



wwPDB EM Validation Summary Report ⓘ

Nov 17, 2022 – 05:34 AM EST

PDB ID : 6WJN
EMDB ID : EMD-21696
Title : SD-like state of human 26S Proteasome with non-cleavable M1-linked hex-
aubiquitin and E3 ubiquitin ligase E6AP/UBE3A
Authors : Chen, X.; Walters, K.J.
Deposited on : 2020-04-14
Resolution : 5.70 Å(reported)
Based on initial model : 5VFR

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

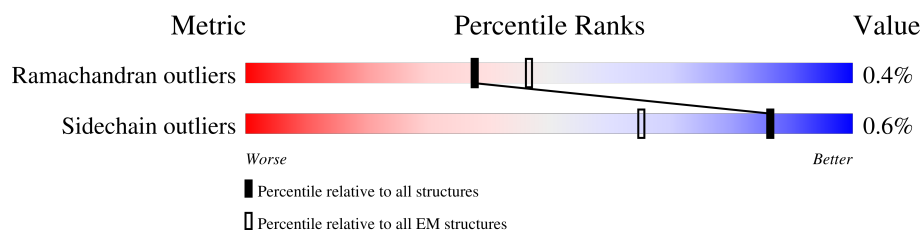
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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


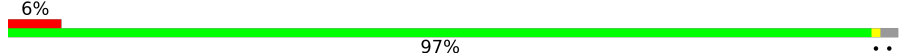
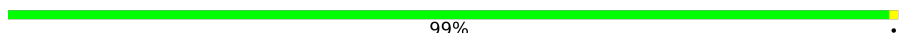
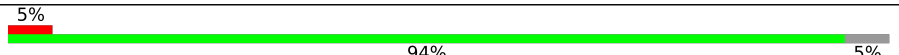
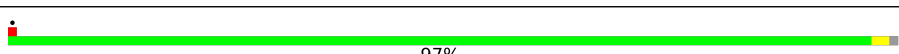
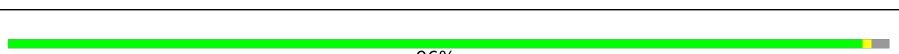
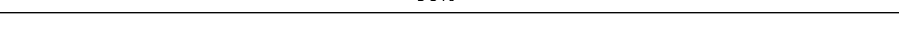
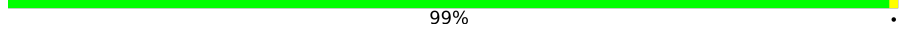

The reported resolution of this entry is 5.70 Å.

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.



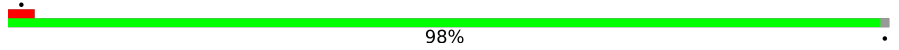

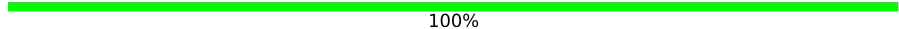
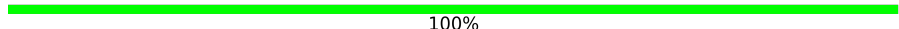
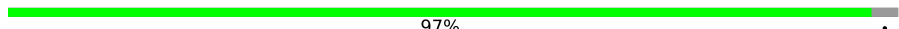
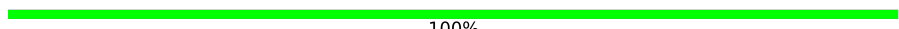
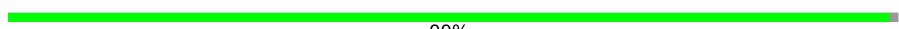










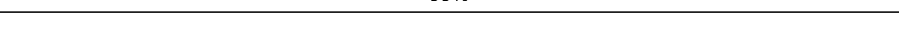
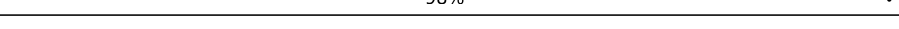
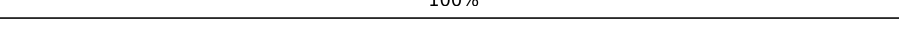
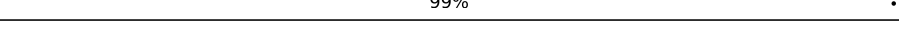
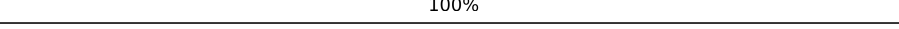
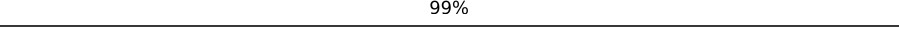

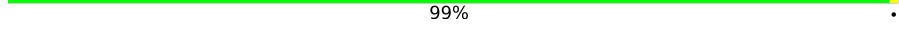
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	U	911	 88% 12%
2	V	480	 97% ..
3	W	456	 99% .
4	X	380	 94% 5%
5	Y	378	 97% ..
6	Z	286	 96% ..
7	a	373	 99% .
8	b	191	 100%
9	c	287	 94% . .

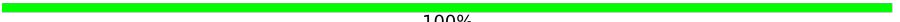











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Mol	Chain	Length	Quality of chain
10	d	257	 98%
11	e	70	 54% 46%
12	G	240	 100%
12	g	240	 100%
13	H	232	 97%
13	h	232	 100%
14	I	250	 99%
14	i	250	 99%
15	J	243	 96%
15	j	243	 97%
16	K	234	 96%
16	k	234	 97%
17	L	238	 100%
17	l	238	 100%
18	M	245	 98%
18	m	245	 98%
19	N	191	 99%
19	n	191	 98%
20	O	220	 100%
20	o	220	 99%
21	P	204	 100%
21	p	204	 99%
22	Q	199	 99%
22	q	199	 99%
23	R	201	 100%

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Mol	Chain	Length	Quality of chain
23	r	201	 100%
24	S	213	 100%
24	s	213	 100%
25	T	215	 100%
25	t	215	 100%
26	A	399	 82% • 16%
27	B	389	 87% • 11%
28	C	392	 87% • 12%
29	D	380	 95% • •
30	E	375	 98% • •
31	F	396	 93% • 6%
32	f	908	 6% 75% • 25%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 95283 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	802	Total	C	N	O	S	0	0
			6143	3889	1054	1158	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	468	Total	C	N	O	S	0	0
			3688	2333	660	683	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3308	2075	564	650	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	360	Total	C	N	O	S	0	0
			2594	1623	449	514	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	374	Total	C	N	O	S	0	0
			2729	1709	479	534	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	279	Total	C	N	O	S	0	0
			1935	1224	341	366	4		

- 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
			2943	1874	504	551	14		

- 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
			1425	887	255	275	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	275	Total	C	N	O	S	0	0
			1880	1180	336	352	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	254	Total	C	N	O	S	0	0
			2067	1340	342	378	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	38	Total	C	N	O	S	0	0
			275	163	47	63	2		

- Molecule 12 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	239	Total	C	N	O	S	0	0
			1773	1124	297	339	13		
12	g	240	Total	C	N	O	S	0	0
			1769	1128	295	335	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	226	Total	C	N	O	S	0	0
			1631	1033	277	317	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	h	232	Total	C	N	O	S	0	0
			1668	1055	279	330	4		

- Molecule 14 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	248	Total	C	N	O	S	0	0
			1869	1181	321	359	8		
14	i	250	Total	C	N	O	S	0	0
			1863	1170	324	361	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	236	Total	C	N	O	S	0	0
			1622	1009	290	318	5		
15	j	236	Total	C	N	O	S	0	0
			1630	1008	297	321	4		

- Molecule 16 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	227	Total	C	N	O	S	0	0
			1653	1033	277	336	7		
16	k	228	Total	C	N	O	S	0	0
			1671	1048	279	337	7		

- Molecule 17 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	238	Total	C	N	O	S	0	0
			1846	1156	333	346	11		
17	l	238	Total	C	N	O	S	0	0
			1838	1152	331	344	11		

- Molecule 18 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	240	Total	C	N	O	S	0	0
			1808	1150	304	347	7		
18	m	240	Total	C	N	O	S	0	0
			1834	1169	307	350	8		

- Molecule 19 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	191	Total	C	N	O	S	0	0
			1408	872	245	279	12		
19	n	191	Total	C	N	O	S	0	0
			1417	886	242	277	12		

- Molecule 20 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	220	Total	C	N	O	S	0	0
			1614	1014	277	311	12		
20	o	218	Total	C	N	O	S	0	0
			1600	1003	278	309	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	204	Total	C	N	O	S	0	0
			1554	992	261	282	19		
21	p	203	Total	C	N	O	S	0	0
			1549	988	259	283	19		

- Molecule 22 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	199	Total	C	N	O	S	0	0
			1561	1000	265	288	8		
22	q	199	Total	C	N	O	S	0	0
			1538	982	260	287	9		

- Molecule 23 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	201	Total	C	N	O	S	0	0
			1526	962	270	285	9		
23	r	201	Total	C	N	O	S	0	0
			1543	969	273	292	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	213	Total	C	N	O	S	0	0
			1614	1023	278	303	10		
24	s	213	Total	C	N	O	S	0	0
			1639	1034	282	313	10		

- Molecule 25 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	215	Total	C	N	O	S	0	0
			1655	1043	282	318	12		
25	t	215	Total	C	N	O	S	0	0
			1652	1043	279	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	337	Total	C	N	O	S	0	0
			2375	1476	429	458	12		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	347	Total	C	N	O	S	0	0
			2426	1510	414	493	9		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	345	Total	C	N	O	S	0	0
			2415	1510	432	459	14		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	375	Total	C	N	O	S	0	0
			2560	1599	452	501	8		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	372	Total	C	N	O	S	0	0
			2563	1601	454	500	8		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	371	Total	C	N	O	S	0	0
			2481	1546	446	478	11		

