



## wwPDB EM Validation Summary Report ⓘ

Jun 9, 2026 – 09:48 PM JST

PDB ID : 9VUF / pdb\_00009vuf  
EMDB ID : EMD-65361  
Title : Structure of human proteasome ATPase-CP intermediate assemblies with 90min rapaprotin addition  
Authors : Wang, W.L.; Yin, D.Y.; Mao, Y.D.  
Deposited on : 2025-07-13  
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.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

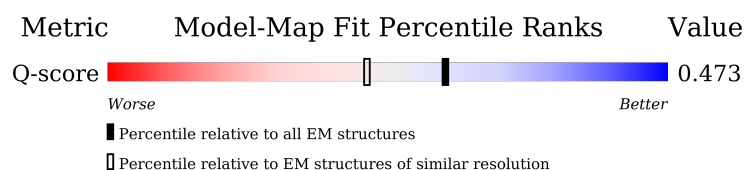
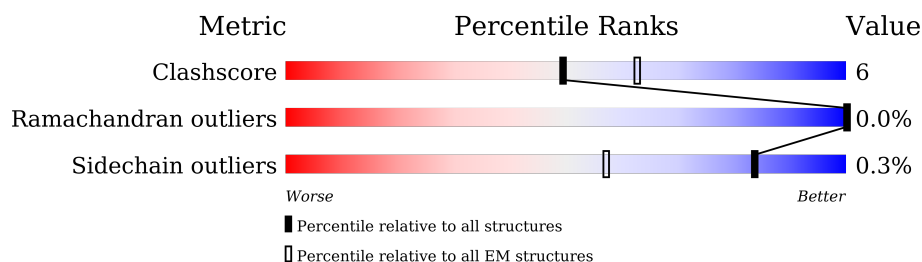
# 1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 ( 2.60 - 3.60 )

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	A	433	<div> <div>10%</div> <div>71%</div> <div>10%</div> <div>18%</div> </div>
2	B	440	<div> <div>16%</div> <div>64%</div> <div>13%</div> <div>23%</div> </div>
3	C	406	<div> <div>23%</div> <div>62%</div> <div>16%</div> <div>22%</div> </div>
4	D	418	<div> <div>24%</div> <div>63%</div> <div>17%</div> <div>19%</div> </div>






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Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	269	
12	l	269	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 63361 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	354	Total	C	N	O	S	0	0
			2776	1749	490	519	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	339	Total	C	N	O	S	0	0
			2638	1658	450	518	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	316	Total	C	N	O	S	0	0
			2464	1559	437	452	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	338	Total	C	N	O	S	0	0
			2666	1684	464	505	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	338	Total	C	N	O	S	0	0
			2664	1678	473	497	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	337	Total	C	N	O	S	0	0
			2627	1660	452	500	15		

- 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
			1826	1160	305	348	13		
7	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	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
			1708	1081	289	333	5		
8	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
9	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- 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
			1713	1062	311	335	5		
10	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
11	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
14	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	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
			1643	1033	280	318	12		
15	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	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
			1591	1013	265	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	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
			1570	1006	265	290	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	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
			1548	974	273	292	9		
18	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

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

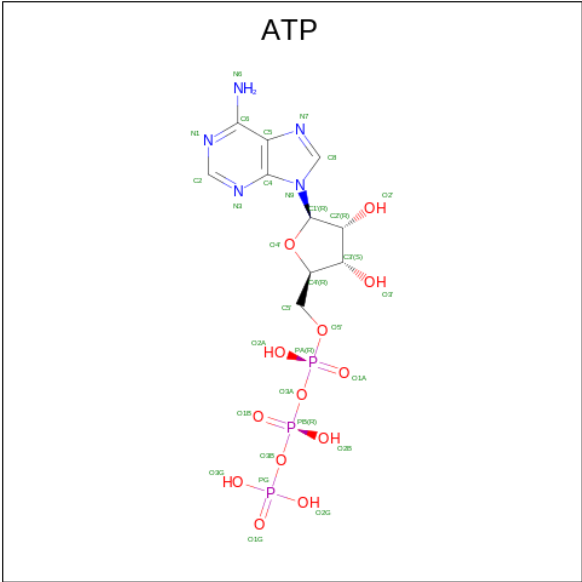
Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
19	s	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
20	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

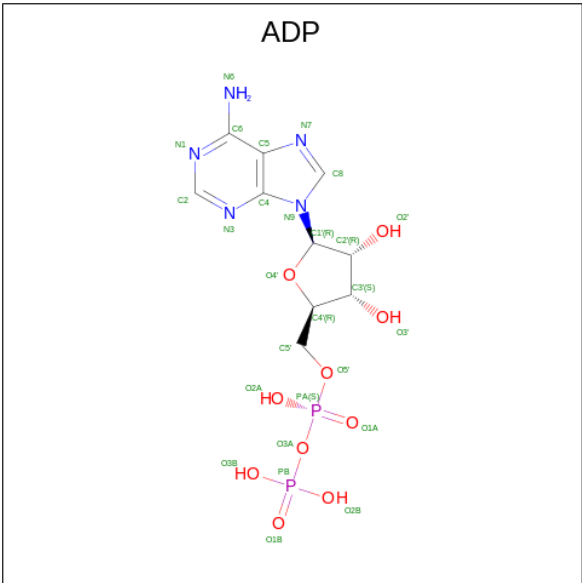
- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





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

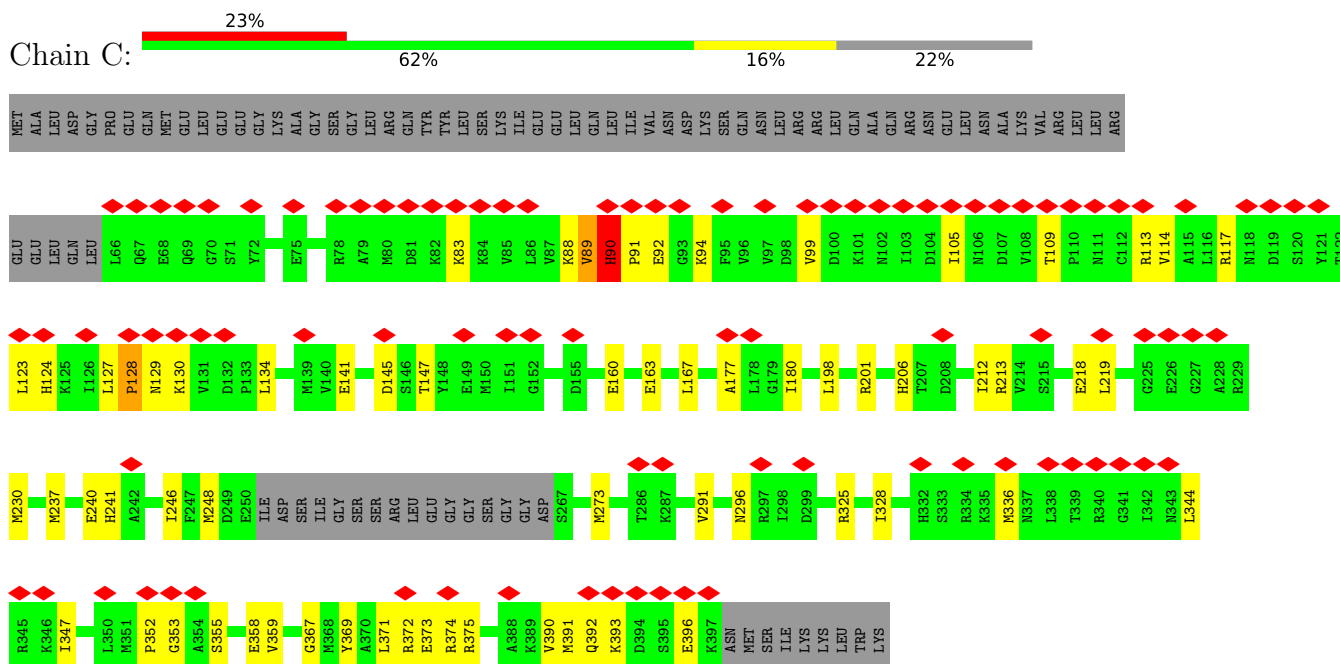
- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



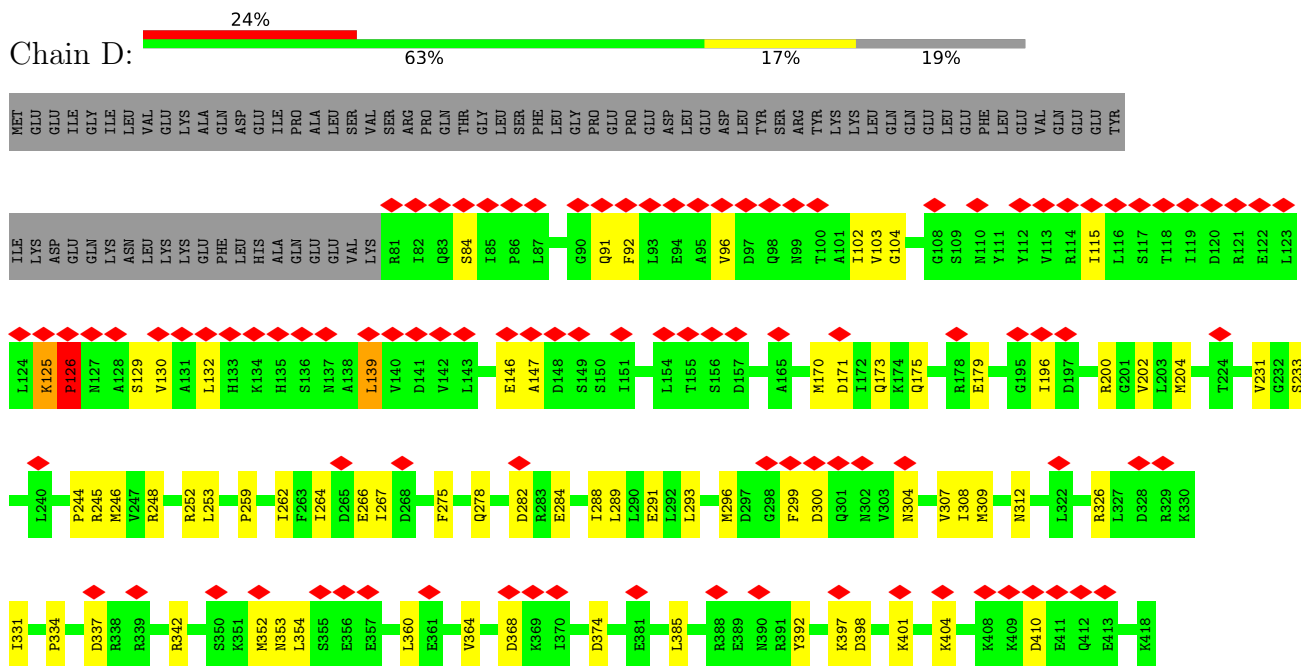
Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total 27	C 10	N 5	O 10	P 2	0
22	F	1	Total 27	C 10	N 5	O 10	P 2	0



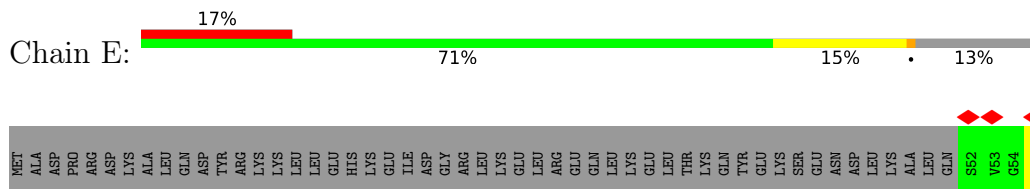
- Molecule 3: 26S proteasome regulatory subunit 8

