



wwPDB EM Validation Summary Report ⓘ

Aug 8, 2026 – 04:18 PM EDT

PDB ID : 9PMJ / pdb_00009pmj
EMDB ID : EMD-71737
Title : Human 19S proteasome bound to TXNL1 PITH domain without C-terminus
Authors : Chen, X.; Negi, H.; Walters, K.J.
Deposited on : 2025-07-17
Resolution : 4.22 Å(reported)
Based on initial models : 1WWY, 7WSI

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:

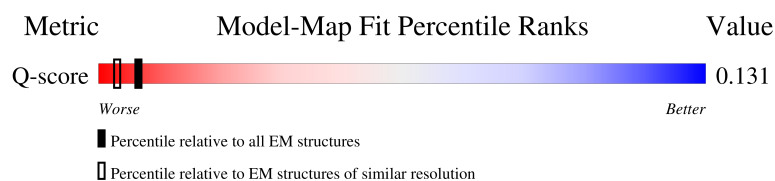
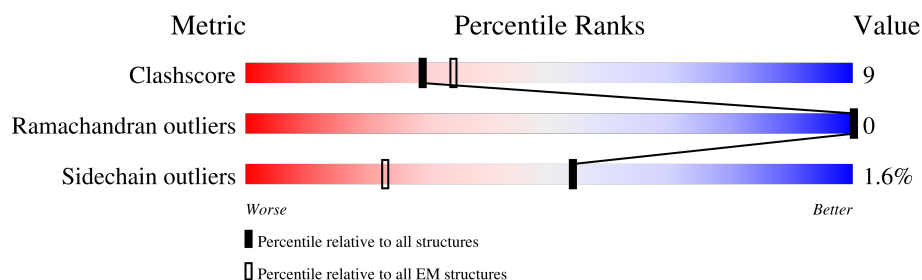
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 4.22 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4772 (3.72 - 4.72)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	406	
4	D	418	

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Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	U	953	
8	V	534	
9	W	456	
10	X	422	
11	Y	389	
12	Z	324	
13	a	376	
14	b	377	
15	c	310	
16	d	350	
17	e	70	
18	f	908	
19	g	289	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 54955 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	403	Total	C	N	O	S	0	0
			3170	1995	556	601	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	387	Total	C	N	O	S	0	0
			3038	1915	522	586	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	379	Total	C	N	O	S	0	0
			2985	1876	535	557	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	372	Total	C	N	O	S	0	0
			2961	1873	512	563	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	385	Total	C	N	O	S	0	0
			3070	1930	548	576	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	360	Total	C	N	O	S	0	0
			2808	1769	486	537	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	806	Total	C	N	O	S	0	0
			6288	3988	1071	1185	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	105	Total	C	N	O	S	0	0
			844	542	140	160	2		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	377	Total	C	N	O	S	0	0
			3106	1982	532	576	16		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	274	Total	C	N	O	S	0	0
			2191	1402	376	408	5		

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

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

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

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

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 17 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	e	49	Total	C	N	O	0	0
			417	256	64	97		

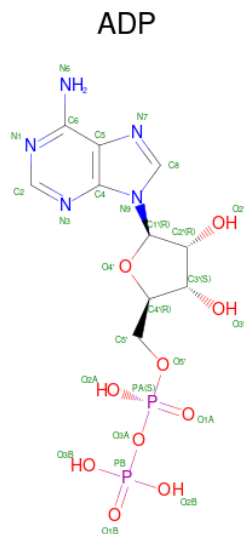
- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	885	Total	C	N	O	S	0	0
			6830	4295	1167	1323	45		

- Molecule 19 is a protein called Thioredoxin-like protein 1.

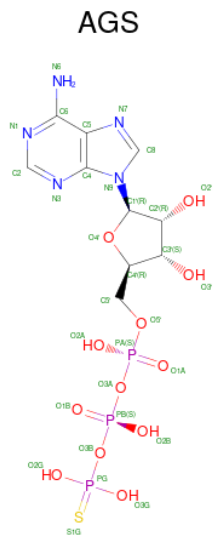
Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	132	Total	C	N	O	S	0	0
			1065	671	172	218	4		

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	D	1	Total	Mg	0
			1	1	
22	E	1	Total	Mg	0
			1	1	

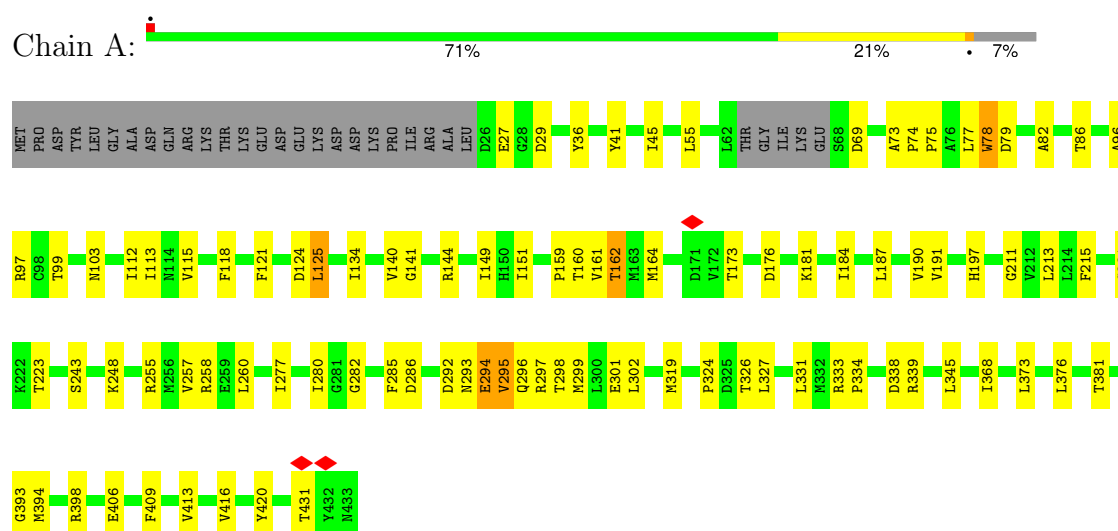
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

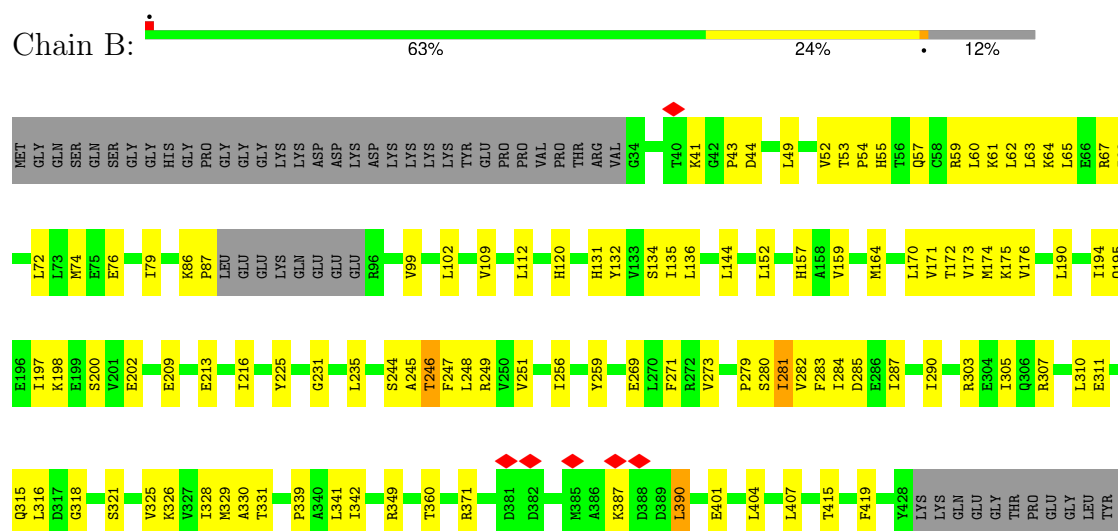
3 Residue-property plots [i](#)

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 regulatory subunit 7

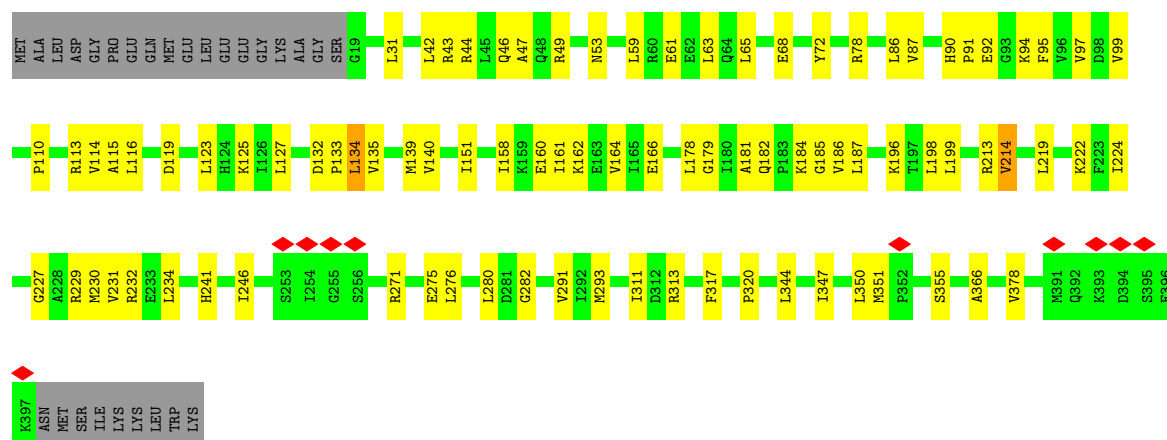


- Molecule 2: 26S proteasome regulatory subunit 4



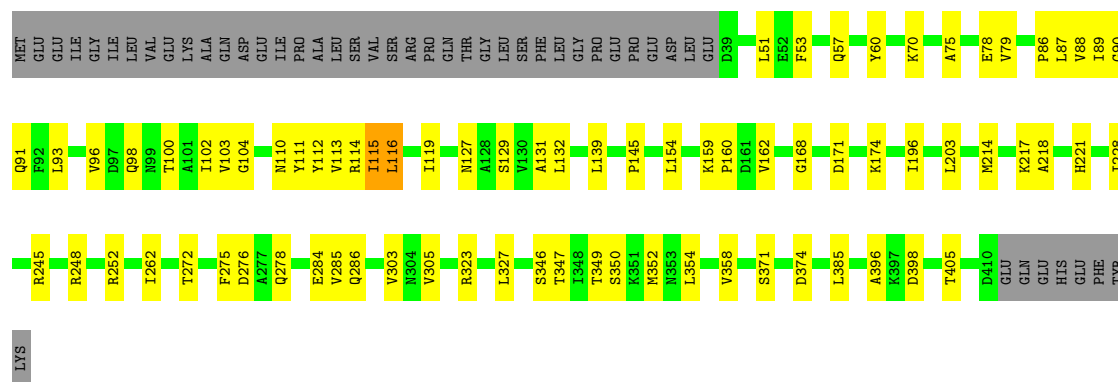
- Molecule 3: 26S protease regulatory subunit 8

Chain C: 



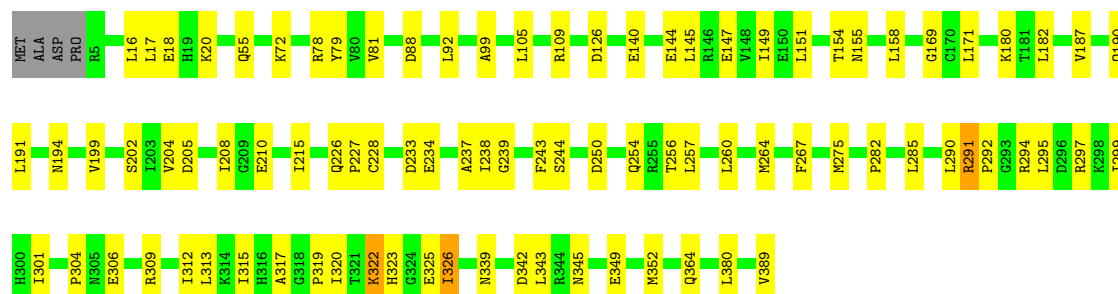
- Molecule 4: 26S proteasome regulatory subunit 6B

Chain D: 