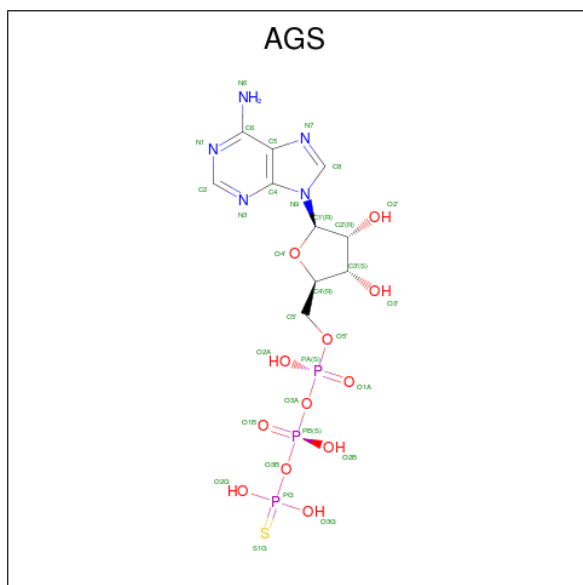
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	684	Total	C	N	O	S	0	0
			5006	3124	858	996	28		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

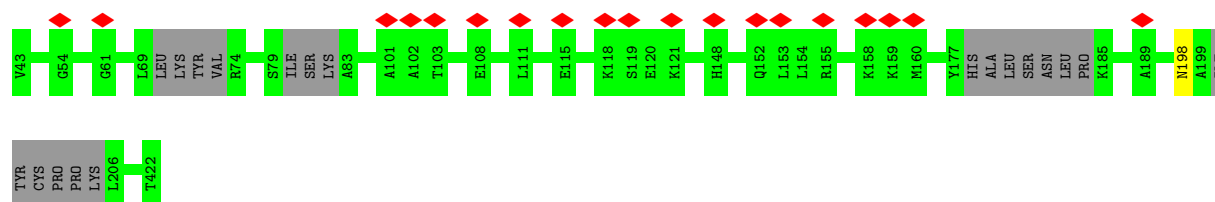
Mol	Chain	Residues	Atoms		AltConf
33	c	1	Total	Zn	0
			1	1	

- Molecule 34 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
34	F	1	31	10	5	12	3	1	0



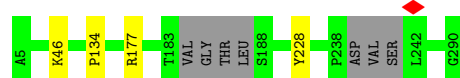
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 97%



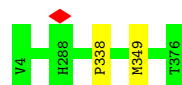
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 96%



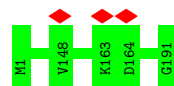
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 99%



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

Chain b: 100%



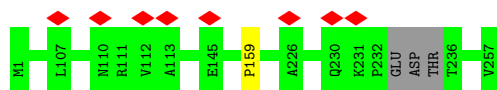
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 94%



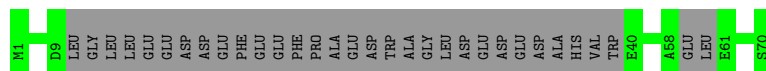
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 98%



- Molecule 11: 26S proteasome complex subunit SEM1

Chain e: 54% 46%



- Molecule 12: Proteasome subunit alpha type-6

Chain G: 100%



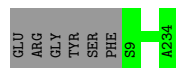
- Molecule 12: Proteasome subunit alpha type-6

Chain g: 100%

There are no outlier residues recorded for this chain.

- Molecule 13: Proteasome subunit alpha type-2

Chain H: 97%



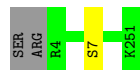
- Molecule 13: Proteasome subunit alpha type-2

Chain h: 100%

There are no outlier residues recorded for this chain.

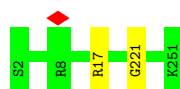
- Molecule 14: Proteasome subunit alpha type-4

Chain I: 99%



- Molecule 14: Proteasome subunit alpha type-4

Chain i: 99%



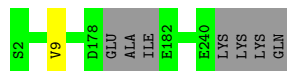
- Molecule 15: Proteasome subunit alpha type-7

Chain J:  96%



- Molecule 15: Proteasome subunit alpha type-7

Chain j:  97%



- Molecule 16: Proteasome subunit alpha type-5

Chain K:  96%



- Molecule 16: Proteasome subunit alpha type-5

Chain k:  97%



- Molecule 17: Proteasome subunit alpha type-1

Chain L:  100%

There are no outlier residues recorded for this chain.

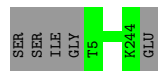
- Molecule 17: Proteasome subunit alpha type-1

Chain l:  100%

There are no outlier residues recorded for this chain.

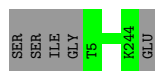
- Molecule 18: Proteasome subunit alpha type-3

Chain M:  98%



- Molecule 18: Proteasome subunit alpha type-3

Chain m:  98%



- Molecule 19: Proteasome subunit beta type-6

Chain N: 99%



- Molecule 19: Proteasome subunit beta type-6

Chain n: 98%



- Molecule 20: Proteasome subunit beta type-7

Chain O: 100%

There are no outlier residues recorded for this chain.

- Molecule 20: Proteasome subunit beta type-7

Chain o: 99%



- Molecule 21: Proteasome subunit beta type-3

Chain P: 100%



- Molecule 21: Proteasome subunit beta type-3

Chain p: 99%



- Molecule 22: Proteasome subunit beta type-2

Chain Q: 99%



- Molecule 22: Proteasome subunit beta type-2

Chain q:  99%



- Molecule 23: Proteasome subunit beta type-5

Chain R:  100%



- Molecule 23: Proteasome subunit beta type-5

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: Proteasome subunit beta type-1

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: Proteasome subunit beta type-1

Chain s:  100%



- Molecule 25: Proteasome subunit beta type-4

Chain T:  100%




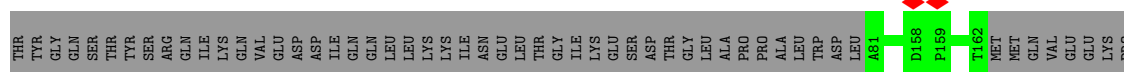
- Molecule 25: Proteasome subunit beta type-4

Chain t:  100%


There are no outlier residues recorded for this chain.

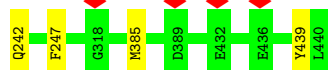
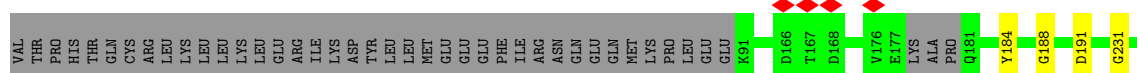
- Molecule 26: 26S proteasome regulatory subunit 7

Chain A:  82% 16%




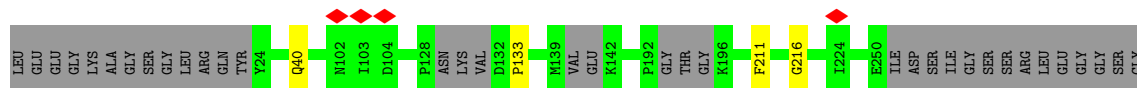
- Molecule 27: 26S proteasome regulatory subunit 4

Chain B:  87% 11%



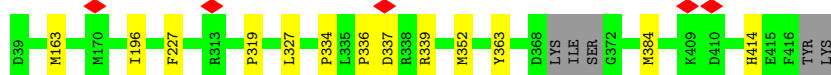
- Molecule 28: 26S proteasome regulatory subunit 8

Chain C:  87% 12%



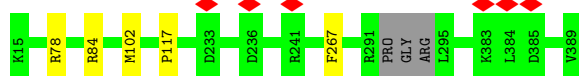
- Molecule 29: 26S proteasome regulatory subunit 6B

Chain D:  95% 5%

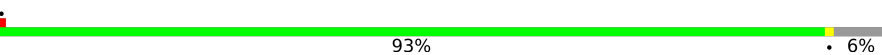


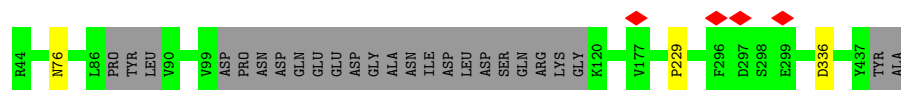
- Molecule 30: 26S proteasome regulatory subunit 10B

Chain E:  98% 2%

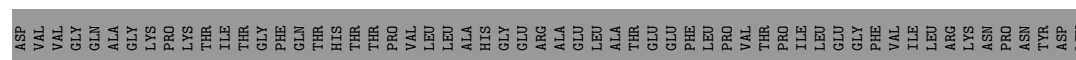
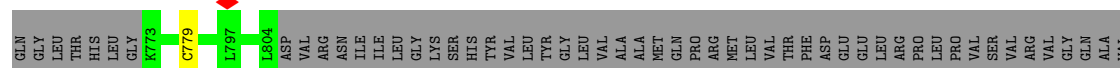
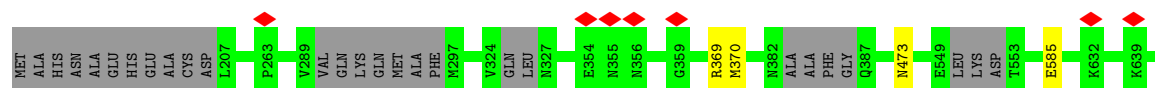
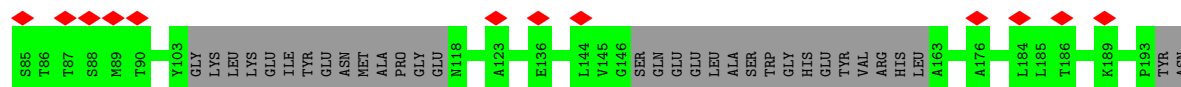
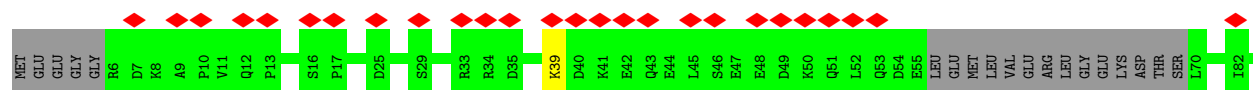
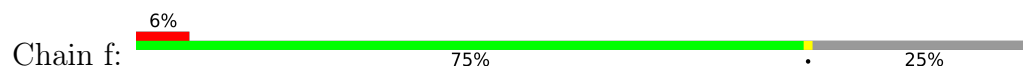