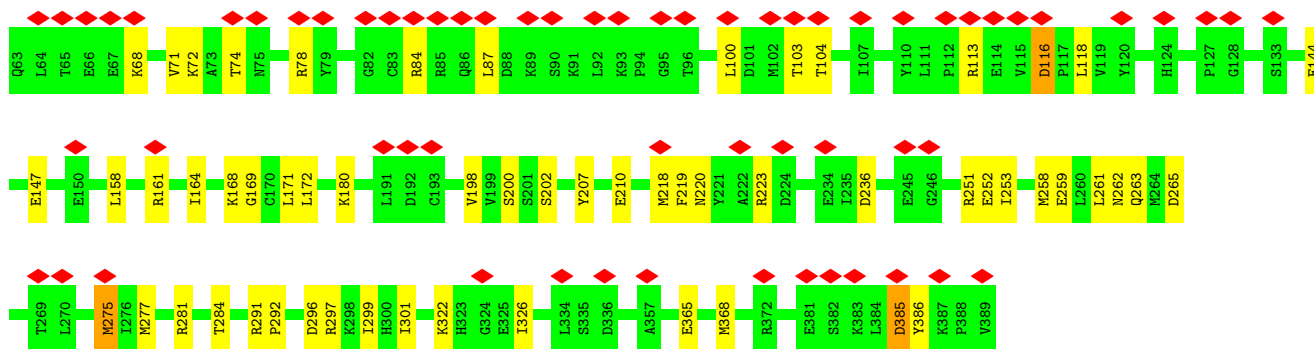


- Molecule 4: 26S proteasome regulatory subunit 6B

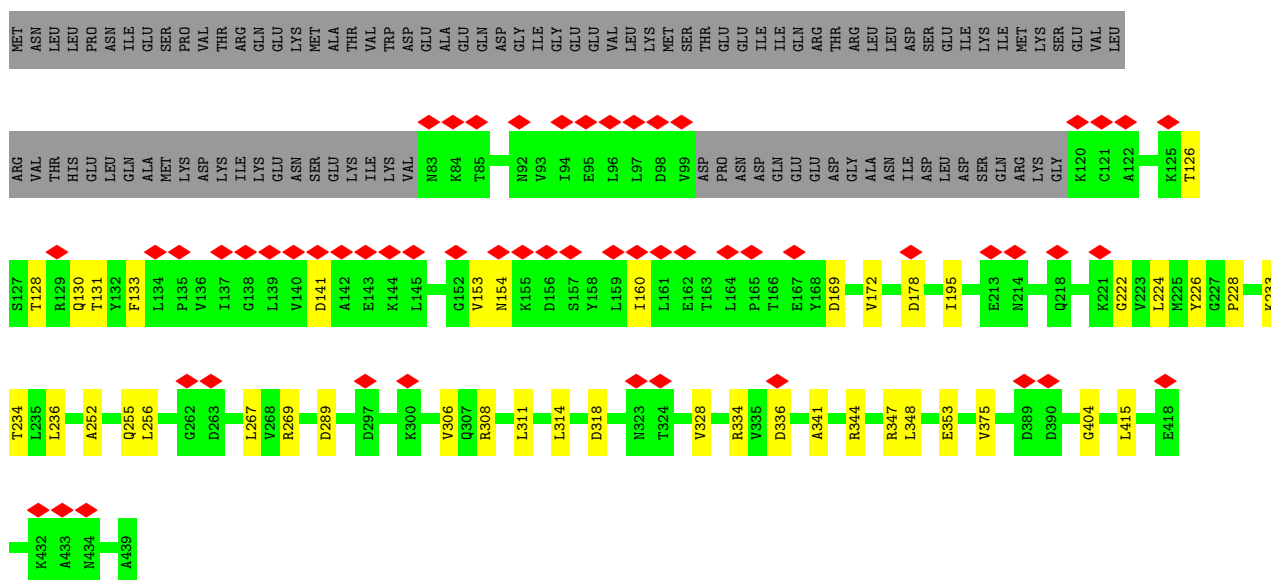


- Molecule 5: 26S proteasome regulatory subunit 10B

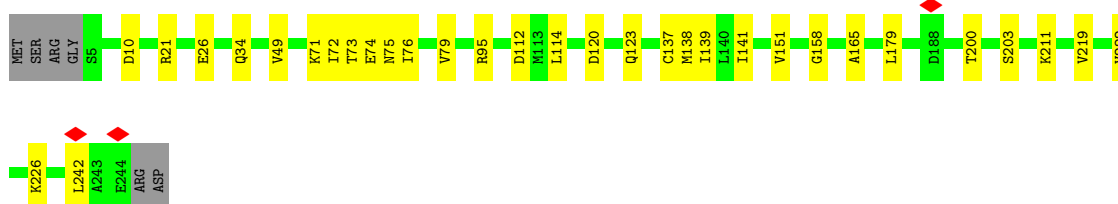
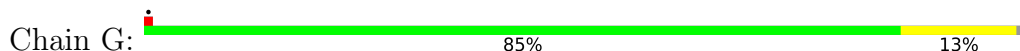




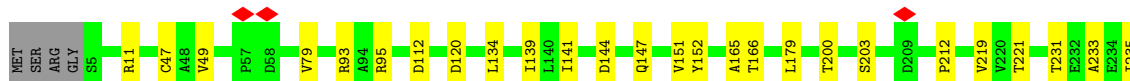
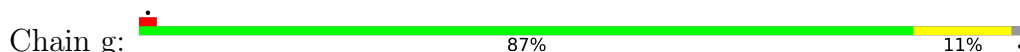
• Molecule 6: 26S proteasome regulatory subunit 6A

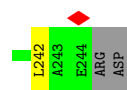


• Molecule 7: Proteasome subunit alpha type-6

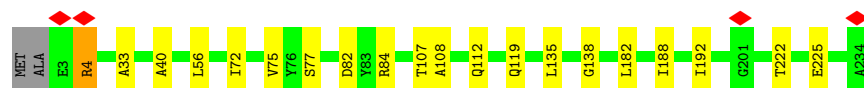


• Molecule 7: Proteasome subunit alpha type-6





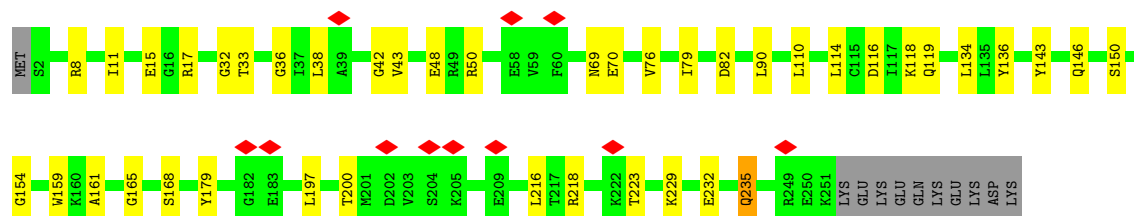
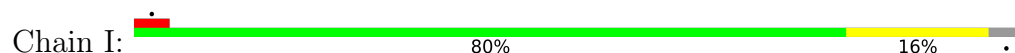
• Molecule 8: Proteasome subunit alpha type-2



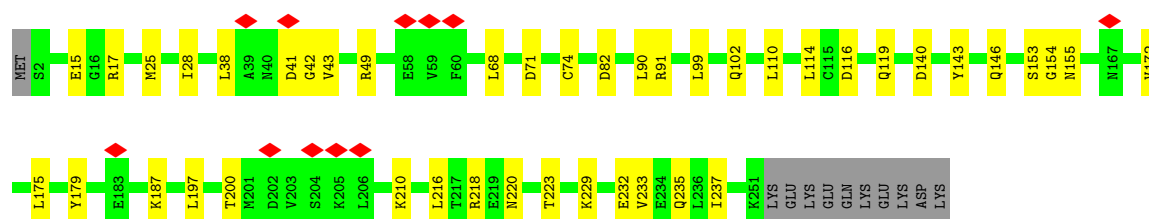
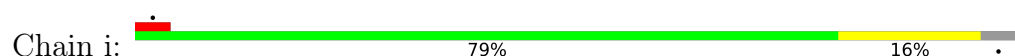
• Molecule 8: Proteasome subunit alpha type-2



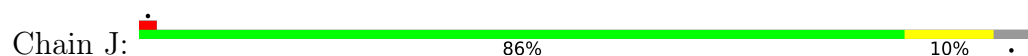
• Molecule 9: Proteasome subunit alpha type-4

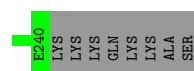


• Molecule 9: Proteasome subunit alpha type-4

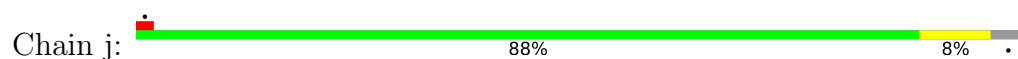


• Molecule 10: Proteasome subunit alpha type-7

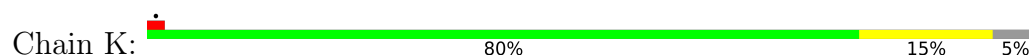




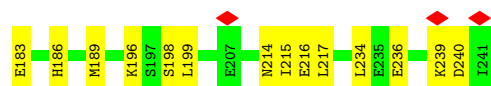
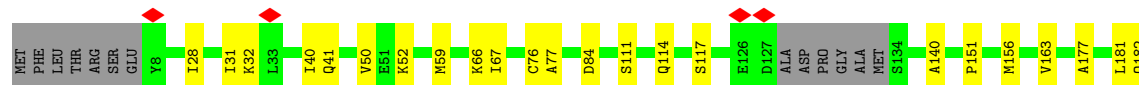
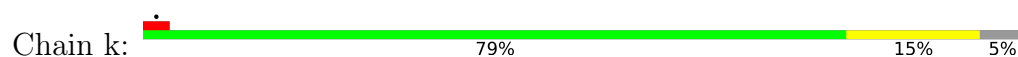
- Molecule 10: Proteasome subunit alpha type-7



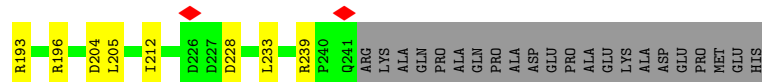
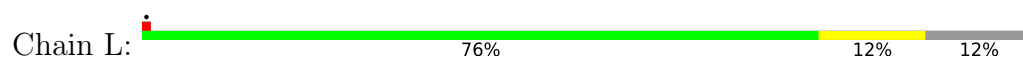
- Molecule 11: Proteasome subunit alpha type-5



- Molecule 11: Proteasome subunit alpha type-5

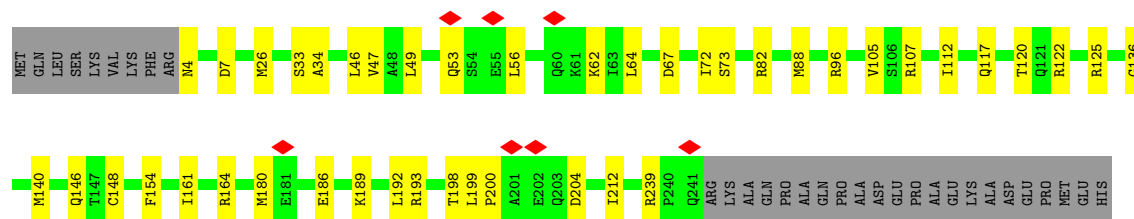


- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

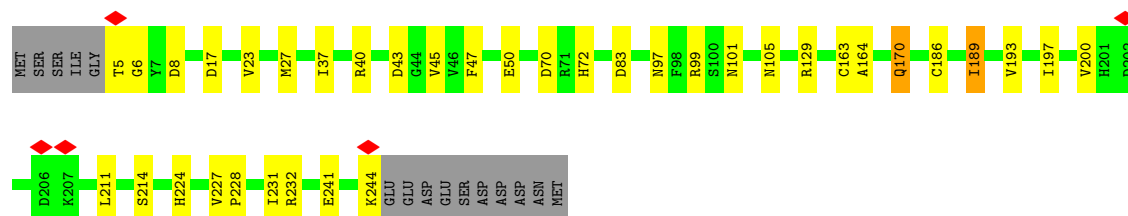
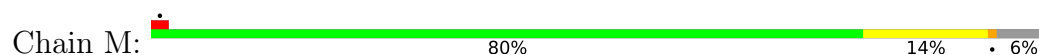


- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

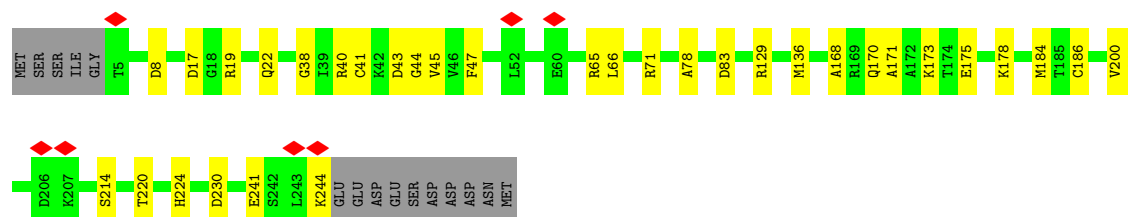
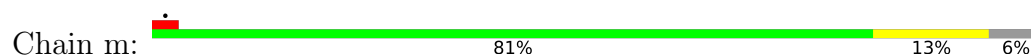




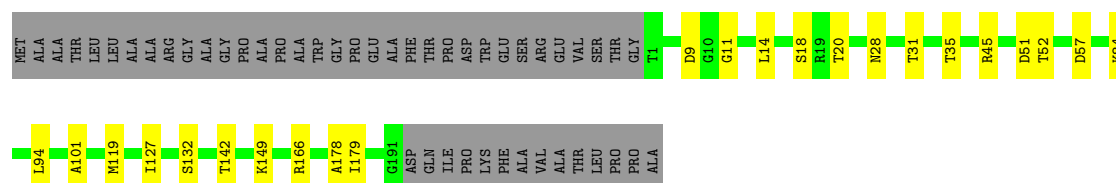
- Molecule 13: Proteasome subunit alpha type-3



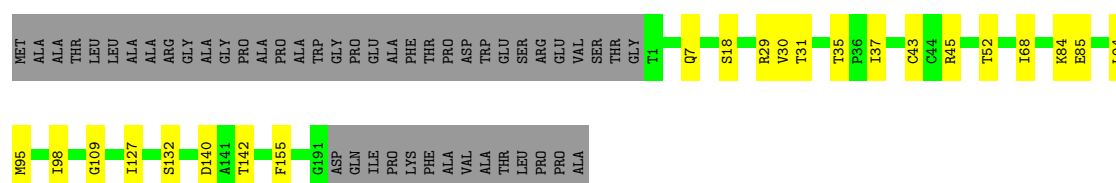
- Molecule 13: Proteasome subunit alpha type-3



- Molecule 14: Proteasome subunit beta type-6

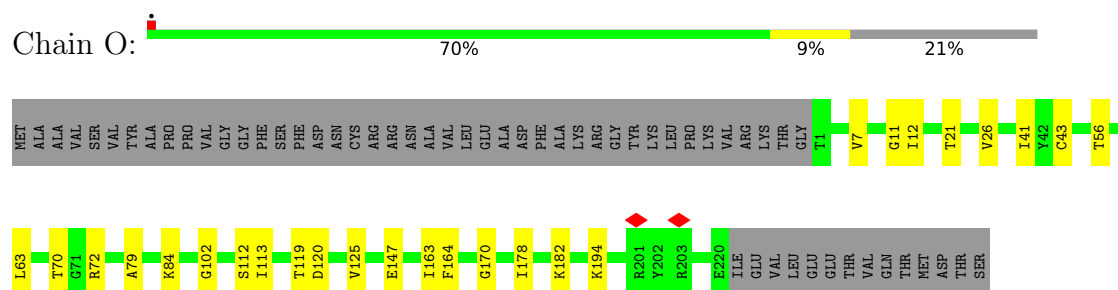


- Molecule 14: Proteasome subunit beta type-6

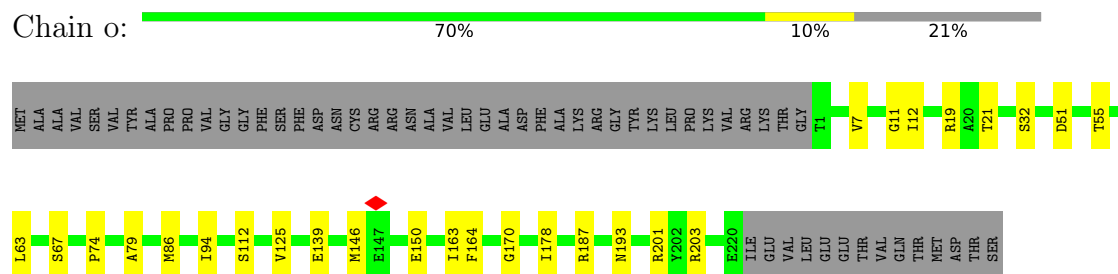




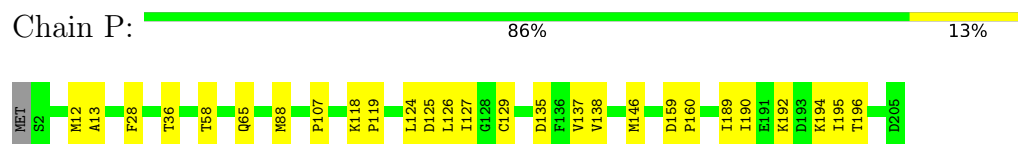
- Molecule 15: Proteasome subunit beta type-7



