



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 09:29 PM UTC

PDB ID : 9U4M / pdb_00009u4m
EMDB ID : EMD-63850
Title : Focused refinement of 19S in the substrate-engaged human 26S proteasome bound to midnolin with RPT6 at top of spiral staircase
Authors : Zhu, C.; Qin, L.; Liang, L.
Deposited on : 2025-03-19
Resolution : 4.14 Å(reported)

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

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

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:

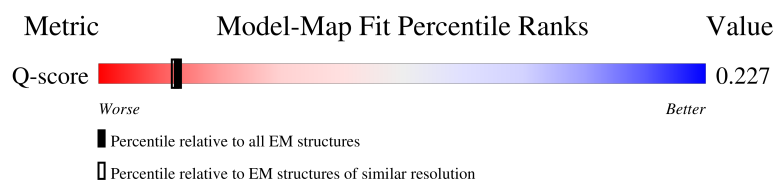
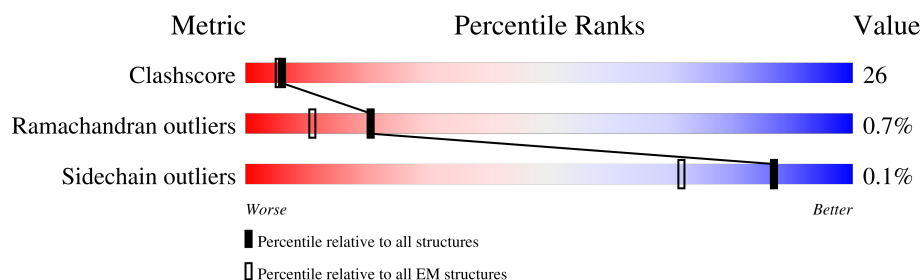
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.14 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	5577 (3.64 - 4.64)

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	Y	389	
2	a	376	
3	v	8	
4	B	440	

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Mol	Chain	Length	Quality of chain
5	c	309	
6	Z	324	
7	e	70	
8	U	953	
9	W	456	
10	A	433	
11	C	398	
12	D	418	
13	E	403	
14	F	439	
15	X	422	
16	V	533	
17	d	349	
18	b	377	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 46918 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 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	380	Total	C	N	O	S	0	0
			3121	1992	532	580	17		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	346	Total	C	N	O	S	0	0
			2764	1760	471	518	15		

- Molecule 3 is a protein called substrate peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	v	8	Total	C	N	O	0	0
			40	24	8	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	320	Total	C	N	O	S	0	0
			2497	1572	426	488	11		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	271	Total	C	N	O	S	0	0
			2134	1353	363	401	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	282	Total	C	N	O	S	0	0
			2251	1440	387	419	5		

- Molecule 7 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	e	32	Total	C	N	O	0	0
			271	162	46	63		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	811	Total	C	N	O	S	0	0
			6300	4000	1072	1184	44		

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

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

- Molecule 10 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	325	Total	C	N	O	S	0	0
			2558	1619	453	471	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	364	Total	C	N	O	S	0	0
			2878	1814	514	533	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	366	Total	C	N	O	S	0	0
			2912	1843	505	553	11		

- Molecule 13 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	360	Total	C	N	O	S	0	0
			2859	1799	509	535	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	357	Total	C	N	O	S	0	0
			2790	1761	483	529	17		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	378	Total	C	N	O	S	0	0
			2988	1906	504	566	12		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	439	Total	C	N	O	S	0	0
			3504	2222	623	646	13		

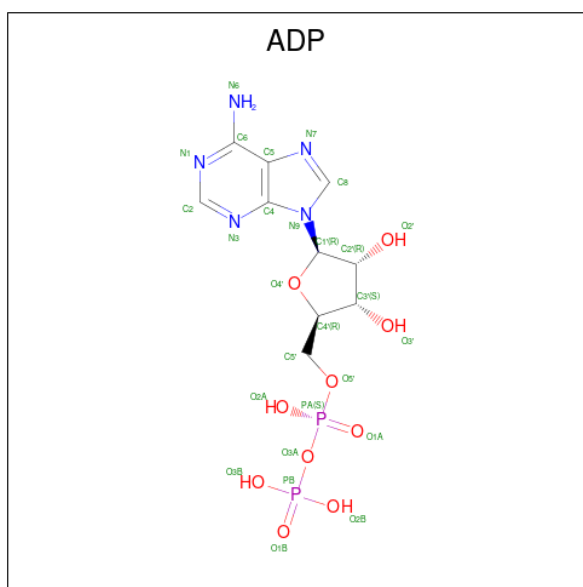
- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	269	Total	C	N	O	S	0	0
			2180	1409	358	404	9		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	148	Total	C	N	O	S	0	0
			1125	702	203	215	5		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

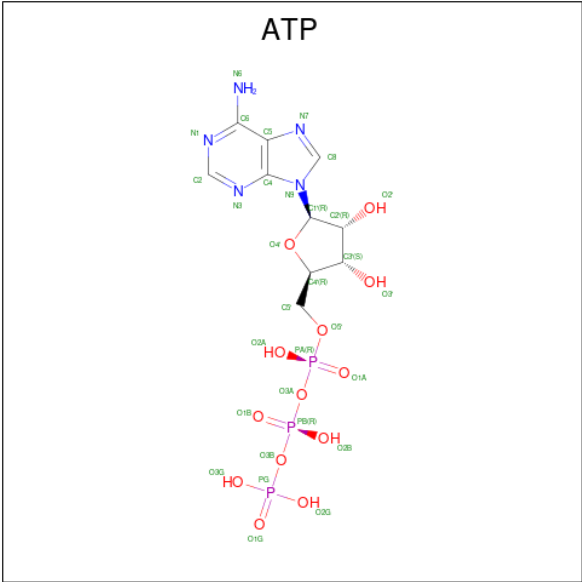


Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

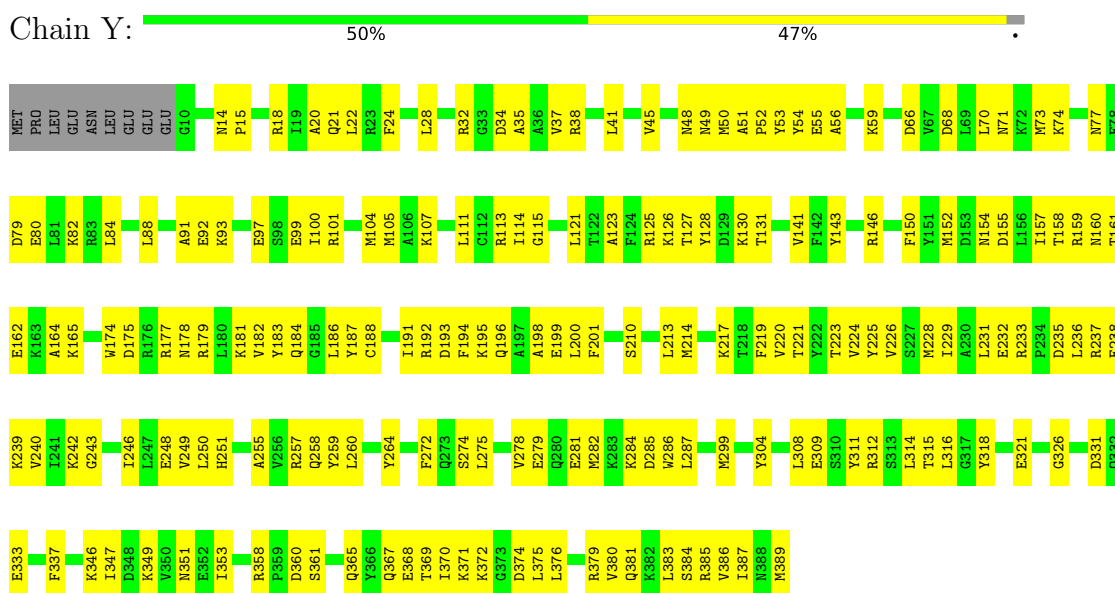
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	C	1	Total	Mg	0
			1	1	

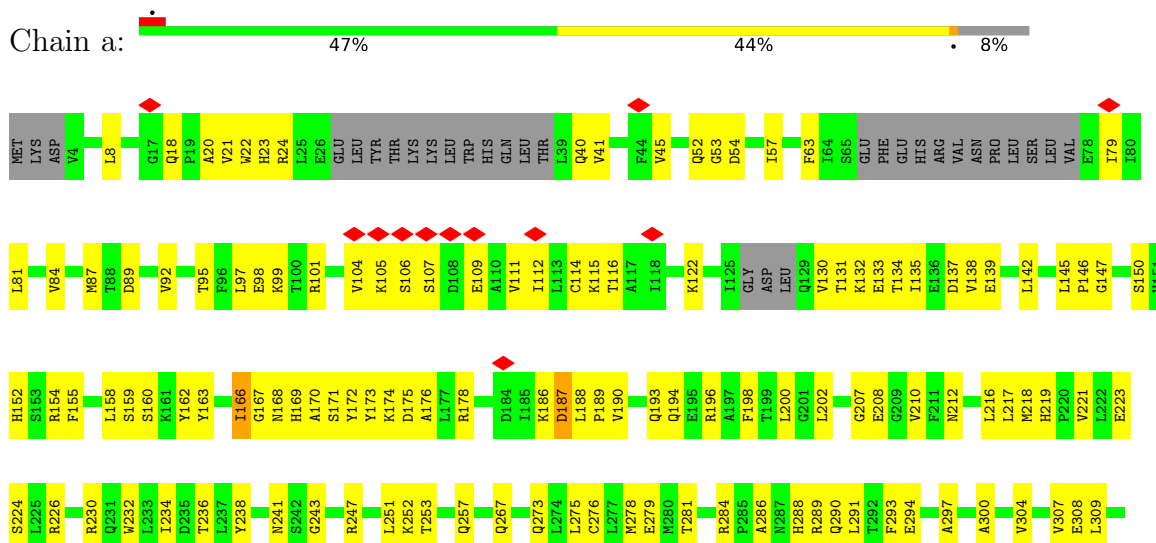
3 Residue-property plots

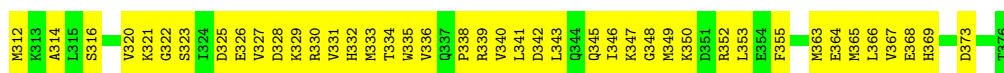
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 6