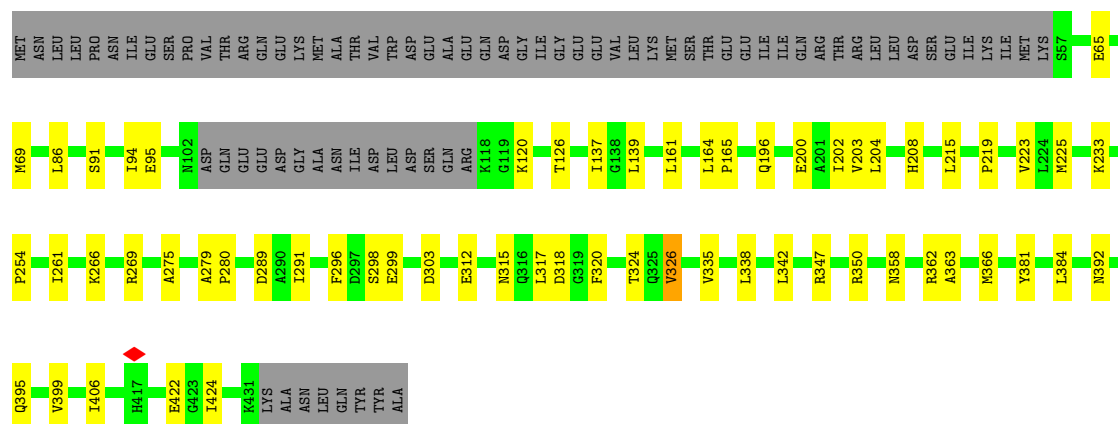
- Molecule 5: 26S protease regulatory subunit 10B

Chain E: 



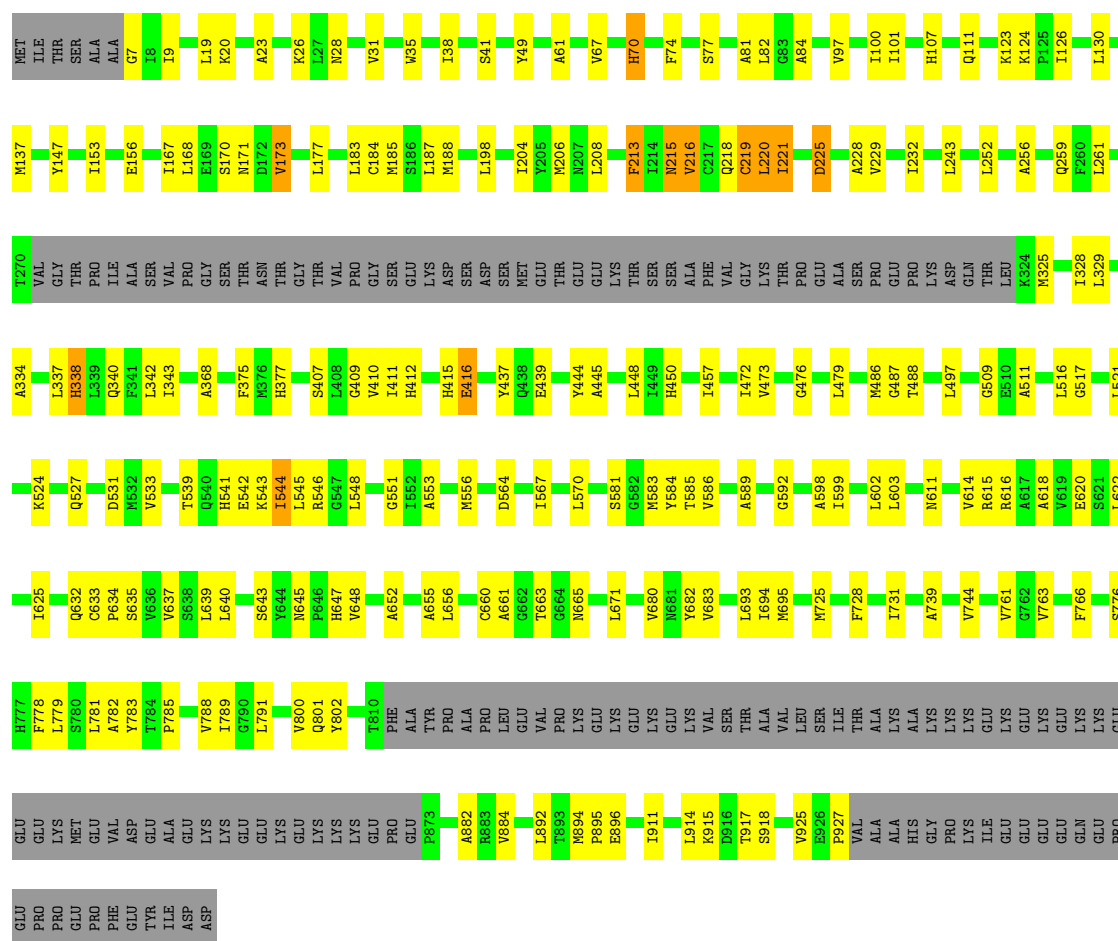
- Molecule 6: 26S proteasome regulatory subunit 6A

Chain F: 



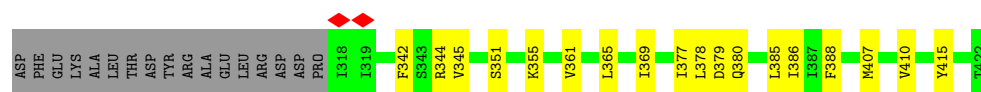
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 64% 20% 15%

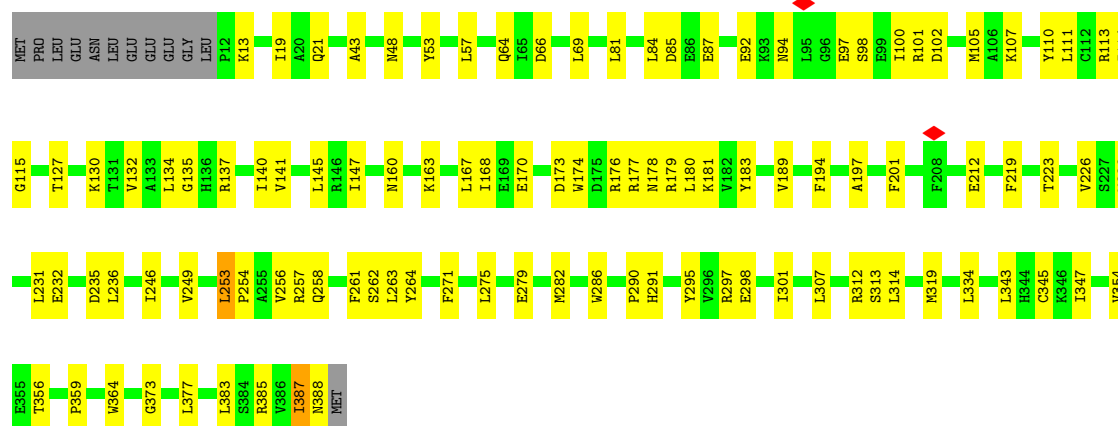


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 3

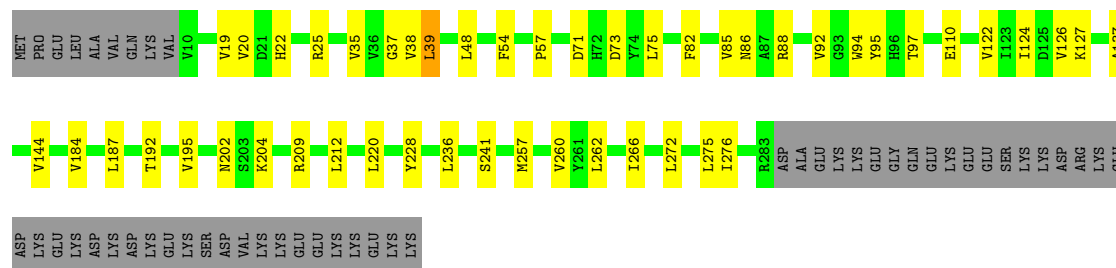
Chain V: 68% 14% 17%



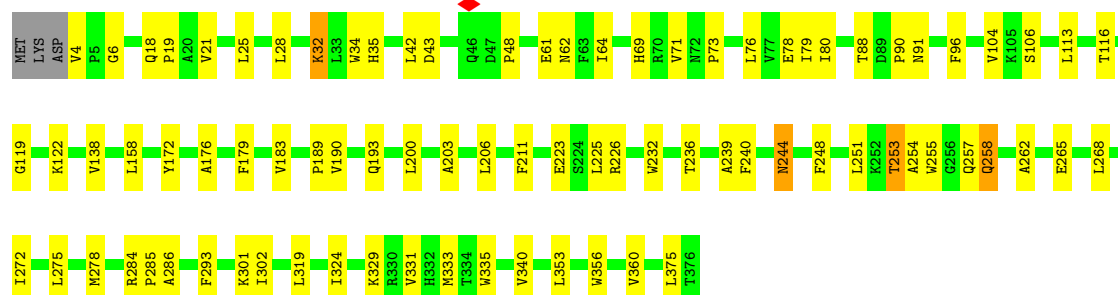
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6



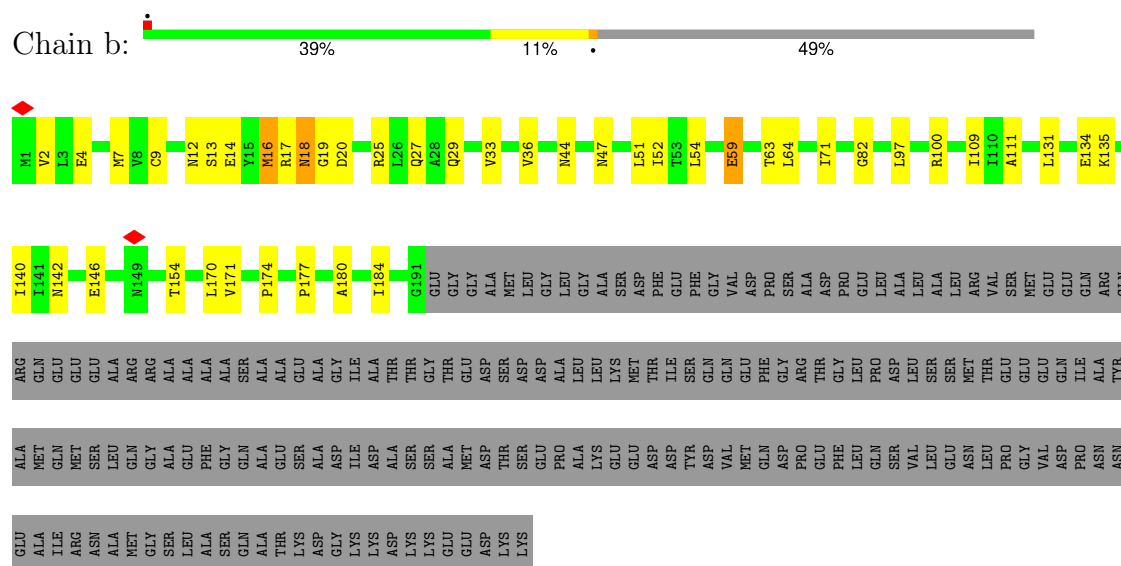
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 7



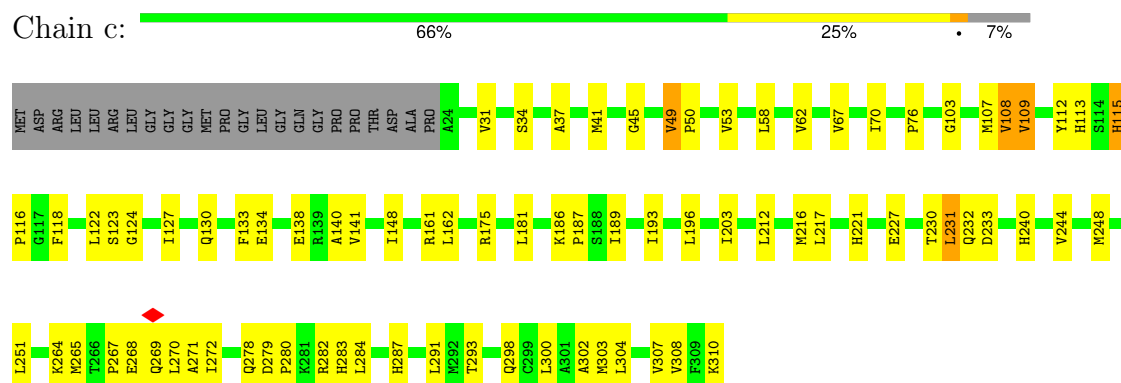
- Molecule 13: 26S proteasome non-ATPase regulatory subunit 13