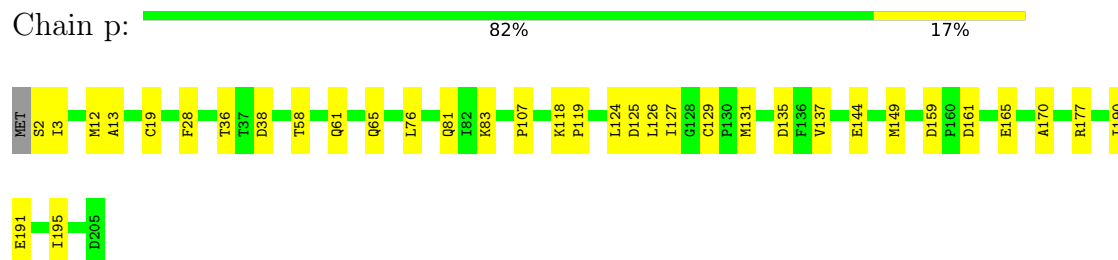
- Molecule 15: Proteasome subunit beta type-7



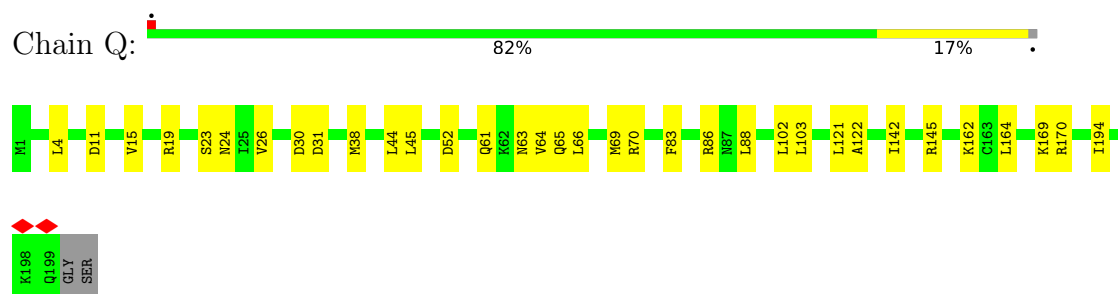
- Molecule 16: Proteasome subunit beta type-3



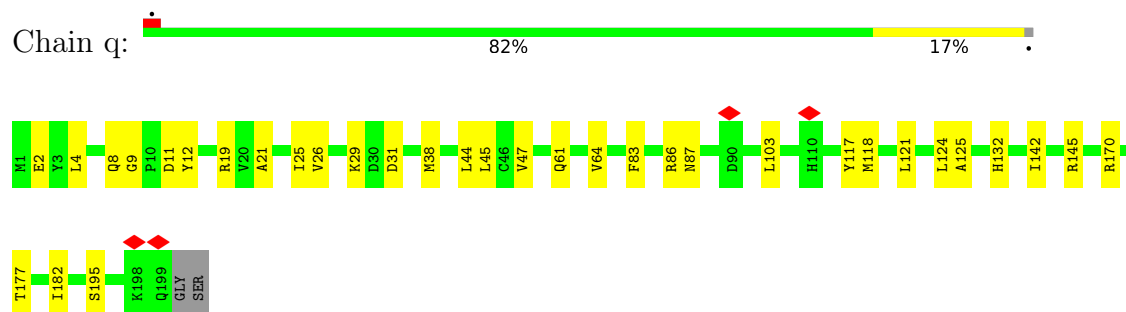
- Molecule 16: Proteasome subunit beta type-3



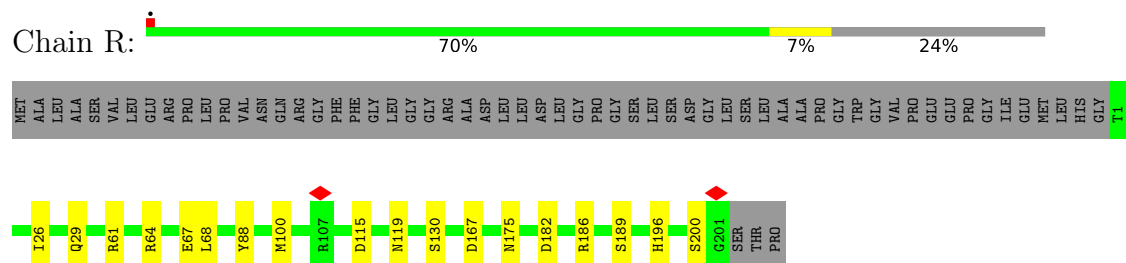
- Molecule 17: Proteasome subunit beta type-2



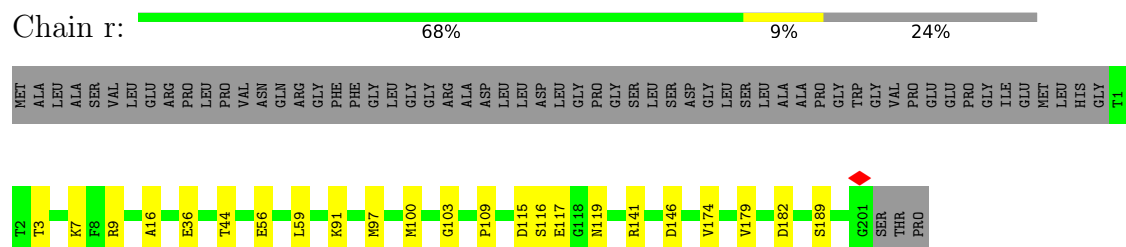
- Molecule 17: Proteasome subunit beta type-2



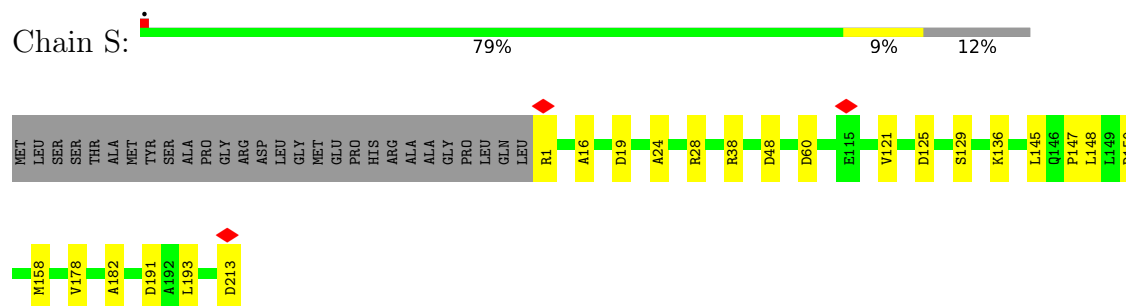
- Molecule 18: Proteasome subunit beta type-5



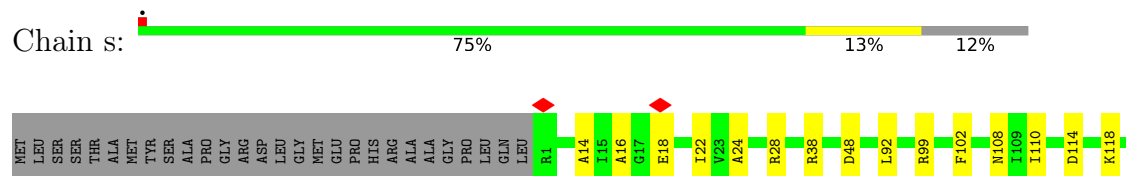
- Molecule 18: Proteasome subunit beta type-5

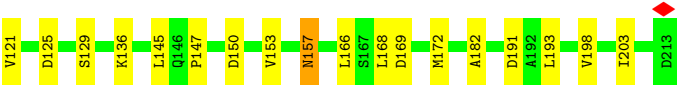


- Molecule 19: Proteasome subunit beta type-1

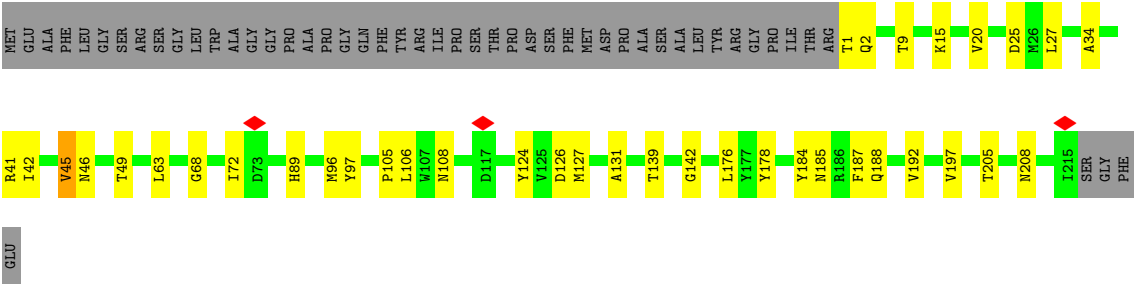


- Molecule 19: Proteasome subunit beta type-1

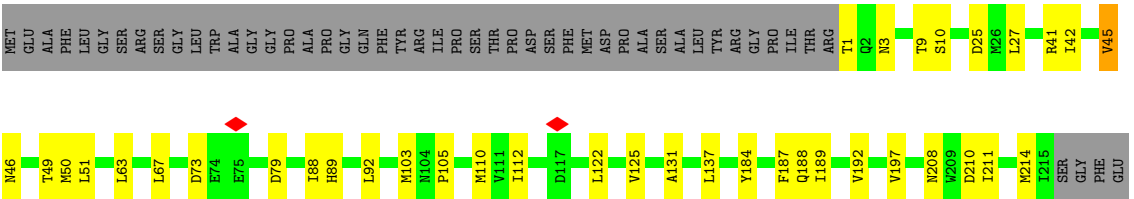




• Molecule 20: Proteasome subunit beta type-4



• Molecule 20: Proteasome subunit beta type-4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88200	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)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	369.59998, 369.59998, 369.59998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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, 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	A	0.18	0/2823	0.55	1/3809 (0.0%)
2	B	0.19	0/2675	0.54	0/3611
3	C	0.22	0/2500	0.57	0/3366
4	D	0.22	0/2710	0.61	2/3663 (0.1%)
5	E	0.20	0/2708	0.55	0/3653
6	F	0.19	0/2665	0.50	0/3597
7	G	0.17	0/1859	0.46	0/2523
7	g	0.19	0/1859	0.51	0/2523
8	H	0.16	0/1743	0.45	0/2372
8	h	0.16	0/1743	0.47	1/2372 (0.0%)
9	I	0.17	0/1942	0.50	1/2628 (0.0%)
9	i	0.17	0/1942	0.50	0/2628
10	J	0.17	0/1737	0.48	0/2369
10	j	0.16	0/1728	0.49	0/2358
11	K	0.17	0/1747	0.49	1/2364 (0.0%)
11	k	0.18	0/1747	0.49	0/2364
12	L	0.17	0/1885	0.48	0/2552
12	l	0.18	0/1885	0.51	0/2552
13	M	0.20	0/1891	0.53	0/2552
13	m	0.17	0/1891	0.48	0/2552
14	N	0.15	0/1454	0.43	0/1967
14	n	0.19	0/1454	0.54	0/1967
15	O	0.18	0/1670	0.53	0/2265
15	o	0.16	0/1670	0.46	0/2265
16	P	0.17	0/1620	0.47	0/2184
16	p	0.18	0/1620	0.48	0/2184
17	Q	0.18	0/1603	0.50	0/2174
17	q	0.18	0/1603	0.51	0/2174
18	R	0.16	0/1579	0.46	0/2134
18	r	0.18	0/1579	0.47	0/2134
19	S	0.17	0/1671	0.44	0/2253
19	s	0.19	0/1674	0.49	0/2257

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.17	0/1700	0.46	0/2305
20	t	0.17	0/1700	0.47	0/2305
All	All	0.18	0/64277	0.50	6/86976 (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
3	C	0	5
4	D	0	3
5	E	0	2
7	G	0	1
10	J	0	1
10	j	0	1
20	T	0	1
20	t	0	1
All	All	0	15

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(°)
11	K	32	LYS	CB-CG-CD	5.59	124.16	111.30
1	A	400	ARG	CA-CB-CG	5.33	124.75	114.10
9	I	235	GLN	CA-CB-CG	5.20	124.49	114.10
8	h	150	ASP	CB-CA-C	5.03	116.87	109.22
4	D	126	PRO	CA-C-N	5.02	128.35	121.33

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	127	LEU	Peptide
3	C	128	PRO	Peptide
3	C	129	ASN	Peptide
3	C	89	VAL	Peptide
3	C	90	HIS	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	2776	0	2814	33	0
2	B	2638	0	2679	42	0
3	C	2464	0	2546	39	0
4	D	2666	0	2707	50	0
5	E	2664	0	2721	42	0
6	F	2627	0	2688	30	0
7	G	1826	0	1796	21	0
7	g	1826	0	1796	18	0
8	H	1708	0	1594	14	0
8	h	1708	0	1594	9	0
9	I	1912	0	1851	29	0
9	i	1912	0	1851	28	0
10	J	1713	0	1537	21	0
10	j	1704	0	1517	12	0
11	K	1722	0	1673	25	0
11	k	1722	0	1673	22	0
12	L	1850	0	1822	22	0
12	l	1850	0	1822	28	0
13	M	1856	0	1814	23	0
13	m	1856	0	1814	21	0
14	N	1430	0	1398	14	0
14	n	1430	0	1398	14	0
15	O	1643	0	1644	18	0
15	o	1643	0	1644	16	0
16	P	1591	0	1609	17	0
16	p	1591	0	1609	26	0
17	Q	1570	0	1547	29	0
17	q	1570	0	1547	23	0
18	R	1548	0	1499	12	0
18	r	1548	0	1499	15	0
19	S	1641	0	1616	16	0
19	s	1644	0	1625	20	0
20	T	1667	0	1628	22	0
20	t	1667	0	1628	27	0
21	A	31	0	12	1	0
21	B	31	0	12	1	0
21	D	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	E	31	0	12	0	0
22	C	27	0	12	1	0
22	F	27	0	12	2	0
All	All	63361	0	62272	717	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 6.