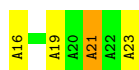


- Molecule 2: 26S proteasome non-ATPase regulatory subunit 13

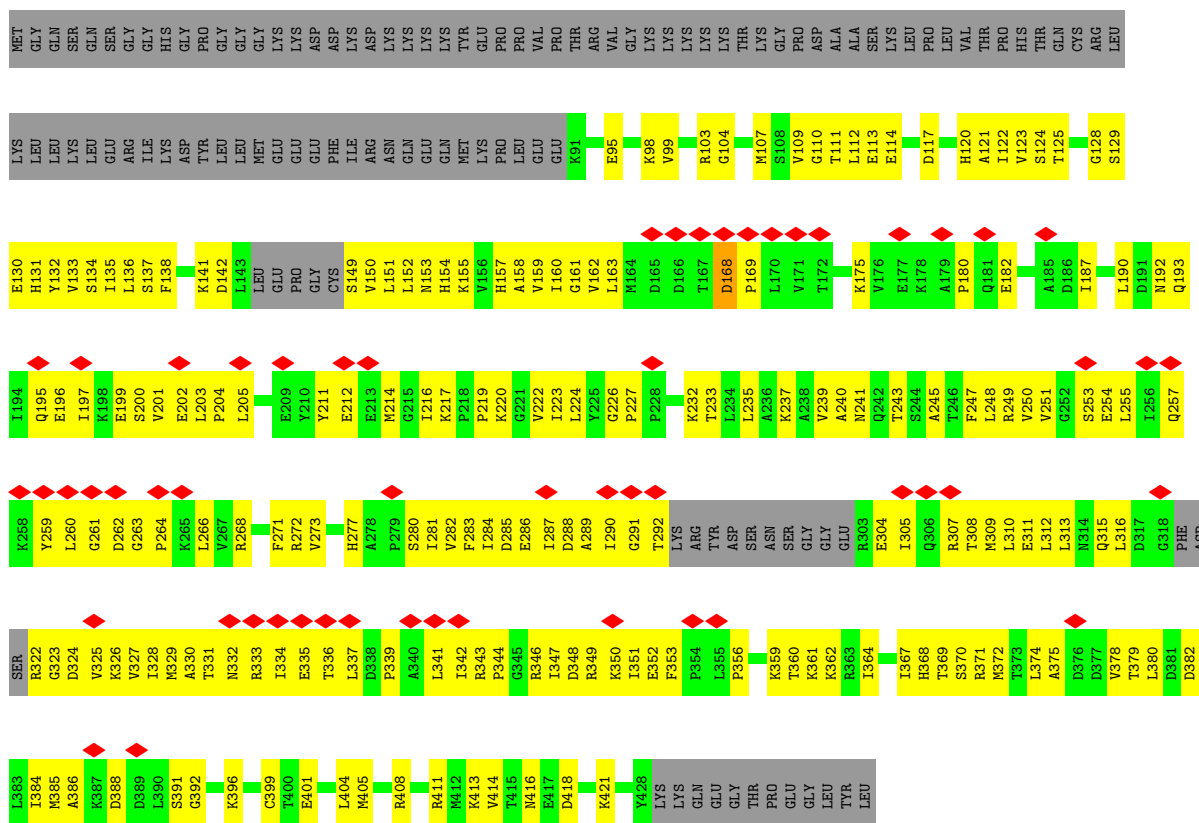




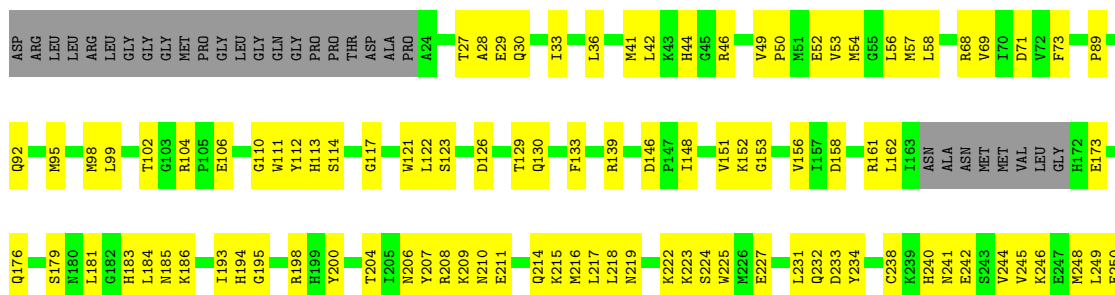
• Molecule 3: substrate peptide

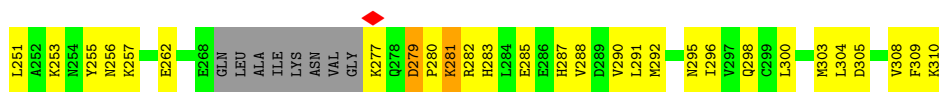


• Molecule 4: 26S proteasome regulatory subunit 4

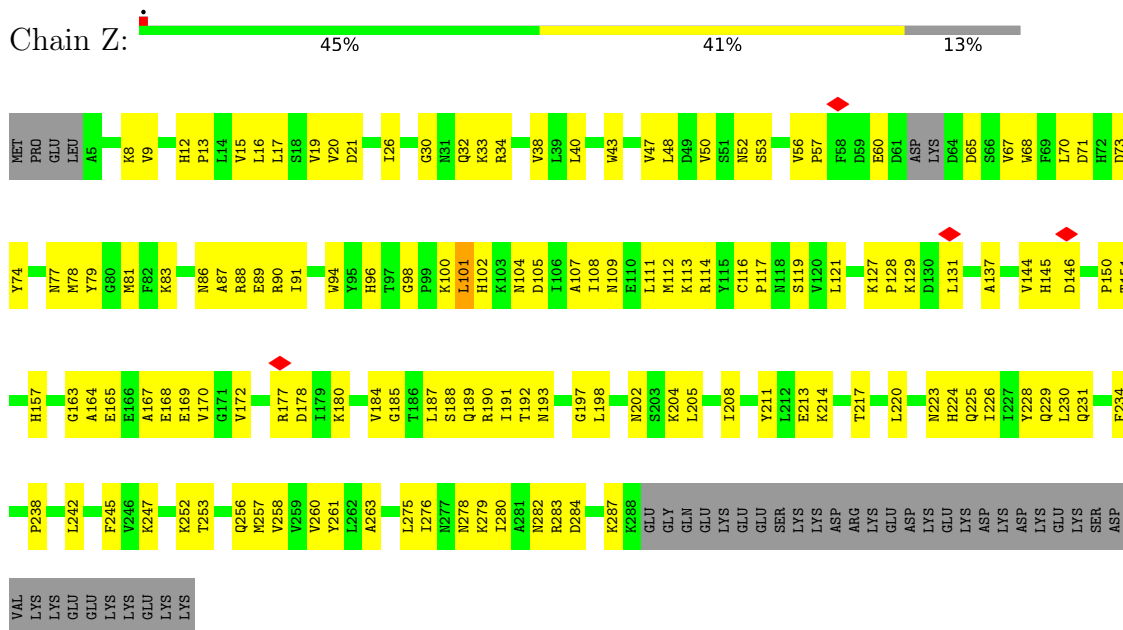


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 14

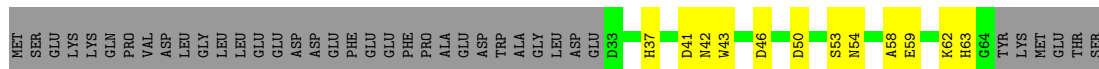
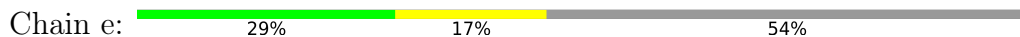




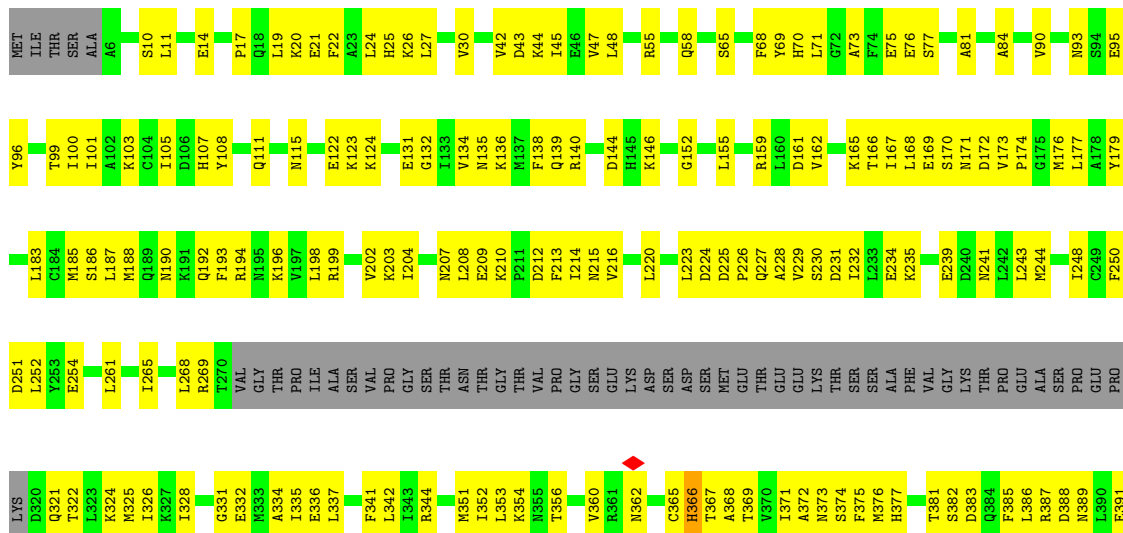
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

