



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 01:09 AM UTC

PDB ID : 8QPK / pdb_00008qpk
EMDB ID : EMD-18555
Title : Cryo-EM Structure of Pre-B+5'ss Complex (core part)
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on : 2023-10-02
Resolution : 4.20 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:

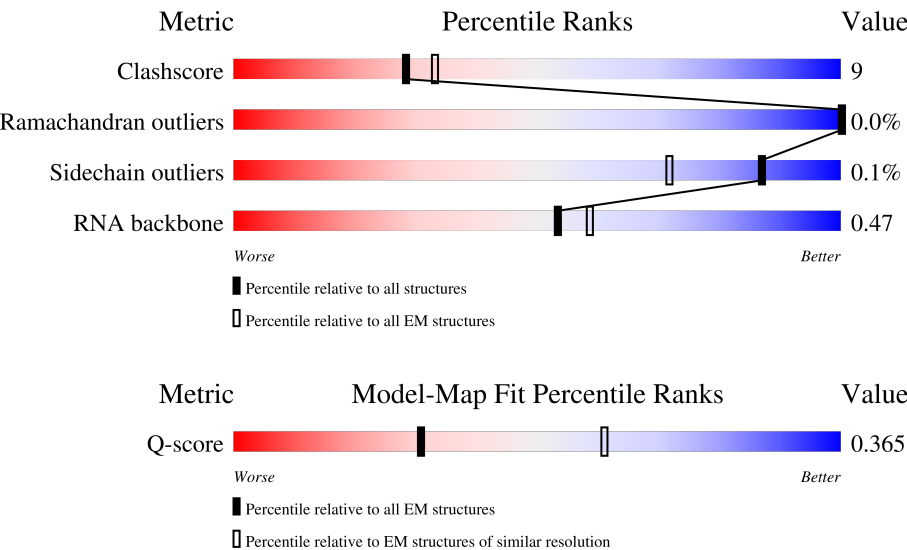
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 4.20 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	G	820	
2	D	142	
3	L	499	

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Mol	Chain	Length	Quality of chain
4	A	2335	
5	R	480	
6	U	565	
7	S	800	
8	C	972	
9	5	117	
10	4	144	
11	X	155	
12	z	11	
13	6	106	
14	N	941	
15	B	2136	
16	7	793	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 29527 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 Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	G	102	Total	C	N	O	0	0
			658	419	128	111		

- Molecule 2 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	141	Total	C	N	O	S	0	0
			1008	648	184	171	5		

- Molecule 3 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	50	Total	C	N	O	0	0
			251	151	50	50		

- Molecule 4 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1947	Total	C	N	O	S	0	0
			13055	8360	2412	2254	29		

- Molecule 5 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	106	Total	C	N	O	S	0	0
			659	412	124	121	2		

- Molecule 6 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	456	Total	C	N	O	0	0
			2320	1404	459	457		

- Molecule 7 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	73	Total	C	N	O	S	0	0
			446	274	90	81	1		

- Molecule 8 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	836	Total	C	N	O	S	0	0
			5163	3262	981	913	7		

- Molecule 9 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	5	77	Total	C	N	O	P	0	0
			1620	726	271	546	77		

- Molecule 10 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	76	Total	C	N	O	P	0	0
			1617	723	286	532	76		

- Molecule 11 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	22	Total	C	N	O	0	0
			124	78	22	24		

- Molecule 12 is a RNA chain called 5'ss oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	z	11	Total	C	N	O	P	0	0
			239	107	46	75	11		

- Molecule 13 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	6	43	Total	C	N	O	P	0	0
			927	414	175	295	43		

- Molecule 14 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	133	Total	C	N	O	0	0
			784	482	157	145		

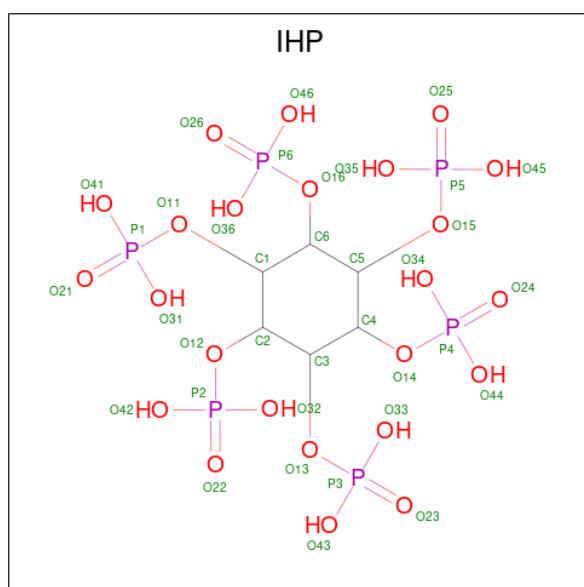
- Molecule 15 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	B	72	Total	C	N	O	0	0
			401	238	86	77		

- Molecule 16 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	7	36	Total	C	N	O	0	0
			219	136	43	40		

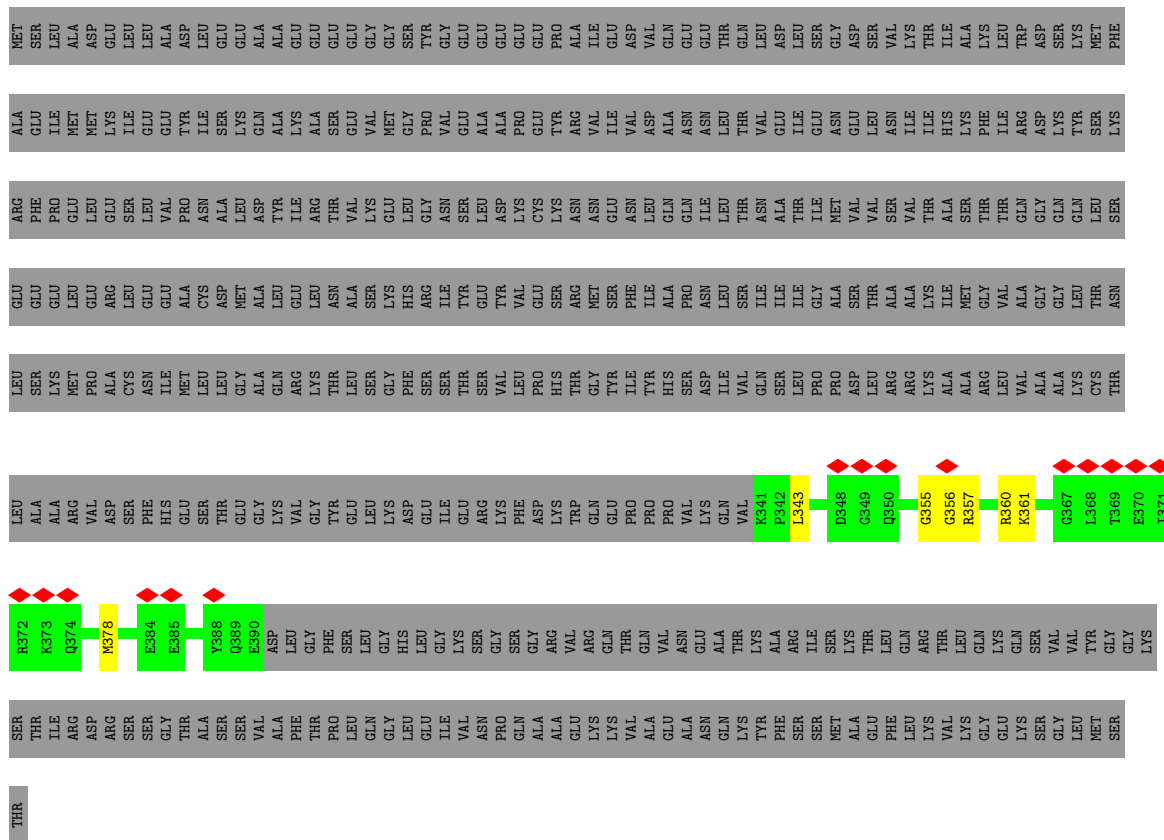
- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



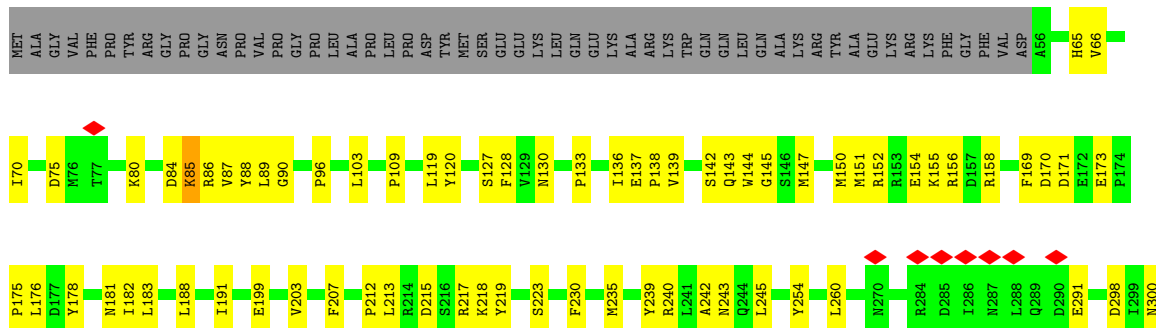
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			36	6	24	6	



Chain L: 9% .