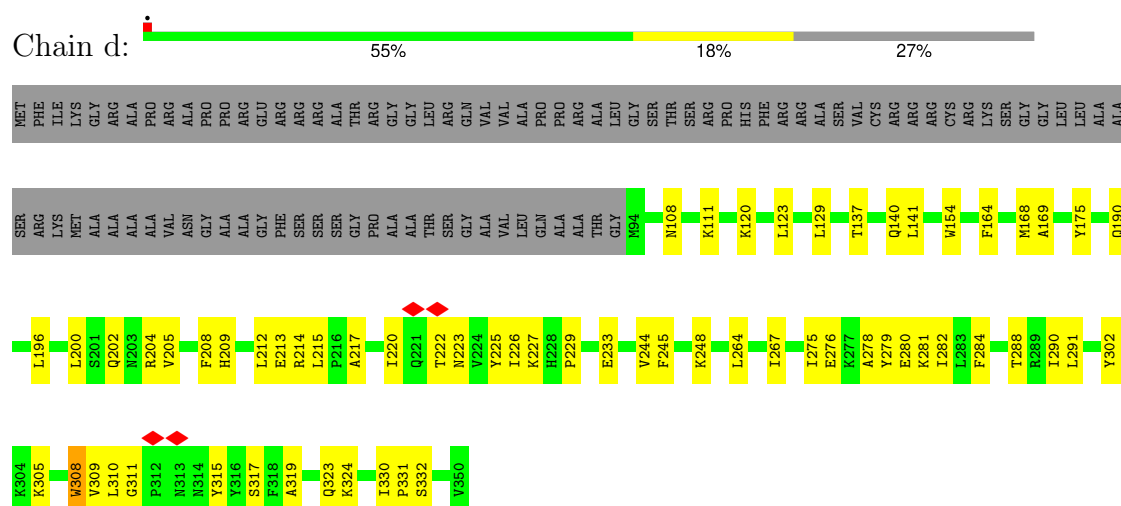
- Molecule 14: 26S proteasome non-ATPase regulatory subunit 4



- Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

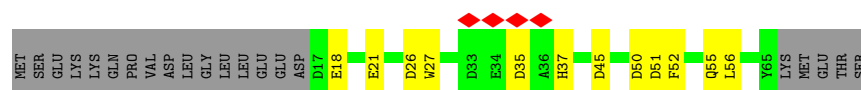


- Molecule 16: 26S proteasome non-ATPase regulatory subunit 8



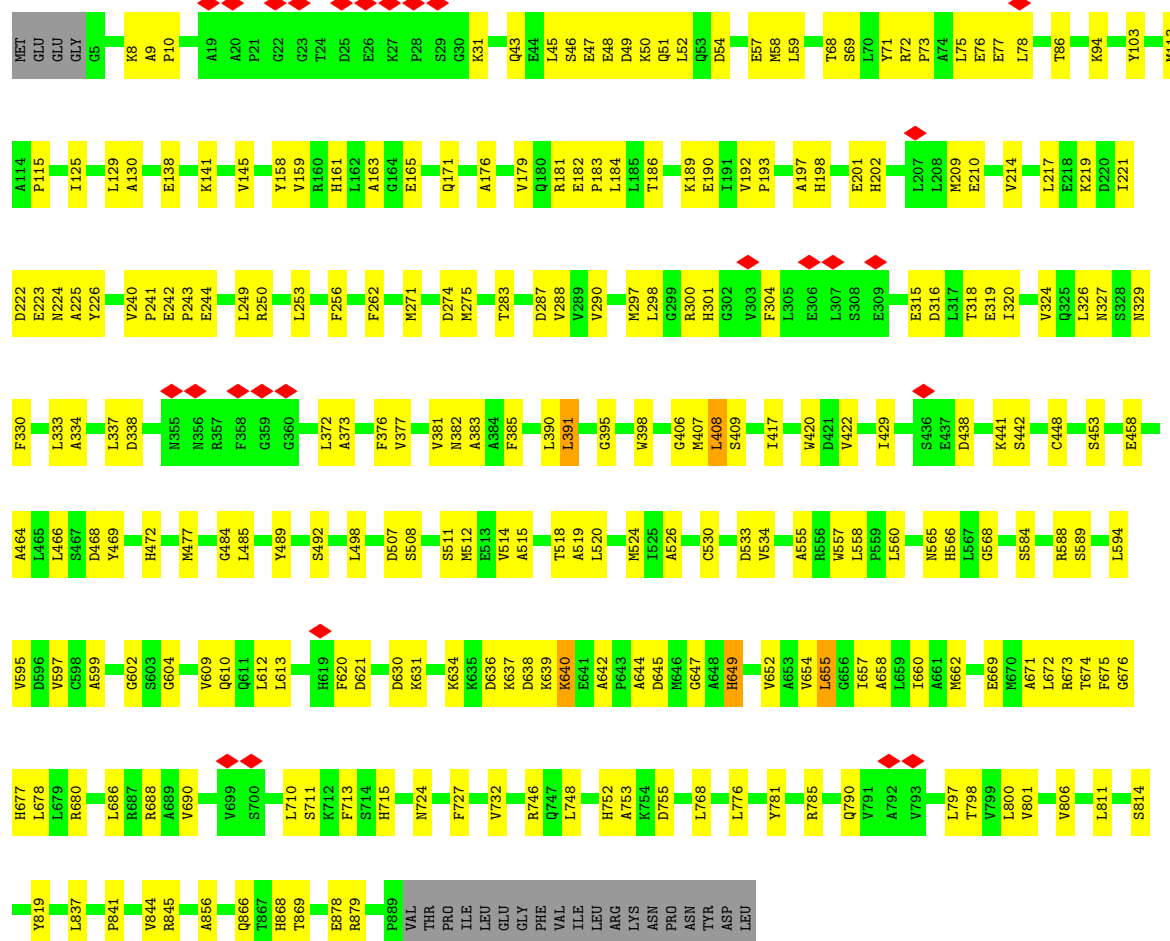
- Molecule 17: 26S proteasome complex subunit SEM1





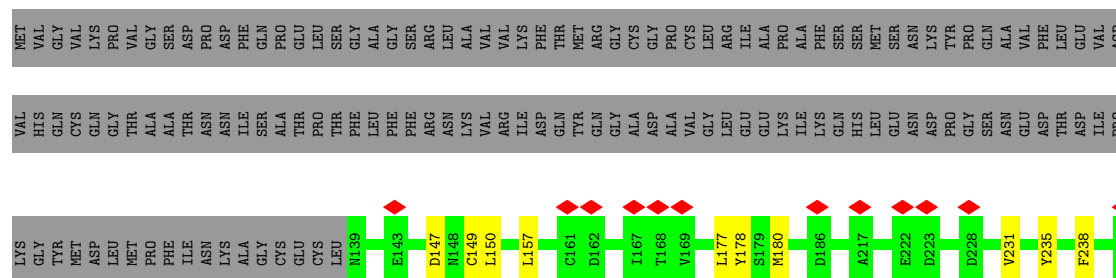
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 70% 27%



• Molecule 19: Thioredoxin-like protein 1

Chain g: 6% 42% 54%



E254	E255	E256	I266	V270	GLN	ALA	THR	ASN	MET	ASN	ASP	PHE	LYS	ARG	VAL	VAL	GLY	LYS	LYS	GLY	GLU	SER	HIS
------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39459	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.467	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.510	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	349.92, 349.92, 349.92	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/3222	0.88	0/4348
2	B	0.53	0/3082	0.90	0/4154
3	C	0.48	0/3024	0.85	0/4067
4	D	0.51	0/3008	0.86	0/4060
5	E	0.55	0/3117	0.87	0/4193
6	F	0.47	0/2846	0.83	0/3837
7	U	0.54	0/6398	0.90	0/8655
8	V	0.42	0/3681	0.78	0/4969
9	W	0.51	0/3612	0.81	0/4858
10	X	0.59	0/855	0.98	0/1150
11	Y	0.58	0/3164	0.90	0/4263
12	Z	0.57	0/2234	0.89	0/3031
13	a	0.62	0/3053	0.90	0/4133
14	b	0.65	0/1478	0.92	0/2001
15	c	0.67	0/2302	0.96	0/3110
16	d	0.51	0/2162	0.87	0/2919
17	e	0.67	0/429	0.94	0/584
18	f	0.51	0/6944	0.89	0/9387
19	g	0.22	0/1086	0.49	0/1470
All	All	0.53	0/55697	0.87	0/75189

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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3170	0	3214	65	0
2	B	3038	0	3127	84	0
3	C	2985	0	3097	75	0
4	D	2961	0	3012	65	0
5	E	3070	0	3146	68	0
6	F	2808	0	2888	44	0
7	U	6288	0	6317	130	0
8	V	3612	0	3682	58	0
9	W	3564	0	3685	43	0
10	X	844	0	886	17	0
11	Y	3106	0	3111	71	0
12	Z	2191	0	2218	41	0
13	a	2995	0	3012	58	0
14	b	1458	0	1505	28	0
15	c	2260	0	2276	58	0
16	d	2116	0	2143	44	0
17	e	417	0	324	9	0
18	f	6830	0	6828	186	0
19	g	1065	0	1015	6	0
20	A	27	0	12	1	0
20	B	27	0	12	1	0
20	C	27	0	12	1	0
21	D	31	0	12	1	0
21	E	31	0	12	1	0
21	F	31	0	12	2	0
22	D	1	0	0	0	0
22	E	1	0	0	0	0
23	c	1	0	0	0	0
All	All	54955	0	55558	1022	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1022 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:45:GLY:HA2	15:c:53:VAL:HG21	1.57	0.85
11:Y:94:ASN:HB2	11:Y:98:SER:HB3	1.63	0.79
18:f:171:GLN:HB3	18:f:179:VAL:HG22	1.65	0.79
7:U:409:GLY:HA3	7:U:445:ALA:HB1	1.65	0.77
2:B:60:LEU:HD11	18:f:222:ASP:HB2	1.67	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/433 (92%)	356 (89%)	43 (11%)	0	100	100
2	B	383/440 (87%)	327 (85%)	56 (15%)	0	100	100
3	C	377/406 (93%)	345 (92%)	32 (8%)	0	100	100
4	D	370/418 (88%)	338 (91%)	32 (9%)	0	100	100
5	E	383/389 (98%)	339 (88%)	44 (12%)	0	100	100
6	F	356/439 (81%)	315 (88%)	41 (12%)	0	100	100
7	U	800/953 (84%)	732 (92%)	68 (8%)	0	100	100
8	V	442/534 (83%)	419 (95%)	23 (5%)	0	100	100
9	W	435/456 (95%)	402 (92%)	33 (8%)	0	100	100
10	X	103/422 (24%)	93 (90%)	10 (10%)	0	100	100
11	Y	375/389 (96%)	340 (91%)	35 (9%)	0	100	100
12	Z	272/324 (84%)	240 (88%)	32 (12%)	0	100	100
13	a	371/376 (99%)	335 (90%)	36 (10%)	0	100	100
14	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
15	c	285/310 (92%)	253 (89%)	32 (11%)	0	100	100
16	d	255/350 (73%)	223 (88%)	32 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	e	47/70 (67%)	39 (83%)	8 (17%)	0	100	100
18	f	883/908 (97%)	733 (83%)	150 (17%)	0	100	100
19	g	130/289 (45%)	123 (95%)	7 (5%)	0	100	100
All	All	6855/8283 (83%)	6123 (89%)	732 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/372 (93%)	335 (97%)	11 (3%)	34	55
2	B	341/385 (89%)	336 (98%)	5 (2%)	57	70
3	C	330/352 (94%)	328 (99%)	2 (1%)	78	80
4	D	325/366 (89%)	322 (99%)	3 (1%)	70	76
5	E	338/341 (99%)	332 (98%)	6 (2%)	51	66
6	F	308/379 (81%)	305 (99%)	3 (1%)	68	75
7	U	688/816 (84%)	673 (98%)	15 (2%)	45	64
8	V	390/460 (85%)	385 (99%)	5 (1%)	61	71
9	W	402/416 (97%)	398 (99%)	4 (1%)	68	75
10	X	97/362 (27%)	97 (100%)	0	100	100
11	Y	333/344 (97%)	329 (99%)	4 (1%)	63	73
12	Z	248/295 (84%)	246 (99%)	2 (1%)	73	77
13	a	333/336 (99%)	324 (97%)	9 (3%)	39	60
14	b	167/312 (54%)	161 (96%)	6 (4%)	31	52
15	c	252/268 (94%)	243 (96%)	9 (4%)	31	52
16	d	231/294 (79%)	226 (98%)	5 (2%)	45	64
17	e	43/63 (68%)	43 (100%)	0	100	100
18	f	741/763 (97%)	733 (99%)	8 (1%)	65	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	g	122/253 (48%)	122 (100%)	0	100	100
All	All	6035/7177 (84%)	5938 (98%)	97 (2%)	54	69

