



wwPDB EM Validation Summary Report ⓘ

Jul 27, 2026 – 05:52 PM EDT

PDB ID : 9PRO / pdb_00009pro
EMDB ID : EMD-71810
Title : Human 19S proteasome bound to TXNL1 PITH domain and PSMD5
Authors : Chen, X.; Negi, H.; Walters, K.J.
Deposited on : 2025-07-24
Resolution : 4.07 Å(reported)
Based on initial models : ., 7WSI, 1WWY

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

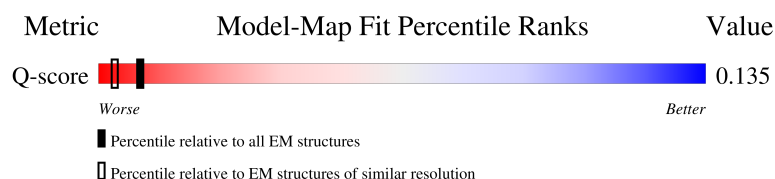
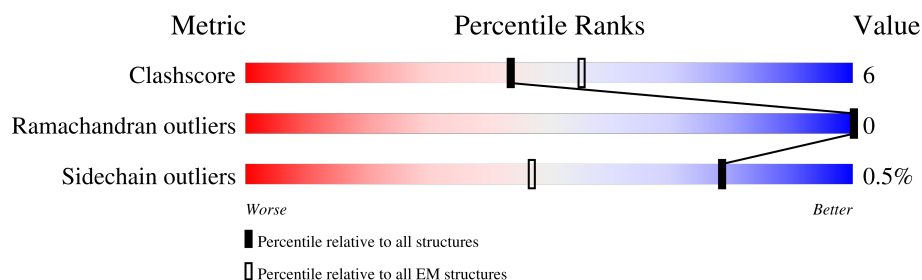
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.07 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.



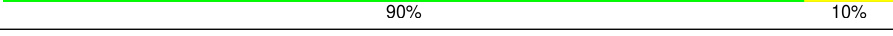
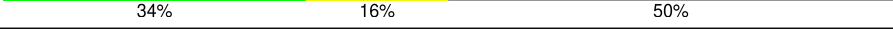
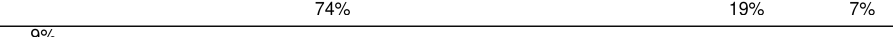
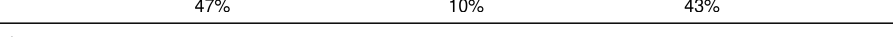
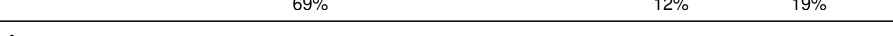
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6427 (3.58 - 4.57)

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	5% 69% 14% 17%
2	B	440	67% 17% 15%
3	C	406	69% 22% 9%
4	D	418	69% 18% 12%

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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	
20	z	504	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 57756 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 RPT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2833	1782	504	530	17		

- Molecule 2 is a protein called RPT2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	373	Total	C	N	O	S	0	0
			2948	1855	502	576	15		

- Molecule 3 is a protein called RPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	0
			2912	1831	523	541	17		

- Molecule 4 is a protein called RPT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	369	Total	C	N	O	S	0	0
			2935	1857	507	558	13		

- Molecule 5 is a protein called RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	380	Total	C	N	O	S	0	0
			3025	1900	542	567	16		

- Molecule 6 is a protein called RPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	374	Total	C	N	O	S	0	0
			2930	1845	506	561	18		

- Molecule 7 is a protein called RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	831	Total	C	N	O	S	0	0
			6472	4108	1099	1221	44		

- Molecule 8 is a protein called RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	463	Total	C	N	O	S	0	0
			3731	2370	665	683	13		

- Molecule 9 is a protein called RPN5.

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 RPN6.

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 RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 12 is a protein called RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

- Molecule 13 is a protein called RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

- Molecule 14 is a protein called RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	189	Total	C	N	O	S	0	0
			1449	905	259	277	8		

- Molecule 15 is a protein called RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	289	Total	C	N	O	S	0	0
			2272	1438	391	424	19		

- Molecule 16 is a protein called RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	265	Total	C	N	O	S	0	0
			2166	1402	355	400	9		

- Molecule 17 is a protein called DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 18 is a protein called RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	736	Total	C	N	O	S	0	0
			5695	3586	973	1096	40		

- Molecule 19 is a protein called TXNL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	173	Total	C	N	O	S	0	0
			1383	869	227	278	9		

- Molecule 20 is a protein called PSMD5.

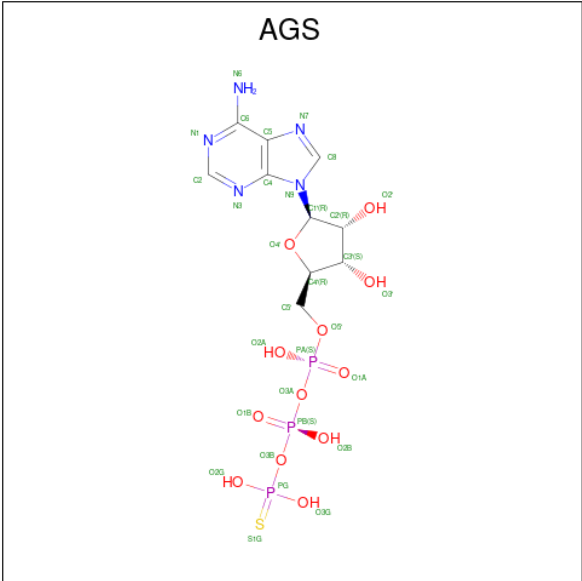
Mol	Chain	Residues	Atoms					AltConf	Trace
20	z	472	Total	C	N	O	S	0	0
			3704	2354	628	706	16		

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	C	1	Total	Mg	0
			1	1	
23	D	1	Total	Mg	0
			1	1	
23	E	1	Total	Mg	0
			1	1	

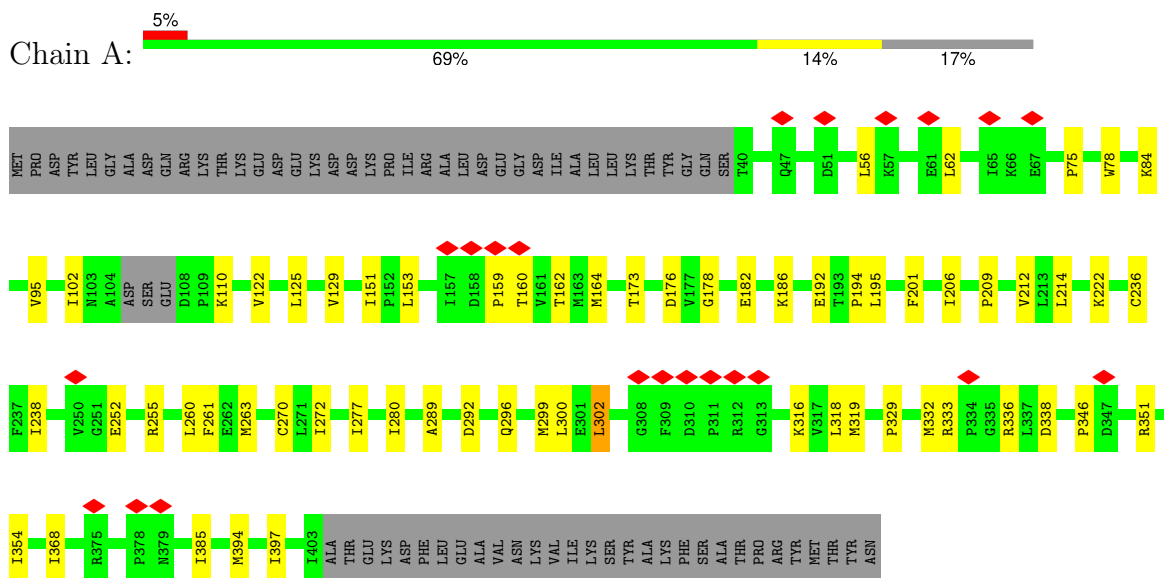
- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

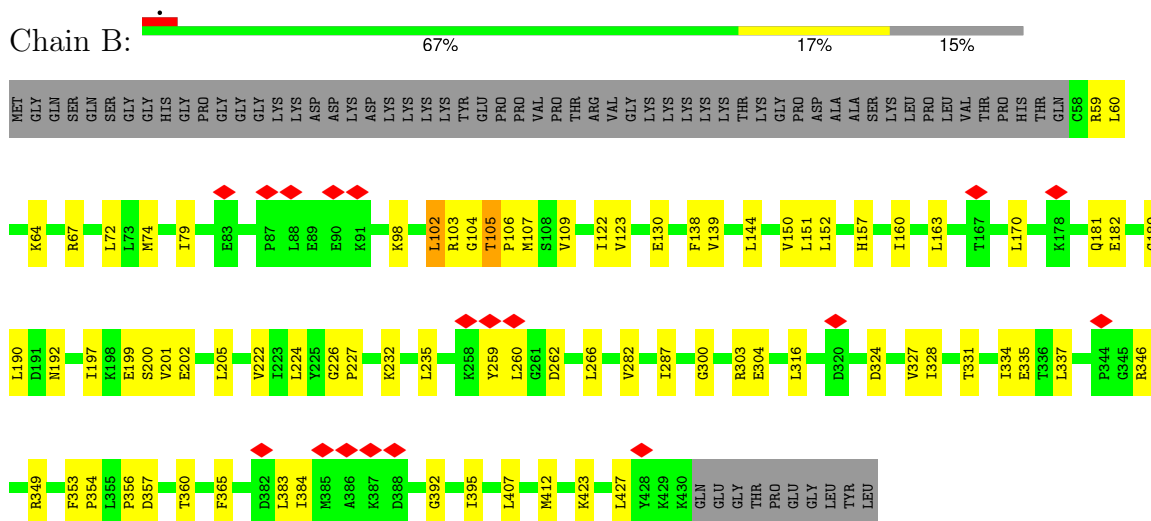
3 Residue-property plots

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: RPT1

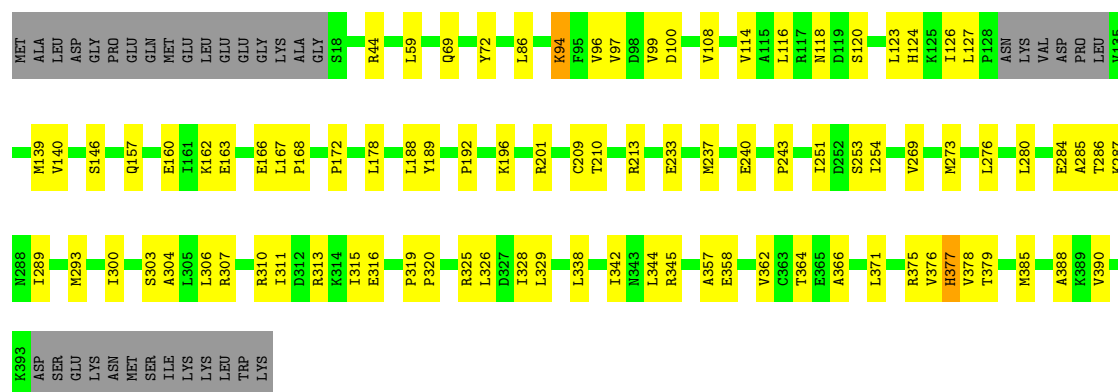


• Molecule 2: RPT2



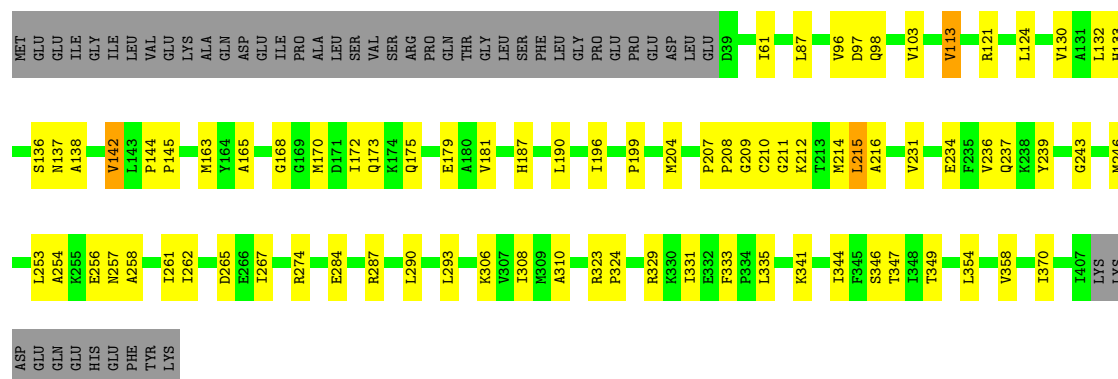
• Molecule 3: RPT6

Chain C: 



