



wwPDB EM Validation Summary Report ⓘ

Feb 26, 2024 – 01:35 AM EST

PDB ID : 6WJD
EMDB ID : EMD-21691
Title : SA-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 : 2020-04-13
Resolution : 4.80 Å(reported)
Based on initial model : 6MSD

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:

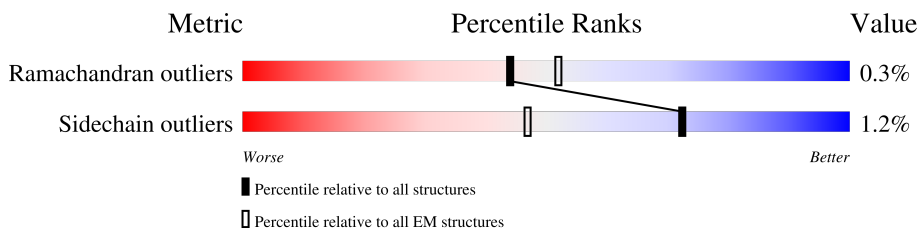
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 4.80 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.



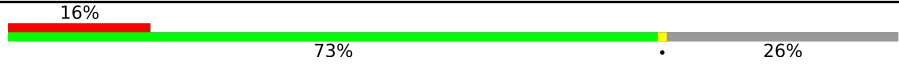
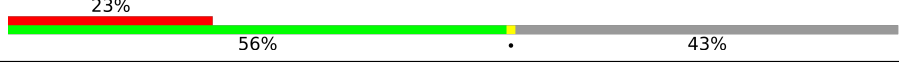
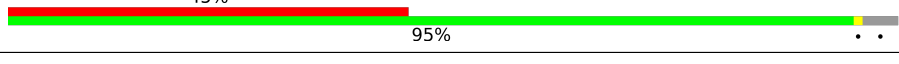
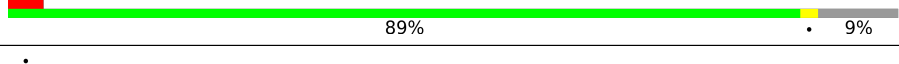

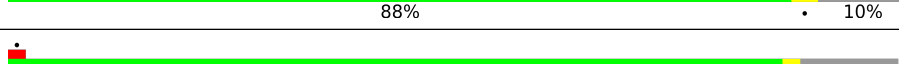
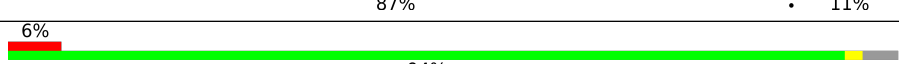
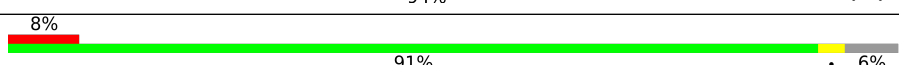
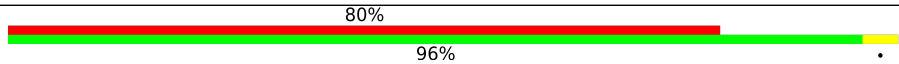
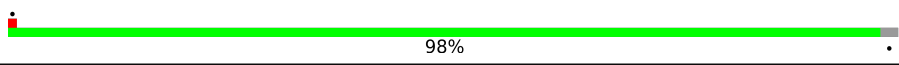
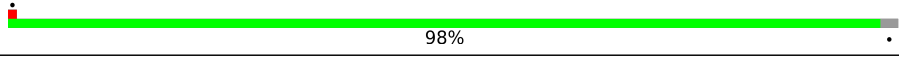
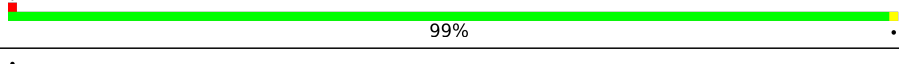
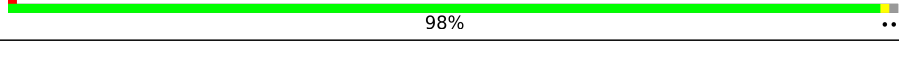
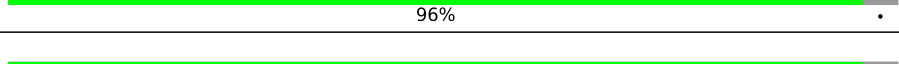
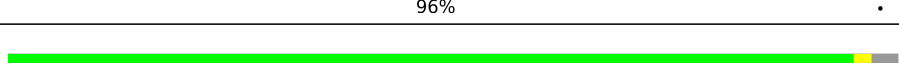
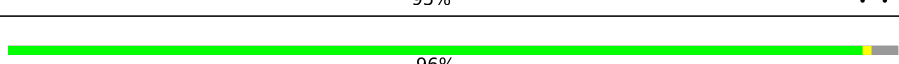
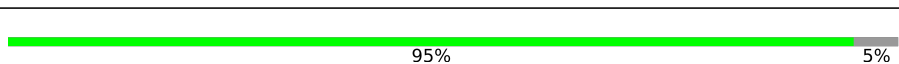
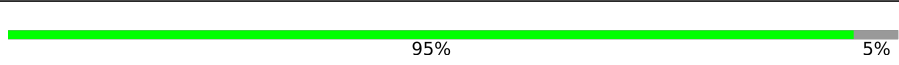
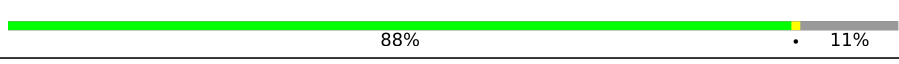
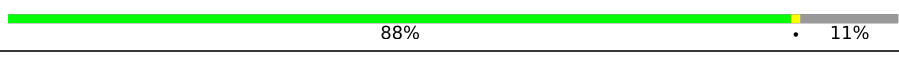
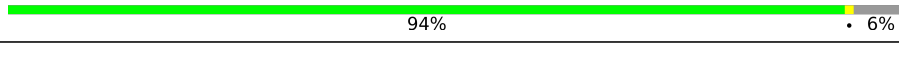
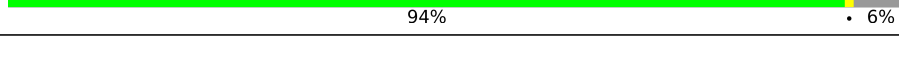



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	953	
2	V	534	
3	W	456	
4	X	422	
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	



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Mol	Chain	Length	Quality of chain
10	d	349	
11	e	70	
12	f	908	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	u	76	
20	G	245	
20	g	245	
21	H	233	
21	h	233	
22	I	260	
22	i	260	
23	J	247	
23	j	247	
24	K	240	
24	k	240	
25	L	268	
25	l	268	
26	M	254	
26	m	254	
27	N	238	

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Mol	Chain	Length	Quality of chain
27	n	238	 80% 20%
28	O	276	 80% 20%
28	o	276	 80% 20%
29	P	204	 100%
29	p	204	 100%
30	Q	201	 99% .
30	q	201	 99% .
31	R	262	 77% 23%
31	r	262	 77% 23%
32	S	240	 89% 11%
32	s	240	 89% 11%
33	T	263	 81% 18%
33	t	263	 81% 18%

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 100757 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
			Total	C	N	O	S		
1	U	812	5815	3666	1006	1109	34	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	480	3785	2394	676	704	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	W	456	3622	2279	631	690	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	380	2967	1885	506	565	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Y	378	3084	1965	524	578	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Z	286	2208	1407	377	419	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	a	373	2964	1892	506	551	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	b	191	1437	899	253	277	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	c	287	2190	1381	386	408	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	d	257	2039	1311	339	381	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e	40	320	189	53	76	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	f	872	6276	3916	1070	1255	35	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A	392	2717	1712	469	526	10	0	0

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B	384	2690	1701	466	513	10	0	0

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	C	360	2529	1593	448	475	13	0	0

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	D	372	2621	1649	468	497	7	0	0

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	E	386	2745	1723	488	523	11	0	0

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	F	414	2918	1813	513	578	14	0	0

- Molecule 19 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	u	76	540	334	100	105	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	G	240	1826	1160	305	348	13	0	0
20	g	240	1818	1155	304	347	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	232	Total	C	N	O	S	0	0
			1697	1076	289	327	5		
21	h	230	Total	C	N	O	S	0	0
			1697	1074	287	331	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	250	Total	C	N	O	S	0	0
			1897	1196	328	365	8		
22	i	250	Total	C	N	O	S	0	0
			1903	1198	328	369	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	239	Total	C	N	O	S	0	0
			1695	1053	307	331	4		
23	j	239	Total	C	N	O	S	0	0
			1696	1053	307	331	5		

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	228	Total	C	N	O	S	0	0
			1709	1072	281	346	10		
24	k	228	Total	C	N	O	S	0	0
			1719	1077	284	348	10		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	238	Total	C	N	O	S	0	0
			1832	1146	331	344	11		
25	l	238	Total	C	N	O	S	0	0
			1832	1146	331	344	11		

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	240	Total	C	N	O	S	0	0
			1853	1178	314	352	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	m	240	Total	C	N	O	S	0	0
			1836	1168	310	350	8		

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
27	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	O	220	Total	C	N	O	S	0	0
			1641	1032	280	317	12		
28	o	220	Total	C	N	O	S	0	0
			1634	1028	277	318	11		

- Molecule 29 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	P	204	Total	C	N	O	S	0	0
			1584	1009	264	293	18		
29	p	204	Total	C	N	O	S	0	0
			1581	1009	264	290	18		

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Q	199	Total	C	N	O	S	0	0
			1556	996	262	289	9		
30	q	199	Total	C	N	O	S	0	0
			1547	992	260	286	9		

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
31	r	201	Total	C	N	O	S	0	0
			1544	972	272	291	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	S	213	Total 1636	C 1035	N 282	O 311	S 8	0	0
32	s	213	Total 1633	C 1035	N 279	O 311	S 8	0	0

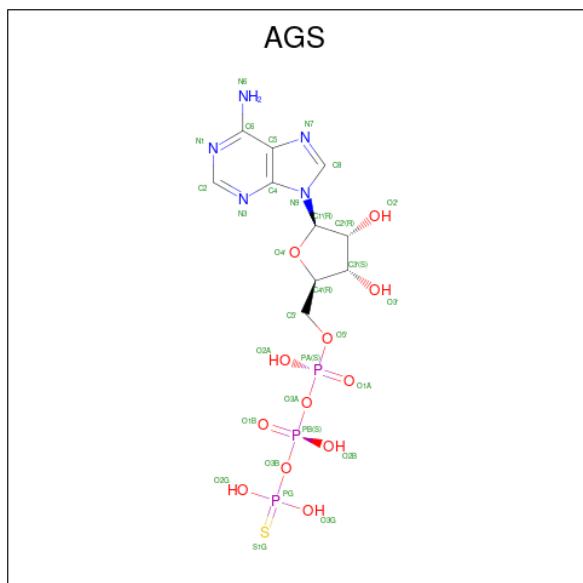
- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	T	215	Total 1665	C 1050	N 285	O 318	S 12	0	0
33	t	215	Total 1667	C 1052	N 285	O 318	S 12	0	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 35 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