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Y	387	ILE
14	b	18	ASN
12	Z	144	VAL
13	a	253	THR
15	c	49	VAL

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

Mol	Chain	Res	Type
14	b	18	ASN
18	f	14	GLN
14	b	142	ASN
15	c	274	ASN
18	f	705	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 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
20	ADP	B	501	-	28,29,29	1.32	3 (10%)	43,45,45	2.08	10 (23%)
20	ADP	A	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.91	9 (20%)
21	AGS	F	501	-	32,33,33	0.68	1 (3%)	45,52,52	0.57	0
21	AGS	D	501	22	32,33,33	0.67	1 (3%)	45,52,52	0.55	0
21	AGS	E	501	22	32,33,33	0.67	1 (3%)	45,52,52	0.50	0
20	ADP	C	501	-	28,29,29	1.47	5 (17%)	43,45,45	1.87	7 (16%)

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
20	ADP	B	501	-	-	5/16/32/32	0/3/3/3
20	ADP	A	501	-	-	0/16/32/32	0/3/3/3
21	AGS	F	501	-	-	8/21/38/38	0/3/3/3
21	AGS	D	501	22	-	8/21/38/38	0/3/3/3
21	AGS	E	501	22	-	0/21/38/38	0/3/3/3
20	ADP	C	501	-	-	5/16/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	ADP	C5-C4	4.79	1.47	1.39
20	A	501	ADP	C5-C4	4.52	1.47	1.39
20	B	501	ADP	C5-C4	4.40	1.46	1.39
20	C	501	ADP	C5-C6	2.72	1.48	1.41
20	A	501	ADP	C5-N7	-2.66	1.34	1.39

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	501	ADP	C5-C4-N3	-6.50	117.77	126.72
20	C	501	ADP	C5-C4-N3	-6.48	117.79	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	501	ADP	C5-C4-N3	-6.29	118.06	126.72
20	B	501	ADP	N3-C4-N9	5.80	137.04	127.17
20	A	501	ADP	N3-C4-N9	5.65	136.78	127.17

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

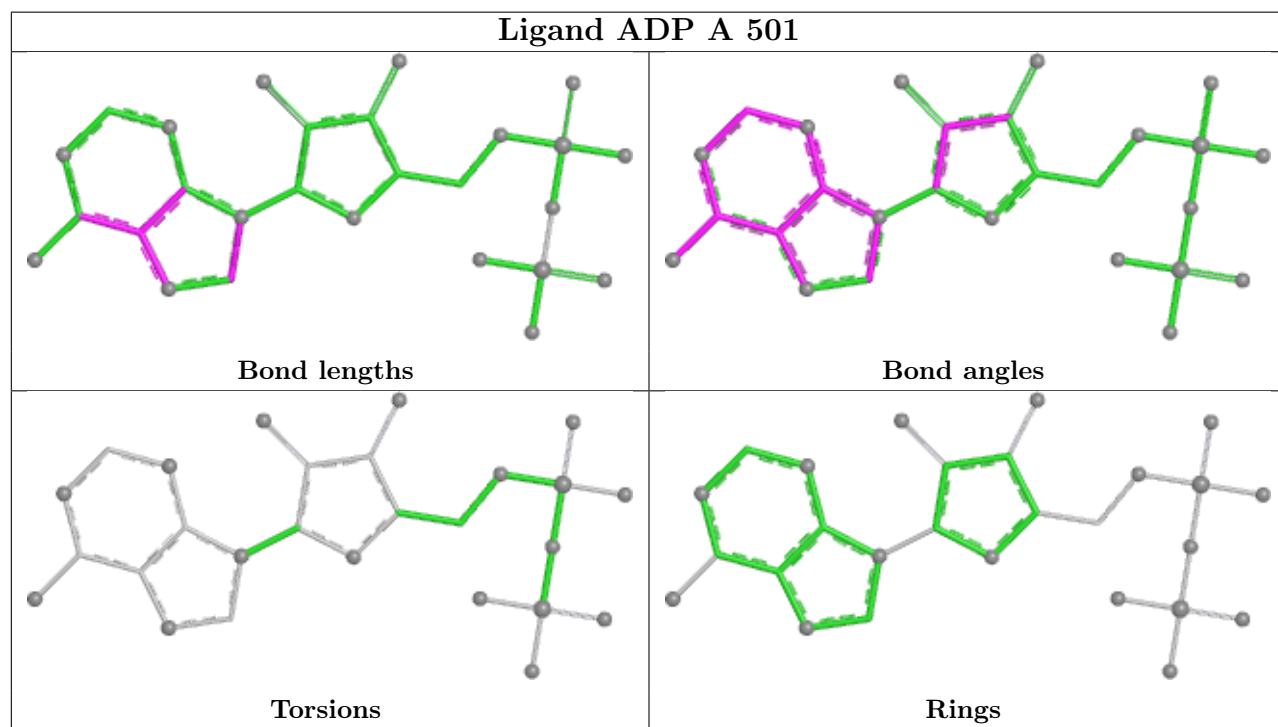
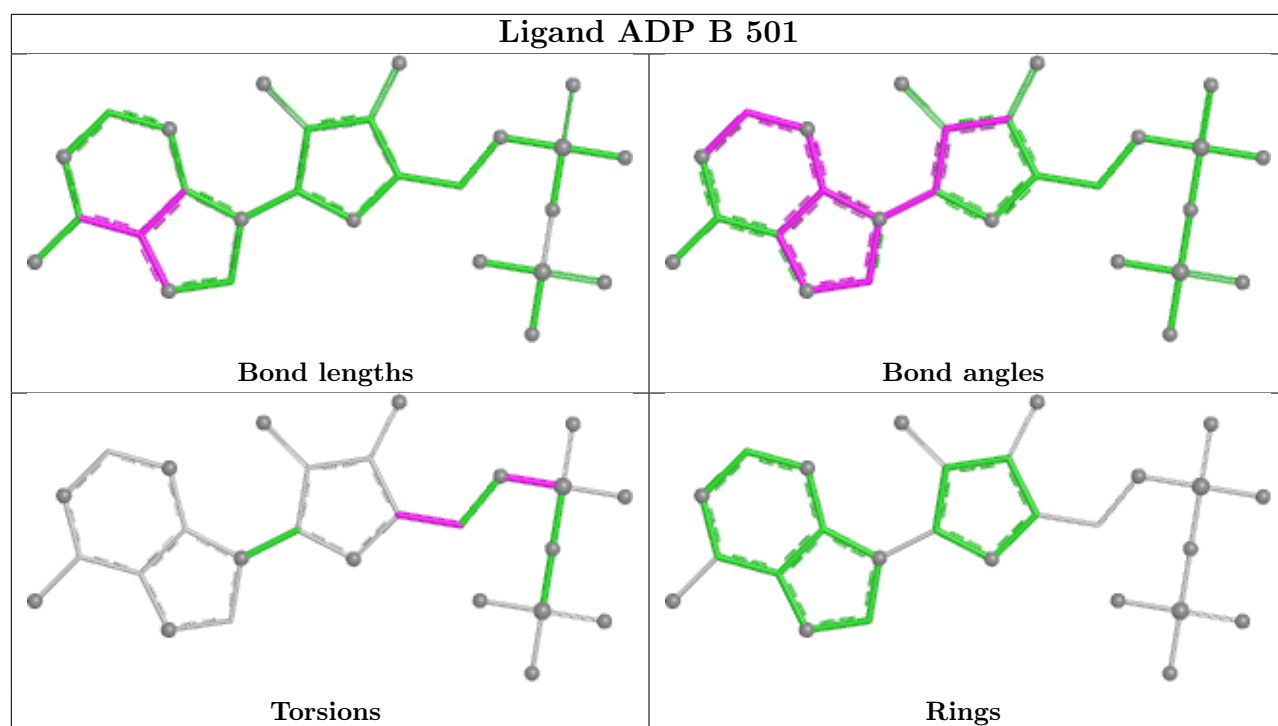
Mol	Chain	Res	Type	Atoms
20	B	501	ADP	C5'-O5'-PA-O1A
20	B	501	ADP	C5'-O5'-PA-O2A
20	B	501	ADP	C5'-O5'-PA-O3A
20	C	501	ADP	C5'-O5'-PA-O1A
20	C	501	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

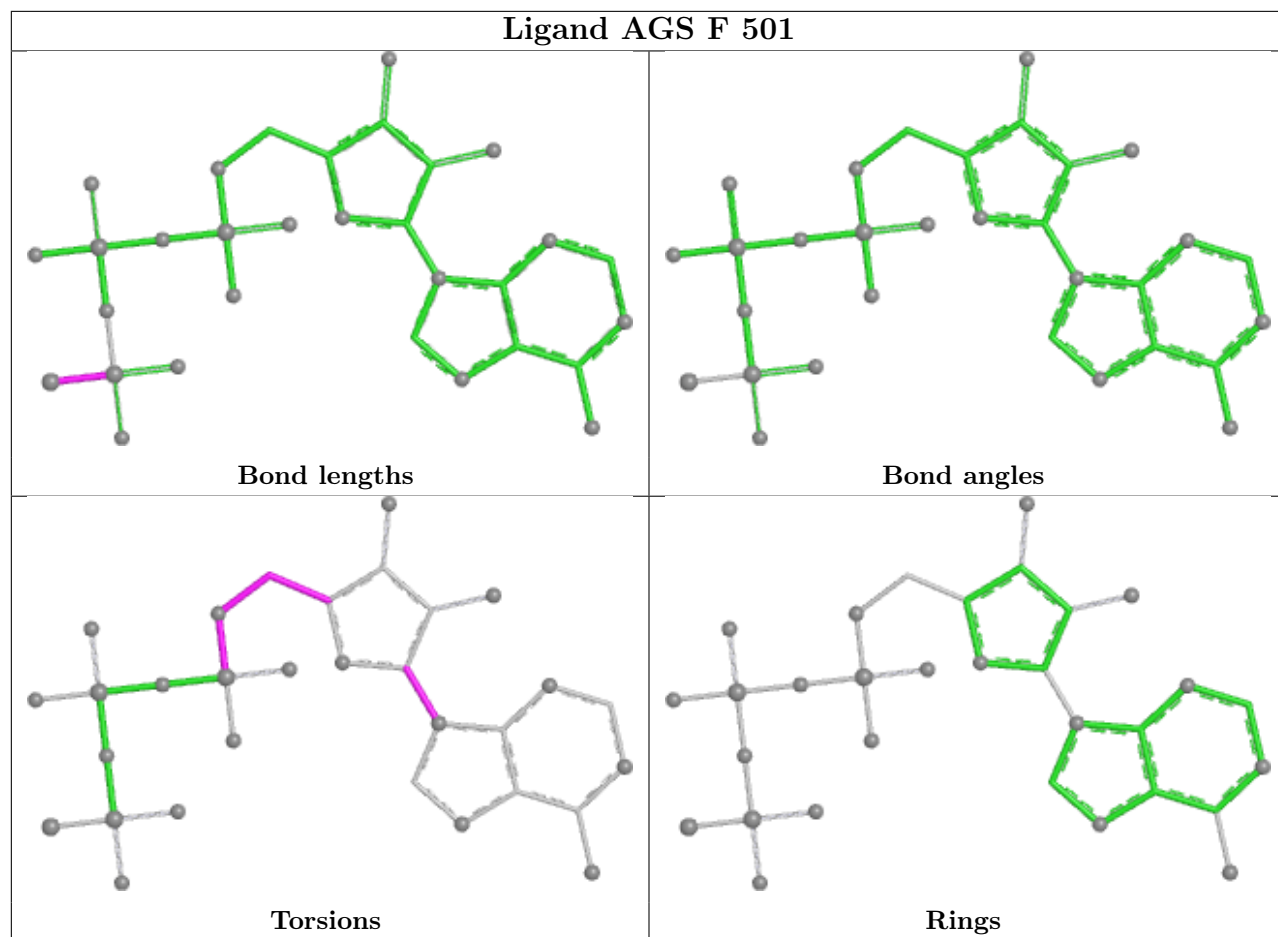
6 monomers are involved in 7 short contacts:

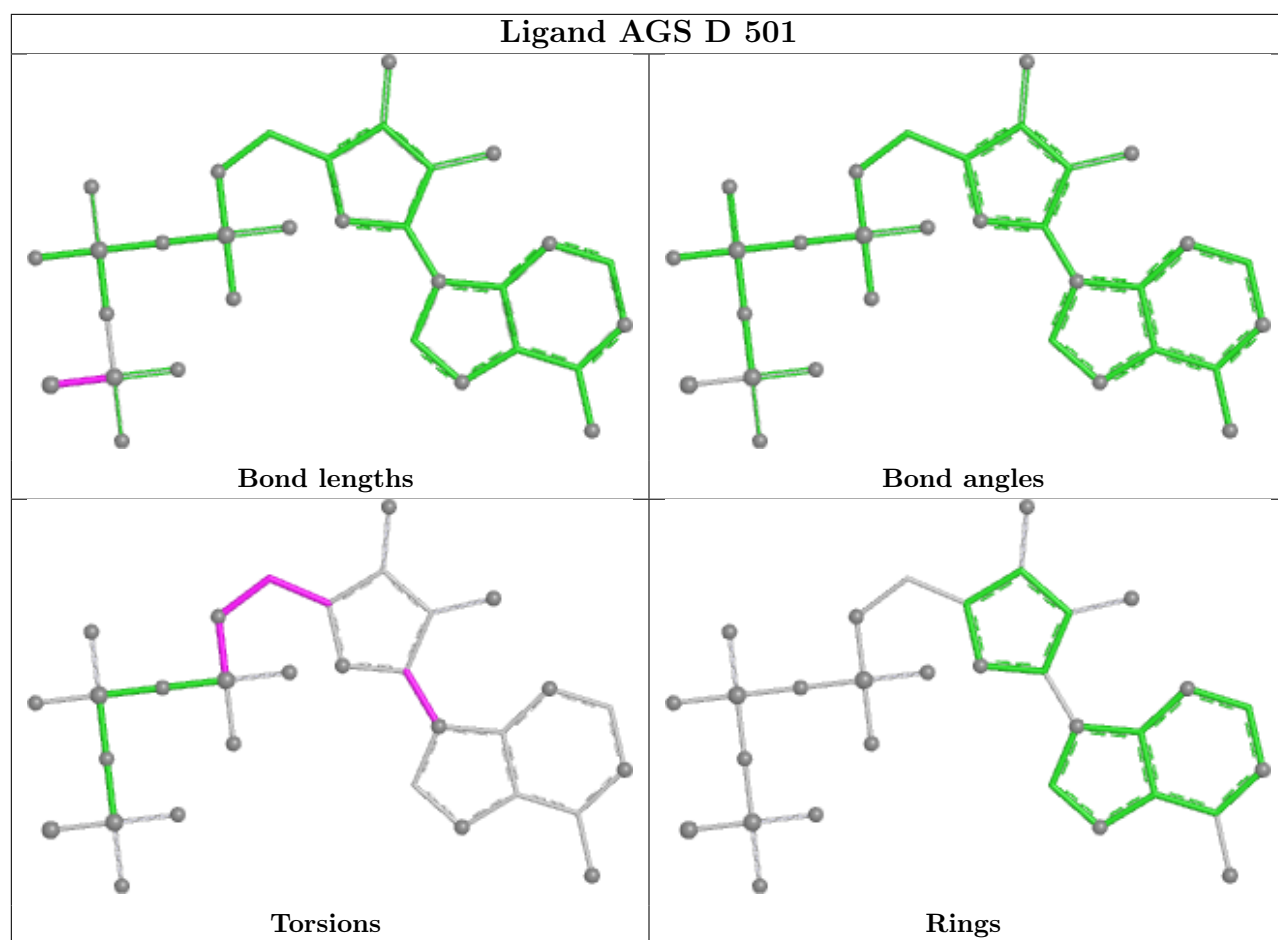
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	501	ADP	1	0
20	A	501	ADP	1	0
21	F	501	AGS	2	0
21	D	501	AGS	1	0
21	E	501	AGS	1	0
20	C	501	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

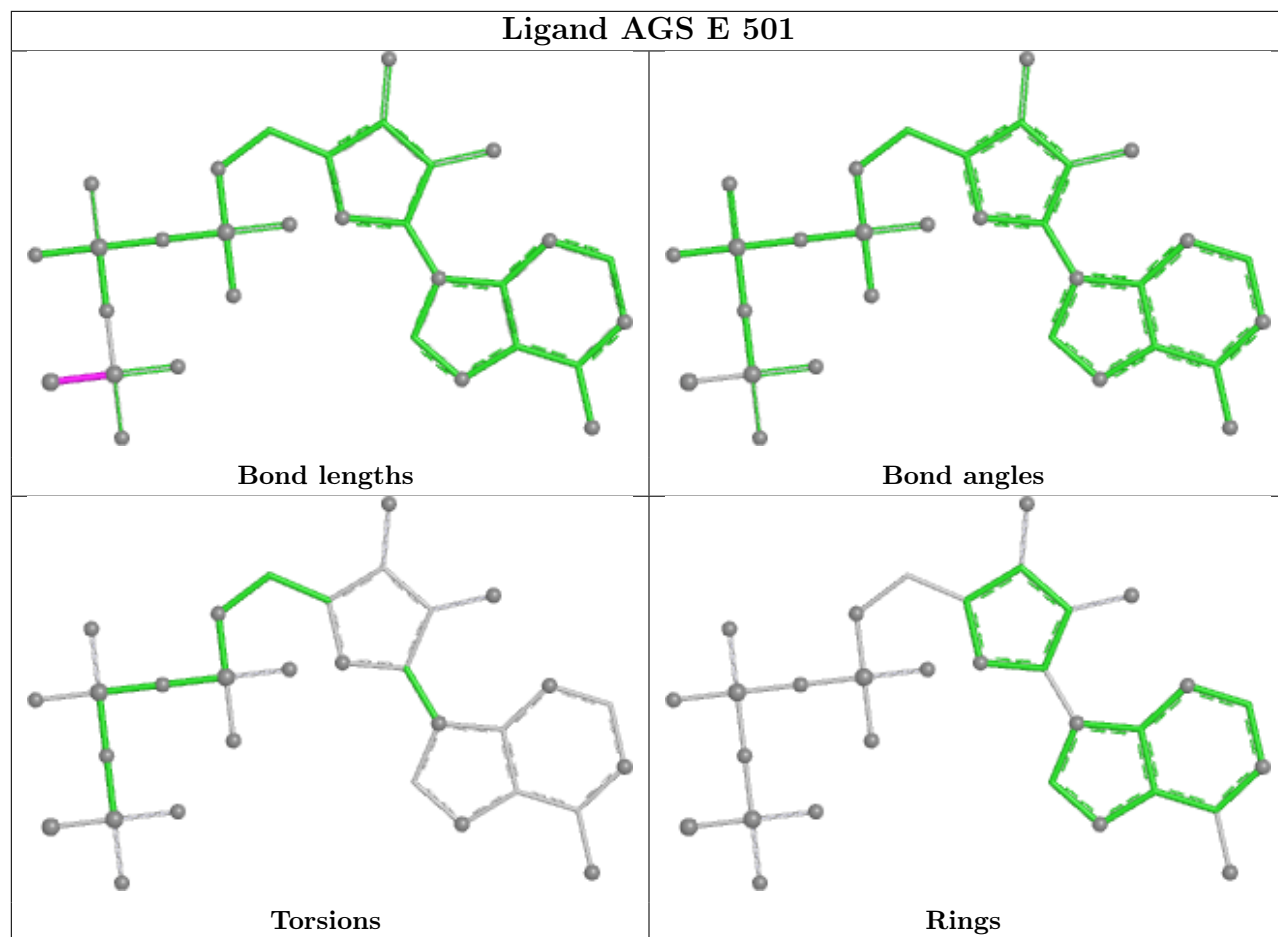


Ligand AGS F 501

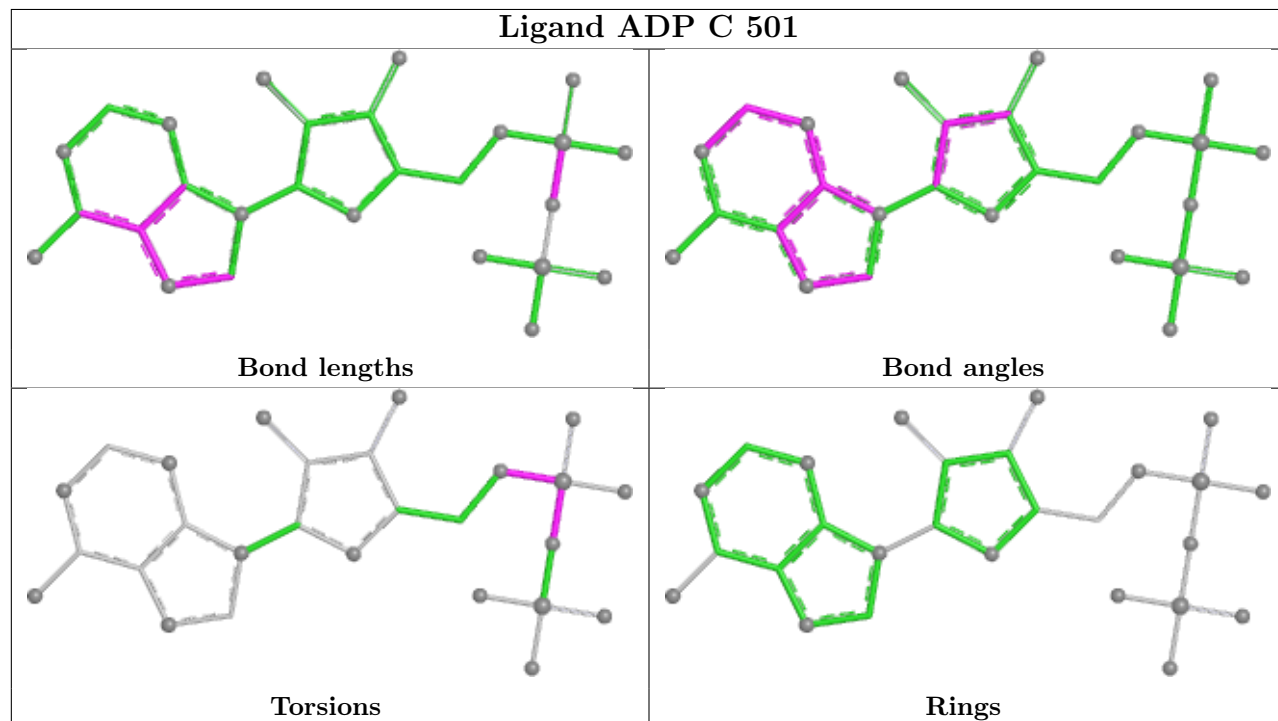




Ligand AGS E 501



Ligand ADP C 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

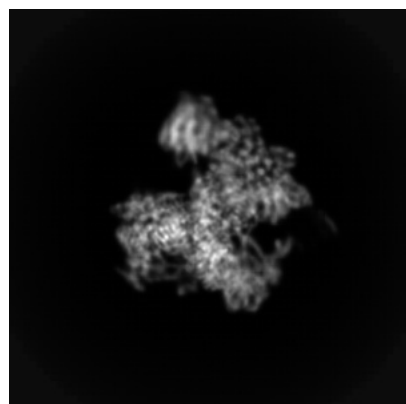
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71737. These allow visual inspection of the internal detail of the map and identification of artifacts.

