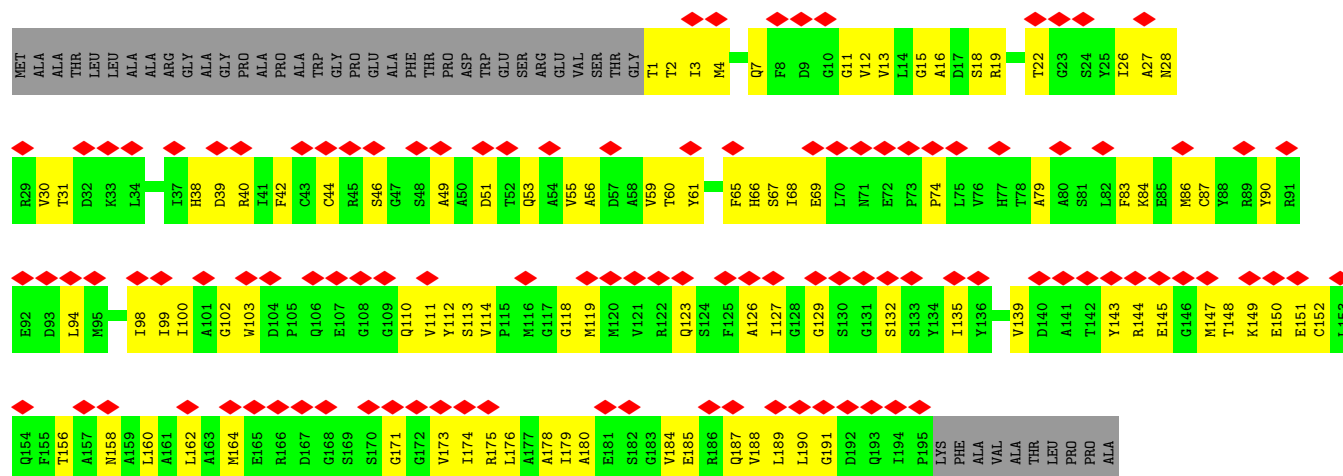




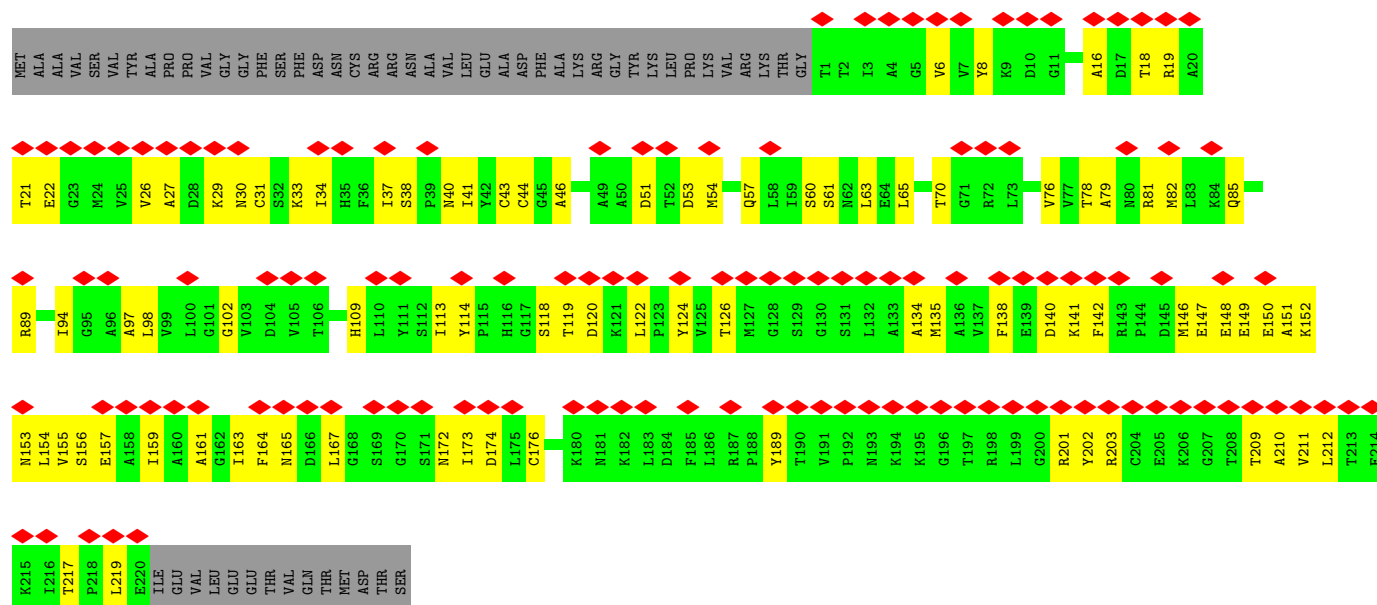
• Molecule 13: Proteasome subunit alpha type-3



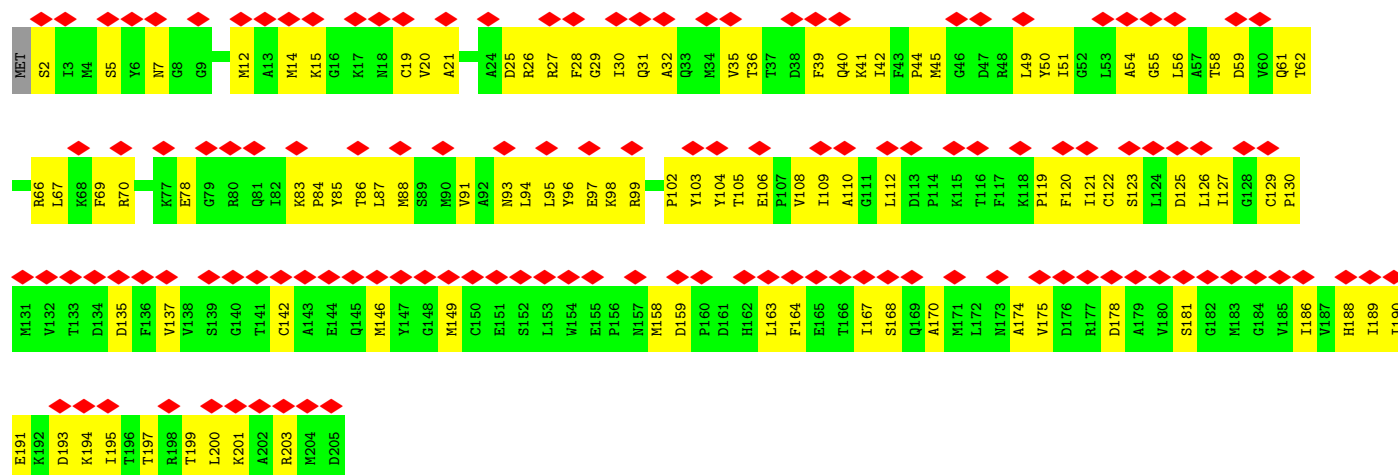
• Molecule 14: Proteasome subunit beta type-6



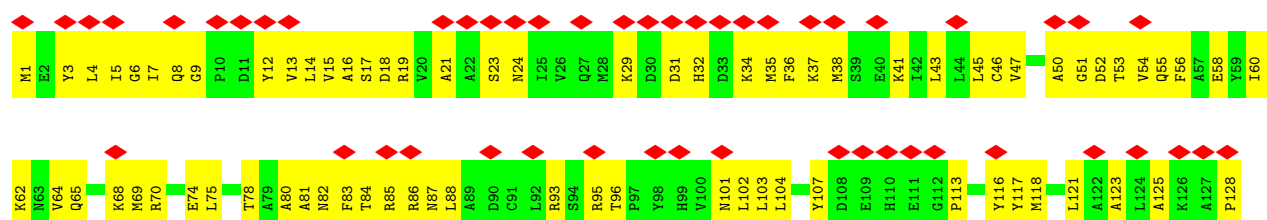
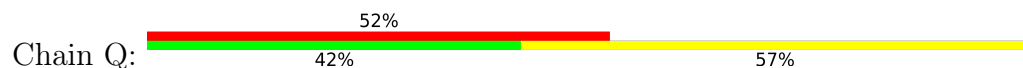
• Molecule 15: Proteasome subunit beta type-7

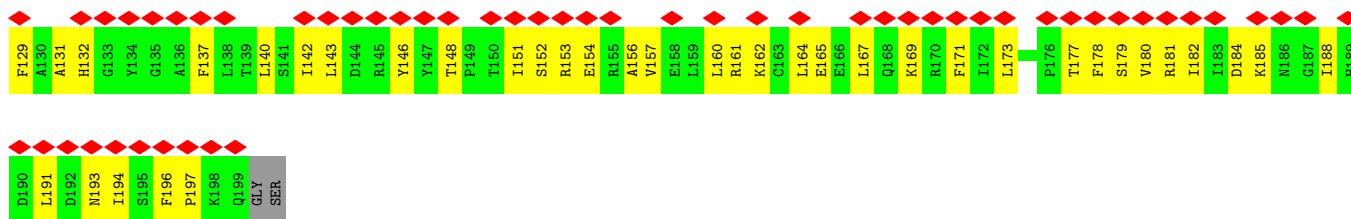


• Molecule 16: Proteasome subunit beta type-3

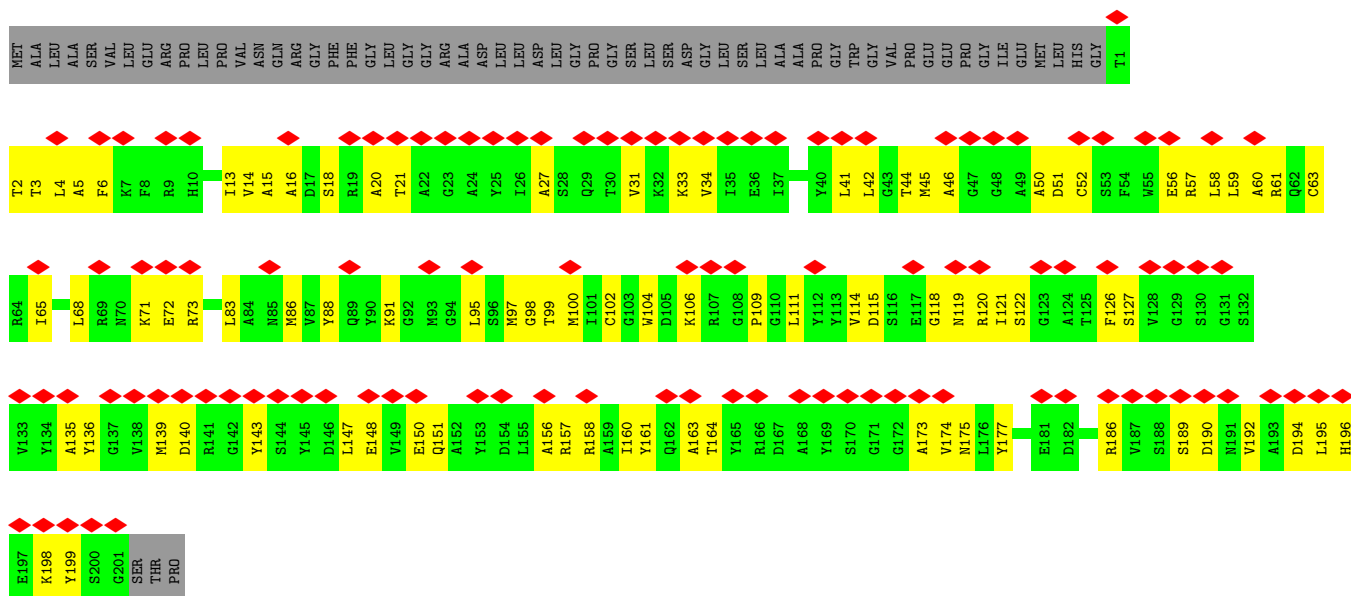
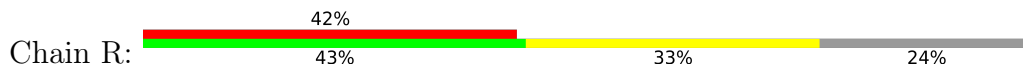


• Molecule 17: Proteasome subunit beta type-2

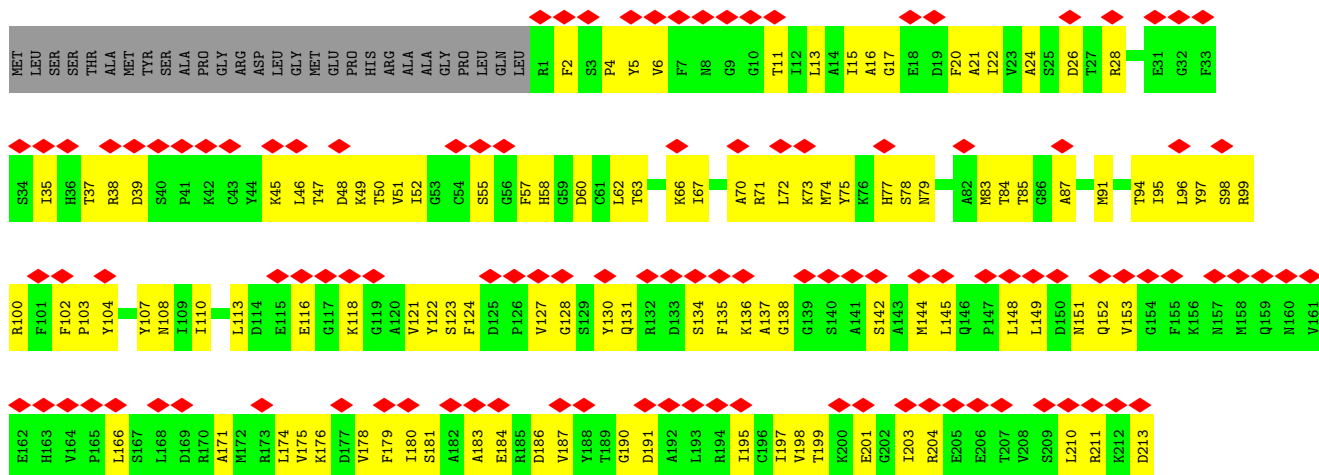
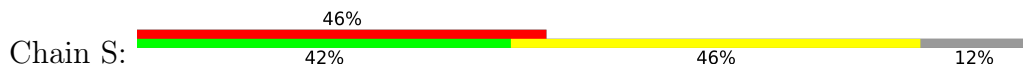