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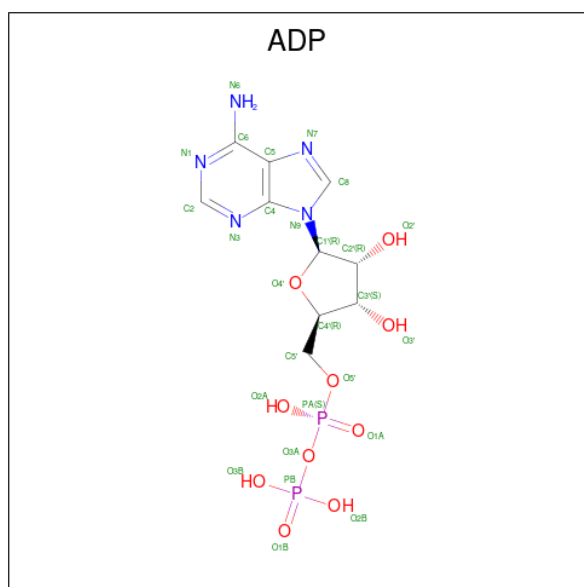
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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
35	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
35	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
35	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	A	1	Total	Mg	0
			1	1	
36	B	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	E	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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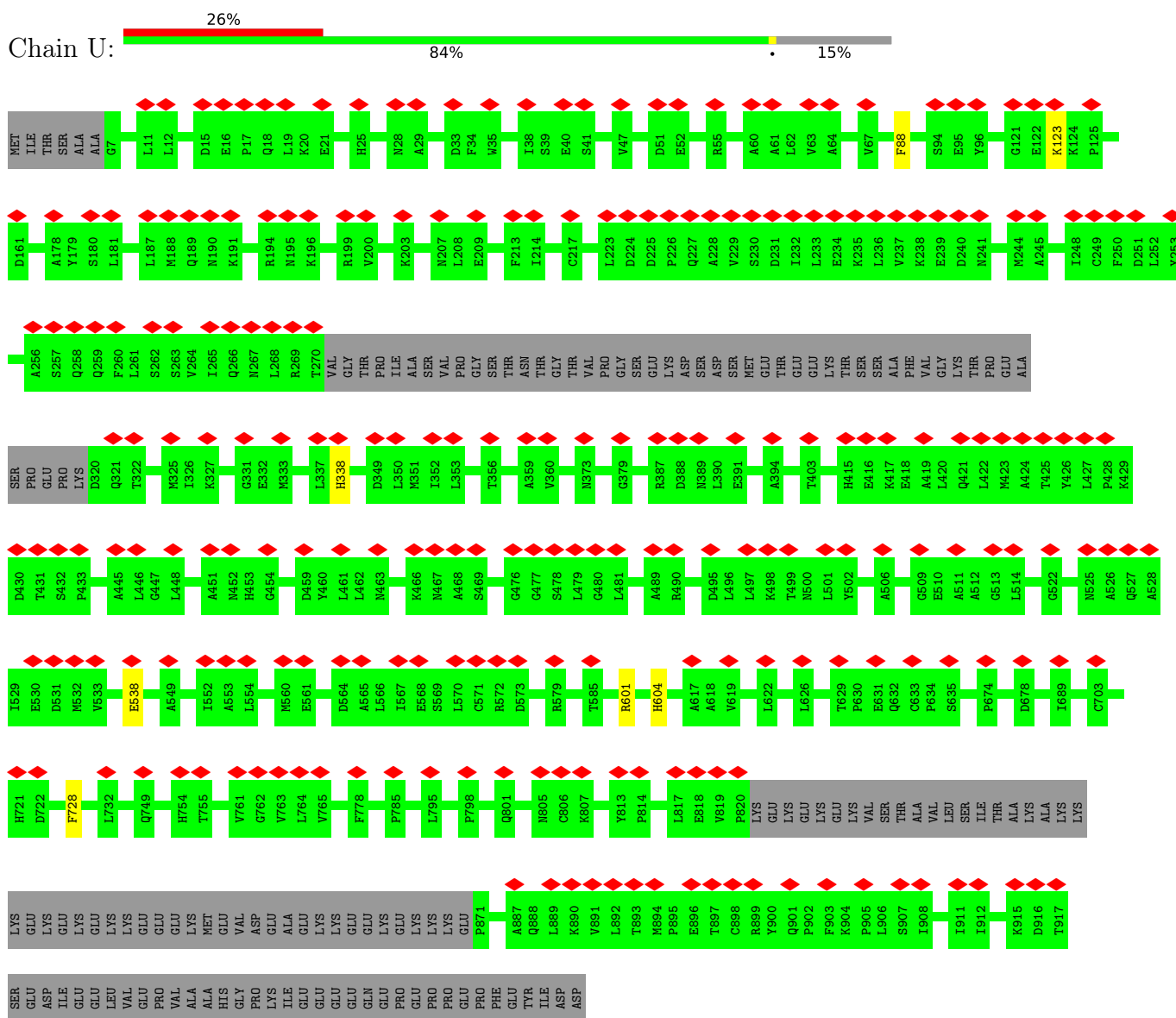
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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
37	F	1	27	10	5	10	2	0

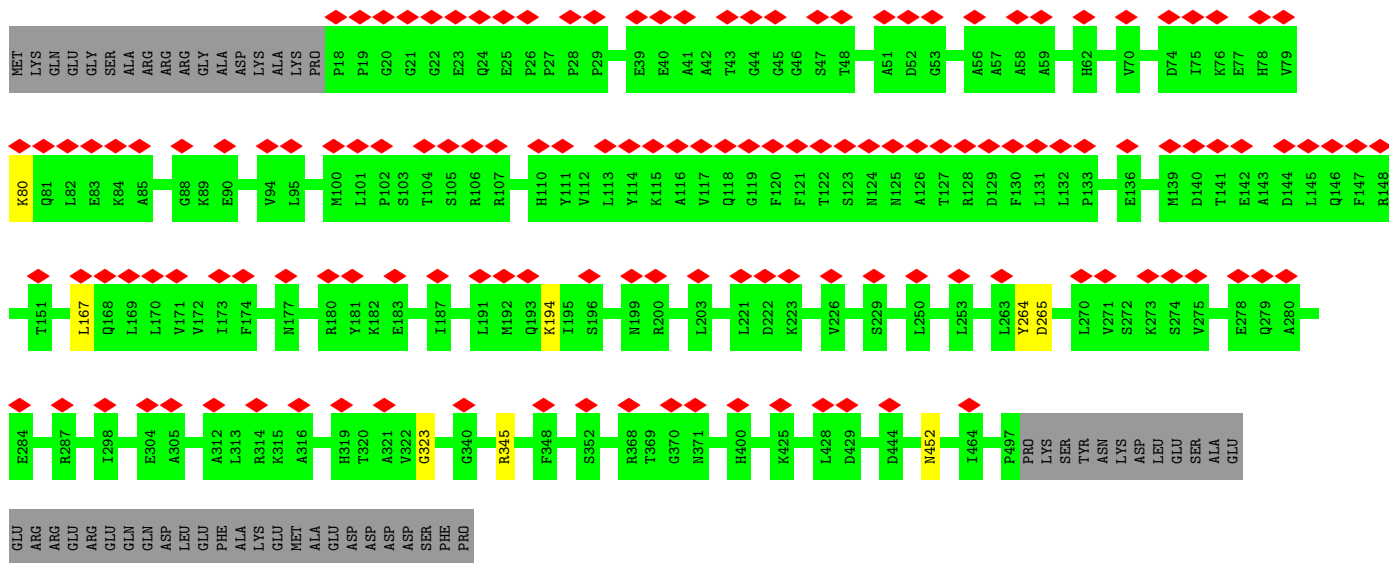
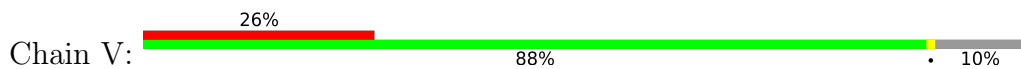
3 Residue-property plots [i](#)

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

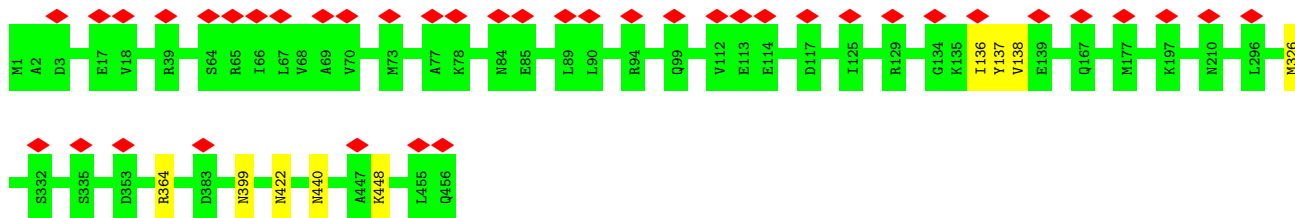
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1



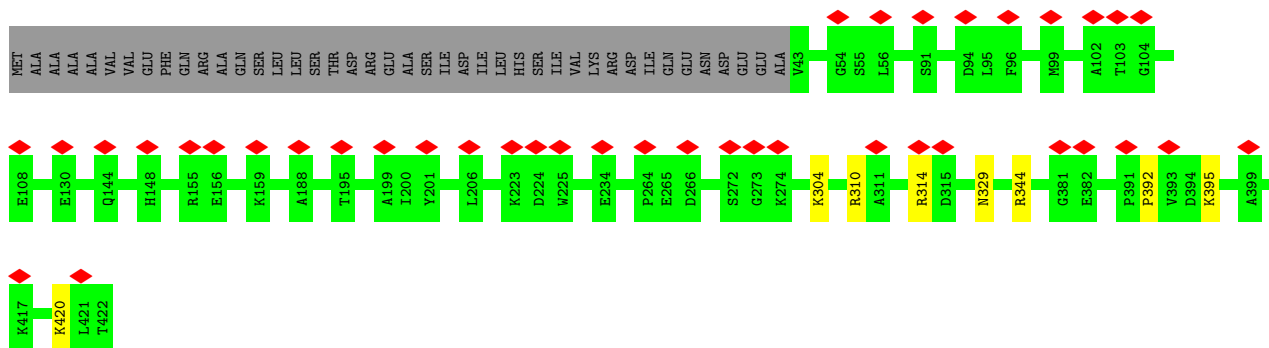
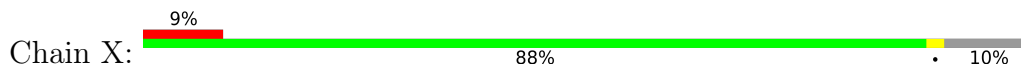
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3



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

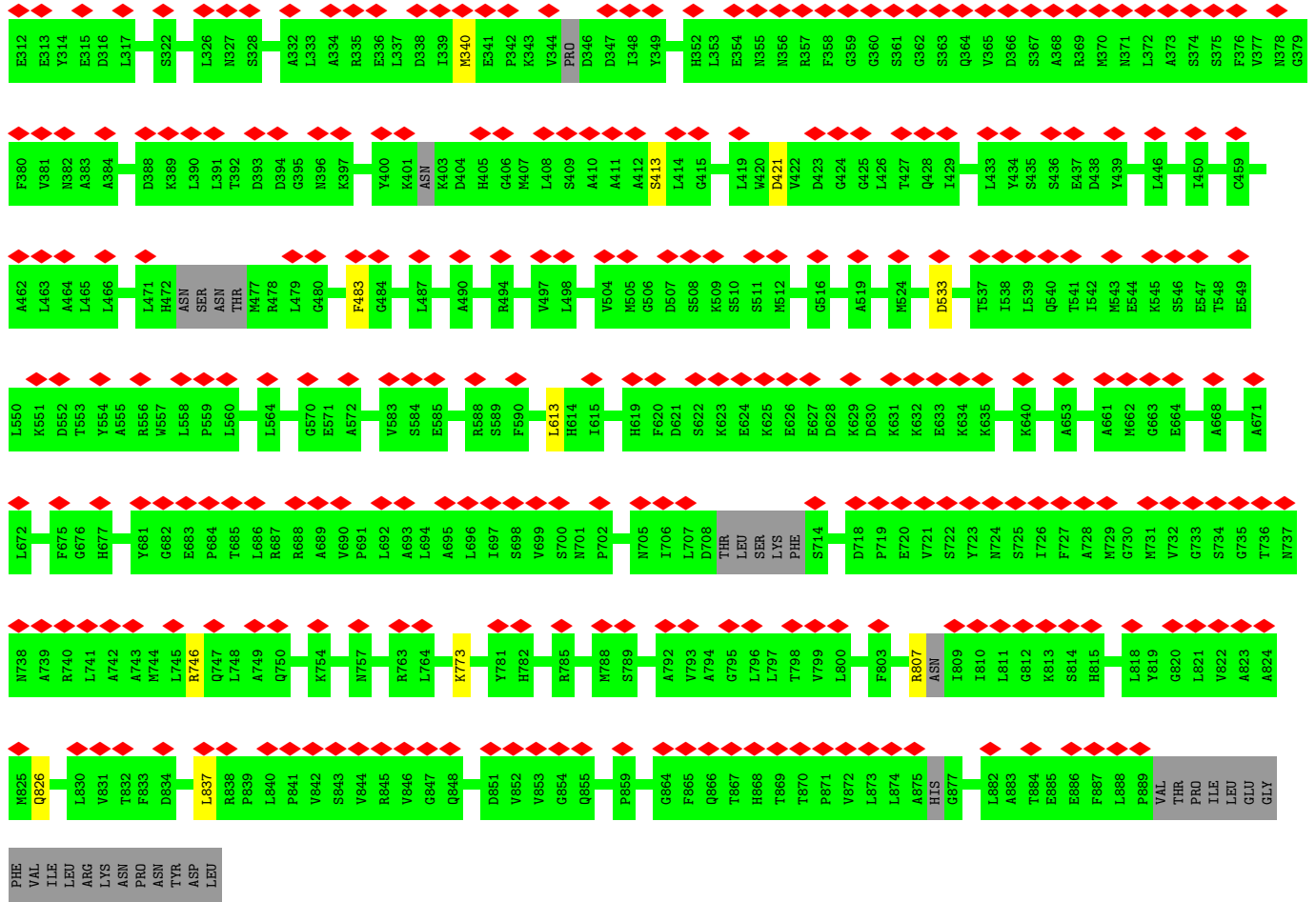


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

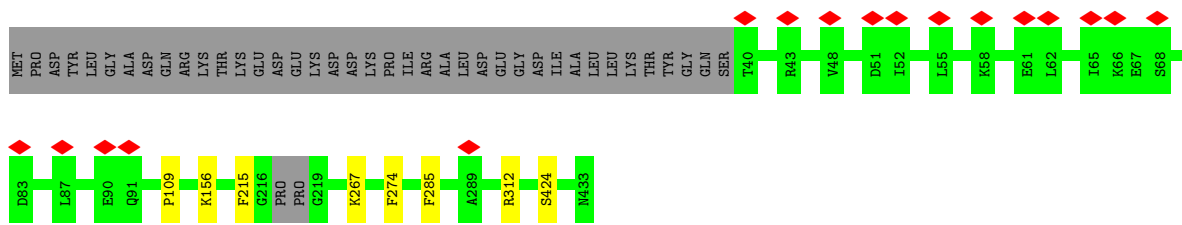
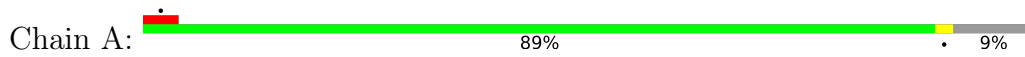