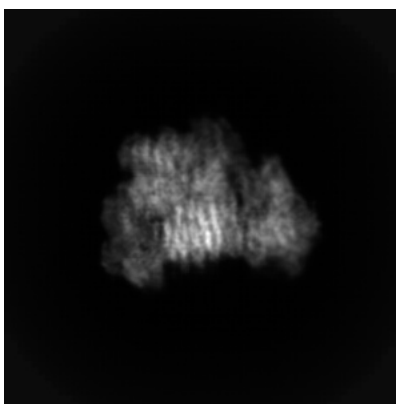
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

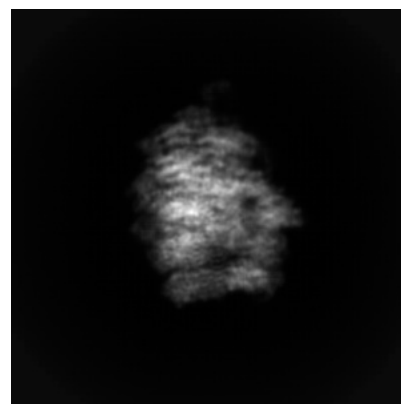
6.1.1 Primary map



X

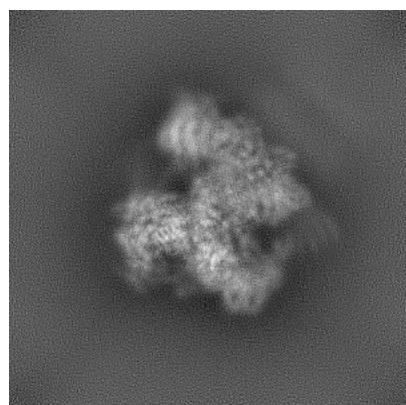


Y

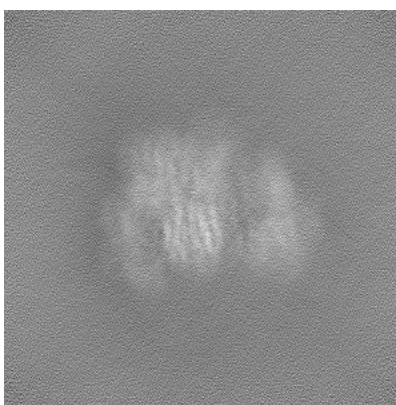


Z

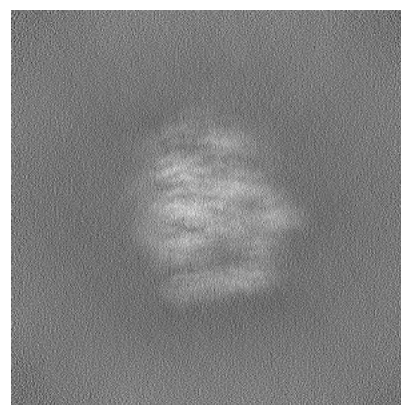
6.1.2 Raw map



X



Y



Z

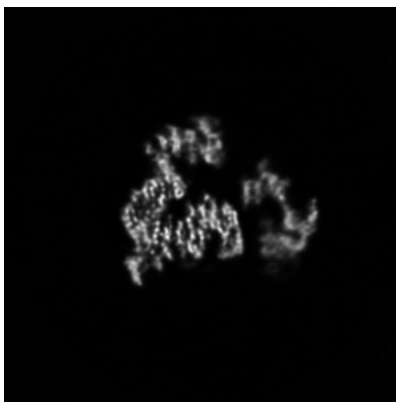
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 216

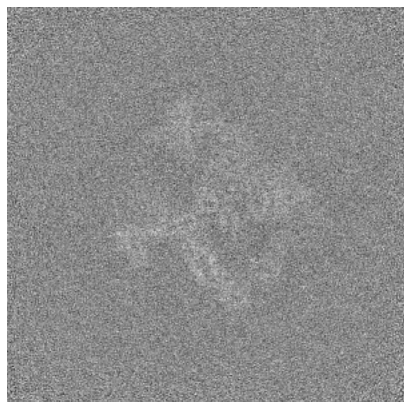


Y Index: 216

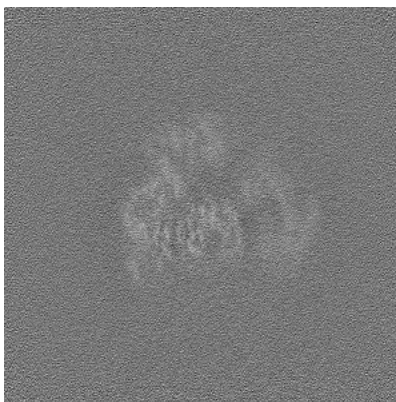


Z Index: 216

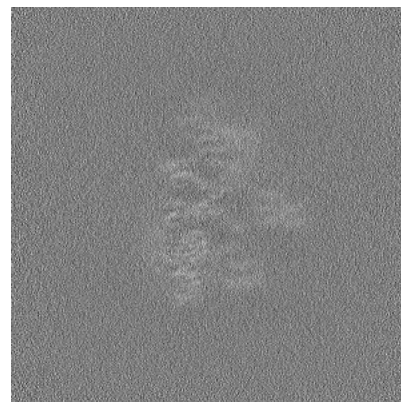
6.2.2 Raw map



X Index: 216



Y Index: 216

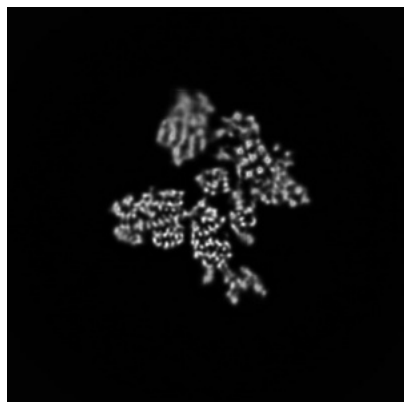


Z Index: 216

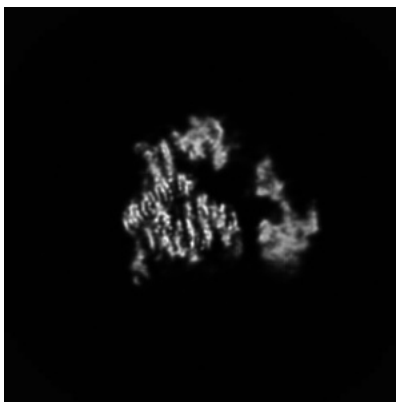
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

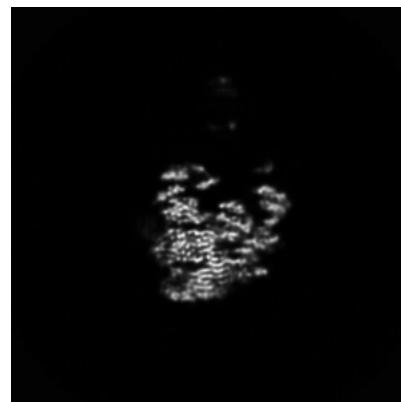
6.3.1 Primary map



X Index: 189

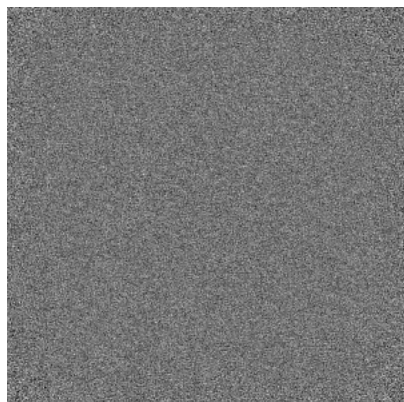


Y Index: 211

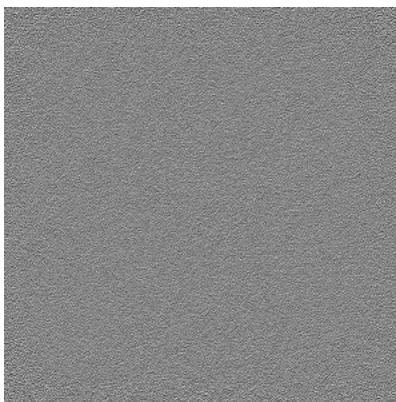


Z Index: 188

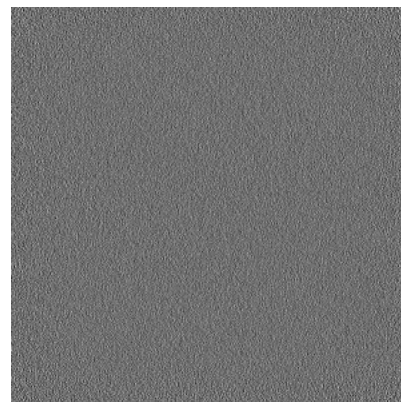
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

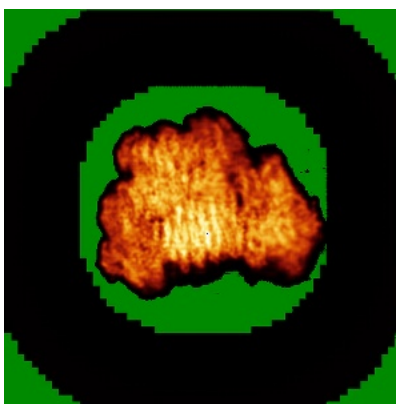
The images above show the largest variance slices of the map in three orthogonal directions.

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

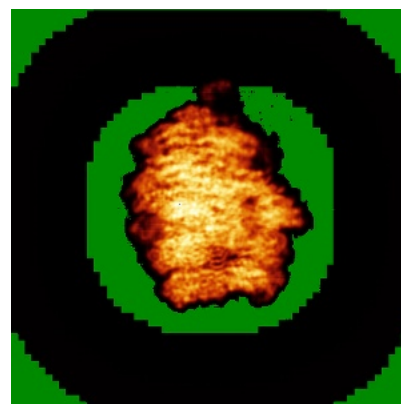
6.4.1 Primary map



X

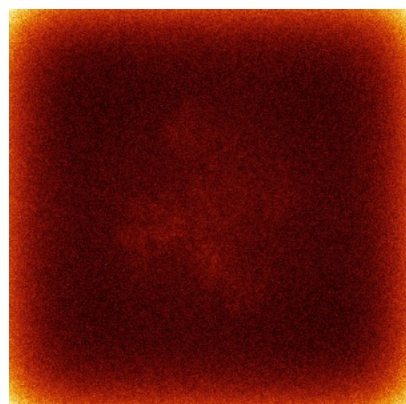


Y

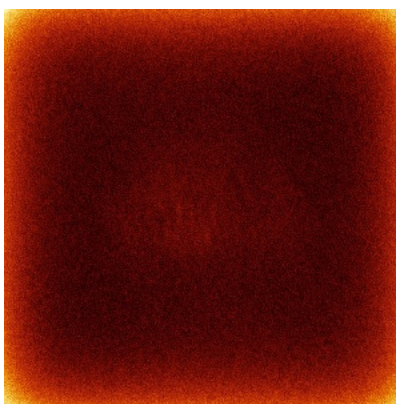


Z

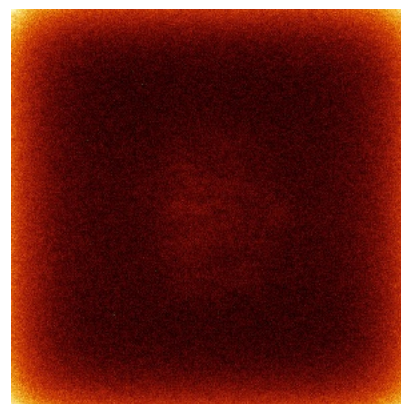
6.4.2 Raw map



X



Y

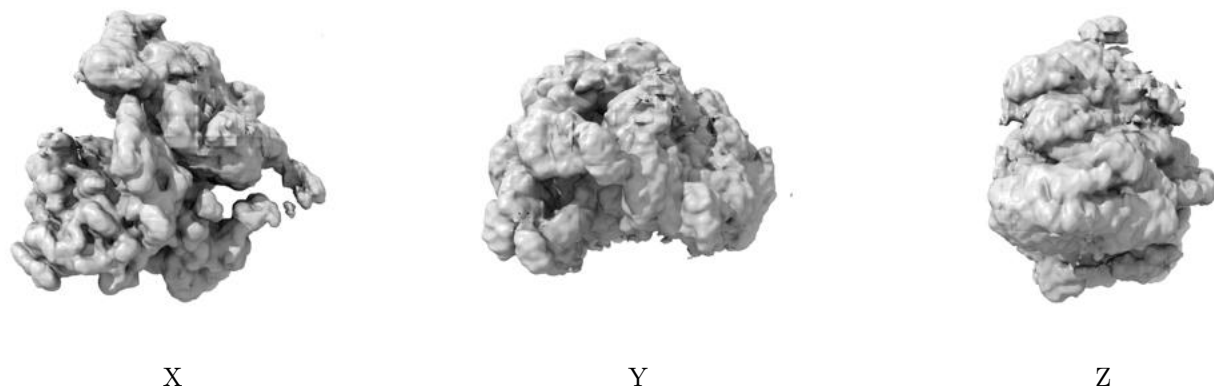


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

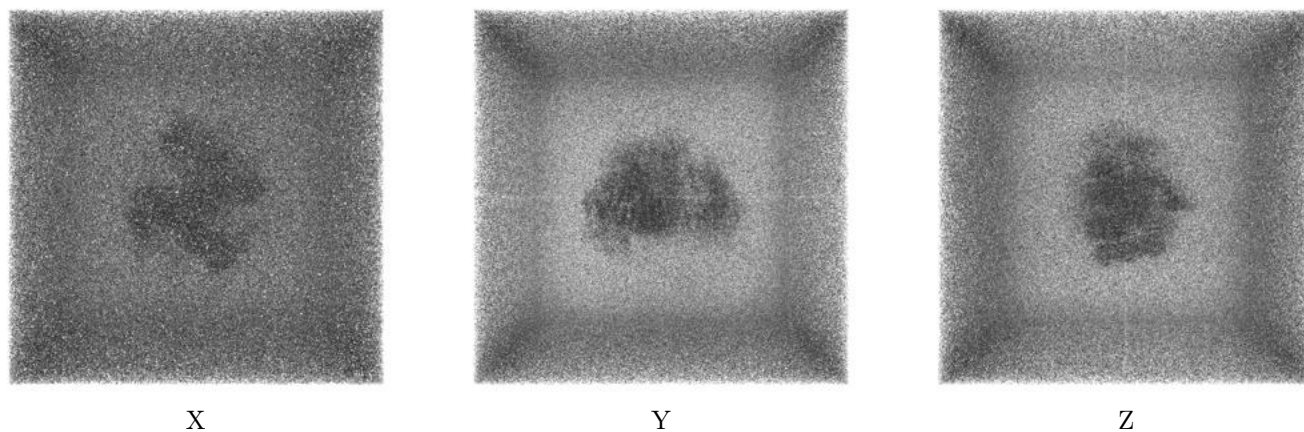
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