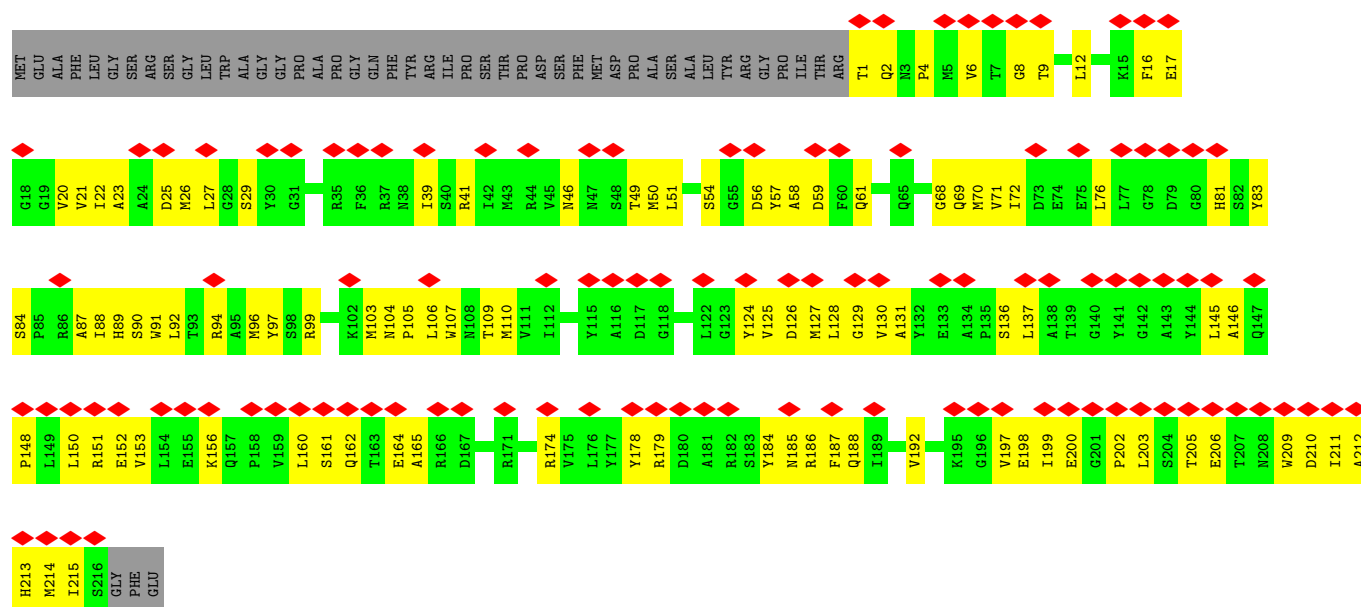
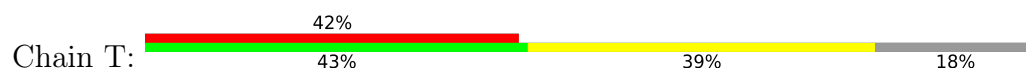
• Molecule 18: Proteasome subunit beta type-5



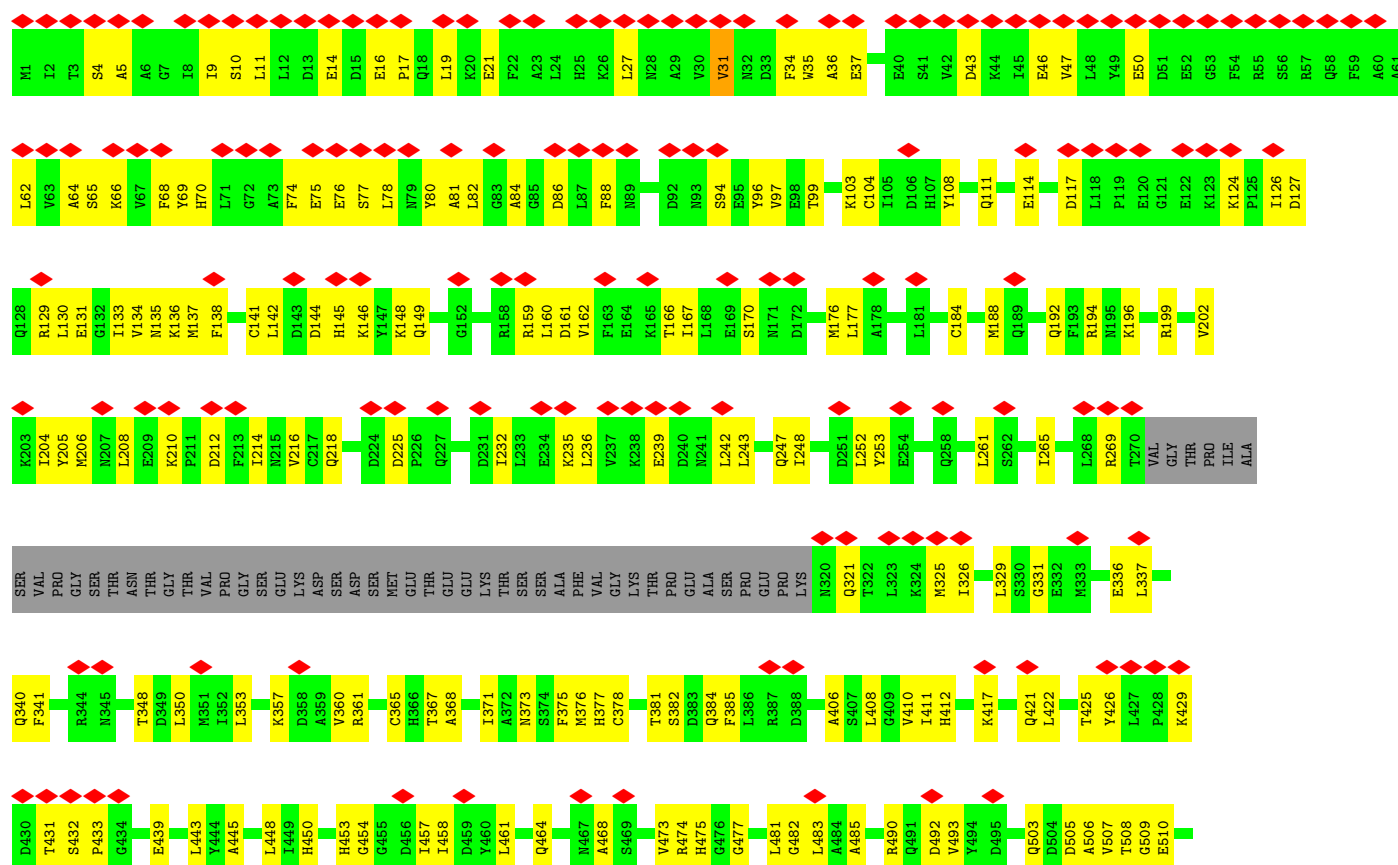
• Molecule 19: Proteasome subunit beta type-1

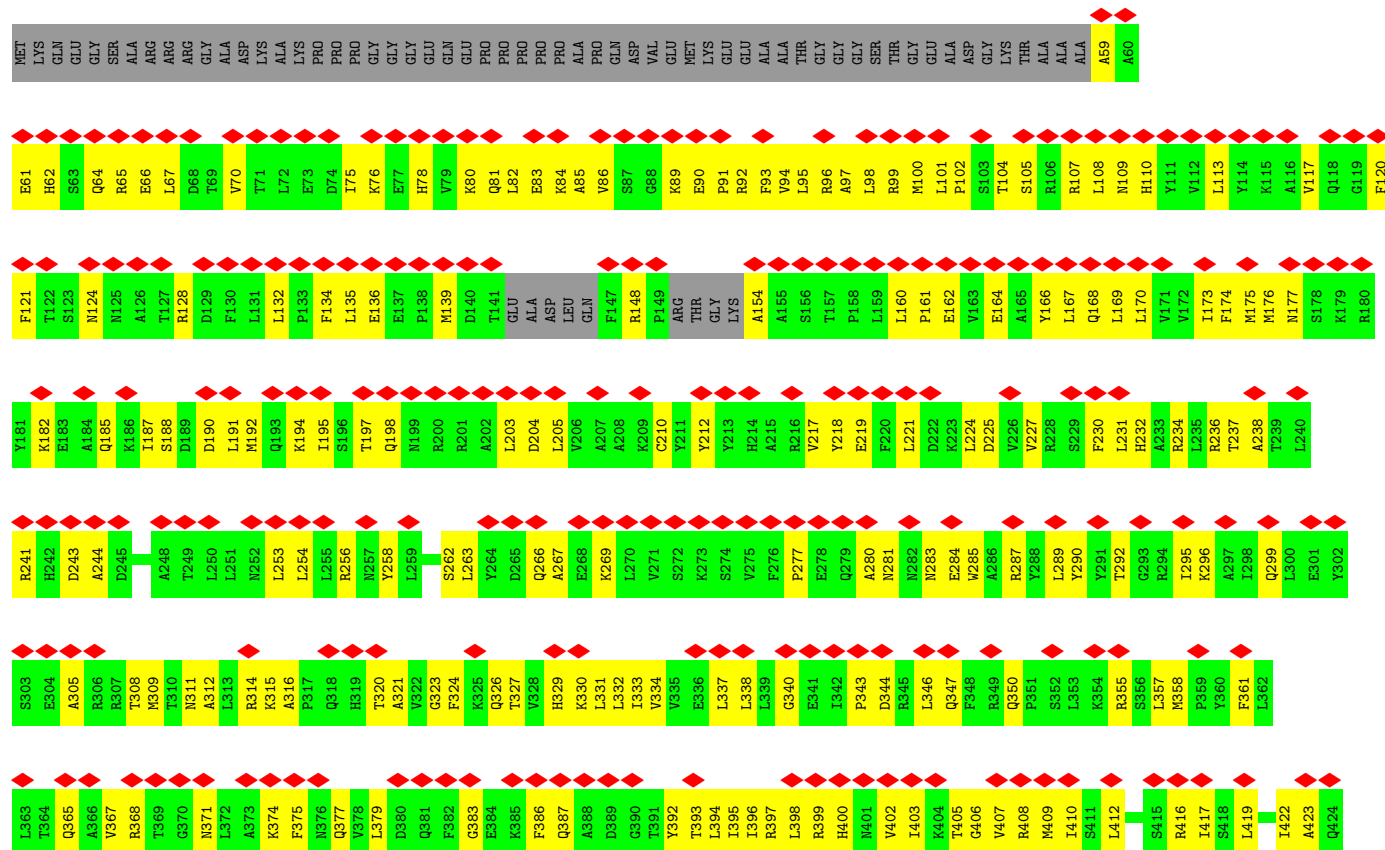


• Molecule 20: Proteasome subunit beta type-4

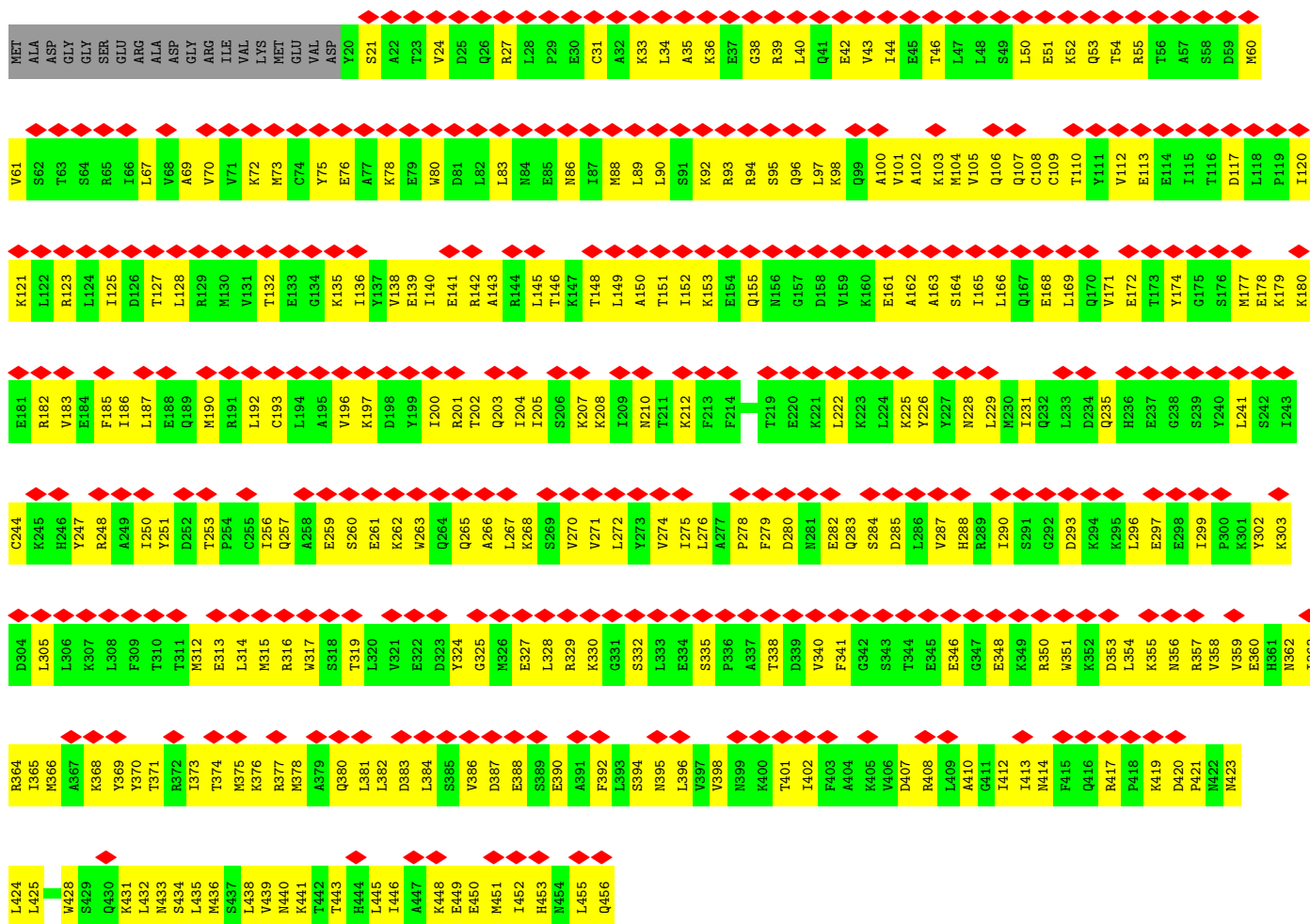
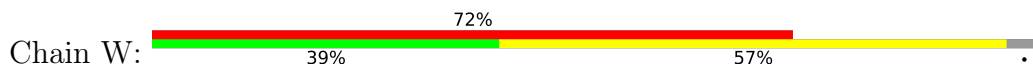


• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

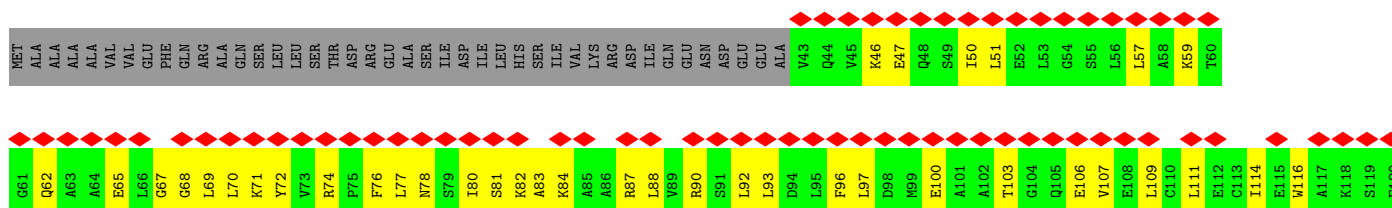


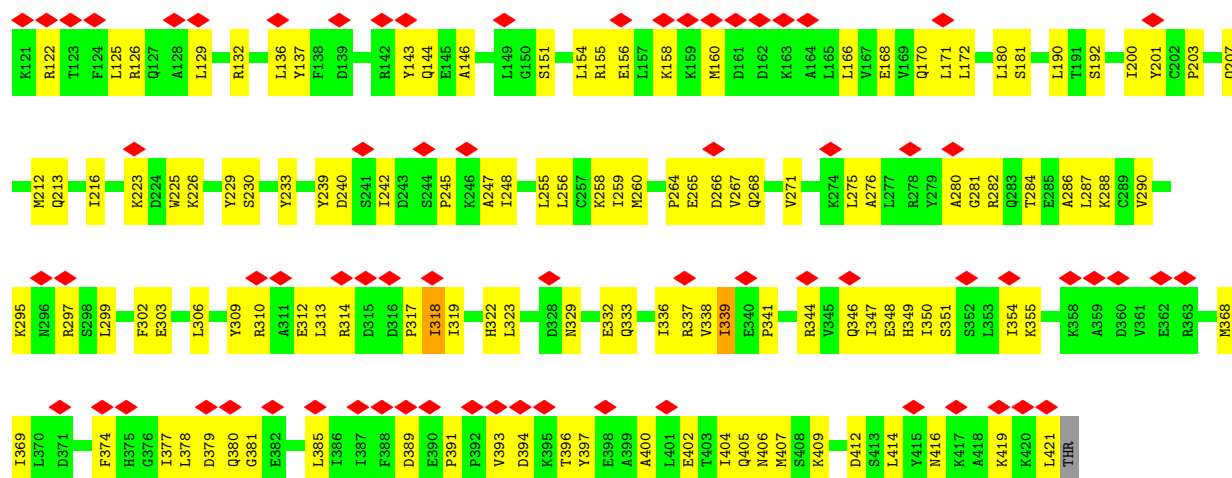


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

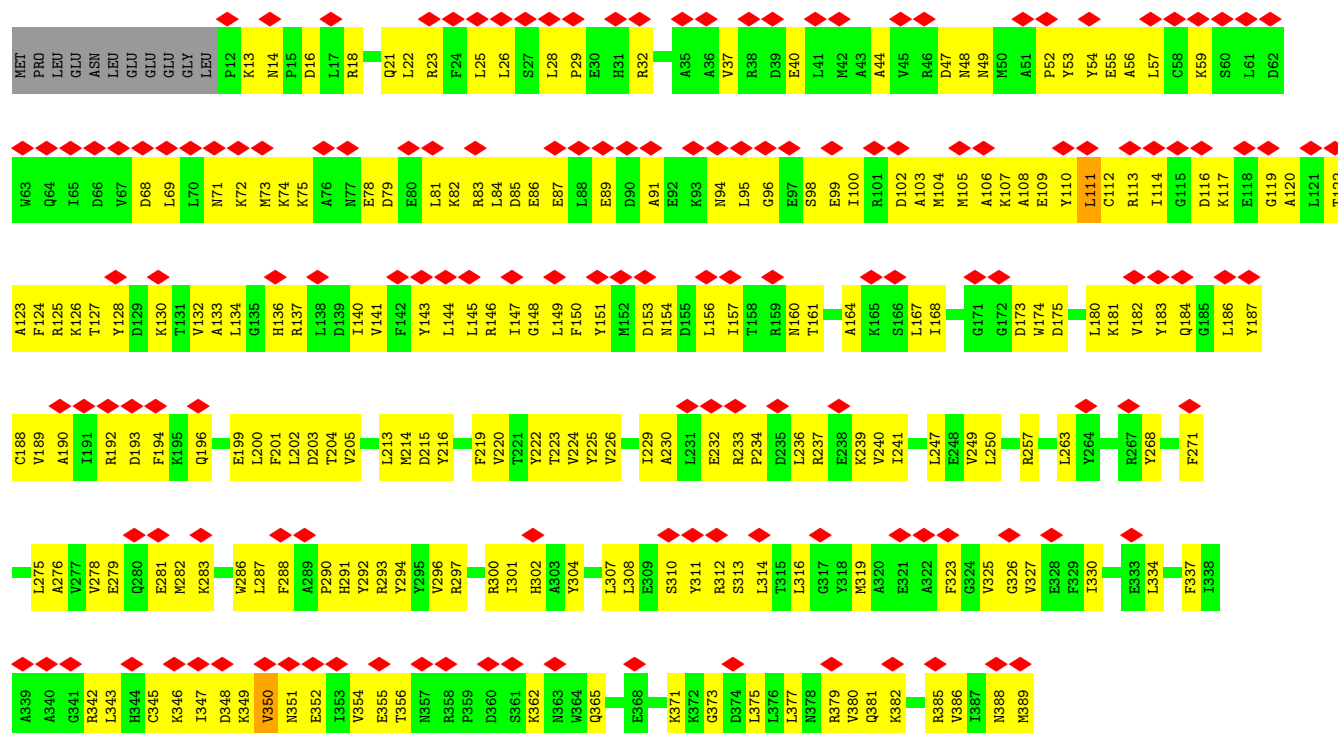


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

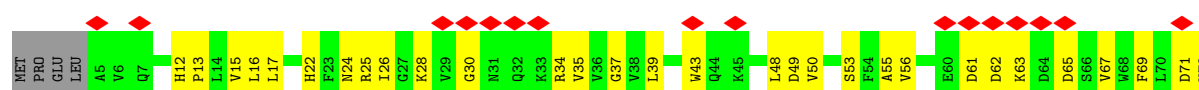




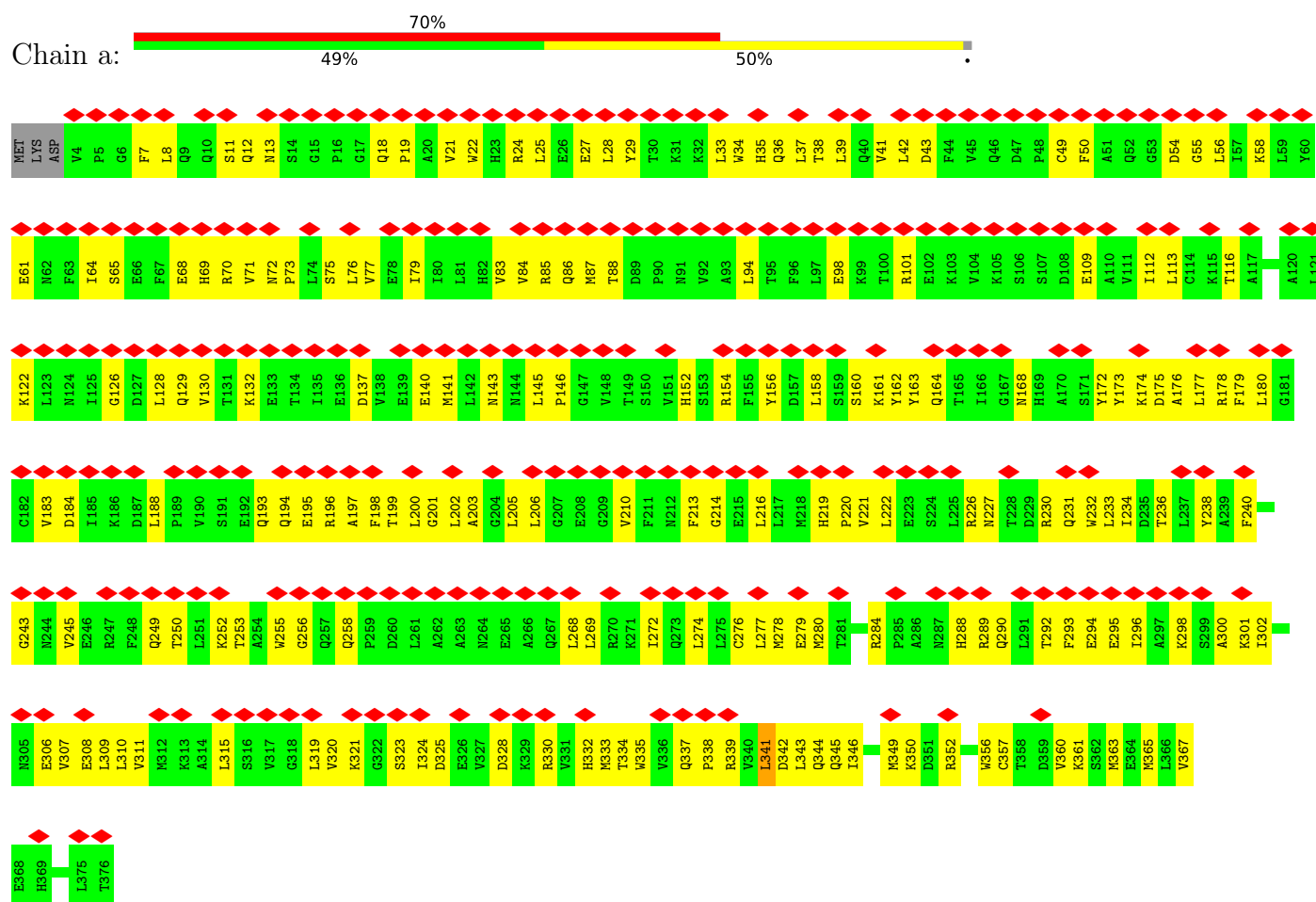
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



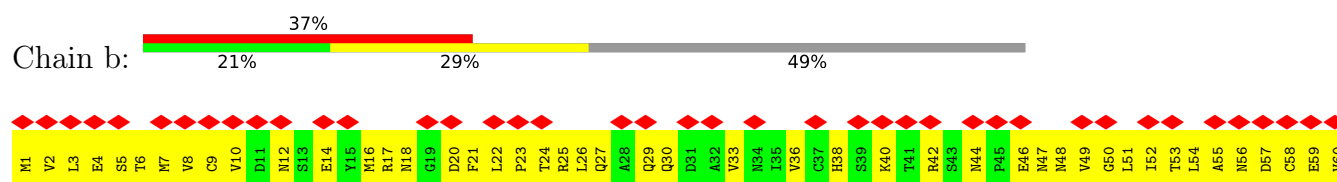
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