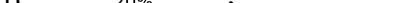
Chain A: 5% 68% 15% 17%





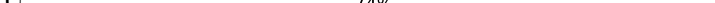
[illegible]

- Molecule 5: RNA-binding protein 42

Chain R:  20% 78%

ARG	THR	LEU	GLY	PRO	LEU	LEU	GLY	ARG	GLY	PRO	PRO	MET
ALA	ALA	LEU	LEU	GLY	LEU	VAL	LEU	MET	VAL	ALA	ALA	ALA
ALA	ALA	VAL	VAL	VAL	VAL	GLY	LEU	ALA	GLY	PRO	GLY	ALA
GLY	GLY	ARG	LEU	ARG	LEU	GLY	LYS	ARG	PHE	THR	GLY	PRO
SER	SER	GLY	GLY	GLY	GLY	PRO	GLY	PRO	PRO	PRO	ALA	ALA
TRP	TRP	LEU	LEU	LEU	LEU	LYS	GLY	HIS	VAL	THR	GLY	PRO
E369	E369	PRO	PRO	PRO	PRO	GLU	GLU	GLN	ASP	PRO	GLY	GLY
C395	C395	PRO	ALA	ALA	ALA	ALA	ALA	ALA	SER	THR	PRO	PRO
C386	C386	LEU	VAL	LEU	VAL	VAL	VAL	LEU	HIS	GLY	GLY	ALA
D387	D387	ARG	VAL	VAL	GLY	GLY	GLY	GLY	ASP	VAL	ALA	GLY
L388	L388	ILE	ALA	ALA	ALA	ALA	ALA	PRO	SER	MET	GLY	GLY
K409	K409	PRO	ALA	ALA	ALA	ALA	ALA	PRO	PRO	GLN	PRO	PRO
R414	R414	LEU	ALA	LEU	ALA	ALA	GLY	LEU	VAL	VAL	VAL	VAL
T421	T421	SER	LEU	LEU	GLY	LEU	GLY	GLY	ARG	PRO	PRO	VAL
K422	K422	LEU	GLU	GLU	GLU	GLU	GLU	PRO	GLU	ALA	ALA	GLY
G423	G423	ARG	ALA	PRO	ALA	ALA	GLY	GLY	MET	VAL	VAL	GLY
A438	A438	ARG	SER	SER	SER	SER	PRO	PRO	PHE	ILE	ALA	ALA
E441	E441	PRO	ALA	ALA	ALA	ALA	MET	MET	LEU	ARG	GLY	GLY
I452	I452	PRO	VAL	VAL	VAL	ALA	LEU	MET	ARG	ILE	PRO	ILE
D465	D465	ARG	ALA	ALA	ALA	ALA	GLY	ALA	ALA	ILE	GLY	GLY
Q471	Q471	PRO	GLY	GLY	GLY	GLY	ALA	ARG	PRO	THR	SER	SER
K472	K472	PRO	GLY	ALA	ALA	ALA	ALA	ALA	GLN	GLN	LYS	GLY
E473	E473	PRO	GLY	PRO	PRO	PRO	GLY	PRO	ALA	VAL	LEU	ARG
K474	K474	LEU	ALA	ALA	ALA	ALA	GLY	GLY	PRO	VAL	LYS	LYS
LYS	LYS	MET	GLY	GLY	PRO	PRO	GLY	PRO	ILE	GLN	GLN	GLU
LYS	LYS	LEU	ALA	ALA	ALA	ALA	LEU	LEU	ARG	GLN	GLY	GLY
LEU	LEU	GLY	VAL	VAL	VAL	VAL	VAL	GLY	PRO	THR	GLY	GLY
LEU	LEU	VAL	ILE	ILE	ILE	ILE	ILE	SER	ALA	GLY	GLY	ALA
GLY	GLY	PRO	GLY	PRO	PRO	PRO	PRO	MET	PHE	ALA	MET	MET
ARG	ARG	GLY	PRO	GLY	GLY	GLY	PRO	ALA	VAL	ARG	ALA	ALA
		PRO	SER	SER	SER	SER	SER	ALA	PRO	ALA	LEU	LEU
		LEU	LEU	LEU	LEU	LEU	LEU	LEU	ALA	ALA	PHE	PHE
		GLY	PRO	GLY	PRO	PRO	PRO	ARG	VAL	ALA	GLN	GLN
		GLY	PRO	GLY	LEU	LEU	LEU	VAL	ALA	ALA	ALA	ALA
		ASP	ALA	ASP	ALA	ALA	ALA	PRO	GLN	THR	VAL	VAL
		LYS	LEU	LYS	LEU	LEU	LEU	LEU	ARG	VAL	LEU	LEU
		LYS	ALA	LYS	ALA	ALA	ALA	GLY	ALA	VAL	GLY	GLY
		LYS	PRO	LYS	PRO	PRO	PRO	GLY	ASP	VAL	GLY	GLY
		LYS	PRO	LYS	PRO	PRO	PRO	GLY	SER	PRO	VAL	VAL
		PRO	PRO	PRO	PRO	PRO	PRO	ALA	ALA	MET	PRO	PRO
		GLY	GLY	GLY	GLY	GLY	GLY	PRO	SER	VAL	VAL	VAL
		LYS	LEU	LYS	LEU	LEU	LEU	ARG	GLY	GLY	GLY	GLY
		LYS	LEU	LYS	LEU	LEU	LEU	GLY	ALA	PRO	THR	THR
		ARG	ARG	ARG	LEU	LEU	LEU	GLY	ALA	ALA	ALA	ALA
		CYS	CYS	CYS	PRO	PRO	PRO	LEU	GLY	PHE	VAL	VAL
		TYR	TYR	TYR	LEU	LEU	LEU	GLY	ARG	VAL	ALA	ALA

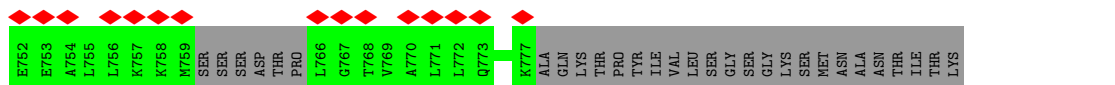
- Molecule 6: Ubiquitin carboxyl-terminal hydrolase 39

Chain U:  74% 7% 19%

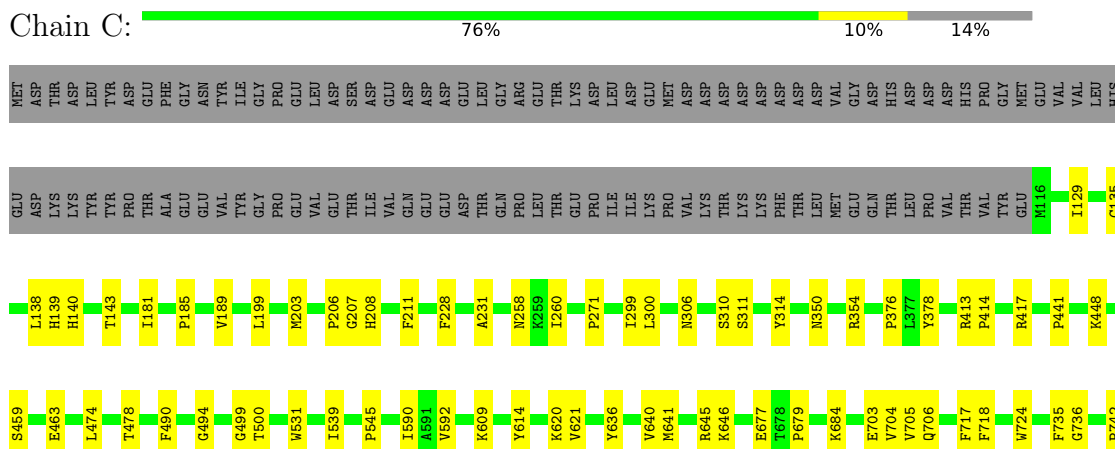
E429	F164	GLU	MET
L438	L165	ALA	SER
K439	N166	PRO	GLY
R440	K171	ALA	SER
F441	F172	VAL	LYS
Q442	Y173	VAL	ARG
L443	Y173	PRO	GLU
K459	E180	PHE	SER
		VAL	ARG
		VAL	GLY
V464	D183	VAL	SER
V504	T198	LYS	THR
		ARG	GLY
S510	I202	GLU	LYS
L529	D206	VAL	GLU
L532	P266	ASP	SER
L544	G267	GLU	ARG
Y548	D268	SER	ARG
	A292	GLU	GLY
R585	M353	ARG	ARG
ASP	R354	VAL	VAL
ASN	T357	ALA	LYS
ASP		ALA	ARG
GLU		LYS	GLU
THR	P366	GLY	ASP
ASN	A367	ARG	ARG
GLN	E368	VAL	GLU
GLN	E369	ASP	ARG
GLY	K370	SER	GLU
ALA	E371	GLU	PRO
	Q372	ASP	GLU
		R100	ALA
			ALA
	H375	Y107	SER
			SER
	T382	T111	ARG
			GLY
	P399	S125	SER
			PRO
	D403	A133	VAL
		Y134	ARG
		A135	VAL
	E406		LYS
	Q407	Y142	ARG
	L408	F143	GLU
	I409	Q144	PHE
	I410	G145	GLU
	P411	R146	PRO
			ALA
	F416	S150	SER
	A420	H151	ALA
		A152	ARG
	G424		
I425			
T426			