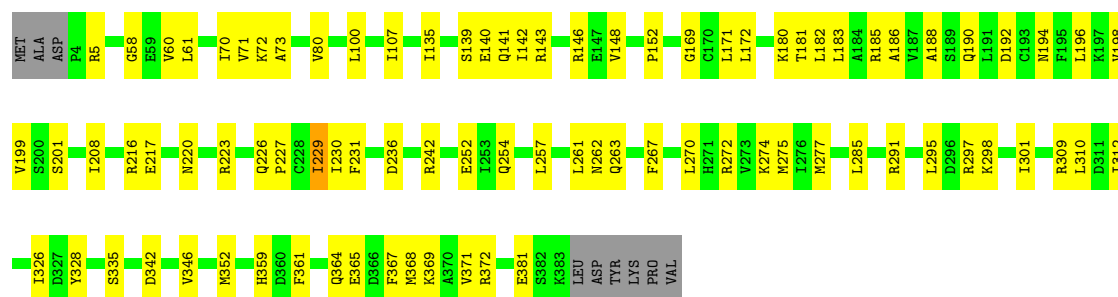
• Molecule 4: RPT3

Chain D: 



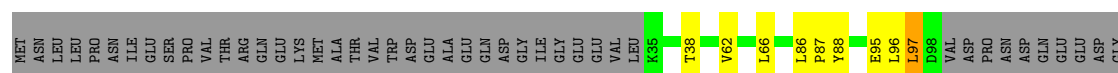
• Molecule 5: RPT4

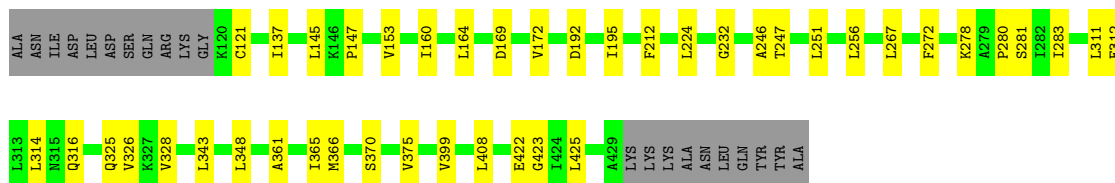
Chain E: 



• Molecule 6: RPT5

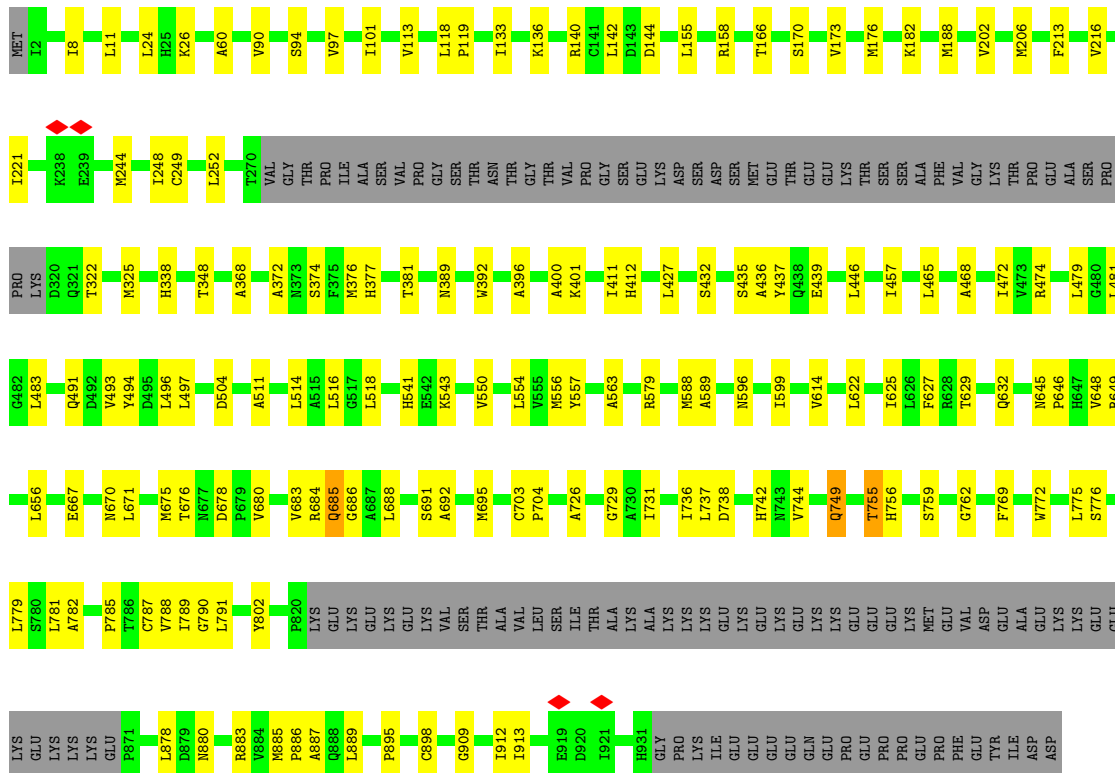
Chain F: 





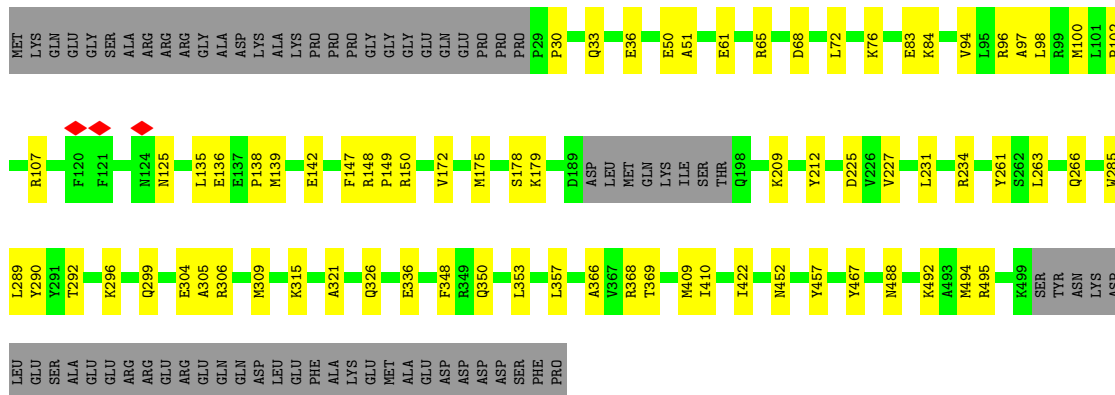
- Molecule 7: RPN2

Chain U: 71% 16% 13%

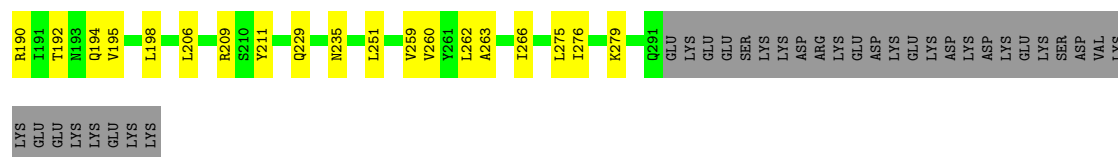


- Molecule 8: RPN3

Chain V: 73% 14% 13%

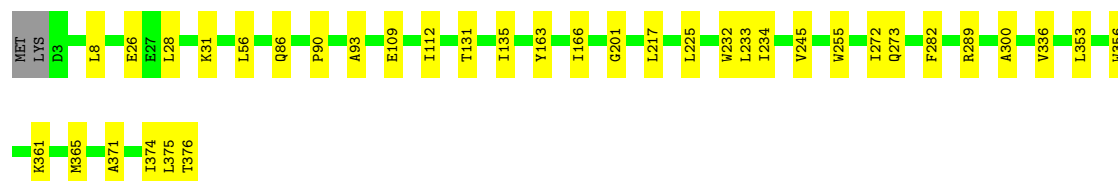


- Molecule 9: RPN5



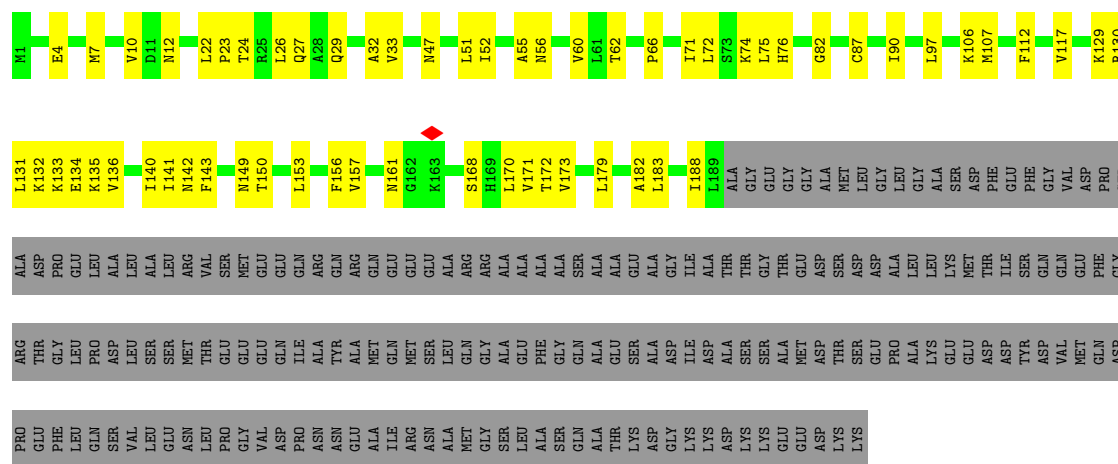
• Molecule 13: RPN9

Chain a: 90% 10%



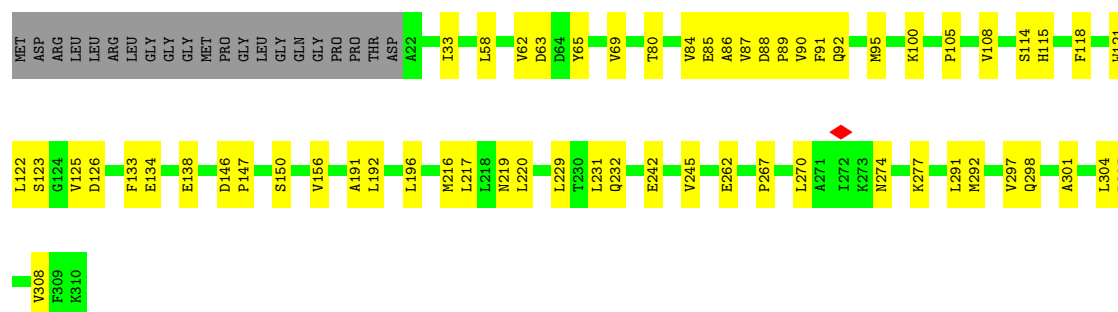
• Molecule 14: RPN10

Chain b: 34% 16% 50%



• Molecule 15: RPN11

Chain c: 74% 19% 7%



• Molecule 16: RPN12

Chain d: 9% 66% 10% 24%

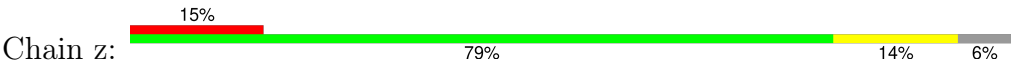


MET VAL VAL GLY VAL LYS PRO VAL GLY ASP ASP ASP PHE GLN PRO GLU LEU SER GLY ALA GLY SER ARG ARG LEU ALA VAL VAL LYS PHE THR MET ARG GLY CYS GLY CYS PRO CYS LEU ARG ILE ALA PRO PHE PHE SER MET SER ASN LYS TYR PRO GLY SER ALA VAL PHE LEU GLU VAL ASP