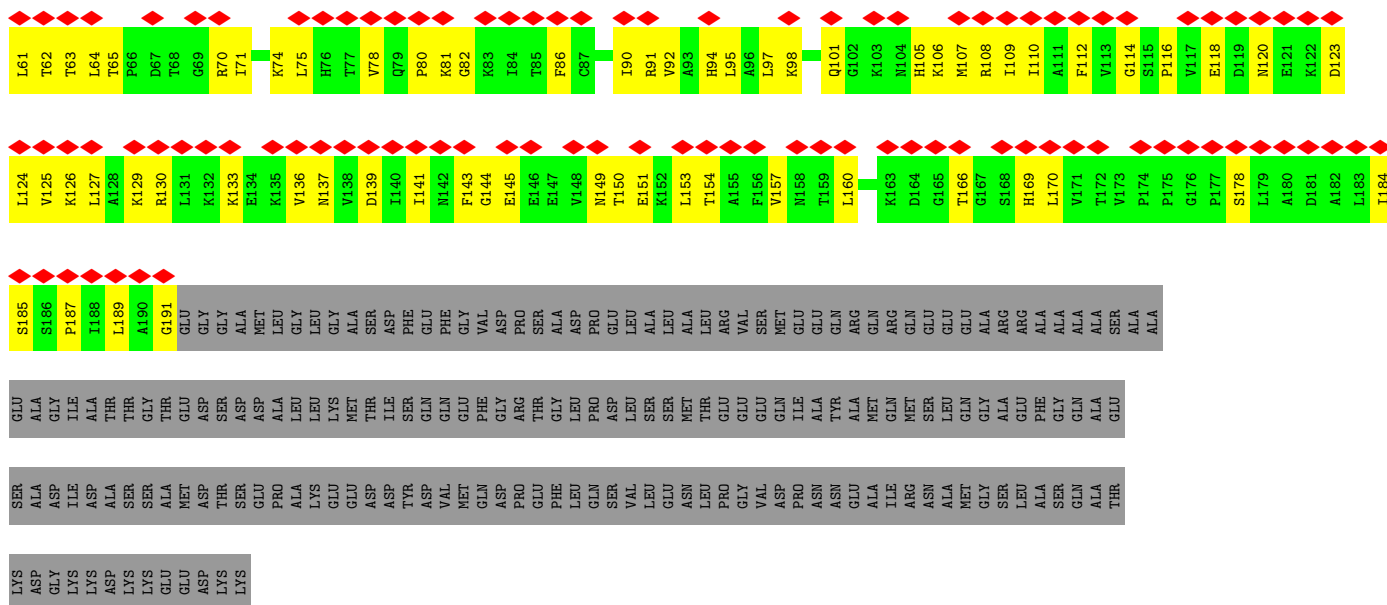


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

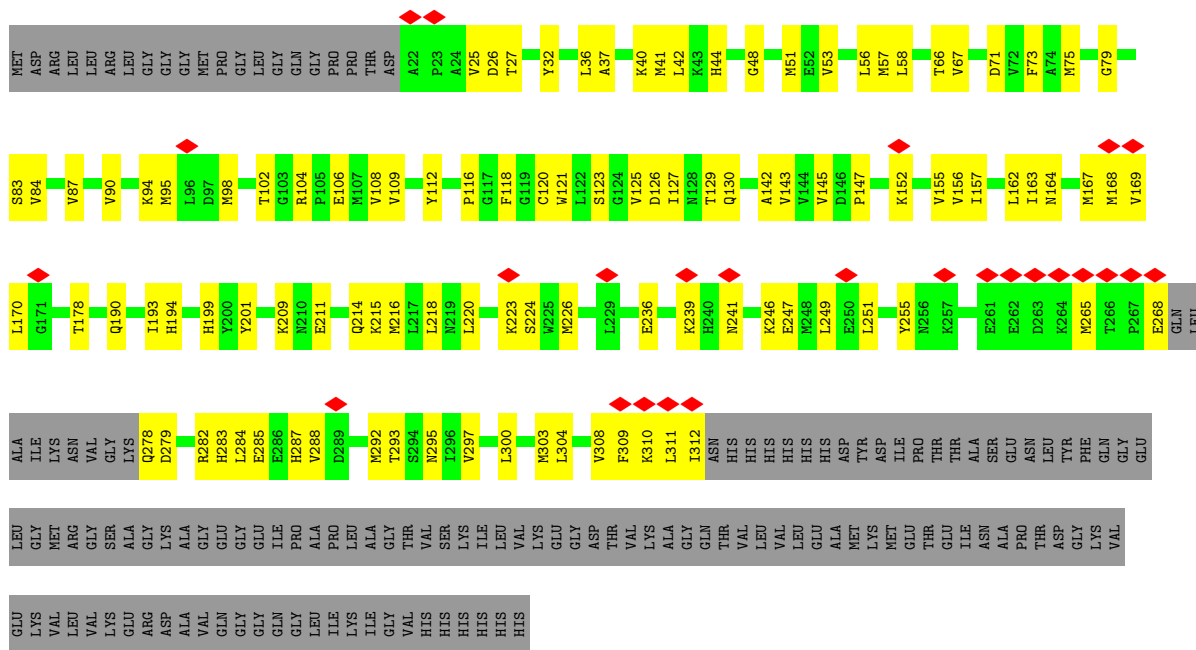


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4



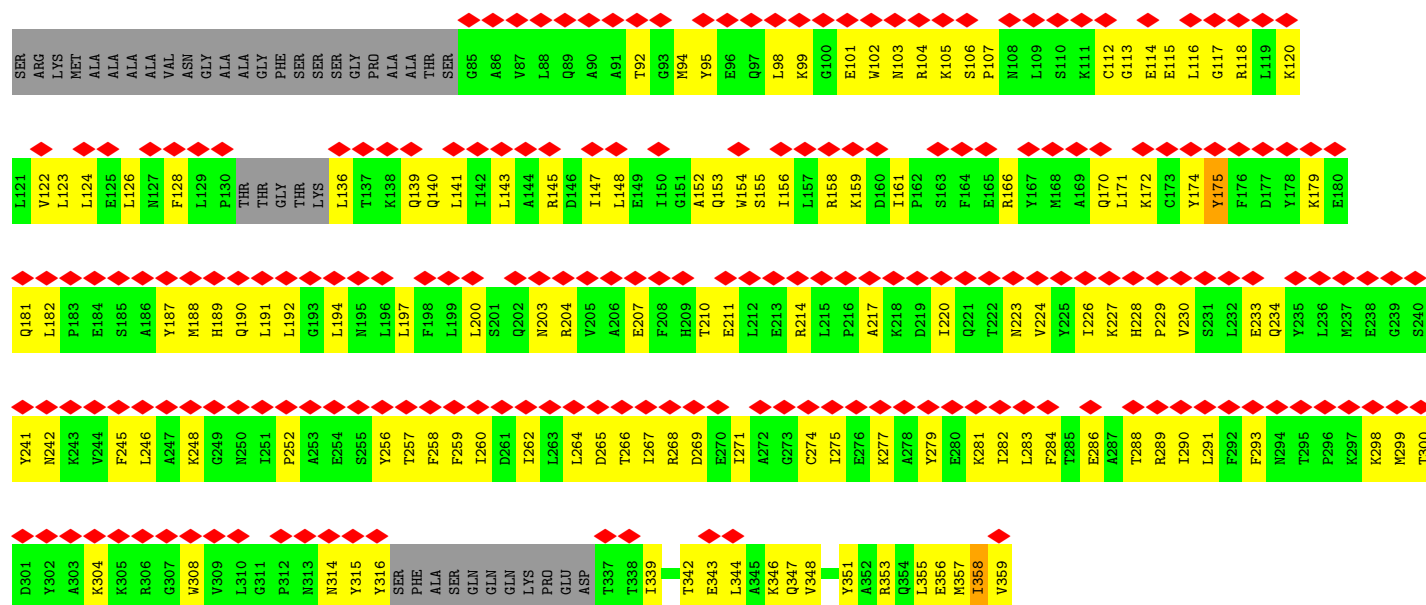


- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8





• Molecule 31: 26S proteasome complex subunit SEM1



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31177	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.937	Depositor
Minimum map value	-0.448	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	356.32, 356.32, 356.32	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/3121	0.51	0/4212
2	B	0.25	0/3170	0.44	1/4278 (0.0%)
3	C	0.26	0/3094	0.38	0/4158
4	D	0.27	0/3090	0.38	0/4168
5	E	0.24	0/2930	0.45	0/3944
6	F	0.23	0/2840	0.59	3/3828 (0.1%)
7	G	0.17	0/1901	0.40	0/2572
8	H	0.16	0/1840	0.33	0/2495
9	I	0.18	0/1963	0.39	0/2650
10	J	0.18	0/1886	0.43	0/2551
11	K	0.21	0/1845	0.40	0/2490
12	L	0.18	0/1911	0.43	0/2584
13	M	0.17	0/1925	0.40	0/2592
14	N	0.17	0/1487	0.44	0/2013
15	O	0.16	0/1672	0.43	0/2267
16	P	0.18	0/1616	0.45	0/2180
17	Q	0.18	0/1621	0.47	0/2194
18	R	0.18	0/1590	0.44	0/2147
19	S	0.17	0/1671	0.41	0/2252
20	T	0.19	0/1716	0.51	0/2323
21	U	0.16	0/6574	0.39	1/8899 (0.0%)
22	V	0.18	0/3595	0.44	0/4851
23	W	0.20	0/3611	0.56	0/4855
24	X	0.16	0/3045	0.43	0/4105
25	Y	0.20	0/3173	0.53	0/4273
26	Z	0.19	0/2323	0.47	1/3147 (0.0%)
27	a	0.17	0/3053	0.49	0/4133
28	b	0.17	0/1478	0.49	0/2001
29	c	0.23	0/2262	0.44	0/3059
30	d	0.20	0/2090	0.53	1/2820 (0.0%)
31	e	0.19	0/437	0.55	0/595
32	f	0.21	0/6948	0.55	0/9387

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.20	0/81478	0.46	7/110023 (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
27	a	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	400	CYS	CA-CB-SG	11.37	140.54	114.40
21	U	31	VAL	N-CA-C	-7.79	106.31	113.71
6	F	400	CYS	N-CA-CB	-6.89	98.84	110.49
2	B	340	ALA	N-CA-C	-5.74	107.27	114.56
30	d	175	TYR	CA-CB-CG	5.26	123.36	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	a	341	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3074	0	3152	188	0
2	B	3124	0	3187	146	0
3	C	3053	0	3173	123	0
4	D	3040	0	3075	138	0
5	E	2887	0	2951	144	0
6	F	2803	0	2896	190	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1867	0	1867	90	0
8	H	1801	0	1773	81	0
9	I	1933	0	1923	98	0
10	J	1860	0	1846	106	0
11	K	1817	0	1804	79	0
12	L	1876	0	1856	80	0
13	M	1890	0	1880	92	0
14	N	1462	0	1428	80	0
15	O	1645	0	1648	79	0
16	P	1587	0	1598	101	0
17	Q	1588	0	1584	112	0
18	R	1559	0	1523	80	0
19	S	1641	0	1639	104	0
20	T	1683	0	1662	101	0
21	U	6459	0	6484	249	0
22	V	3527	0	3595	208	0
23	W	3564	0	3684	267	0
24	X	3001	0	3106	154	0
25	Y	3115	0	3120	244	0
26	Z	2281	0	2311	144	0
27	a	2995	0	3012	177	0
28	b	1458	0	1505	111	0
29	c	2220	0	2230	106	0
30	d	2048	0	2082	129	0
31	e	425	0	328	32	0
32	f	6836	0	6841	559	0
33	v	110	0	28	0	0
34	A	27	0	12	6	0
34	D	27	0	12	2	0
34	E	27	0	12	3	0
34	F	27	0	12	5	0
35	B	31	0	12	4	0
35	C	31	0	12	4	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
37	c	1	0	0	0	0
All	All	80403	0	80863	4158	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 26.

The worst 5 of 4158 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)
32:f:103:TYR:HB2	32:f:141:LYS:HB2	1.41	1.02
32:f:610:GLN:O	32:f:614:HIS:HB2	1.57	1.01
12:L:173:GLU:HA	12:L:176:MET:HE1	1.48	0.95
25:Y:23:ARG:HH12	25:Y:59:LYS:HB3	1.31	0.94
2:B:208:PRO:HD2	32:f:722:SER:HB2	1.47	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/433 (89%)	348 (90%)	37 (10%)	2 (0%)	24	55
2	B	393/440 (89%)	350 (89%)	38 (10%)	5 (1%)	9	36
3	C	384/406 (95%)	355 (92%)	29 (8%)	0	100	100
4	D	378/418 (90%)	358 (95%)	19 (5%)	1 (0%)	36	64
5	E	360/389 (92%)	342 (95%)	18 (5%)	0	100	100
6	F	353/439 (80%)	311 (88%)	38 (11%)	4 (1%)	11	39
7	G	238/246 (97%)	228 (96%)	10 (4%)	0	100	100
8	H	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
9	I	246/261 (94%)	230 (94%)	16 (6%)	0	100	100
10	J	237/248 (96%)	221 (93%)	16 (7%)	0	100	100
11	K	236/241 (98%)	233 (99%)	3 (1%)	0	100	100
12	L	238/263 (90%)	226 (95%)	12 (5%)	0	100	100
13	M	240/255 (94%)	234 (98%)	6 (2%)	0	100	100
14	N	193/239 (81%)	188 (97%)	5 (3%)	0	100	100
15	O	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
16	P	202/205 (98%)	193 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
18	R	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
20	T	214/264 (81%)	203 (95%)	11 (5%)	0	100	100
21	U	823/953 (86%)	796 (97%)	27 (3%)	0	100	100
22	V	426/534 (80%)	408 (96%)	18 (4%)	0	100	100
23	W	433/456 (95%)	401 (93%)	32 (7%)	0	100	100
24	X	377/422 (89%)	363 (96%)	12 (3%)	2 (0%)	24	55
25	Y	376/389 (97%)	322 (86%)	52 (14%)	2 (0%)	24	55
26	Z	283/324 (87%)	245 (87%)	38 (13%)	0	100	100
27	a	371/376 (99%)	340 (92%)	30 (8%)	1 (0%)	36	64
28	b	189/377 (50%)	164 (87%)	25 (13%)	0	100	100
29	c	278/424 (66%)	260 (94%)	18 (6%)	0	100	100
30	d	244/350 (70%)	221 (91%)	22 (9%)	1 (0%)	30	59
31	e	48/70 (69%)	39 (81%)	9 (19%)	0	100	100
32	f	880/908 (97%)	726 (82%)	154 (18%)	0	100	100
All	All	10082/11546 (87%)	9311 (92%)	753 (8%)	18 (0%)	44	71

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	86	LEU
24	X	318	ILE
24	X	339	ILE
30	d	358	ILE
2	B	156	VAL

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
34	ADP	D	501	36	28,29,29	1.38	4 (14%)	43,45,45	1.88	8 (18%)
35	ATP	C	501	36	32,33,33	0.73	1 (3%)	48,52,52	0.41	0
34	ADP	E	501	-	28,29,29	1.43	5 (17%)	43,45,45	1.73	9 (20%)
34	ADP	F	501	-	28,29,29	1.44	4 (14%)	43,45,45	1.81	9 (20%)
35	ATP	B	501	36	32,33,33	0.86	2 (6%)	48,52,52	0.39	0
34	ADP	A	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.90	8 (18%)

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	D	501	36	-	2/16/32/32	0/3/3/3
35	ATP	C	501	36	-	3/22/38/38	0/3/3/3
34	ADP	E	501	-	-	9/16/32/32	0/3/3/3
34	ADP	F	501	-	-	6/16/32/32	0/3/3/3
35	ATP	B	501	36	-	4/22/38/38	0/3/3/3
34	ADP	A	501	-	-	5/16/32/32	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	501	ADP	C5-C4	4.87	1.47	1.39
34	E	501	ADP	C5-C4	4.58	1.47	1.39
34	D	501	ADP	C5-C4	4.52	1.47	1.39
34	A	501	ADP	C5-C4	4.41	1.46	1.39
35	B	501	ATP	PA-O3A	-3.37	1.55	1.59

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	501	ADP	C5-C4-N3	-6.35	117.97	126.72
34	D	501	ADP	C5-C4-N3	-6.14	118.26	126.72
34	F	501	ADP	C5-C4-N3	-6.13	118.28	126.72
34	E	501	ADP	C5-C4-N3	-5.51	119.13	126.72
34	A	501	ADP	N3-C4-N9	5.02	135.70	127.17

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ADP	C5'-O5'-PA-O1A
34	A	501	ADP	C5'-O5'-PA-O2A
34	A	501	ADP	C5'-O5'-PA-O3A
34	D	501	ADP	C3'-C4'-C5'-O5'
34	E	501	ADP	C5'-O5'-PA-O1A

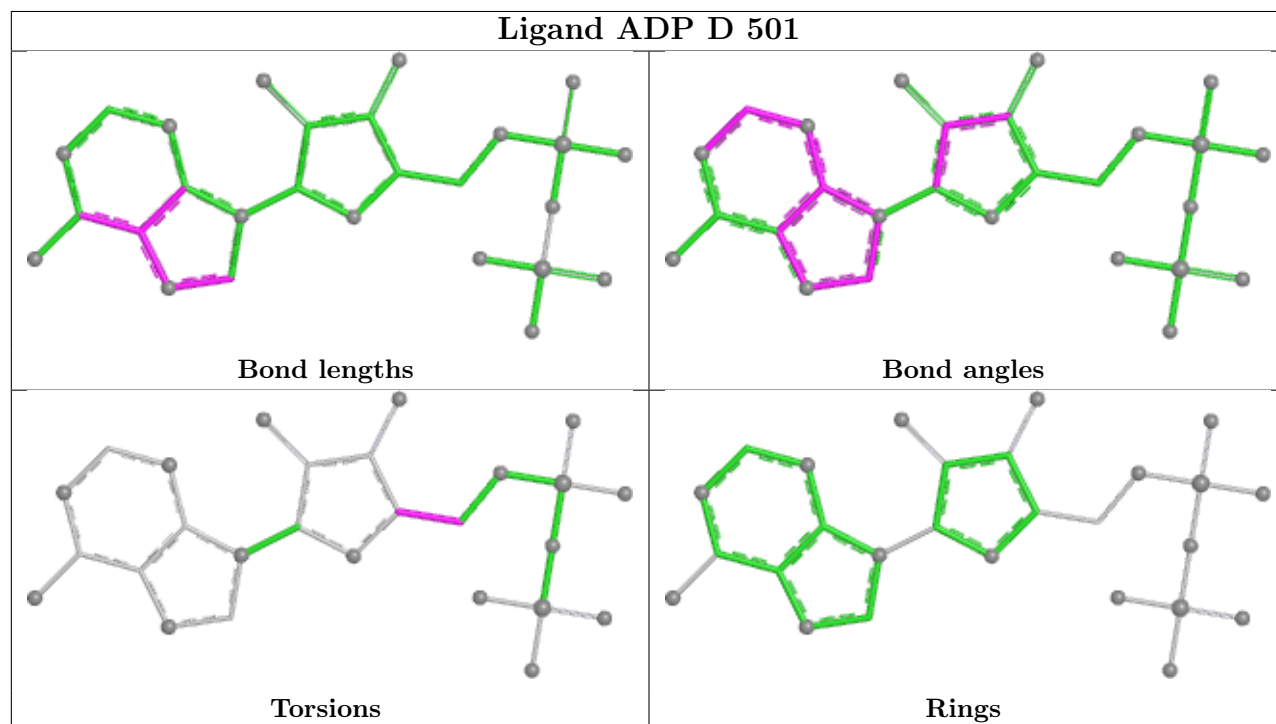
There are no ring outliers.