- Molecule 7: U4/U6.U5 tri-snRNP-associated protein 1

Chain S: 8% 91%



- Molecule 8: 116 kDa U5 small nuclear ribonucleoprotein component



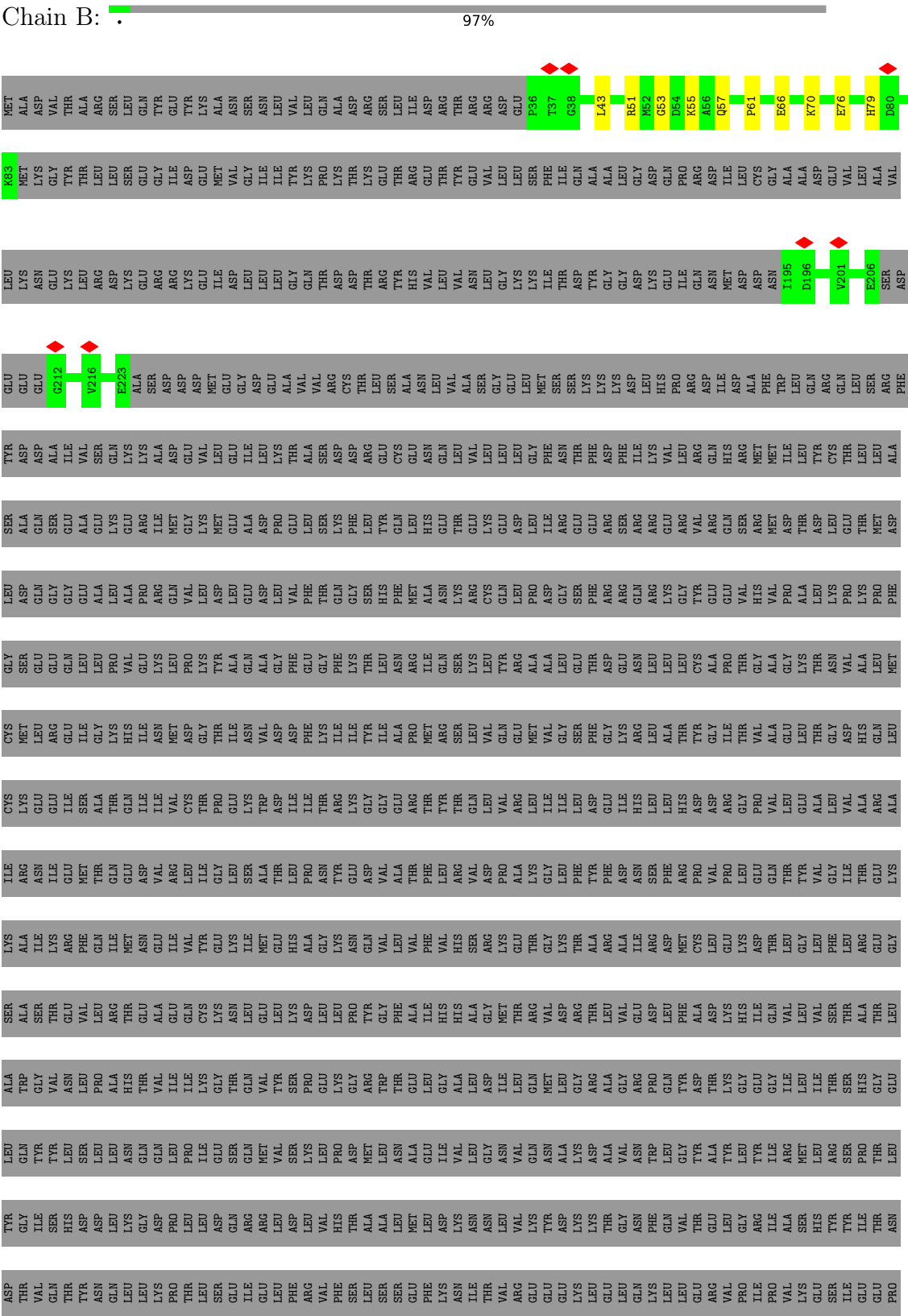


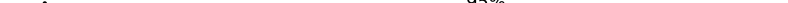
- Molecule 14: Pre-mRNA-processing factor 6

Chain N: 13% . 86%



● Molecule 15: U5 small nuclear ribonucleoprotein 200 kDa helicase



Chain 7:  95%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176879	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0165	Depositor
Map size (Å)	580.0, 580.0, 580.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

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

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	G	0.09	0/667	0.26	0/906
2	D	0.10	0/1032	0.27	0/1409
3	L	0.06	0/253	0.20	0/352
4	A	0.13	0/13400	0.30	1/18475 (0.0%)
5	R	0.08	0/668	0.25	0/913
6	U	0.09	0/2343	0.25	0/3285
7	S	0.08	0/450	0.21	0/610
8	C	0.09	0/5286	0.27	0/7297
9	5	0.08	0/1806	0.18	0/2807
10	4	0.05	0/1805	0.13	0/2805
11	X	0.06	0/126	0.20	0/174
12	z	0.07	0/268	0.17	0/416
13	6	0.05	0/1038	0.10	0/1615
14	N	0.06	0/794	0.19	0/1086
15	B	0.08	0/401	0.25	0/544
16	7	0.06	0/220	0.17	0/300
All	All	0.10	0/30557	0.26	1/42994 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	85	LYS	CB-CA-C	-5.91	109.75	116.54

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	G	658	0	505	11	0
2	D	1008	0	877	22	0
3	L	251	0	128	6	0
4	A	13055	0	10358	265	0
5	R	659	0	511	7	0
6	U	2320	0	1124	24	0
7	S	446	0	330	7	0
8	C	5163	0	3686	66	0
9	5	1620	0	822	29	0
10	4	1617	0	819	30	0
11	X	124	0	64	0	0
12	z	239	0	119	4	0
13	6	927	0	467	15	0
14	N	784	0	517	12	0
15	B	401	0	244	14	0
16	7	219	0	171	2	0
17	A	36	0	6	0	0
All	All	29527	0	20748	449	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 449 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)
6:U:164:PHE:H	6:U:173:TYR:H	1.29	0.81
4:A:1536:LEU:HD22	4:A:1572:SER:HB3	1.64	0.77
4:A:1571:ILE:HD12	4:A:1574:ILE:HD11	1.70	0.73
4:A:136:ILE:HG13	4:A:418:THR:HG22	1.69	0.73
4:A:596:TYR:HE1	9:5:46:U:H5'	1.54	0.73

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	G	98/820 (12%)	96 (98%)	2 (2%)	0	100	100
2	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
3	L	48/499 (10%)	48 (100%)	0	0	100	100
4	A	1943/2335 (83%)	1861 (96%)	81 (4%)	1 (0%)	48	82
5	R	104/480 (22%)	101 (97%)	3 (3%)	0	100	100
6	U	454/565 (80%)	441 (97%)	13 (3%)	0	100	100
7	S	69/800 (9%)	68 (99%)	1 (1%)	0	100	100
8	C	834/972 (86%)	814 (98%)	20 (2%)	0	100	100
11	X	20/155 (13%)	20 (100%)	0	0	100	100
14	N	127/941 (14%)	125 (98%)	2 (2%)	0	100	100
15	B	66/2136 (3%)	66 (100%)	0	0	100	100
16	7	34/793 (4%)	34 (100%)	0	0	100	100
All	All	3936/10638 (37%)	3810 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	80	LYS