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

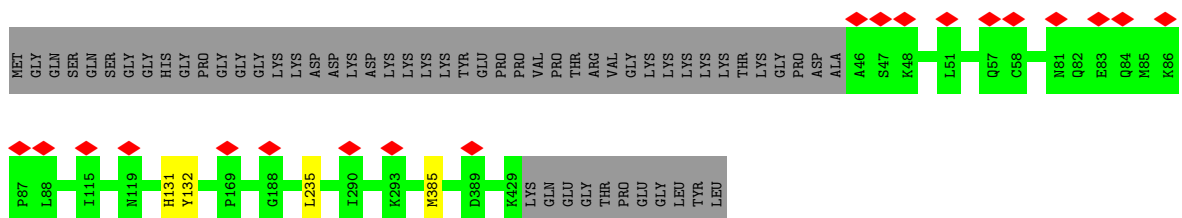
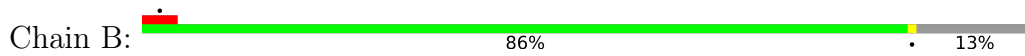




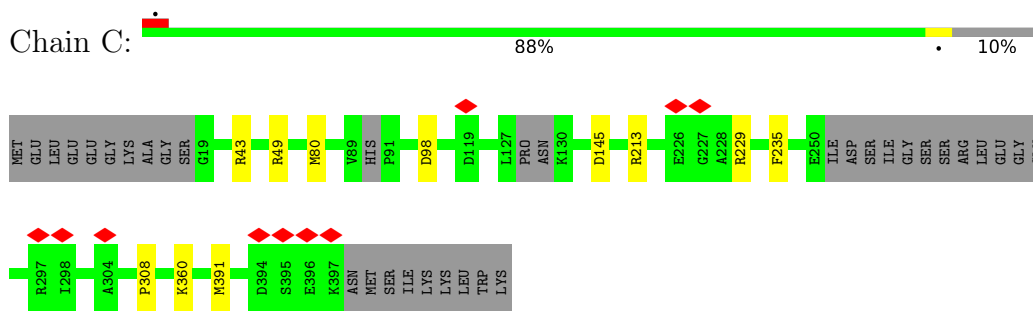
• Molecule 13: 26S proteasome regulatory subunit 7



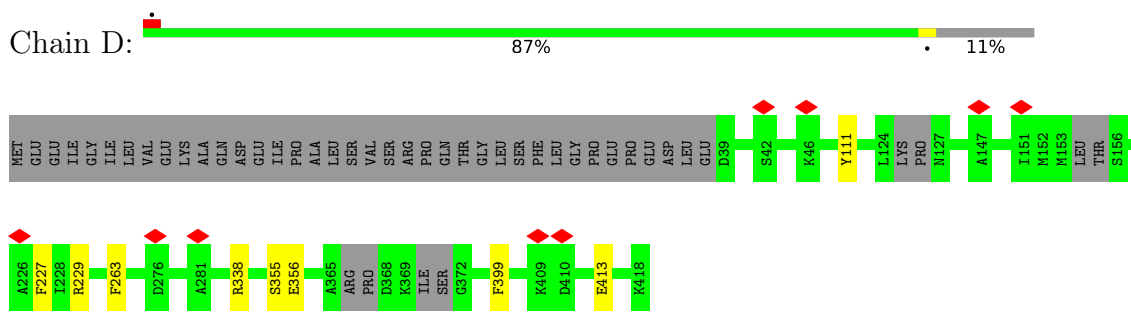
• Molecule 14: 26S proteasome regulatory subunit 4



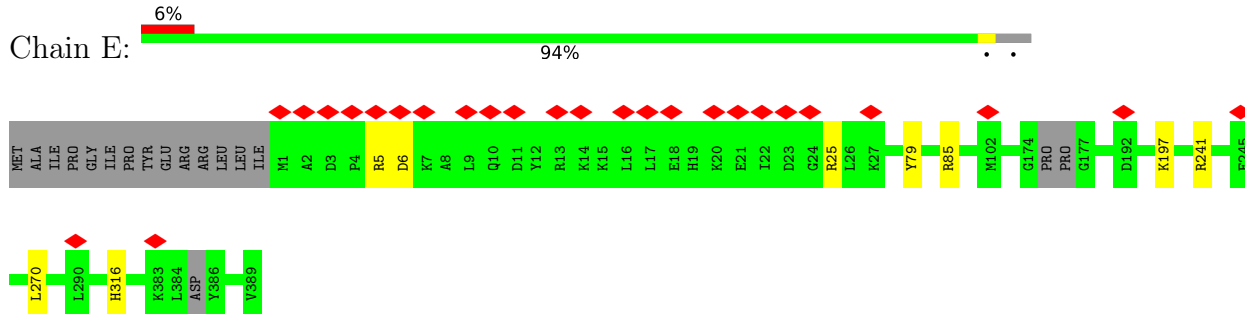
• Molecule 15: 26S proteasome regulatory subunit 8



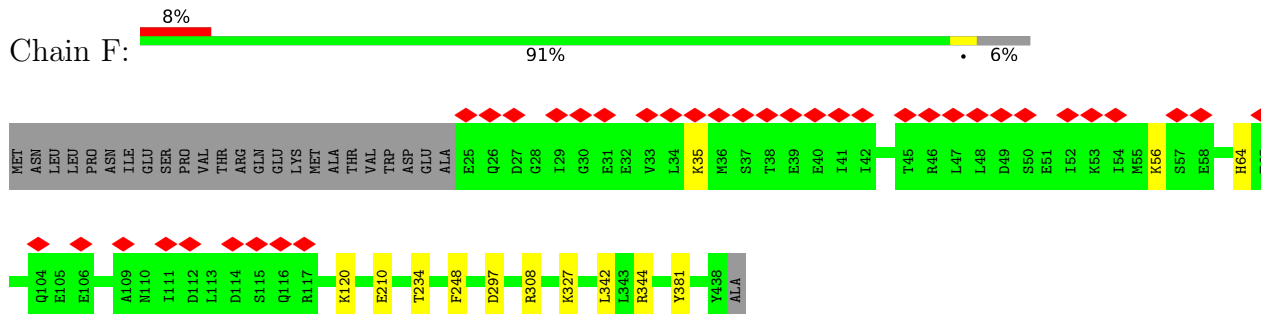
• Molecule 16: 26S proteasome regulatory subunit 6B



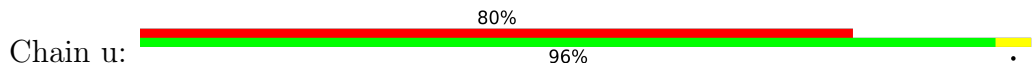
• Molecule 17: 26S proteasome regulatory subunit 10B

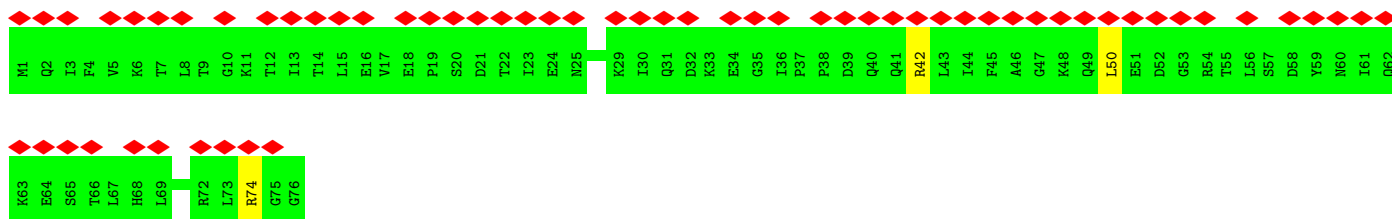


• Molecule 18: 26S proteasome regulatory subunit 6A

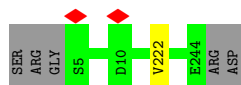


• Molecule 19: Ubiquitin

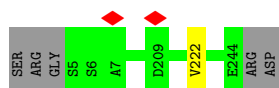




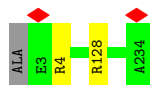
- Molecule 20: Proteasome subunit alpha type-6



- Molecule 20: Proteasome subunit alpha type-6



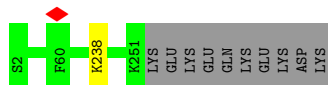
- Molecule 21: Proteasome subunit alpha type-2



- Molecule 21: Proteasome subunit alpha type-2

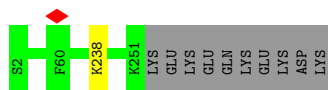


- Molecule 22: Proteasome subunit alpha type-4



- Molecule 22: Proteasome subunit alpha type-4





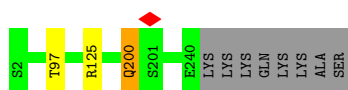
- Molecule 23: Proteasome subunit alpha type-7

Chain J: 95%



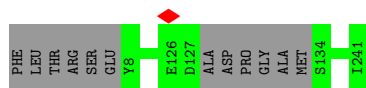
- Molecule 23: Proteasome subunit alpha type-7

Chain j: 96%



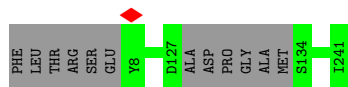
- Molecule 24: Proteasome subunit alpha type-5

Chain K: 95% 5%



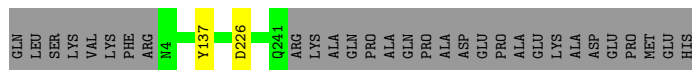
- Molecule 24: Proteasome subunit alpha type-5

Chain k: 95% 5%



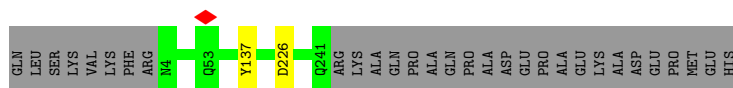
- Molecule 25: Proteasome subunit alpha type-1

Chain L: 88% 11%



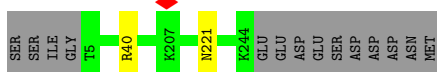
- Molecule 25: Proteasome subunit alpha type-1

Chain l: 88% 11%



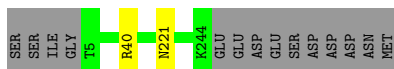
- Molecule 26: Proteasome subunit alpha type-3

Chain M:  94% • 6%




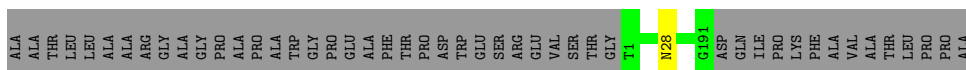
- Molecule 26: Proteasome subunit alpha type-3

Chain m:  94% • 6%




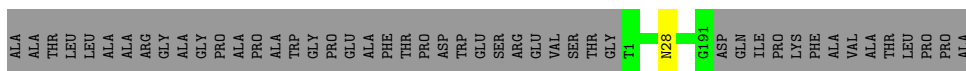
- Molecule 27: Proteasome subunit beta type-6

Chain N:  80% 20%




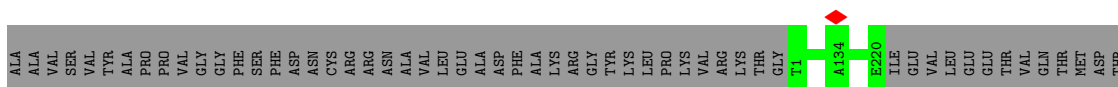
- Molecule 27: Proteasome subunit beta type-6

Chain n:  80% 20%




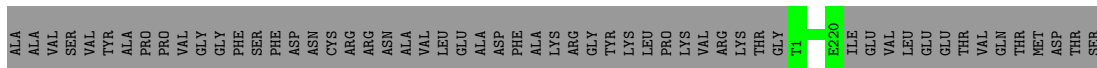
- Molecule 28: Proteasome subunit beta type-7

Chain O:  80% 20%



- Molecule 28: Proteasome subunit beta type-7

Chain o:  80% 20%



- Molecule 29: Proteasome subunit beta type-3

Chain P:  100%

There are no outlier residues recorded for this chain.

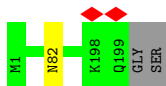
- Molecule 29: Proteasome subunit beta type-3

Chain p: 100%

There are no outlier residues recorded for this chain.