- Molecule 31: 26S proteasome regulatory subunit 6A

Chain F:  93% 6%



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52593	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 ($e^-/\text{\AA}^2$)	36.64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (\AA)	614.25, 614.25, 614.25	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.365, 1.365, 1.365	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	U	0.33	0/6243	0.64	0/8443
2	V	0.35	0/3757	0.68	0/5082
3	W	0.26	0/3348	0.47	0/4537
4	X	0.33	0/2619	0.55	0/3543
5	Y	0.29	0/2774	0.47	0/3771
6	Z	0.32	0/1965	0.51	0/2685
7	a	0.32	0/3001	0.68	0/4066
8	b	0.33	0/1444	0.68	0/1957
9	c	0.31	0/1913	0.50	0/2611
10	d	0.32	0/2112	0.69	0/2851
11	e	0.26	0/276	0.49	0/369
12	G	0.35	0/1803	0.65	0/2449
12	g	0.34	0/1801	0.61	0/2451
13	H	0.35	0/1664	0.59	0/2270
13	h	0.34	0/1703	0.59	0/2324
14	I	0.35	0/1899	0.71	0/2572
14	i	0.34	0/1891	0.66	0/2562
15	J	0.39	0/1643	0.64	0/2248
15	j	0.34	0/1651	0.69	0/2256
16	K	0.35	0/1676	0.61	0/2275
16	k	0.34	0/1694	0.60	0/2296
17	L	0.36	0/1881	0.63	0/2548
17	l	0.34	0/1873	0.62	0/2537
18	M	0.36	0/1840	0.58	0/2488
18	m	0.36	0/1868	0.59	0/2524
19	N	0.34	0/1430	0.60	0/1935
19	n	0.36	0/1441	0.61	0/1951
20	O	0.36	0/1641	0.59	0/2227
20	o	0.35	0/1624	0.65	0/2201
21	P	0.33	0/1582	0.56	0/2136
21	p	0.34	0/1576	0.57	0/2125
22	Q	0.40	0/1594	0.70	0/2163

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	q	0.38	0/1570	0.68	0/2131
23	R	0.36	0/1557	0.56	0/2106
23	r	0.34	0/1574	0.55	0/2127
24	S	0.35	0/1643	0.59	0/2216
24	s	0.35	0/1669	0.59	0/2250
25	T	0.35	0/1688	0.57	0/2290
25	t	0.35	0/1685	0.57	0/2287
26	A	0.31	0/2409	0.51	0/3267
27	B	0.35	0/2459	0.48	0/3342
28	C	0.29	0/2442	0.49	0/3307
29	D	0.35	0/2596	0.52	0/3547
30	E	0.31	0/2602	0.47	0/3551
31	F	0.32	0/2507	0.50	0/3407
32	f	0.25	0/5074	0.47	0/6861
All	All	0.33	0/96702	0.59	0/131142

There are no bond length outliers.

There are no bond angle outliers.

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	U	790/911 (87%)	726 (92%)	63 (8%)	1 (0%)	51	85
2	V	464/480 (97%)	397 (86%)	65 (14%)	2 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	W	454/456 (100%)	393 (87%)	58 (13%)	3 (1%)	22	62
4	X	350/380 (92%)	314 (90%)	36 (10%)	0	100	100
5	Y	370/378 (98%)	310 (84%)	59 (16%)	1 (0%)	41	76
6	Z	273/286 (96%)	228 (84%)	44 (16%)	1 (0%)	34	72
7	a	371/373 (100%)	339 (91%)	31 (8%)	1 (0%)	41	76
8	b	189/191 (99%)	160 (85%)	29 (15%)	0	100	100
9	c	269/287 (94%)	206 (77%)	60 (22%)	3 (1%)	14	51
10	d	250/257 (97%)	215 (86%)	34 (14%)	1 (0%)	34	72
11	e	32/70 (46%)	25 (78%)	7 (22%)	0	100	100
12	G	237/240 (99%)	215 (91%)	22 (9%)	0	100	100
12	g	238/240 (99%)	220 (92%)	18 (8%)	0	100	100
13	H	224/232 (97%)	209 (93%)	15 (7%)	0	100	100
13	h	230/232 (99%)	219 (95%)	11 (5%)	0	100	100
14	I	246/250 (98%)	222 (90%)	23 (9%)	1 (0%)	34	72
14	i	248/250 (99%)	218 (88%)	29 (12%)	1 (0%)	34	72
15	J	232/243 (96%)	218 (94%)	13 (6%)	1 (0%)	34	72
15	j	232/243 (96%)	218 (94%)	13 (6%)	1 (0%)	34	72
16	K	223/234 (95%)	205 (92%)	16 (7%)	2 (1%)	17	56
16	k	224/234 (96%)	202 (90%)	20 (9%)	2 (1%)	17	56
17	L	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
17	l	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
18	M	238/245 (97%)	214 (90%)	24 (10%)	0	100	100
18	m	238/245 (97%)	219 (92%)	19 (8%)	0	100	100
19	N	189/191 (99%)	179 (95%)	9 (5%)	1 (0%)	29	69
19	n	189/191 (99%)	179 (95%)	7 (4%)	3 (2%)	9	43
20	O	218/220 (99%)	204 (94%)	14 (6%)	0	100	100
20	o	214/220 (97%)	205 (96%)	9 (4%)	0	100	100
21	P	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
21	p	199/204 (98%)	187 (94%)	12 (6%)	0	100	100
22	Q	197/199 (99%)	181 (92%)	15 (8%)	1 (0%)	29	69
22	q	197/199 (99%)	179 (91%)	16 (8%)	2 (1%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	R	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
23	r	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
24	S	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
24	s	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
25	T	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
25	t	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
26	A	331/399 (83%)	266 (80%)	60 (18%)	5 (2%)	10	45
27	B	343/389 (88%)	276 (80%)	63 (18%)	4 (1%)	13	49
28	C	331/392 (84%)	267 (81%)	61 (18%)	3 (1%)	17	56
29	D	371/380 (98%)	278 (75%)	85 (23%)	8 (2%)	6	35
30	E	368/375 (98%)	316 (86%)	50 (14%)	2 (0%)	29	69
31	F	365/396 (92%)	316 (87%)	48 (13%)	1 (0%)	41	76
32	f	660/908 (73%)	568 (86%)	92 (14%)	0	100	100
All	All	12714/13558 (94%)	11307 (89%)	1356 (11%)	51 (0%)	38	72

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	K	10	ARG
19	n	91	ARG
19	n	92	GLU
15	J	176	TYR
16	k	12	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	652/779 (84%)	650 (100%)	2 (0%)	92	94
2	V	382/414 (92%)	381 (100%)	1 (0%)	92	94
3	W	307/416 (74%)	304 (99%)	3 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	242/327 (74%)	241 (100%)	1 (0%)	91	94
5	Y	236/334 (71%)	230 (98%)	6 (2%)	47	68
6	Z	168/257 (65%)	165 (98%)	3 (2%)	59	77
7	a	316/333 (95%)	315 (100%)	1 (0%)	92	94
8	b	158/167 (95%)	158 (100%)	0	100	100
9	c	155/252 (62%)	152 (98%)	3 (2%)	57	75
10	d	219/231 (95%)	219 (100%)	0	100	100
11	e	25/63 (40%)	25 (100%)	0	100	100
12	G	180/205 (88%)	180 (100%)	0	100	100
12	g	174/205 (85%)	174 (100%)	0	100	100
13	H	153/190 (80%)	153 (100%)	0	100	100
13	h	153/190 (80%)	153 (100%)	0	100	100
14	I	183/210 (87%)	183 (100%)	0	100	100
14	i	180/210 (86%)	179 (99%)	1 (1%)	86	92
15	J	135/207 (65%)	132 (98%)	3 (2%)	52	71
15	j	136/207 (66%)	136 (100%)	0	100	100
16	K	167/196 (85%)	167 (100%)	0	100	100
16	k	170/196 (87%)	170 (100%)	0	100	100
17	L	197/204 (97%)	197 (100%)	0	100	100
17	l	195/204 (96%)	195 (100%)	0	100	100
18	M	178/202 (88%)	178 (100%)	0	100	100
18	m	184/202 (91%)	184 (100%)	0	100	100
19	N	143/148 (97%)	143 (100%)	0	100	100
19	n	144/148 (97%)	144 (100%)	0	100	100
20	O	167/181 (92%)	167 (100%)	0	100	100
20	o	167/181 (92%)	167 (100%)	0	100	100
21	P	162/173 (94%)	161 (99%)	1 (1%)	86	92
21	p	164/173 (95%)	163 (99%)	1 (1%)	86	92
22	Q	161/170 (95%)	160 (99%)	1 (1%)	86	92
22	q	156/170 (92%)	156 (100%)	0	100	100
23	R	146/156 (94%)	145 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	r	151/156 (97%)	151 (100%)	0	100	100
24	S	165/178 (93%)	165 (100%)	0	100	100
24	s	173/178 (97%)	172 (99%)	1 (1%)	86	92
25	T	172/178 (97%)	171 (99%)	1 (1%)	86	92
25	t	172/178 (97%)	172 (100%)	0	100	100
26	A	209/343 (61%)	204 (98%)	5 (2%)	49	69
27	B	224/345 (65%)	220 (98%)	4 (2%)	59	77
28	C	216/340 (64%)	214 (99%)	2 (1%)	78	87
29	D	212/333 (64%)	207 (98%)	5 (2%)	49	69
30	E	221/329 (67%)	218 (99%)	3 (1%)	67	80
31	F	198/340 (58%)	196 (99%)	2 (1%)	76	86
32	f	491/763 (64%)	484 (99%)	7 (1%)	67	80
All	All	9259/11562 (80%)	9201 (99%)	58 (1%)	86	92