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	G	35/721 (5%)	35 (100%)	0	100	100
2	D	82/130 (63%)	82 (100%)	0	100	100
3	L	3/424 (1%)	3 (100%)	0	100	100
4	A	877/2108 (42%)	876 (100%)	1 (0%)	88	88
5	R	40/369 (11%)	40 (100%)	0	100	100
6	U	26/511 (5%)	26 (100%)	0	100	100
7	S	23/681 (3%)	23 (100%)	0	100	100
8	C	266/866 (31%)	266 (100%)	0	100	100
11	X	3/144 (2%)	3 (100%)	0	100	100
14	N	29/792 (4%)	29 (100%)	0	100	100
15	B	12/1908 (1%)	12 (100%)	0	100	100
16	7	11/709 (2%)	11 (100%)	0	100	100
All	All	1407/9363 (15%)	1406 (100%)	1 (0%)	87	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	616	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	723	ASN
4	A	1083	HIS
7	S	731	HIS
4	A	1586	HIS
5	R	463	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	4	74/144 (51%)	16 (21%)	2 (2%)
12	z	10/11 (90%)	5 (50%)	0
13	6	41/106 (38%)	5 (12%)	0
9	5	76/117 (64%)	27 (35%)	1 (1%)
All	All	201/378 (53%)	53 (26%)	3 (1%)

5 of 53 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	5	8	G
9	5	9	G
9	5	10	U
9	5	12	U
9	5	14	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	5	19	A
10	4	1	A
10	4	68	A

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](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
17	IHP	A	2401	-	36,36,36	1.22	4 (11%)	60,60,60	1.63	7 (11%)

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
17	IHP	A	2401	-	-	1/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	2401	IHP	P5-O15	2.67	1.64	1.59
17	A	2401	IHP	P1-O11	2.31	1.63	1.59
17	A	2401	IHP	C4-C3	2.20	1.56	1.52
17	A	2401	IHP	C5-C4	2.18	1.56	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	2401	IHP	C5-C6-C1	5.03	121.47	110.43
17	A	2401	IHP	C3-C2-C1	4.59	120.50	110.43
17	A	2401	IHP	C5-C4-C3	4.37	120.01	110.43
17	A	2401	IHP	C4-C3-C2	3.45	118.00	110.43
17	A	2401	IHP	O15-C5-C4	2.65	114.40	108.76

There are no chirality outliers.

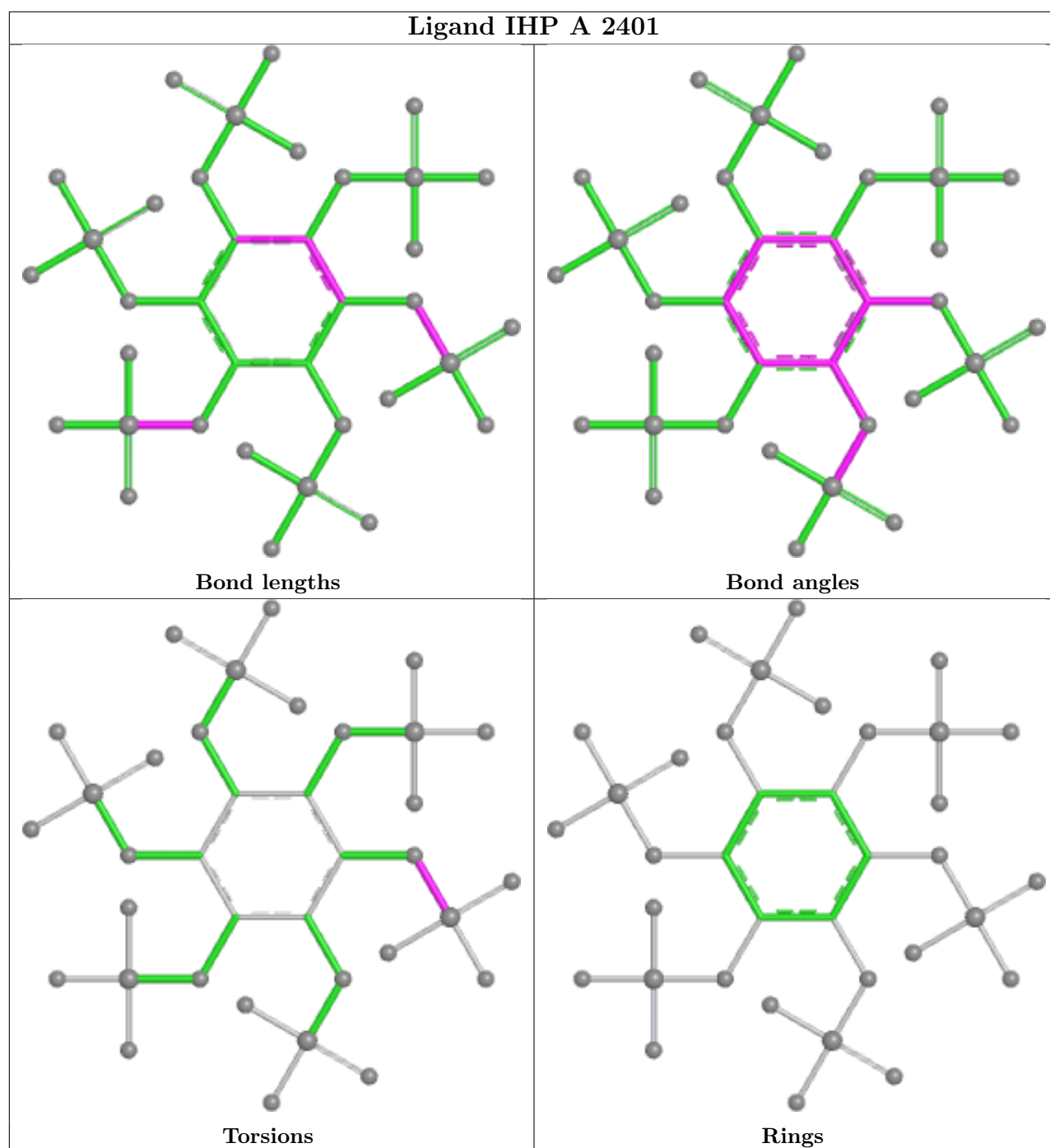
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	2401	IHP	C5-O15-P5-O35

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

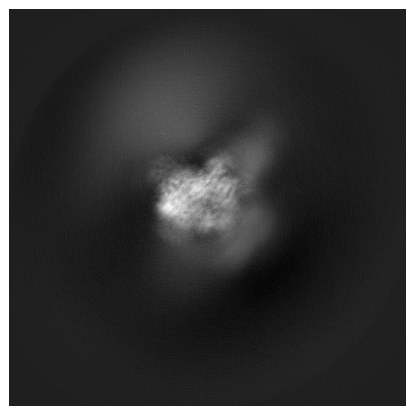
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18555. These allow visual inspection of the internal detail of the map and identification of artifacts.

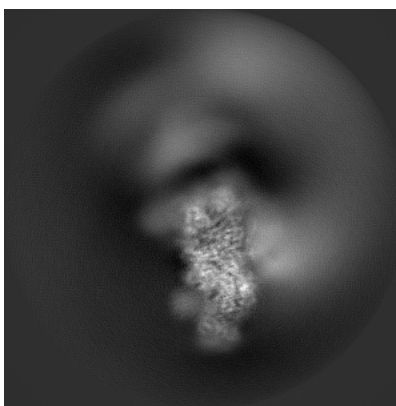
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