VAL HIS GLN CYS GLY THR ALA THR ASN TLE SER ALA THR PRO PHE LEU PHE PHE ASN LYS VAL ARG ILE LYS ASP GLN TYR GLN GLY ALA LYS ILE LYS HIS LEU GLU ASN ASP PRO GLY SER ASN GLU ASP T117 D118 I119 P120

L126 F129 I130 N131 L138 D153 L157 L166 I167 T168 V169 A170 K176 P185 D186 Q189 E222 Y235 Q239 T245 G253 E254 R259 I260 R280 E287 S288 H289

● Molecule 20: PSMD5



MET ALA ALA GLN ALA LEU LEU ARG GLU VAL ARG LEU LEU ALA HIS SER VAL LEU GLN ALA V32 P33 L34 N35 E36 L49 E55 N56 H57 R58 E59 K60 T61 T62 L63 C64 V65 S66 I67 R70 L71 L72 E76 P77

V80 L84 D87 P95 D96 K100 I101 L102 D115 I120 L126 I127 K128 Y132 N138 L139 S140 V141 Q156 L159 E164 L168 L171 I180 R184 V185 Y186 I189 S199 T204 T205 L208 V209 T210 Q211 L212 L213 R214 E215

L222 S233 L234 Q242 I250 P264 Y269 L270 P271 S285 P286 Q287 Q288 E291 R292 Y293 E298 K299 V300 I304 V314 D317 G320 I321 L322 G323 S324 N325 V326 Q333 T337 L342 I346 Q349 S350 A353 P354 L357 L362 D363

S367 F372 P373 E374 Q375 T377 D378 D379 L380 M383 W387 R393 R400 P406 K416 T419 F437 V438 E439 Y440 V441 V442 E458 L459 V460 K461 A462 L463 A464 M465 I469 A470 E471 I472 F473 G474 M475 P476 M477 Y478 L479 R480 L481 R482 T483 T497

T498 E501 G502 A503 GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54253	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	0.194	Depositor
Minimum map value	-0.073	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.01	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: ZN, MG, AGS, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/2878	0.69	0/3884
2	B	0.40	0/2989	0.73	0/4028
3	C	0.50	0/2949	0.82	0/3964
4	D	0.52	0/2982	0.77	0/4027
5	E	0.45	0/3071	0.76	0/4131
6	F	0.39	0/2967	0.68	0/3997
7	U	0.34	0/6589	0.71	0/8922
8	V	0.25	0/3803	0.58	0/5134
9	W	0.33	0/3612	0.69	0/4858
10	X	0.36	0/855	0.57	0/1150
11	Y	0.37	0/3173	0.69	0/4273
12	Z	0.31	0/2333	0.59	0/3162
13	a	0.26	0/3061	0.56	0/4144
14	b	0.52	0/1469	0.79	0/1989
15	c	0.34	0/2315	0.68	0/3129
16	d	0.26	0/2212	0.60	0/2988
17	e	0.26	0/338	0.58	0/450
18	f	0.28	0/5776	0.59	0/7791
19	g	0.25	0/1410	0.55	0/1902
20	z	0.29	0/3768	0.56	0/5111
All	All	0.36	0/58550	0.67	0/79034

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	2833	0	2894	42	0
2	B	2948	0	3012	57	0
3	C	2912	0	3023	62	0
4	D	2935	0	2982	64	0
5	E	3025	0	3101	59	0
6	F	2930	0	3023	31	0
7	U	6472	0	6494	98	0
8	V	3731	0	3780	43	0
9	W	3564	0	3685	37	0
10	X	844	0	886	10	0
11	Y	3115	0	3120	32	0
12	Z	2290	0	2320	39	0
13	a	3003	0	3016	22	0
14	b	1449	0	1497	43	0
15	c	2272	0	2288	42	0
16	d	2166	0	2196	19	0
17	e	334	0	294	5	0
18	f	5695	0	5718	63	0
19	g	1383	0	1331	15	0
20	z	3704	0	3762	42	0
21	A	27	0	12	3	0
21	F	27	0	12	1	0
22	C	31	0	12	0	0
22	D	31	0	12	4	0
22	E	31	0	12	0	0
23	C	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
24	c	1	0	0	0	0
All	All	57756	0	58482	751	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 751 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)
14:b:140:ILE:HG21	14:b:153:LEU:HB3	1.67	0.75
12:Z:195:VAL:HG21	13:a:375:LEU:HD11	1.69	0.74
4:D:231:VAL:HG13	5:E:262:ASN:HD21	1.56	0.70
10:X:354:ILE:HG22	10:X:356:LEU:HB2	1.74	0.69
7:U:749:GLN:HA	7:U:755:THR:HA	1.75	0.68

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	357/433 (82%)	315 (88%)	42 (12%)	0	100	100
2	B	371/440 (84%)	326 (88%)	45 (12%)	0	100	100
3	C	366/406 (90%)	330 (90%)	36 (10%)	0	100	100
4	D	367/418 (88%)	339 (92%)	28 (8%)	0	100	100
5	E	378/389 (97%)	356 (94%)	22 (6%)	0	100	100
6	F	370/439 (84%)	345 (93%)	25 (7%)	0	100	100
7	U	825/953 (87%)	756 (92%)	69 (8%)	0	100	100
8	V	459/534 (86%)	428 (93%)	31 (7%)	0	100	100
9	W	435/456 (95%)	406 (93%)	29 (7%)	0	100	100
10	X	103/422 (24%)	101 (98%)	2 (2%)	0	100	100
11	Y	376/389 (97%)	346 (92%)	30 (8%)	0	100	100
12	Z	285/324 (88%)	275 (96%)	10 (4%)	0	100	100
13	a	372/376 (99%)	361 (97%)	11 (3%)	0	100	100
14	b	187/377 (50%)	165 (88%)	22 (12%)	0	100	100
15	c	287/310 (93%)	268 (93%)	19 (7%)	0	100	100
16	d	263/350 (75%)	244 (93%)	19 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	e	36/70 (51%)	30 (83%)	6 (17%)	0	100	100
18	f	716/908 (79%)	650 (91%)	66 (9%)	0	100	100
19	g	171/289 (59%)	158 (92%)	13 (8%)	0	100	100
20	z	470/504 (93%)	443 (94%)	27 (6%)	0	100	100
All	All	7194/8787 (82%)	6642 (92%)	552 (8%)	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	310/372 (83%)	308 (99%)	2 (1%)	78	81
2	B	331/385 (86%)	327 (99%)	4 (1%)	63	73
3	C	321/352 (91%)	317 (99%)	4 (1%)	63	73
4	D	322/366 (88%)	317 (98%)	5 (2%)	55	70
5	E	333/341 (98%)	331 (99%)	2 (1%)	78	81
6	F	323/379 (85%)	321 (99%)	2 (1%)	78	81
7	U	707/816 (87%)	702 (99%)	5 (1%)	76	79
8	V	400/460 (87%)	400 (100%)	0	100	100
9	W	402/416 (97%)	401 (100%)	1 (0%)	87	87
10	X	97/362 (27%)	97 (100%)	0	100	100
11	Y	334/344 (97%)	334 (100%)	0	100	100
12	Z	258/295 (88%)	258 (100%)	0	100	100
13	a	334/336 (99%)	334 (100%)	0	100	100
14	b	167/312 (54%)	166 (99%)	1 (1%)	78	81
15	c	253/268 (94%)	249 (98%)	4 (2%)	55	70
16	d	235/294 (80%)	235 (100%)	0	100	100
17	e	38/63 (60%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	f	620/763 (81%)	620 (100%)	0	100	100
19	g	157/253 (62%)	157 (100%)	0	100	100
20	z	417/441 (95%)	414 (99%)	3 (1%)	76	79
All	All	6359/7618 (84%)	6326 (100%)	33 (0%)	78	82

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	c	90	VAL
15	c	298	GLN
20	z	215	GLU
4	D	215	LEU
4	D	142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
13	a	72	ASN
18	f	198	HIS
13	a	144	ASN
14	b	149	ASN
18	f	371	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	ADP	A	501	-	28,29,29	1.41	5 (17%)	43,45,45	1.98	9 (20%)
22	AGS	E	501	23	32,33,33	0.67	1 (3%)	45,52,52	0.58	0
22	AGS	C	501	23	32,33,33	0.65	1 (3%)	45,52,52	0.53	0
21	ADP	F	501	-	28,29,29	0.45	0	43,45,45	0.49	0
22	AGS	D	501	23	32,33,33	0.68	1 (3%)	45,52,52	0.50	0

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	ADP	A	501	-	-	5/16/32/32	0/3/3/3
22	AGS	E	501	23	-	3/21/38/38	0/3/3/3
22	AGS	C	501	23	-	2/21/38/38	0/3/3/3
21	ADP	F	501	-	-	3/16/32/32	0/3/3/3
22	AGS	D	501	23	-	2/21/38/38	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)
21	A	501	ADP	C5-C4	4.56	1.47	1.39
21	A	501	ADP	C5-N7	-2.65	1.34	1.39
21	A	501	ADP	C5-C6	2.41	1.47	1.41
21	A	501	ADP	PA-O3A	2.31	1.62	1.59
22	D	501	AGS	PG-S1G	2.14	1.95	1.90

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	501	ADP	C5-C4-N3	-6.59	117.65	126.72
21	A	501	ADP	N3-C4-N9	5.53	136.58	127.17
21	A	501	ADP	C2-N3-C4	3.93	121.43	111.83
21	A	501	ADP	N3-C2-N1	-3.19	123.75	128.58
21	A	501	ADP	C4-C5-N7	-2.88	107.29	110.58