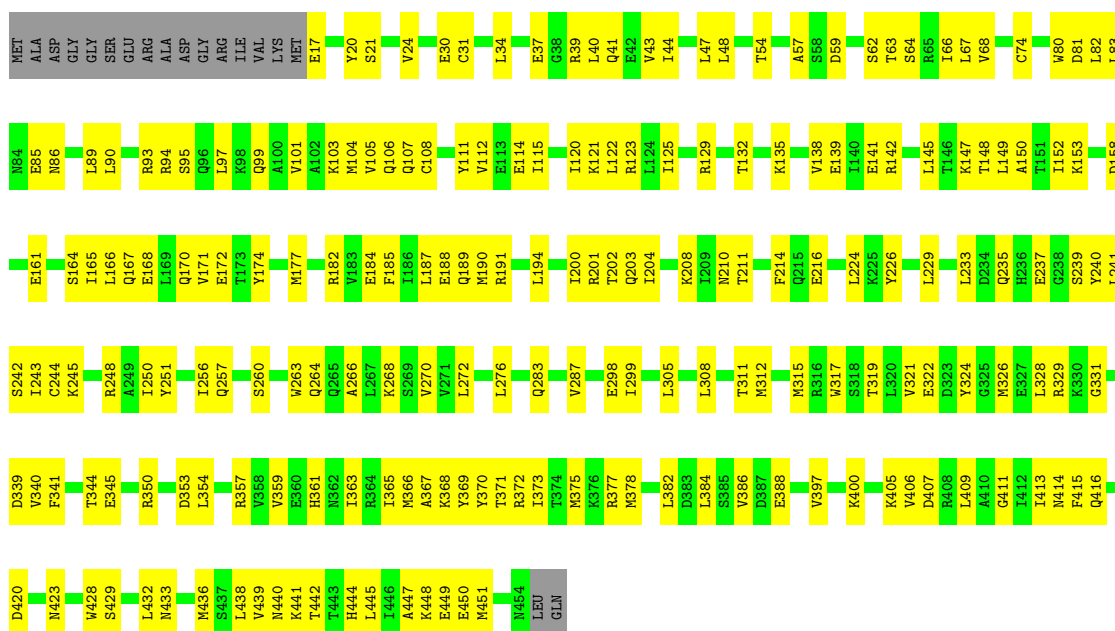


• Molecule 7: 26S proteasome complex subunit SEM1

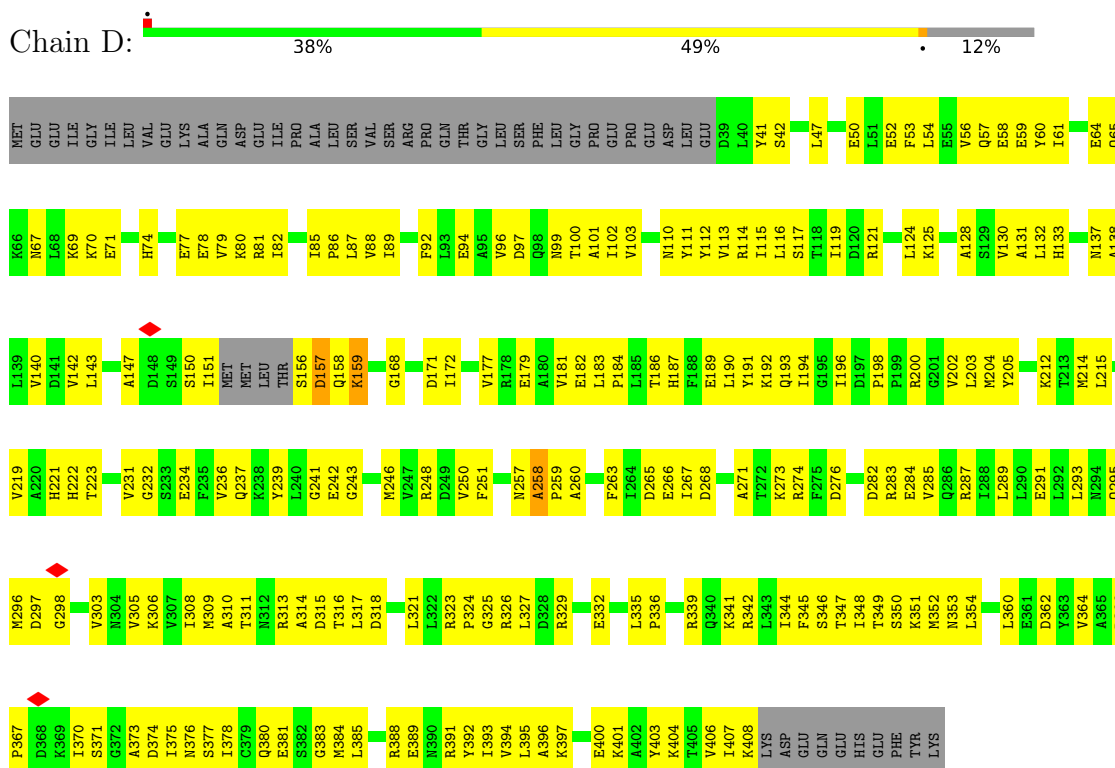


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 1

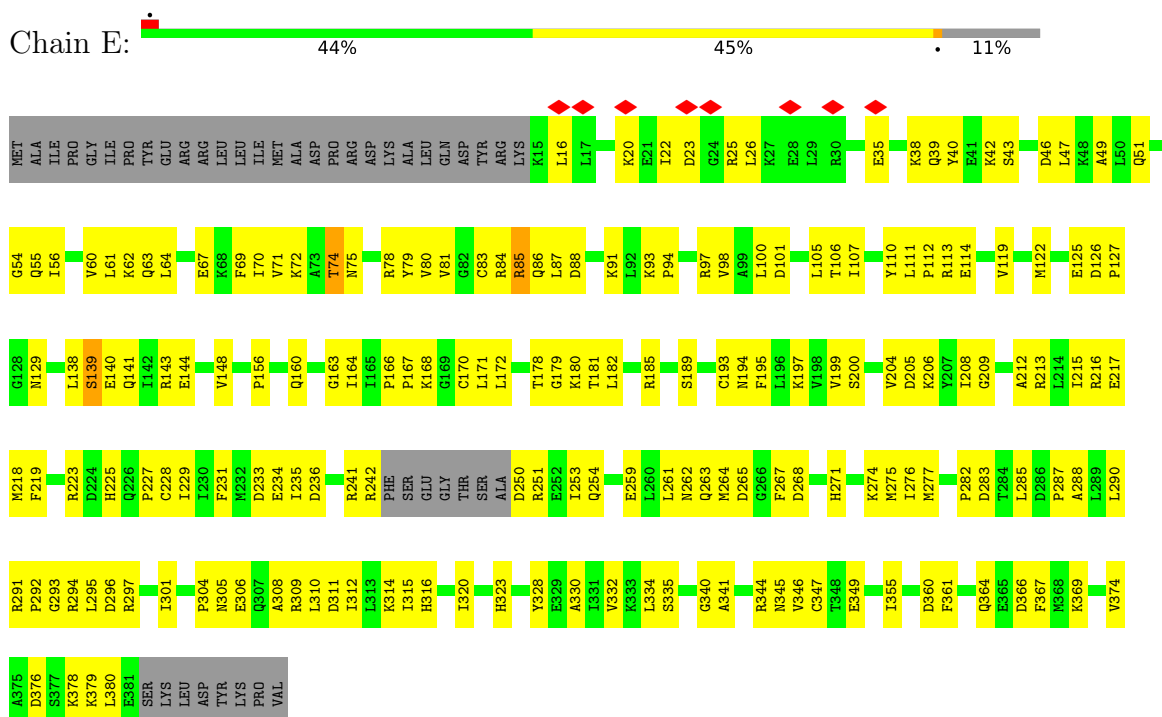






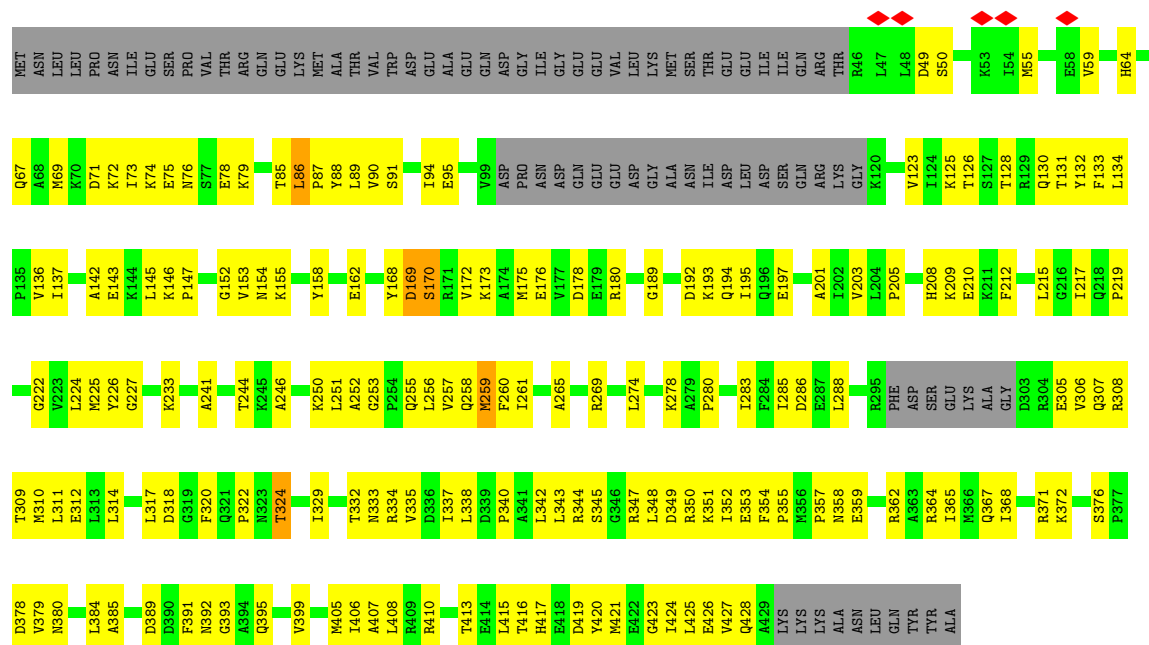


• Molecule 13: Proteasome 26S subunit, ATPase 6

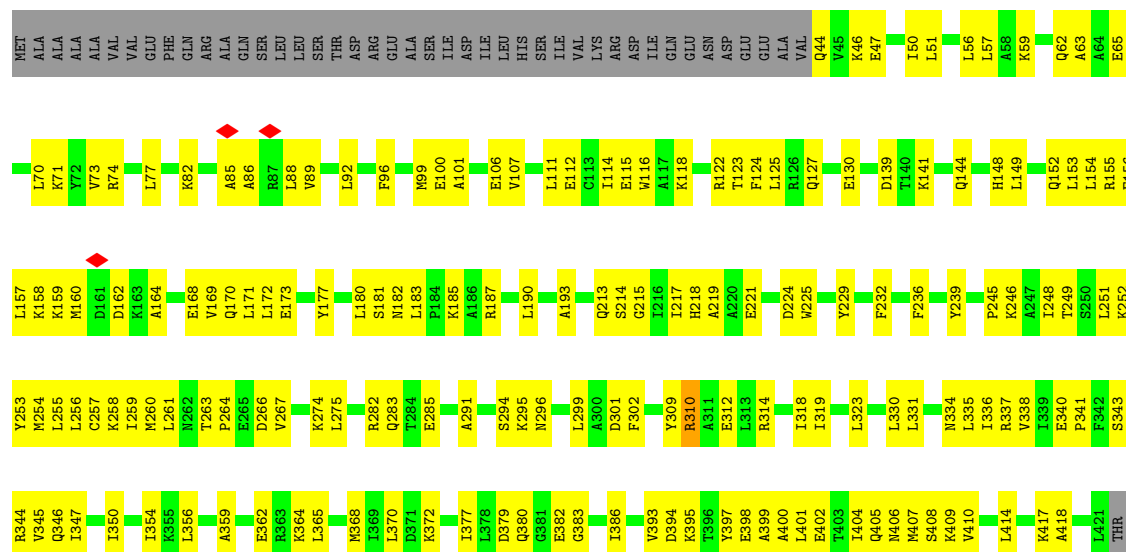


• Molecule 14: 26S proteasome regulatory subunit 6A

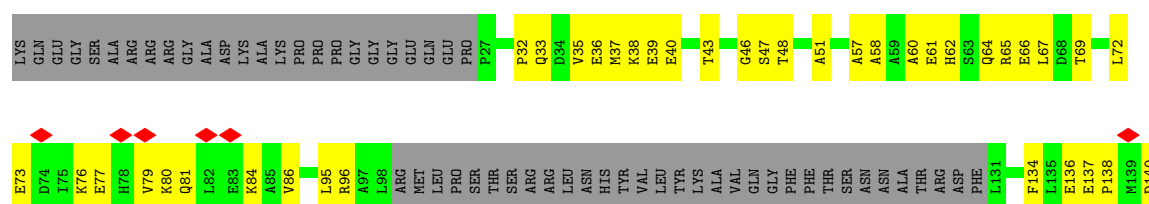
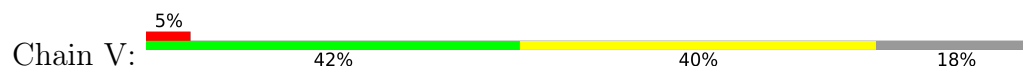


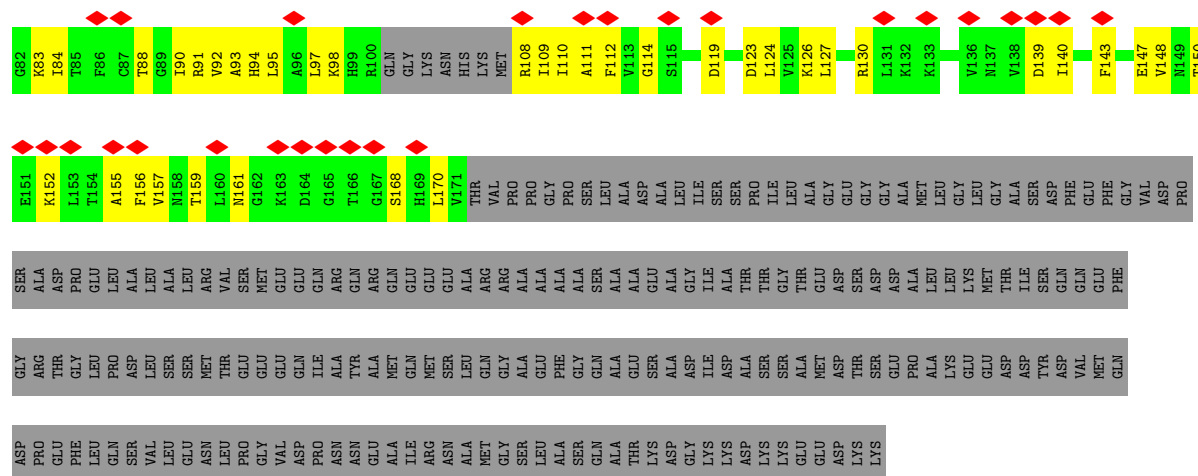


• Molecule 15: 26S proteasome non-ATPase regulatory subunit 11



• Molecule 16: 26S proteasome non-ATPase regulatory subunit 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.228	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	306.0, 306.0, 306.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	Y	0.16	0/3179	0.42	0/4283
2	a	0.16	0/2812	0.47	0/3800
3	v	0.32	0/39	0.65	0/53
4	B	0.20	0/2529	0.45	0/3413
5	c	0.23	0/2173	0.52	0/2936
6	Z	0.19	0/2293	0.50	0/3108
7	e	0.12	0/277	0.38	0/376
8	U	0.22	0/6410	0.50	1/8675 (0.0%)
9	W	0.15	0/3618	0.37	0/4868
10	A	0.22	0/2601	0.46	0/3510
11	C	0.17	0/2916	0.44	0/3925
12	D	0.19	0/2958	0.48	0/3993
13	E	0.17	0/2901	0.40	0/3905
14	F	0.15	0/2825	0.38	0/3808
15	X	0.16	0/3032	0.40	0/4088
16	V	0.25	0/3568	0.54	0/4818
17	d	0.17	0/2226	0.42	0/3009
18	b	0.15	0/1133	0.44	0/1527
All	All	0.19	0/47490	0.45	1/64095 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	891	VAL	N-CA-C	-5.03	107.80	112.43

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	Y	3121	0	3122	156	0
2	a	2764	0	2779	146	0
3	v	40	0	39	4	0
4	B	2497	0	2547	235	0
5	c	2134	0	2134	134	0
6	Z	2251	0	2285	142	0
7	e	271	0	214	9	0
8	U	6300	0	6319	299	0
9	W	3570	0	3685	170	0
10	A	2558	0	2623	192	0
11	C	2878	0	2988	196	0
12	D	2912	0	2955	203	0
13	E	2859	0	2930	181	0
14	F	2790	0	2886	158	0
15	X	2988	0	3086	145	0
16	V	3504	0	3549	207	0
17	d	2180	0	2201	95	0
18	b	1125	0	1161	48	0
19	A	27	0	12	2	0
19	B	27	0	12	4	0
19	F	27	0	12	4	0
20	c	1	0	0	0	0
21	C	31	0	12	2	0
21	D	31	0	12	3	0
21	E	31	0	12	8	0
22	C	1	0	0	1	0
All	All	46918	0	47575	2495	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 26.

