



## wwPDB EM Validation Summary Report ⓘ

Apr 14, 2025 – 02:27 PM EDT

PDB ID : 8USC / pdb\_00008usc  
EMDB ID : EMD-42507  
Title : Nub1/Fat10-processing human 26S proteasome  
Authors : Arkinson, C.; Gee, C.L.; Martin, A.  
Deposited on : 2023-10-27  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

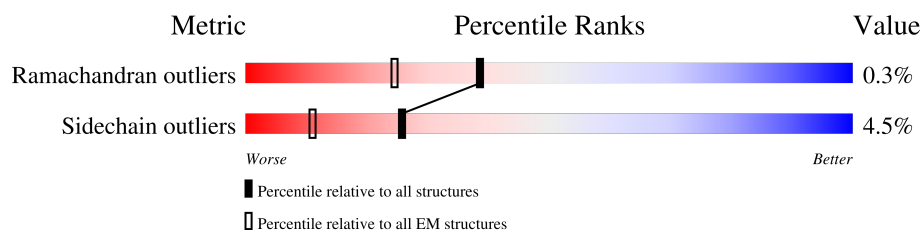
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

# 1 Overall quality at a glance

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

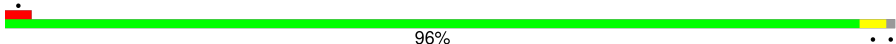








The reported resolution of this entry is 3.10 Å.

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




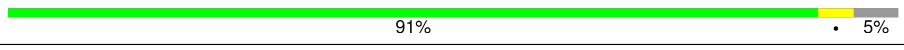


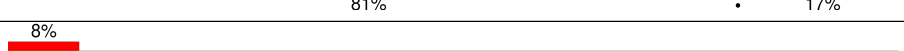
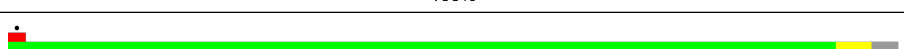
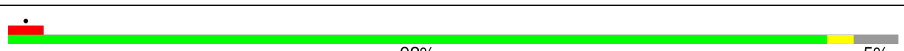

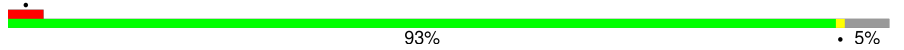


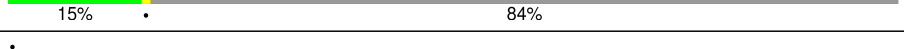
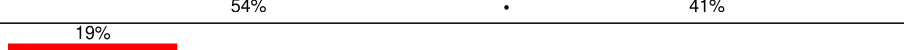






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	H	234	 96% ..
2	Y	389	 96% ..
3	f	908	 19% 90% . 7%
4	X	422	 6% 84% 5% 10%
5	U	953	 6% 83% 5% 12%
6	Z	324	 83% 5% 12%
7	a	376	 13% 93% 6% .
8	b	377	 7% 48% . 49%
9	A	433	 5% 92% . .

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Mol	Chain	Length	Quality of chain
10	B	440	
11	C	406	
12	D	418	
13	E	389	
14	F	439	
15	v	12	
16	G	246	
17	I	261	
18	J	248	
19	K	241	
20	L	263	
21	M	255	
22	O	277	
23	e	70	
24	d	350	
25	W	456	
26	g	601	
27	V	534	
28	c	424	

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 70061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	380	Total	C	N	O	S	0	0
			3127	1995	535	580	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	842	Total	C	N	O	S	0	0
			6512	4117	1105	1245	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	378	Total	C	N	O	S	0	0
			2994	1909	507	566	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	841	Total	C	N	O	S	0	0
			6559	4162	1115	1238	44		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	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
			1458	910	261	279	8		

- Molecule 9 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	415	Total	C	N	O	S	0	0
			3261	2053	573	617	18		

- Molecule 10 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	398	Total	C	N	O	S	0	0
			3122	1966	532	609	15		

- Molecule 11 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	386	Total	C	N	O	S	0	0
			3051	1919	547	567	18		

- Molecule 12 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 13 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	360	Total	C	N	O	S	0	0
			2859	1805	505	533	16		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	364	Total	C	N	O	S	0	0
			2850	1803	492	538	17		

- Molecule 15 is a protein called substrate peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	v	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 16 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		

- Molecule 17 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	248	Total	C	N	O	S	0	0
			1911	1207	325	370	9		

- Molecule 18 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	236	Total	C	N	O	S	0	0
			1749	1090	318	336	5		

- Molecule 19 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	228	Total	C	N	O	S	0	0
			1733	1089	285	349	10		

- Molecule 20 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 21 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 22 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	44	Total	C	N	O	S	0	0
			355	222	64	66	3		

- Molecule 23 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	e	41	Total	C	N	O	S	0	0
			353	217	55	81			

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	269	Total	C	N	O	S	0	0
			2188	1414	359	406	9		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	438	Total	C	N	O	S	0	0
			3570	2261	609	677	23		

- Molecule 26 is a protein called Isoform 2 of NEDD8 ultimate buster 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	95	Total	C	N	O	S	0	0
			771	487	139	144	1		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	441	Total	C	N	O	S	0	0
			3593	2290	641	649	13		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	273	Total	C	N	O	S	0	0
			2150	1362	369	401	18		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	LEU	-	insertion	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

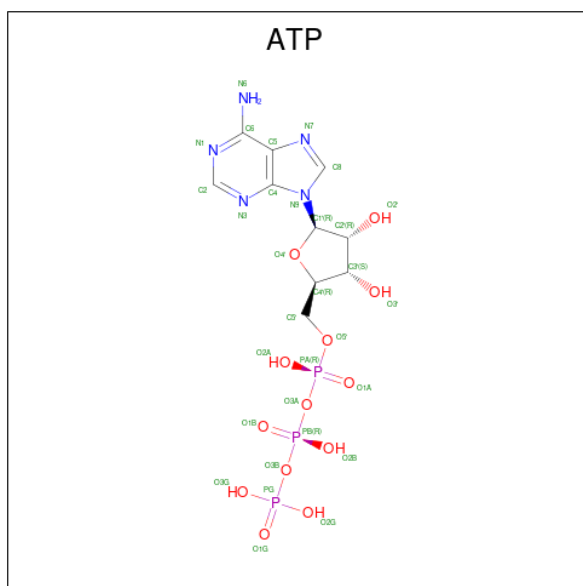
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total Mg 1 1	0

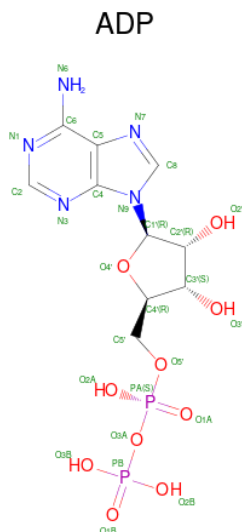
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Mol	Chain	Residues	Atoms		AltConf
29	B	1	Total	Mg	0
			1	1	
29	C	1	Total	Mg	0
			1	1	
29	D	1	Total	Mg	0
			1	1	
29	F	1	Total	Mg	0
			1	1	

- Molecule 30 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

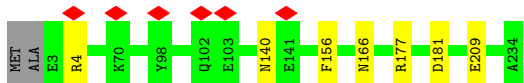
Mol	Chain	Residues	Atoms	AltConf
32	c	1	Total Zn 1 1	0

### 3 Residue-property plots [i](#)

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

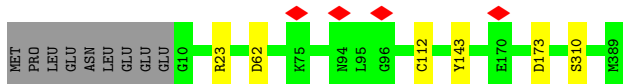
- Molecule 1: Proteasome subunit alpha type-2

Chain H:  96%




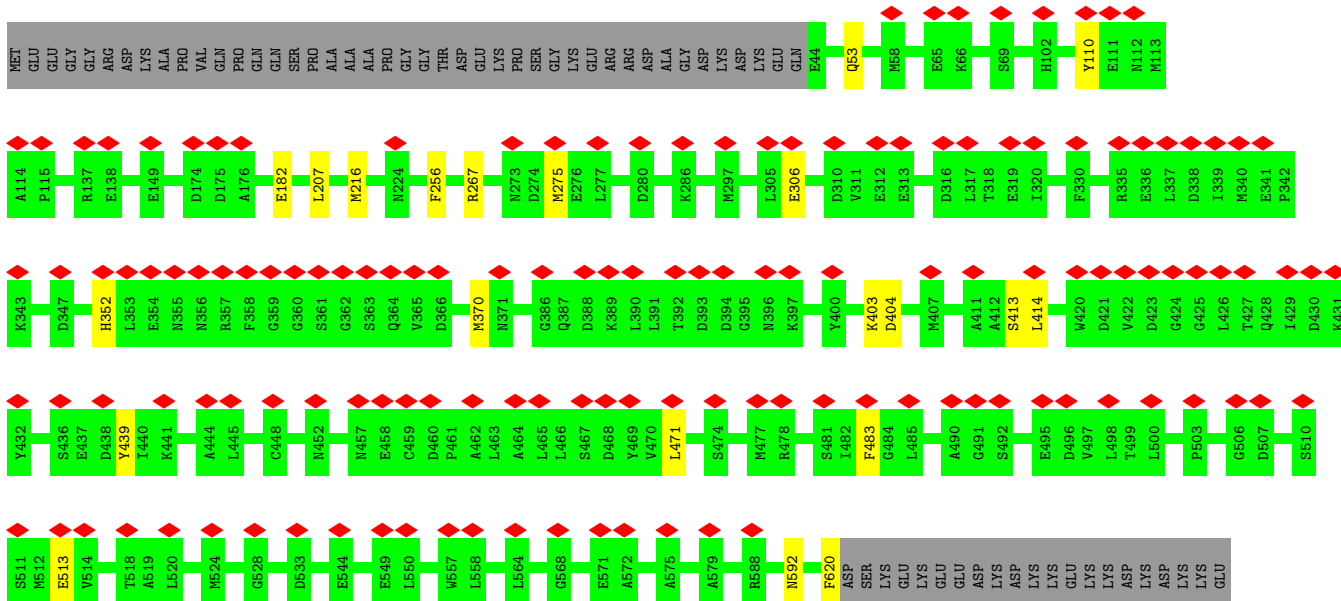
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 6

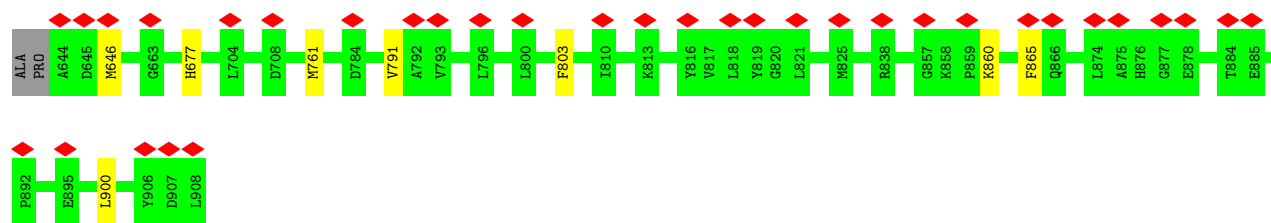
Chain Y:  96%



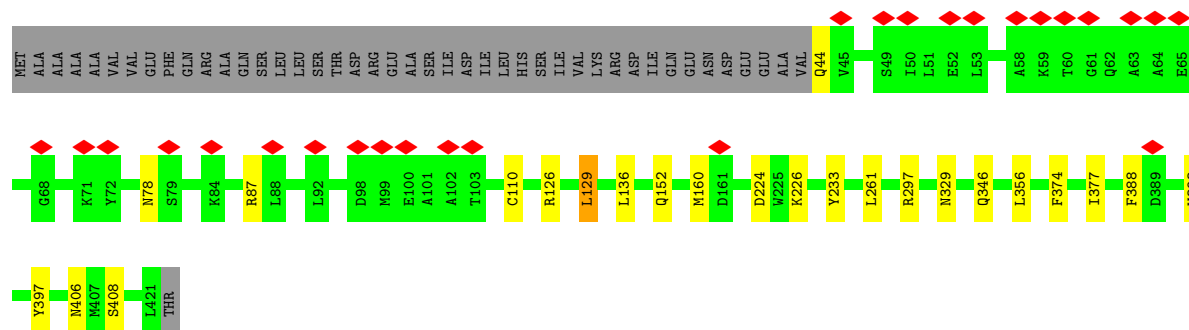
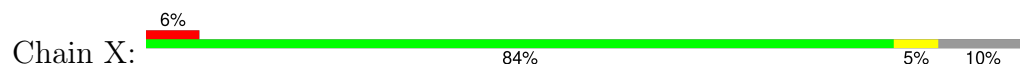
- Molecule 3: 26S proteasome non-ATPase regulatory subunit 2