The worst 5 of 717 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)
9:I:42:GLY:HA2	9:I:216:LEU:O	1.78	0.82
9:i:42:GLY:HA2	9:i:216:LEU:O	1.86	0.74
13:M:47:PHE:HB2	13:M:214:SER:HB3	1.70	0.72
11:k:236:GLU:HA	11:k:239:LYS:HE3	1.72	0.71
10:J:86:ARG:HE	10:J:114:LEU:HD11	1.58	0.68

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	352/433 (81%)	309 (88%)	43 (12%)	0	100	100
2	B	337/440 (77%)	321 (95%)	16 (5%)	0	100	100
3	C	312/406 (77%)	290 (93%)	20 (6%)	2 (1%)	21	52
4	D	336/418 (80%)	294 (88%)	41 (12%)	1 (0%)	36	67
5	E	336/389 (86%)	305 (91%)	31 (9%)	0	100	100
6	F	333/439 (76%)	304 (91%)	29 (9%)	0	100	100
7	G	238/246 (97%)	227 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	238/246 (97%)	224 (94%)	14 (6%)	0	100	100
8	H	230/234 (98%)	224 (97%)	6 (3%)	0	100	100
8	h	230/234 (98%)	222 (96%)	8 (4%)	0	100	100
9	I	248/261 (95%)	231 (93%)	17 (7%)	0	100	100
9	i	248/261 (95%)	232 (94%)	16 (6%)	0	100	100
10	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
10	j	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
11	K	224/241 (93%)	214 (96%)	10 (4%)	0	100	100
11	k	224/241 (93%)	217 (97%)	7 (3%)	0	100	100
12	L	236/269 (88%)	222 (94%)	14 (6%)	0	100	100
12	l	236/269 (88%)	221 (94%)	15 (6%)	0	100	100
13	M	238/255 (93%)	228 (96%)	10 (4%)	0	100	100
13	m	238/255 (93%)	229 (96%)	9 (4%)	0	100	100
14	N	189/239 (79%)	182 (96%)	7 (4%)	0	100	100
14	n	189/239 (79%)	180 (95%)	9 (5%)	0	100	100
15	O	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
15	o	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
16	P	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
16	p	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
17	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
17	q	197/201 (98%)	185 (94%)	12 (6%)	0	100	100
18	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
18	r	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
19	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
19	s	211/241 (88%)	207 (98%)	4 (2%)	0	100	100
20	T	213/264 (81%)	204 (96%)	9 (4%)	0	100	100
20	t	213/264 (81%)	202 (95%)	11 (5%)	0	100	100
All	All	8166/9413 (87%)	7705 (94%)	458 (6%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	90	HIS

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Mol	Chain	Res	Type
4	D	126	PRO
3	C	128	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/372 (81%)	299 (99%)	2 (1%)	76	82
2	B	295/385 (77%)	294 (100%)	1 (0%)	86	87
3	C	270/352 (77%)	268 (99%)	2 (1%)	76	82
4	D	292/366 (80%)	289 (99%)	3 (1%)	68	79
5	E	294/341 (86%)	293 (100%)	1 (0%)	86	87
6	F	285/379 (75%)	284 (100%)	1 (0%)	84	86
7	G	193/210 (92%)	193 (100%)	0	100	100
7	g	193/210 (92%)	192 (100%)	1 (0%)	81	85
8	H	164/191 (86%)	163 (99%)	1 (1%)	78	83
8	h	164/191 (86%)	164 (100%)	0	100	100
9	I	193/221 (87%)	193 (100%)	0	100	100
9	i	193/221 (87%)	193 (100%)	0	100	100
10	J	154/211 (73%)	154 (100%)	0	100	100
10	j	152/211 (72%)	151 (99%)	1 (1%)	76	82
11	K	186/203 (92%)	186 (100%)	0	100	100
11	k	186/203 (92%)	186 (100%)	0	100	100
12	L	198/230 (86%)	196 (99%)	2 (1%)	68	79
12	l	198/230 (86%)	198 (100%)	0	100	100
13	M	192/212 (91%)	190 (99%)	2 (1%)	68	79
13	m	192/212 (91%)	191 (100%)	1 (0%)	81	85
14	N	148/181 (82%)	147 (99%)	1 (1%)	76	82
14	n	148/181 (82%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	177/228 (78%)	176 (99%)	1 (1%)	78	83
15	o	177/228 (78%)	177 (100%)	0	100	100
16	P	173/174 (99%)	172 (99%)	1 (1%)	78	83
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	164/171 (96%)	164 (100%)	0	100	100
17	q	164/171 (96%)	164 (100%)	0	100	100
18	R	153/202 (76%)	153 (100%)	0	100	100
18	r	153/202 (76%)	153 (100%)	0	100	100
19	S	174/199 (87%)	174 (100%)	0	100	100
19	s	175/199 (88%)	174 (99%)	1 (1%)	78	83
20	T	175/215 (81%)	175 (100%)	0	100	100
20	t	175/215 (81%)	175 (100%)	0	100	100
All	All	6624/7891 (84%)	6602 (100%)	22 (0%)	84	87

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	189	ILE
16	P	194	LYS
15	O	194	LYS
7	g	166	THR
4	D	170	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
9	i	146	GLN
16	p	93	ASN
10	j	116	GLN
12	l	146	GLN
19	s	163	HIS

### 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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
22	ADP	F	501	-	27,29,29	1.35	4 (14%)	42,45,45	1.95	10 (23%)
21	ATP	D	501	-	29,33,33	0.29	0	44,52,52	0.52	1 (2%)
21	ATP	E	401	-	29,33,33	0.27	0	44,52,52	0.46	1 (2%)
21	ATP	B	501	-	29,33,33	0.27	0	44,52,52	0.44	1 (2%)
22	ADP	C	501	-	27,29,29	1.36	4 (14%)	42,45,45	2.00	9 (21%)
21	ATP	A	501	-	29,33,33	0.29	0	44,52,52	0.46	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ADP	F	501	-	-	7/16/32/32	0/3/3/3
21	ATP	D	501	-	-	9/22/38/38	0/3/3/3
21	ATP	E	401	-	-	7/22/38/38	0/3/3/3
21	ATP	B	501	-	-	4/22/38/38	0/3/3/3
22	ADP	C	501	-	-	7/16/32/32	0/3/3/3
21	ATP	A	501	-	-	7/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	ADP	C5-C4	4.60	1.47	1.39
22	F	501	ADP	C5-C4	4.49	1.47	1.39
22	C	501	ADP	C5-C6	2.68	1.48	1.41
22	F	501	ADP	C5-C6	2.62	1.48	1.41
22	F	501	ADP	C8-N7	2.37	1.36	1.31

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	501	ADP	C5-C4-N3	-6.61	118.12	126.75
22	F	501	ADP	C5-C4-N3	-6.14	118.74	126.75
22	C	501	ADP	N3-C4-N9	5.20	135.66	127.08
22	F	501	ADP	N3-C4-N9	4.74	134.90	127.08
22	C	501	ADP	C2-N3-C4	3.98	121.14	111.75

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	501	ATP	C5'-O5'-PA-O1A
21	A	501	ATP	C3'-C4'-C5'-O5'
21	B	501	ATP	PB-O3B-PG-O3G
21	B	501	ATP	C5'-O5'-PA-O1A
21	B	501	ATP	C5'-O5'-PA-O2A

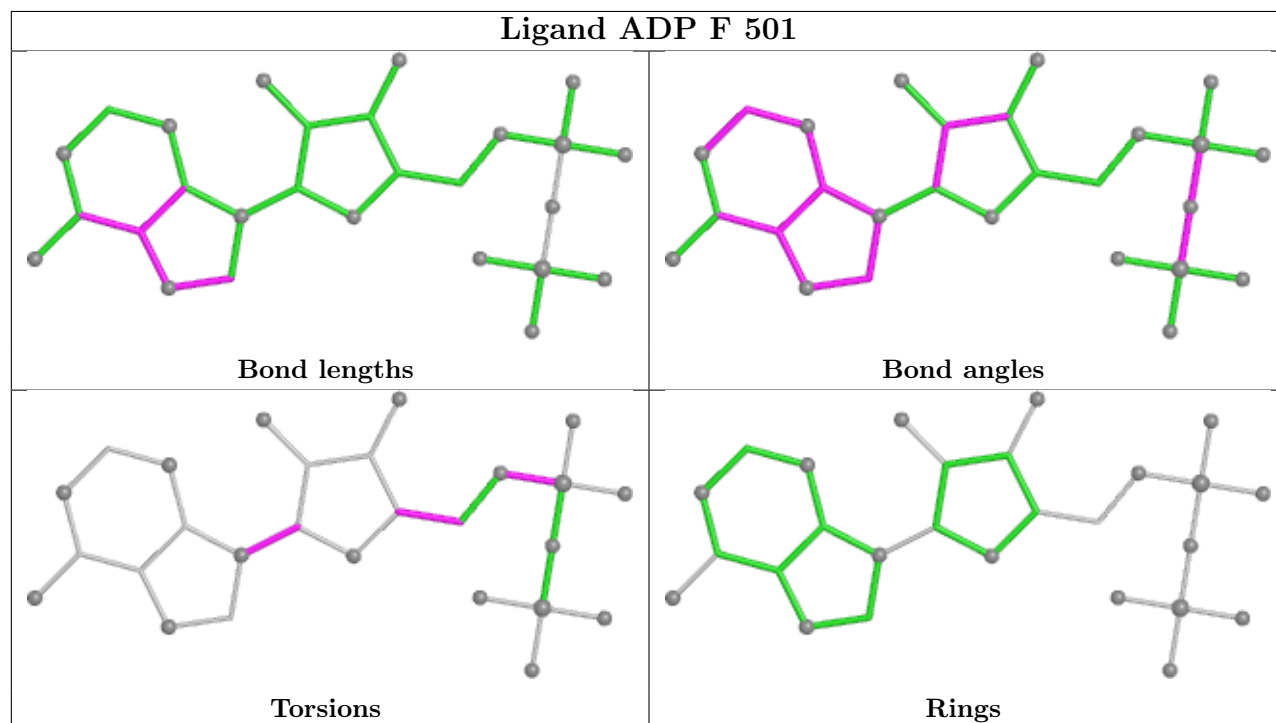
There are no ring outliers.

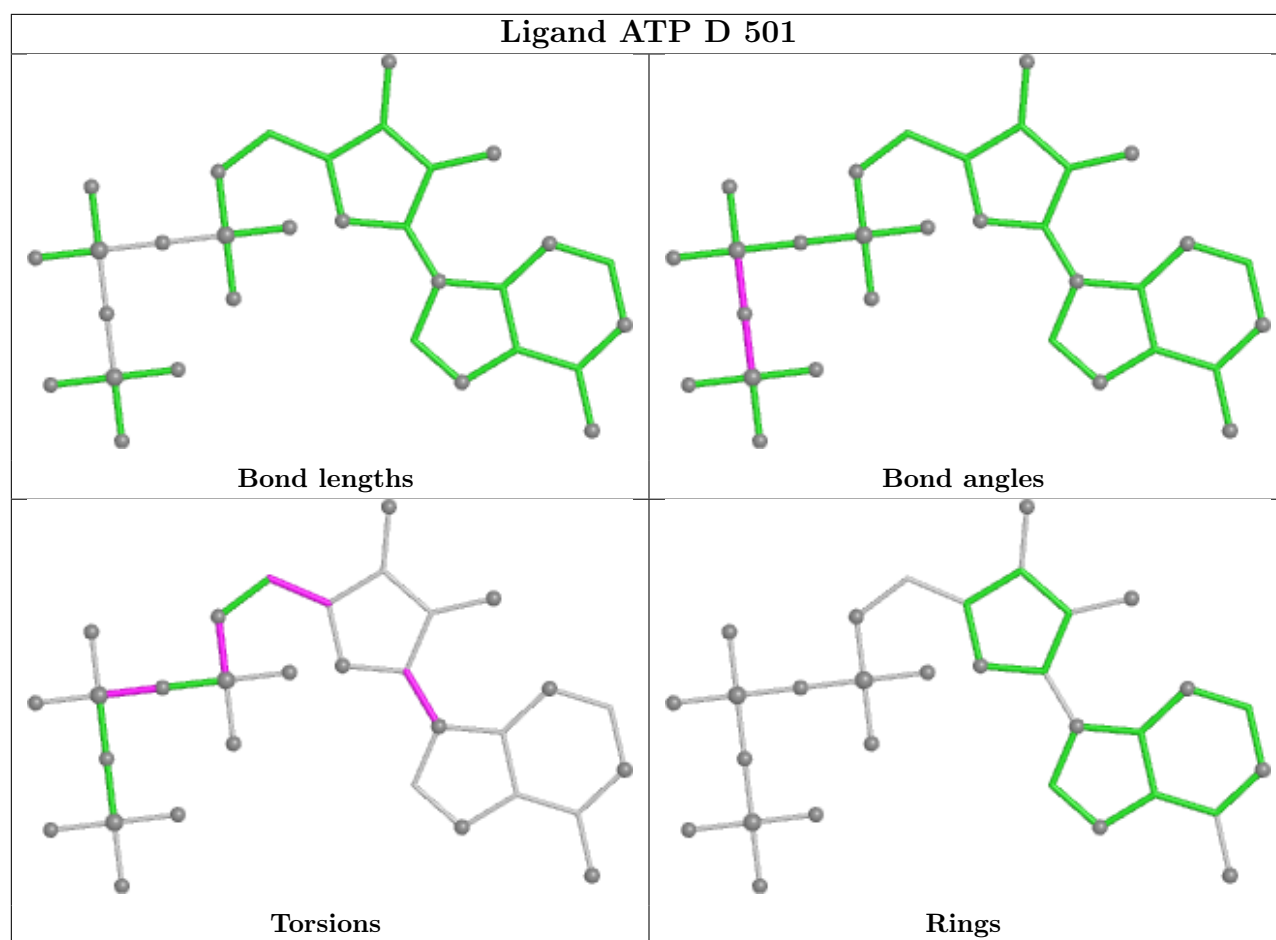
4 monomers are involved in 5 short contacts:

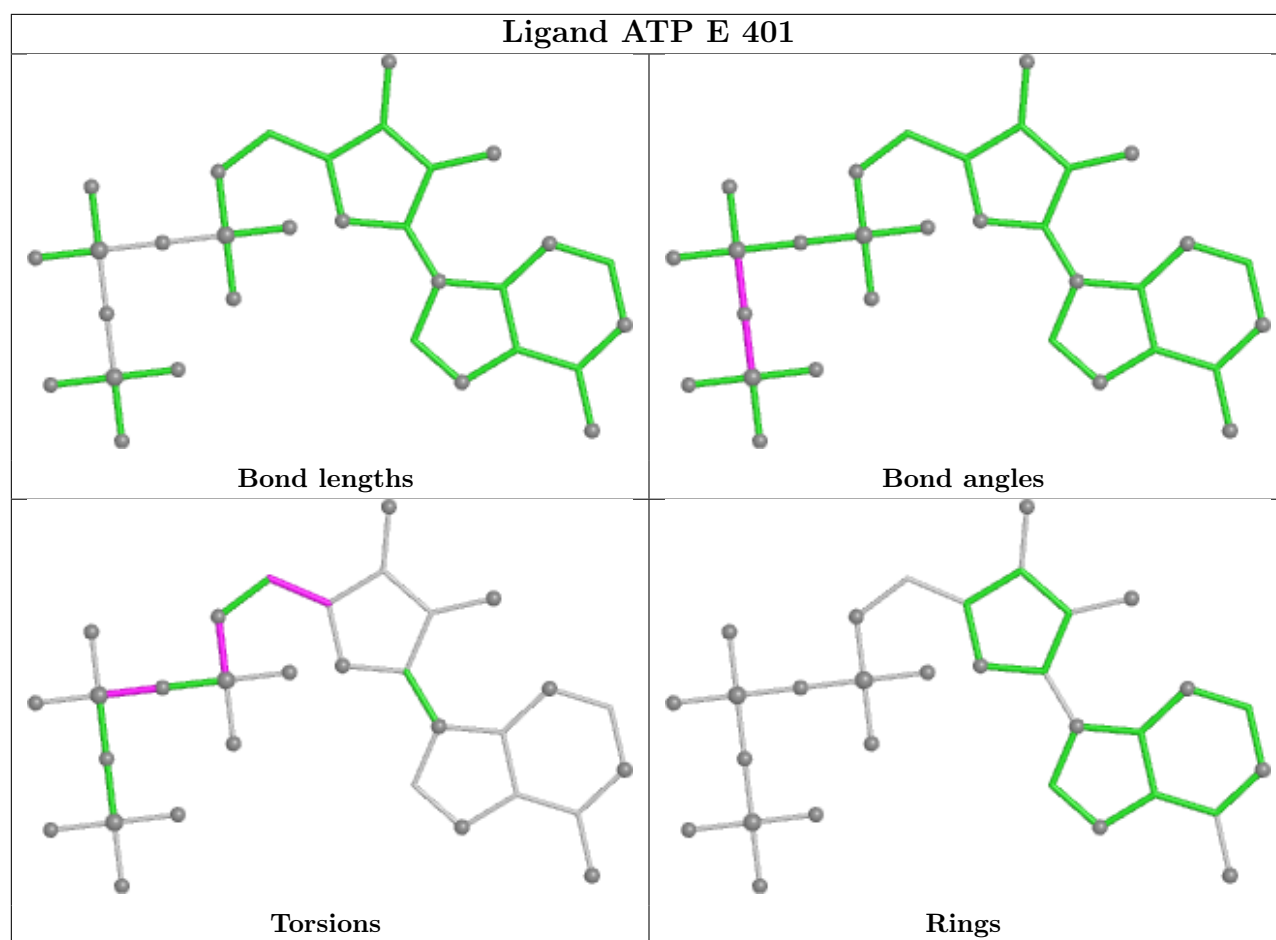
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	501	ADP	2	0
21	B	501	ATP	1	0
22	C	501	ADP	1	0
21	A	501	ATP	1	0

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.

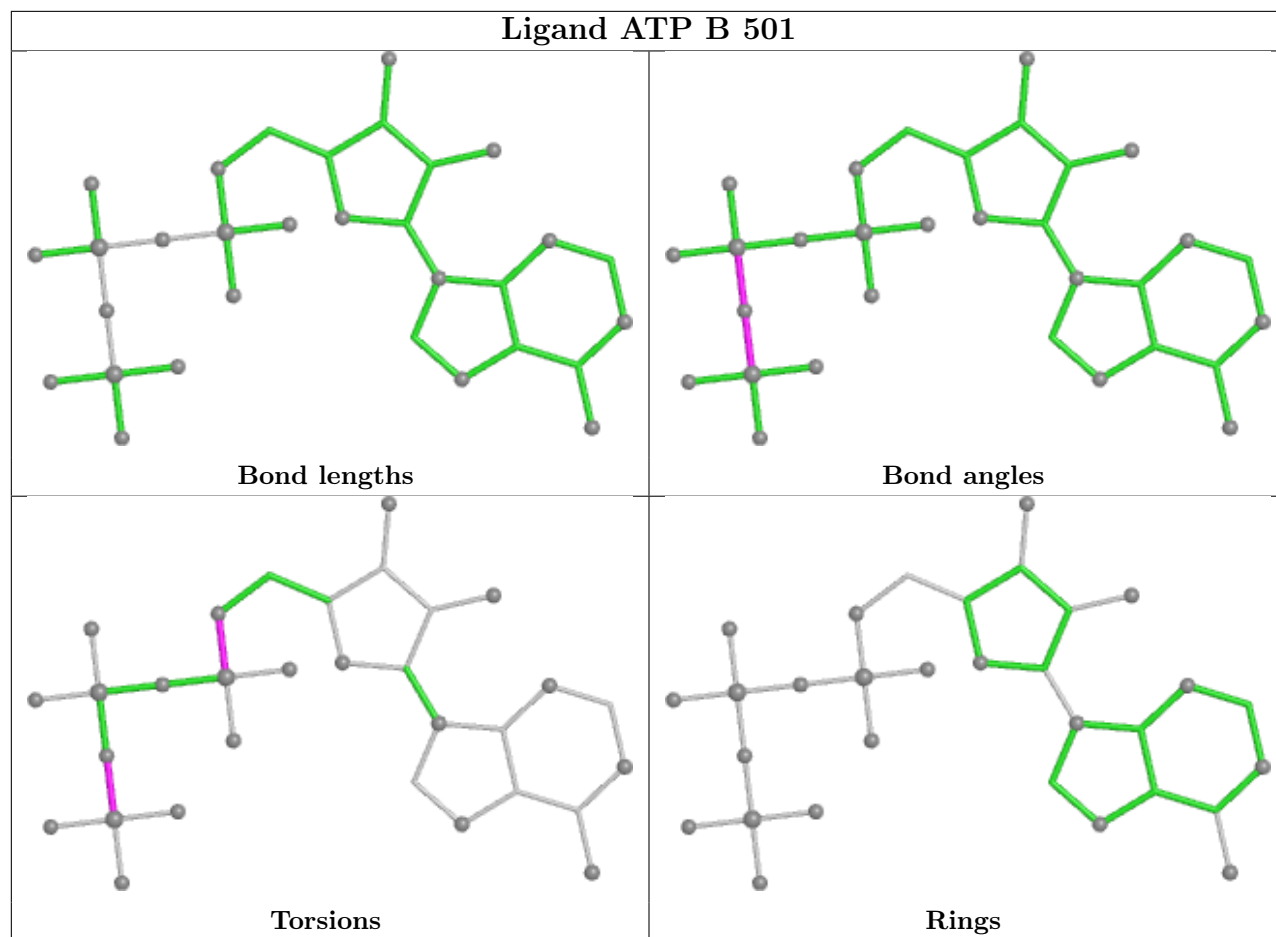




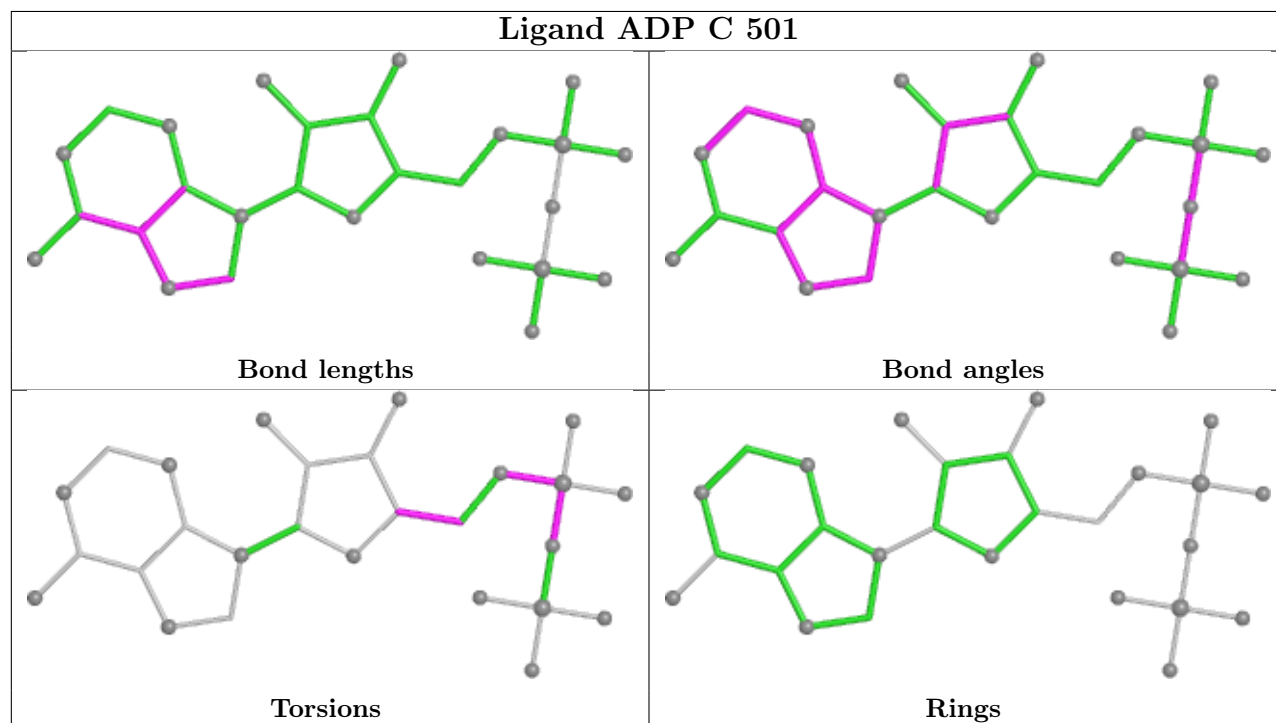


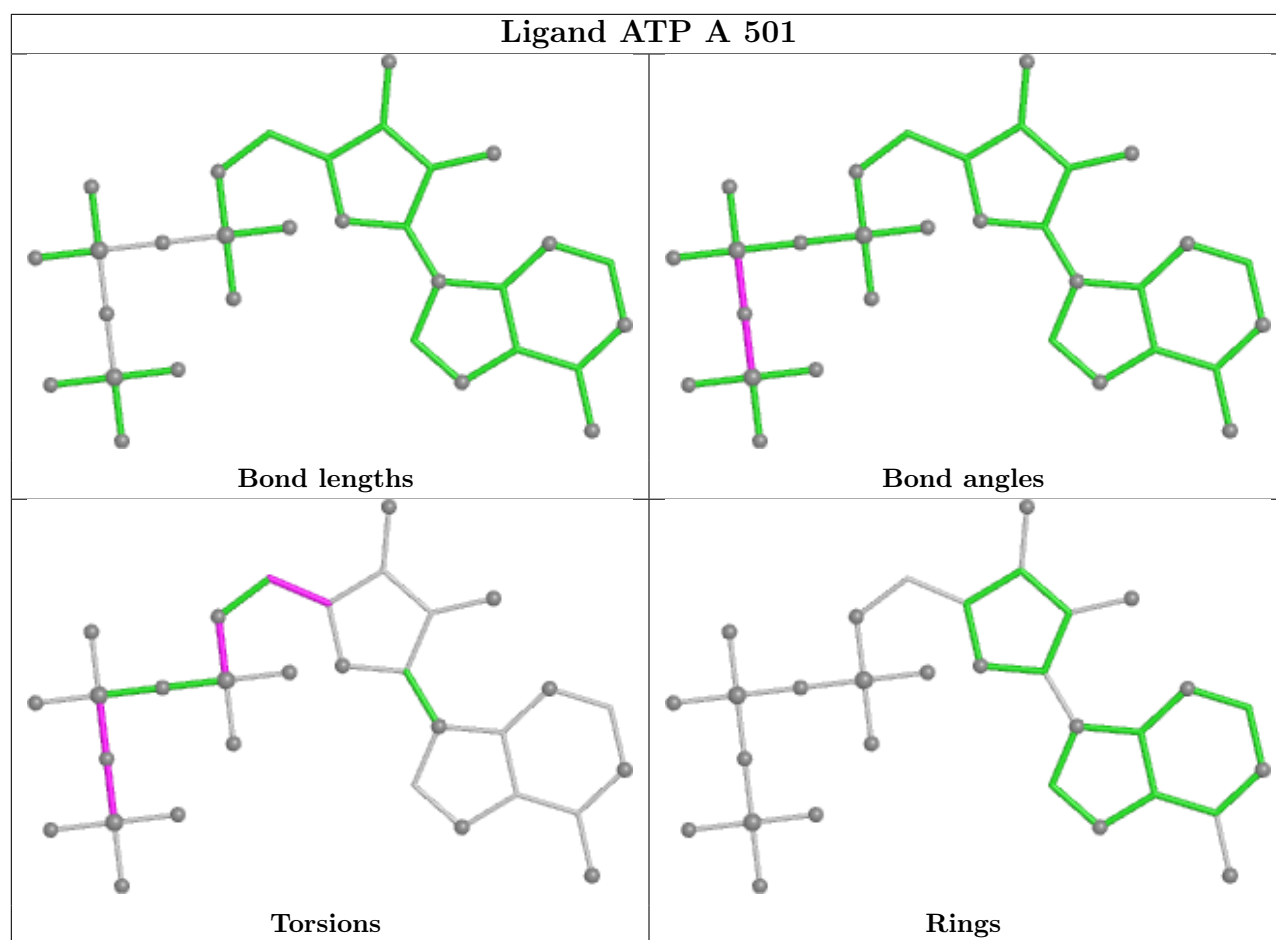


## Ligand ATP B 501



## Ligand ADP C 501





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

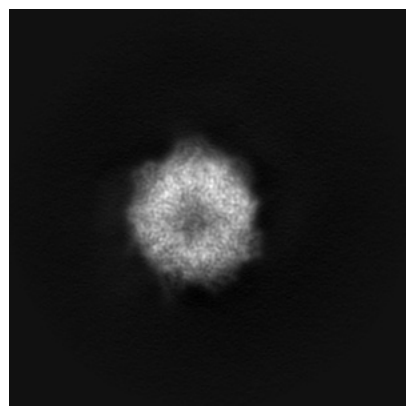
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65361. These allow visual inspection of the internal detail of the map and identification of artifacts.