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

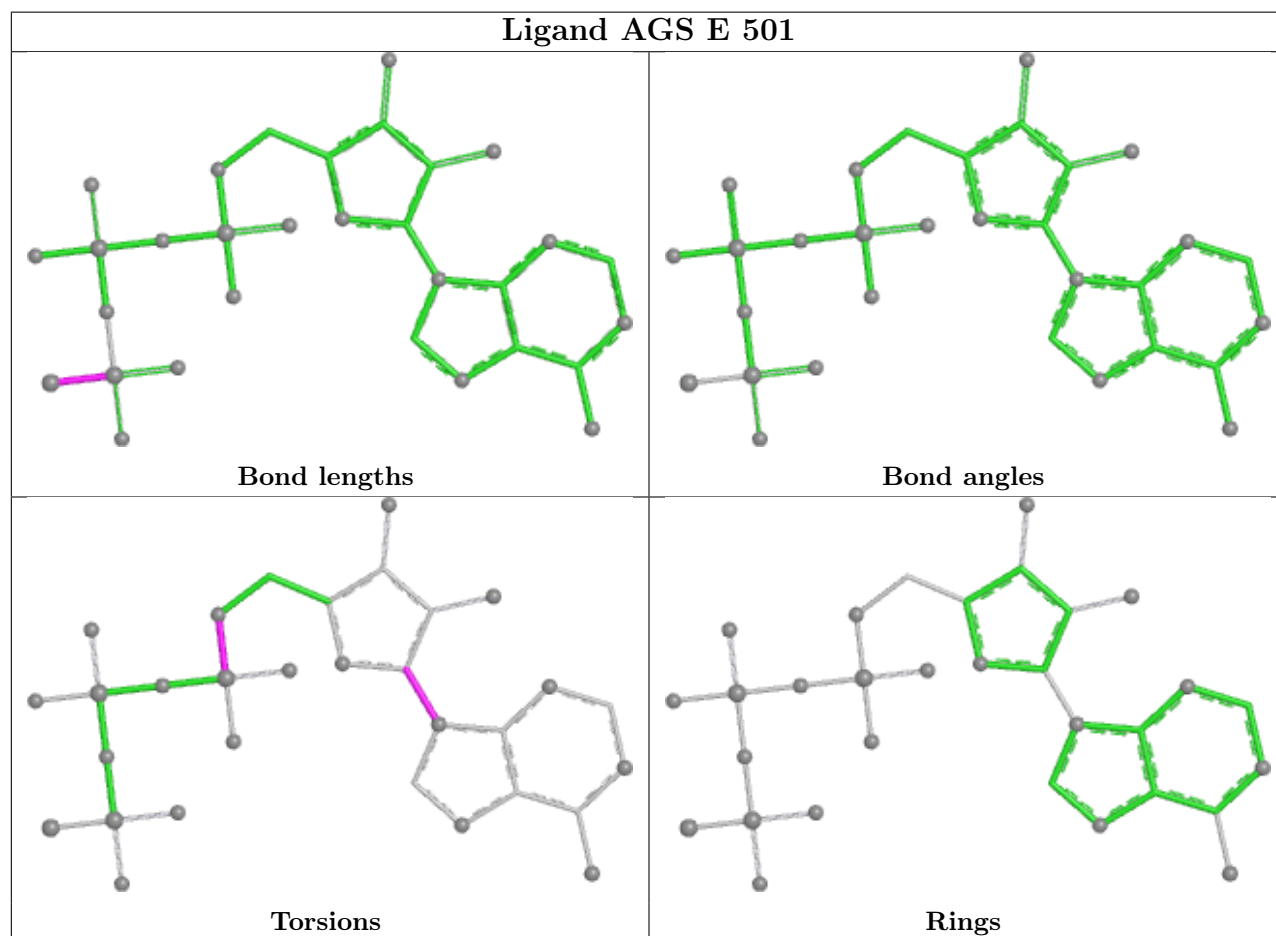
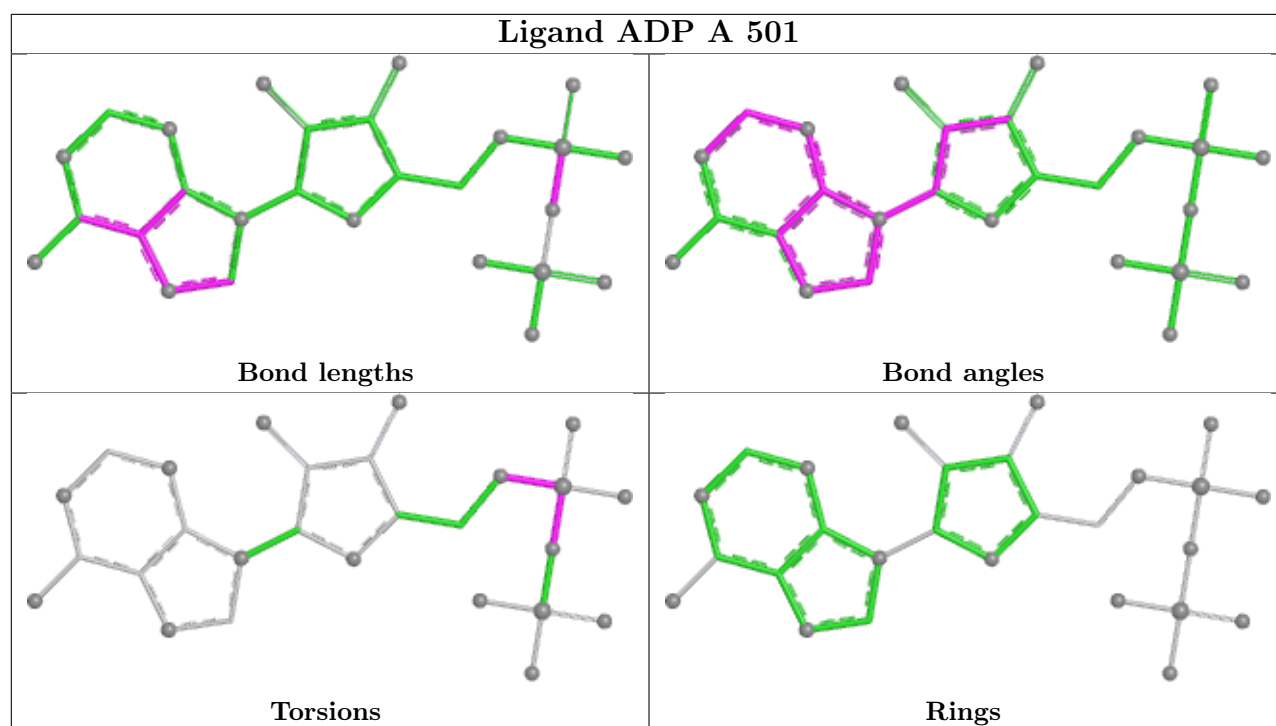
Mol	Chain	Res	Type	Atoms
21	A	501	ADP	C5'-O5'-PA-O1A
21	A	501	ADP	C5'-O5'-PA-O2A
21	A	501	ADP	C5'-O5'-PA-O3A
22	D	501	AGS	PB-O3A-PA-O5'
22	E	501	AGS	C5'-O5'-PA-O2A

There are no ring outliers.

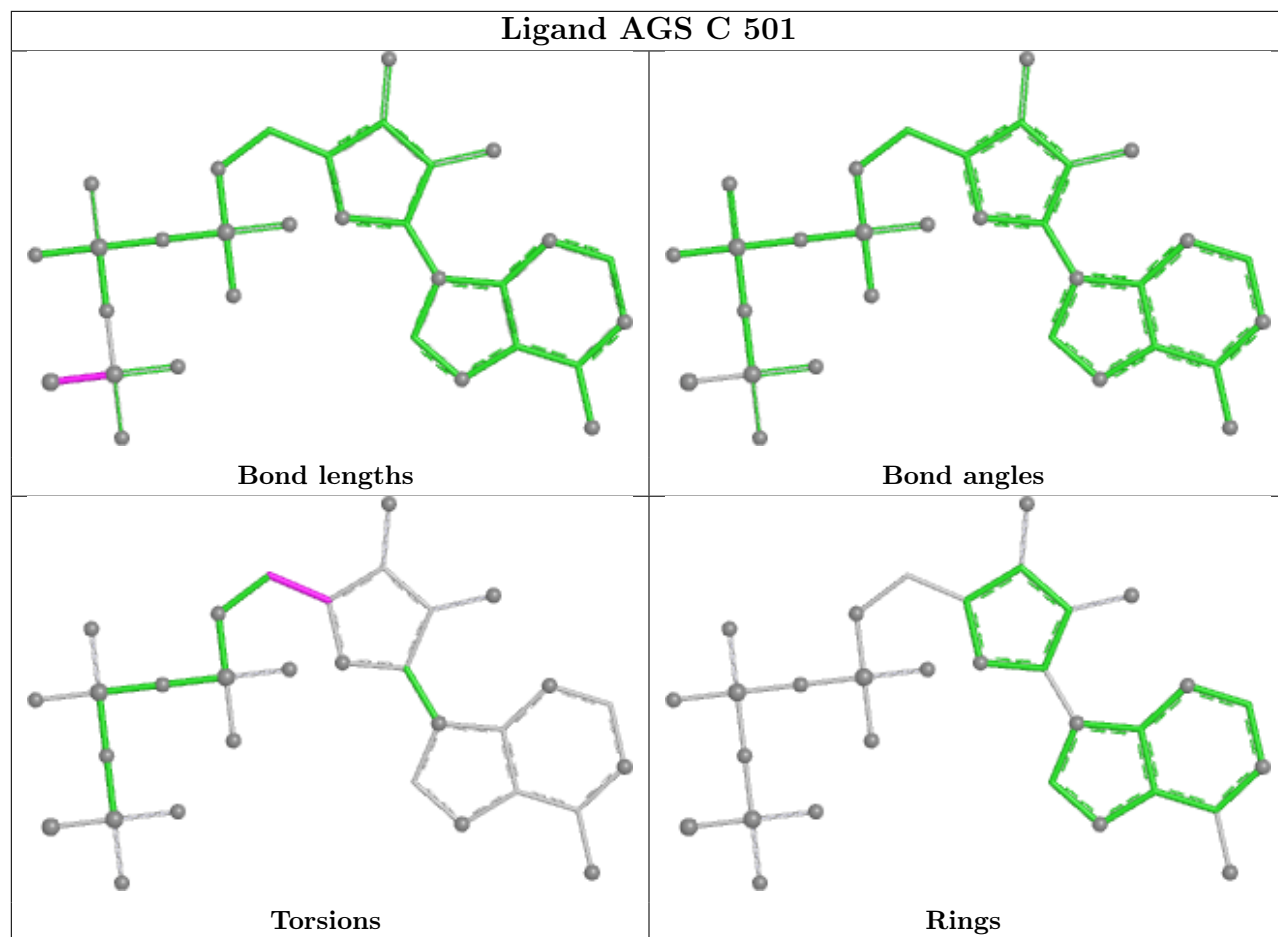
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	501	ADP	3	0
21	F	501	ADP	1	0
22	D	501	AGS	4	0

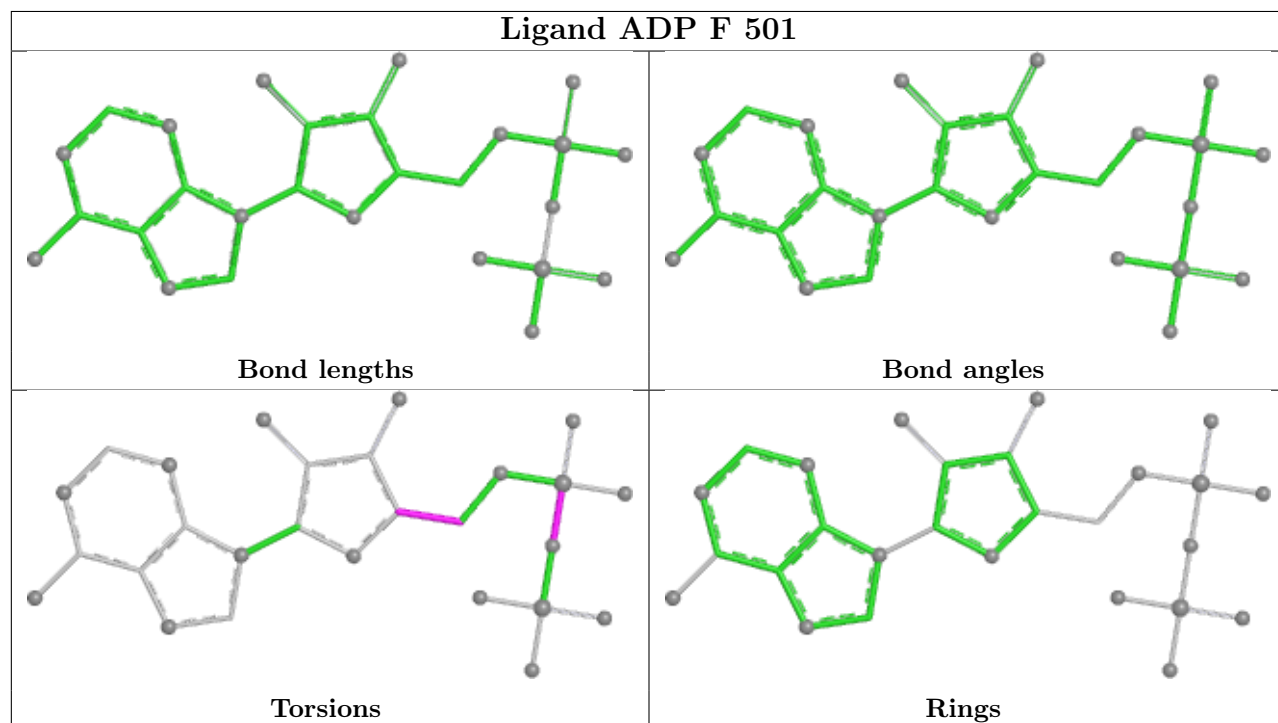
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