Chain f:  19% 90% 7%

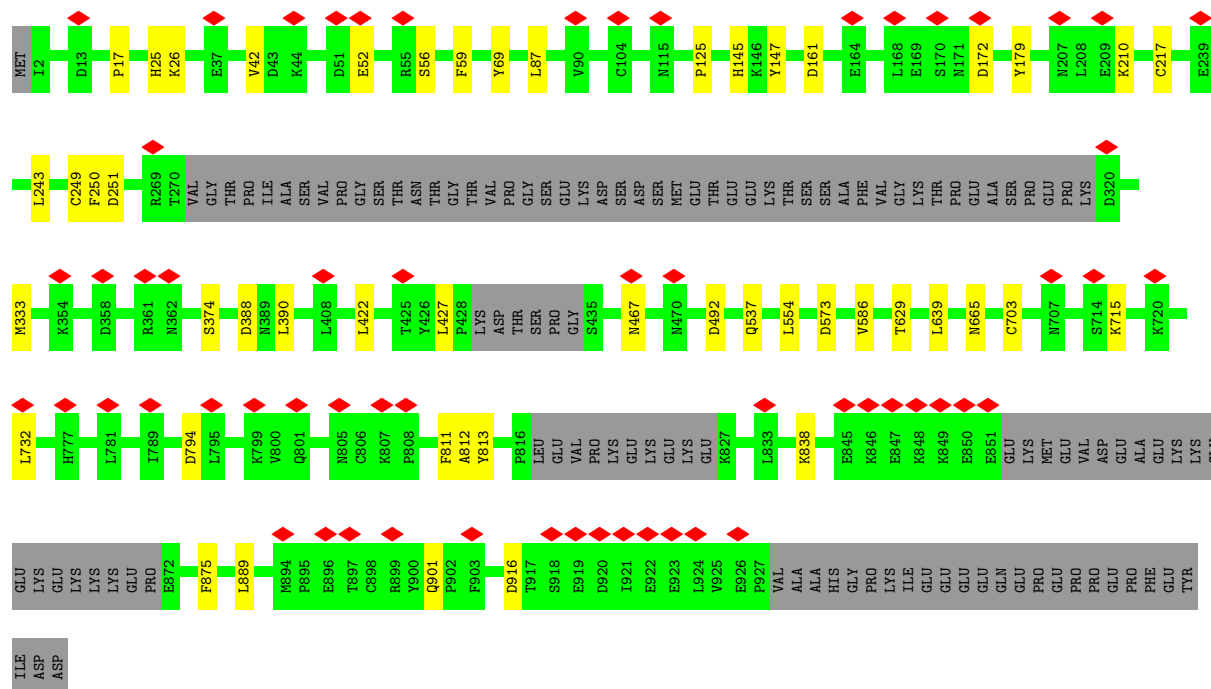
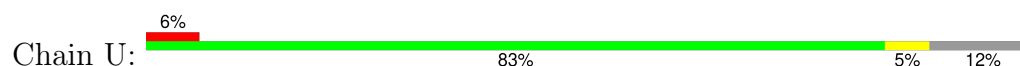




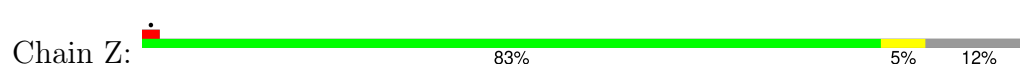
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

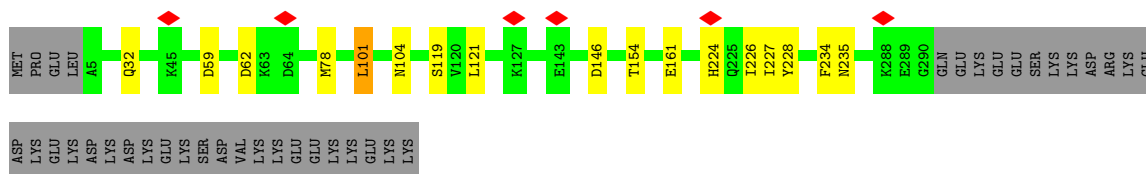


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 1



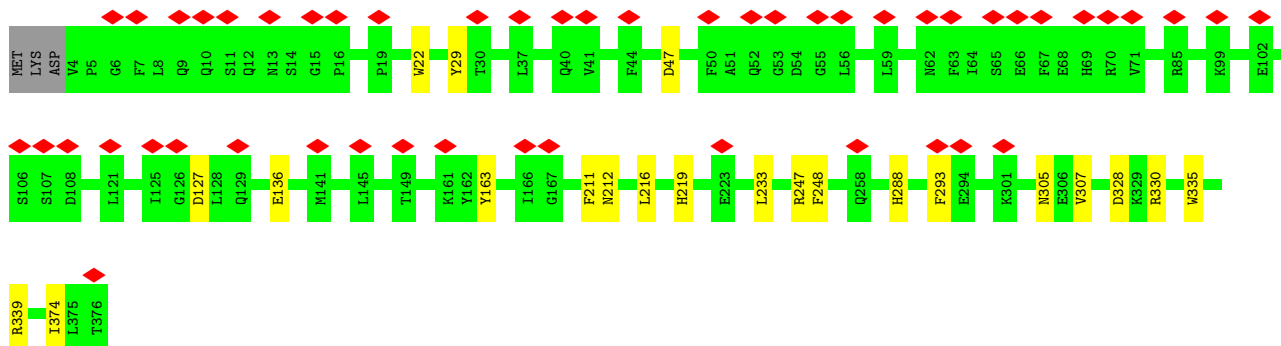
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7





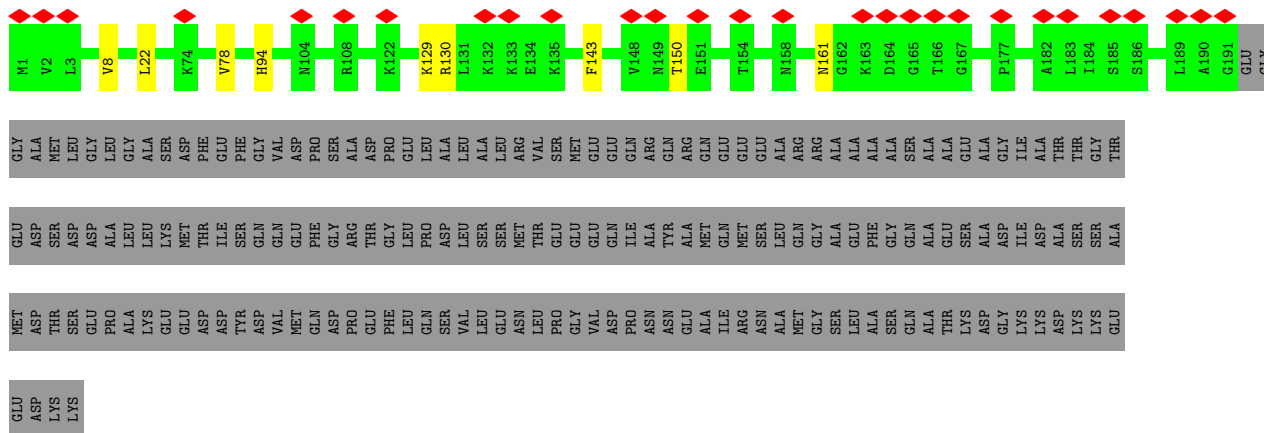
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 13% 93% 6% .



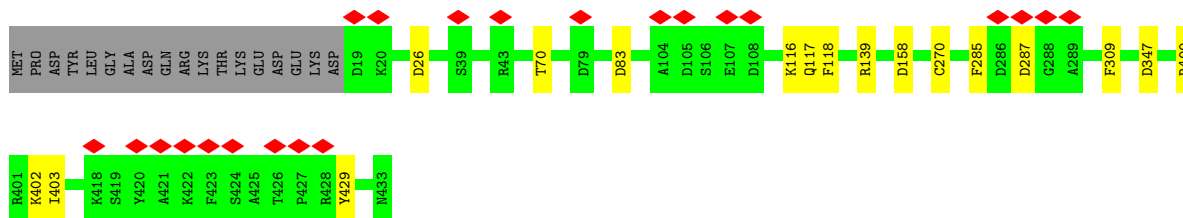
- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 7% 48% 49% .



- Molecule 9: 26S proteasome regulatory subunit 7

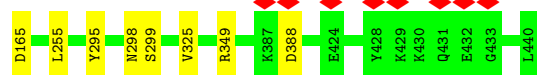
Chain A: 5% 92% . .



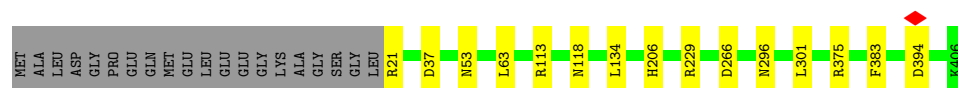
- Molecule 10: 26S proteasome regulatory subunit 4

A horizontal bar chart with a green bar representing 88% and a yellow bar representing 10%. The x-axis is labeled with '88%' and '10%'.

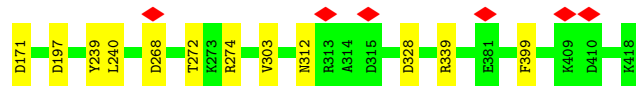
Response	Percentage
Yes	88%
No	10%



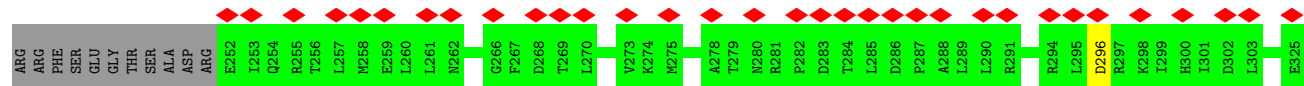
- 91% • 5%



- 
- | Response   | Percentage |
|------------|------------|
| Yes        | 86%        |
| No         | 5%         |
| Don't know | 9%         |

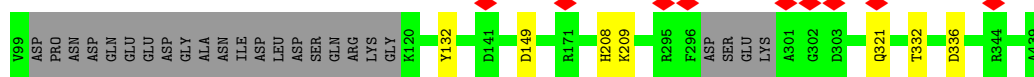
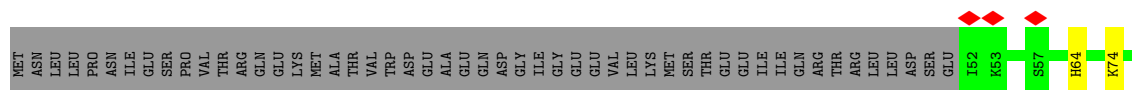


- 
- | Country | Percentage |
|---------|------------|
| U.S.    | 28%        |
| U.S.    | 85%        |
| U.S.    | 7%         |
| U.S.    | 7%         |



- 
- | Response | Percentage |
|----------|------------|
| Yes      | 81%        |
| No       | 17%        |





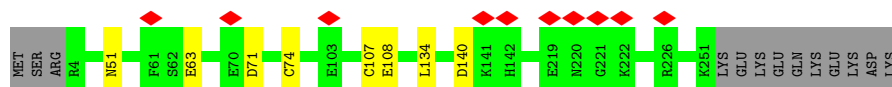
- Molecule 15: substrate peptide



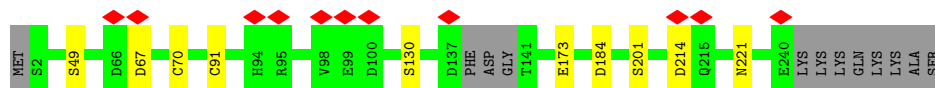
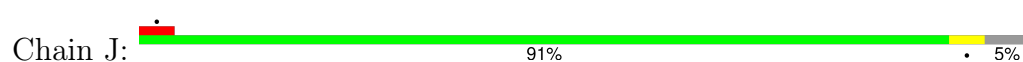
- Molecule 16: Proteasome subunit alpha type-6



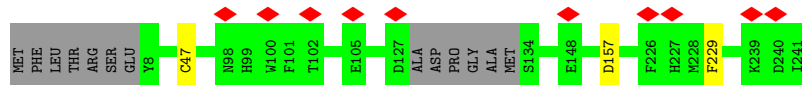
- Molecule 17: Proteasome subunit alpha type-4



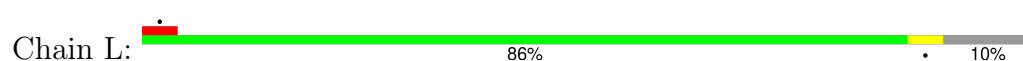
- Molecule 18: Proteasome subunit alpha type-7



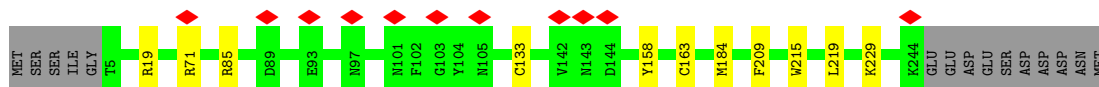
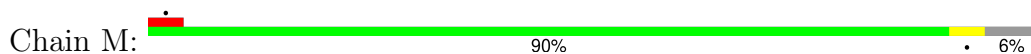
- Molecule 19: Proteasome subunit alpha type-5



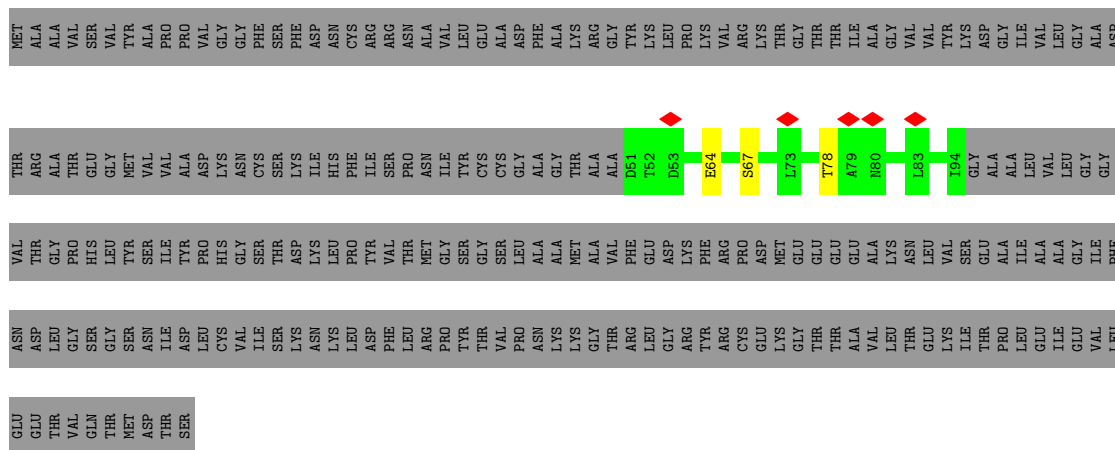
- Molecule 20: Proteasome subunit alpha type-1