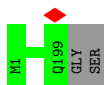
- Molecule 30: Proteasome subunit beta type-2

Chain Q: 99%



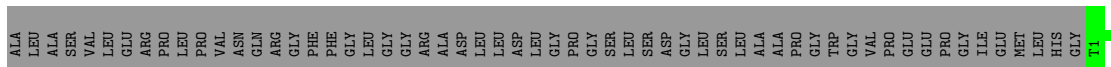
- Molecule 30: Proteasome subunit beta type-2

Chain q: 99%



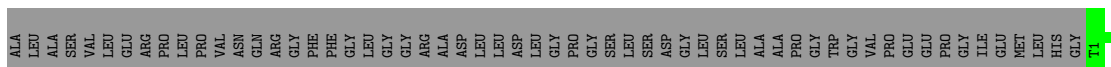
- Molecule 31: Proteasome subunit beta type-5

Chain R: 77% 23%



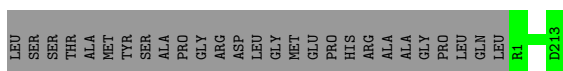
- Molecule 31: Proteasome subunit beta type-5

Chain r: 77% 23%



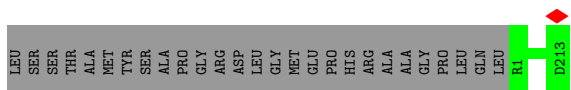
- Molecule 32: Proteasome subunit beta type-1

Chain S: 89% 11%

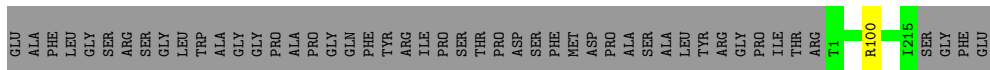
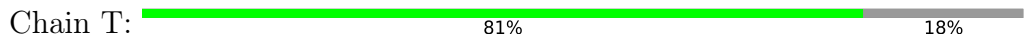


- Molecule 32: Proteasome subunit beta type-1

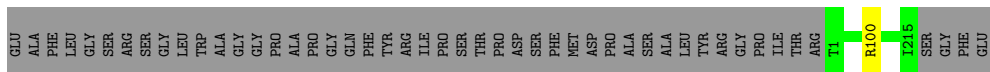
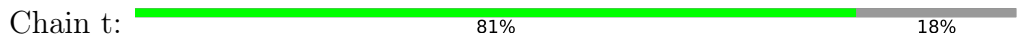
Chain s: 89% 11%



- Molecule 33: Proteasome subunit beta type-4



- Molecule 33: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37698	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	0.054	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	614.25, 614.25, 614.25	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MG, ZN, ADP, 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	0.28	0/5916	0.47	0/8044
2	V	0.32	0/3859	0.65	0/5221
3	W	0.33	0/3667	0.60	0/4934
4	X	0.31	0/3011	0.57	0/4064
5	Y	0.34	0/3142	0.60	0/4234
6	Z	0.32	0/2247	0.63	0/3049
7	a	0.29	0/3022	0.58	0/4093
8	b	0.31	0/1455	0.60	0/1971
9	c	0.37	0/2231	0.66	0/3020
10	d	0.31	0/2082	0.63	0/2820
11	e	0.28	0/324	0.57	0/433
12	f	0.27	0/6364	0.49	0/8634
13	A	0.37	0/2760	0.50	0/3768
14	B	0.35	0/2729	0.50	0/3717
15	C	0.35	0/2561	0.49	0/3476
16	D	0.38	0/2659	0.50	0/3611
17	E	0.37	0/2788	0.50	0/3786
18	F	0.37	0/2955	0.50	0/4018
19	u	0.34	0/546	0.49	0/738
20	G	0.37	0/1859	0.55	0/2523
20	g	0.38	0/1851	0.55	0/2513
21	H	0.42	0/1732	0.53	0/2358
21	h	0.40	0/1731	0.53	0/2354
22	I	0.36	0/1927	0.58	0/2608
22	i	0.35	0/1933	0.57	0/2616
23	J	0.41	0/1719	0.58	0/2347
23	j	0.33	0/1720	0.55	0/2347
24	K	0.34	0/1734	0.55	0/2348
24	k	0.35	0/1744	0.56	0/2360
25	L	0.38	0/1867	0.58	0/2529
25	l	0.38	0/1867	0.59	0/2529
26	M	0.38	0/1888	0.55	0/2549

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	m	0.38	0/1871	0.55	0/2529
27	N	0.35	0/1454	0.51	0/1967
27	n	0.35	0/1454	0.50	0/1967
28	O	0.36	0/1668	0.53	0/2262
28	o	0.36	0/1661	0.53	0/2255
29	P	0.36	0/1613	0.52	0/2176
29	p	0.36	0/1610	0.52	0/2173
30	Q	0.37	0/1589	0.54	0/2156
30	q	0.37	0/1580	0.54	0/2145
31	R	0.37	0/1579	0.49	0/2134
31	r	0.37	0/1575	0.49	0/2129
32	S	0.35	0/1666	0.51	0/2247
32	s	0.35	0/1663	0.50	0/2244
33	T	0.37	0/1698	0.52	0/2302
33	t	0.37	0/1700	0.52	0/2305
All	All	0.35	0/102271	0.55	0/138603

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	806/953 (85%)	707 (88%)	99 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	478/534 (90%)	418 (87%)	56 (12%)	4 (1%)	19	59
3	W	454/456 (100%)	408 (90%)	43 (10%)	3 (1%)	22	62
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	41	76
5	Y	376/389 (97%)	346 (92%)	30 (8%)	0	100	100
6	Z	284/324 (88%)	246 (87%)	37 (13%)	1 (0%)	34	72
7	a	371/376 (99%)	334 (90%)	36 (10%)	1 (0%)	41	76
8	b	189/377 (50%)	175 (93%)	13 (7%)	1 (0%)	29	68
9	c	285/309 (92%)	241 (85%)	40 (14%)	4 (1%)	11	46
10	d	255/349 (73%)	217 (85%)	37 (14%)	1 (0%)	34	72
11	e	36/70 (51%)	25 (69%)	11 (31%)	0	100	100
12	f	854/908 (94%)	696 (82%)	158 (18%)	0	100	100
13	A	388/433 (90%)	309 (80%)	76 (20%)	3 (1%)	19	59
14	B	382/440 (87%)	313 (82%)	69 (18%)	0	100	100
15	C	352/398 (88%)	291 (83%)	60 (17%)	1 (0%)	41	76
16	D	362/418 (87%)	296 (82%)	63 (17%)	3 (1%)	19	59
17	E	380/403 (94%)	313 (82%)	65 (17%)	2 (0%)	29	68
18	F	412/439 (94%)	342 (83%)	68 (16%)	2 (0%)	29	68
19	u	74/76 (97%)	65 (88%)	8 (11%)	1 (1%)	11	46
20	G	238/245 (97%)	223 (94%)	14 (6%)	1 (0%)	34	72
20	g	238/245 (97%)	223 (94%)	14 (6%)	1 (0%)	34	72
21	H	230/233 (99%)	223 (97%)	7 (3%)	0	100	100
21	h	226/233 (97%)	219 (97%)	7 (3%)	0	100	100
22	I	248/260 (95%)	227 (92%)	21 (8%)	0	100	100
22	i	248/260 (95%)	226 (91%)	22 (9%)	0	100	100
23	J	237/247 (96%)	217 (92%)	18 (8%)	2 (1%)	19	59
23	j	237/247 (96%)	221 (93%)	14 (6%)	2 (1%)	19	59
24	K	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
24	k	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
25	L	236/268 (88%)	221 (94%)	14 (6%)	1 (0%)	34	72
25	l	236/268 (88%)	220 (93%)	15 (6%)	1 (0%)	34	72
26	M	238/254 (94%)	223 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	m	238/254 (94%)	223 (94%)	15 (6%)	0	100	100
27	N	189/238 (79%)	182 (96%)	7 (4%)	0	100	100
27	n	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
28	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
28	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
30	Q	197/201 (98%)	180 (91%)	17 (9%)	0	100	100
30	q	197/201 (98%)	180 (91%)	17 (9%)	0	100	100
31	R	199/262 (76%)	191 (96%)	8 (4%)	0	100	100
31	r	199/262 (76%)	191 (96%)	8 (4%)	0	100	100
32	S	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
32	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
33	T	213/263 (81%)	205 (96%)	8 (4%)	0	100	100
33	t	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
All	All	13272/14936 (89%)	11908 (90%)	1328 (10%)	36 (0%)	44	76

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	167	LEU
2	V	265	ASP
3	W	137	TYR
9	c	156	VAL
9	c	108	VAL

5.3.2 Protein sidechains [i](#)

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	542/816 (66%)	535 (99%)	7 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	394/460 (86%)	390 (99%)	4 (1%)	76	86
3	W	394/416 (95%)	388 (98%)	6 (2%)	65	80
4	X	313/362 (86%)	306 (98%)	7 (2%)	52	71
5	Y	326/344 (95%)	324 (99%)	2 (1%)	86	92
6	Z	238/295 (81%)	233 (98%)	5 (2%)	53	72
7	a	324/336 (96%)	324 (100%)	0	100	100
8	b	162/312 (52%)	161 (99%)	1 (1%)	86	92
9	c	225/267 (84%)	220 (98%)	5 (2%)	52	71
10	d	211/293 (72%)	209 (99%)	2 (1%)	78	87
11	e	34/63 (54%)	33 (97%)	1 (3%)	42	64
12	f	608/763 (80%)	595 (98%)	13 (2%)	53	72
13	A	235/372 (63%)	230 (98%)	5 (2%)	53	72
14	B	246/385 (64%)	242 (98%)	4 (2%)	62	79
15	C	226/346 (65%)	216 (96%)	10 (4%)	28	54
16	D	223/366 (61%)	217 (97%)	6 (3%)	44	66
17	E	246/353 (70%)	239 (97%)	7 (3%)	43	65
18	F	266/379 (70%)	255 (96%)	11 (4%)	30	55
19	u	49/68 (72%)	47 (96%)	2 (4%)	30	55
20	G	193/209 (92%)	193 (100%)	0	100	100
20	g	190/209 (91%)	190 (100%)	0	100	100
21	H	161/190 (85%)	159 (99%)	2 (1%)	71	84
21	h	163/190 (86%)	161 (99%)	2 (1%)	71	84
22	I	188/220 (86%)	187 (100%)	1 (0%)	88	93
22	i	190/220 (86%)	189 (100%)	1 (0%)	88	93
23	J	149/210 (71%)	147 (99%)	2 (1%)	69	82
23	j	149/210 (71%)	147 (99%)	2 (1%)	69	82
24	K	183/202 (91%)	183 (100%)	0	100	100
24	k	185/202 (92%)	185 (100%)	0	100	100
25	L	193/229 (84%)	192 (100%)	1 (0%)	88	93
25	l	193/229 (84%)	192 (100%)	1 (0%)	88	93
26	M	189/211 (90%)	187 (99%)	2 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	m	184/211 (87%)	182 (99%)	2 (1%)	73	85
27	N	148/180 (82%)	147 (99%)	1 (1%)	84	90
27	n	148/180 (82%)	147 (99%)	1 (1%)	84	90
28	O	176/227 (78%)	176 (100%)	0	100	100
28	o	175/227 (77%)	175 (100%)	0	100	100
29	P	171/173 (99%)	171 (100%)	0	100	100
29	p	170/173 (98%)	170 (100%)	0	100	100
30	Q	160/171 (94%)	159 (99%)	1 (1%)	86	92
30	q	158/171 (92%)	158 (100%)	0	100	100
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	152/201 (76%)	152 (100%)	0	100	100
32	S	171/198 (86%)	171 (100%)	0	100	100
32	s	171/198 (86%)	171 (100%)	0	100	100
33	T	174/214 (81%)	173 (99%)	1 (1%)	86	92
33	t	175/214 (82%)	174 (99%)	1 (1%)	86	92
All	All	10074/12666 (80%)	9955 (99%)	119 (1%)	72	84

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	A	285	PHE
21	h	128	ARG
15	C	391	MET
21	h	4	ARG
33	t	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
13	A	44	GLN
17	E	271	HIS
30	q	71	ASN
13	A	322	ASN
16	D	49	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	AGS	B	501	36	26,33,33	0.88	2 (7%)	26,52,52	1.23	2 (7%)
37	ADP	F	501	36	24,29,29	0.80	1 (4%)	29,45,45	0.90	2 (6%)
35	AGS	D	501	36	26,33,33	0.97	1 (3%)	26,52,52	1.64	4 (15%)
37	ADP	C	501	-	24,29,29	0.82	1 (4%)	29,45,45	0.94	2 (6%)
35	AGS	E	401	36	26,33,33	0.87	2 (7%)	26,52,52	1.20	1 (3%)
35	AGS	A	501	36	26,33,33	0.83	1 (3%)	26,52,52	1.21	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	AGS	B	501	36	-	5/17/38/38	0/3/3/3
37	ADP	F	501	36	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	AGS	D	501	36	-	6/17/38/38	0/3/3/3
37	ADP	C	501	-	-	7/12/32/32	0/3/3/3
35	AGS	E	401	36	-	3/17/38/38	0/3/3/3
35	AGS	A	501	36	-	6/17/38/38	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)
37	C	501	ADP	C5-C4	2.21	1.46	1.40
37	F	501	ADP	C5-C4	2.11	1.46	1.40
35	D	501	AGS	PG-O2G	2.06	1.61	1.54
35	B	501	AGS	PG-O3G	-2.02	1.48	1.54
35	E	401	AGS	PG-O3G	-2.02	1.48	1.54

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	401	AGS	N3-C2-N1	-4.66	121.39	128.68
35	B	501	AGS	N3-C2-N1	-4.63	121.43	128.68
35	A	501	AGS	N3-C2-N1	-4.63	121.45	128.68
35	D	501	AGS	N3-C2-N1	-4.53	121.60	128.68
35	D	501	AGS	PA-O3A-PB	-4.41	117.71	132.83