The worst 5 of 2495 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)
17:d:185:SER:H	17:d:188:MET:HE3	1.27	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:216:GLY:HA3	10:A:343:PHE:HB2	1.48	0.95
4:B:203:LEU:HD23	4:B:211:TYR:HE1	1.30	0.93
2:a:174:LYS:HG2	2:a:178:ARG:HH12	1.29	0.92
6:Z:257:MET:HE1	16:V:476:PHE:HB3	1.50	0.91

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	Y	378/389 (97%)	365 (97%)	13 (3%)	0	100	100
2	a	338/376 (90%)	310 (92%)	26 (8%)	2 (1%)	21	58
3	v	6/8 (75%)	2 (33%)	3 (50%)	1 (17%)	0	2
4	B	312/440 (71%)	280 (90%)	31 (10%)	1 (0%)	36	70
5	c	265/309 (86%)	248 (94%)	14 (5%)	3 (1%)	11	44
6	Z	278/324 (86%)	255 (92%)	22 (8%)	1 (0%)	30	65
7	e	30/70 (43%)	28 (93%)	2 (7%)	0	100	100
8	U	803/953 (84%)	748 (93%)	50 (6%)	5 (1%)	21	58
9	W	436/456 (96%)	426 (98%)	9 (2%)	1 (0%)	43	76
10	A	319/433 (74%)	279 (88%)	39 (12%)	1 (0%)	36	70
11	C	360/398 (90%)	314 (87%)	45 (12%)	1 (0%)	36	70
12	D	362/418 (87%)	321 (89%)	37 (10%)	4 (1%)	11	44
13	E	356/403 (88%)	334 (94%)	17 (5%)	5 (1%)	9	39
14	F	351/439 (80%)	320 (91%)	25 (7%)	6 (2%)	7	36
15	X	376/422 (89%)	363 (96%)	10 (3%)	3 (1%)	16	52
16	V	435/533 (82%)	392 (90%)	42 (10%)	1 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	d	267/349 (76%)	254 (95%)	11 (4%)	2 (1%)	18	54
18	b	140/377 (37%)	133 (95%)	5 (4%)	2 (1%)	9	39
All	All	5812/7097 (82%)	5372 (92%)	401 (7%)	39 (1%)	20	54

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	187	ASP
5	c	279	ASP
5	c	281	LYS
8	U	416	GLU
11	C	167	LEU

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	Y	334/344 (97%)	334 (100%)	0	100	100
2	a	307/336 (91%)	307 (100%)	0	100	100
4	B	279/385 (72%)	279 (100%)	0	100	100
5	c	238/267 (89%)	238 (100%)	0	100	100
6	Z	254/295 (86%)	253 (100%)	1 (0%)	84	83
7	e	29/63 (46%)	29 (100%)	0	100	100
8	U	685/816 (84%)	683 (100%)	2 (0%)	86	84
9	W	403/416 (97%)	402 (100%)	1 (0%)	87	86
10	A	280/372 (75%)	280 (100%)	0	100	100
11	C	319/346 (92%)	319 (100%)	0	100	100
12	D	318/366 (87%)	318 (100%)	0	100	100
13	E	315/353 (89%)	315 (100%)	0	100	100
14	F	307/379 (81%)	306 (100%)	1 (0%)	86	84
15	X	324/362 (90%)	324 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	374/459 (82%)	374 (100%)	0	100	100
17	d	235/293 (80%)	234 (100%)	1 (0%)	84	83
18	b	128/312 (41%)	128 (100%)	0	100	100
All	All	5129/6164 (83%)	5123 (100%)	6 (0%)	87	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	W	416	GLN
14	F	255	GLN
17	d	221	GLN
8	U	366	HIS
6	Z	101	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
9	W	107	GLN
11	C	48	GLN
18	b	161	ASN
16	V	347	GLN
9	W	228	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 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
21	ATP	C	501	22	32,33,33	0.31	0	48,52,52	0.34	0
19	ADP	A	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)
21	ATP	E	501	-	32,33,33	0.36	0	48,52,52	0.31	0
19	ADP	B	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.87	8 (18%)
21	ATP	D	501	-	32,33,33	0.29	0	48,52,52	0.53	0
19	ADP	F	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.86	8 (18%)

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
21	ATP	C	501	22	-	3/22/38/38	0/3/3/3
19	ADP	A	501	-	-	5/16/32/32	0/3/3/3
21	ATP	E	501	-	-	12/22/38/38	0/3/3/3
19	ADP	B	501	-	-	0/16/32/32	0/3/3/3
21	ATP	D	501	-	-	6/22/38/38	0/3/3/3
19	ADP	F	501	-	-	8/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	501	ADP	C5-C4	4.77	1.47	1.39
19	B	501	ADP	C5-C4	4.77	1.47	1.39
19	A	501	ADP	C5-C4	4.65	1.47	1.39
19	A	501	ADP	C5-C6	2.75	1.48	1.41
19	B	501	ADP	C5-C6	2.72	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	501	ADP	C5-C4-N3	-6.09	118.33	126.72
19	F	501	ADP	C5-C4-N3	-5.94	118.54	126.72
19	A	501	ADP	C5-C4-N3	-5.81	118.72	126.72
19	B	501	ADP	N3-C4-N9	4.97	135.62	127.17
19	F	501	ADP	N3-C4-N9	4.85	135.42	127.17

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	501	ADP	C5'-O5'-PA-O1A
19	A	501	ADP	C5'-O5'-PA-O3A
19	F	501	ADP	C5'-O5'-PA-O1A
19	F	501	ADP	C5'-O5'-PA-O2A
19	F	501	ADP	C5'-O5'-PA-O3A

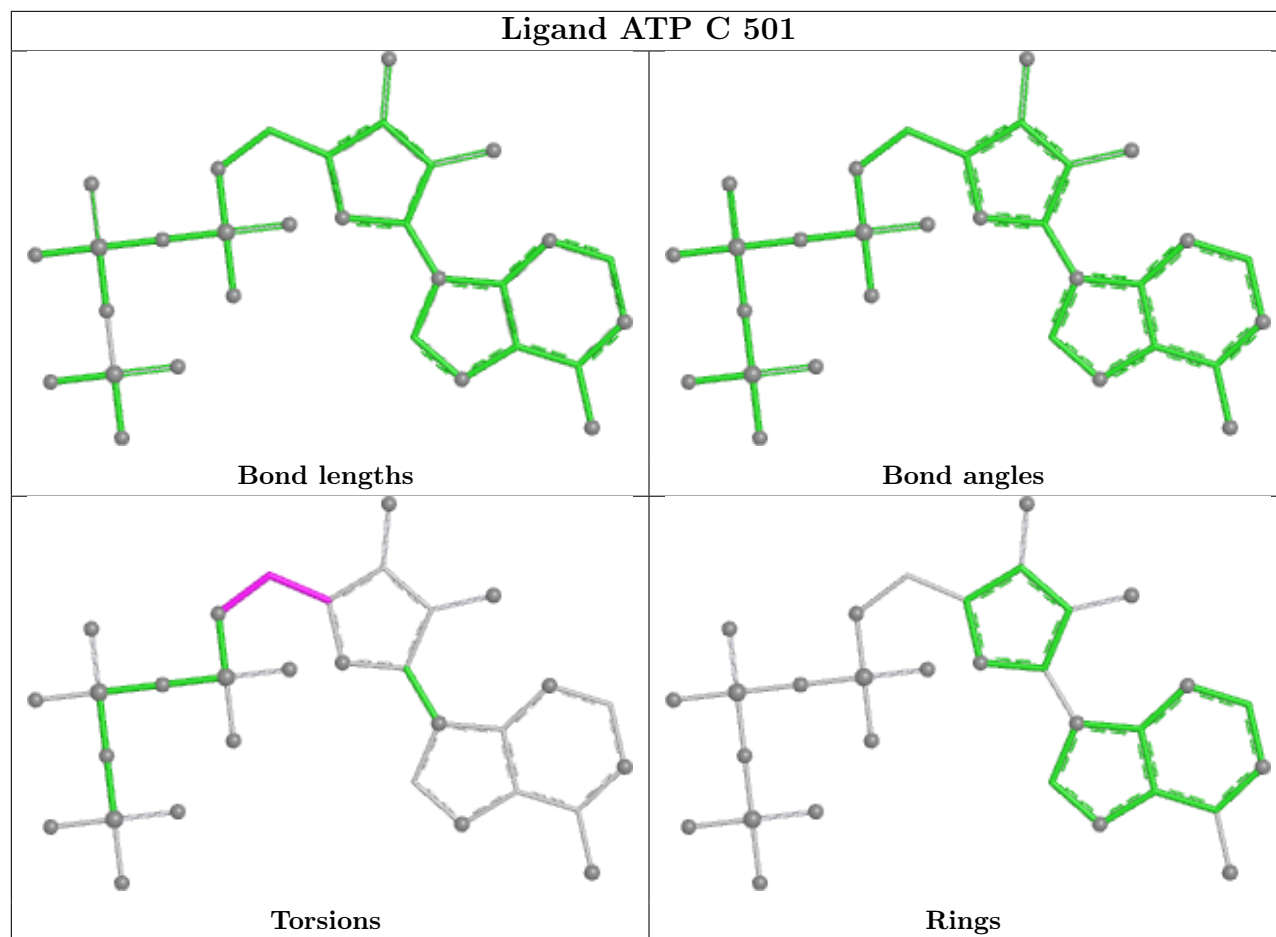
There are no ring outliers.

6 monomers are involved in 23 short contacts:

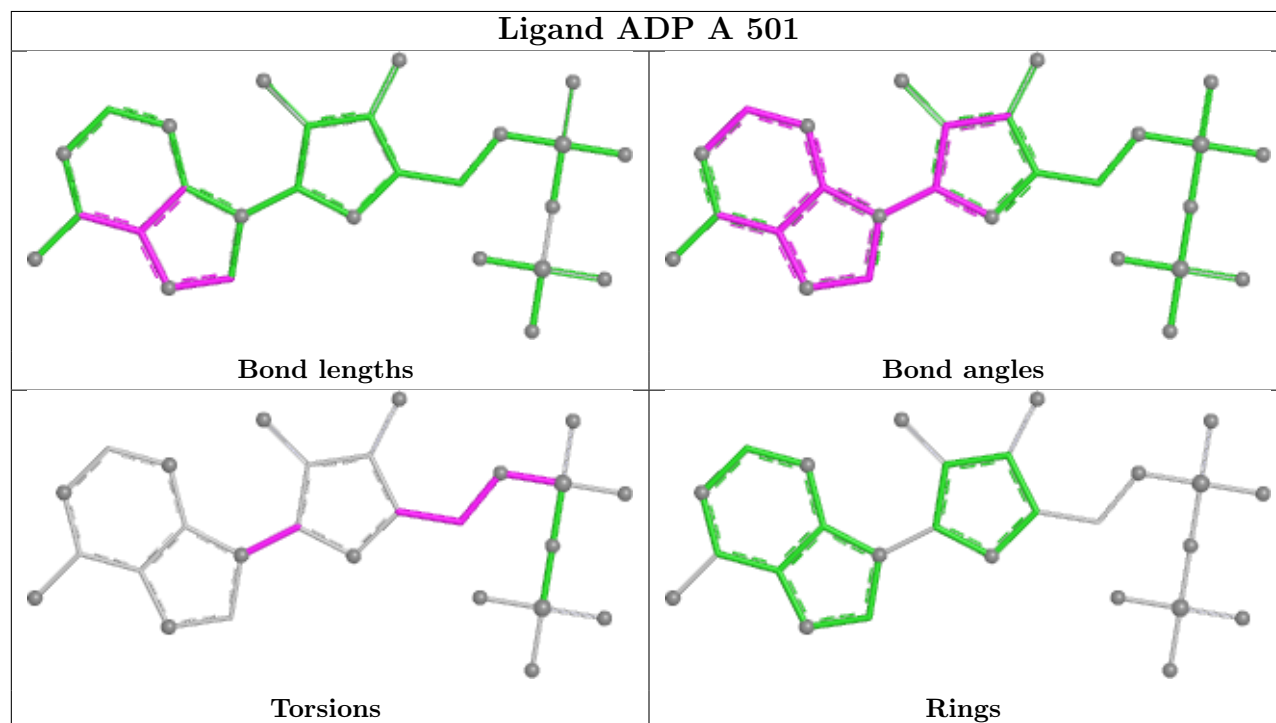
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	501	ATP	2	0
19	A	501	ADP	2	0
21	E	501	ATP	8	0
19	B	501	ADP	4	0
21	D	501	ATP	3	0
19	F	501	ADP	4	0