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	p	93	ASN
32	f	585	GLU
27	B	184	TYR
32	f	473	ASN
31	F	76	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
21	P	93	ASN
32	f	53	GLN
20	o	66	HIS
31	F	315	ASN
30	E	300	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	AGS	D	501	-	26,33,33	0.99	3 (11%)	26,52,52	1.64	4 (15%)
34	AGS	A	501	-	26,33,33	1.00	3 (11%)	26,52,52	1.64	4 (15%)
34	AGS	B	501	-	26,33,33	0.99	3 (11%)	26,52,52	1.63	4 (15%)
34	AGS	F	501	-	26,33,33	1.00	3 (11%)	26,52,52	1.64	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	AGS	D	501	-	-	9/17/38/38	0/3/3/3
34	AGS	A	501	-	-	2/17/38/38	0/3/3/3
34	AGS	B	501	-	-	5/17/38/38	0/3/3/3
34	AGS	F	501	-	-	6/17/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	501	AGS	PG-S1G	2.19	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	501	AGS	PG-S1G	2.16	1.95	1.90
34	F	501	AGS	PG-S1G	2.16	1.95	1.90
34	D	501	AGS	PG-S1G	2.14	1.95	1.90
34	A	501	AGS	PG-O2G	2.04	1.61	1.54

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	501	AGS	N3-C2-N1	-4.55	121.57	128.68
34	B	501	AGS	N3-C2-N1	-4.54	121.59	128.68
34	A	501	AGS	N3-C2-N1	-4.53	121.61	128.68
34	F	501	AGS	N3-C2-N1	-4.52	121.61	128.68
34	A	501	AGS	PA-O3A-PB	-3.64	120.34	132.83

There are no chirality outliers.

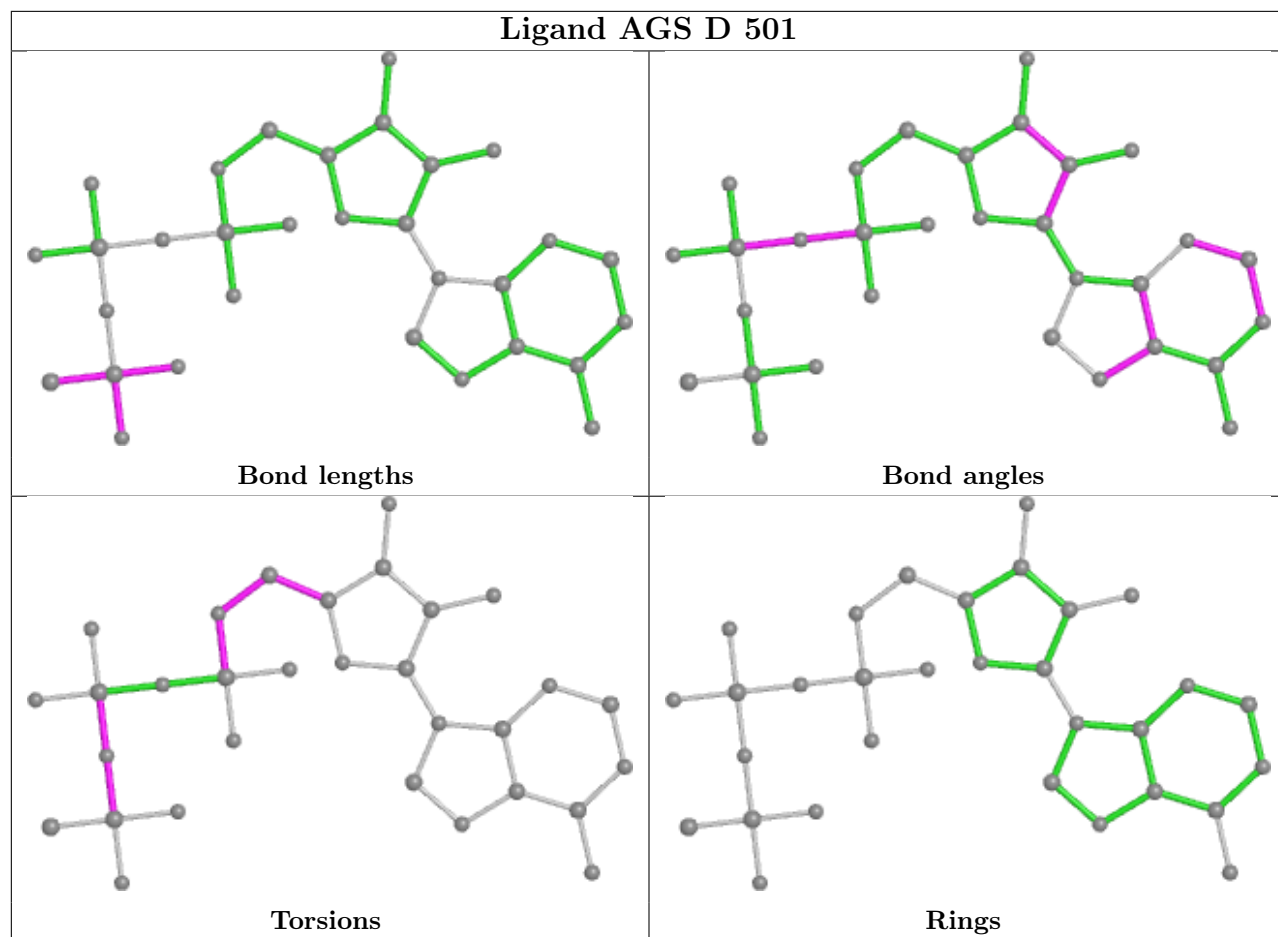
5 of 22 torsion outliers are listed below:

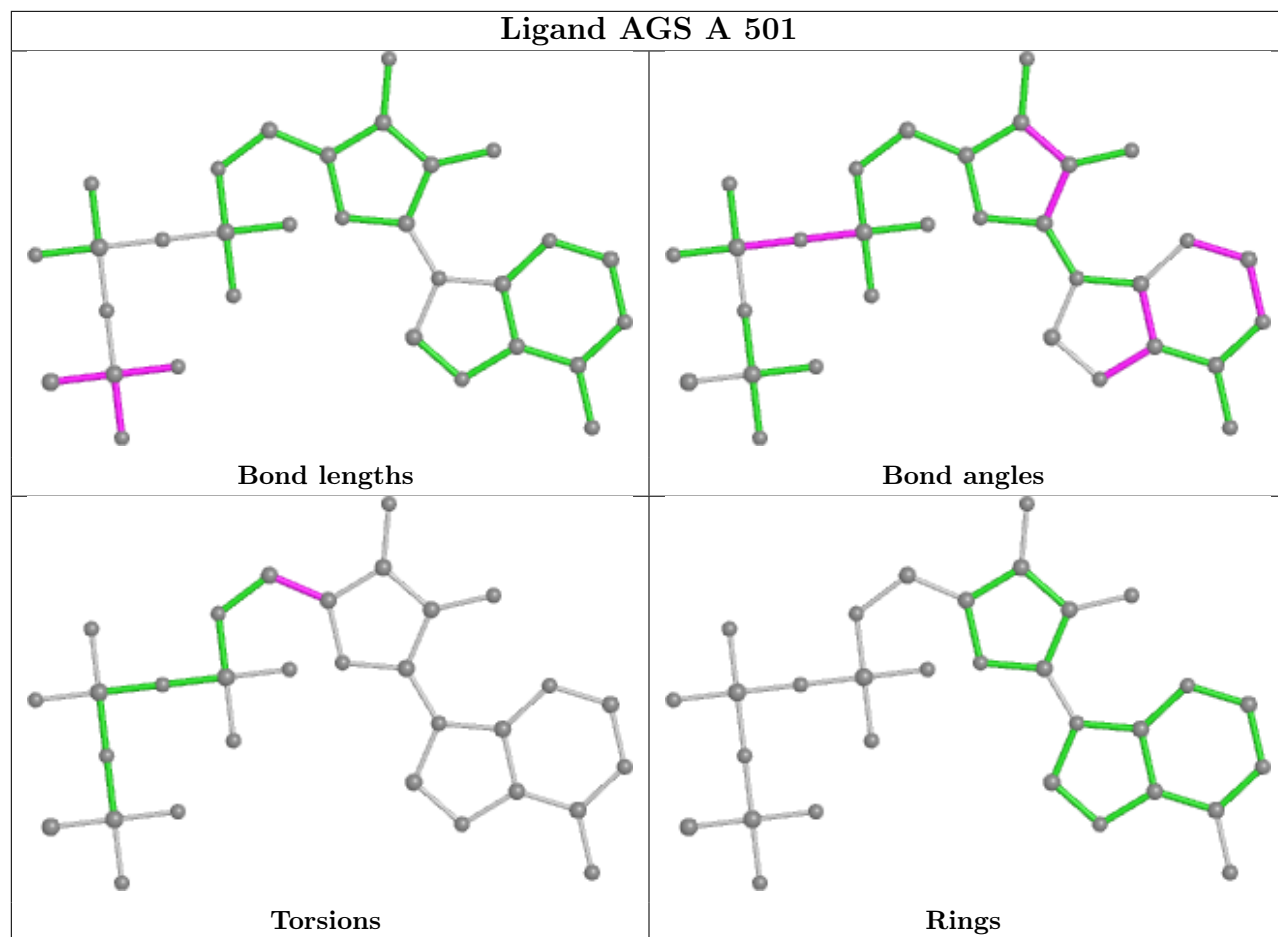
Mol	Chain	Res	Type	Atoms
34	D	501	AGS	PB-O3B-PG-O2G
34	D	501	AGS	C5'-O5'-PA-O1A
34	D	501	AGS	C5'-O5'-PA-O2A
34	F	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O2A

There are no ring outliers.