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

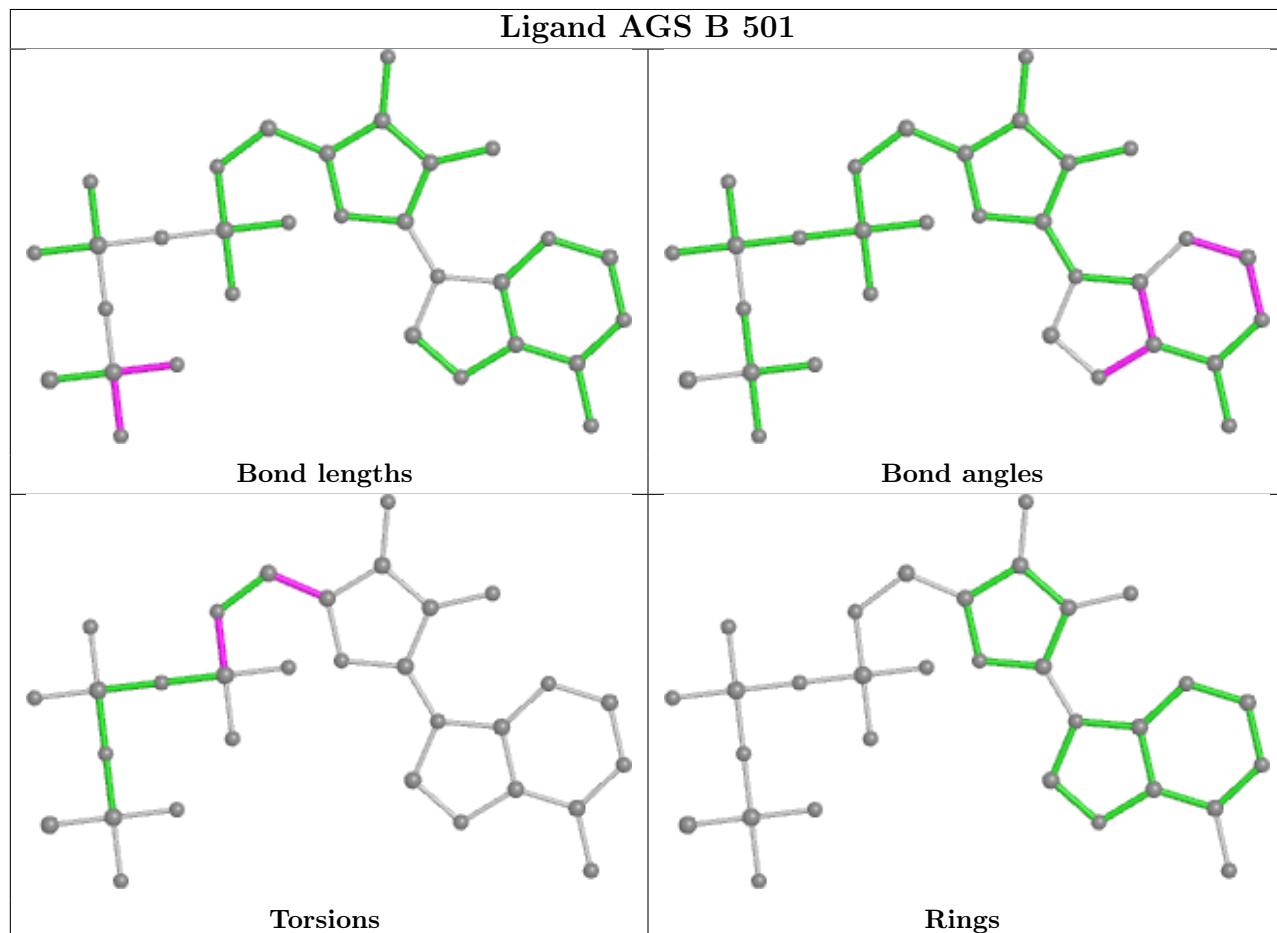
Mol	Chain	Res	Type	Atoms
35	B	501	AGS	C5'-O5'-PA-O2A
35	D	501	AGS	C5'-O5'-PA-O1A
35	D	501	AGS	C5'-O5'-PA-O3A
37	C	501	ADP	PA-O3A-PB-O3B
37	C	501	ADP	C5'-O5'-PA-O2A

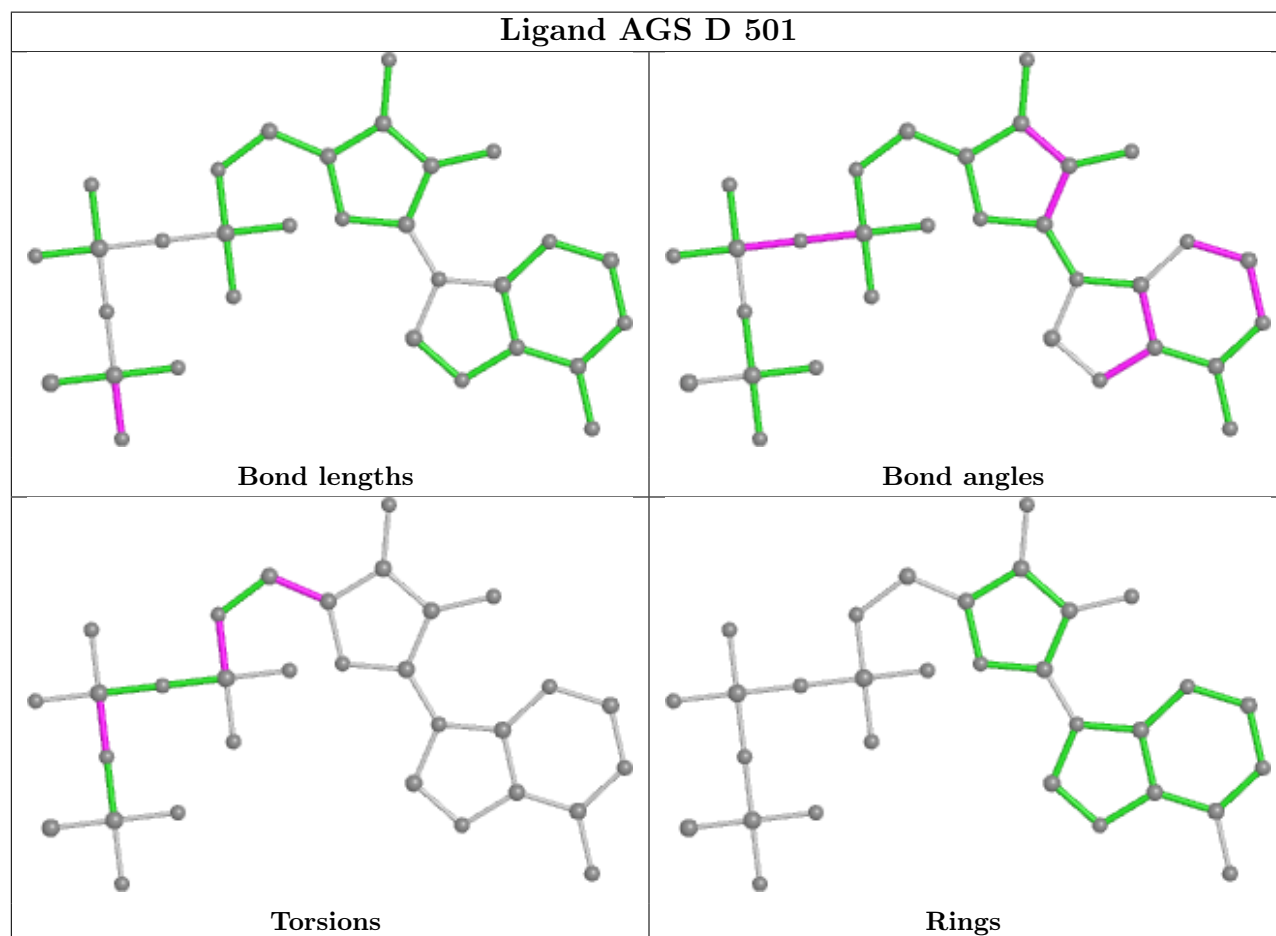
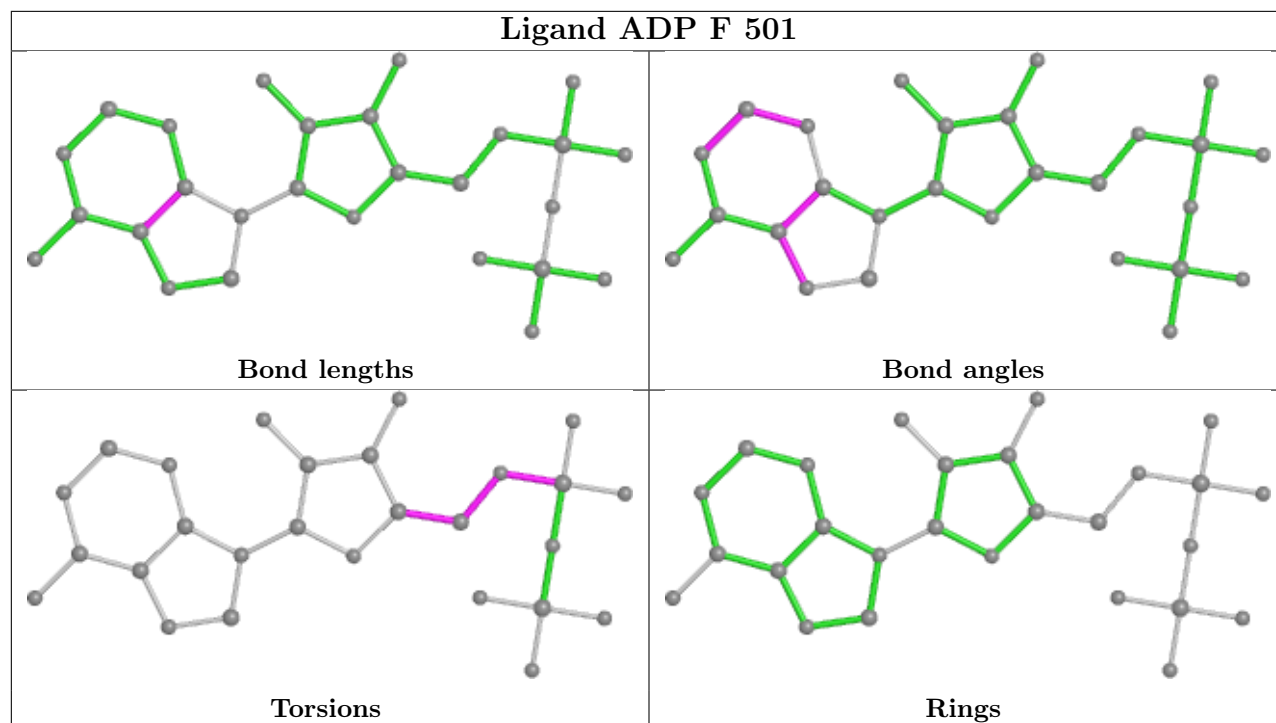
There are no ring outliers.

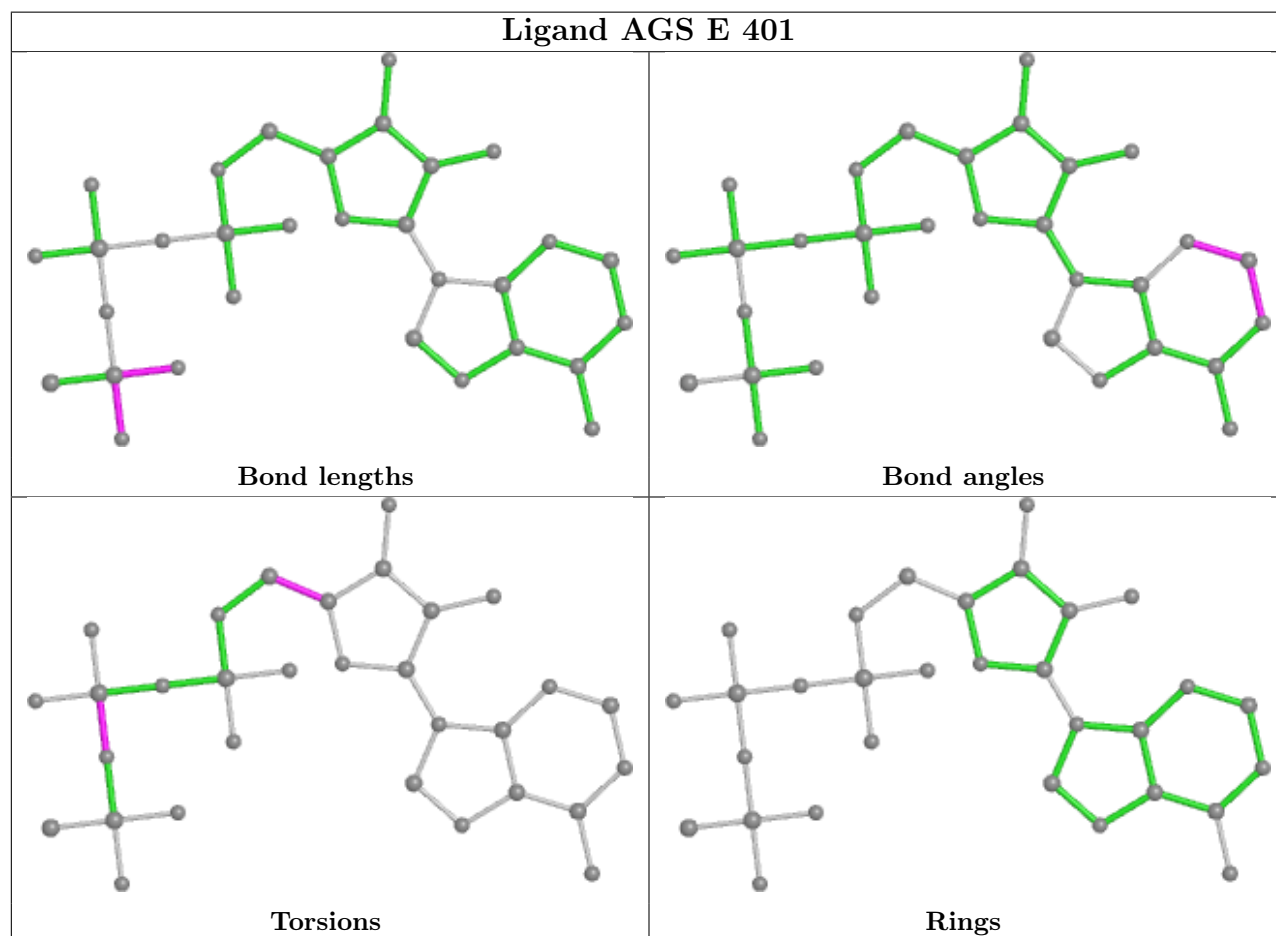
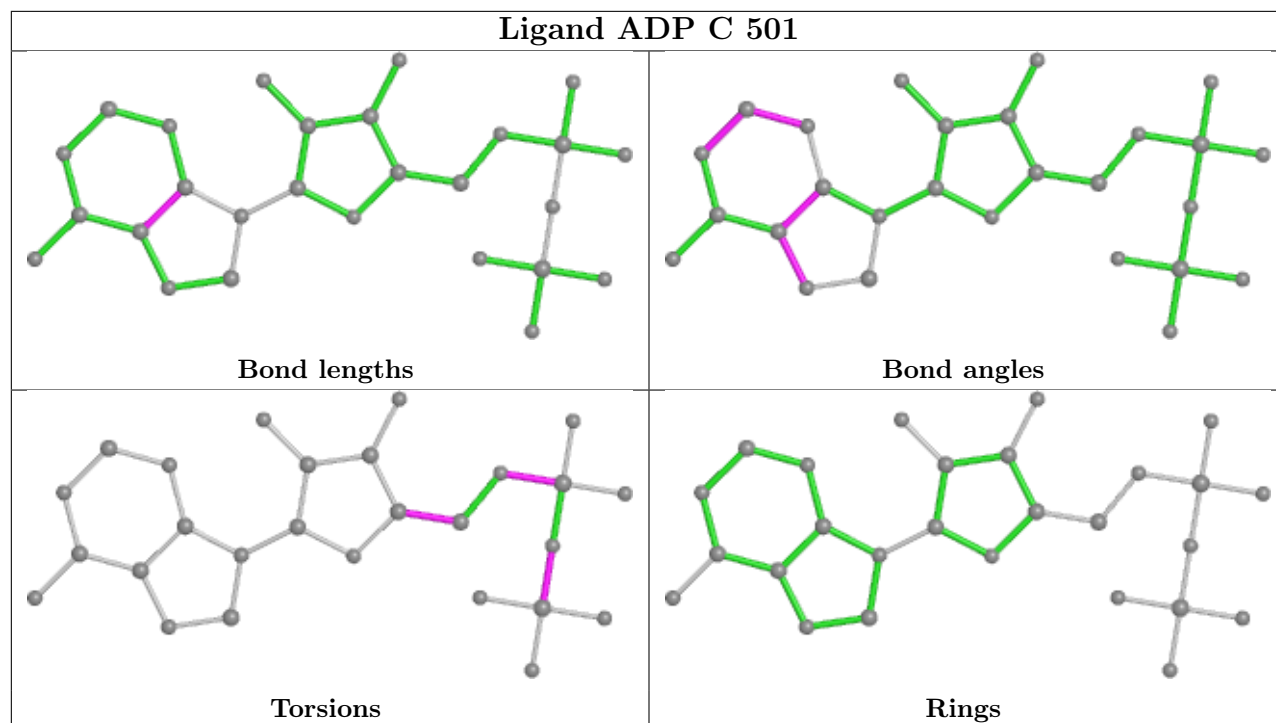
No monomer is involved in short contacts.