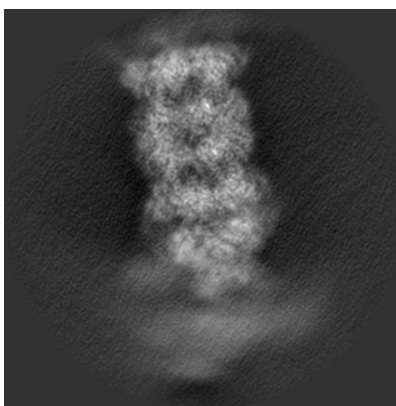
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

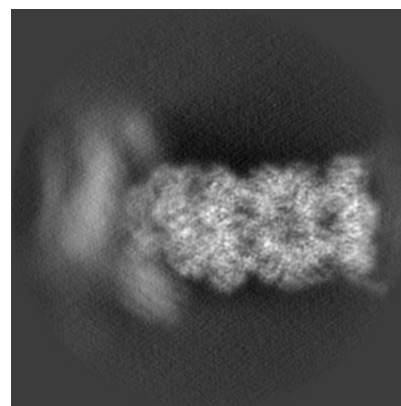
#### 6.1.1 Primary map



X

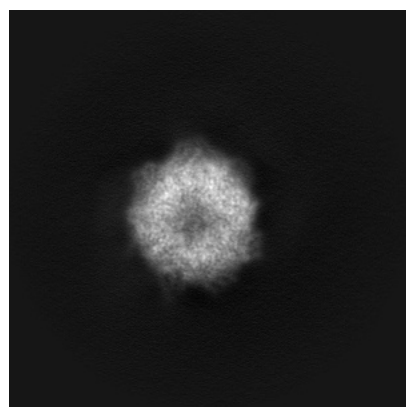


Y

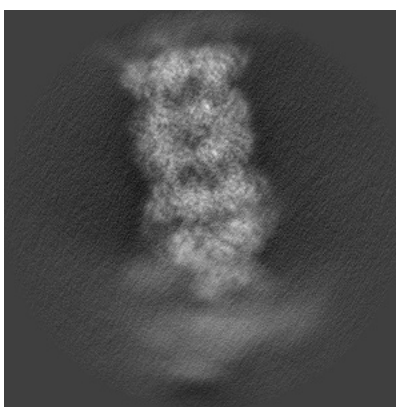


Z

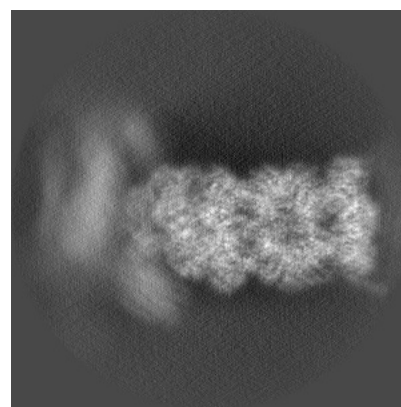
#### 6.1.2 Raw map



X



Y

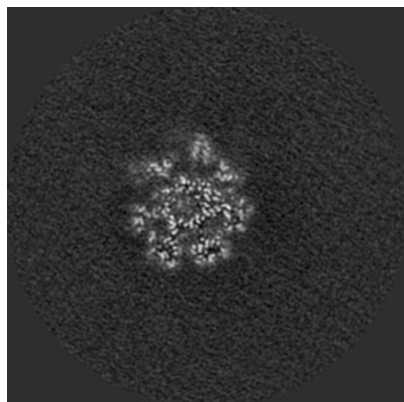


Z

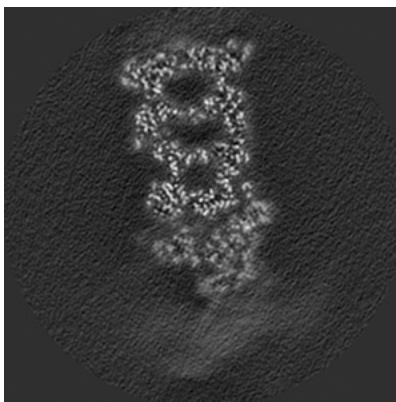
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

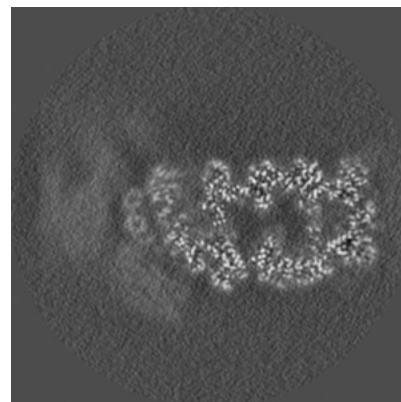
### 6.2.1 Primary map



X Index: 220

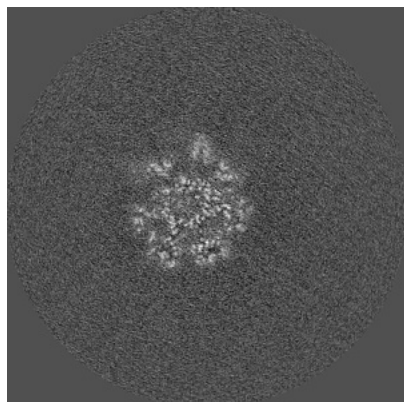


Y Index: 220

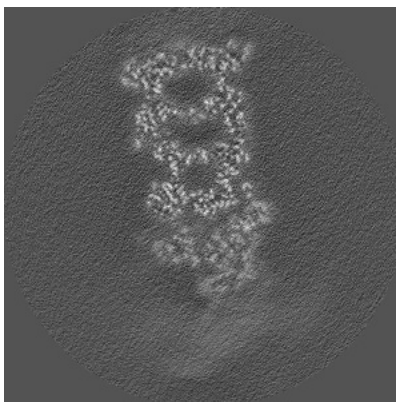


Z Index: 220

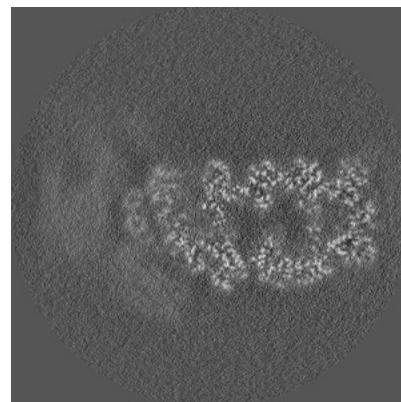
### 6.2.2 Raw map



X Index: 220



Y Index: 220

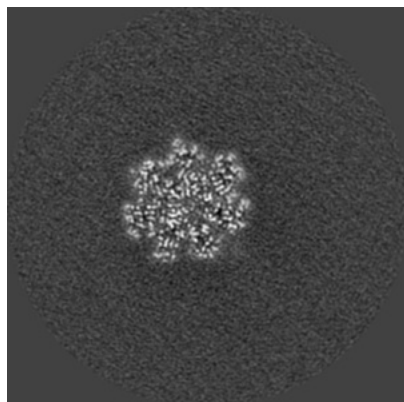


Z Index: 220

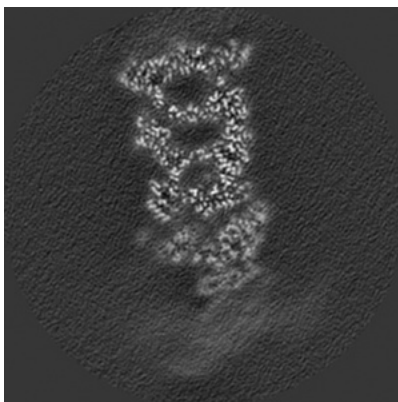
The images above show central slices of the map in three orthogonal directions.

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

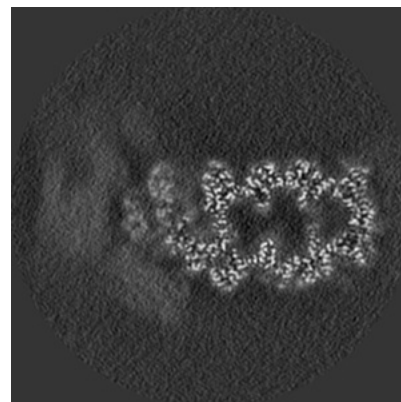
### 6.3.1 Primary map



X Index: 236

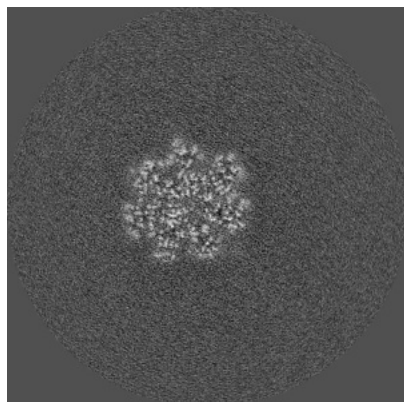


Y Index: 223

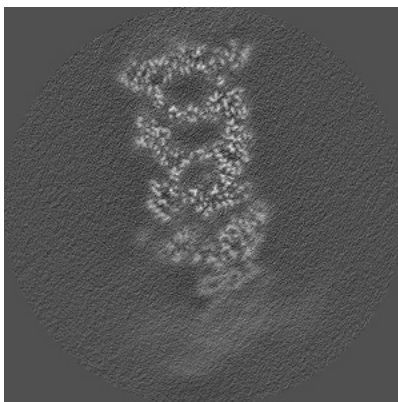


Z Index: 217

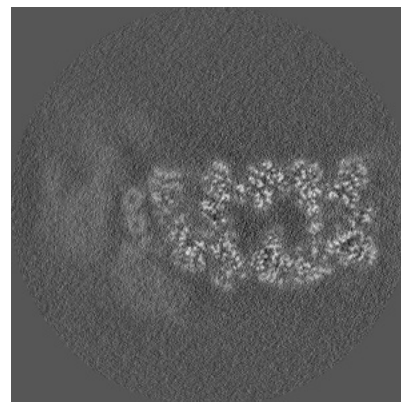
### 6.3.2 Raw map



X Index: 236



Y Index: 223



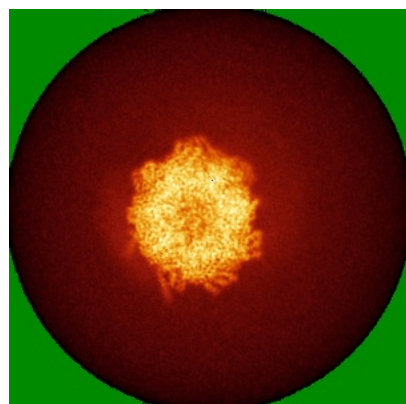
Z Index: 222

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

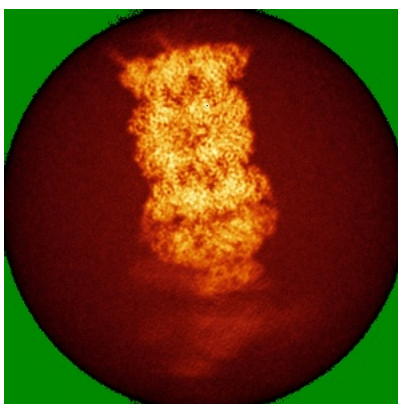


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

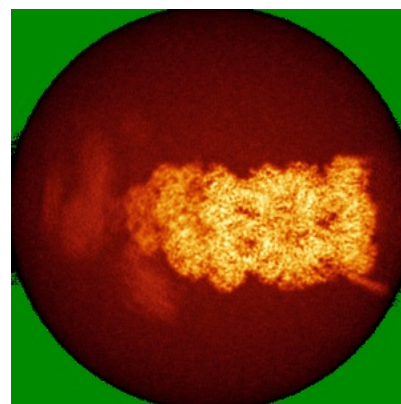
### 6.4.1 Primary map



X

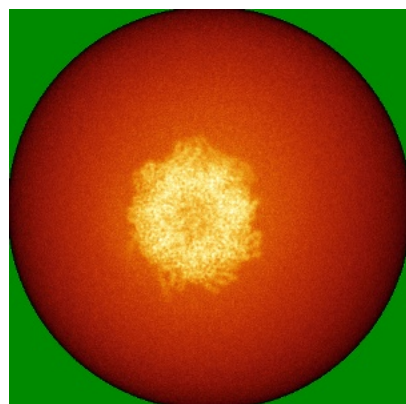


Y

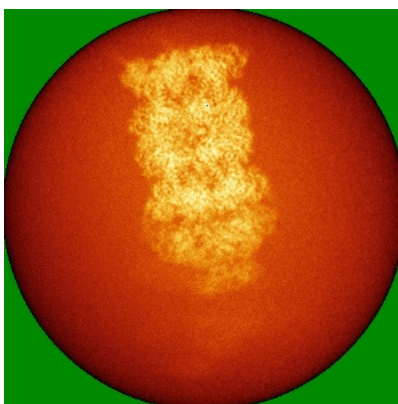


Z

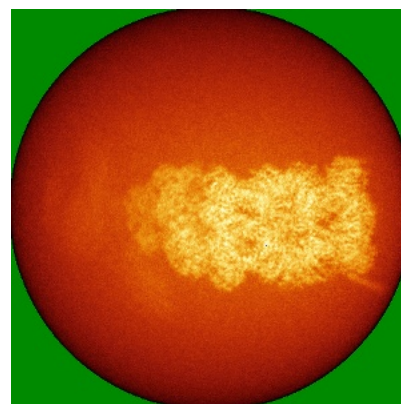
### 6.4.2 Raw map



X



Y

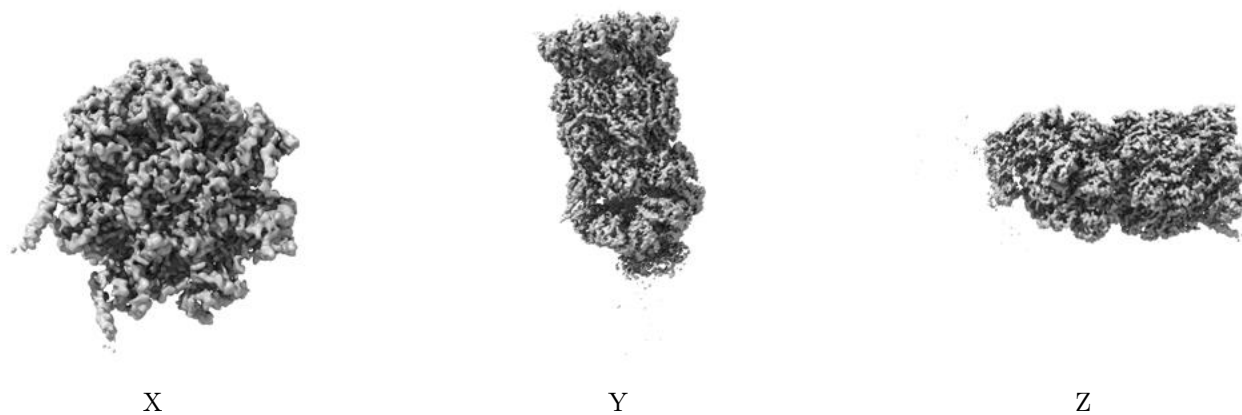


Z

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.