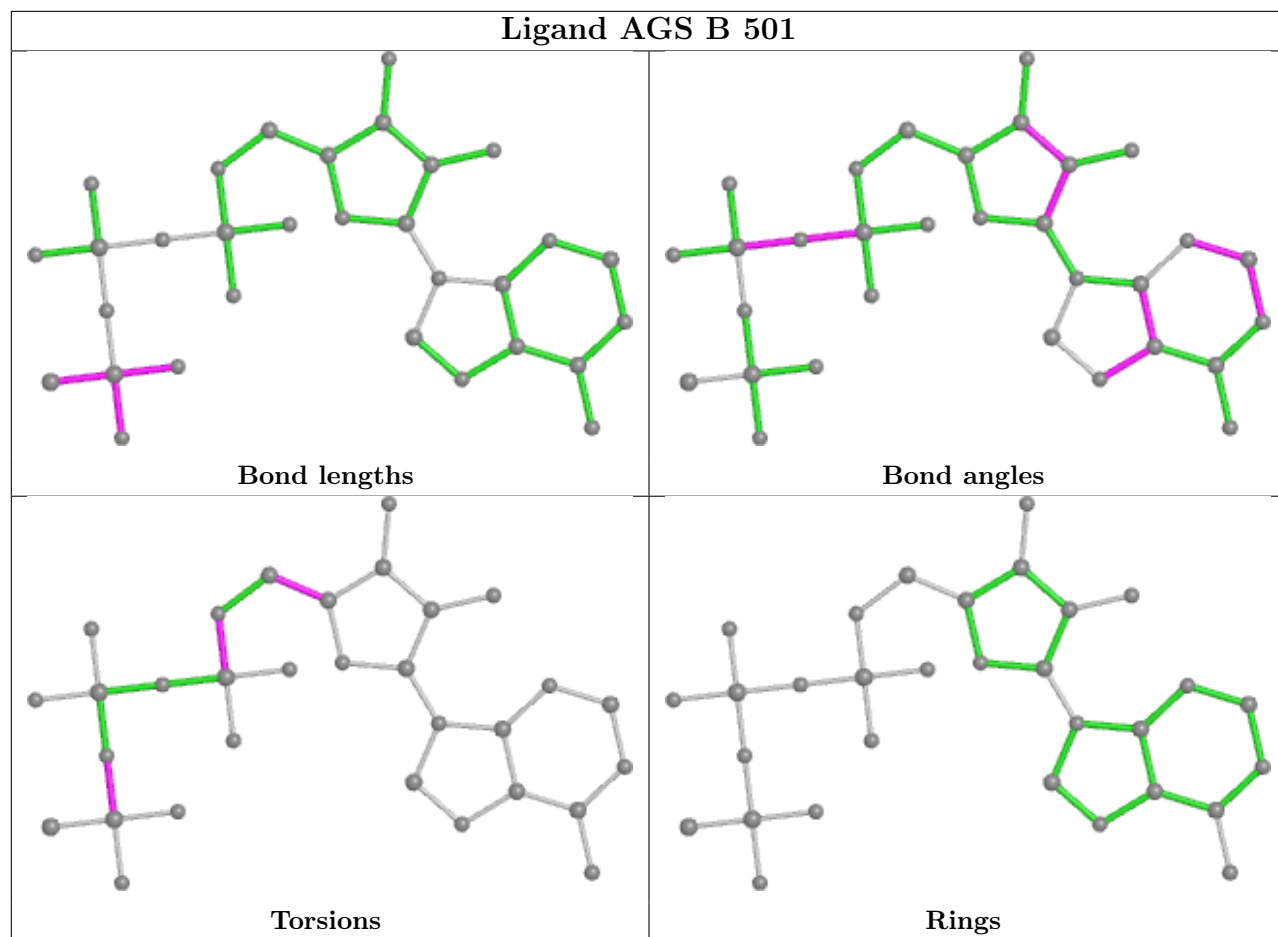
No monomer is involved in short contacts.

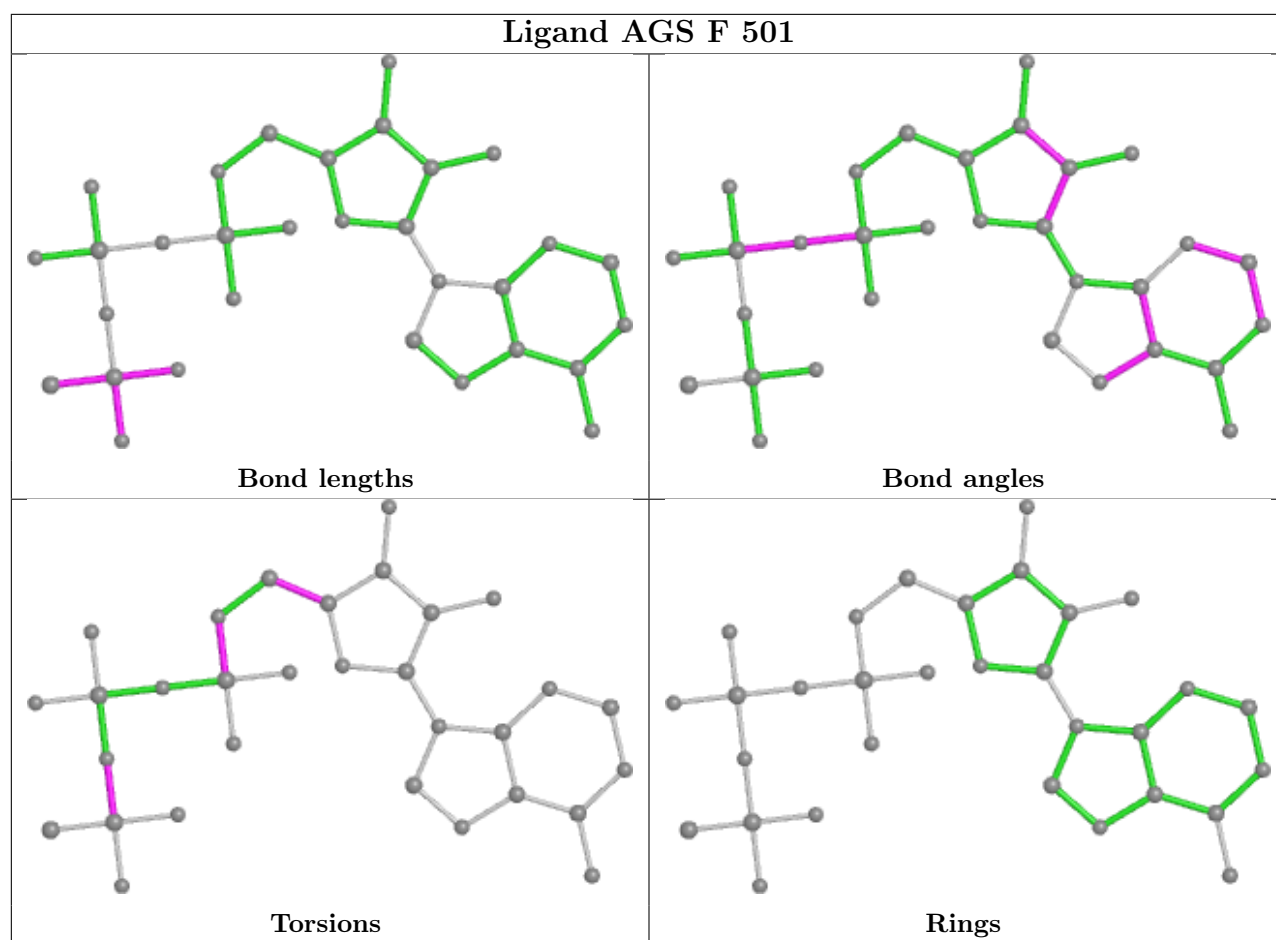
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand AGS B 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.

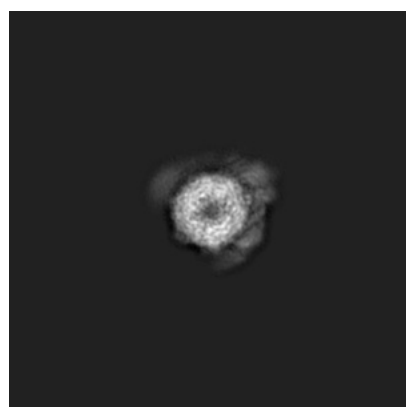
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21696. These allow visual inspection of the internal detail of the map and identification of artifacts.