- Molecule 21: Proteasome subunit alpha type-3



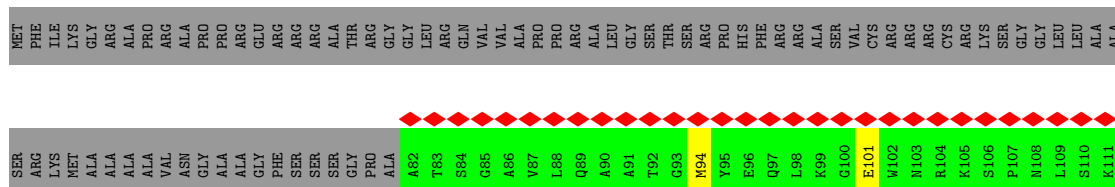
- Molecule 22: Proteasome subunit beta type-7

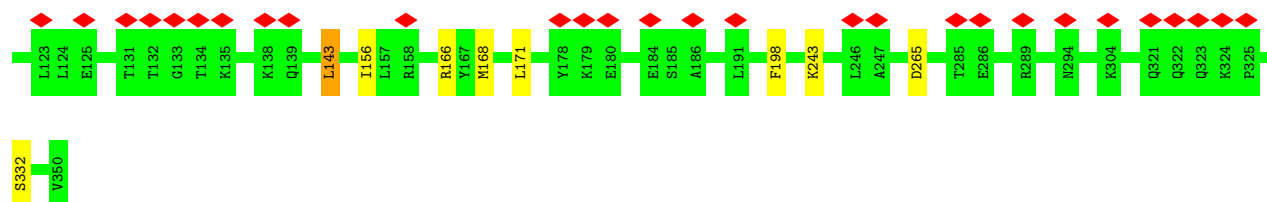


- Molecule 23: 26S proteasome complex subunit SEM1



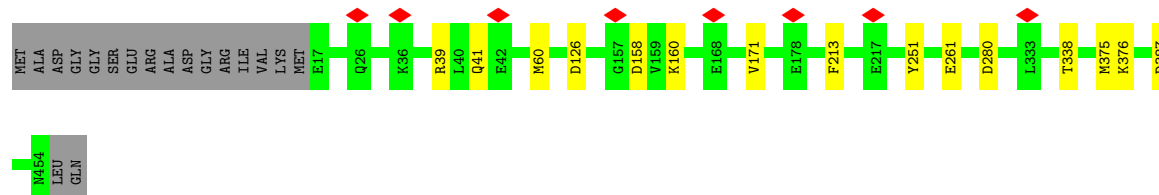
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 8





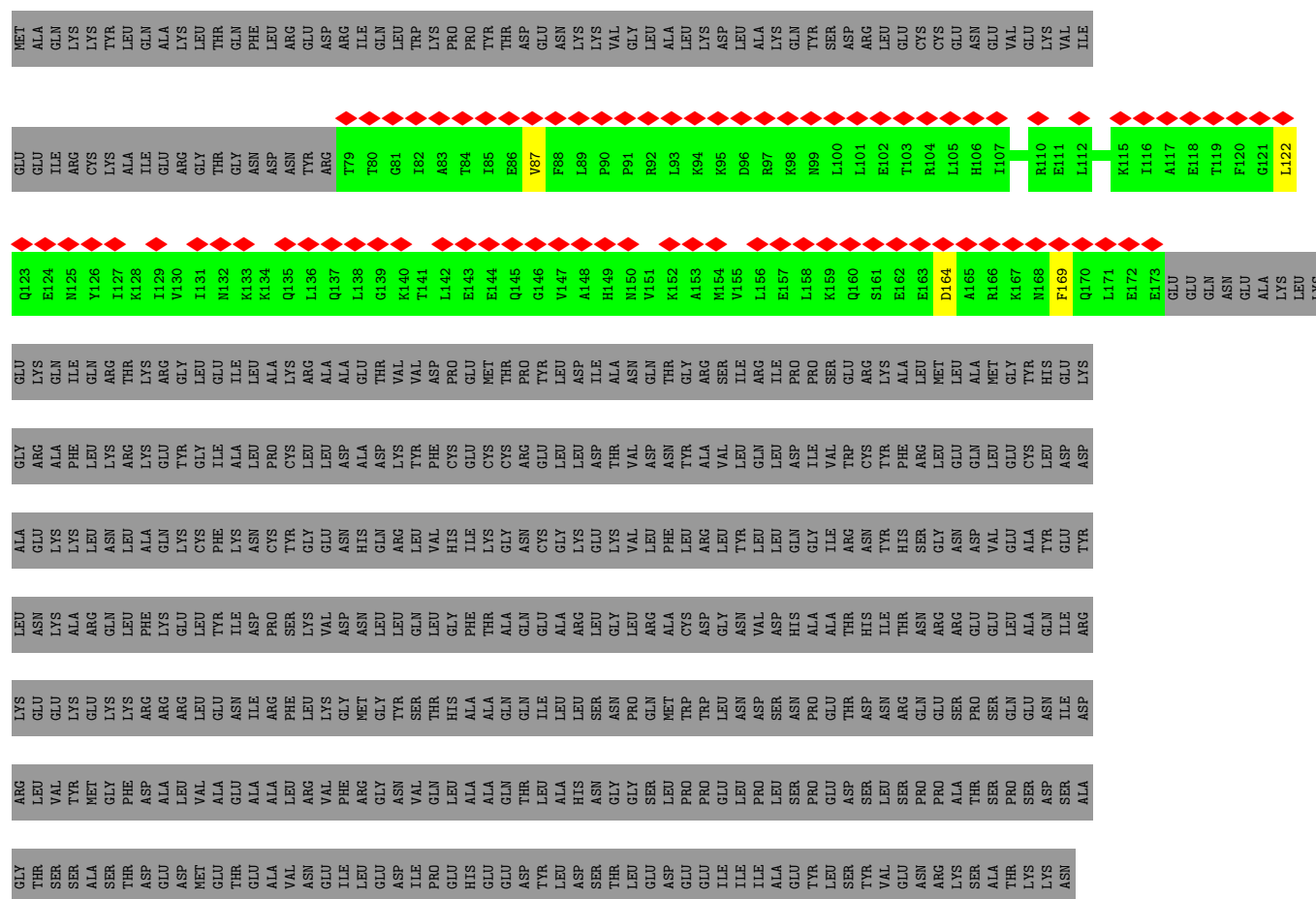
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 93%

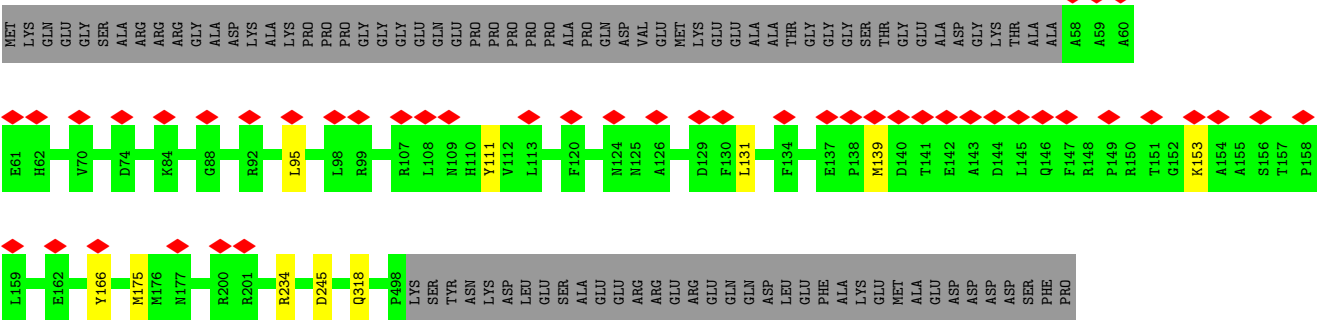
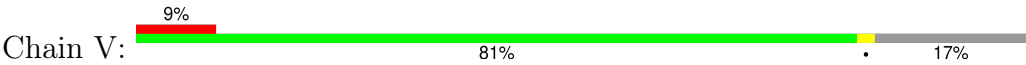


- Molecule 26: Isoform 2 of NEDD8 ultimate buster 1

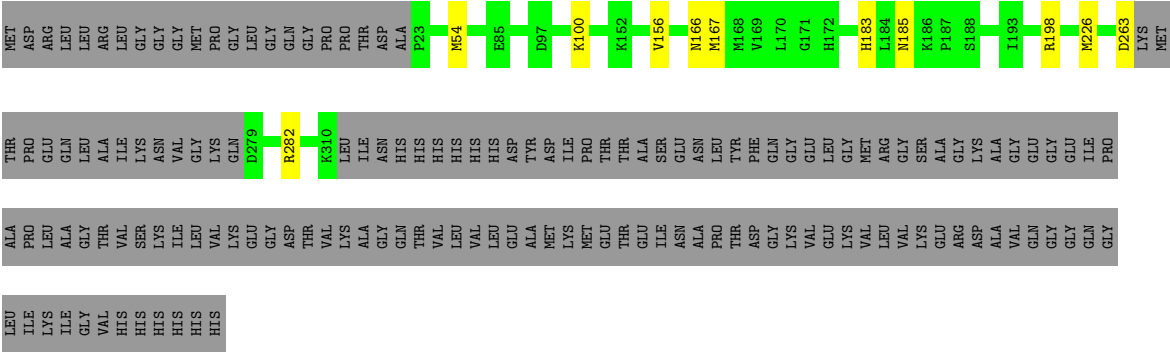
Chain g: 14% 15% 84%



- Molecule 27: 26S proteasome non-ATPase regulatory subunit 3



• Molecule 28: 26S proteasome non-ATPase regulatory subunit 14



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41903	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	0.758	Depositor
Minimum map value	-0.411	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.13	Depositor
Map size ( $\text{\AA}$ )	293.44, 293.44, 293.44	wwPDB
Map dimensions	280, 280, 280	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ZN, 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	H	0.27	0/1852	0.47	0/2507
2	Y	0.25	0/3185	0.47	0/4290
3	f	0.25	0/6623	0.49	0/8965
4	X	0.25	0/3038	0.50	1/4095 (0.0%)
5	U	0.25	0/6670	0.49	1/9017 (0.0%)
6	Z	0.27	0/2324	0.55	2/3150 (0.1%)
7	a	0.25	0/3053	0.50	0/4133
8	b	0.26	0/1478	0.54	0/2001
9	A	0.25	0/3315	0.50	0/4475
10	B	0.26	0/3167	0.51	0/4271
11	C	0.25	0/3092	0.51	0/4154
12	D	0.26	0/3090	0.50	0/4168
13	E	0.26	0/2902	0.56	1/3904 (0.0%)
14	F	0.25	0/2888	0.48	0/3889
16	G	0.26	0/1853	0.47	0/2515
17	I	0.25	0/1941	0.50	0/2626
18	J	0.26	0/1773	0.53	0/2407
19	K	0.26	0/1759	0.51	0/2379
20	L	0.25	0/1885	0.51	0/2552
21	M	0.26	0/1891	0.49	0/2552
22	O	0.23	0/359	0.50	0/483
23	e	0.26	0/362	0.43	0/490
24	d	0.25	0/2234	0.49	1/3018 (0.0%)
25	W	0.25	0/3618	0.50	0/4868
26	g	0.25	0/778	0.52	0/1041
27	V	0.25	0/3663	0.51	0/4946
28	c	0.25	0/2191	0.49	0/2962
All	All	0.25	0/70984	0.50	6/95858 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	143	LEU	CA-CB-CG	6.16	129.47	115.30
6	Z	78	MET	CB-CG-SD	5.96	130.28	112.40
4	X	129	LEU	CA-CB-CG	5.77	128.57	115.30
6	Z	101	LEU	CA-CB-CG	5.63	128.26	115.30
13	E	172	LEU	CA-CB-CG	5.37	127.65	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	230/234 (98%)	224 (97%)	6 (3%)	0	100	100
2	Y	378/389 (97%)	369 (98%)	9 (2%)	0	100	100
3	f	838/908 (92%)	793 (95%)	44 (5%)	1 (0%)	48	79
4	X	376/422 (89%)	353 (94%)	22 (6%)	1 (0%)	37	68
5	U	831/953 (87%)	768 (92%)	60 (7%)	3 (0%)	30	63
6	Z	284/324 (88%)	256 (90%)	25 (9%)	3 (1%)	12	39
7	a	371/376 (99%)	341 (92%)	30 (8%)	0	100	100
8	b	189/377 (50%)	170 (90%)	18 (10%)	1 (0%)	25	58
9	A	413/433 (95%)	379 (92%)	33 (8%)	1 (0%)	44	74
10	B	394/440 (90%)	368 (93%)	26 (7%)	0	100	100
11	C	384/406 (95%)	354 (92%)	29 (8%)	1 (0%)	37	68
12	D	378/418 (90%)	341 (90%)	34 (9%)	3 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	E	354/389 (91%)	308 (87%)	41 (12%)	5 (1%)	9	34
14	F	358/439 (82%)	338 (94%)	18 (5%)	2 (1%)	22	53
16	G	237/246 (96%)	231 (98%)	5 (2%)	1 (0%)	30	63
17	I	246/261 (94%)	235 (96%)	10 (4%)	1 (0%)	30	63
18	J	232/248 (94%)	216 (93%)	16 (7%)	0	100	100
19	K	224/241 (93%)	207 (92%)	17 (8%)	0	100	100
20	L	236/263 (90%)	231 (98%)	5 (2%)	0	100	100
21	M	238/255 (93%)	228 (96%)	10 (4%)	0	100	100
22	O	42/277 (15%)	42 (100%)	0	0	100	100
23	e	37/70 (53%)	37 (100%)	0	0	100	100
24	d	267/350 (76%)	253 (95%)	13 (5%)	1 (0%)	30	63
25	W	436/456 (96%)	423 (97%)	12 (3%)	1 (0%)	44	74
26	g	93/601 (16%)	91 (98%)	2 (2%)	0	100	100
27	V	439/534 (82%)	421 (96%)	17 (4%)	1 (0%)	44	74
28	c	269/424 (63%)	253 (94%)	16 (6%)	0	100	100
All	All	8774/10734 (82%)	8230 (94%)	518 (6%)	26 (0%)	38	68