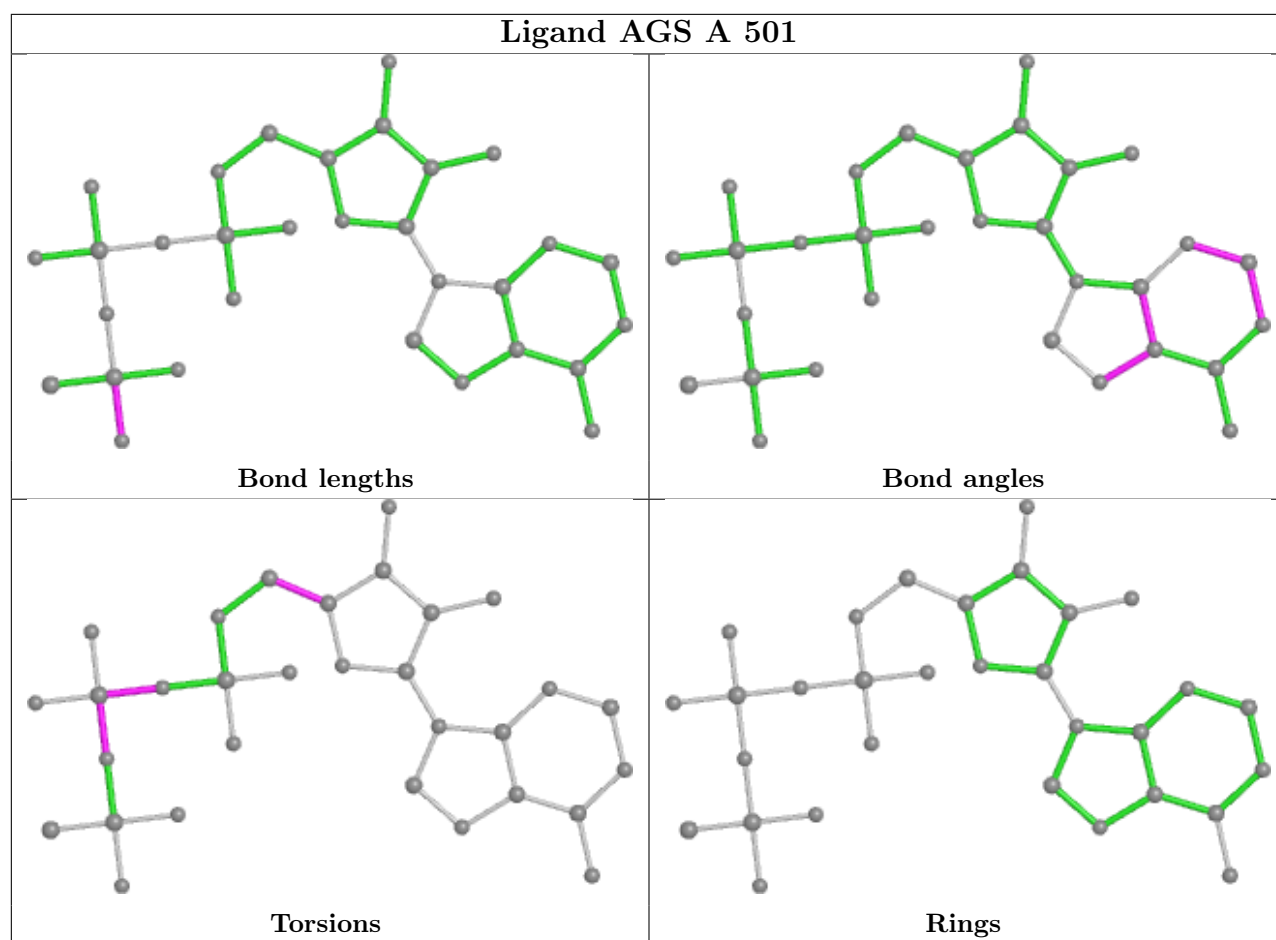
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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.

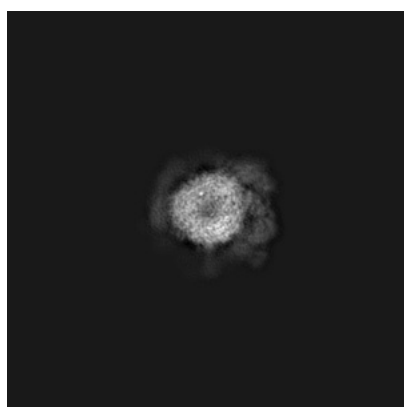
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21691. These allow visual inspection of the internal detail of the map and identification of artifacts.

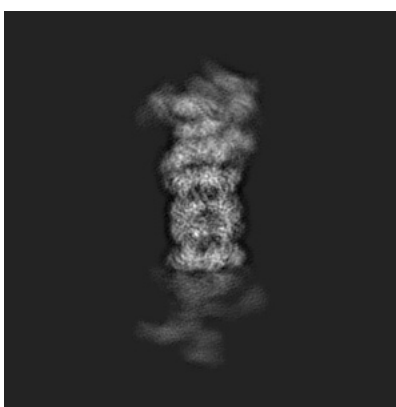
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

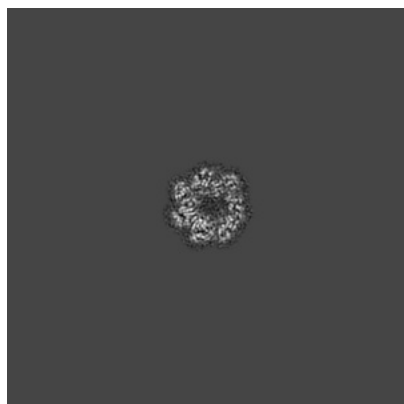


Z

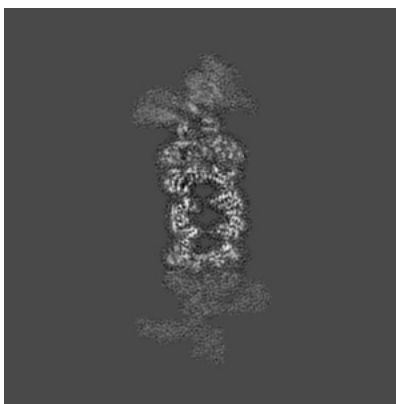
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

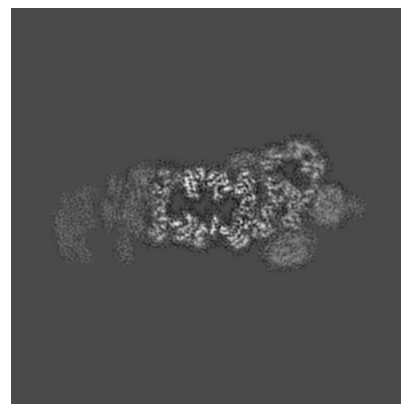
6.2.1 Primary map



X Index: 225



Y Index: 225

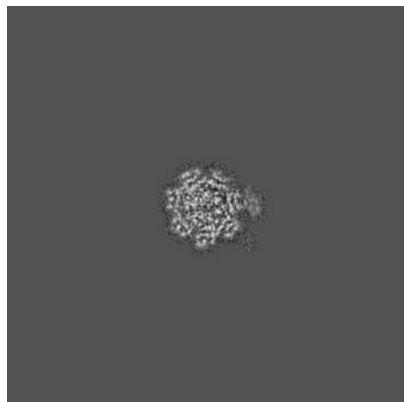


Z Index: 225

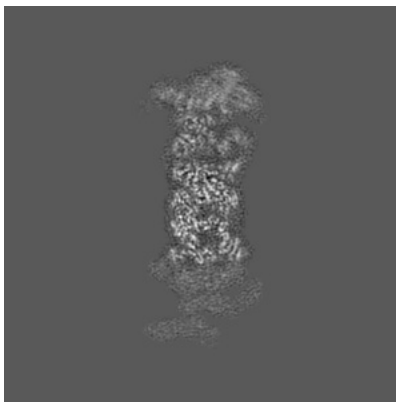
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

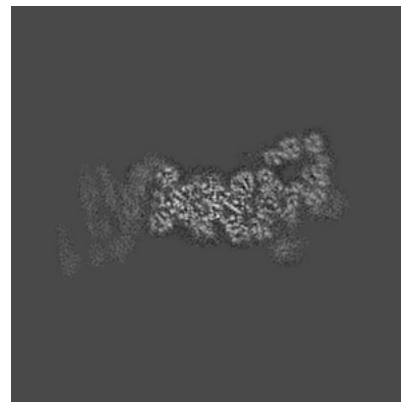
6.3.1 Primary map



X Index: 258



Y Index: 245

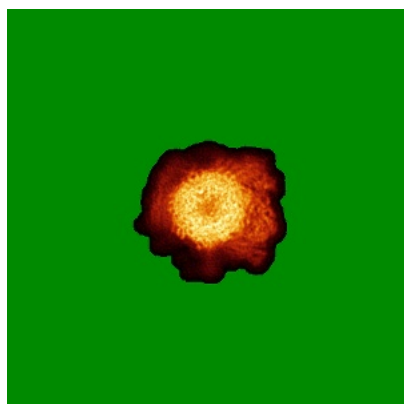


Z Index: 205

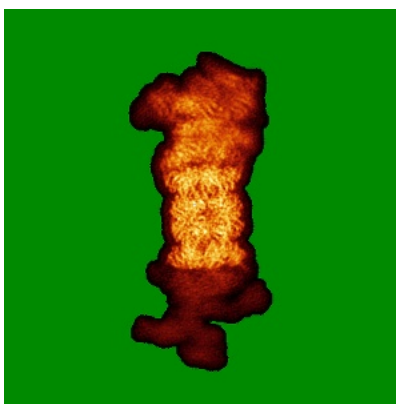
The images above show the largest variance slices of the map in three orthogonal directions.