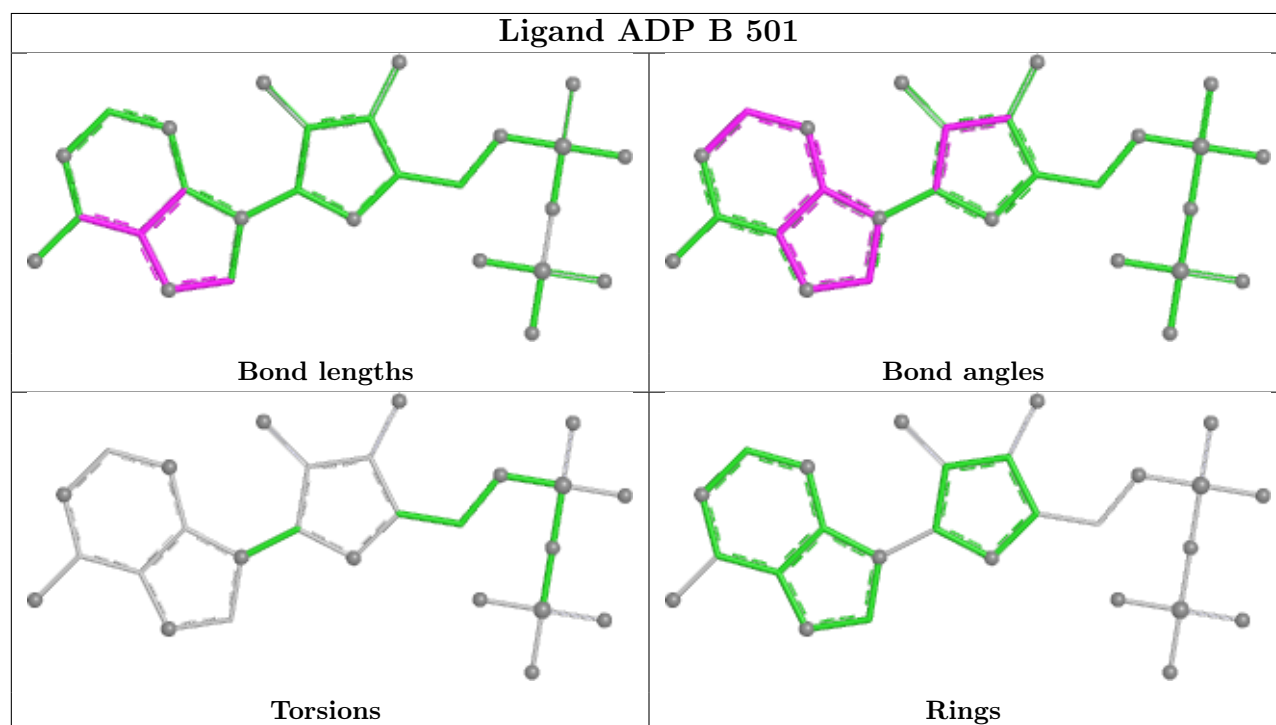
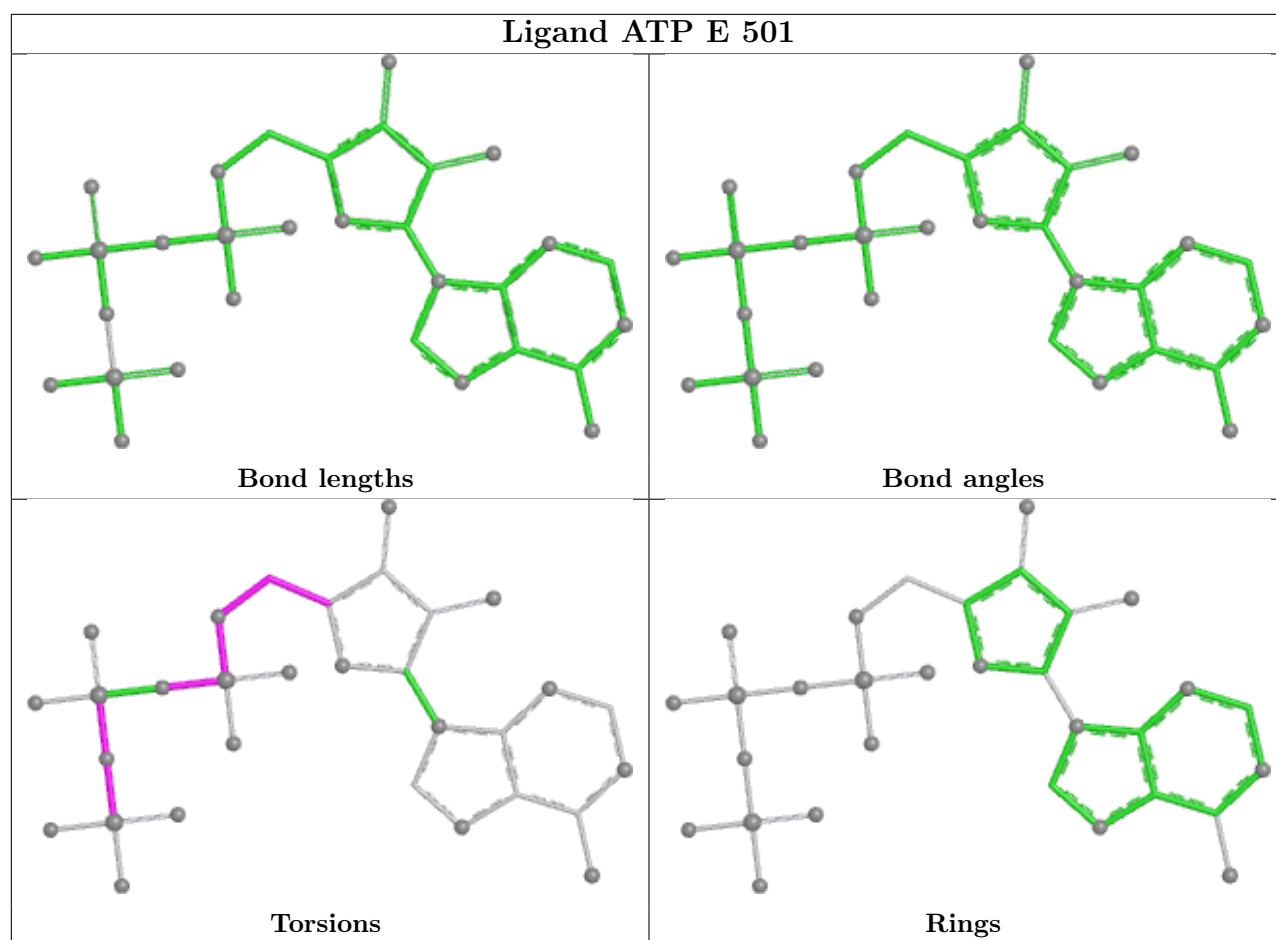
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

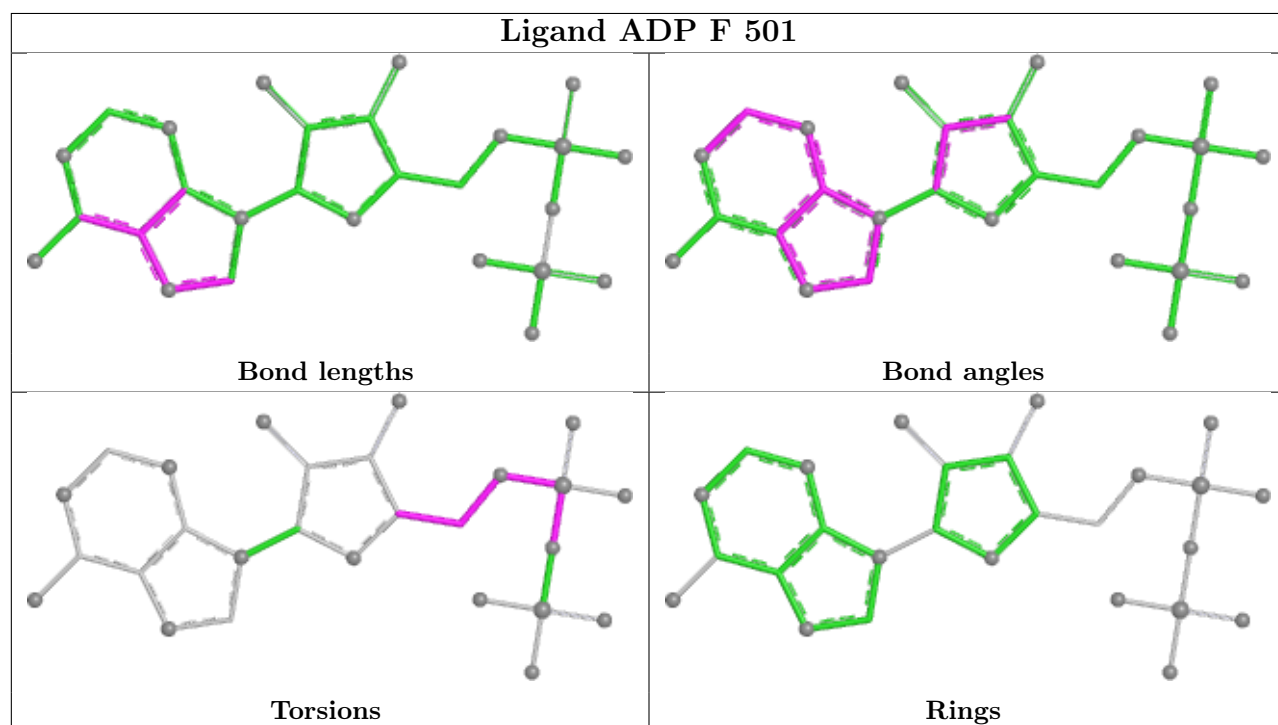
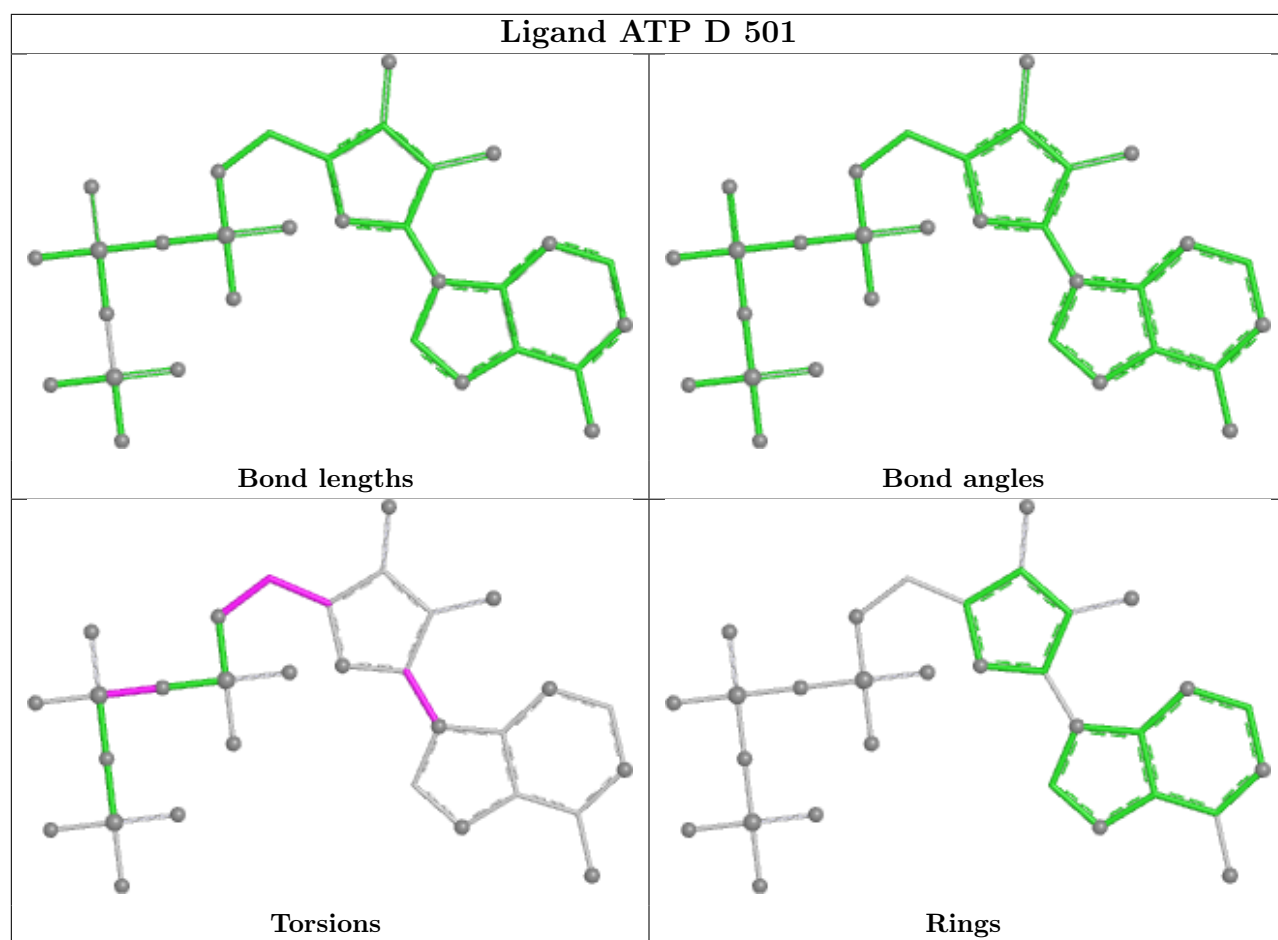
Ligand ATP C 501



Ligand ADP A 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.

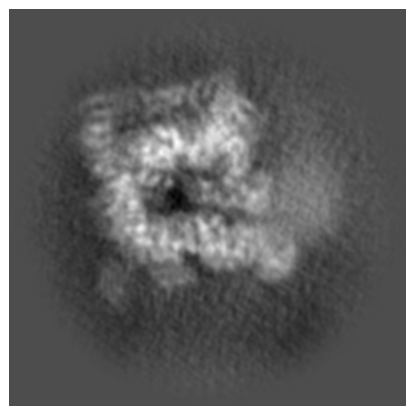
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63850. These allow visual inspection of the internal detail of the map and identification of artifacts.