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	393	VAL
5	U	42	VAL
5	U	812	ALA
6	Z	146	ASP
12	D	339	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	190/191 (100%)	183 (96%)	7 (4%)	29	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	335/344 (97%)	329 (98%)	6 (2%)	54	76
3	f	709/763 (93%)	681 (96%)	28 (4%)	27	58
4	X	325/362 (90%)	302 (93%)	23 (7%)	12	39
5	U	715/816 (88%)	671 (94%)	44 (6%)	15	43
6	Z	257/295 (87%)	244 (95%)	13 (5%)	20	49
7	a	333/336 (99%)	311 (93%)	22 (7%)	14	41
8	b	167/312 (54%)	159 (95%)	8 (5%)	21	51
9	A	356/372 (96%)	340 (96%)	16 (4%)	23	53
10	B	350/385 (91%)	338 (97%)	12 (3%)	32	62
11	C	338/352 (96%)	324 (96%)	14 (4%)	26	57
12	D	333/366 (91%)	316 (95%)	17 (5%)	20	49
13	E	316/341 (93%)	293 (93%)	23 (7%)	11	37
14	F	311/379 (82%)	304 (98%)	7 (2%)	45	70
16	G	192/210 (91%)	184 (96%)	8 (4%)	25	56
17	I	197/221 (89%)	190 (96%)	7 (4%)	30	60
18	J	167/211 (79%)	157 (94%)	10 (6%)	16	44
19	K	188/203 (93%)	185 (98%)	3 (2%)	58	79
20	L	198/224 (88%)	187 (94%)	11 (6%)	17	46
21	M	192/212 (91%)	181 (94%)	11 (6%)	17	46
22	O	41/228 (18%)	38 (93%)	3 (7%)	11	37
23	e	37/63 (59%)	34 (92%)	3 (8%)	9	33
24	d	237/294 (81%)	227 (96%)	10 (4%)	25	56
25	W	403/416 (97%)	389 (96%)	14 (4%)	31	61
26	g	85/527 (16%)	81 (95%)	4 (5%)	22	52
27	V	389/460 (85%)	380 (98%)	9 (2%)	45	70
28	c	240/359 (67%)	229 (95%)	11 (5%)	23	52
All	All	7601/9242 (82%)	7257 (96%)	344 (4%)	26	53

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	E	371	VAL
21	M	209	PHE

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Mol	Chain	Res	Type
14	F	332	THR
18	J	173	GLU
24	d	166	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
11	C	205	HIS
13	E	121	ASN
28	c	219	ASN
12	D	65	GLN
13	E	316	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 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	$\# Z  > 2$
30	ATP	F	501	29	28,33,33	0.64	0	34,52,52	0.66	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	ADP	D	501	29	24,29,29	0.88	0	29,45,45	1.27	3 (10%)
31	ADP	E	401	-	24,29,29	0.90	0	29,45,45	1.25	2 (6%)
31	ADP	C	502	29	24,29,29	0.88	0	29,45,45	1.20	2 (6%)
30	ATP	B	502	29	28,33,33	0.64	0	34,52,52	0.60	1 (2%)
30	ATP	B	501	29	28,33,33	0.83	1 (3%)	34,52,52	0.69	2 (5%)

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
30	ATP	F	501	29	-	5/18/38/38	0/3/3/3
31	ADP	D	501	29	-	1/12/32/32	0/3/3/3
31	ADP	E	401	-	-	4/12/32/32	0/3/3/3
31	ADP	C	502	29	-	3/12/32/32	0/3/3/3
30	ATP	B	502	29	-	7/18/38/38	0/3/3/3
30	ATP	B	501	29	-	8/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	501	ATP	PA-O3A	2.27	1.62	1.59

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	E	401	ADP	N3-C2-N1	-3.60	123.79	128.67
31	D	501	ADP	N3-C2-N1	-3.58	123.82	128.67
31	C	502	ADP	N3-C2-N1	-3.57	123.83	128.67
31	C	502	ADP	C4-C5-N7	-2.54	106.65	109.34
31	D	501	ADP	C4'-O4'-C1'	2.54	112.25	109.92

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	B	501	ATP	PB-O3B-PG-O2G
30	B	501	ATP	C5'-O5'-PA-O1A

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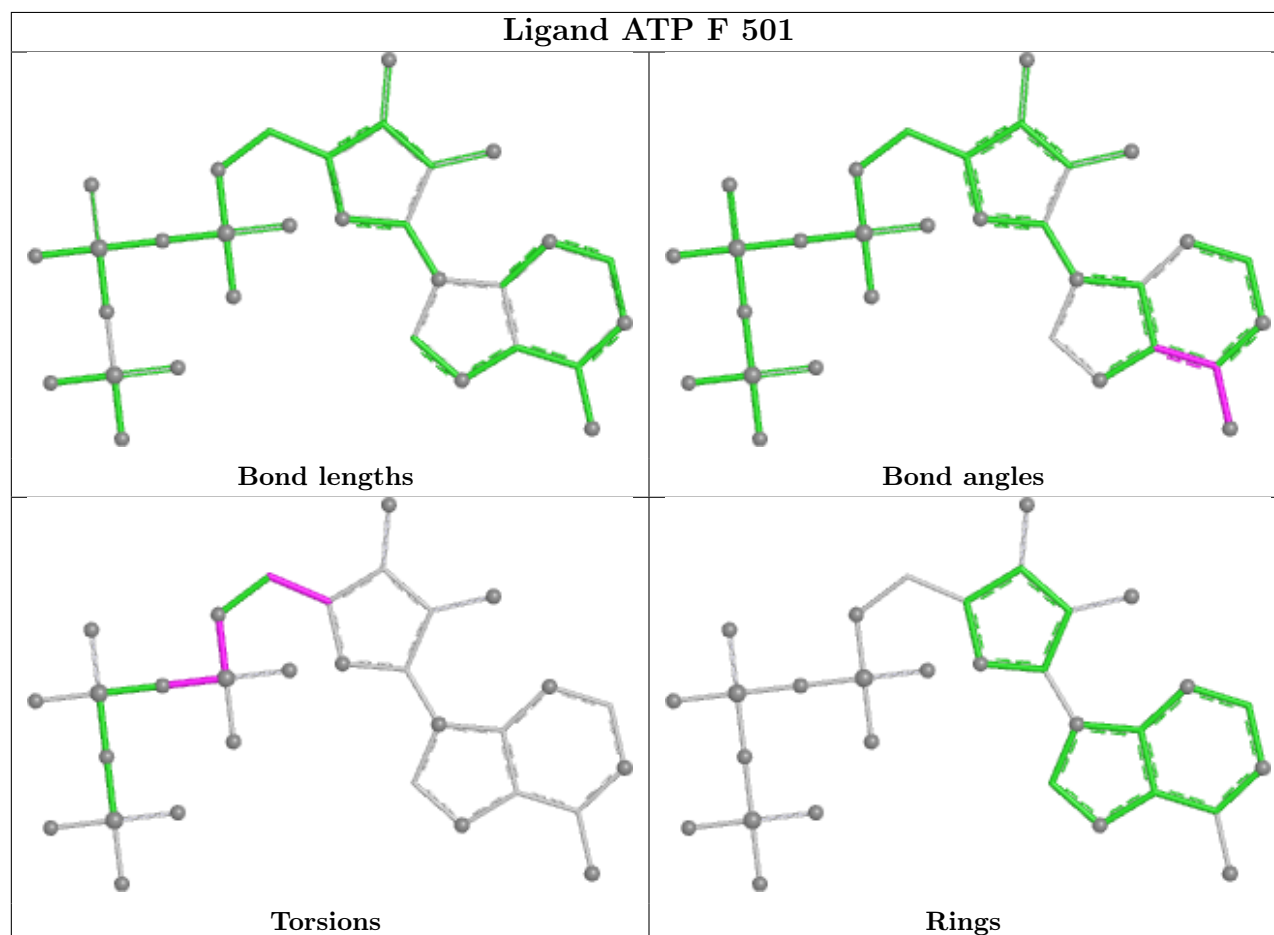
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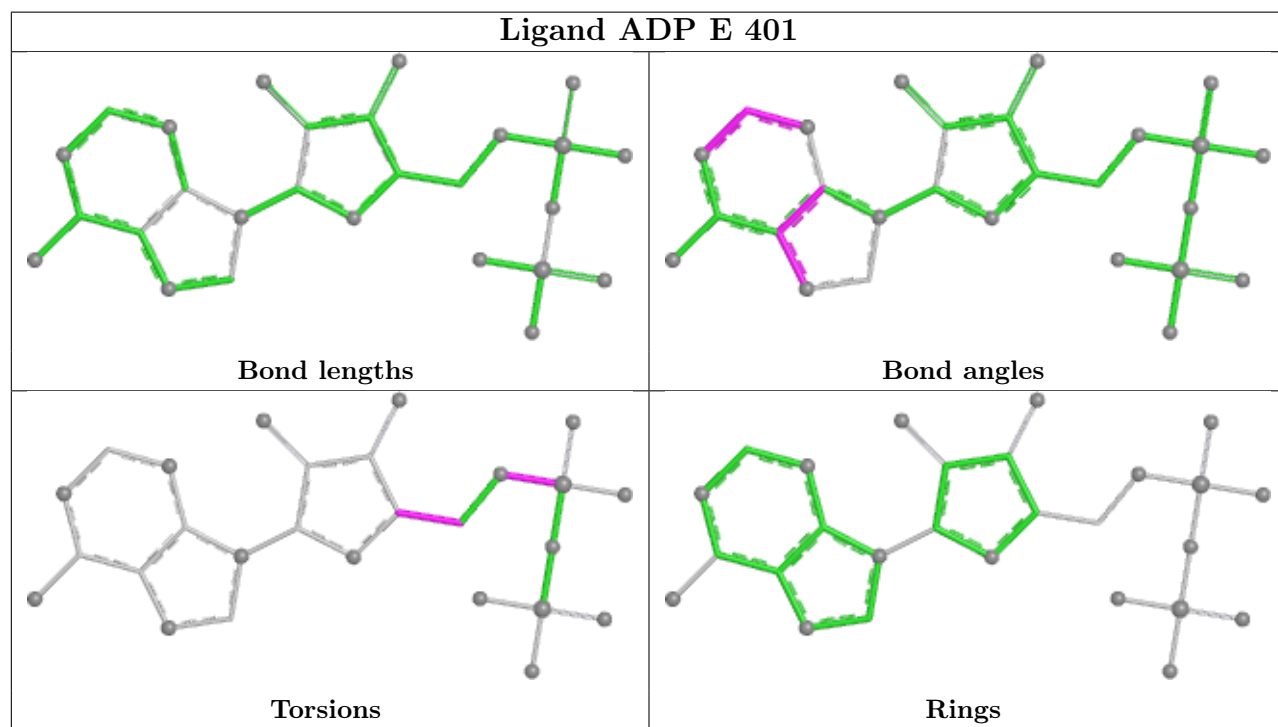
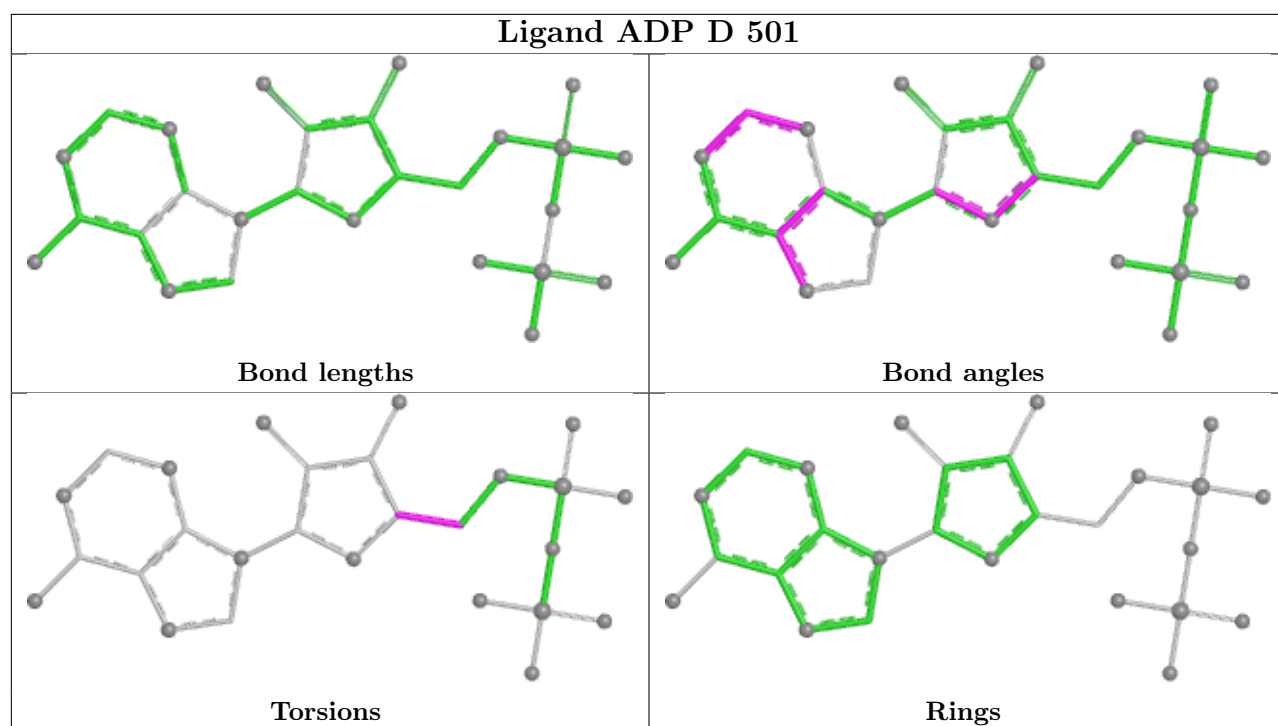
Mol	Chain	Res	Type	Atoms
30	B	501	ATP	C5'-O5'-PA-O3A
30	B	502	ATP	PB-O3B-PG-O2G
30	B	502	ATP	C5'-O5'-PA-O1A