6 monomers are involved in 24 short contacts:

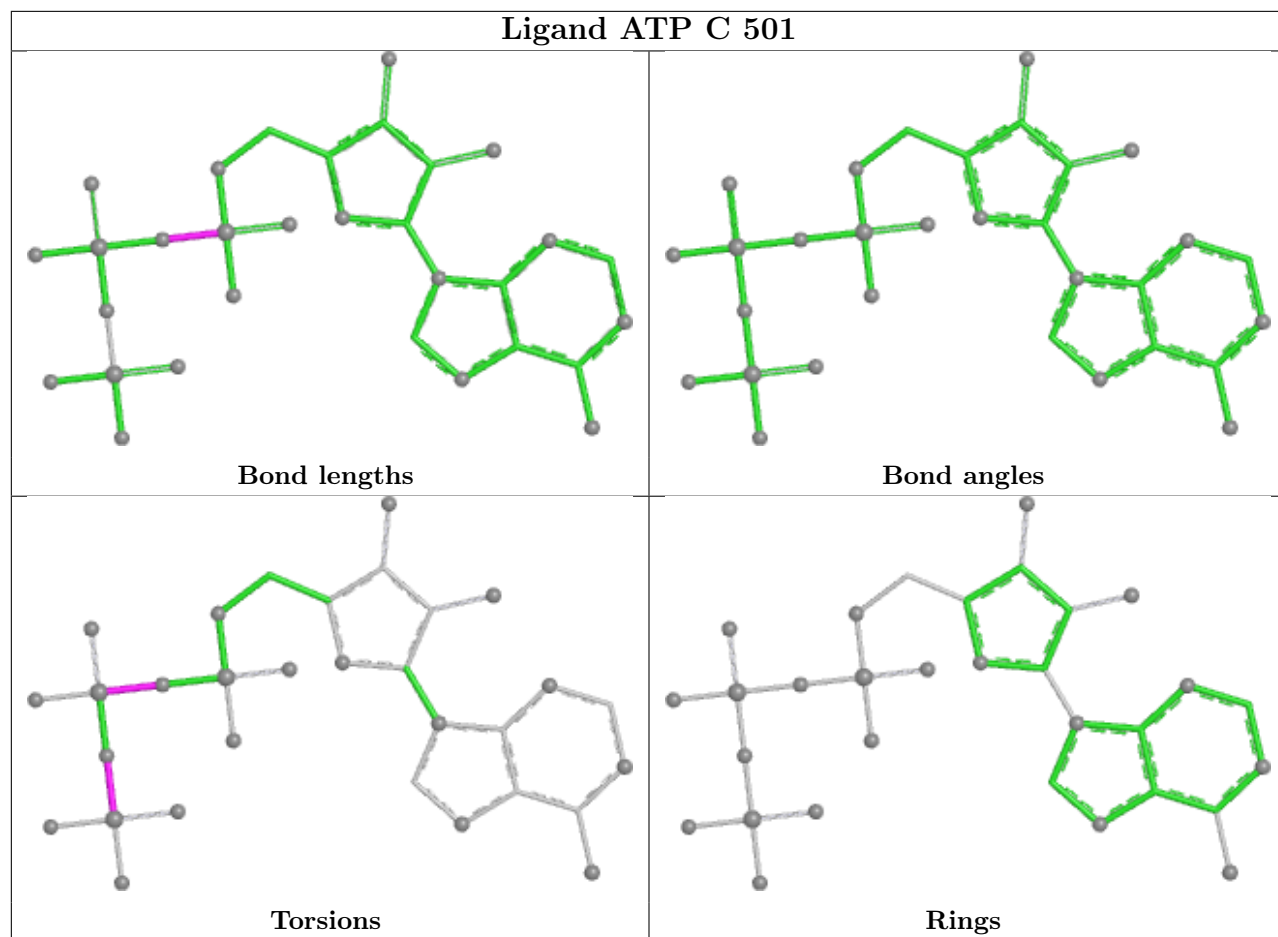
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	D	501	ADP	2	0
35	C	501	ATP	4	0
34	E	501	ADP	3	0
34	F	501	ADP	5	0
35	B	501	ATP	4	0
34	A	501	ADP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

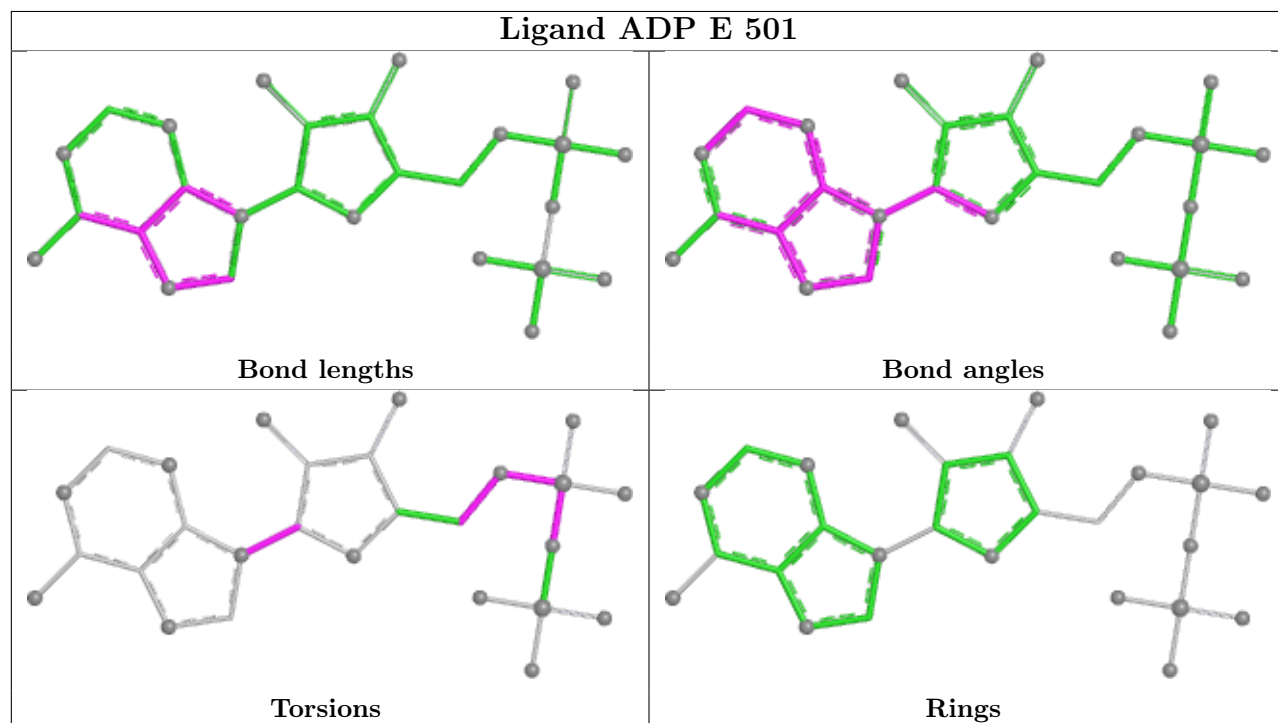
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

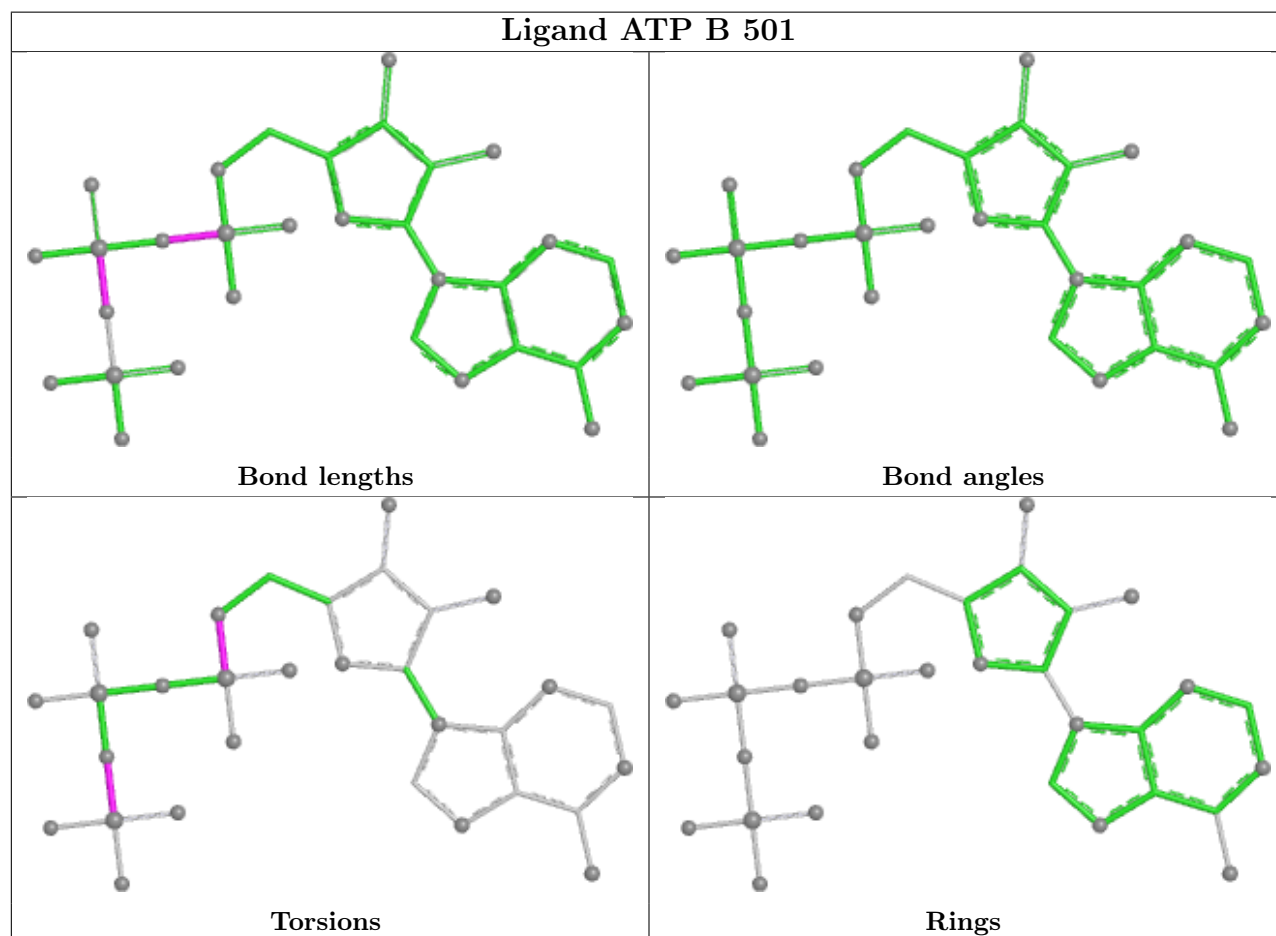
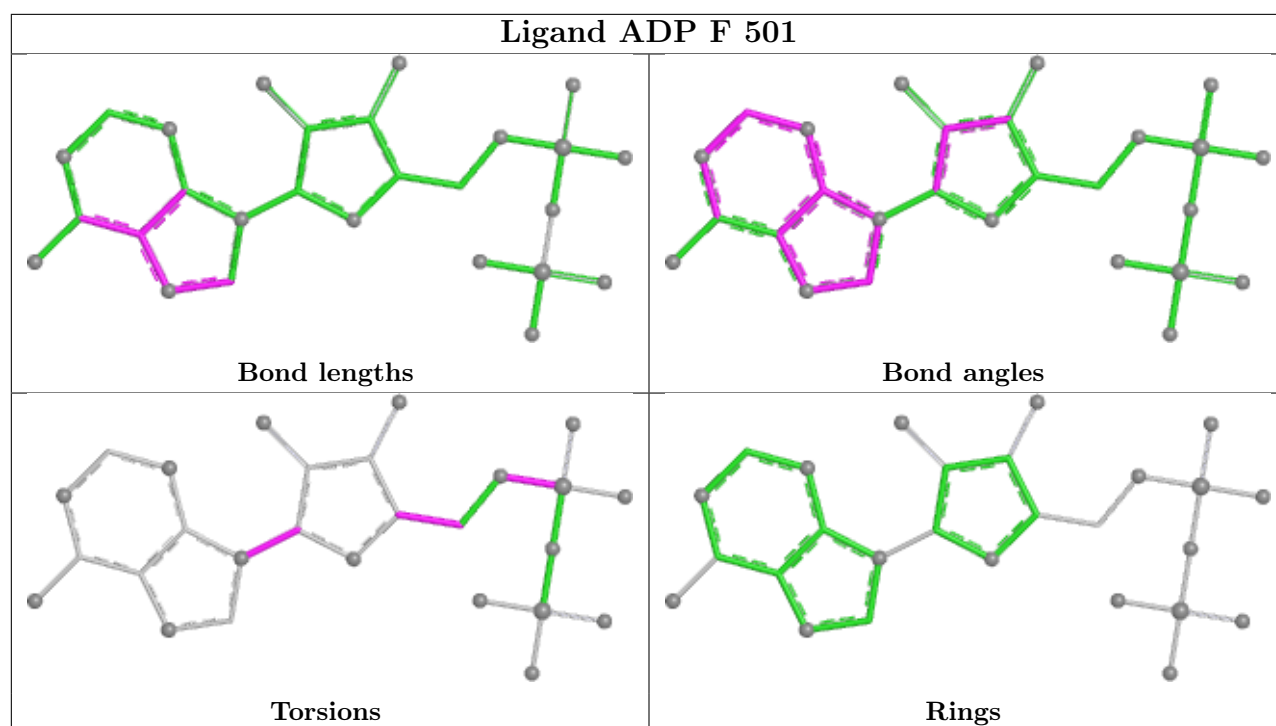