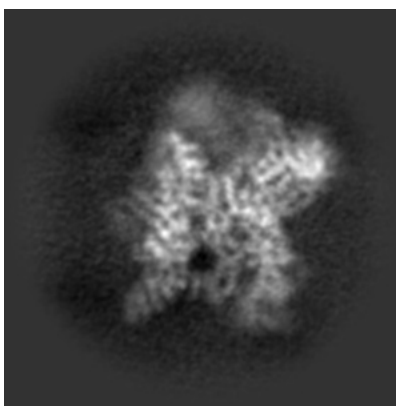
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

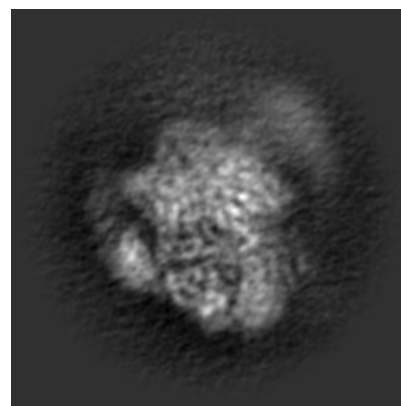
6.1.1 Primary map



X

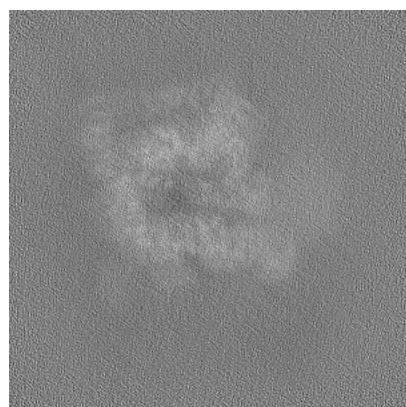


Y

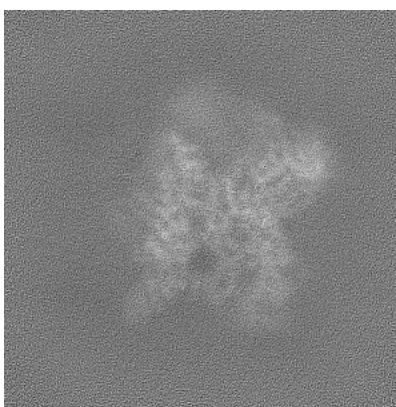


Z

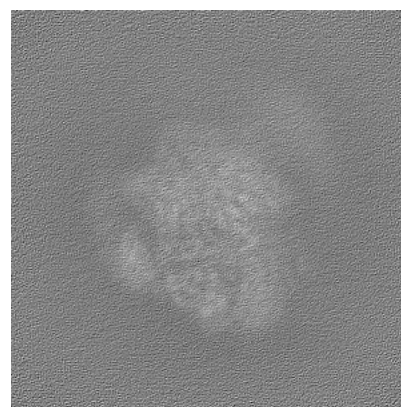
6.1.2 Raw map



X



Y

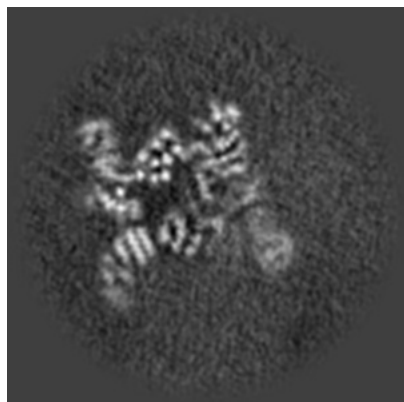


Z

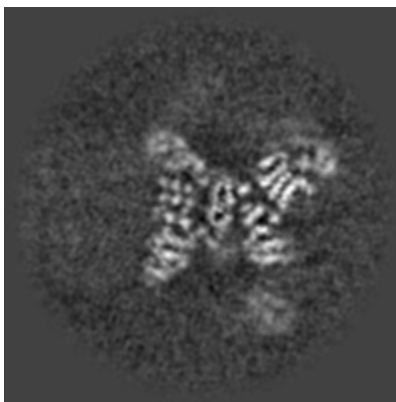
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

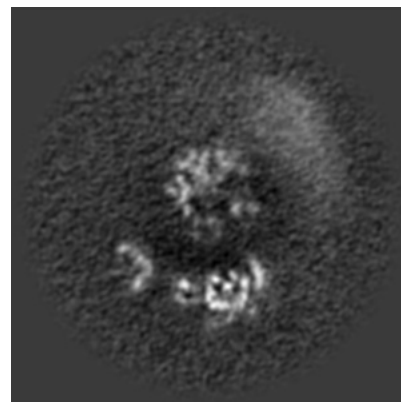
6.2.1 Primary map



X Index: 180

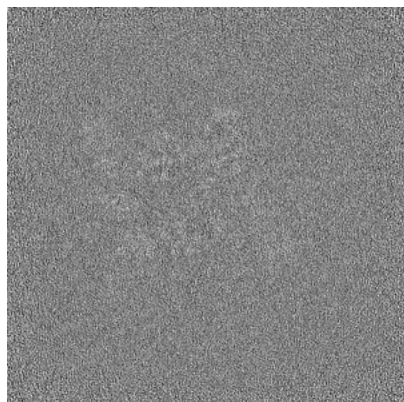


Y Index: 180

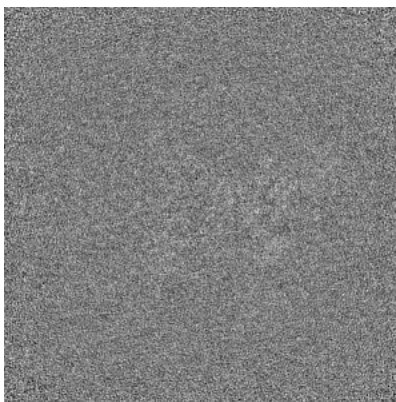


Z Index: 180

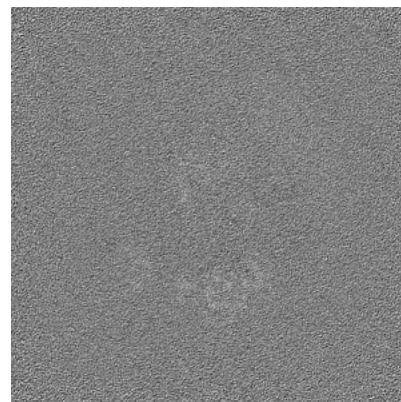
6.2.2 Raw map



X Index: 180



Y Index: 180

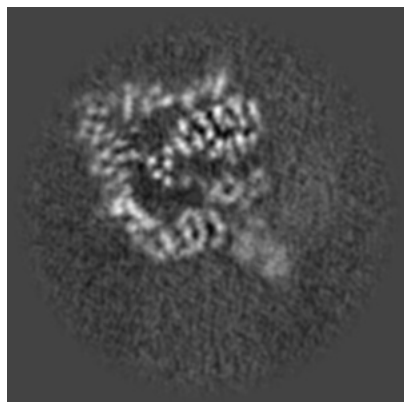


Z Index: 180

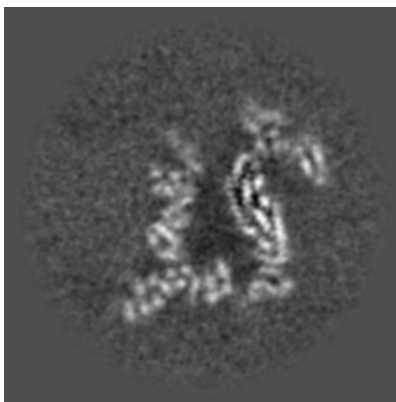
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

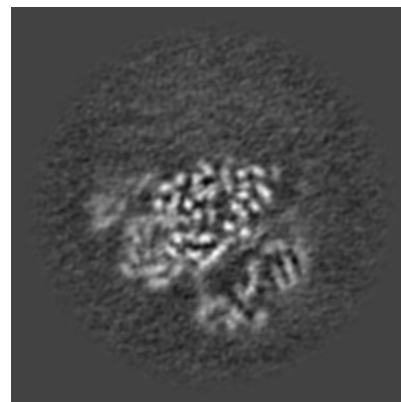
6.3.1 Primary map



X Index: 210

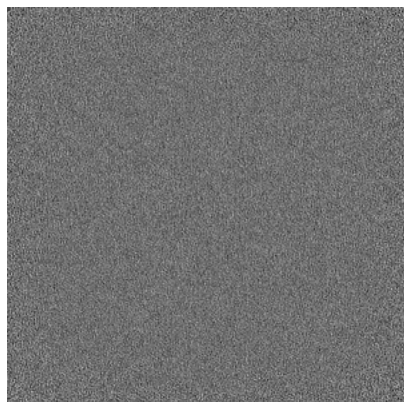


Y Index: 138

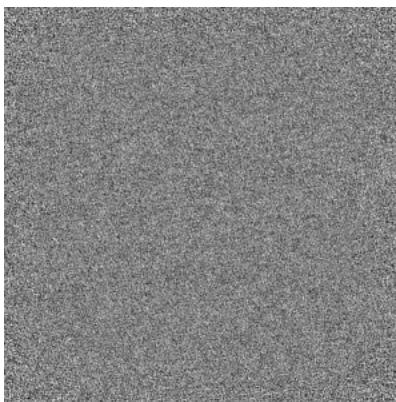


Z Index: 235

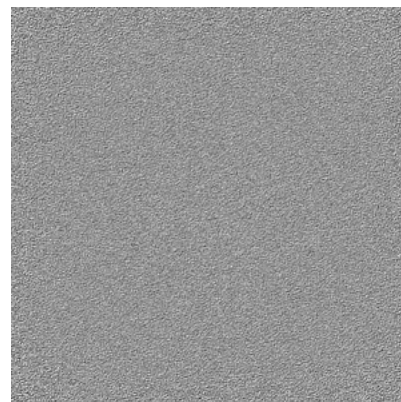
6.3.2 Raw map



X Index: 0



Y Index: 0

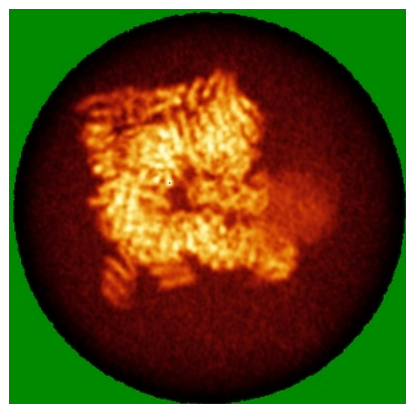


Z Index: 0

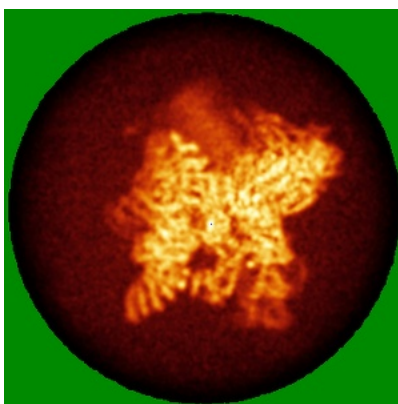
The images above show the largest variance slices of the map in three orthogonal directions.

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

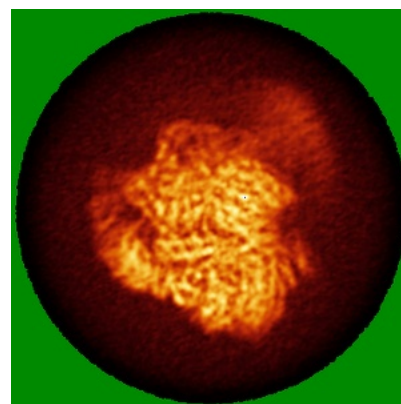
6.4.1 Primary map



X

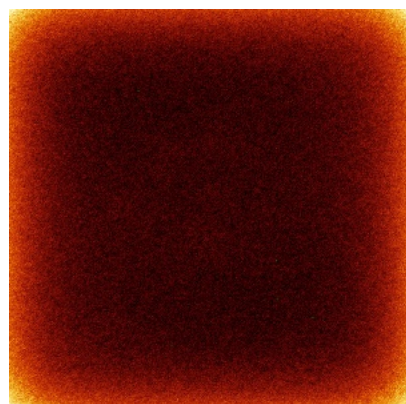


Y

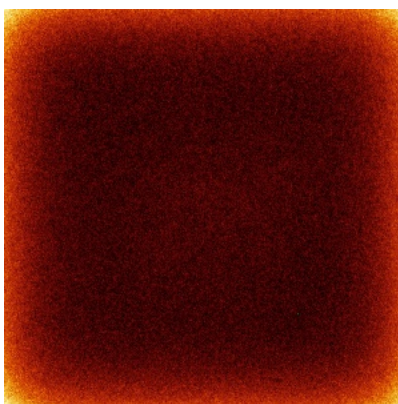


Z

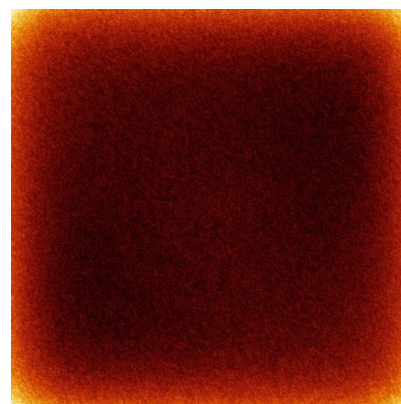
6.4.2 Raw map



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.