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

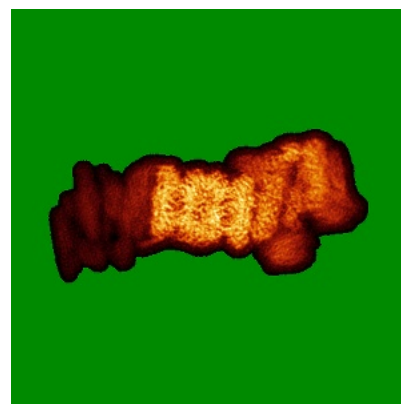
6.4.1 Primary map



X



Y

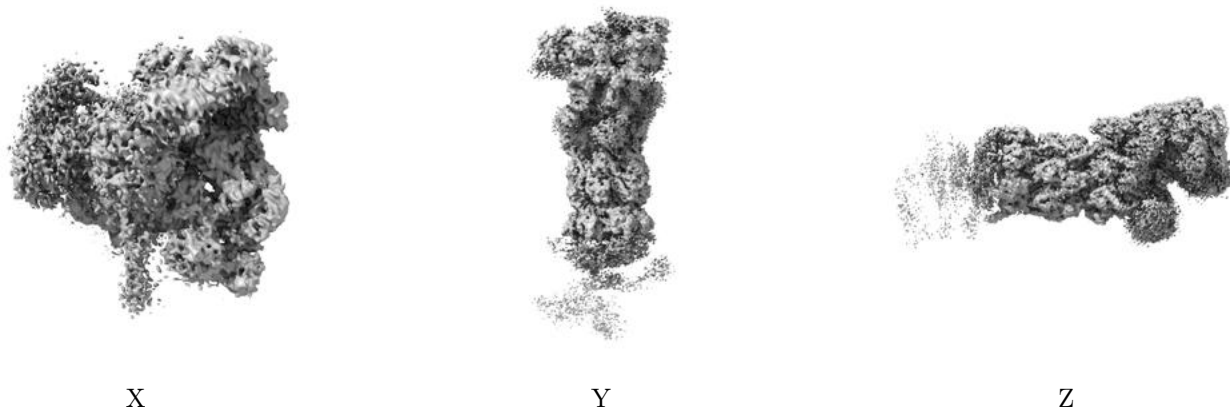


Z

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 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

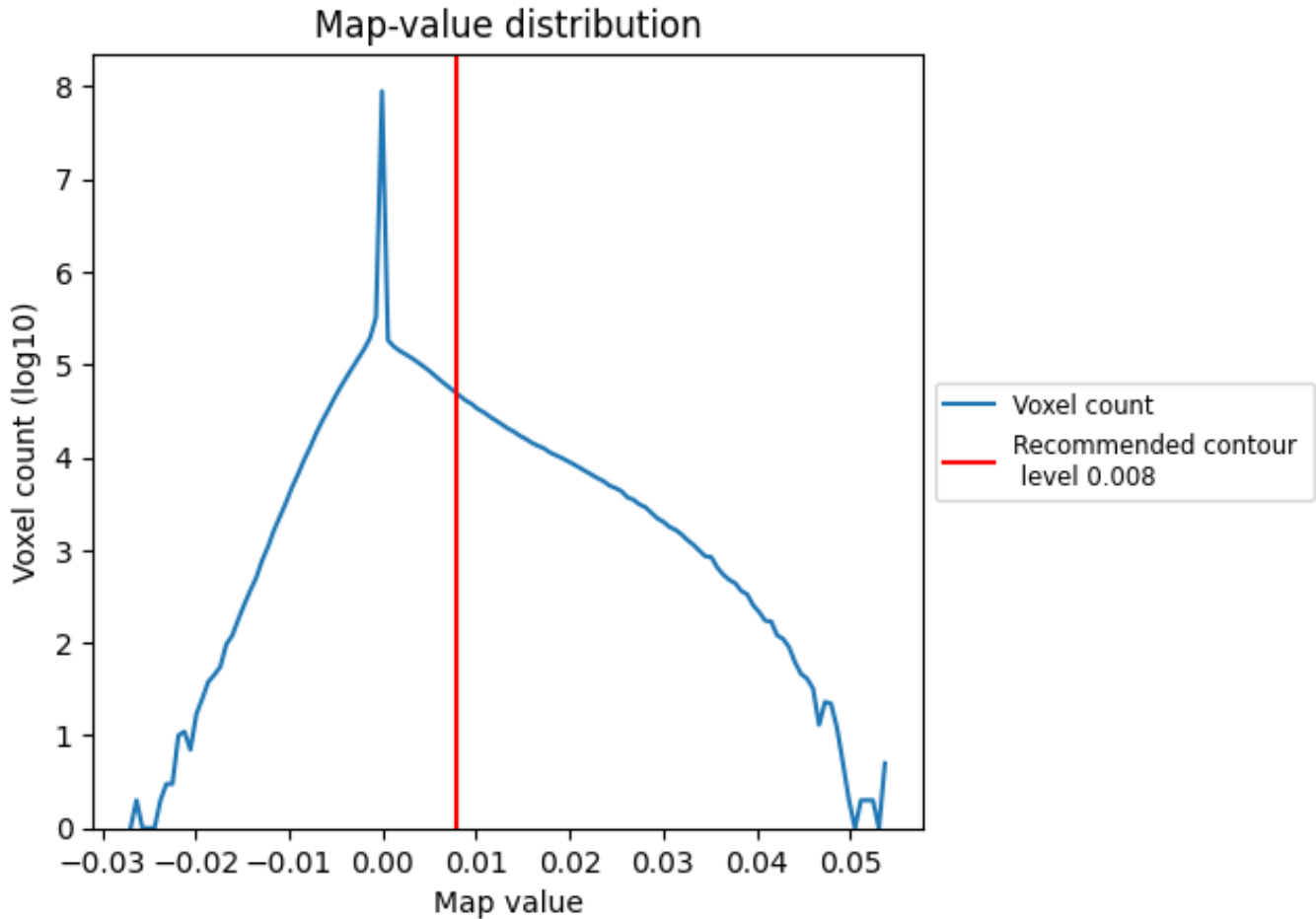
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

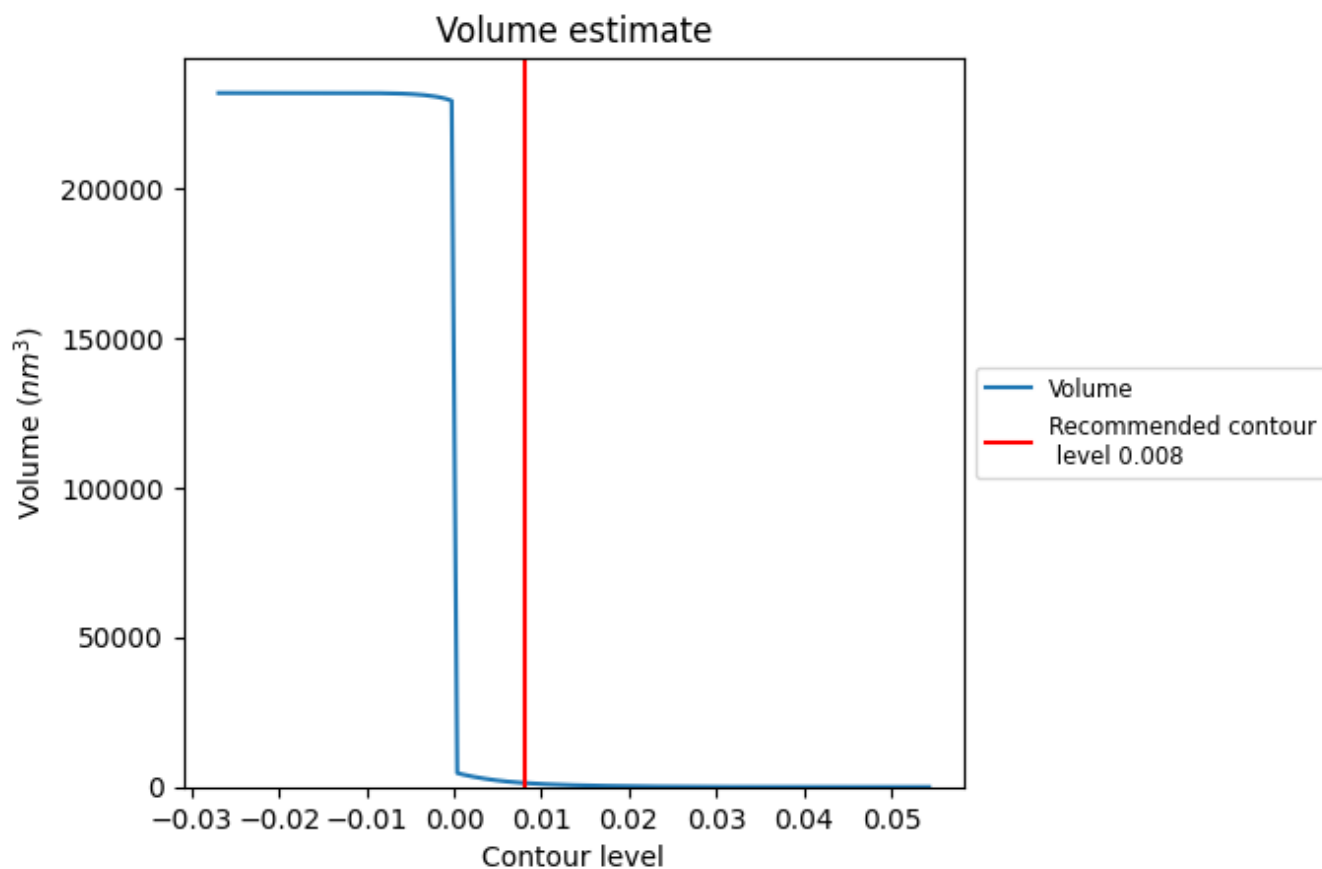
This section contains the results of statistical analysis of the map.

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.

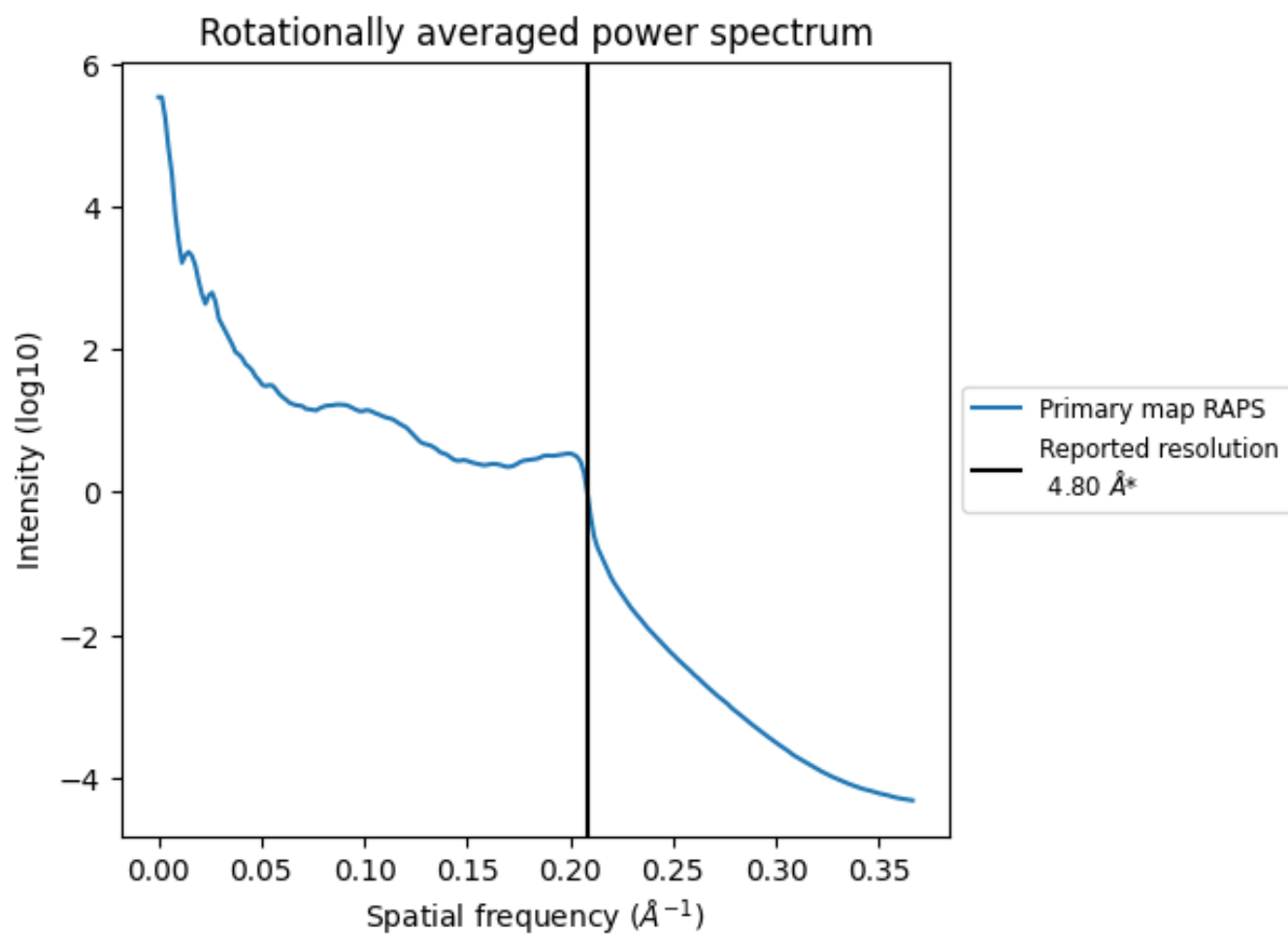
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1336 nm^3 ; this corresponds to an approximate mass of 1207 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 i