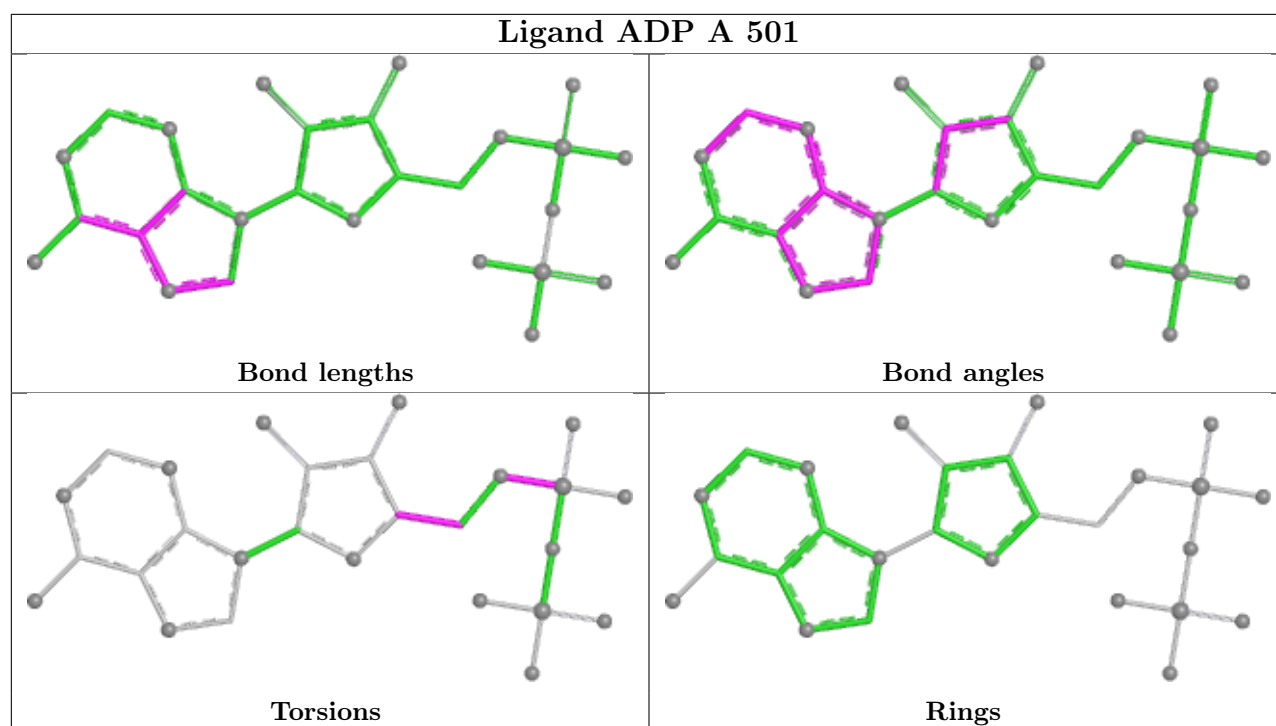
Ligand ATP C 501



Ligand ADP E 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	W	1
5	E	1
26	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	416:GLN	C	417:ARG	N	6.83
1	E	273:VAL	C	274:LYS	N	6.55
1	Z	289:GLU	C	290:GLY	N	3.21

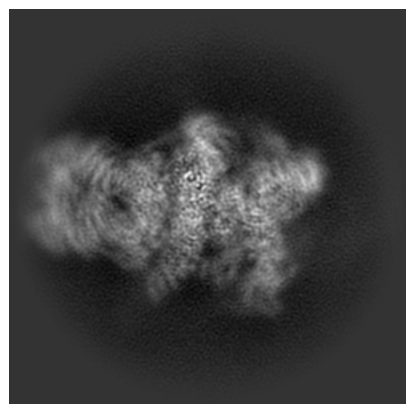
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47727. These allow visual inspection of the internal detail of the map and identification of artifacts.

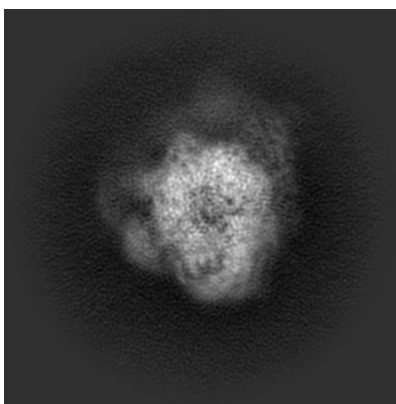
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

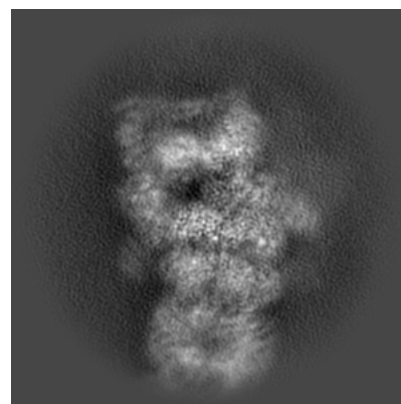
6.1.1 Primary map



X

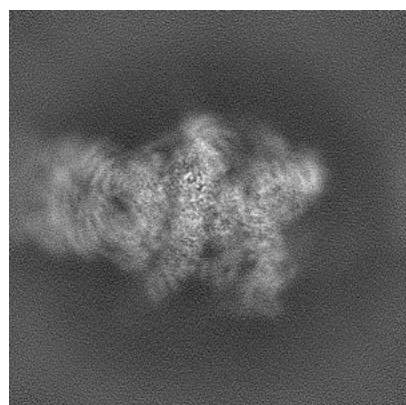


Y

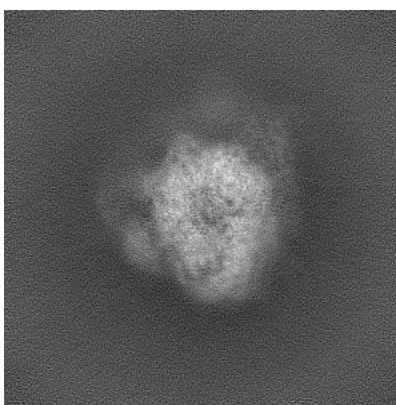


Z

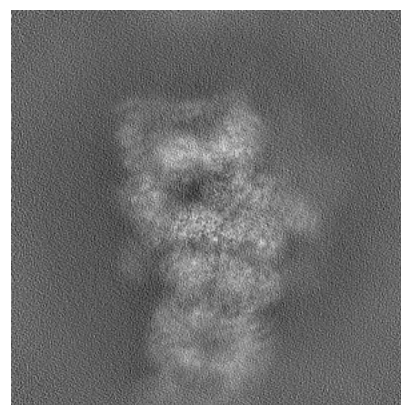
6.1.2 Raw map



X



Y

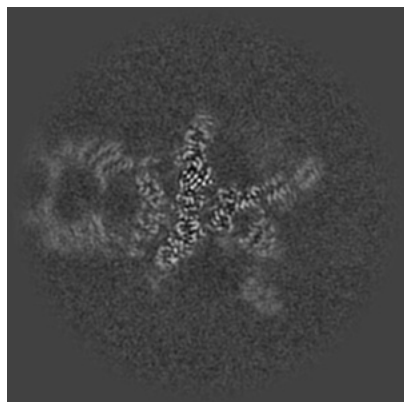


Z

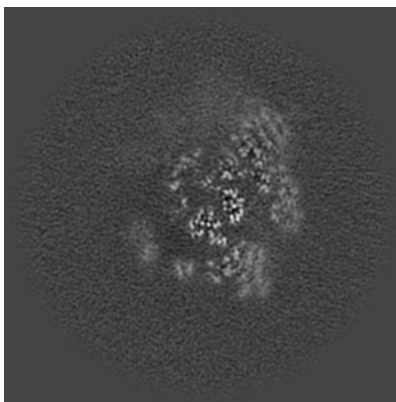
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

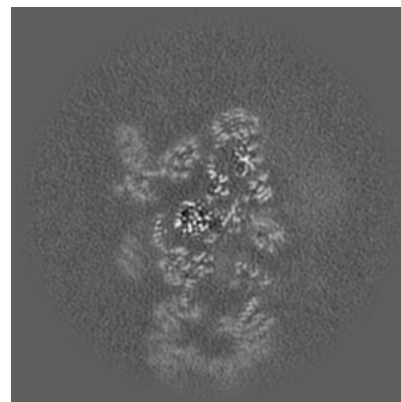
6.2.1 Primary map



X Index: 170

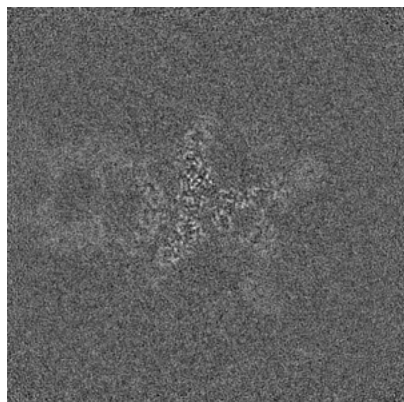


Y Index: 170

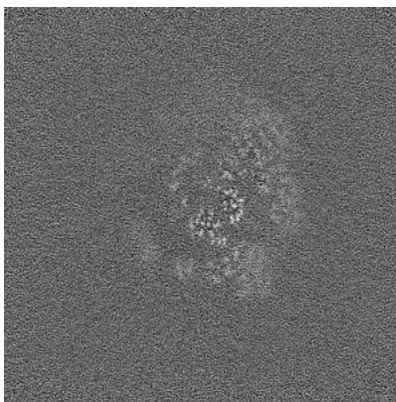


Z Index: 170

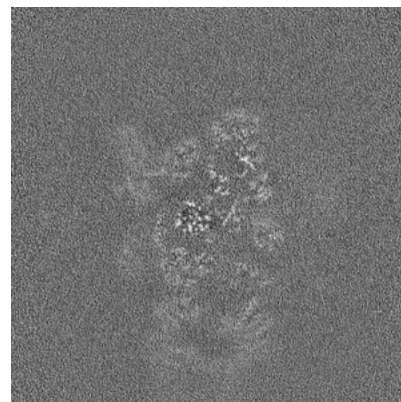
6.2.2 Raw map



X Index: 170



Y Index: 170

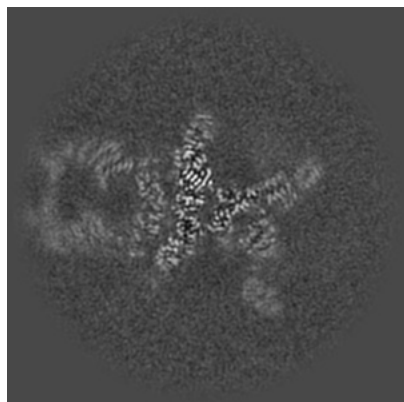


Z Index: 170

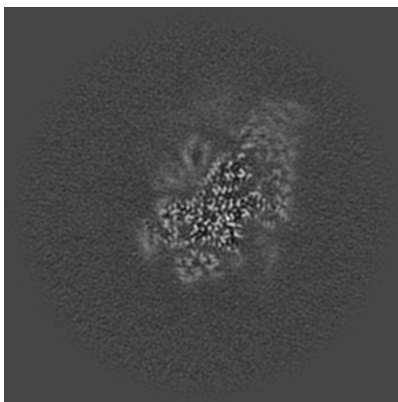
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

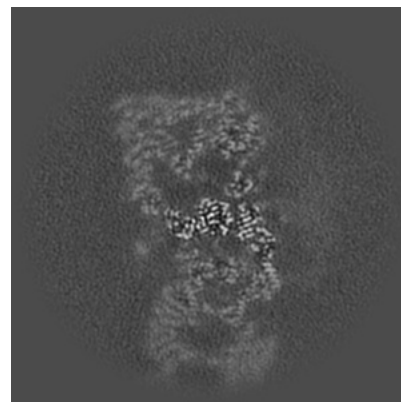
6.3.1 Primary map



X Index: 171

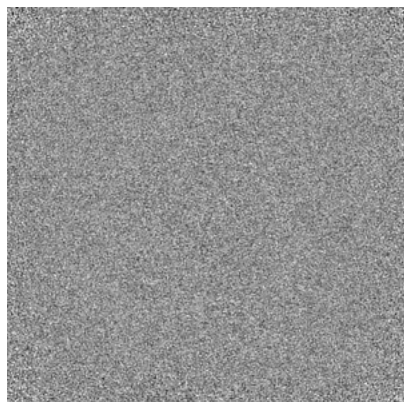


Y Index: 157

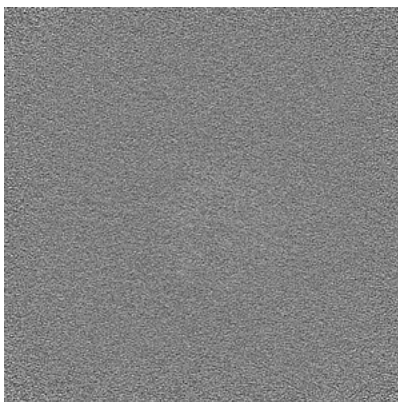


Z Index: 192

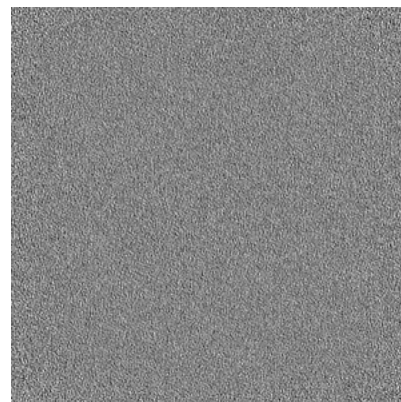
6.3.2 Raw map



X Index: 0



Y Index: 0

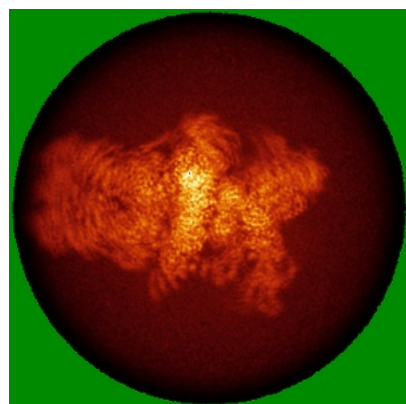


Z Index: 0

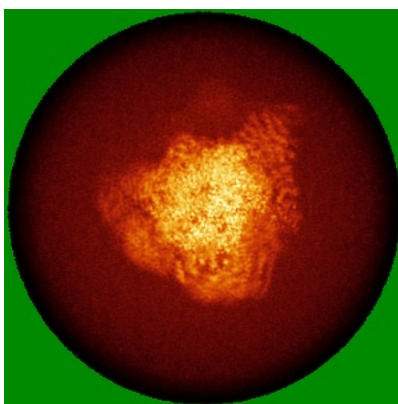
The images above show the largest variance slices of the map in three orthogonal directions.