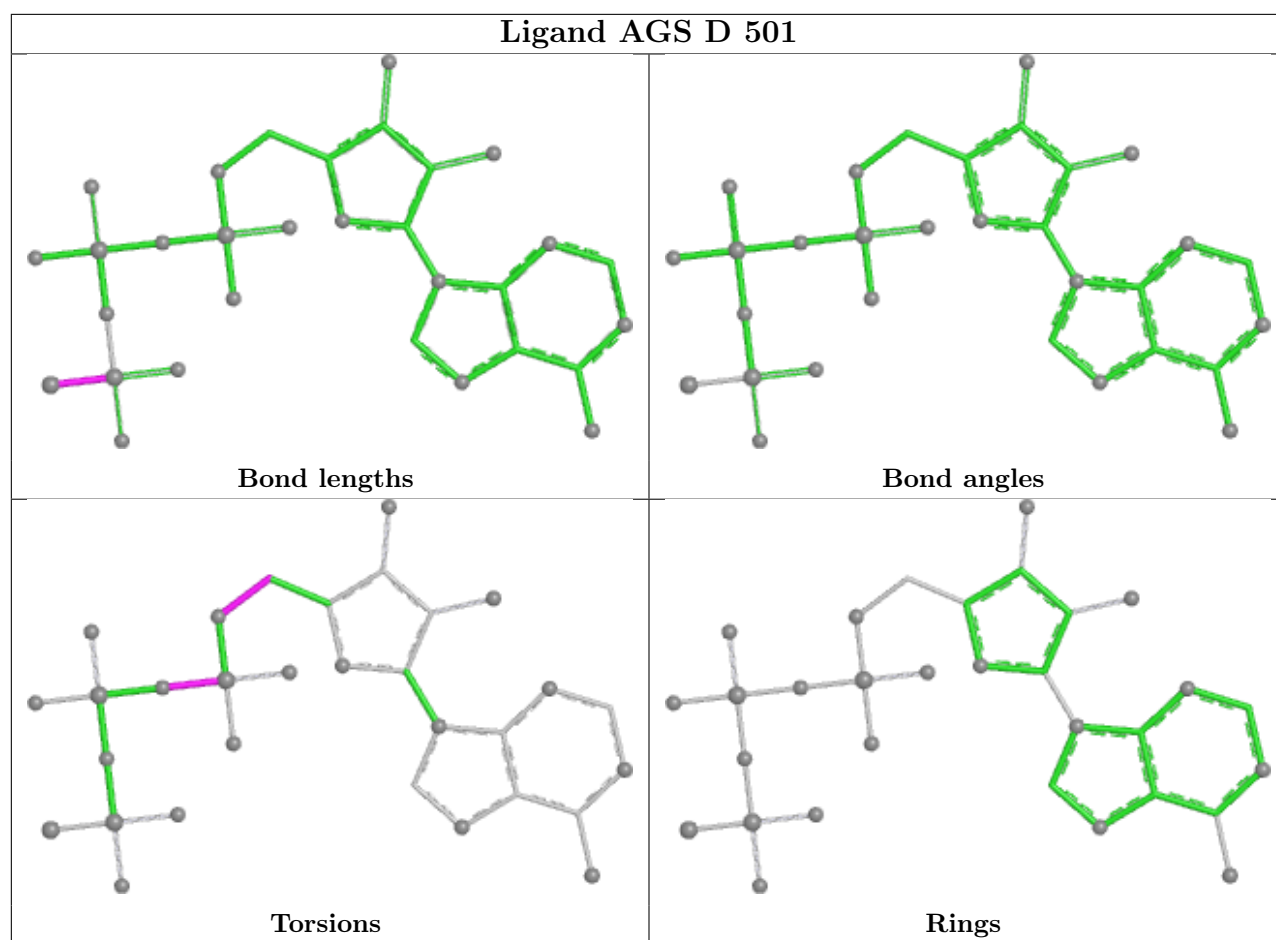


Ligand AGS C 501



Ligand ADP F 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.

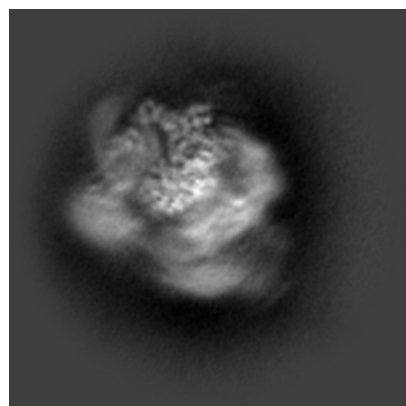
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71810. These allow visual inspection of the internal detail of the map and identification of artifacts.

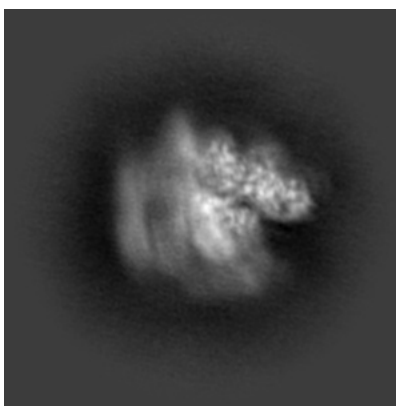
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

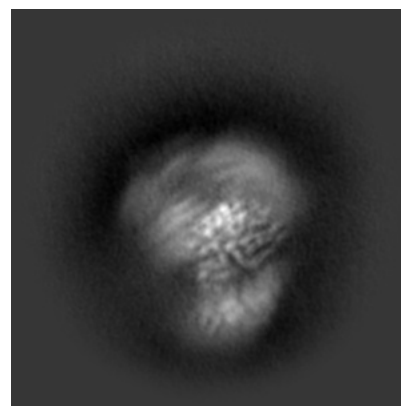
6.1.1 Primary map



X

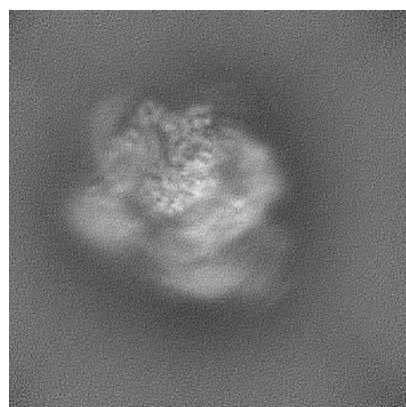


Y

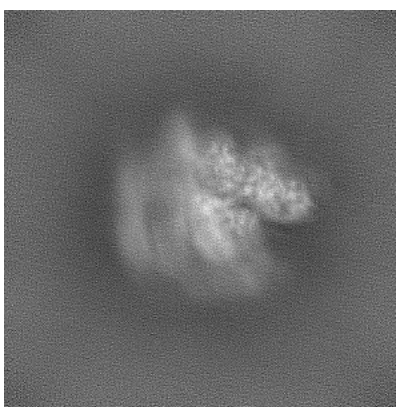


Z

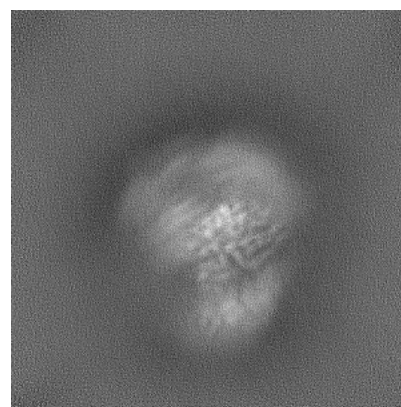
6.1.2 Raw map



X



Y

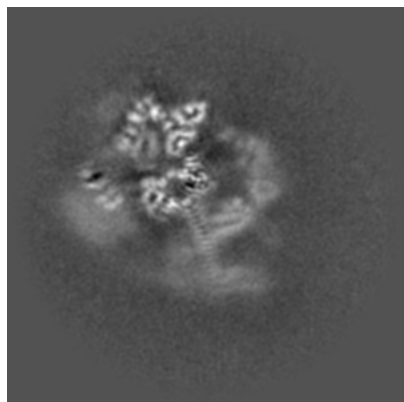


Z

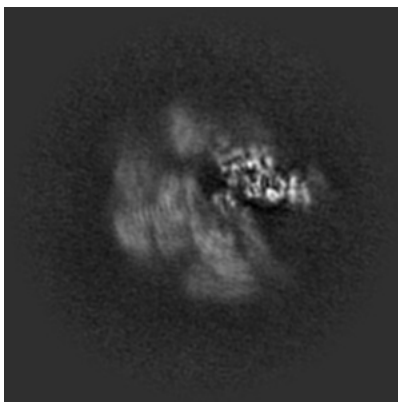
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

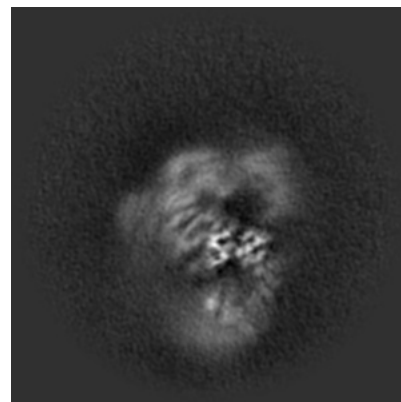
6.2.1 Primary map



X Index: 216

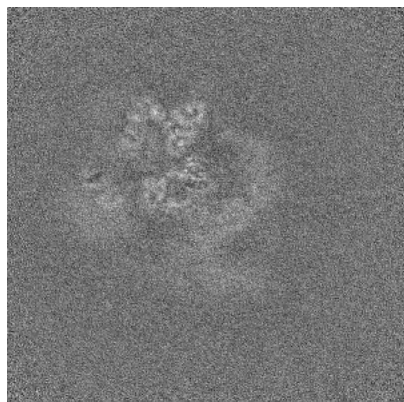


Y Index: 216

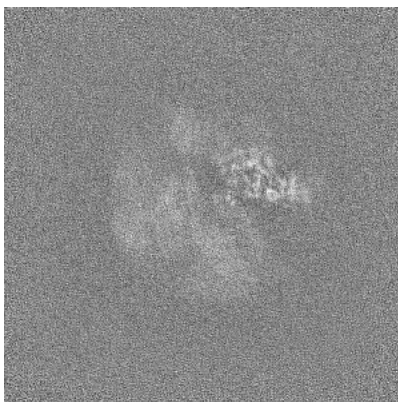


Z Index: 216

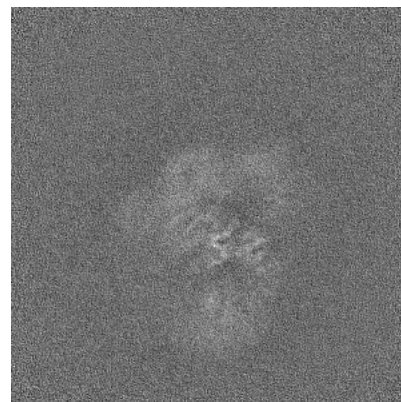
6.2.2 Raw map



X Index: 216



Y Index: 216

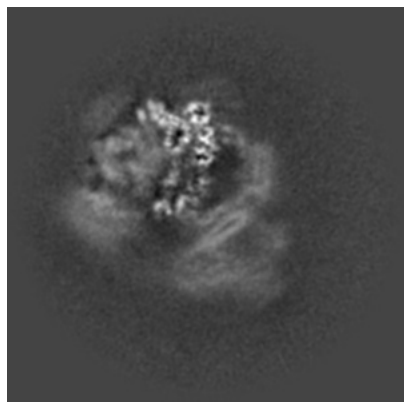


Z Index: 216

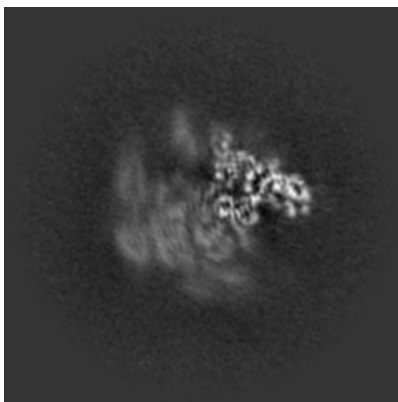
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