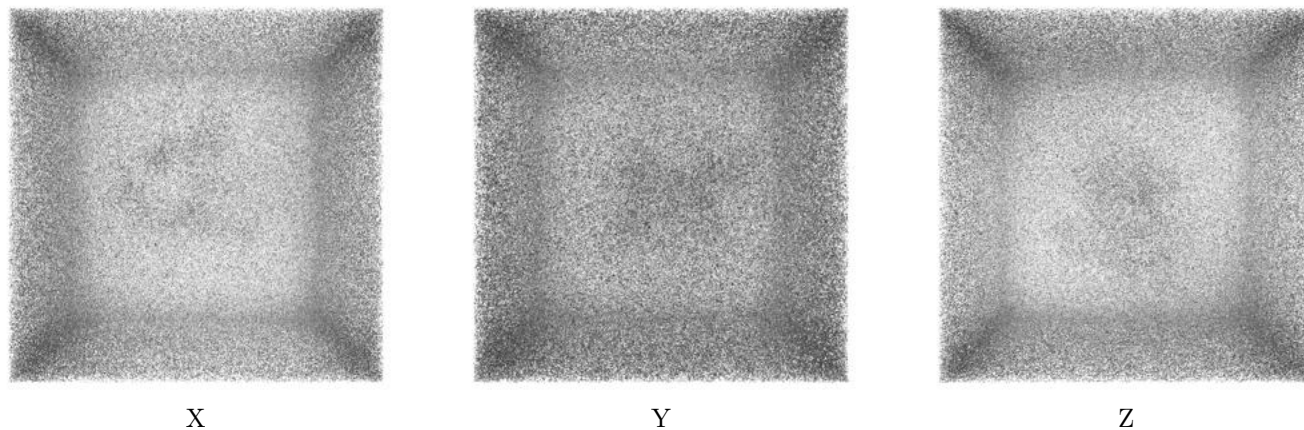
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

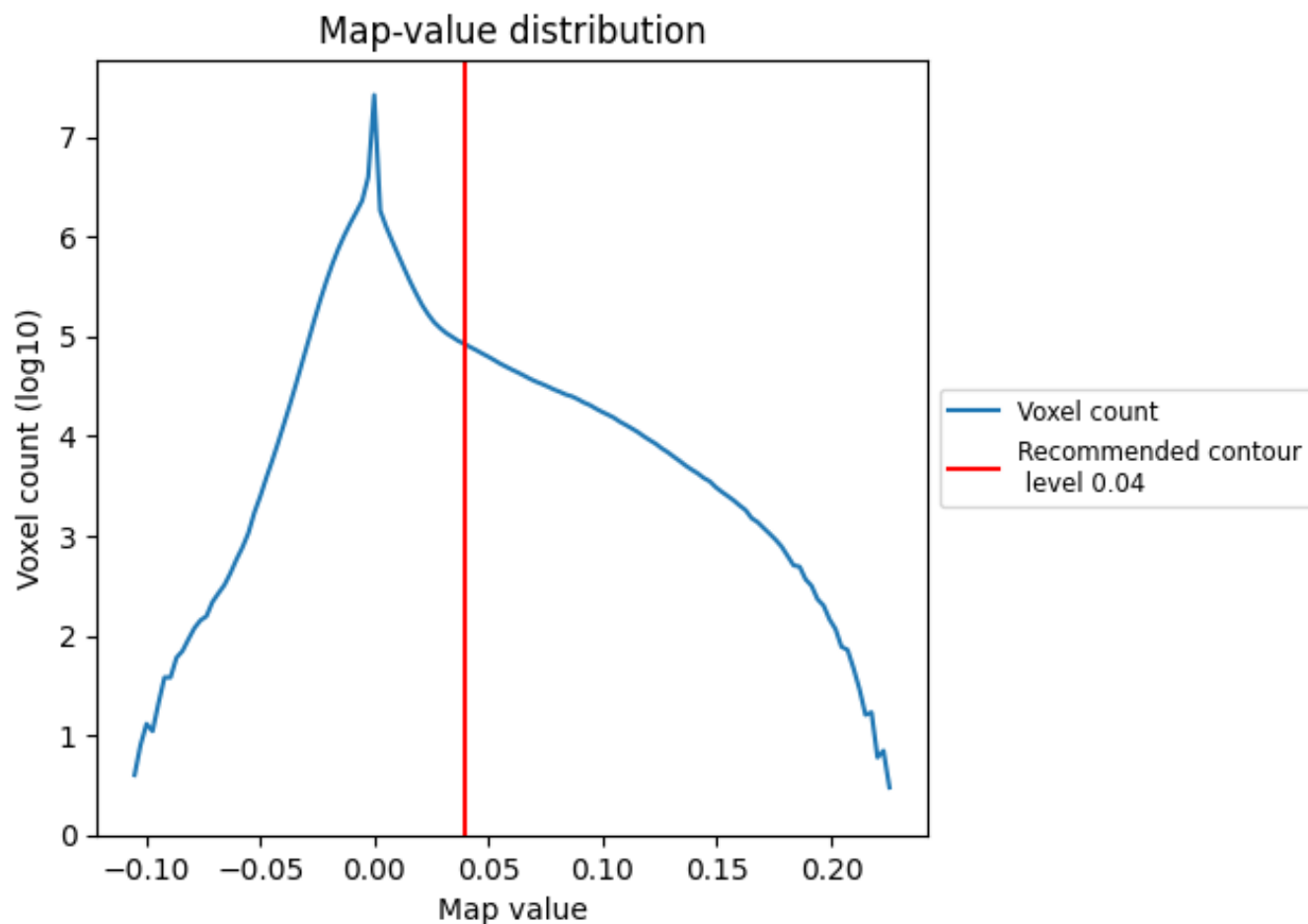
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

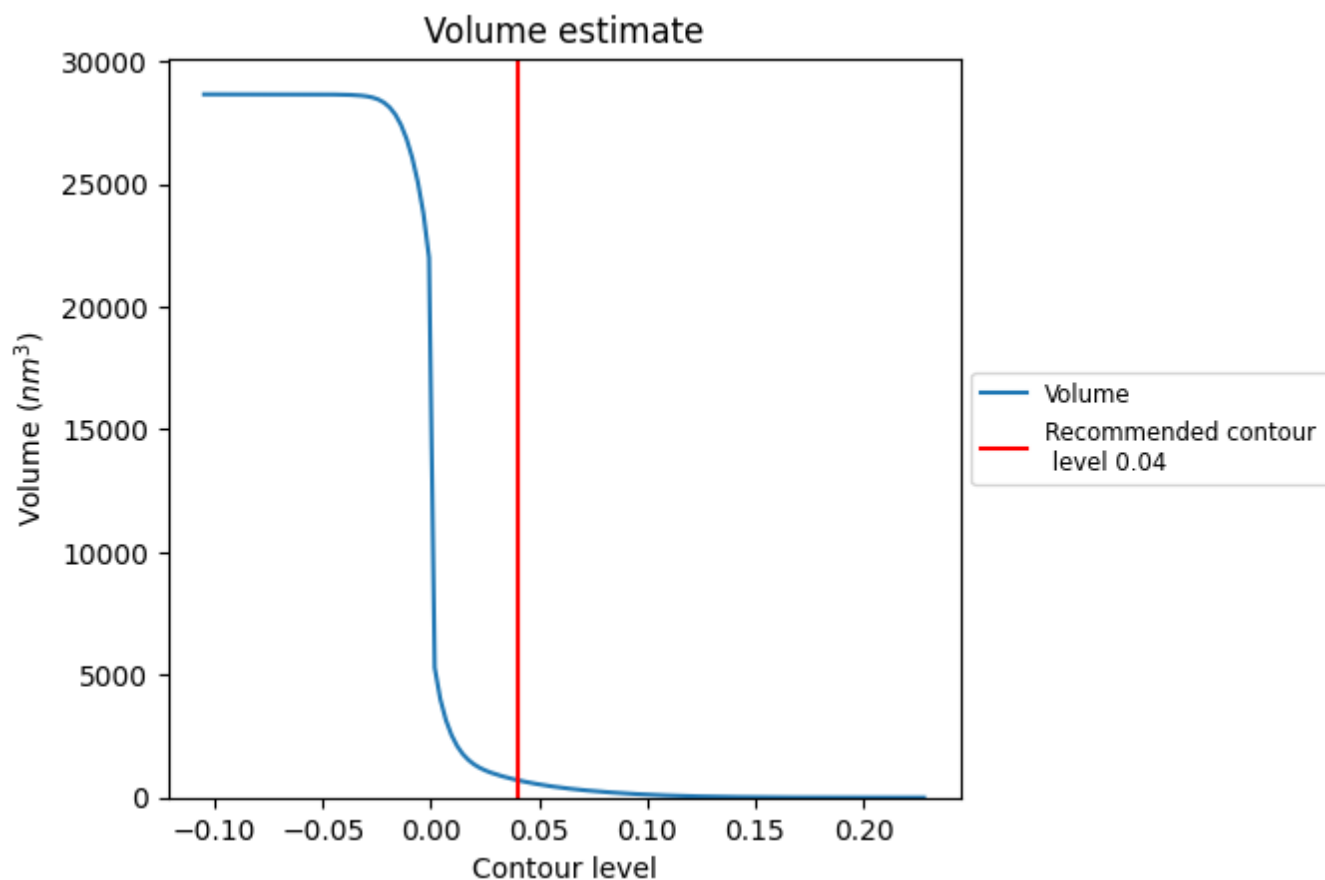
This section contains the results of statistical analysis of the map.

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.

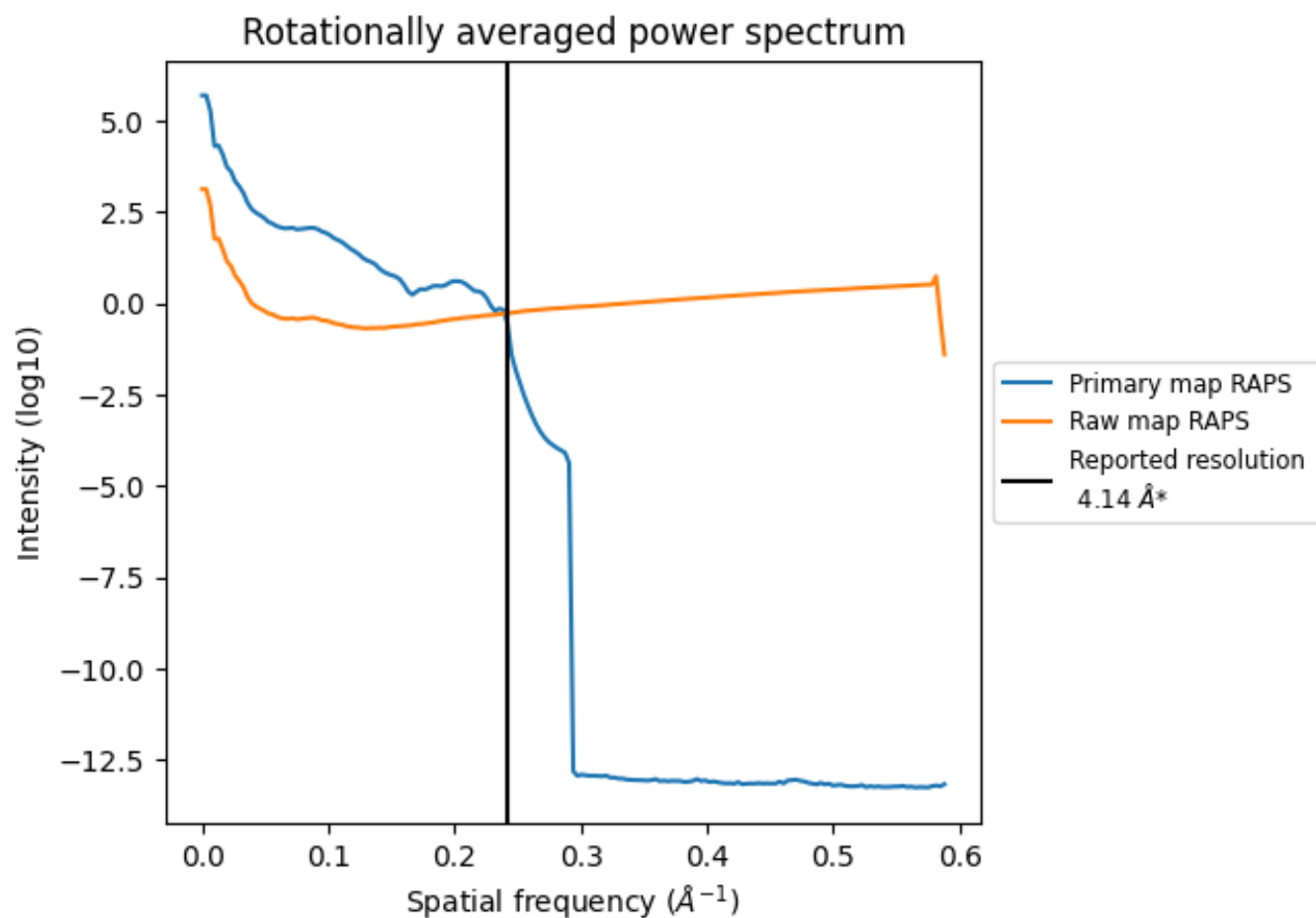
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 713 nm³; this corresponds to an approximate mass of 644 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](#)