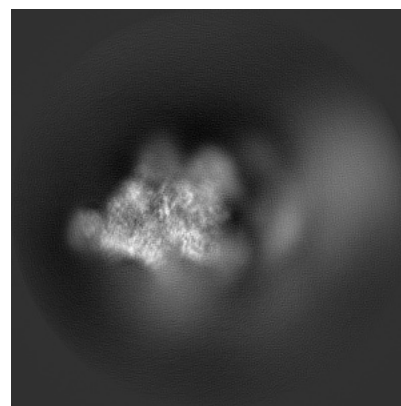
6.1.1 Primary map



X

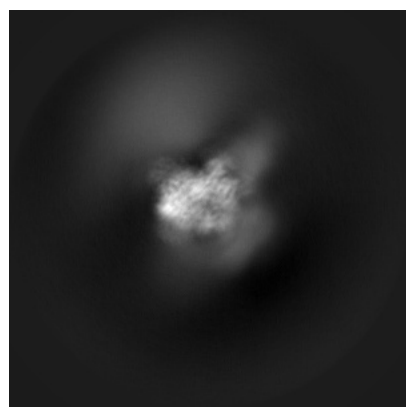


Y

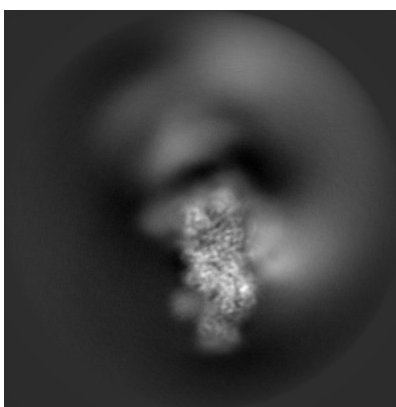


Z

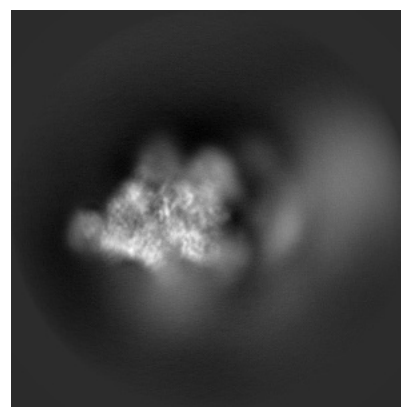
6.1.2 Raw map



X



Y

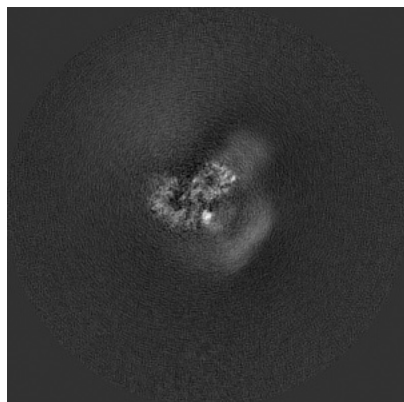


Z

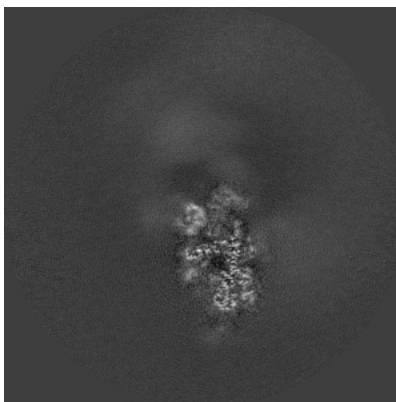
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

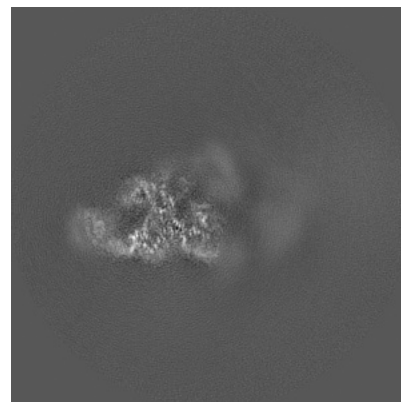
6.2.1 Primary map



X Index: 250

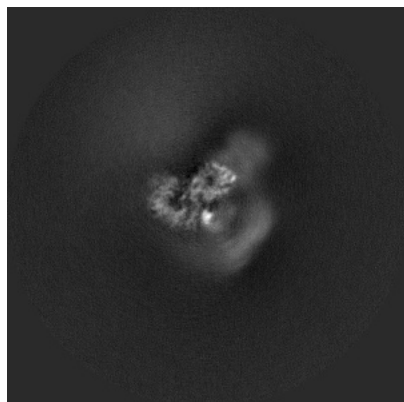


Y Index: 250

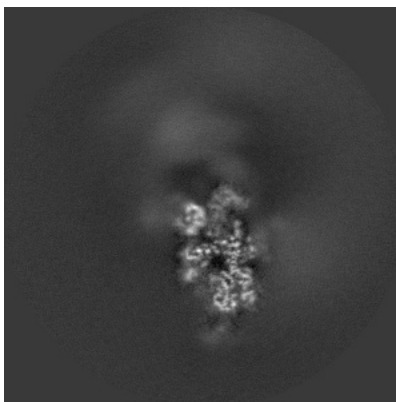


Z Index: 250

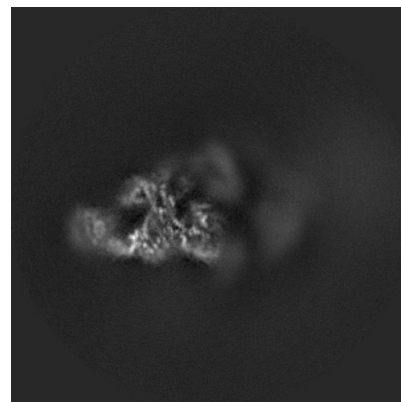
6.2.2 Raw map



X Index: 250



Y Index: 250

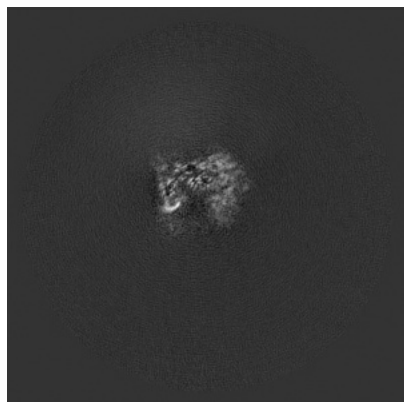


Z Index: 250

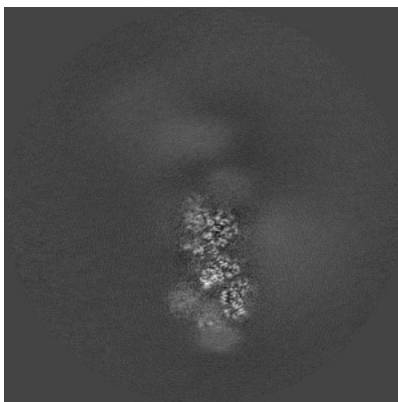
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

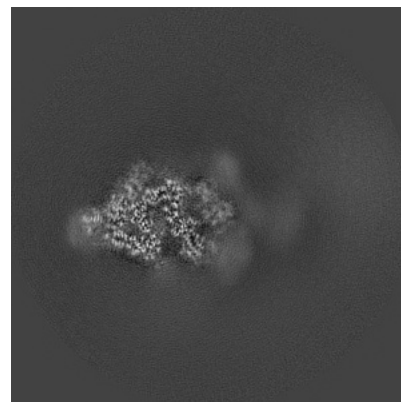
6.3.1 Primary map



X Index: 153

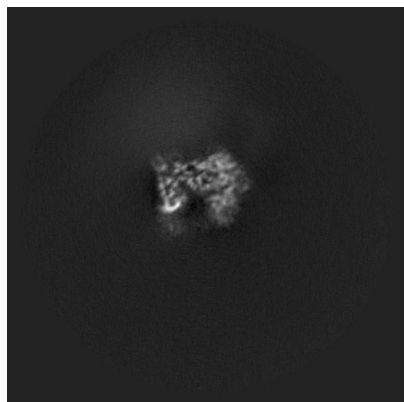


Y Index: 214

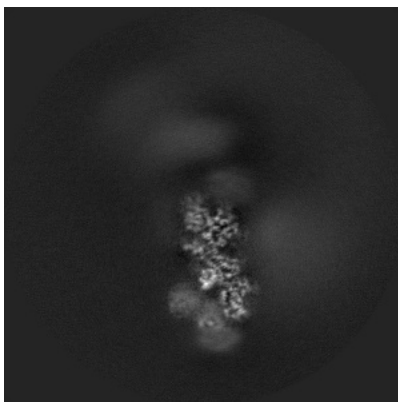


Z Index: 276

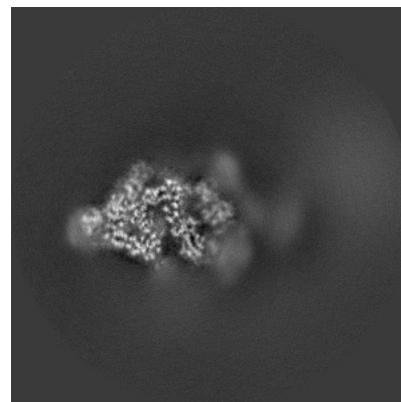
6.3.2 Raw map



X Index: 153



Y Index: 213

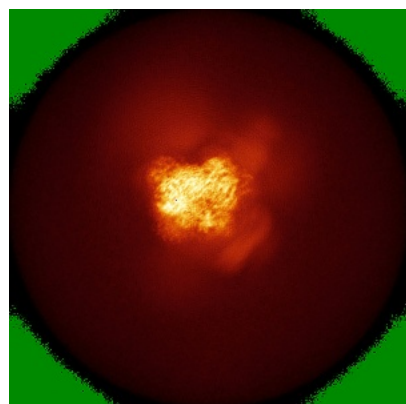


Z Index: 276

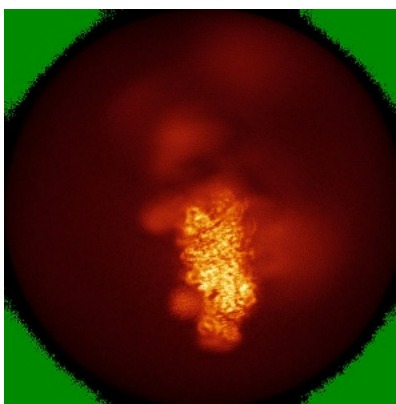
The images above show the largest variance slices of the map in three orthogonal directions.