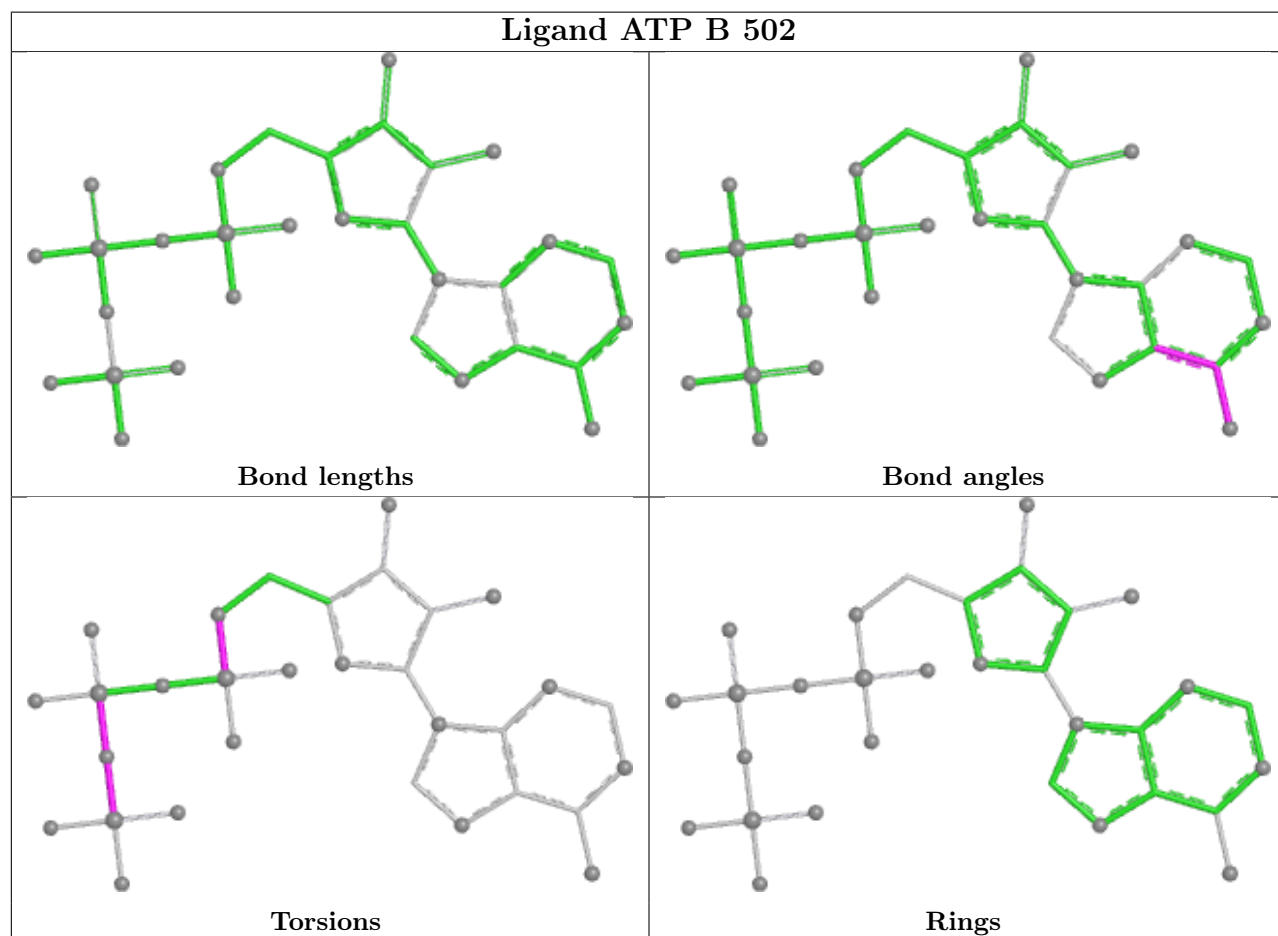
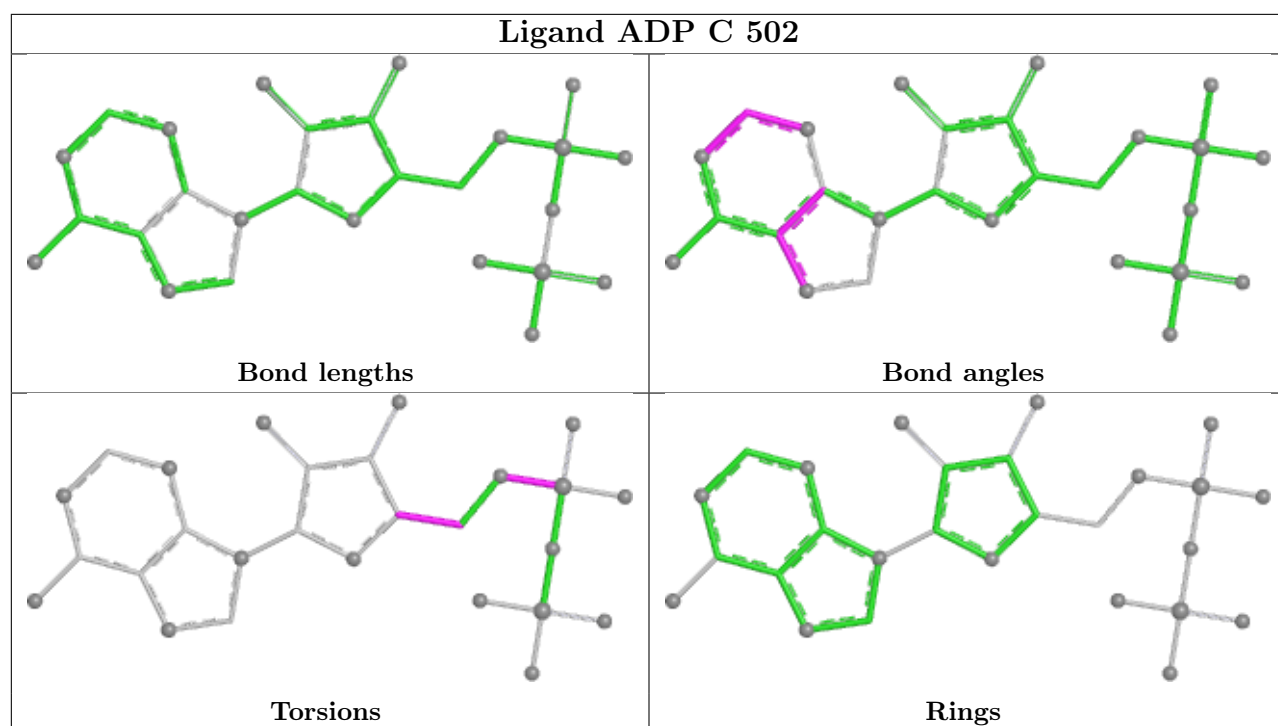
There are no ring outliers.

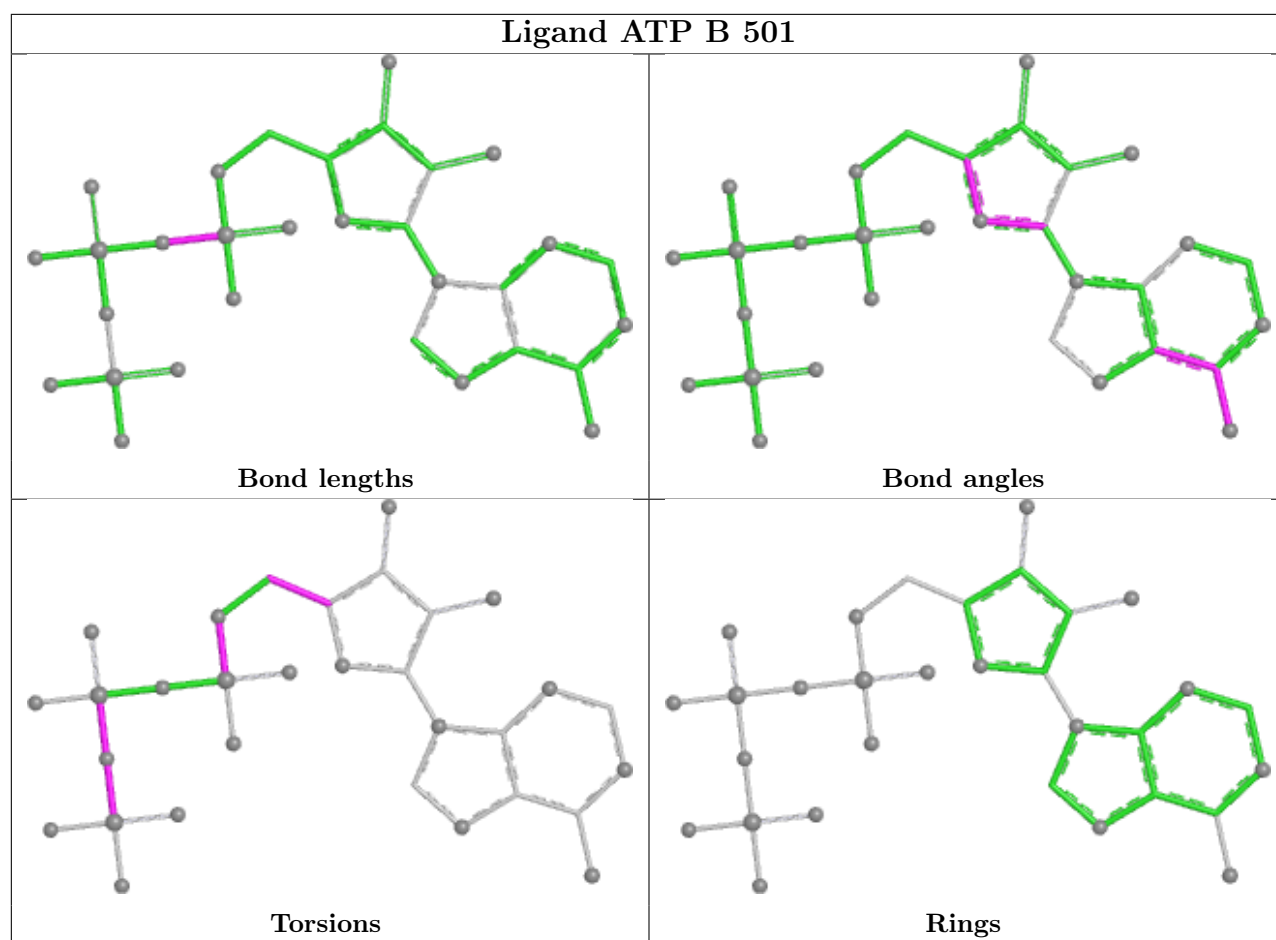
No monomer is involved in short contacts.

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.



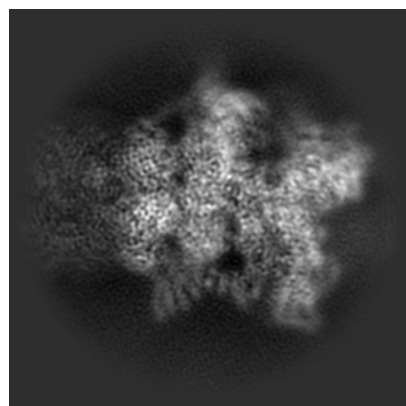
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42507. These allow visual inspection of the internal detail of the map and identification of artifacts.