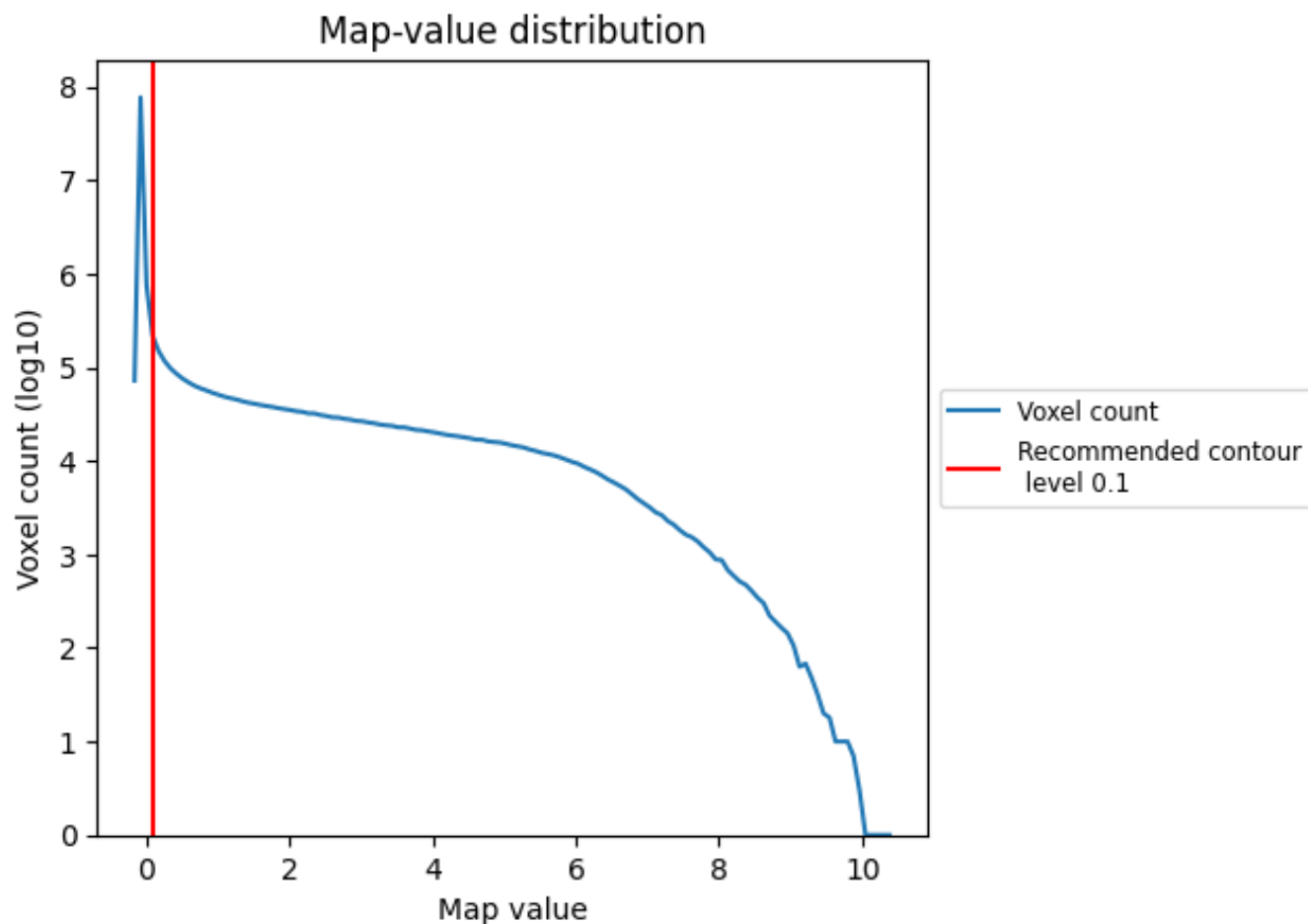
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

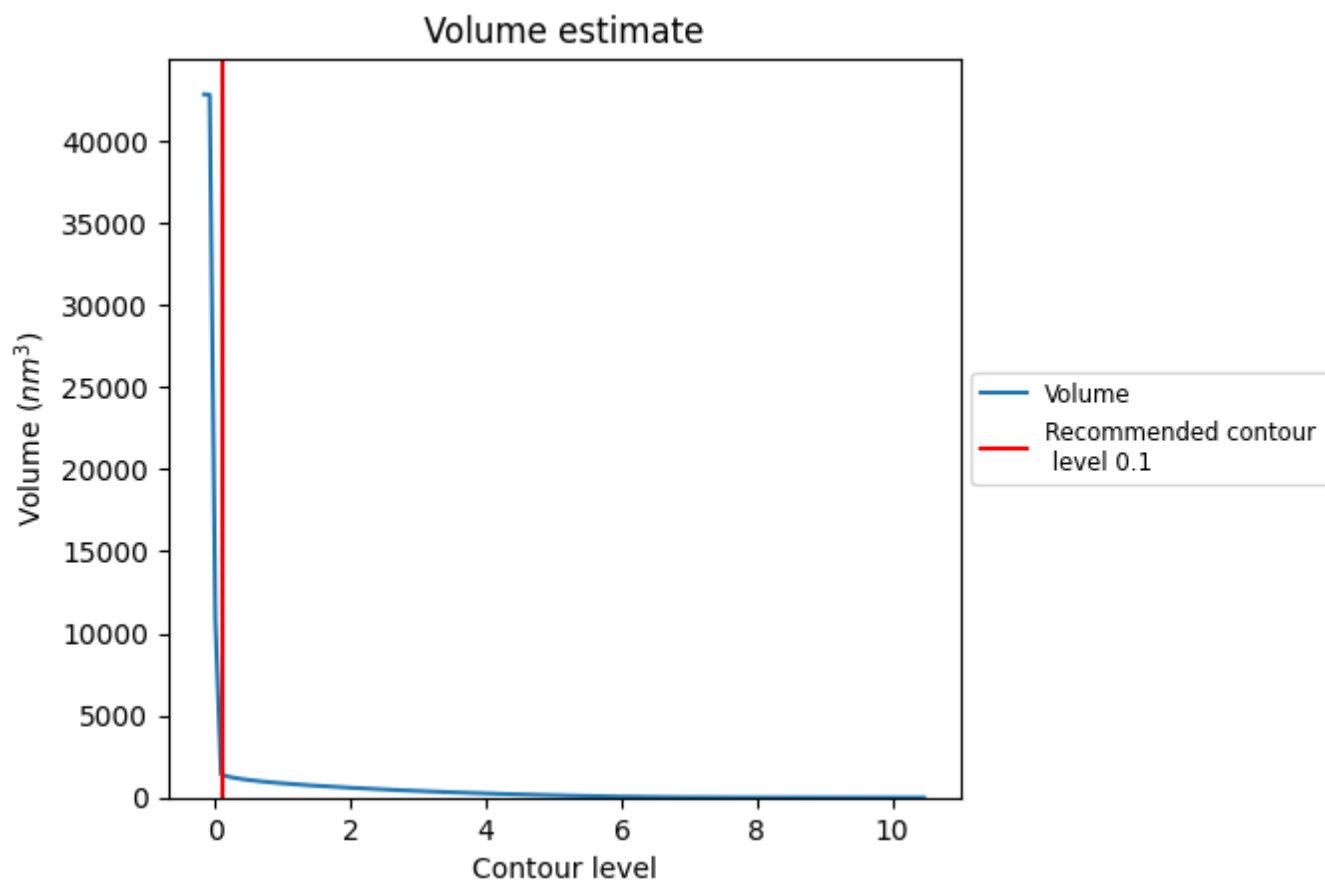
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

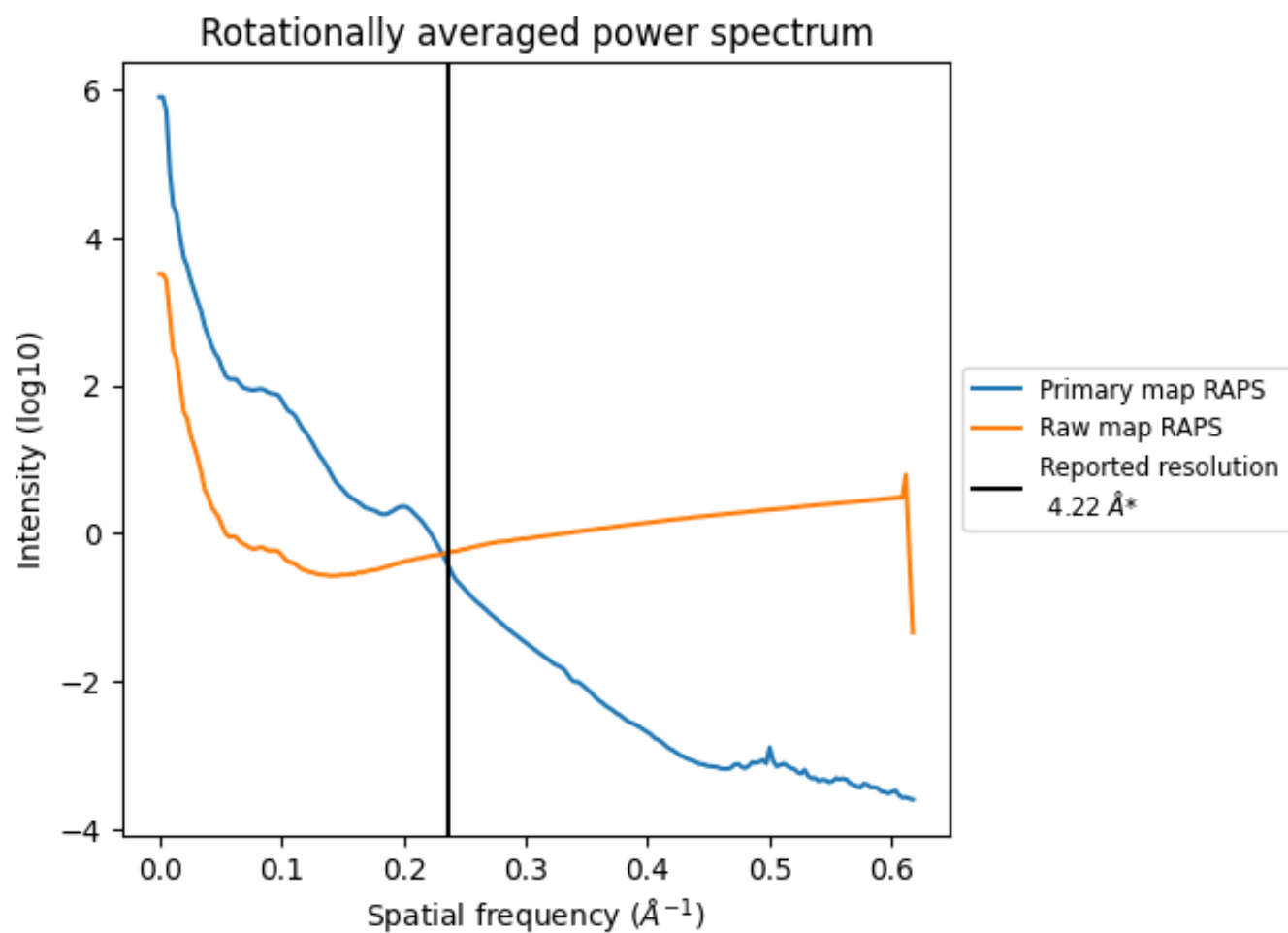
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1397 nm^3 ; this corresponds to an approximate mass of 1262 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](#)