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

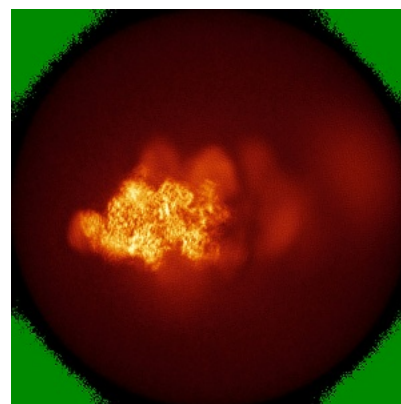
6.4.1 Primary map



X

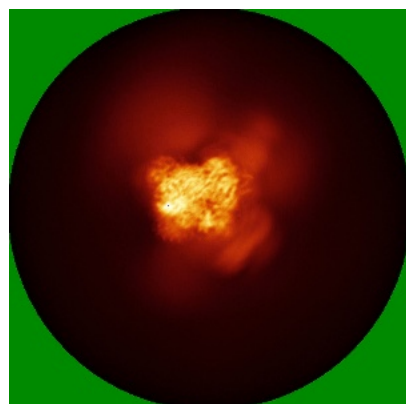


Y

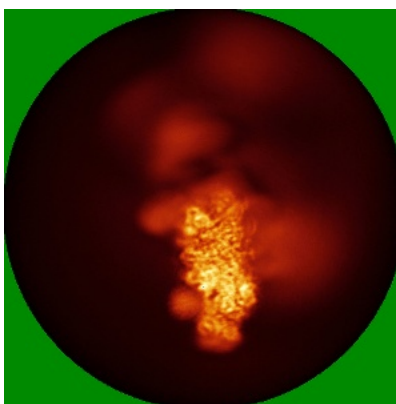


Z

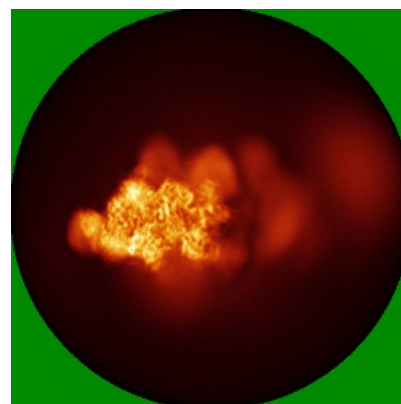
6.4.2 Raw map



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.

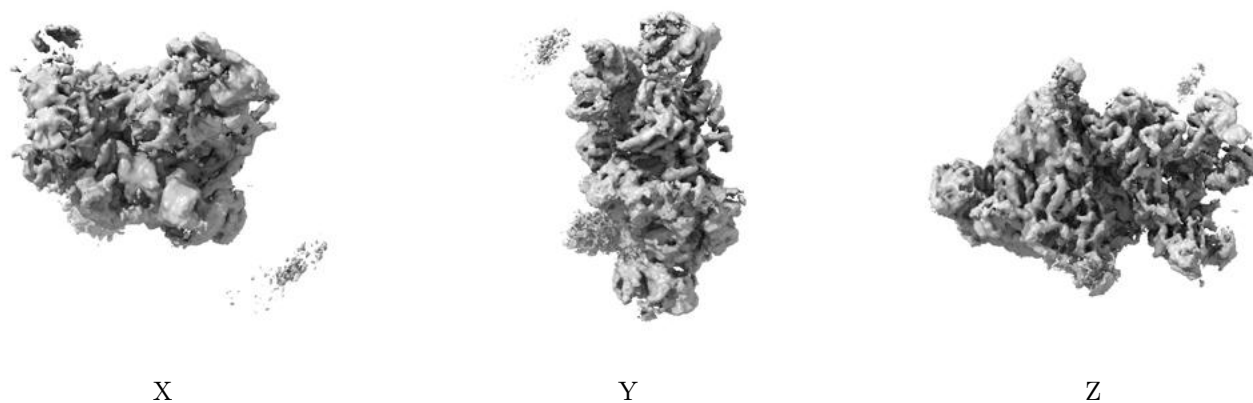
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0165. 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.

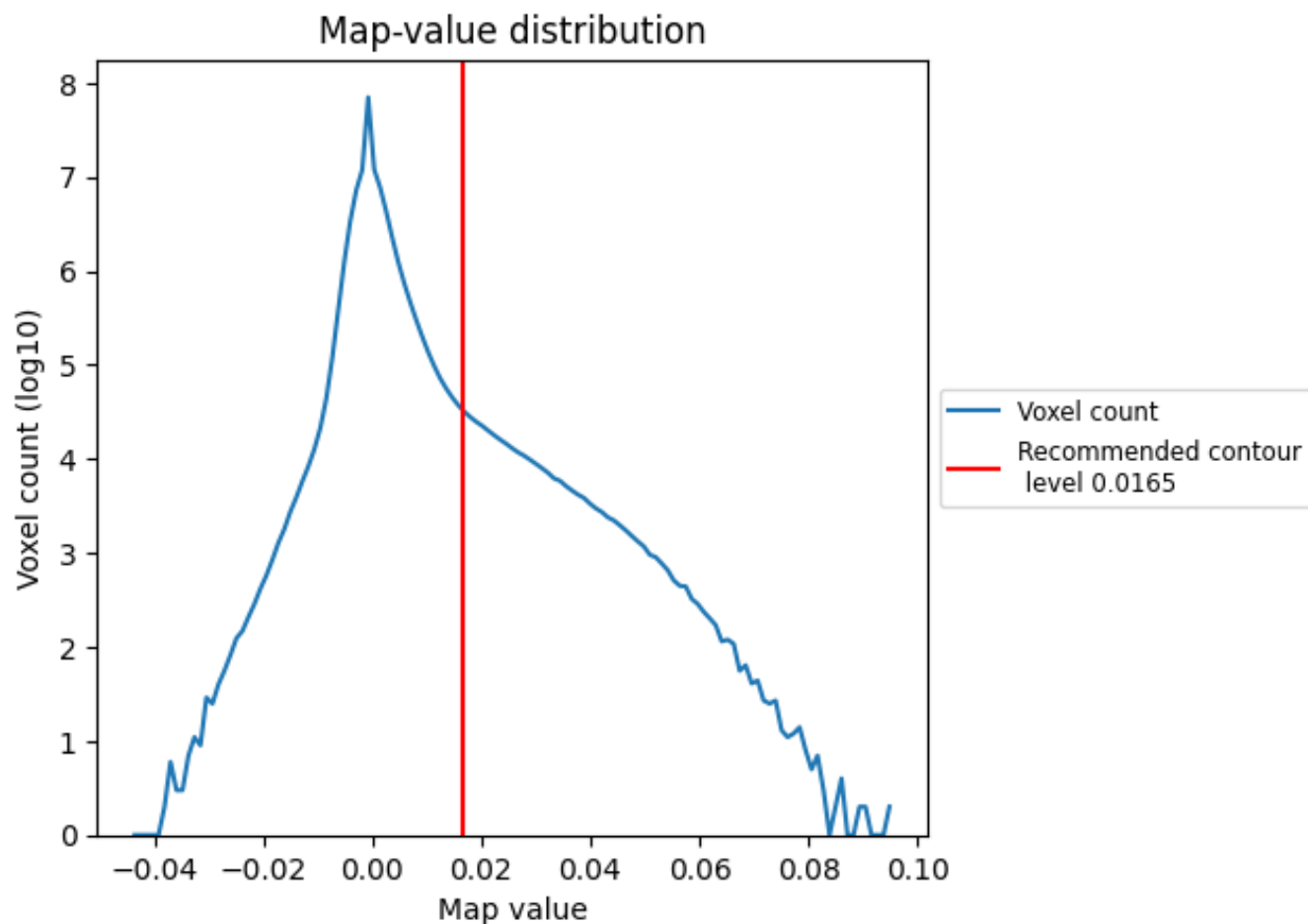
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