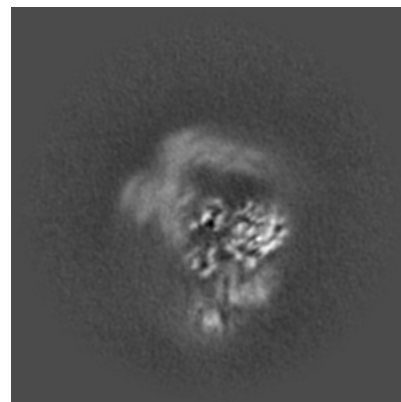
6.3.1 Primary map



X Index: 231

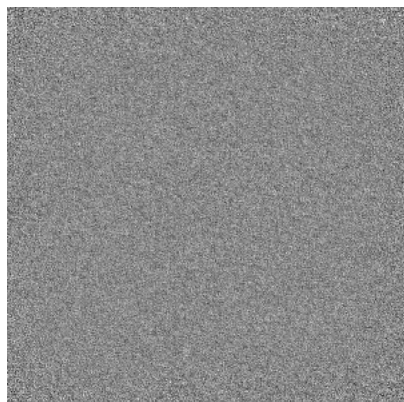


Y Index: 203

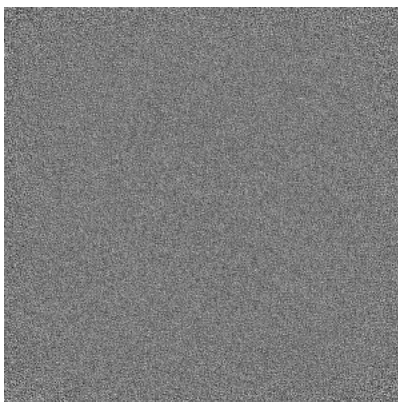


Z Index: 239

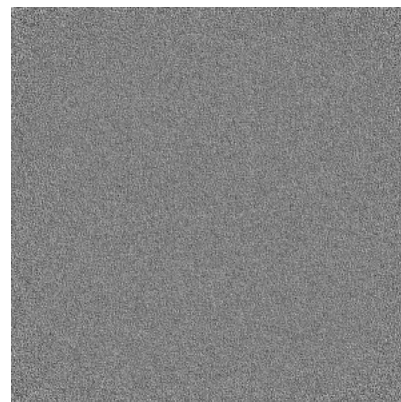
6.3.2 Raw map



X Index: 0



Y Index: 0

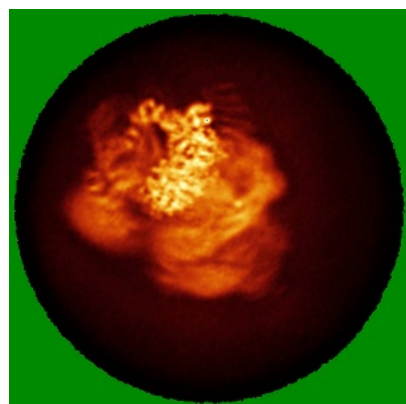


Z Index: 0

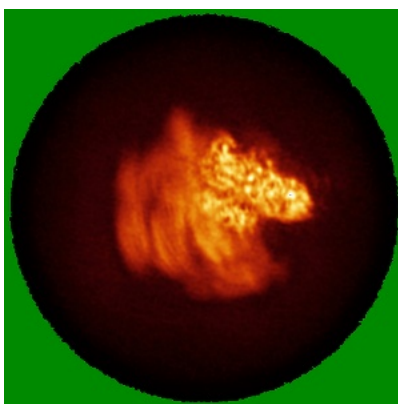
The images above show the largest variance slices of the map in three orthogonal directions.

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

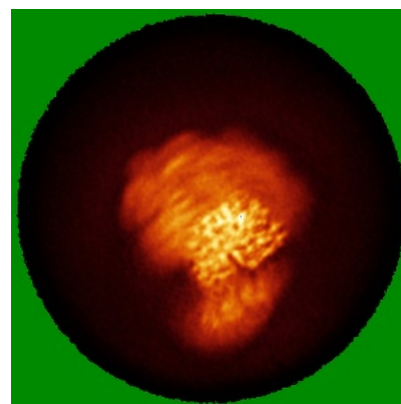
6.4.1 Primary map



X

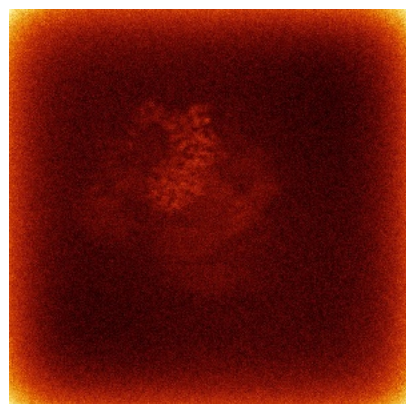


Y

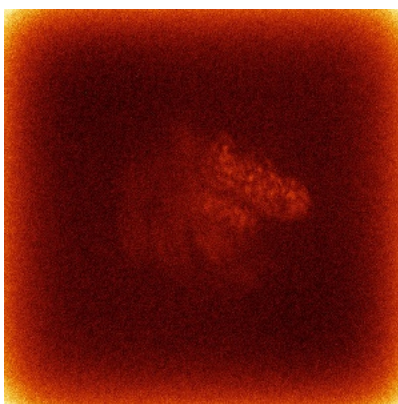


Z

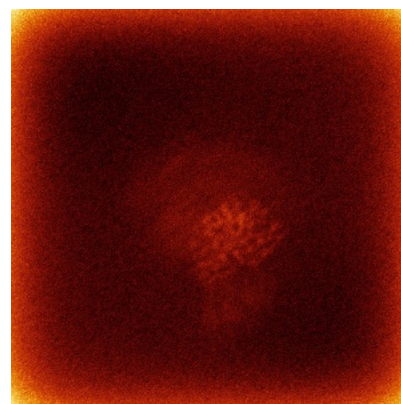
6.4.2 Raw map



X



Y

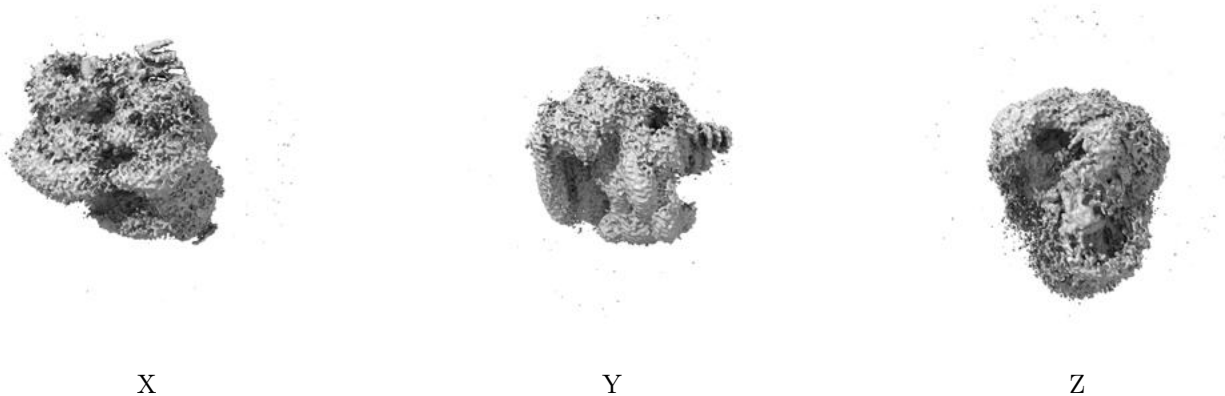


Z

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.

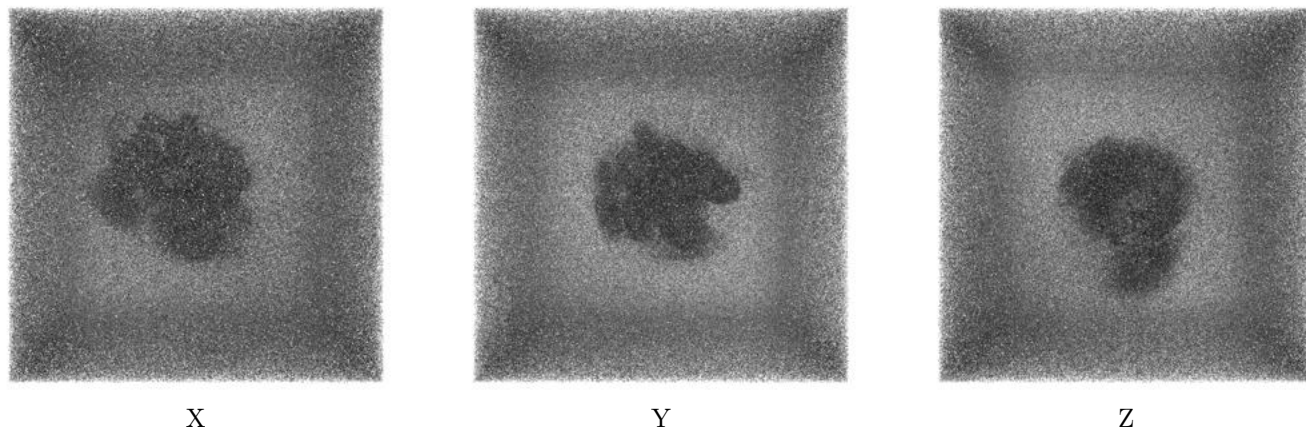
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