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

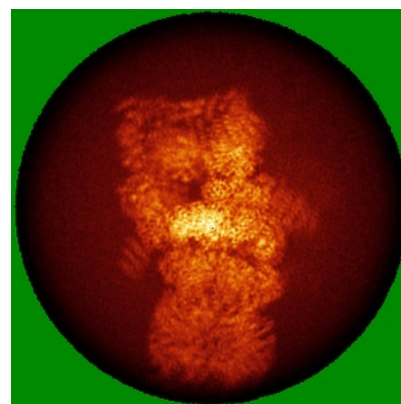
6.4.1 Primary map



X

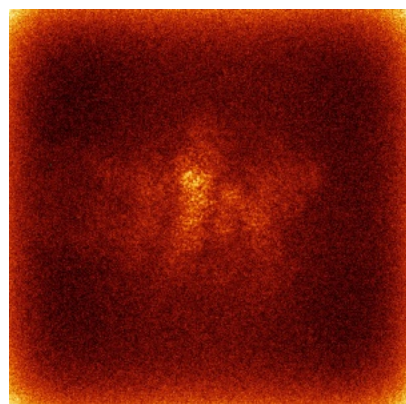


Y

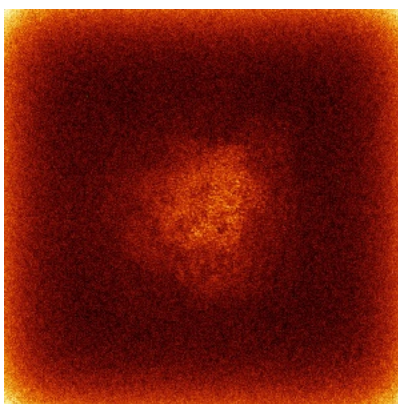


Z

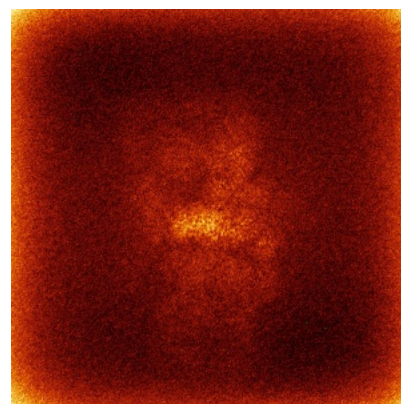
6.4.2 Raw map



X



Y

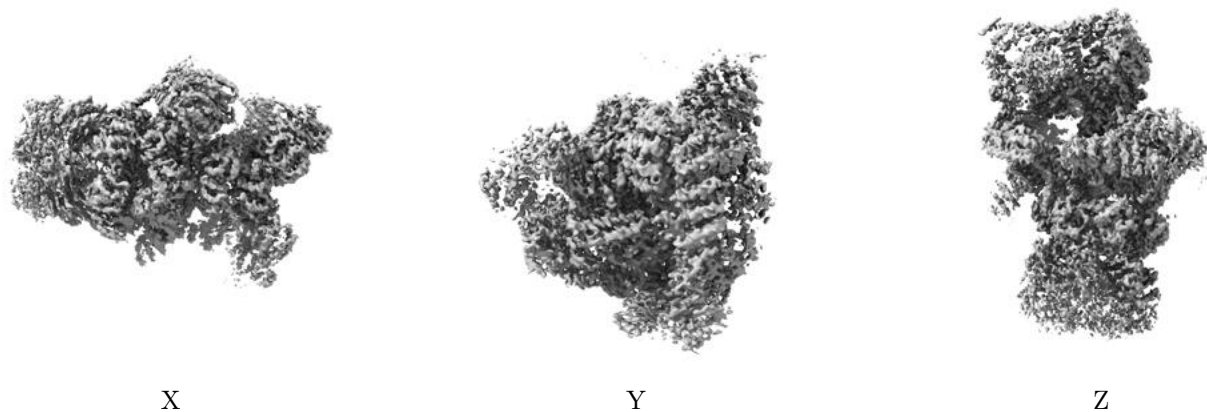


Z

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.

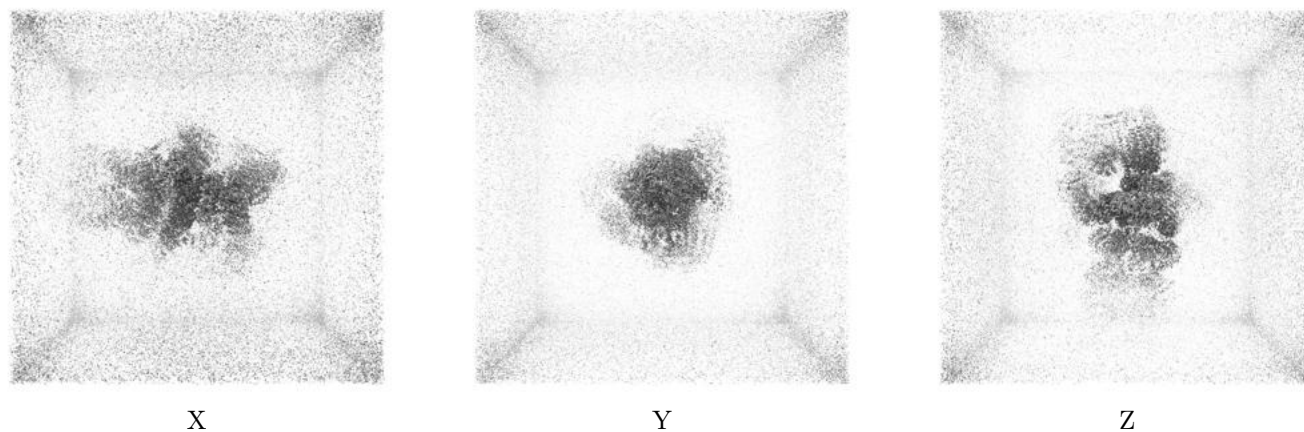
6.5 Orthogonal surface views [i](#)

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.

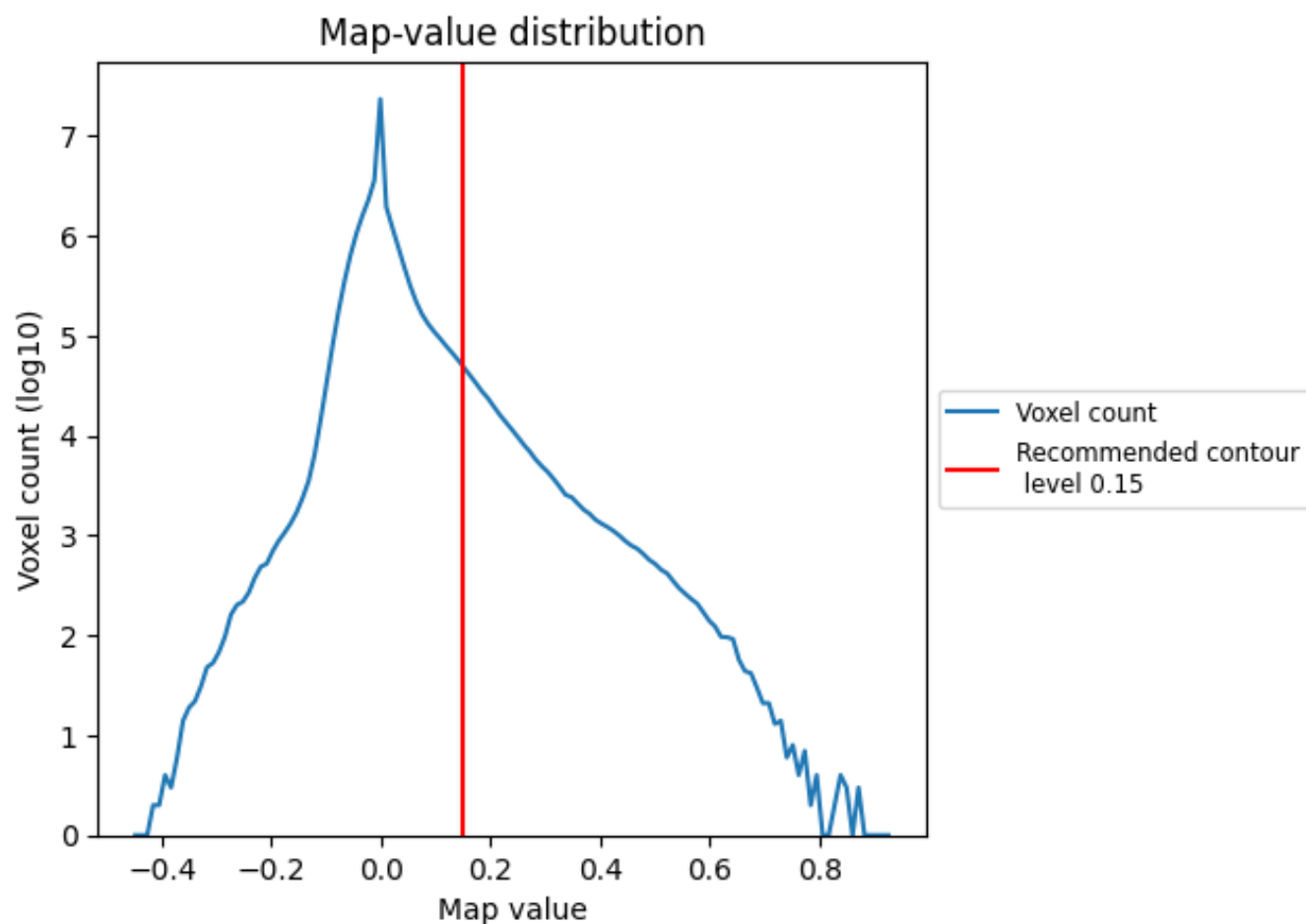
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

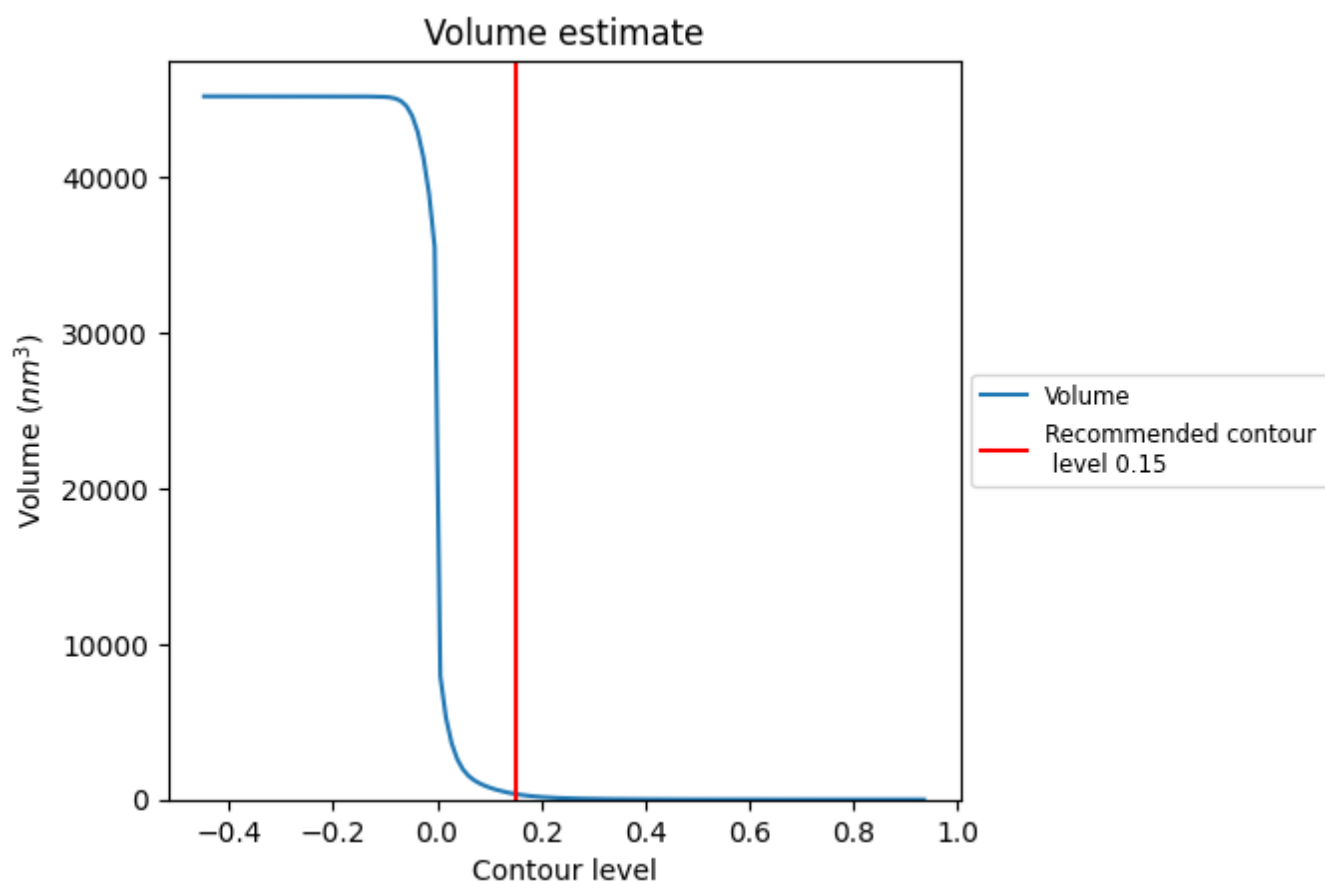
This section contains the results of statistical analysis of the map.

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.

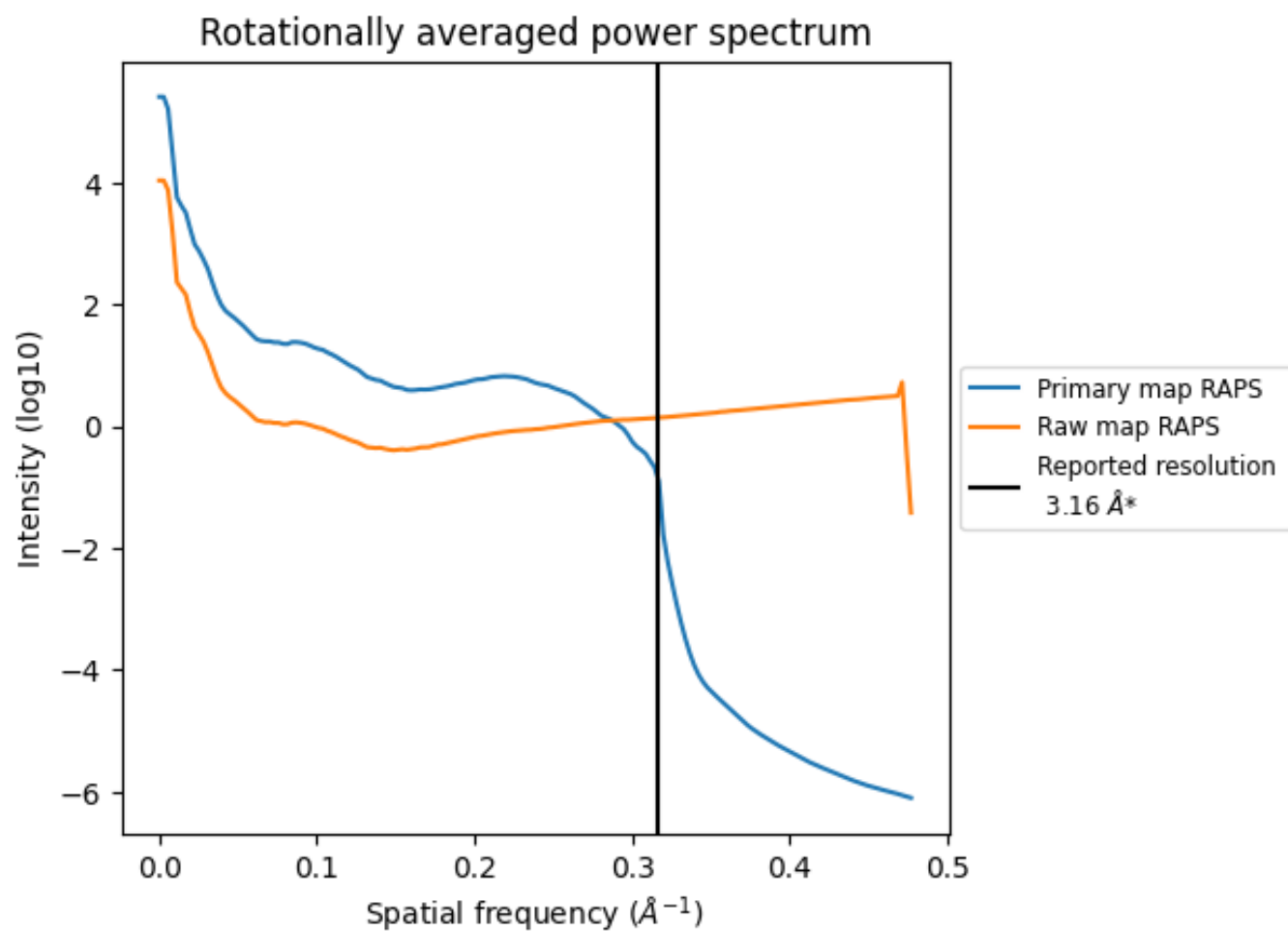
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 361 nm³; this corresponds to an approximate mass of 326 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 ⓘ