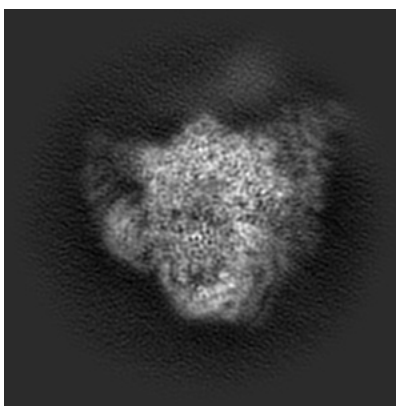
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

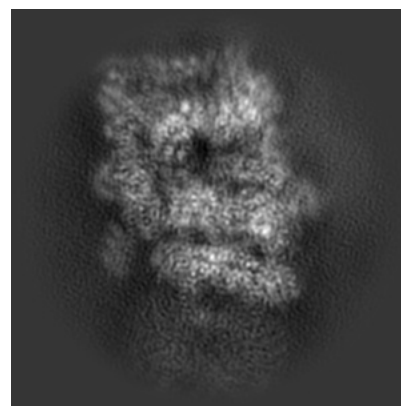
#### 6.1.1 Primary map



X

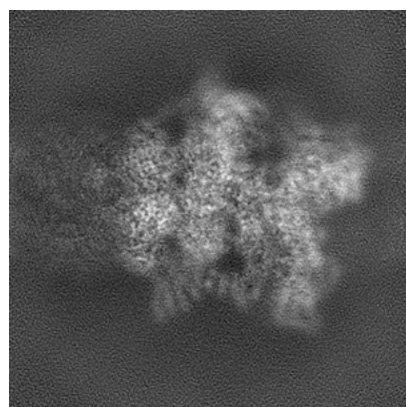


Y

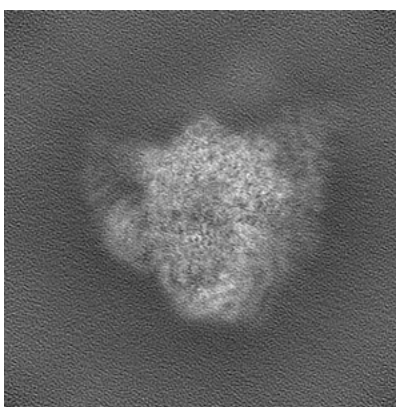


Z

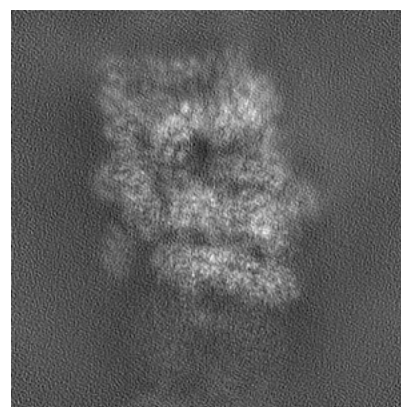
#### 6.1.2 Raw map



X



Y



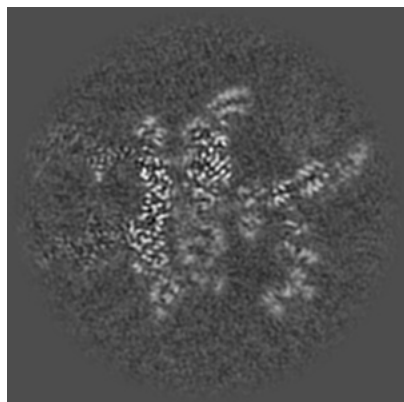
Z

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

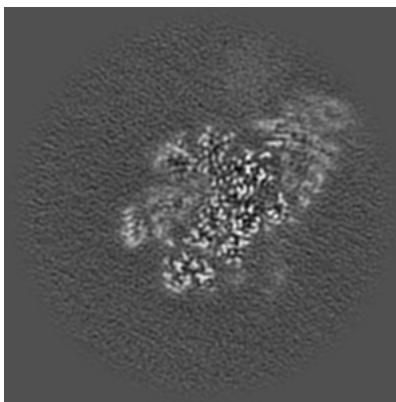


## 6.2 Central slices [i](#)

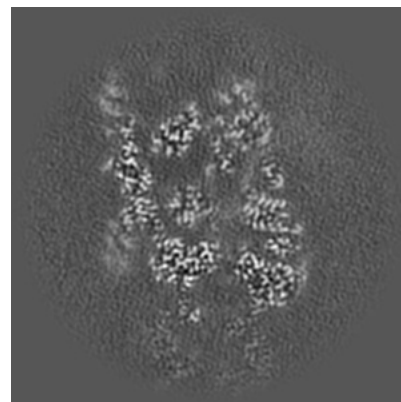
### 6.2.1 Primary map



X Index: 140

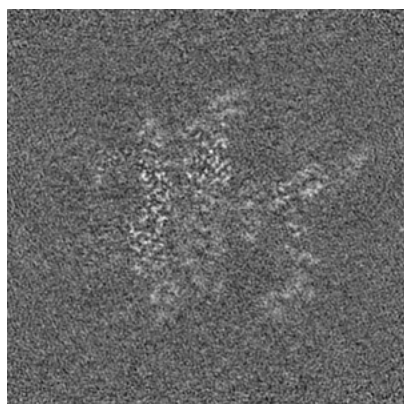


Y Index: 140

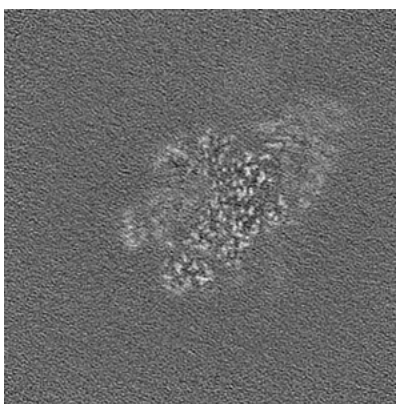


Z Index: 140

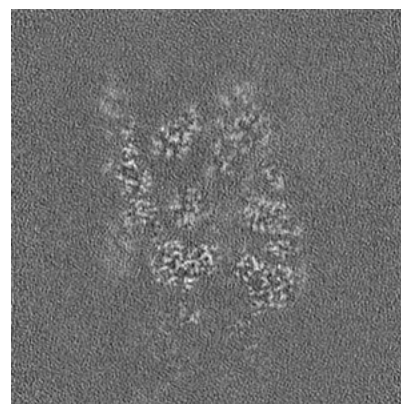
### 6.2.2 Raw map



X Index: 140



Y Index: 140

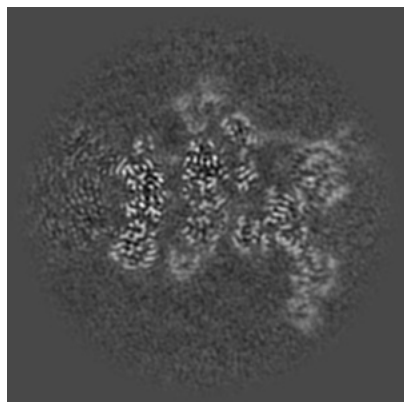


Z Index: 140

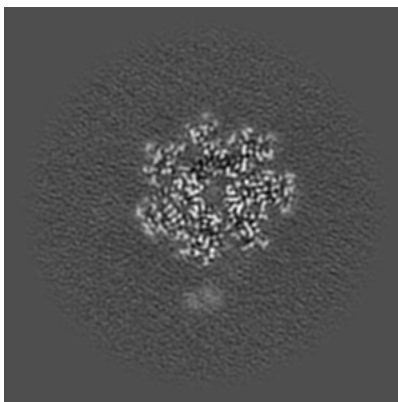
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

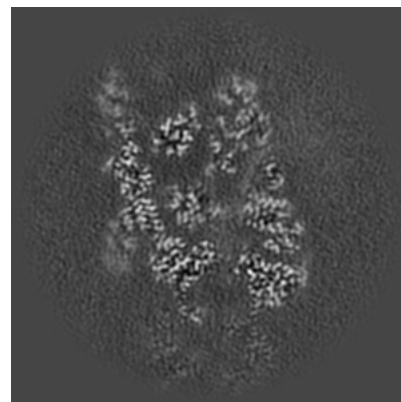
### 6.3.1 Primary map



X Index: 167

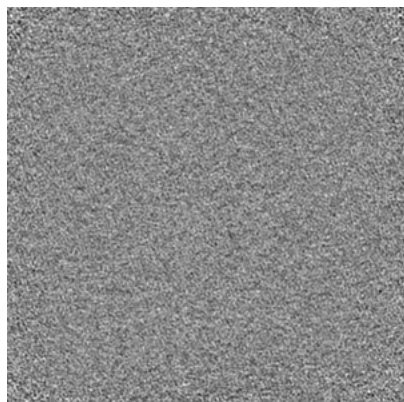


Y Index: 96

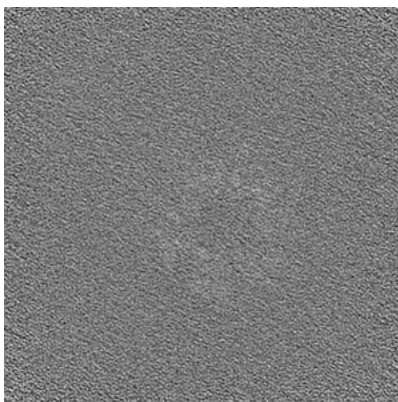


Z Index: 141

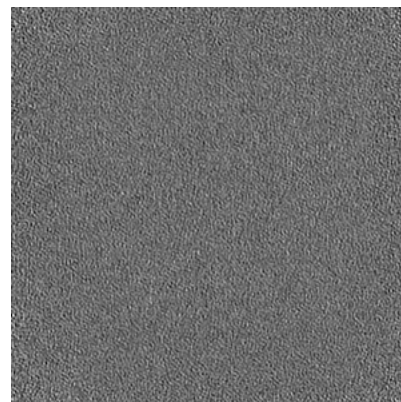
### 6.3.2 Raw map



X Index: 0



Y Index: 0

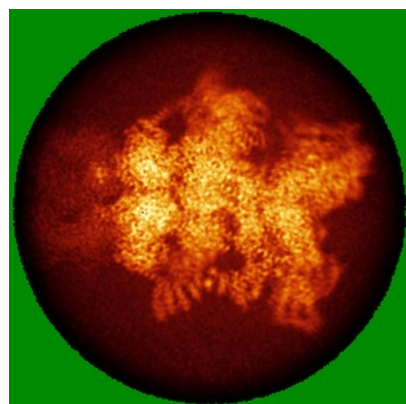


Z Index: 0

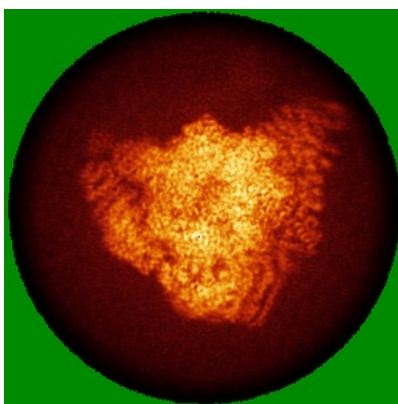
The images above show the largest variance slices of the map in three orthogonal directions.

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

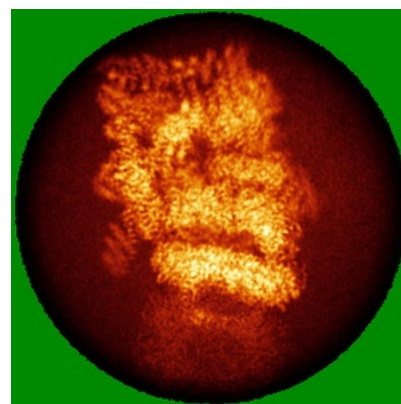
### 6.4.1 Primary map



X

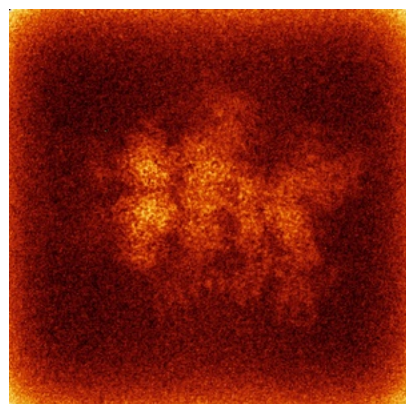


Y

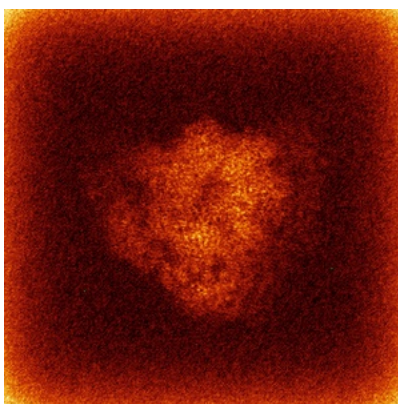


Z

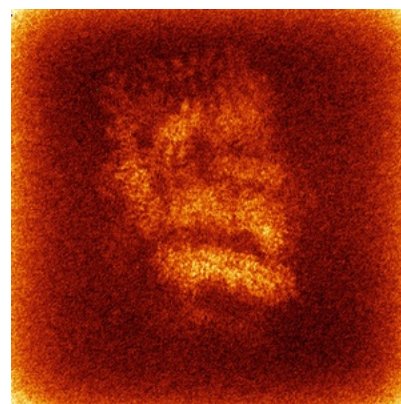
### 6.4.2 Raw map



X



Y



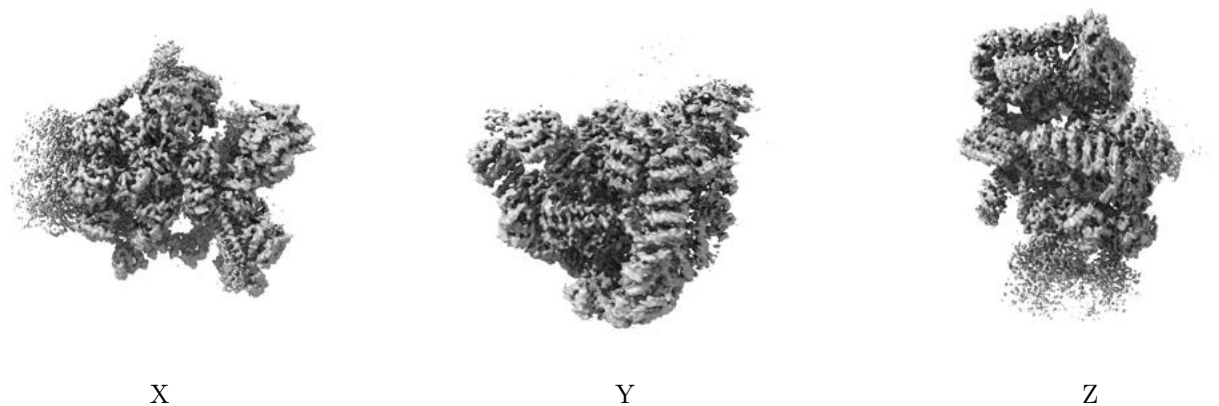
Z

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.