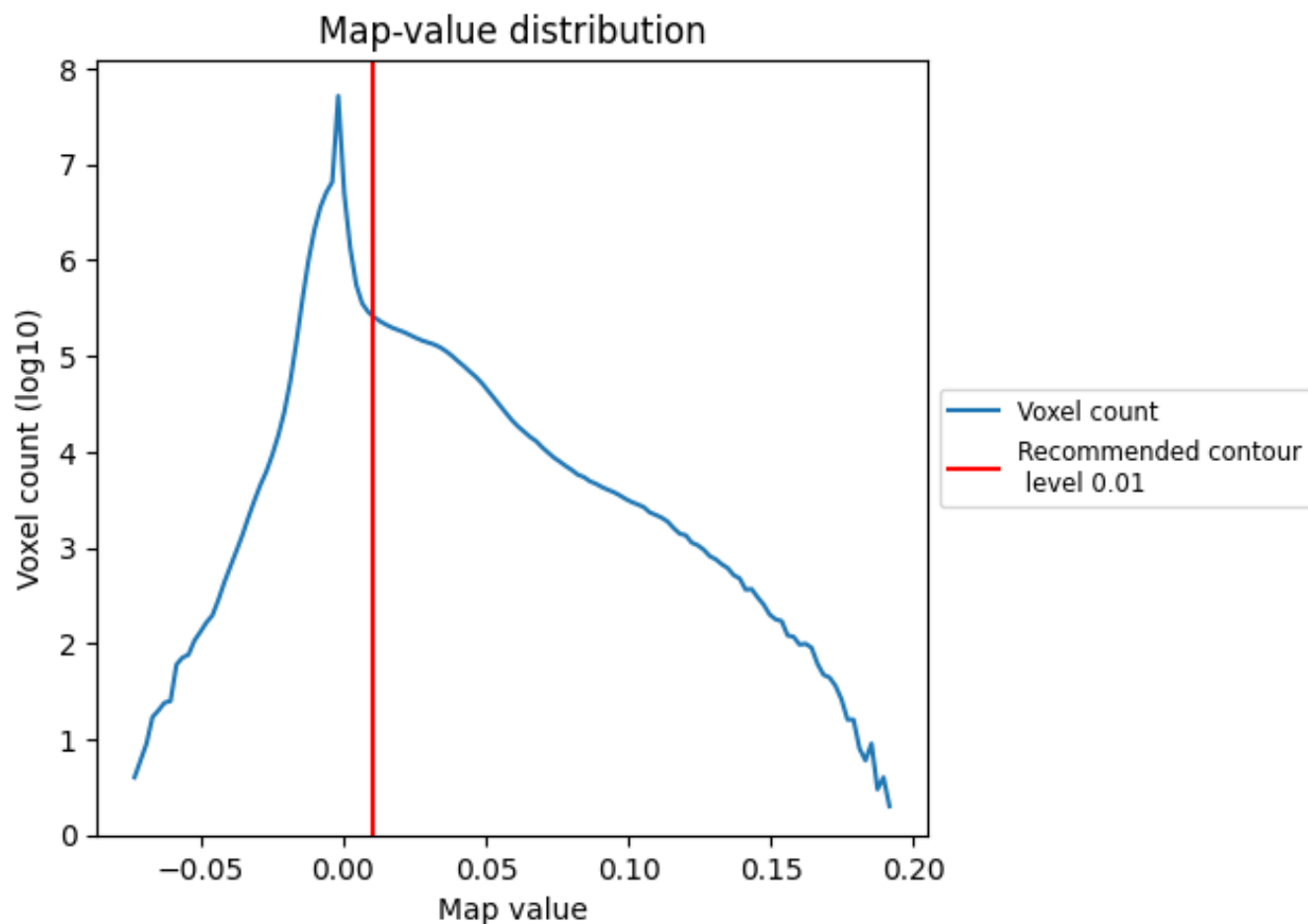
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

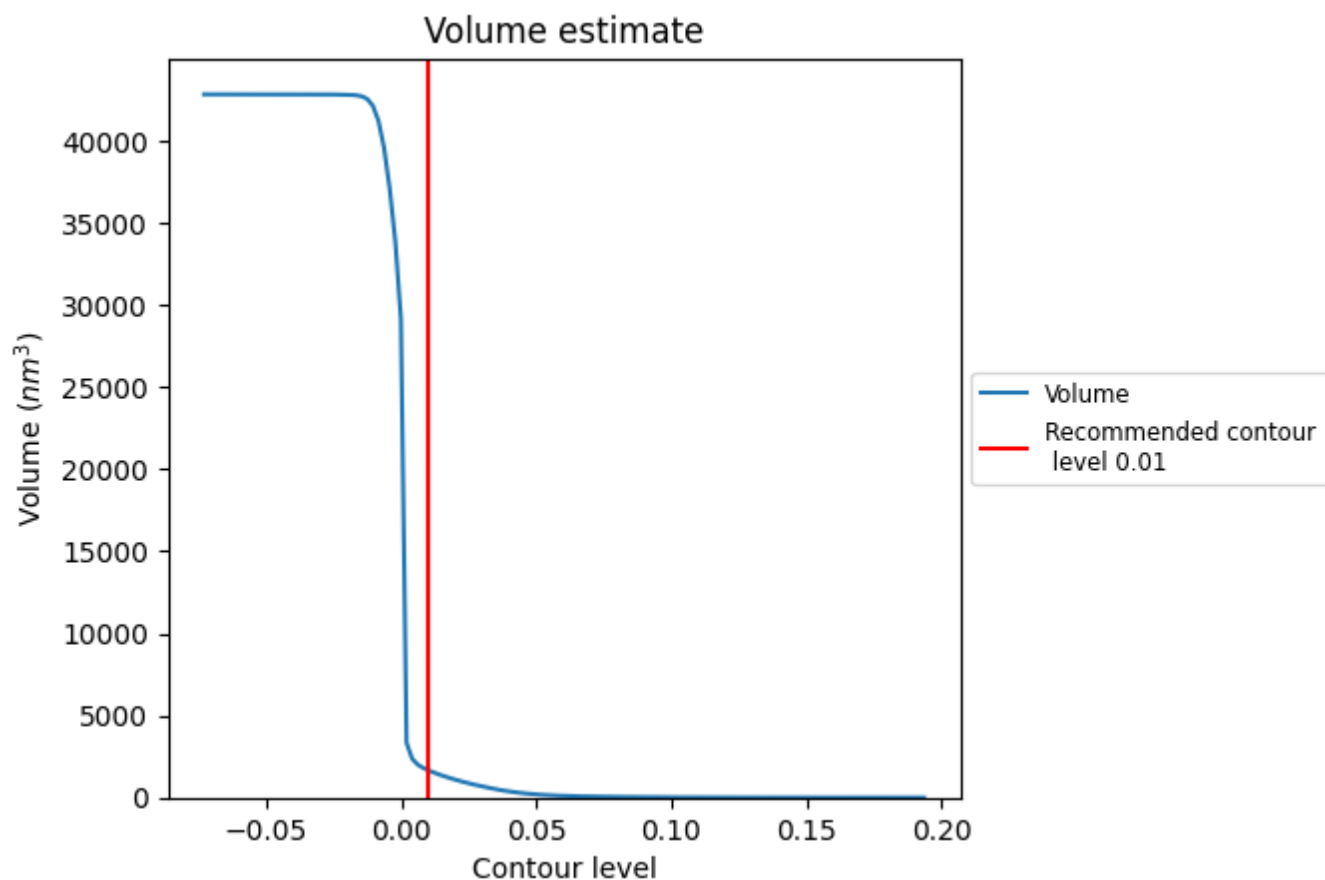
This section contains the results of statistical analysis of the map.

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.

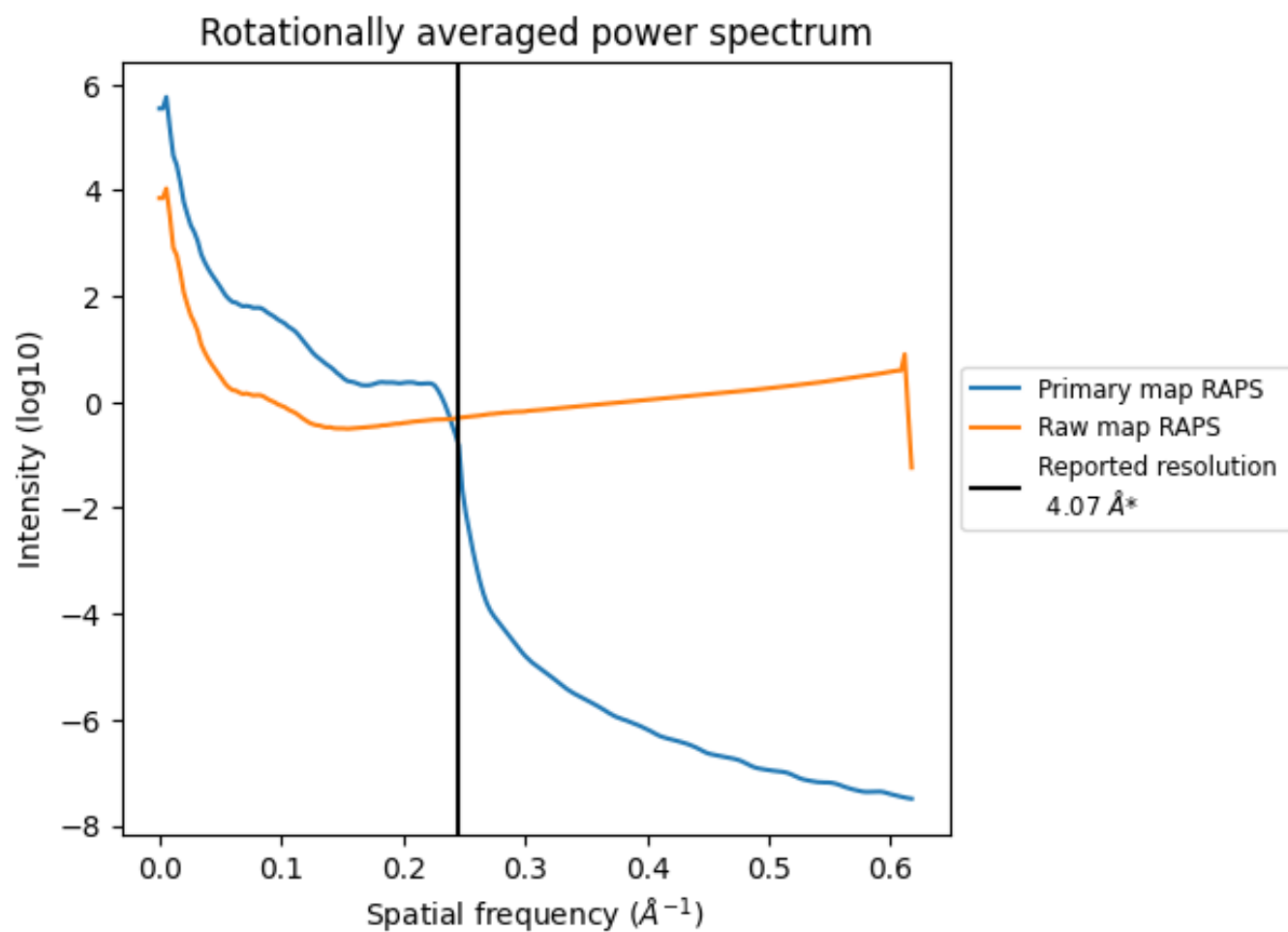
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1654 nm^3 ; this corresponds to an approximate mass of 1494 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