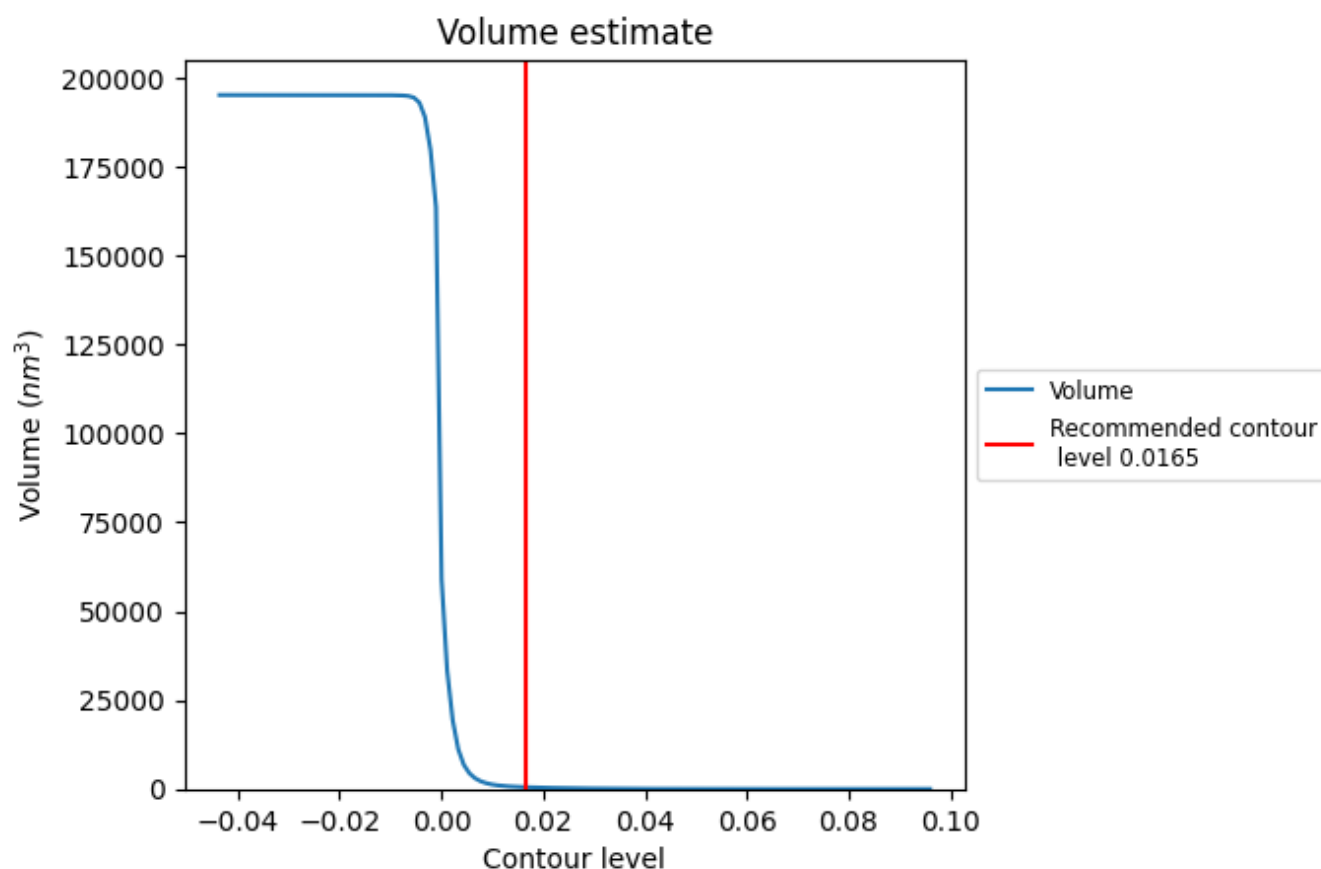
This section contains the results of statistical analysis of the map.

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.

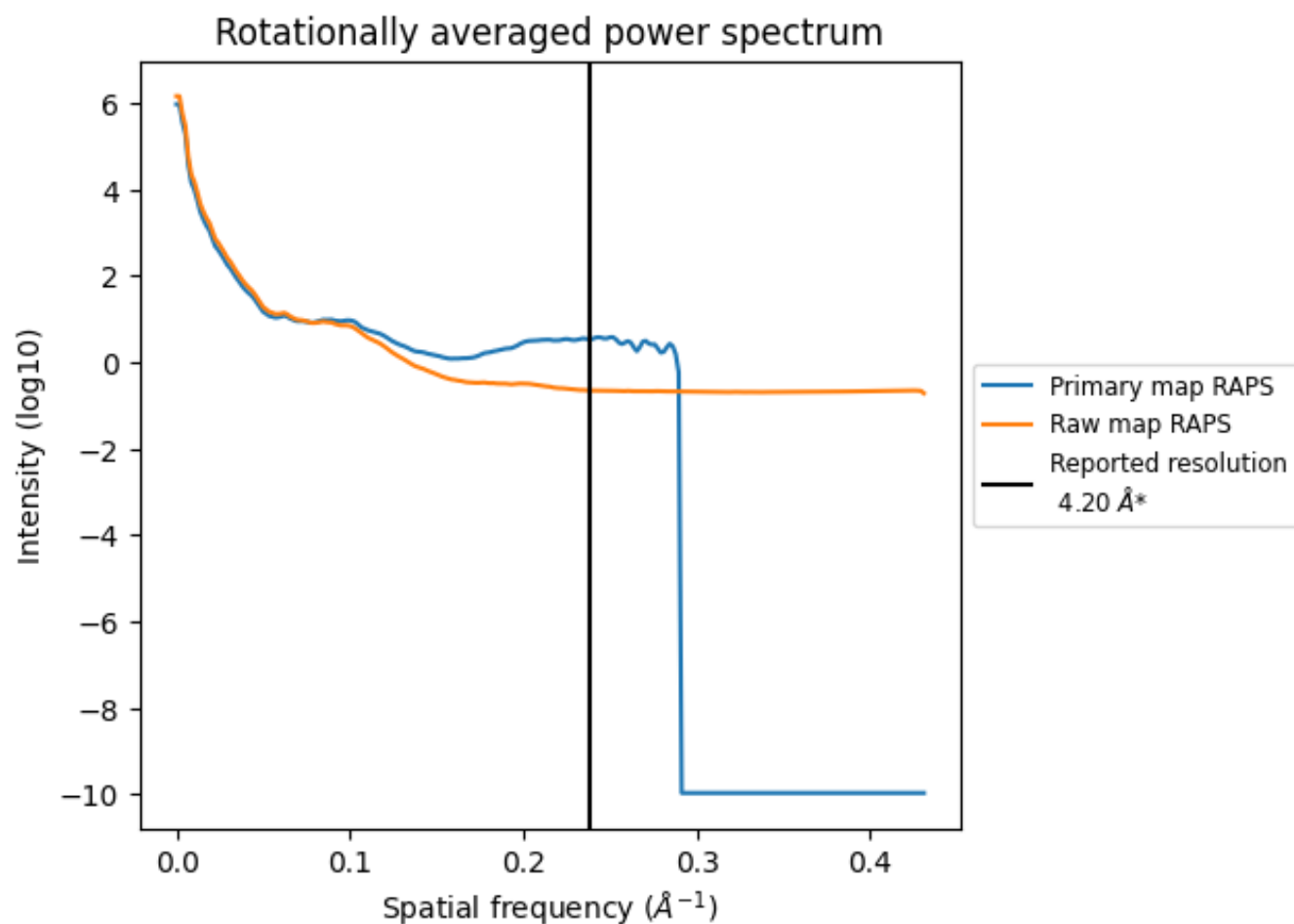
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 494 nm^3 ; this corresponds to an approximate mass of 446 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 ⓘ