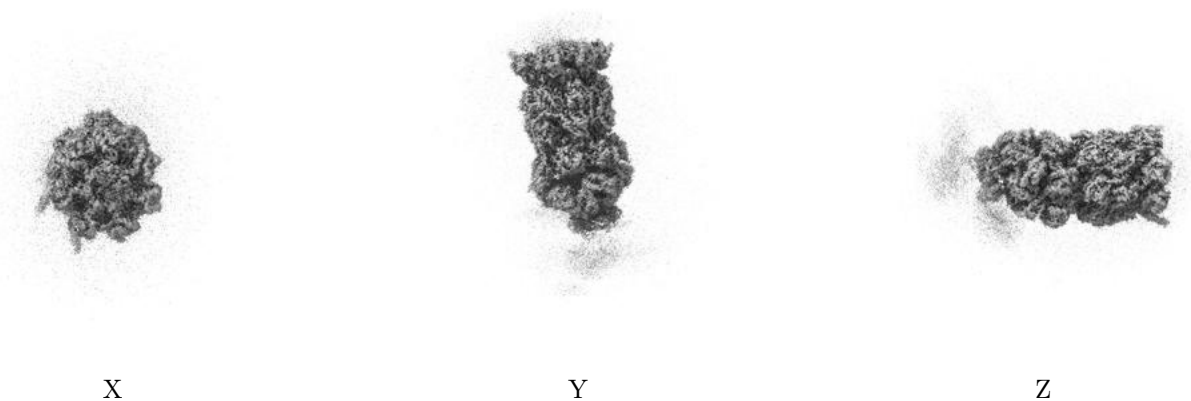
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. 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.

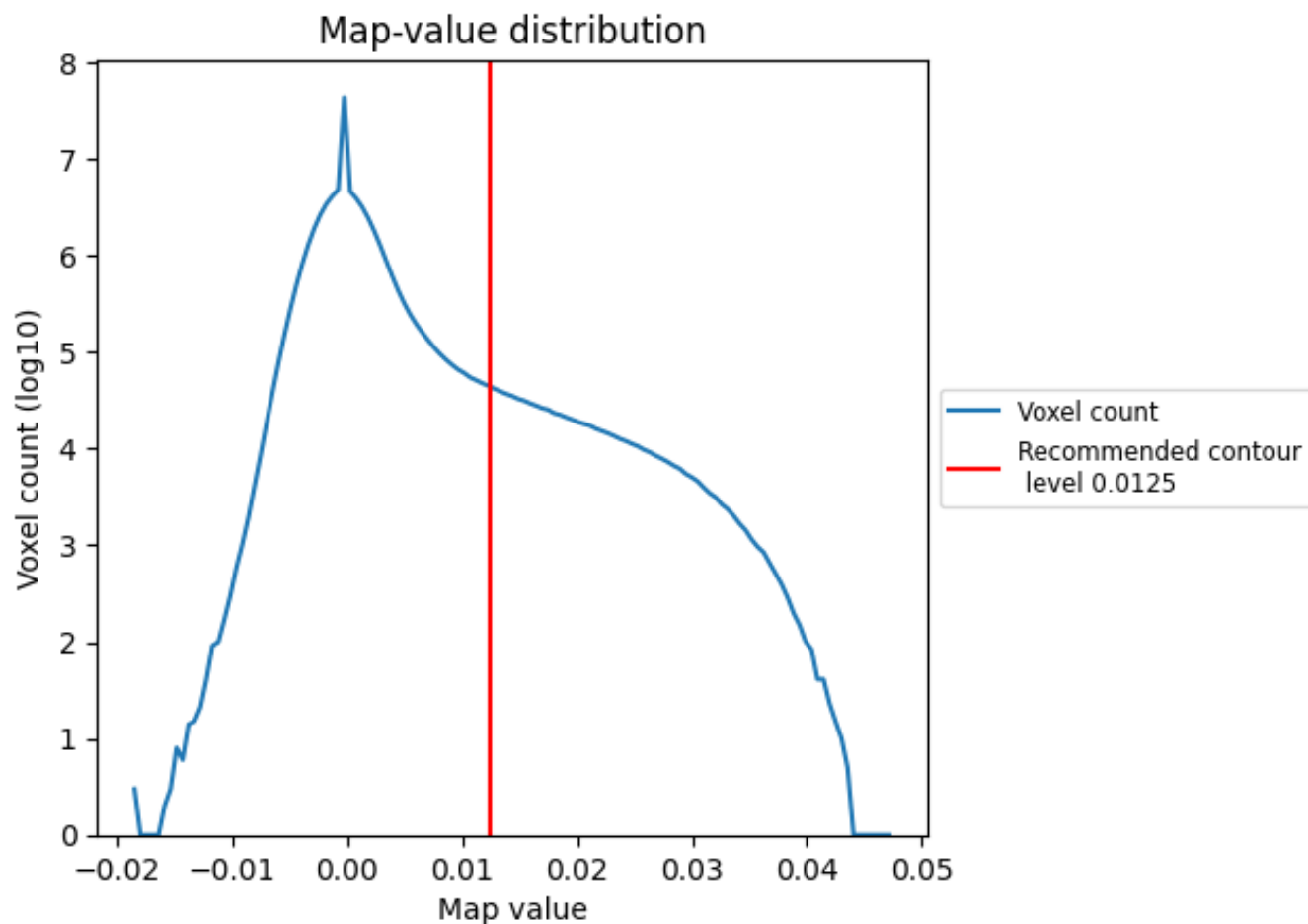
## 6.6 Mask visualisation [i](#)

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.

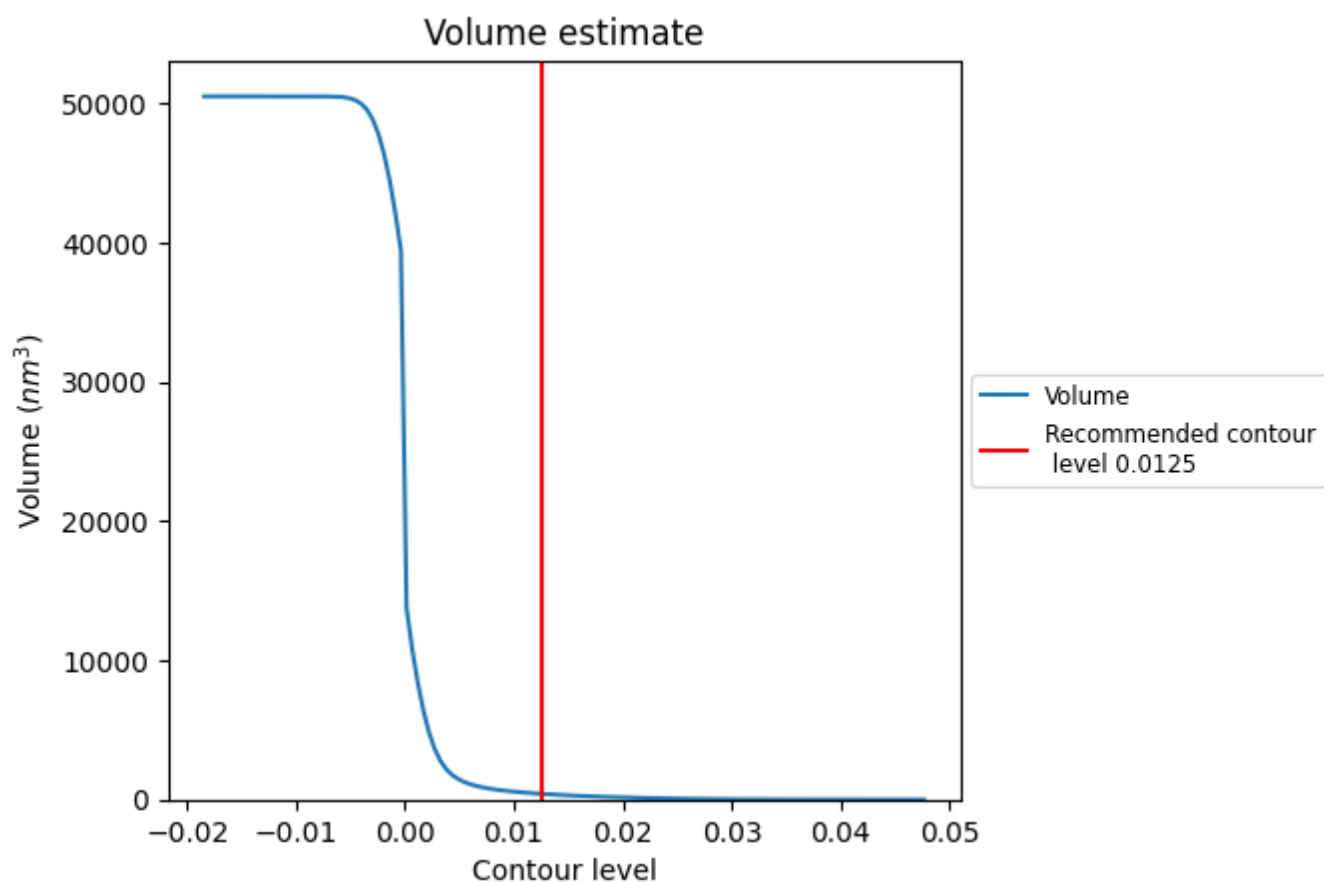
### 7.1 Map-value distribution [i](#)



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.



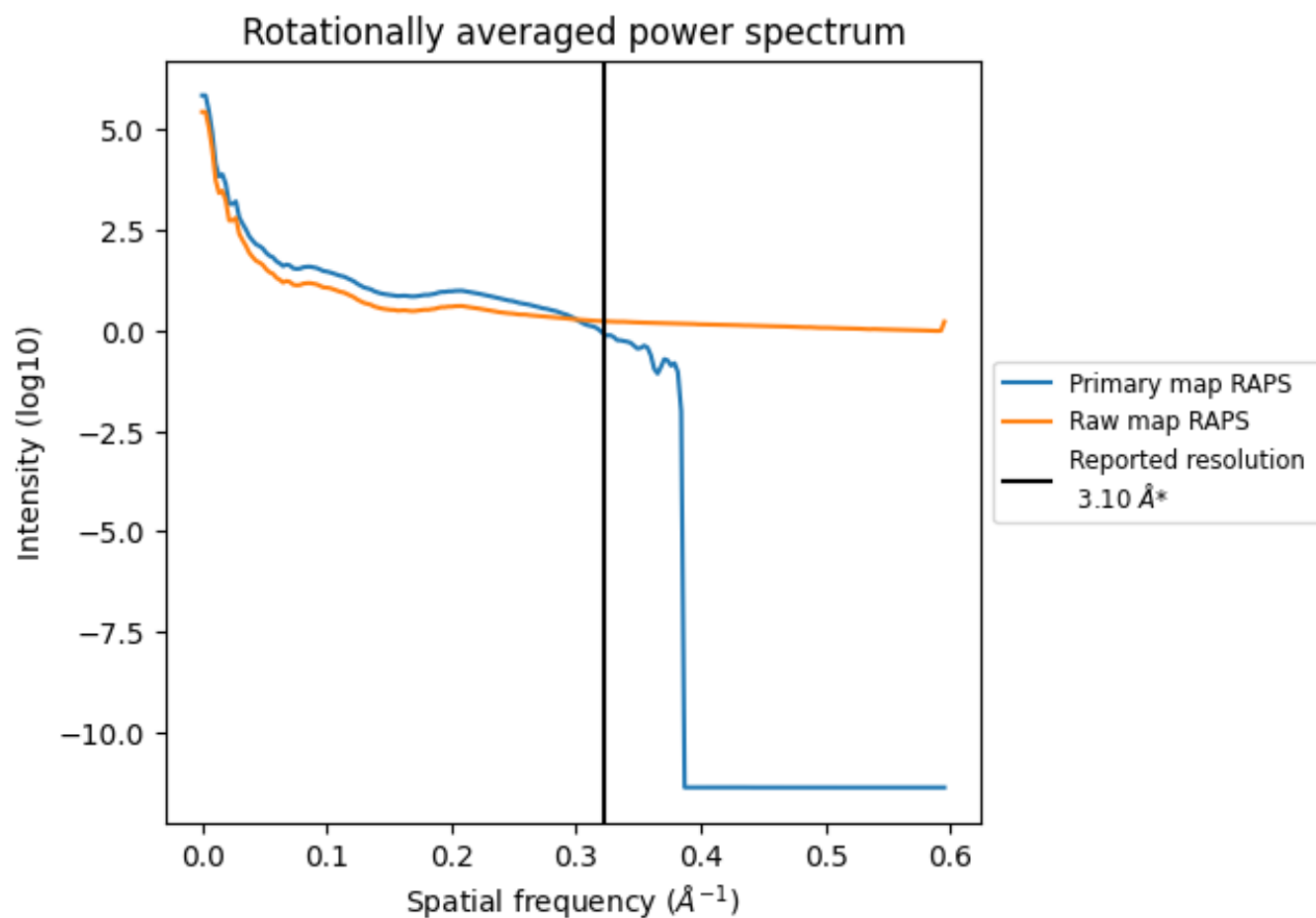
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm<sup>3</sup>; this corresponds to an approximate mass of 373 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 ⓘ