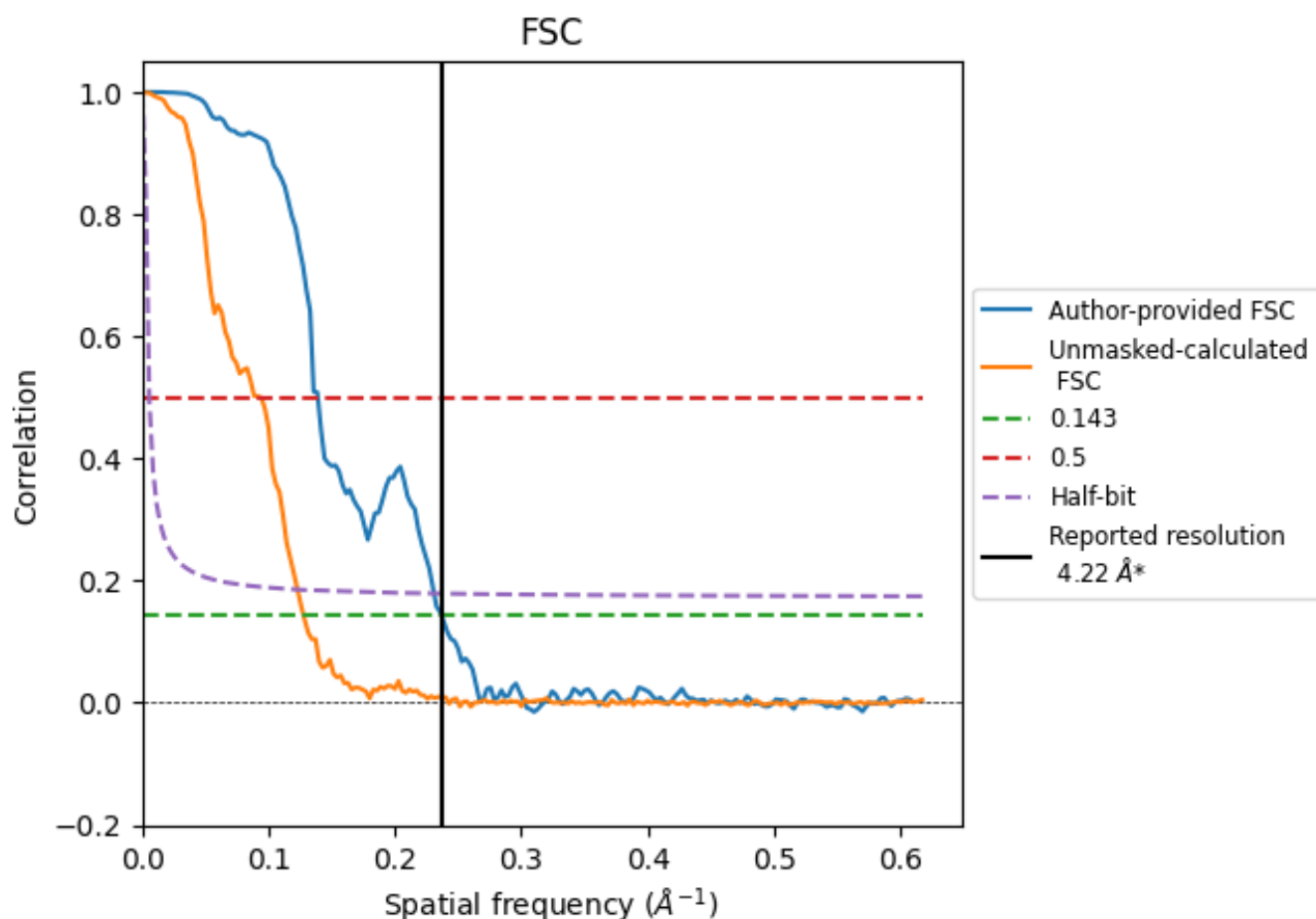


*Reported resolution corresponds to spatial frequency of 0.237 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.237 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

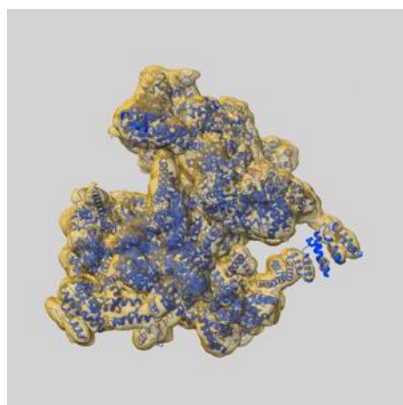
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.22	-	-
Author-provided FSC curve	4.22	7.19	4.33
Unmasked-calculated*	7.83	10.66	8.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.83 differs from the reported value 4.22 by more than 10 %

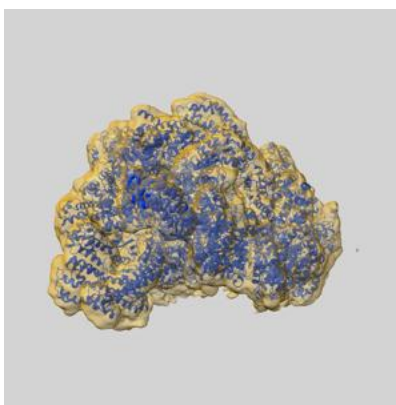
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71737 and PDB model 9PMJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

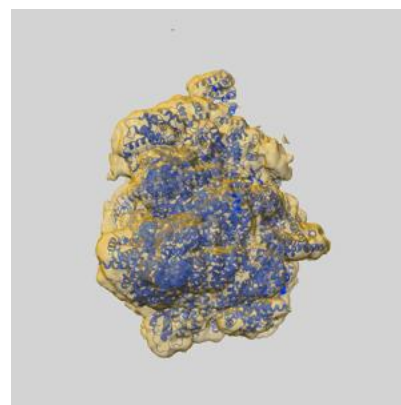
9.1 Map-model overlay [i](#)



X



Y



Z

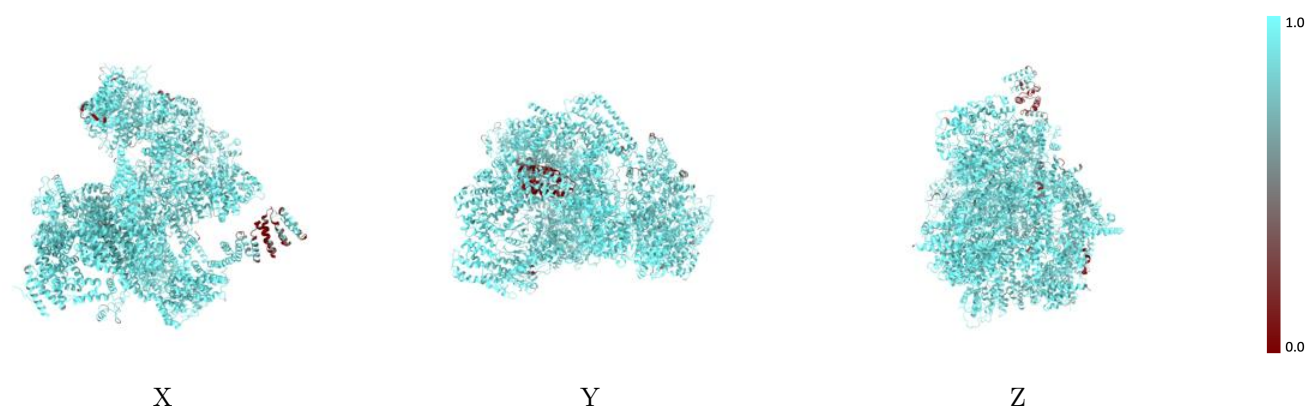
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



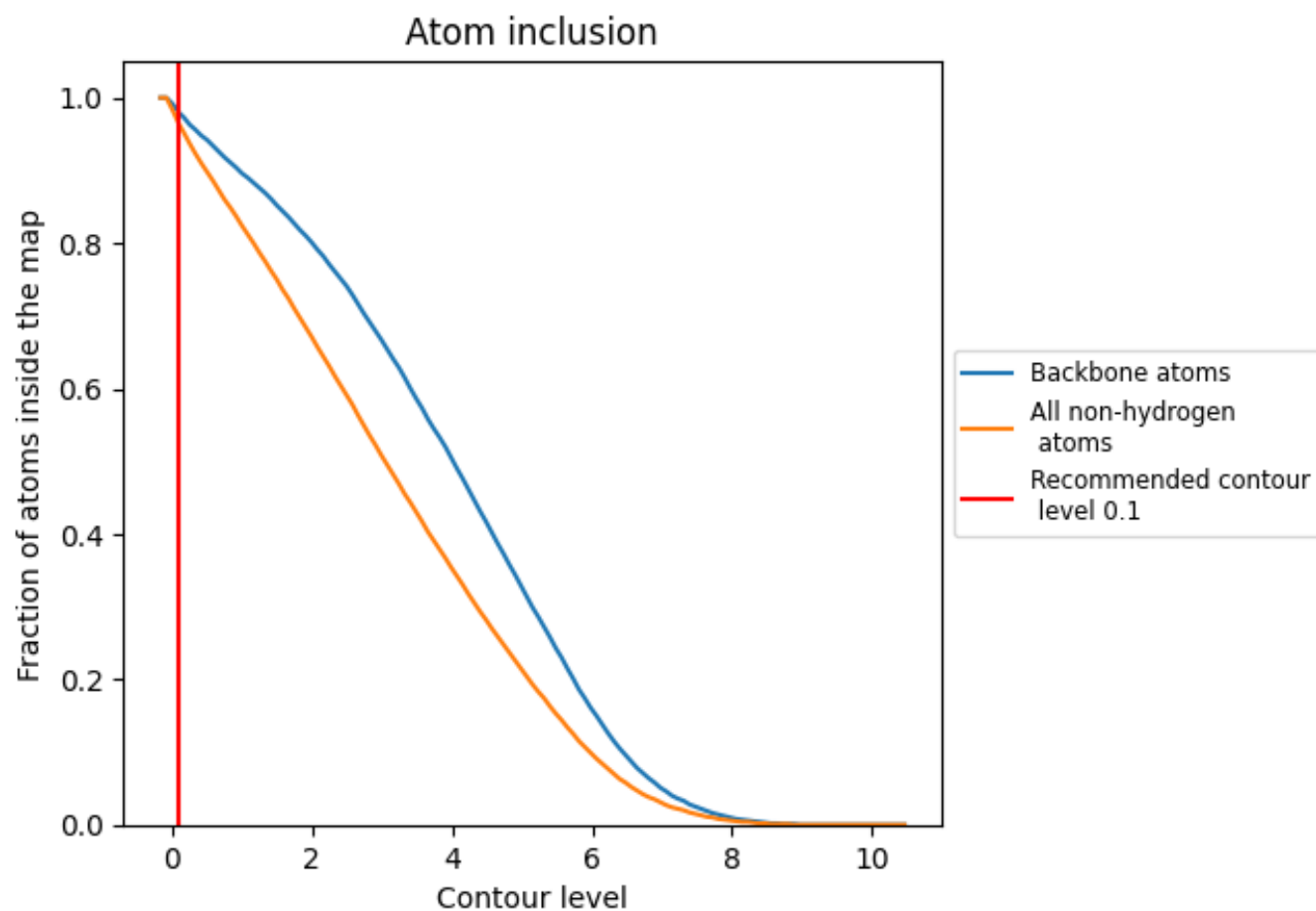
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.1310
A	 0.9770	 0.1440
B	 0.9680	 0.1220
C	 0.9590	 0.1220
D	 0.9950	 0.1360
E	 0.9850	 0.1390
F	 0.9870	 0.1600
U	 0.9920	 0.1740
V	 0.9820	 0.1370
W	 0.7990	 0.1020
X	 0.9770	 0.1390
Y	 0.9810	 0.1180
Z	 0.9970	 0.2200
a	 0.9850	 0.1410
b	 0.9690	 0.1340
c	 0.9840	 0.1870
d	 0.9600	 0.0950
e	 0.8880	 0.0960
f	 0.9610	 0.0630
g	 0.8280	 0.0480