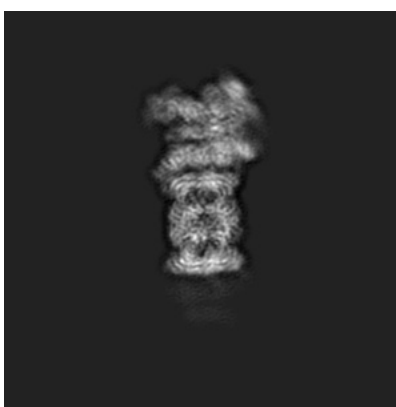
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

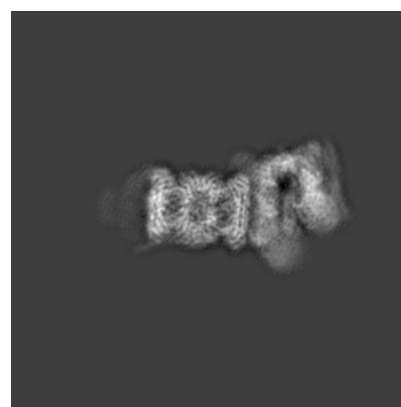
6.1.1 Primary map



X



Y

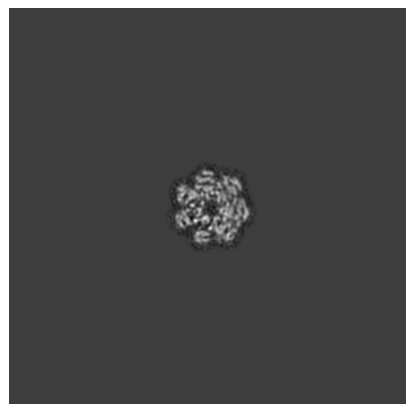


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225



Y Index: 225

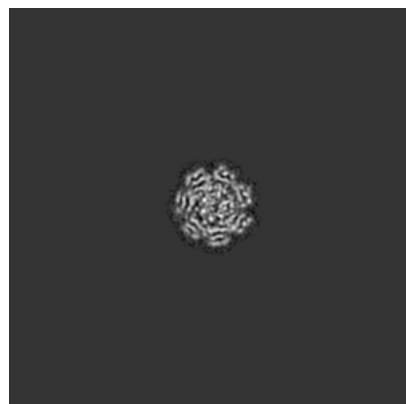


Z Index: 225

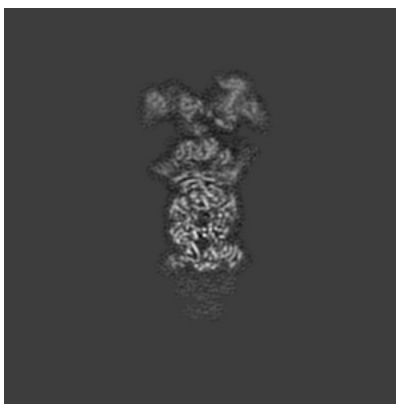
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 167



Y Index: 246



Z Index: 241

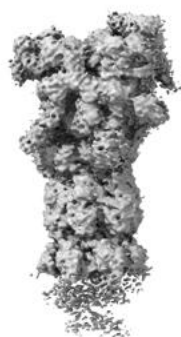
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

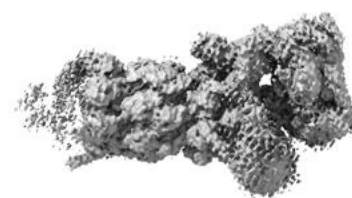
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

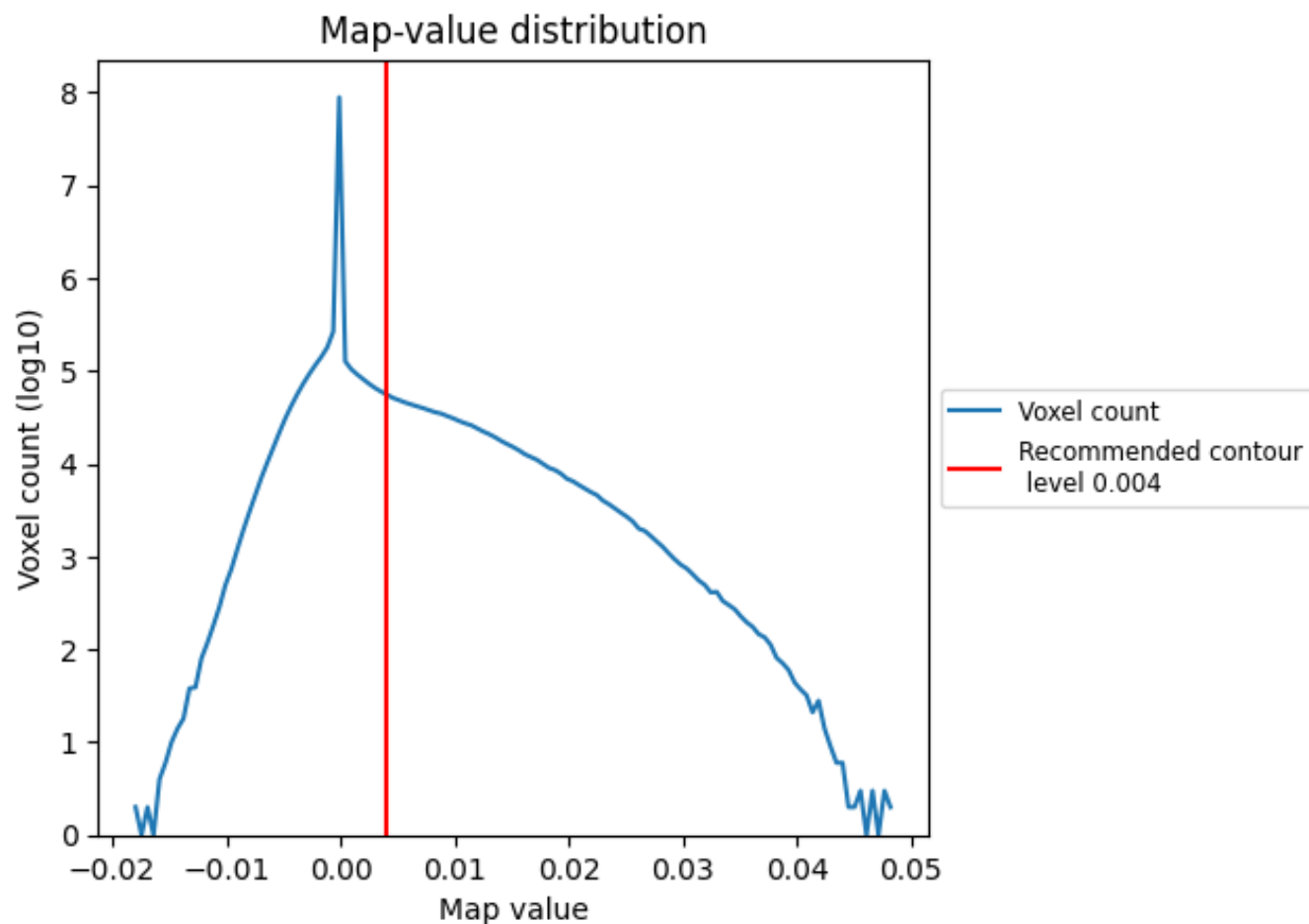
6.5 Mask visualisation

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

7 Map analysis [i](#)

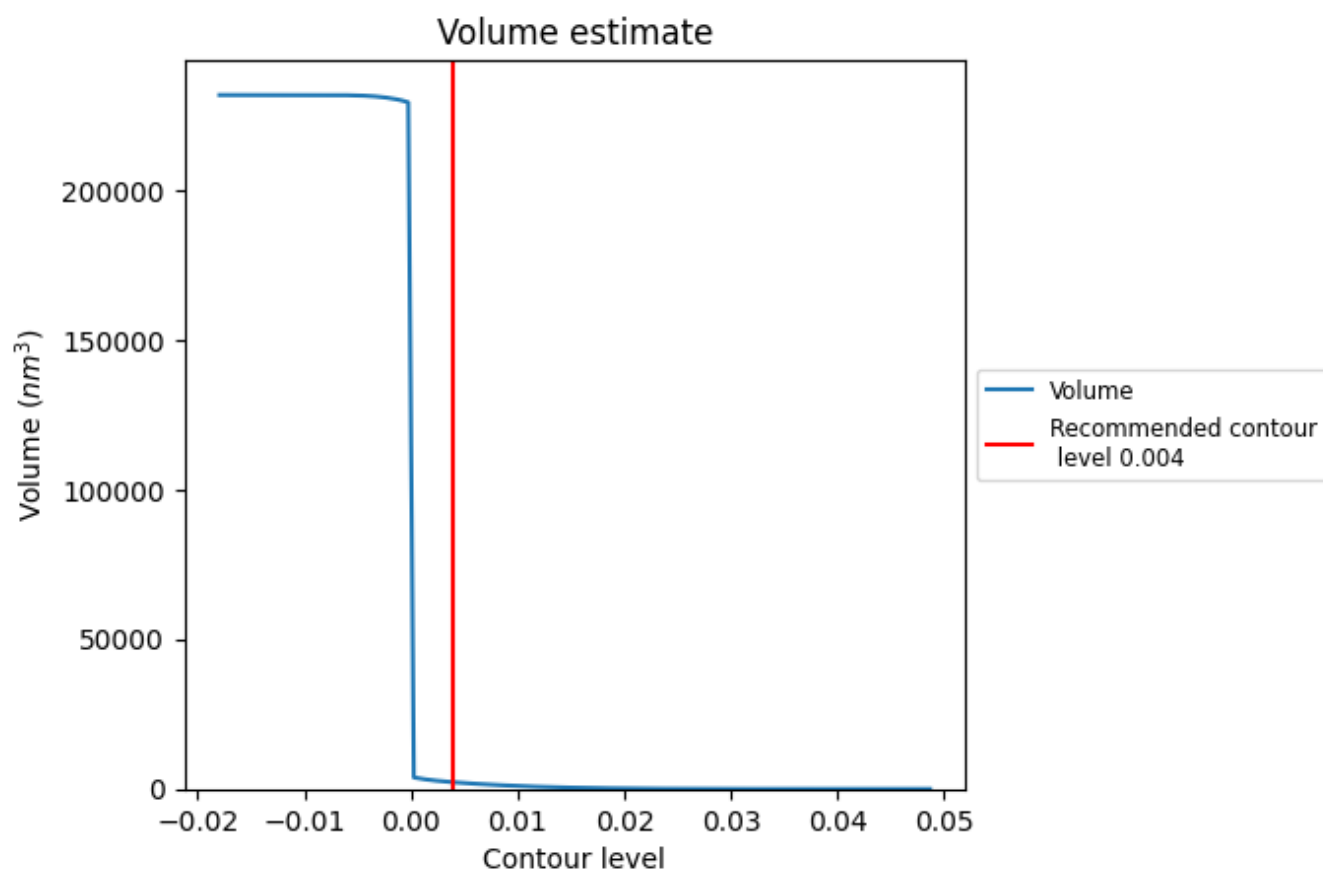
This section contains the results of statistical analysis of the map.