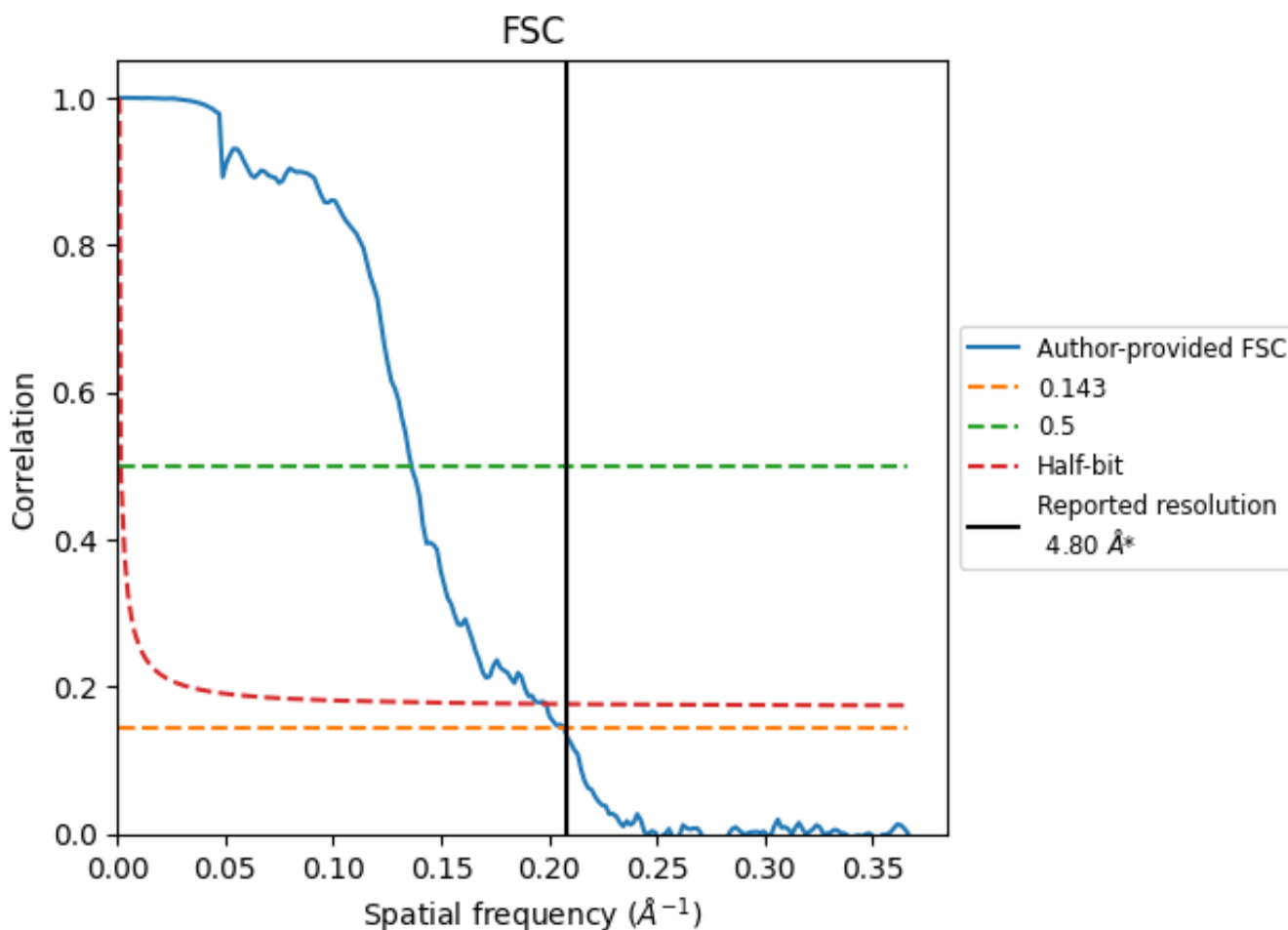


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

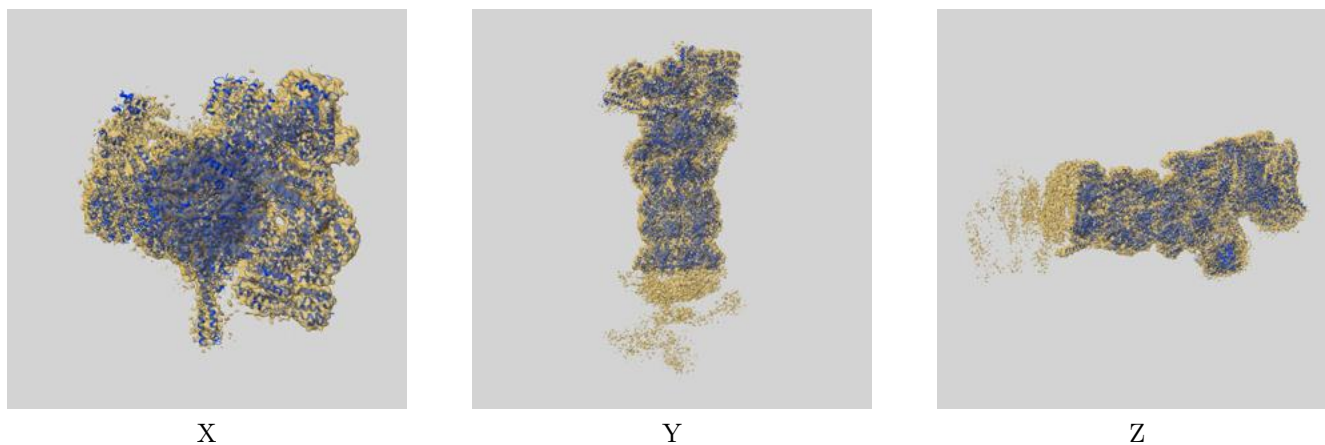
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.83	7.34	5.03
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

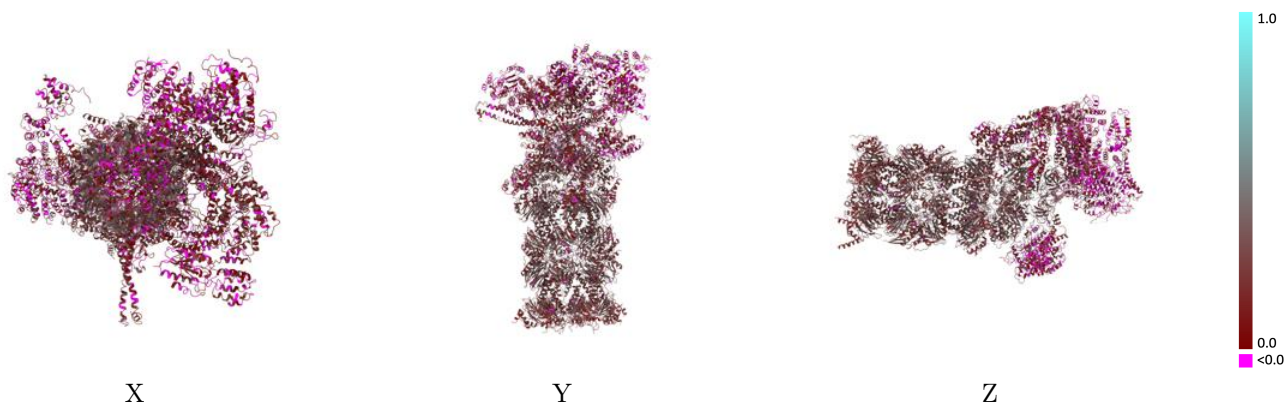
This section contains information regarding the fit between EMDB map EMD-21691 and PDB model 6WJD. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



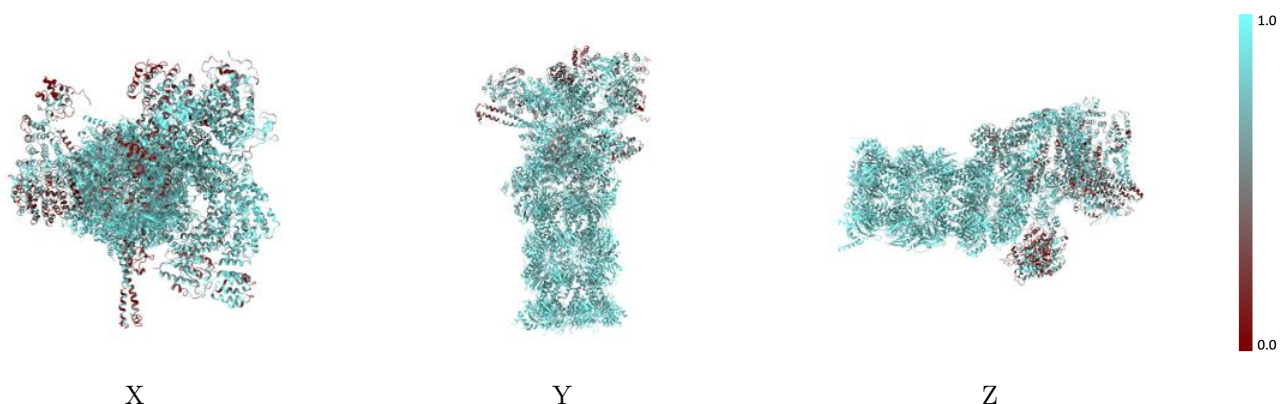
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



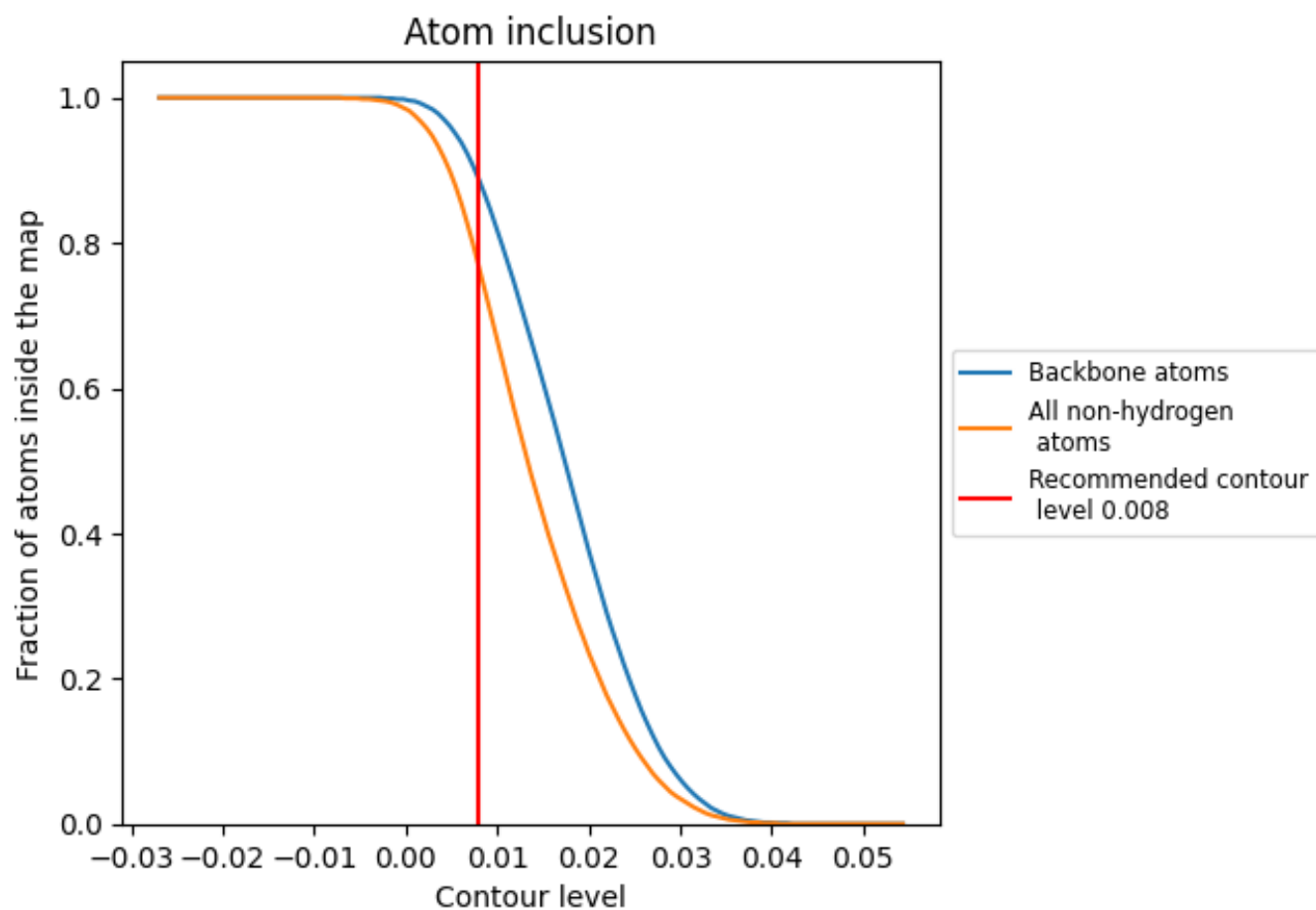
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7670	 0.2300
A	 0.8340	 0.2980
B	 0.7950	 0.2790
C	 0.8250	 0.2910
D	 0.8360	 0.2940
E	 0.8370	 0.2950
F	 0.7990	 0.2950
G	 0.8330	 0.2850
H	 0.8390	 0.2880
I	 0.8390	 0.2730
J	 0.8790	 0.2900
K	 0.8530	 0.2800
L	 0.8580	 0.2740
M	 0.8450	 0.2750
N	 0.8780	 0.2900
O	 0.8600	 0.2860
P	 0.8530	 0.2970
Q	 0.8710	 0.3050
R	 0.8810	 0.2970
S	 0.8580	 0.2950
T	 0.8740	 0.2890
U	 0.6160	 0.1310
V	 0.5920	 0.1010
W	 0.7350	 0.1470
X	 0.6770	 0.1760
Y	 0.6760	 0.1530
Z	 0.7260	 0.1710
a	 0.7440	 0.1470
b	 0.6180	 0.0990
c	 0.7380	 0.1780
d	 0.6120	 0.0850
e	 0.4870	 0.0960
f	 0.4640	 0.1370
g	 0.8450	 0.2610
h	 0.8670	 0.2730



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Chain	Atom inclusion	Q-score
i	 0.8480	 0.2580
j	 0.8700	 0.2690
k	 0.8470	 0.2580
l	 0.8530	 0.2530
m	 0.8550	 0.2590
n	 0.8760	 0.2930
o	 0.8770	 0.2880
p	 0.8630	 0.2950
q	 0.8690	 0.2980
r	 0.8770	 0.2940
s	 0.8570	 0.2930
t	 0.8720	 0.2750
u	 0.2280	 0.1390