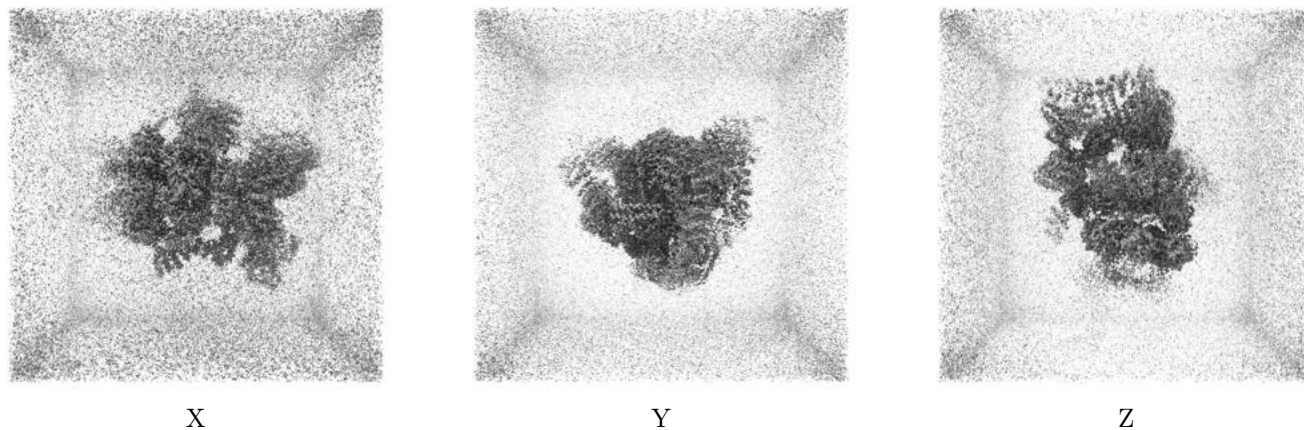
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

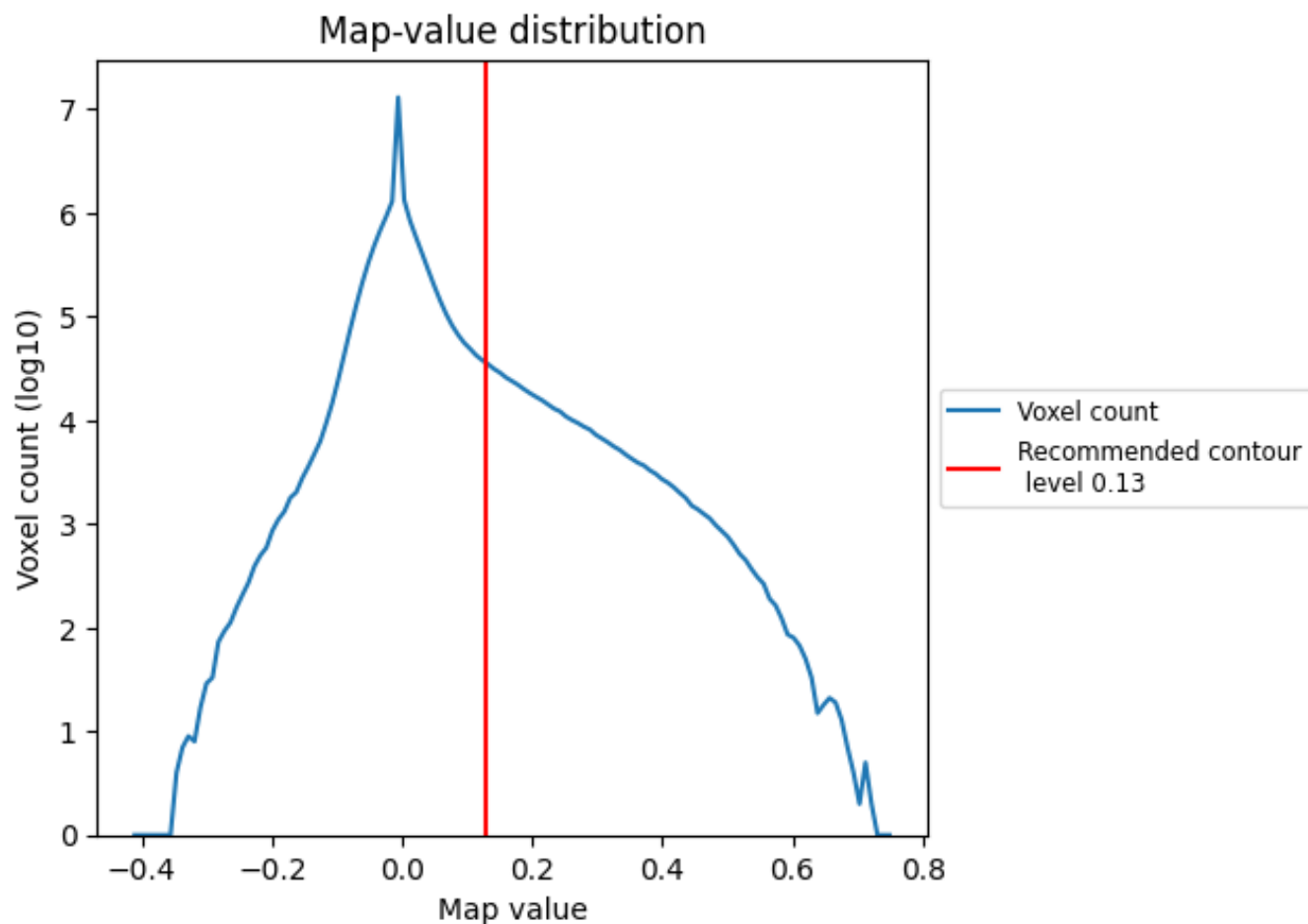
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

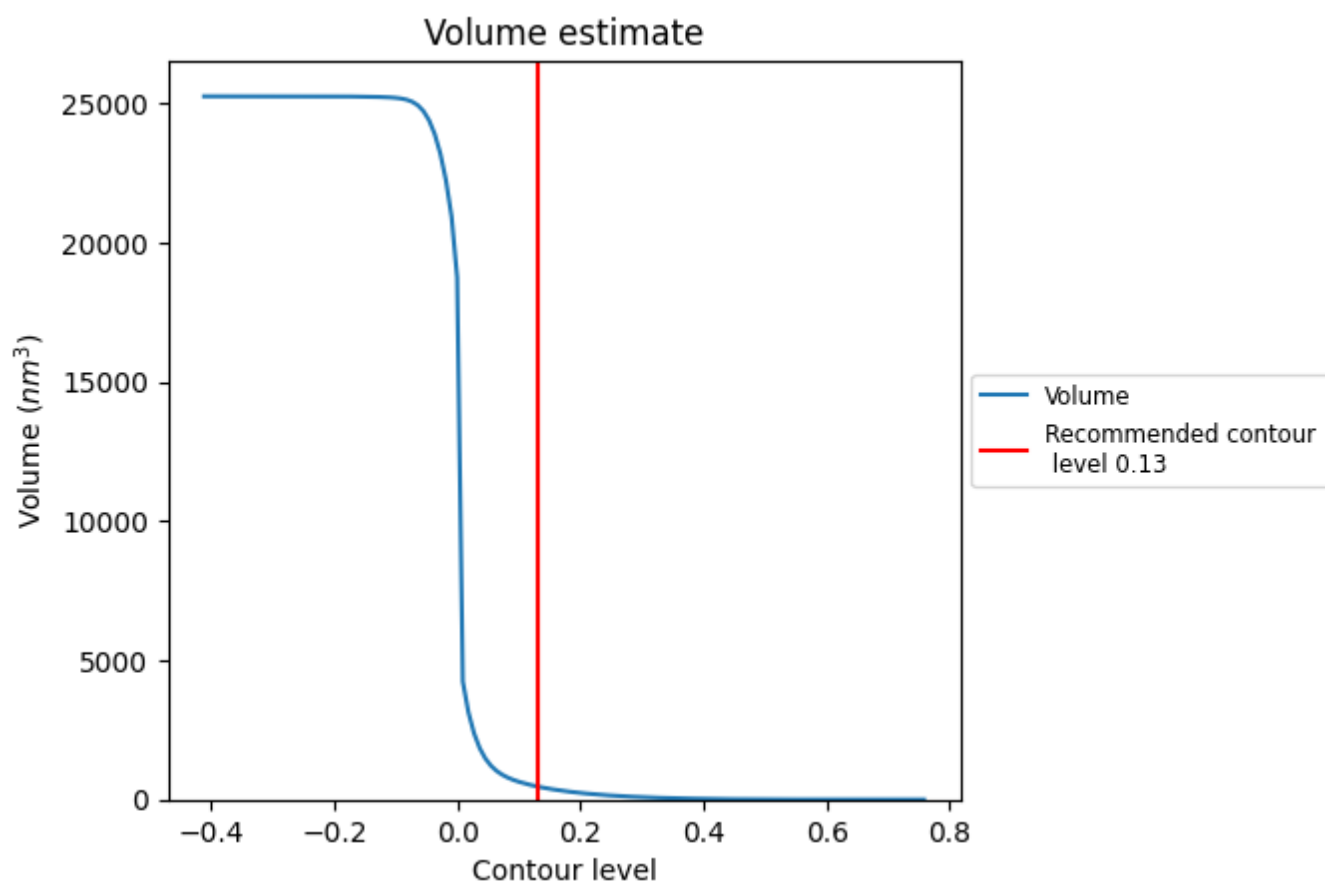
This section contains the results of statistical analysis of the map.

### 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.

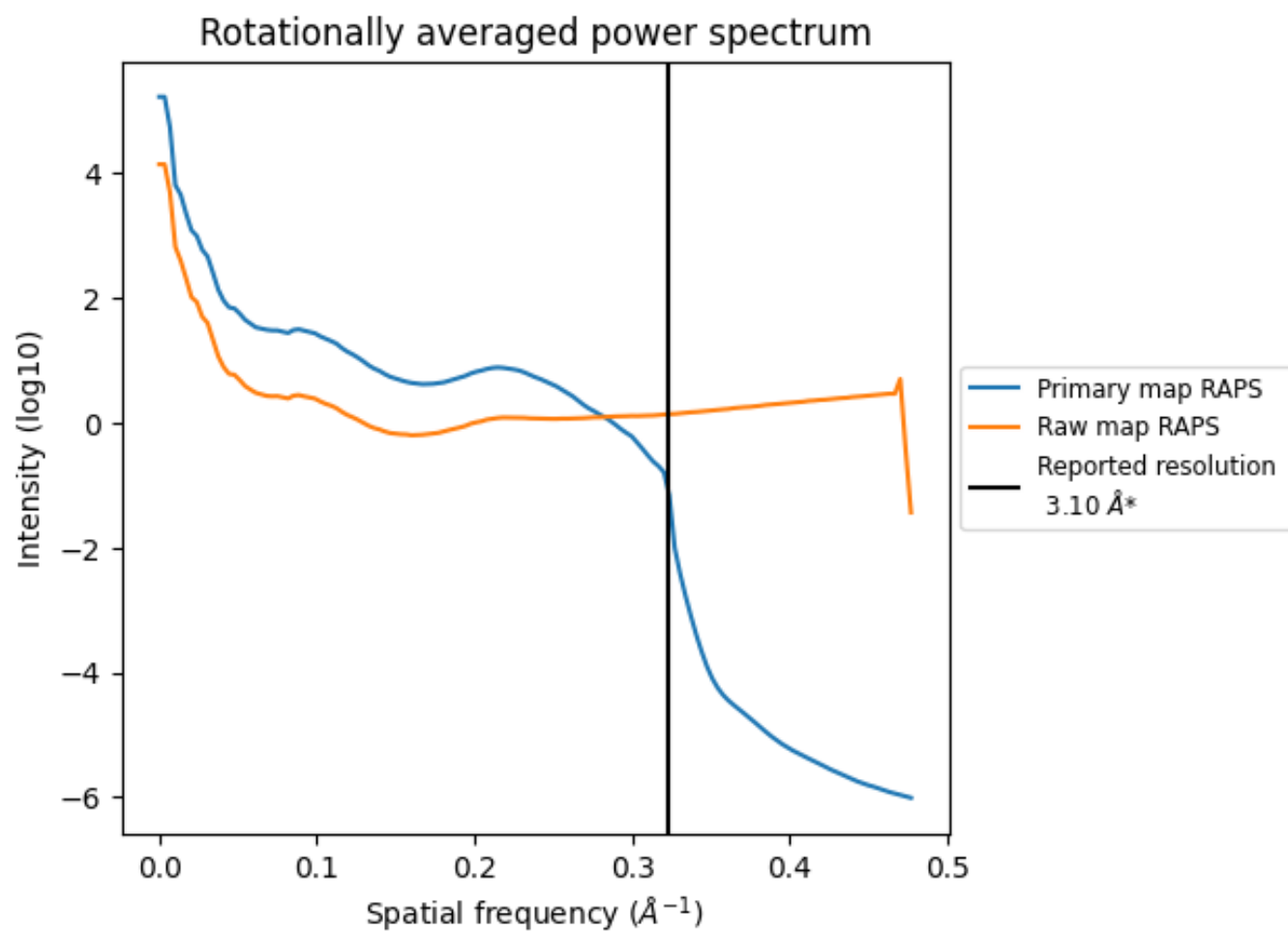
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 471 nm<sup>3</sup>; this corresponds to an approximate mass of 425 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 ⓘ