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.

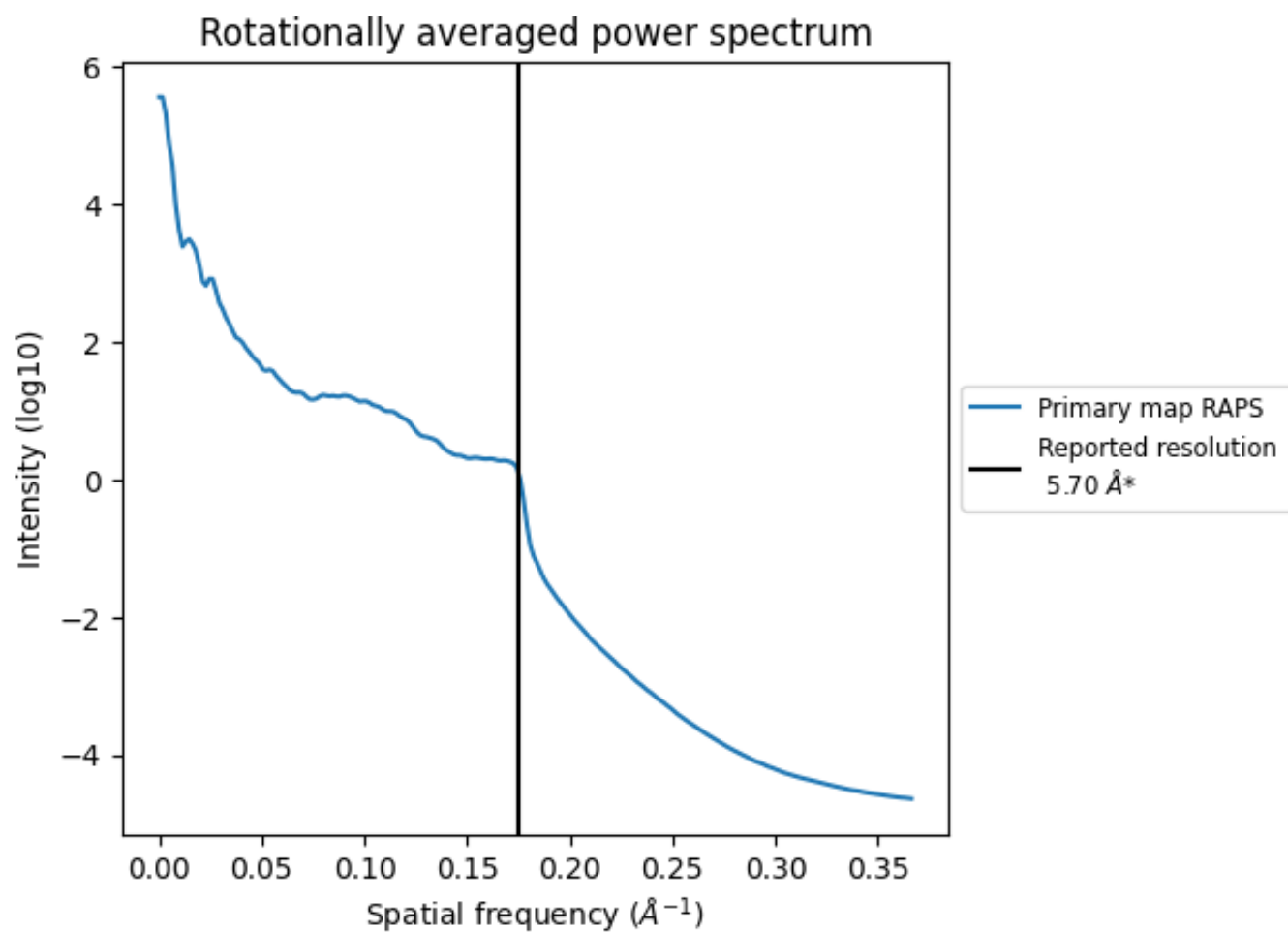
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2235 nm^3 ; this corresponds to an approximate mass of 2019 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 ⓘ

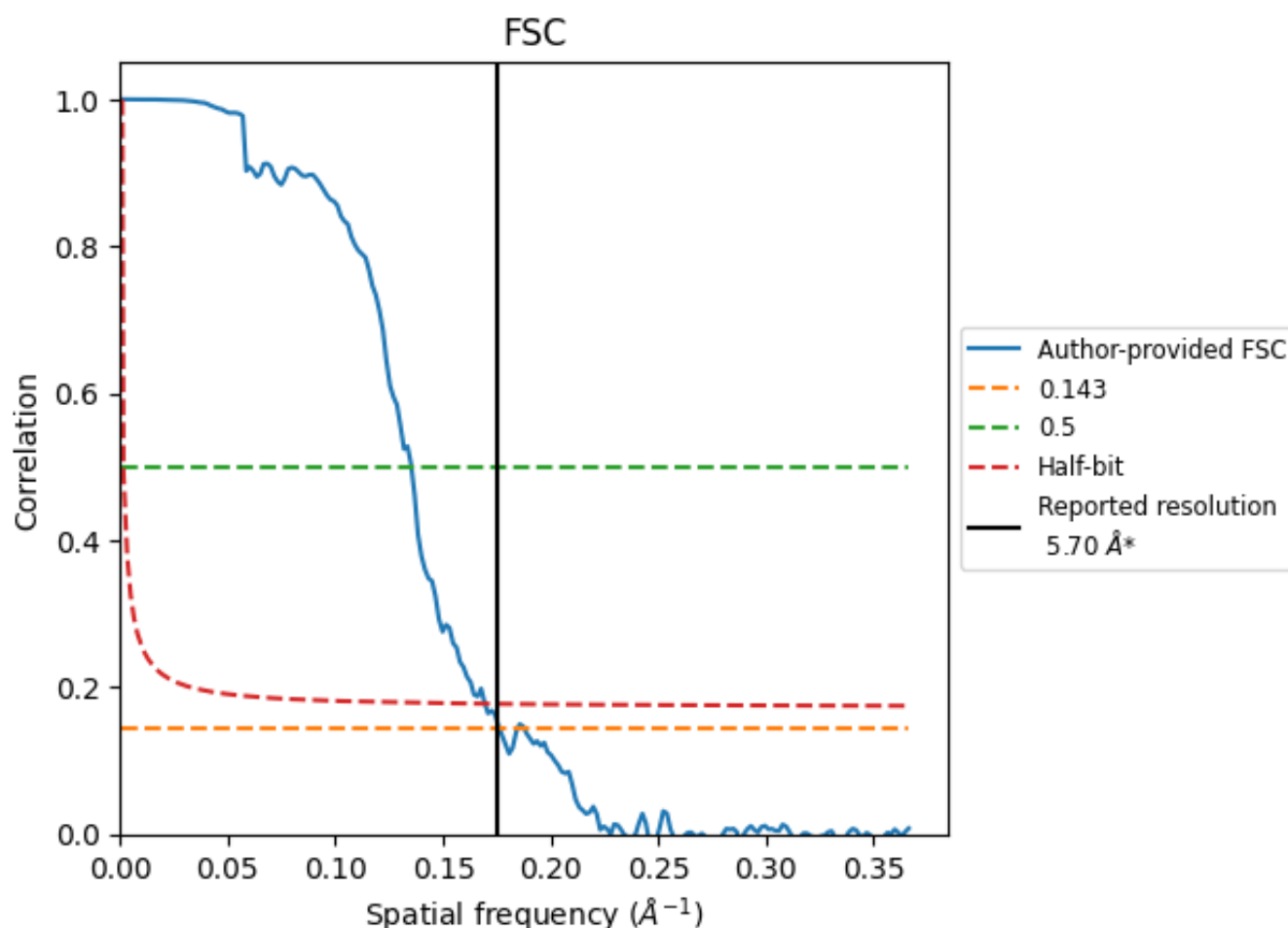


*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

8.2 Resolution estimates [i](#)

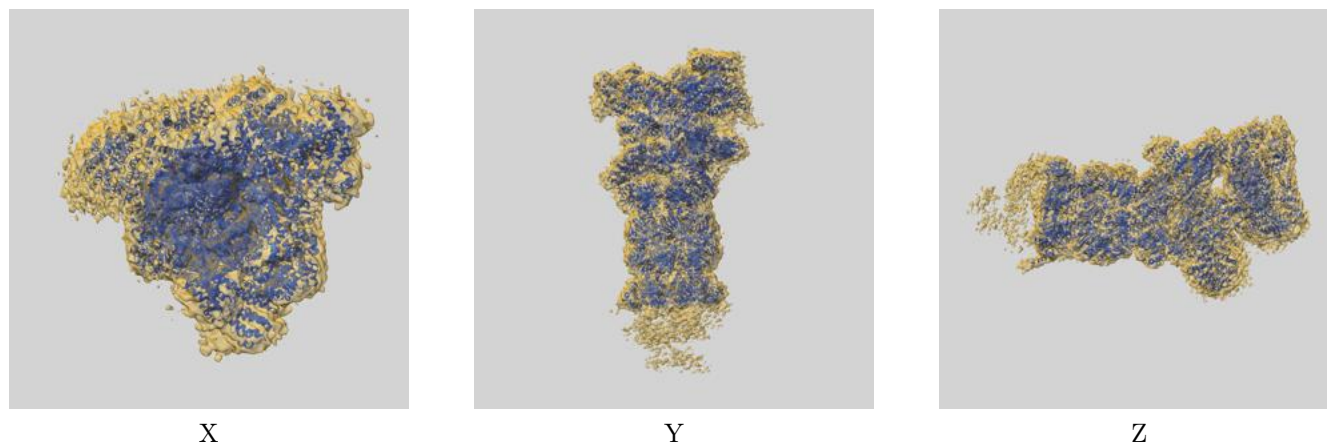
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.68	7.39	5.90
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