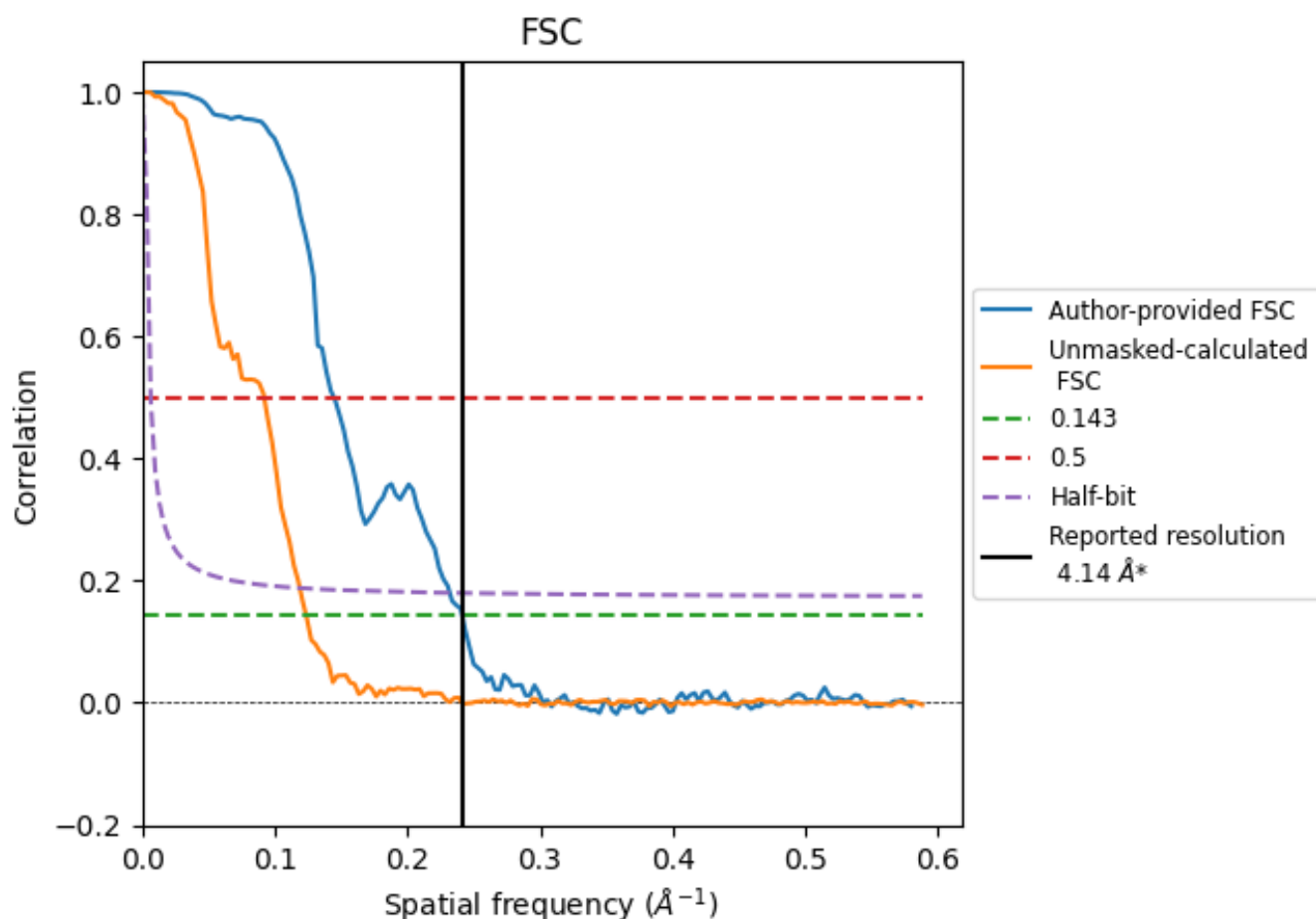


*Reported resolution corresponds to spatial frequency of 0.242 \AA^{-1}

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 0.242 \AA^{-1}

8.2 Resolution estimates [i](#)

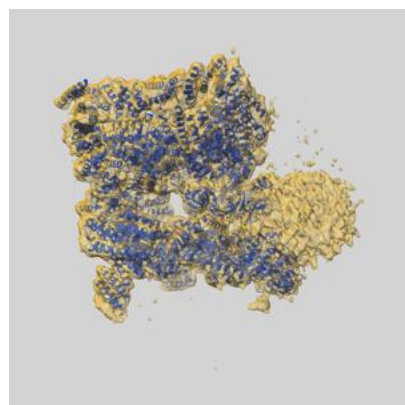
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	4.14	6.92	4.31
Unmasked-calculated*	8.09	10.88	8.41

*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 8.09 differs from the reported value 4.14 by more than 10 %

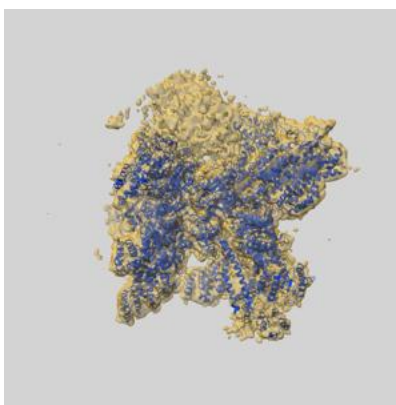
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63850 and PDB model 9U4M. Per-residue inclusion information can be found in section [3](#) on page [9](#).

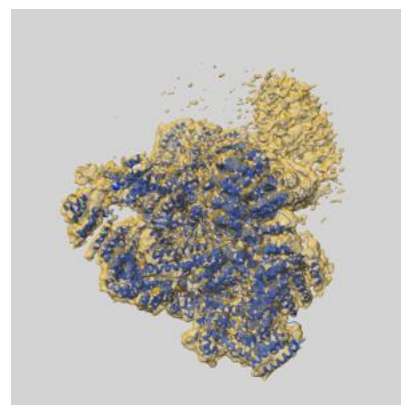
9.1 Map-model overlay [i](#)



X



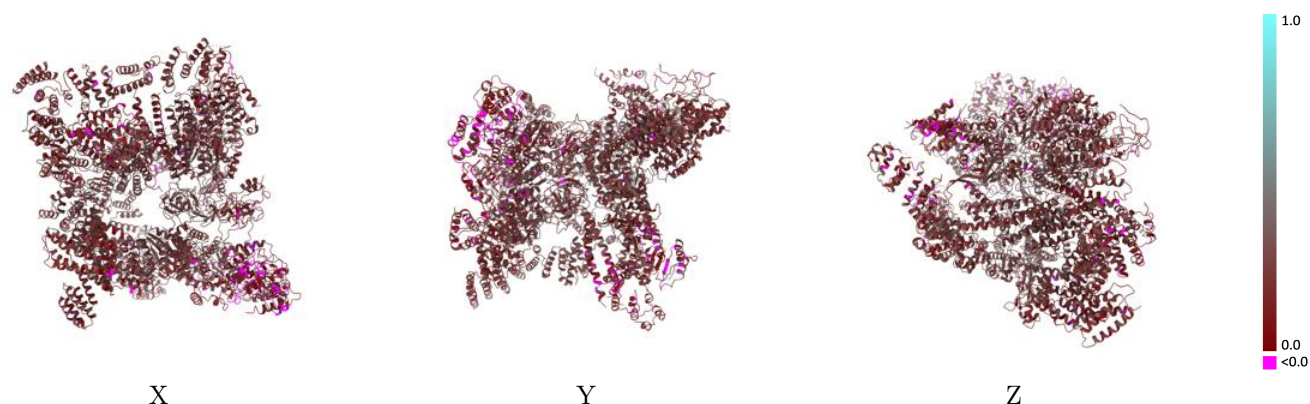
Y



Z

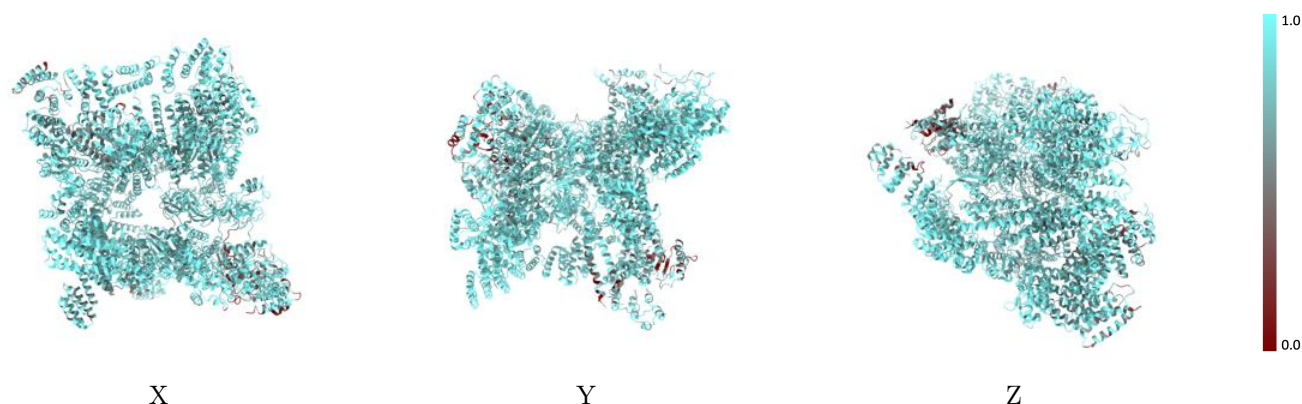
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



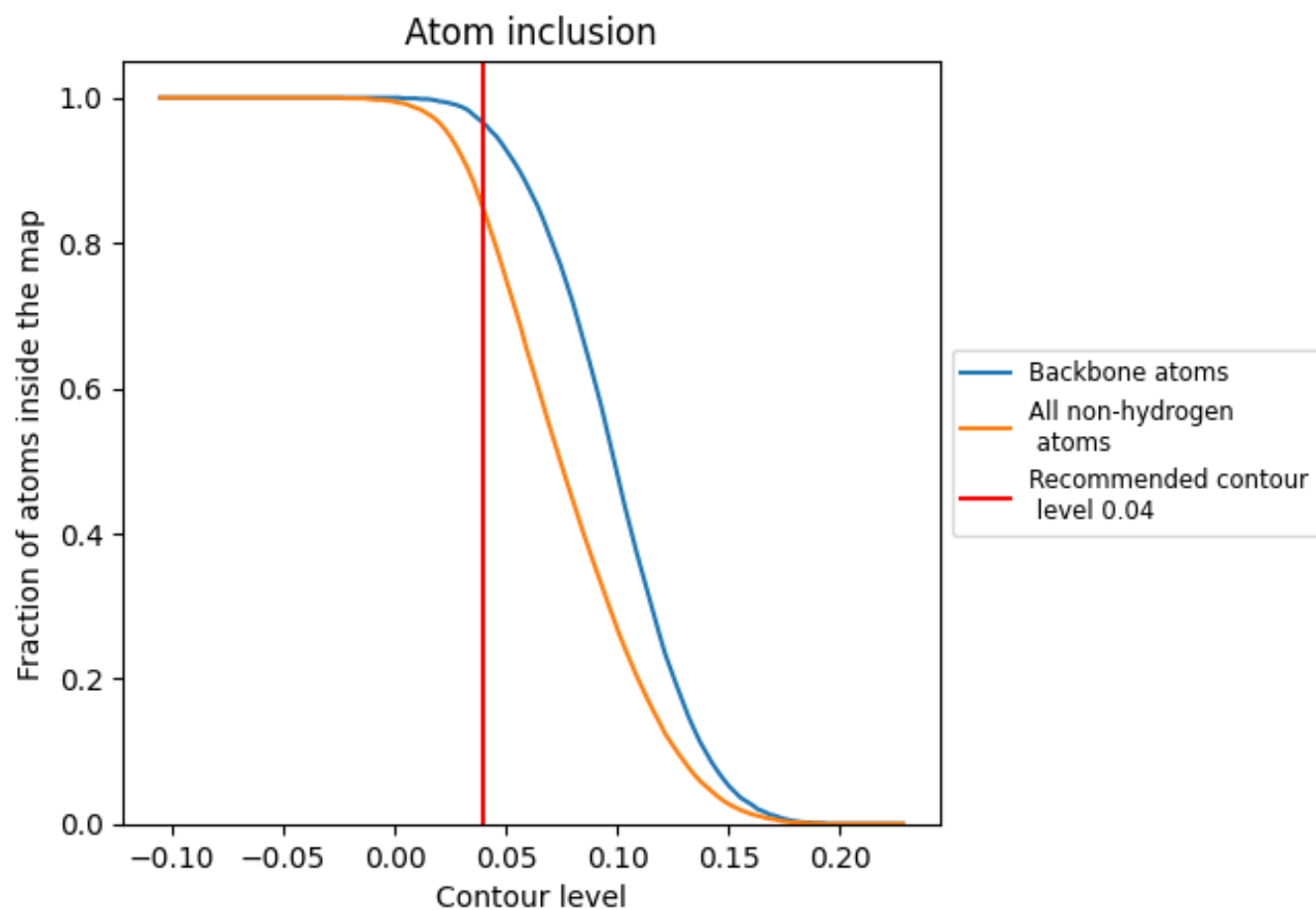
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 85% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.2270
A	 0.7940	 0.1610
B	 0.7150	 0.1340
C	 0.8710	 0.2440
D	 0.8540	 0.2710
E	 0.8520	 0.2580
F	 0.8690	 0.2330
U	 0.8930	 0.2440
V	 0.7890	 0.2160
W	 0.9100	 0.2200
X	 0.8490	 0.2450
Y	 0.9050	 0.2330
Z	 0.8640	 0.2290
a	 0.8530	 0.2010
b	 0.5640	 0.1650
c	 0.8950	 0.2740
d	 0.7980	 0.2310
e	 0.9400	 0.2780
v	 0.9750	 0.2730