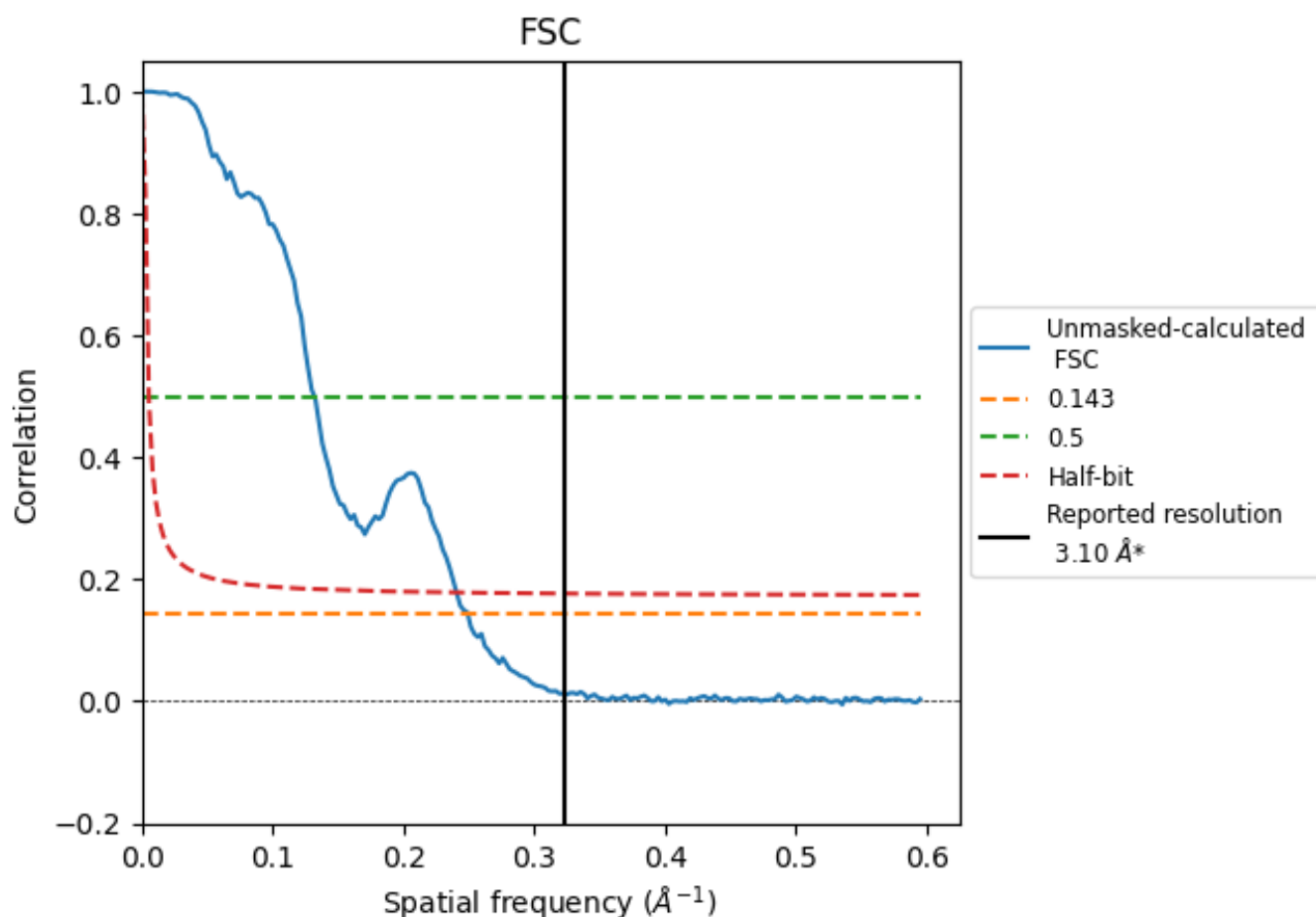


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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](#)

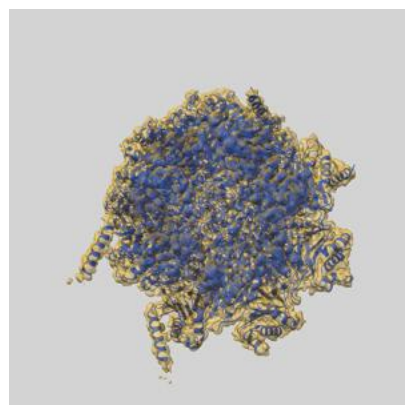
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.58	4.15

\*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 4.01 differs from the reported value 3.1 by more than 10 %

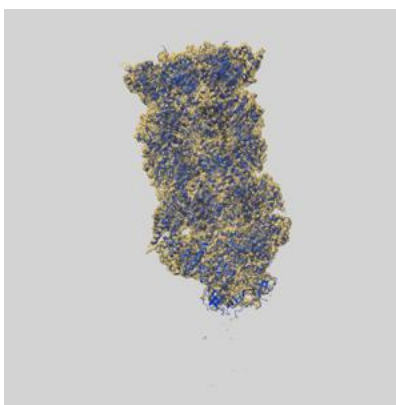
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65361 and PDB model 9VUF. Per-residue inclusion information can be found in section 3 on page 11.

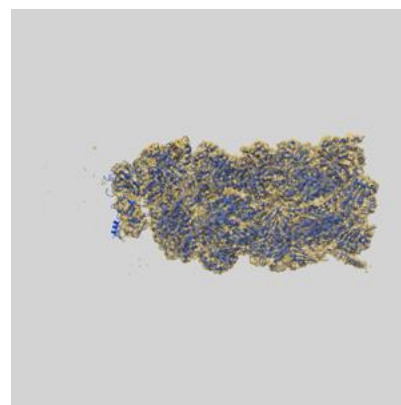
### 9.1 Map-model overlay [i](#)



X



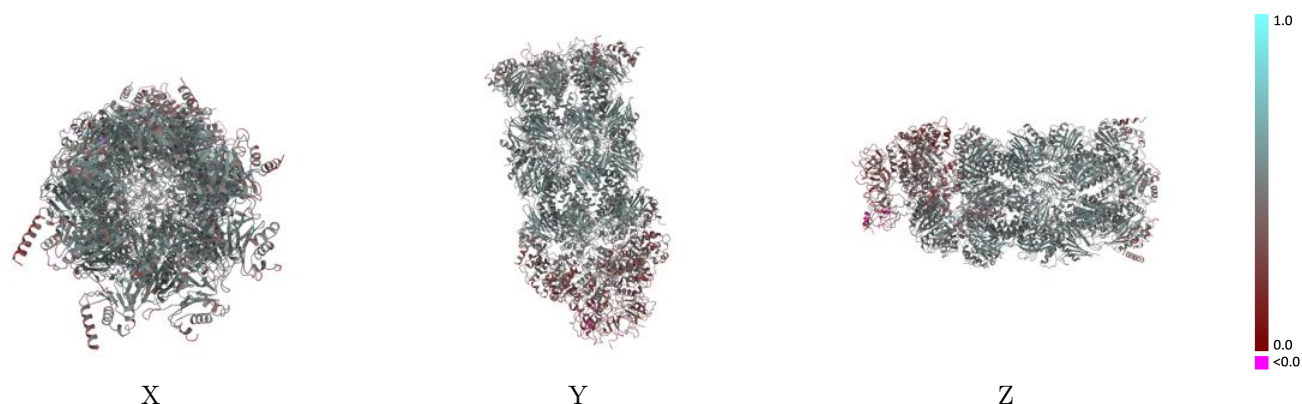
Y



Z

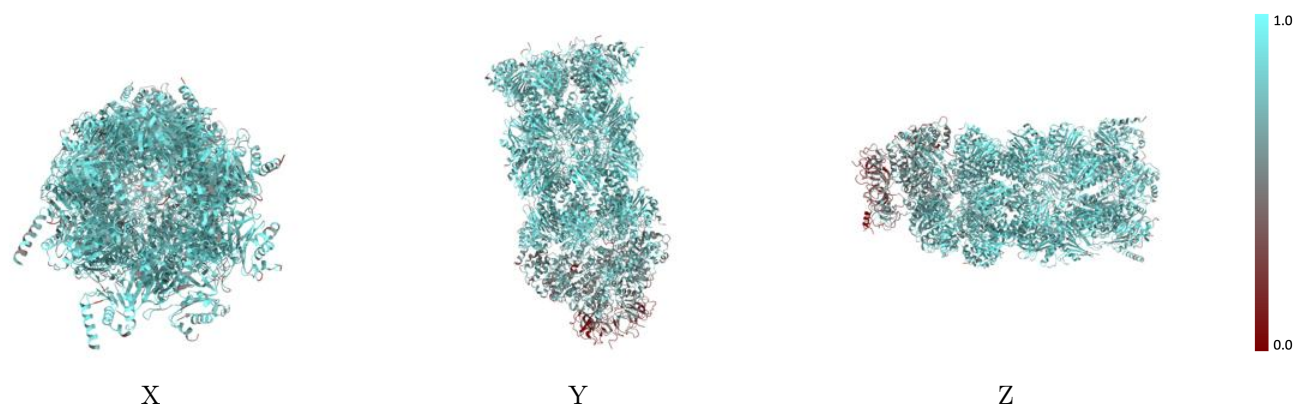
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



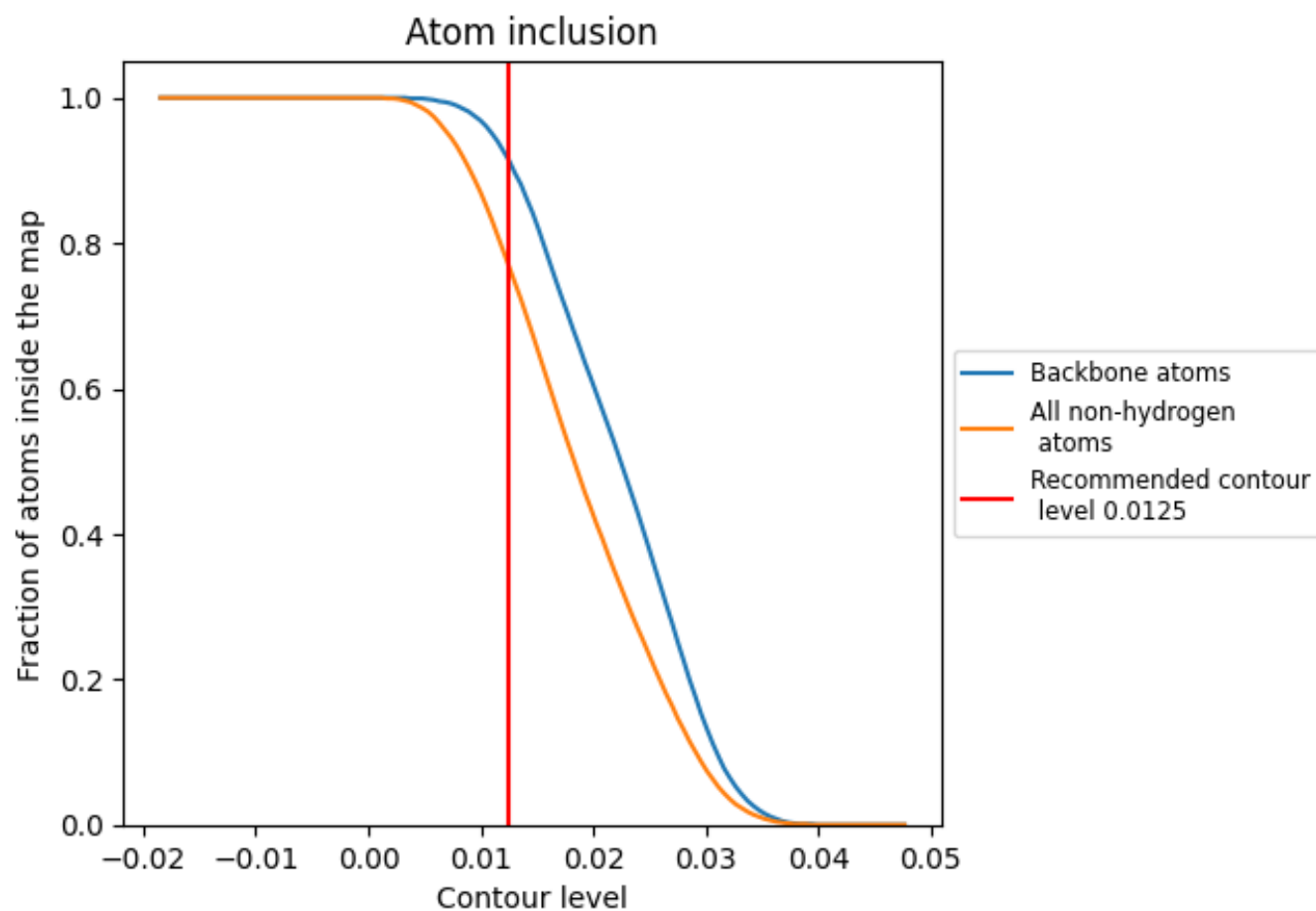
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.4730
A	 0.6750	 0.4370
B	 0.5820	 0.3780
C	 0.5160	 0.3440
D	 0.5300	 0.3290
E	 0.5840	 0.3400
F	 0.6470	 0.4120
G	 0.8350	 0.5110
H	 0.8630	 0.5290
I	 0.8010	 0.4880
J	 0.8340	 0.5050
K	 0.8000	 0.5130
L	 0.8430	 0.5090
M	 0.8200	 0.4900
N	 0.8750	 0.5360
O	 0.8550	 0.5260
P	 0.8620	 0.5370
Q	 0.8530	 0.5290
R	 0.8660	 0.5360
S	 0.8510	 0.5150
T	 0.8630	 0.5280
g	 0.7880	 0.4760
h	 0.7930	 0.4830
i	 0.7610	 0.4590
j	 0.8000	 0.4680
k	 0.7700	 0.4700
l	 0.7950	 0.4750
m	 0.7850	 0.4700
n	 0.8600	 0.5280
o	 0.8480	 0.5230
p	 0.8430	 0.5290
q	 0.8420	 0.5180
r	 0.8740	 0.5290
s	 0.8480	 0.5220
t	 0.8650	 0.5300