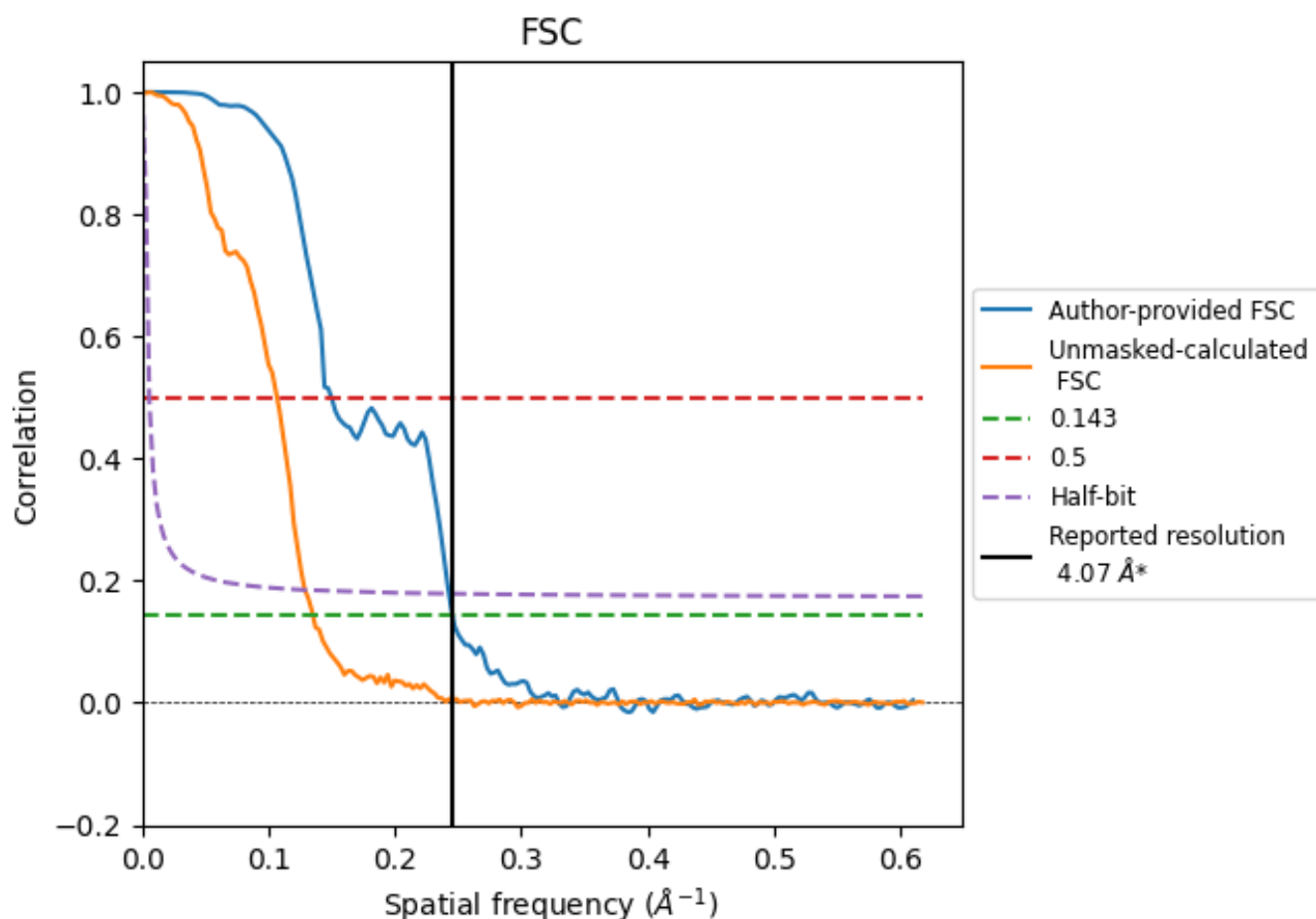


*Reported resolution corresponds to spatial frequency of 0.246 $\text{\AA}^{-1}$

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 $0.246 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

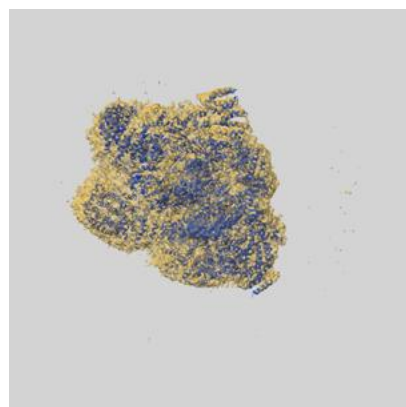
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.07	-	-
Author-provided FSC curve	4.07	6.68	4.12
Unmasked-calculated*	7.40	9.37	7.77

*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 7.40 differs from the reported value 4.07 by more than 10 %

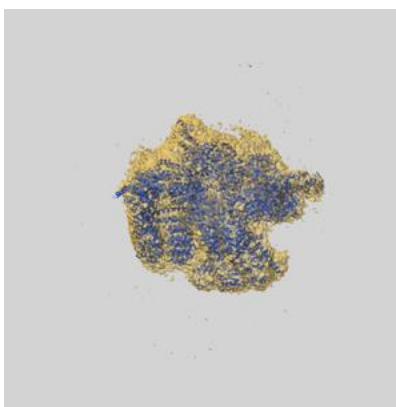
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71810 and PDB model 9PRO. Per-residue inclusion information can be found in section [3](#) on page [9](#).

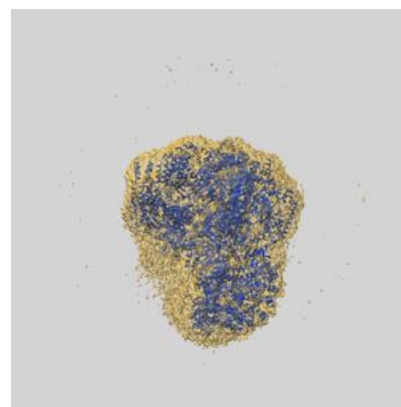
9.1 Map-model overlay [i](#)



X



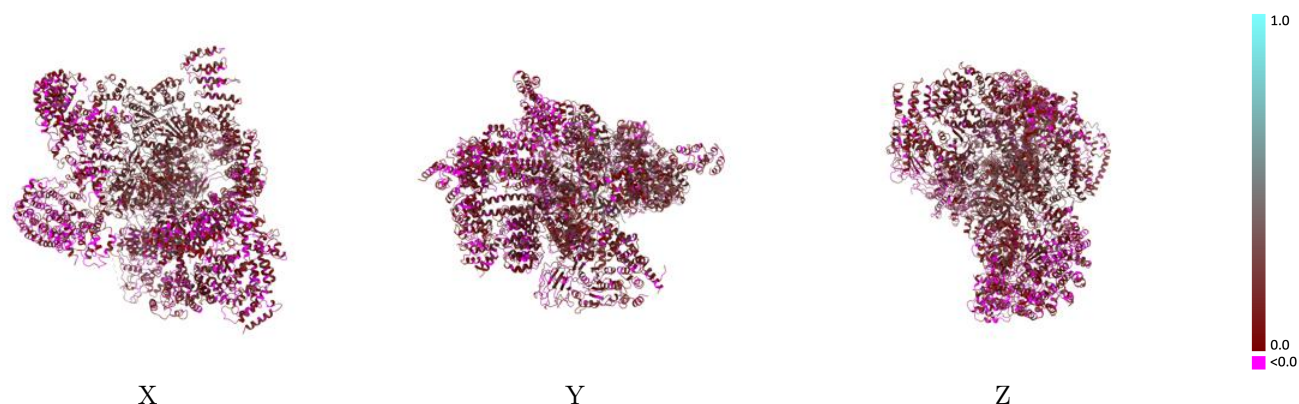
Y



Z

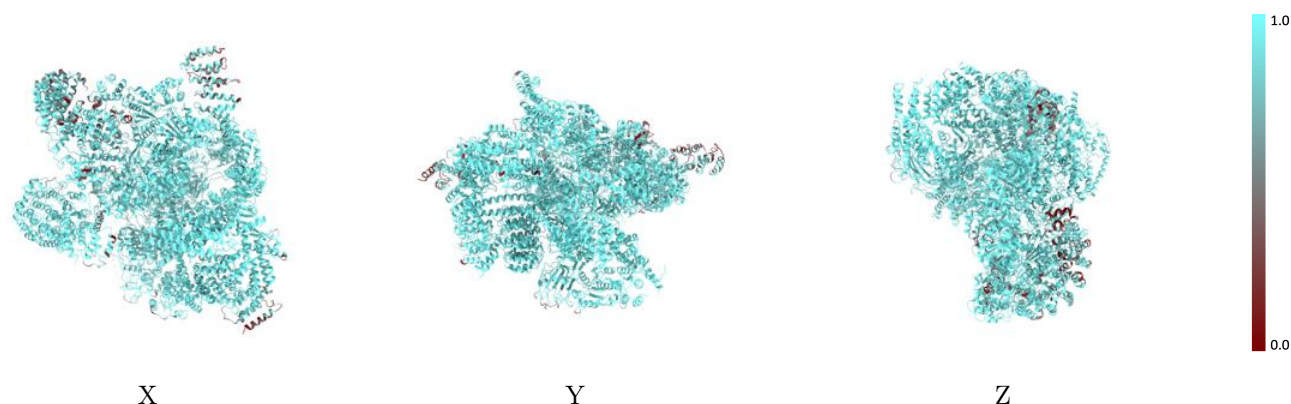
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



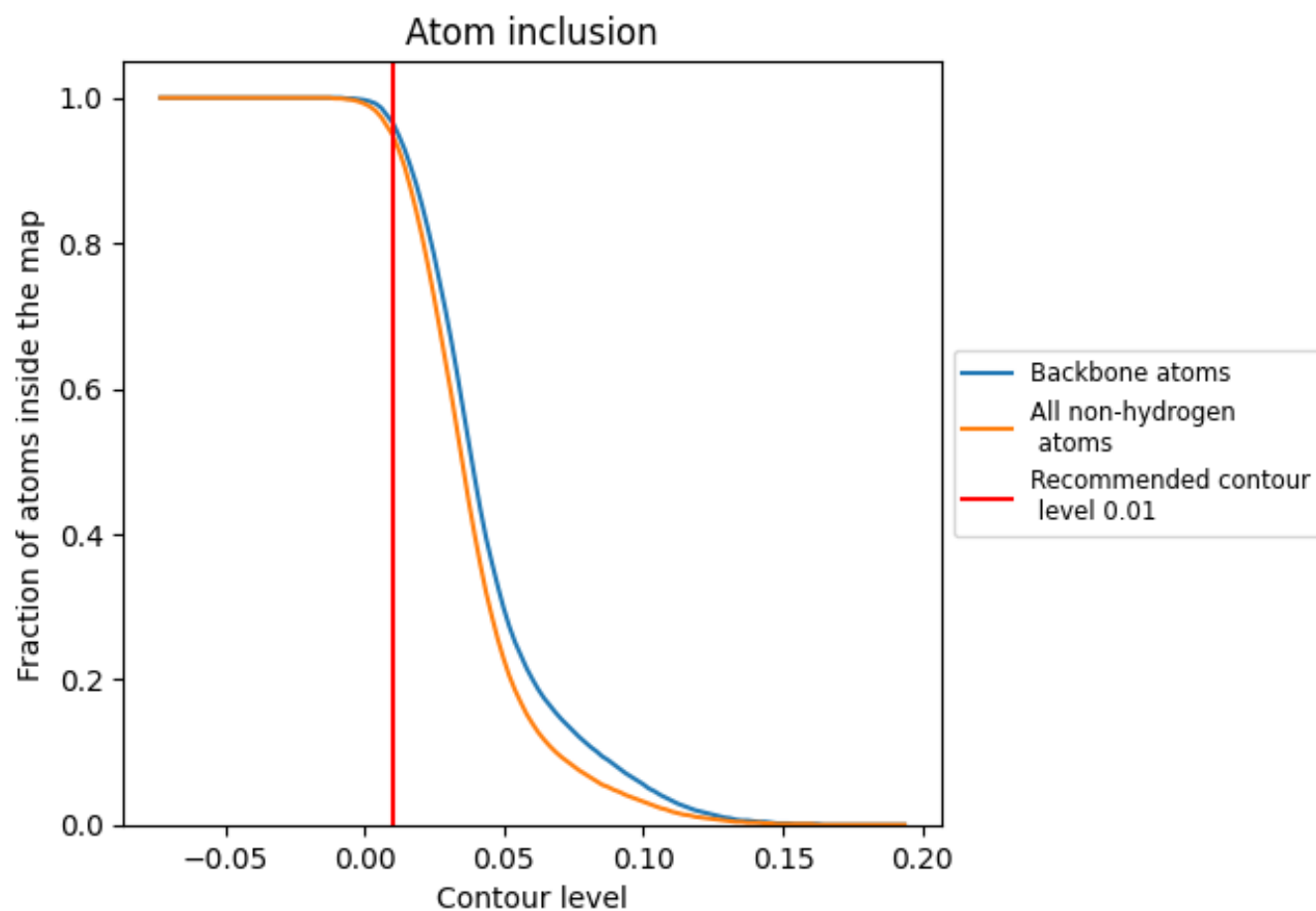
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.1350
A	 0.8990	 0.1360
B	 0.9200	 0.1210
C	 0.9750	 0.2160
D	 0.9800	 0.2440
E	 0.9790	 0.2510
F	 0.9870	 0.2350
U	 0.9880	 0.0970
V	 0.9840	 0.0990
W	 0.8550	 0.1460
X	 0.9860	 0.1220
Y	 0.9880	 0.0810
Z	 1.0000	 0.1790
a	 0.9930	 0.1500
b	 0.9850	 0.1260
c	 0.9810	 0.1590
d	 0.8590	 0.0870
e	 1.0000	 0.0690
f	 0.9740	 0.0510
g	 0.9380	 0.0770
z	 0.7650	 0.0990