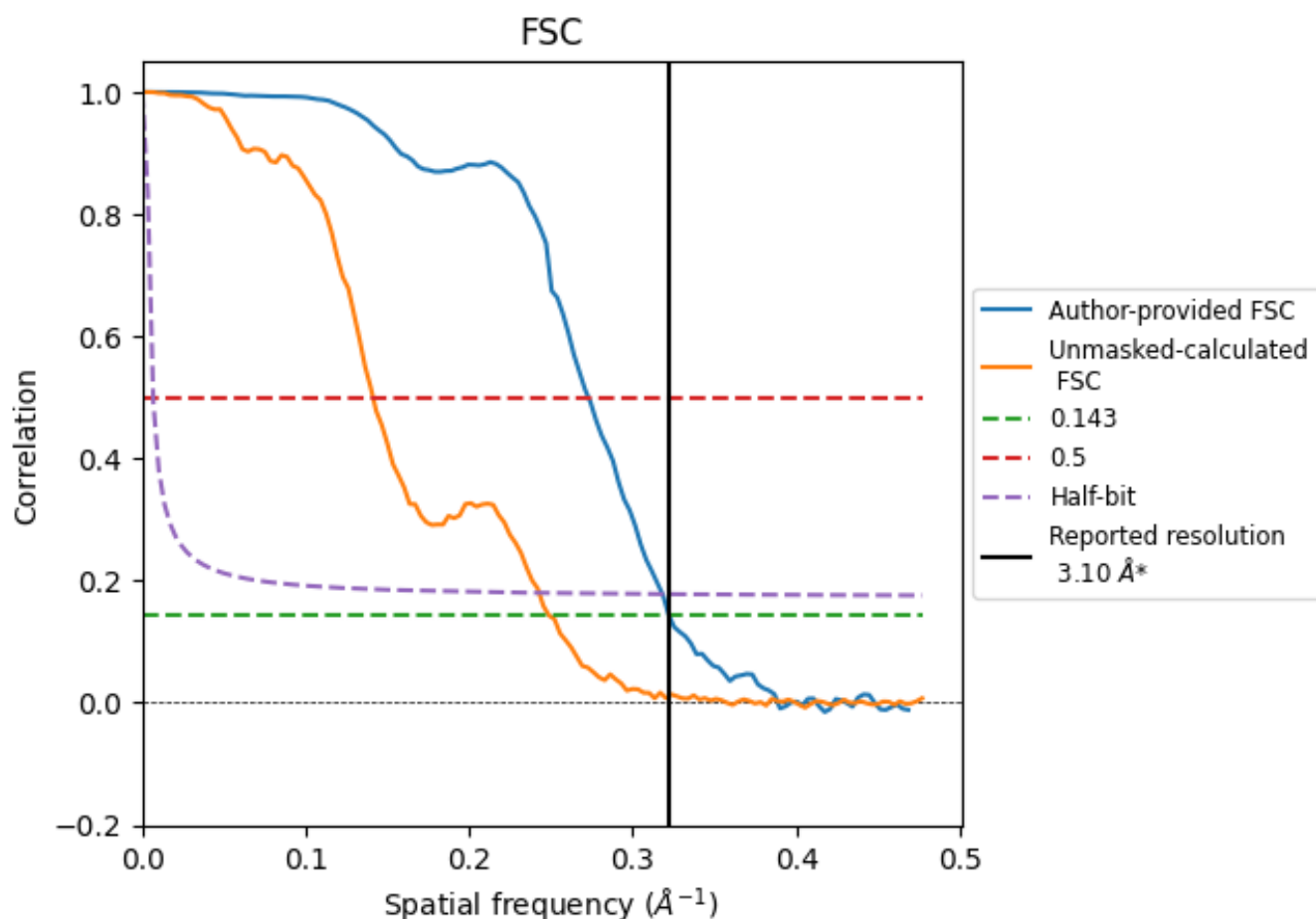


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

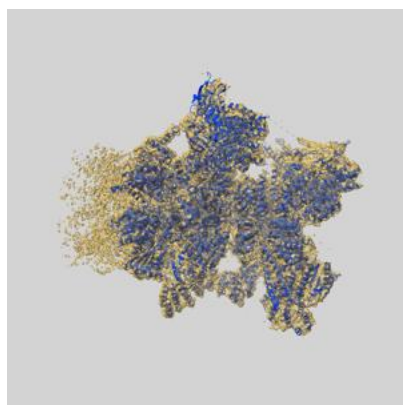
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.66	3.14
Unmasked-calculated*	4.02	7.08	4.12

\*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 4.02 differs from the reported value 3.1 by more than 10 %

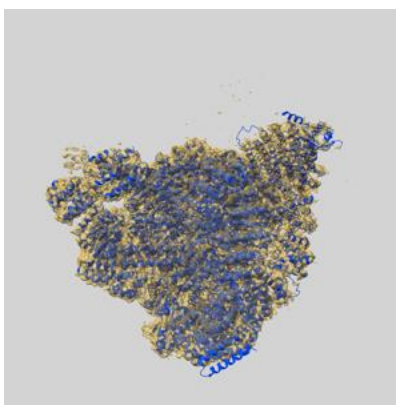
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42507 and PDB model 8USC. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

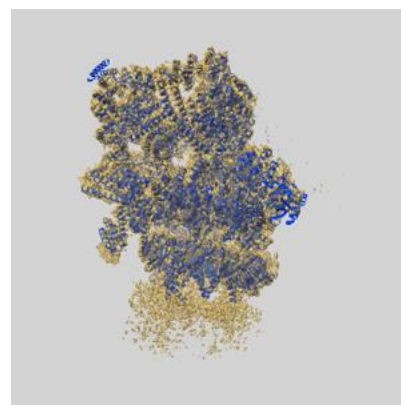
### 9.1 Map-model overlay [i](#)



X



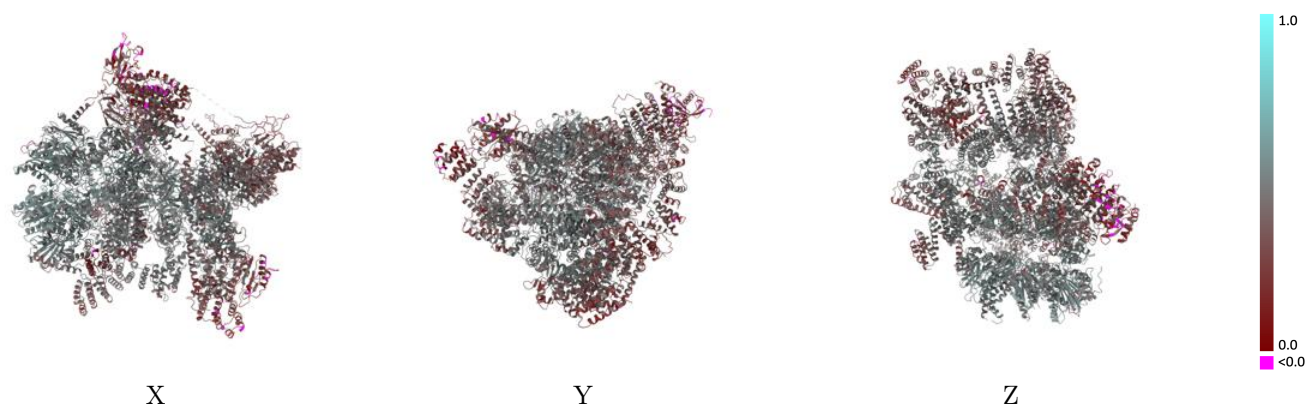
Y



Z

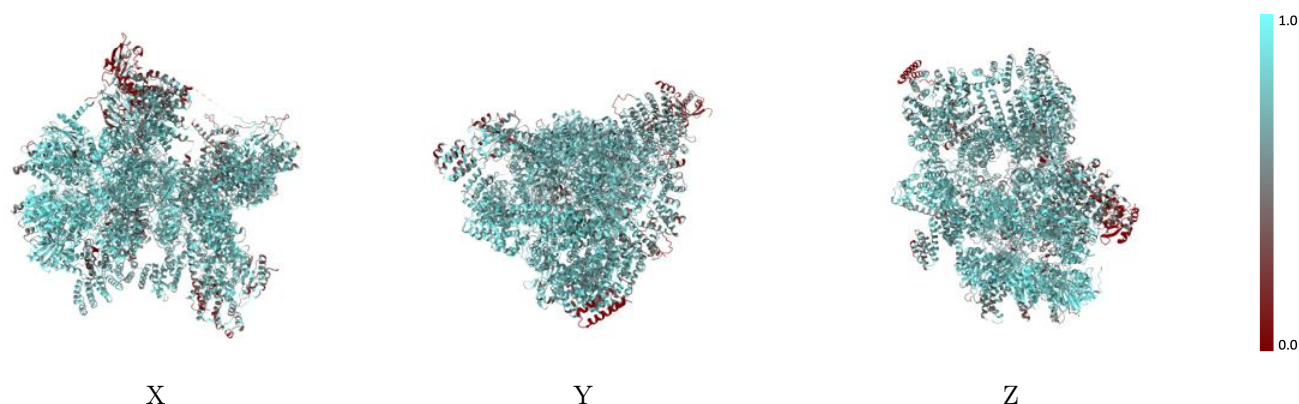
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



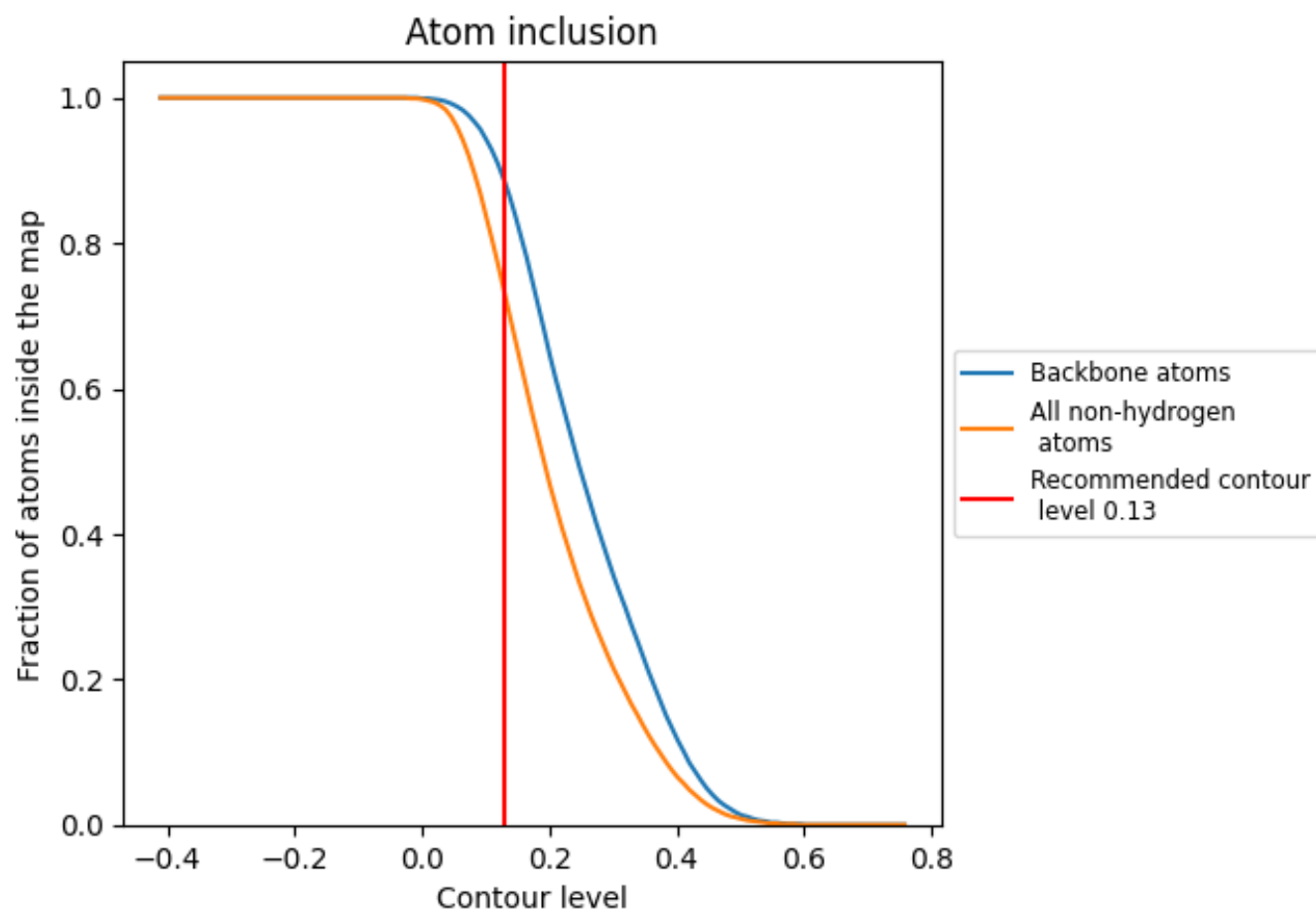
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 73% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 0.4350
A	 0.7730	 0.4910
B	 0.7910	 0.4960
C	 0.8180	 0.5060
D	 0.7800	 0.4900
E	 0.5410	 0.3430
F	 0.7590	 0.4790
G	 0.8230	 0.5210
H	 0.8490	 0.5260
I	 0.7860	 0.5090
J	 0.8260	 0.5160
K	 0.8010	 0.5060
L	 0.8480	 0.5350
M	 0.8000	 0.5100
O	 0.6640	 0.5180
U	 0.7080	 0.3780
V	 0.6970	 0.3930
W	 0.7690	 0.4370
X	 0.7550	 0.4480
Y	 0.8250	 0.4650
Z	 0.7830	 0.4610
a	 0.6840	 0.3380
b	 0.6500	 0.3180
c	 0.7740	 0.4710
d	 0.5840	 0.3270
e	 0.7670	 0.4570
f	 0.6040	 0.3430
g	 0.1370	 0.2010
v	 0.9000	 0.5430