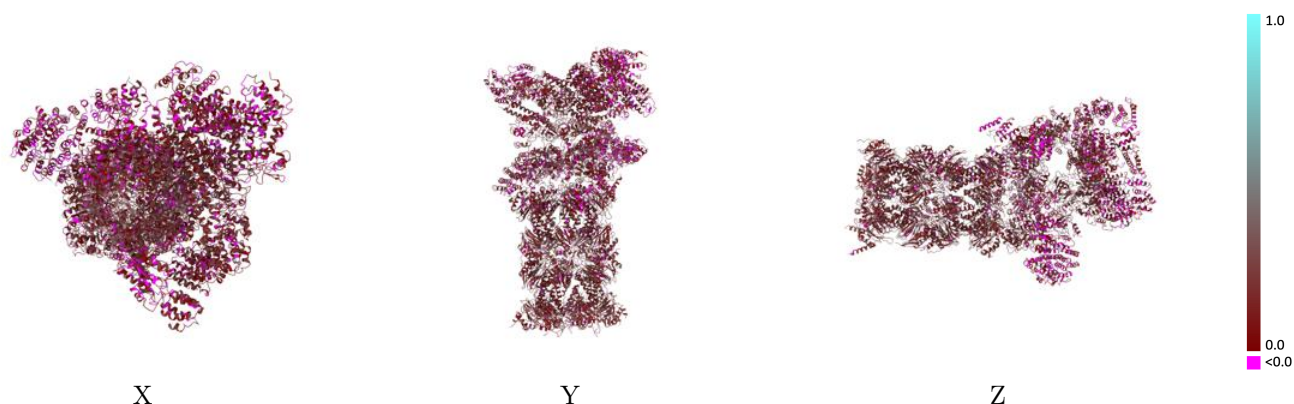
This section contains information regarding the fit between EMDB map EMD-21696 and PDB model 6WJN. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



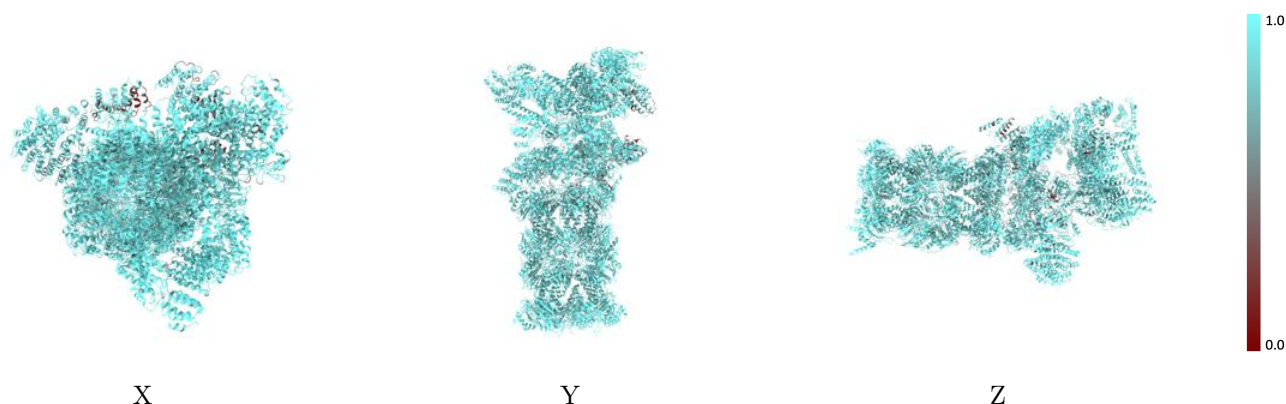
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



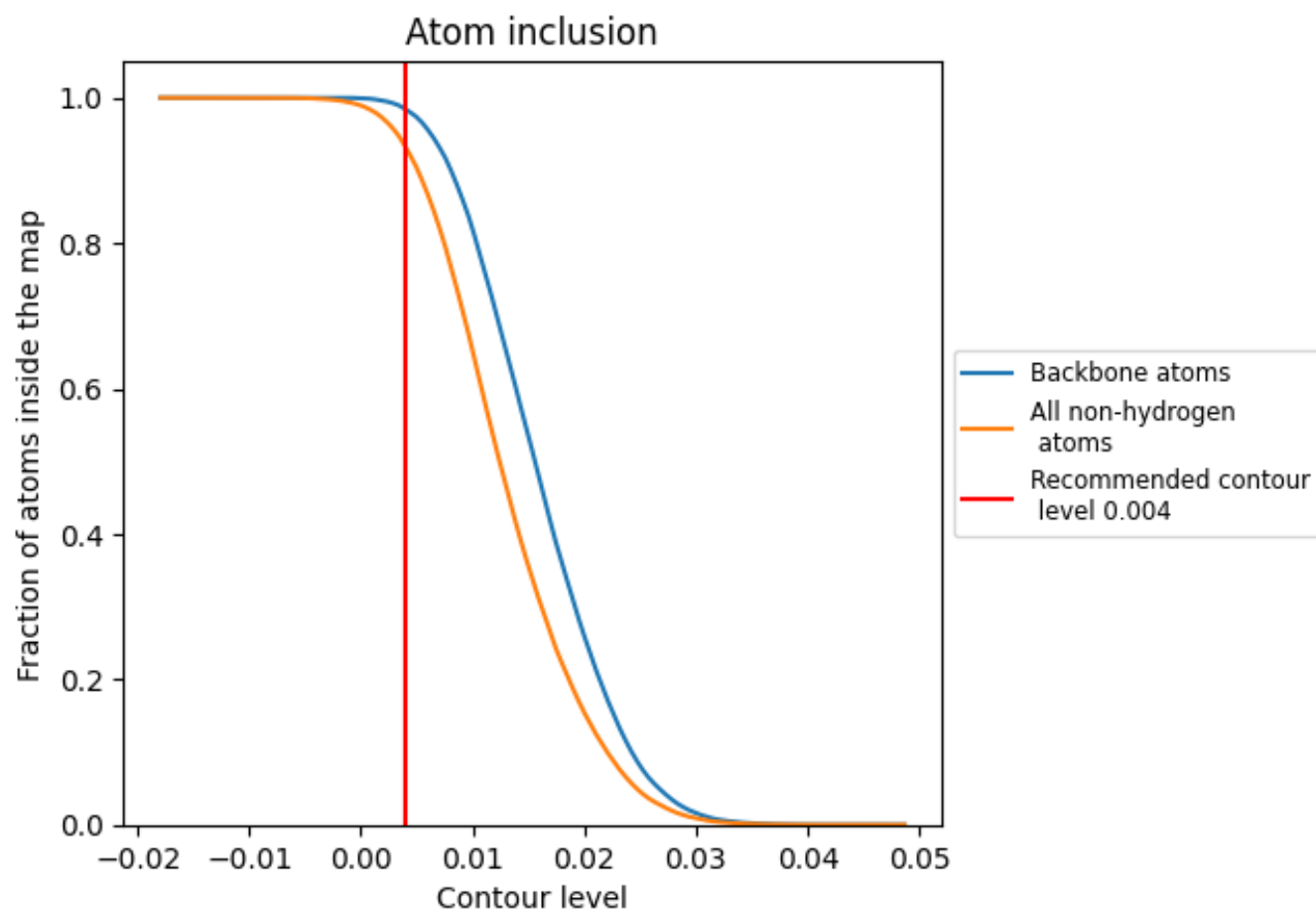
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.1740
A	 0.9611	 0.1930
B	 0.9142	 0.1880
C	 0.9175	 0.1910
D	 0.9352	 0.1980
E	 0.9549	 0.2000
F	 0.9566	 0.1870
G	 0.9353	 0.1790
H	 0.9166	 0.1750
I	 0.9045	 0.1740
J	 0.9252	 0.1900
K	 0.9152	 0.2070
L	 0.9323	 0.2060
M	 0.9211	 0.1840
N	 0.9325	 0.1990
O	 0.9445	 0.1940
P	 0.9339	 0.1820
Q	 0.9384	 0.2000
R	 0.9323	 0.2080
S	 0.9214	 0.2100
T	 0.9293	 0.2060
U	 0.9412	 0.1070
V	 0.8569	 0.1170
W	 0.9718	 0.1750
X	 0.8729	 0.1520
Y	 0.9696	 0.1480
Z	 0.9645	 0.2020
a	 0.9621	 0.1440
b	 0.9362	 0.0820
c	 0.9667	 0.2060
d	 0.9043	 0.1060
e	 0.9815	 0.1930
f	 0.8729	 0.0920
g	 0.9598	 0.2030
h	 0.9659	 0.2070



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Chain	Atom inclusion	Q-score
i	 0.9453	 0.1970
j	 0.9462	 0.1970
k	 0.9462	 0.2110
l	 0.9544	 0.2000
m	 0.9438	 0.1890
n	 0.9315	 0.2040
o	 0.9498	 0.2000
p	 0.9271	 0.1990
q	 0.9329	 0.2100
r	 0.9357	 0.2090
s	 0.9289	 0.2080
t	 0.9225	 0.2020