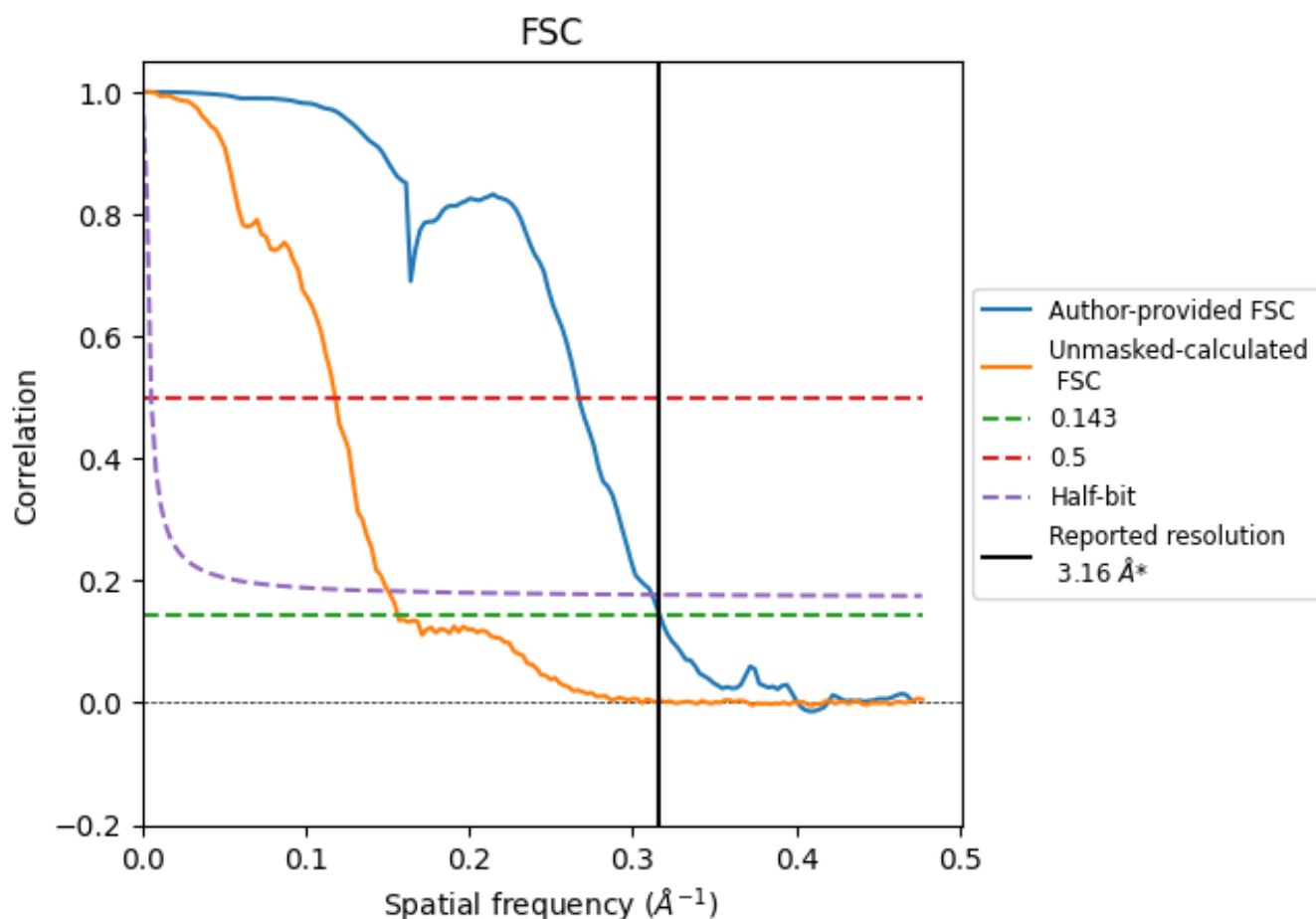


*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

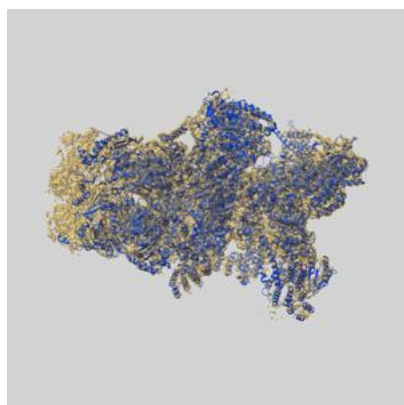
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.74	3.21
Unmasked-calculated*	6.40	8.47	6.64

*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 6.40 differs from the reported value 3.16 by more than 10 %

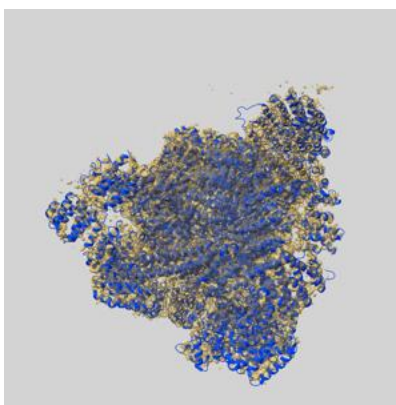
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47727 and PDB model 9E8Q. Per-residue inclusion information can be found in section [3](#) on page [15](#).

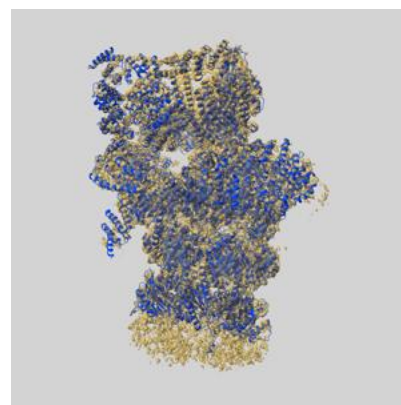
9.1 Map-model overlay [i](#)



X



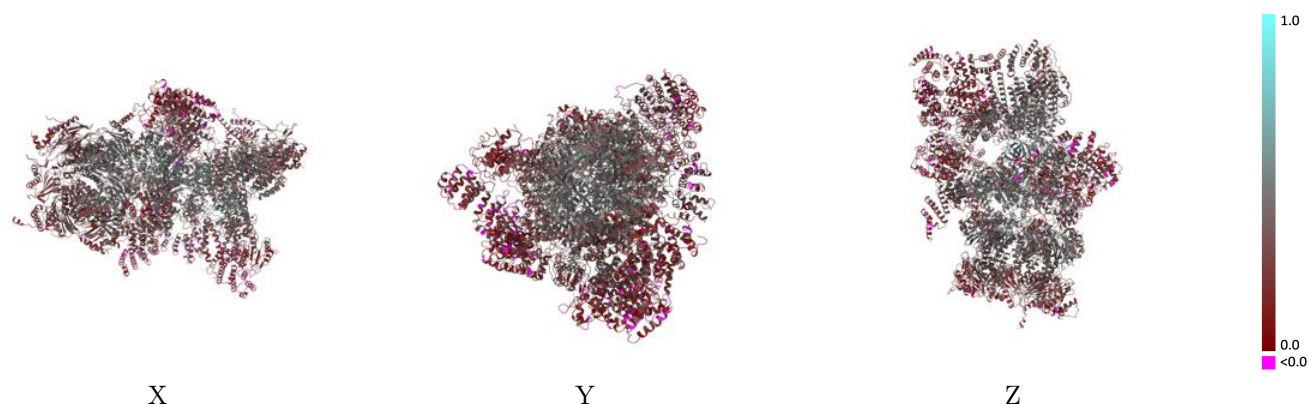
Y



Z

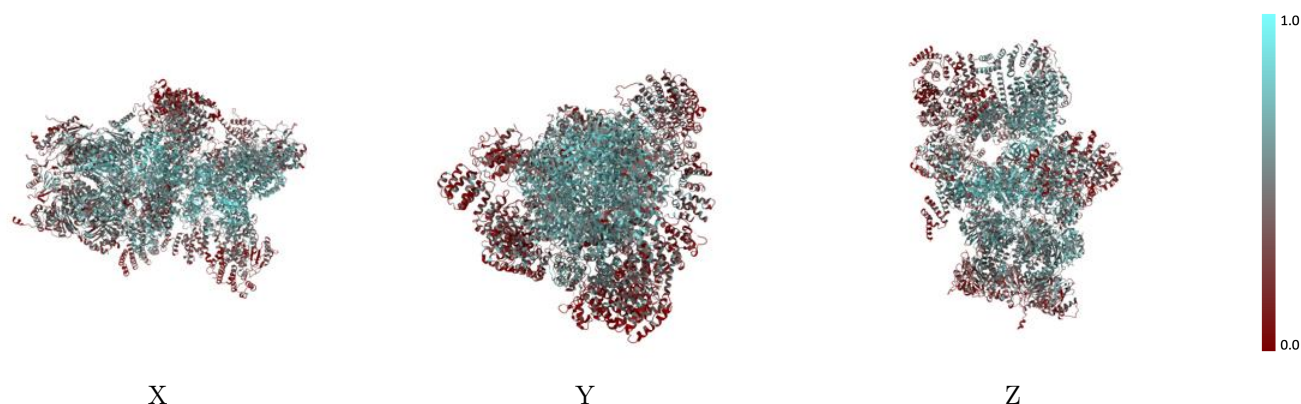
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



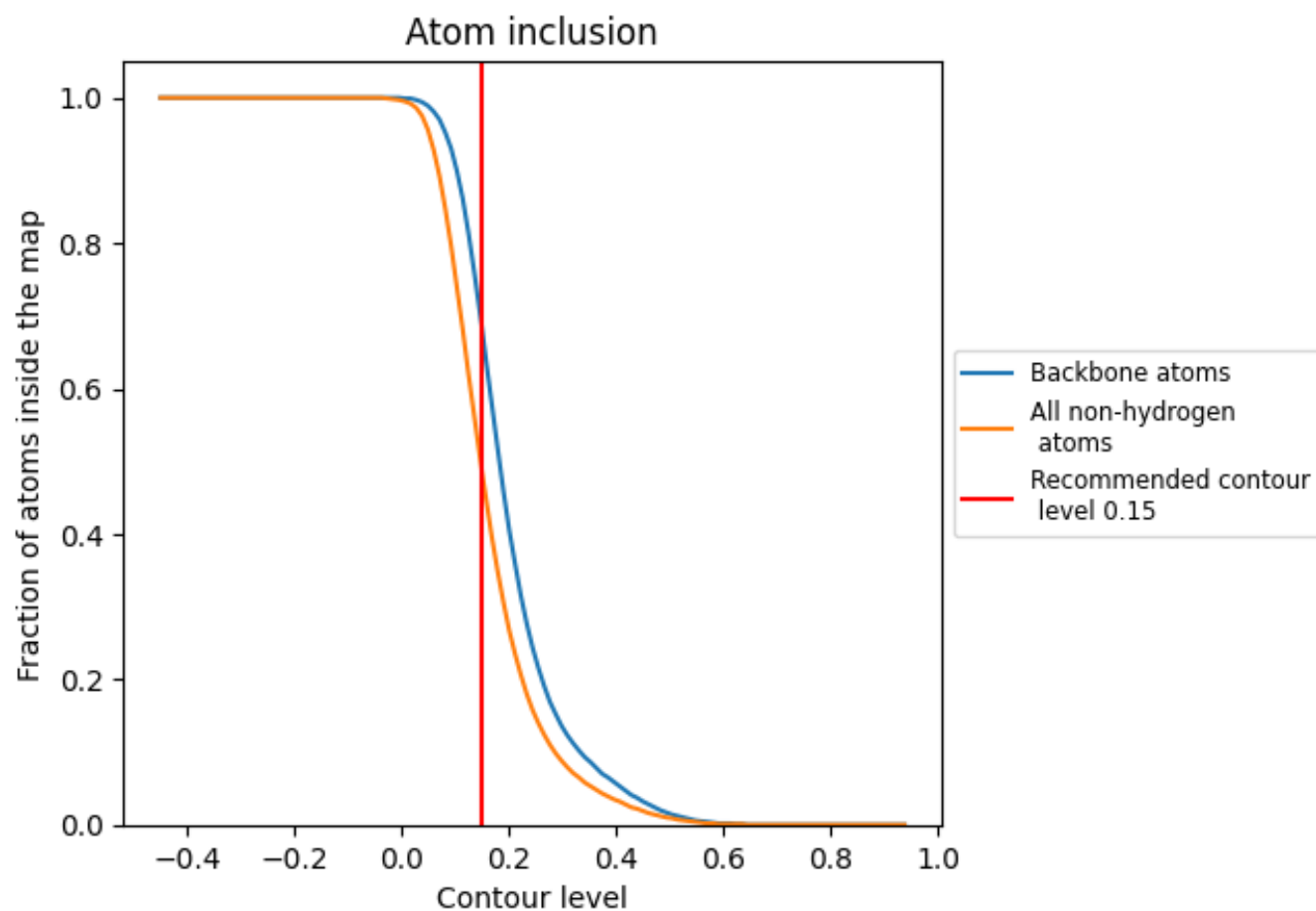
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 68% of all backbone atoms, 49% 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	 0.4860	 0.3390
A	 0.5620	 0.3610
B	 0.7080	 0.4670
C	 0.7880	 0.5070
D	 0.7750	 0.4990
E	 0.7130	 0.4390
F	 0.4380	 0.2920
G	 0.5550	 0.3890
H	 0.6230	 0.4390
I	 0.5860	 0.4180
J	 0.5920	 0.4130
K	 0.6300	 0.4330
L	 0.5630	 0.3820
M	 0.5040	 0.3530
N	 0.3940	 0.3150
O	 0.3270	 0.3130
P	 0.3400	 0.3070
Q	 0.3880	 0.3060
R	 0.4020	 0.2990
S	 0.3850	 0.2940
T	 0.3880	 0.2810
U	 0.5410	 0.3640
V	 0.3170	 0.2420
W	 0.2360	 0.1820
X	 0.4870	 0.3270
Y	 0.4640	 0.2690
Z	 0.5490	 0.3690
a	 0.2920	 0.2170
b	 0.2620	 0.2460
c	 0.7050	 0.4540
d	 0.1820	 0.1940
e	 0.2340	 0.2330
f	 0.3310	 0.2490
v	 0.6180	 0.5270