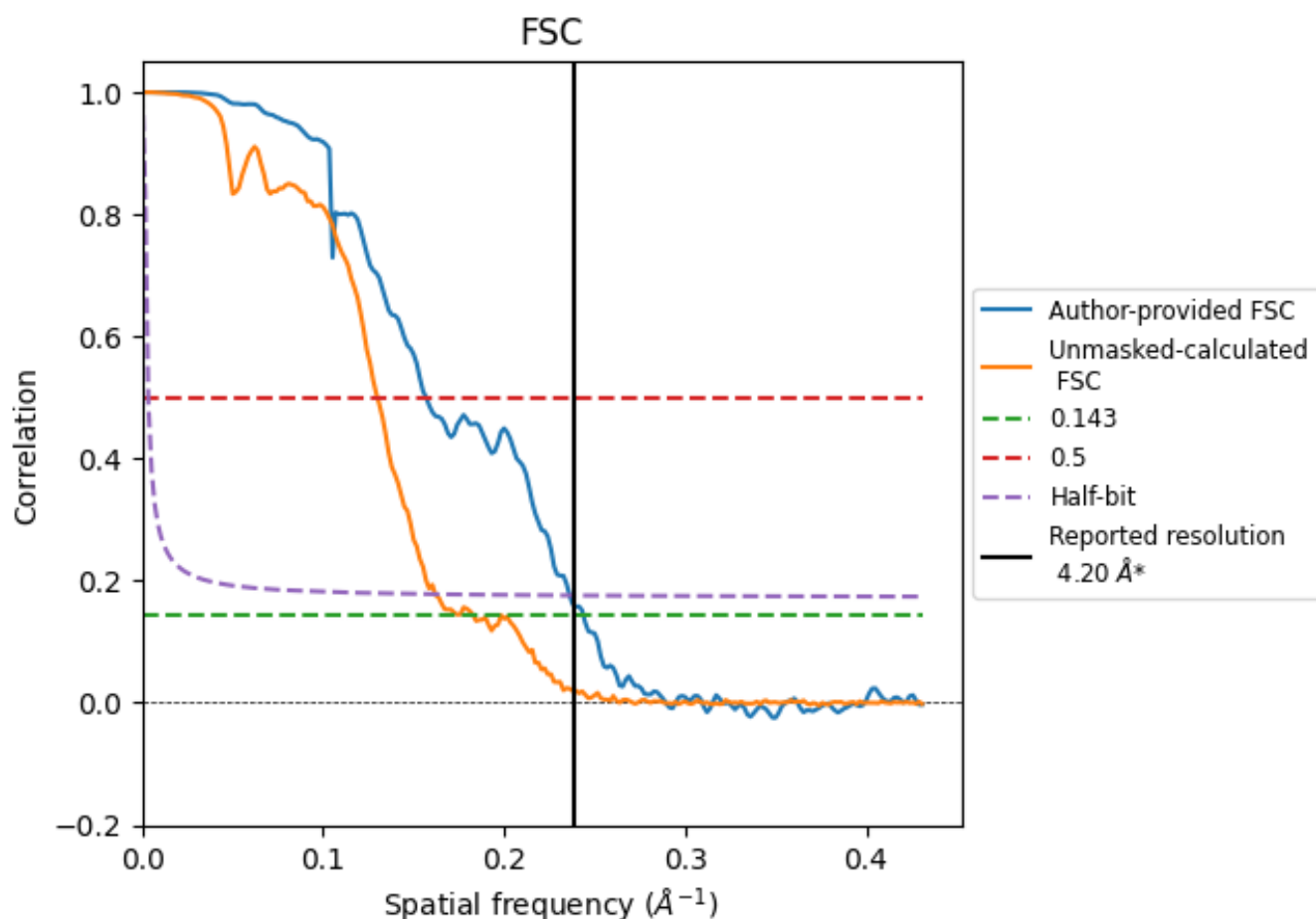


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

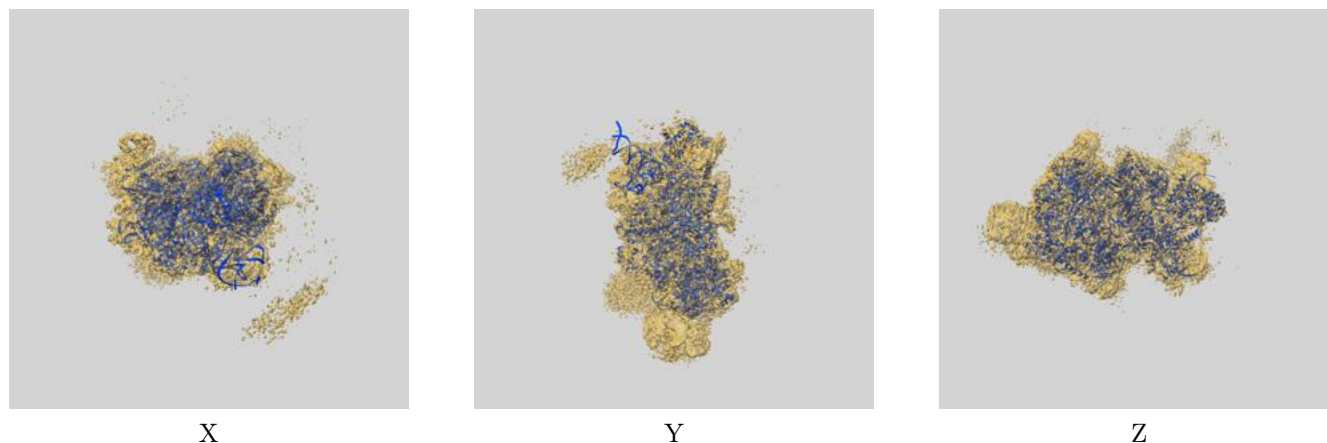
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.10	6.37	4.23
Unmasked-calculated*	5.46	7.69	6.18

*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 5.46 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

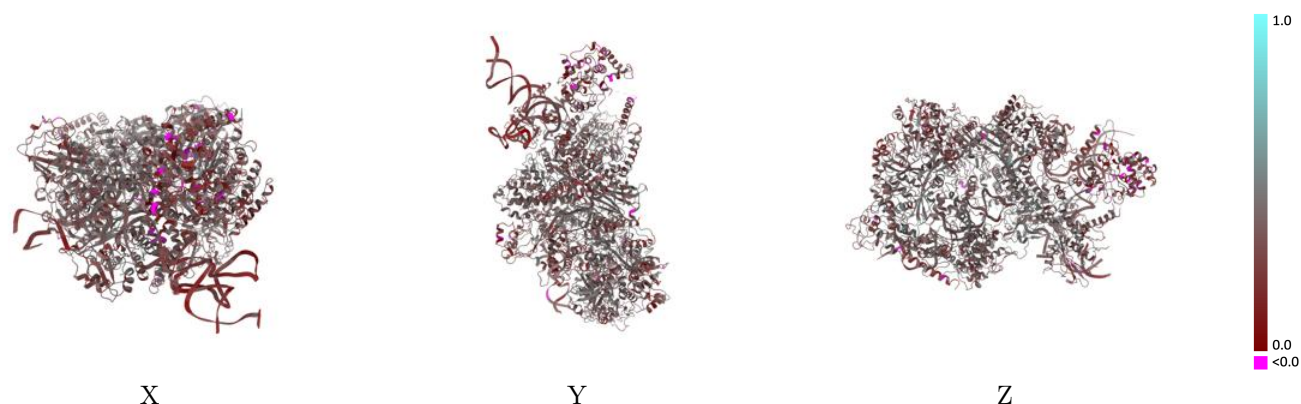
This section contains information regarding the fit between EMDB map EMD-18555 and PDB model 8QPK. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



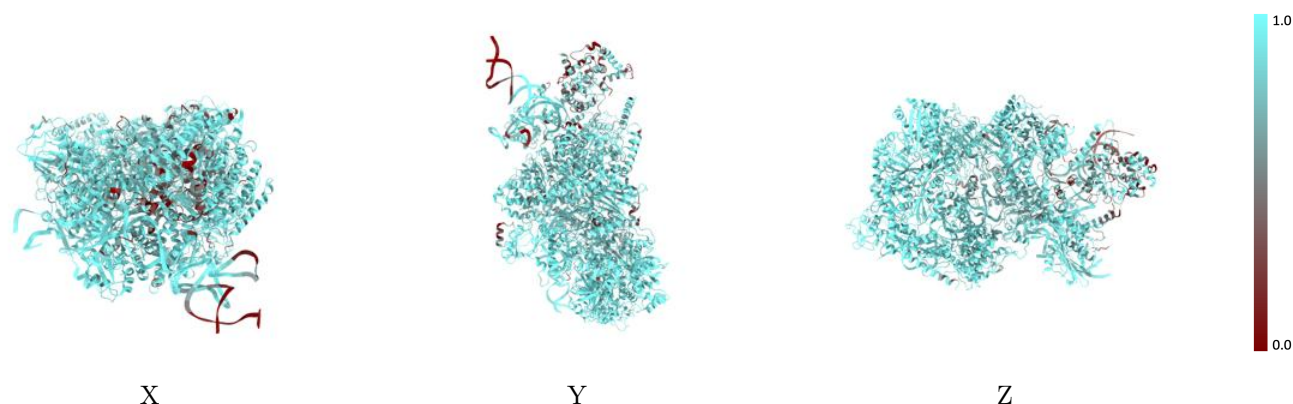
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



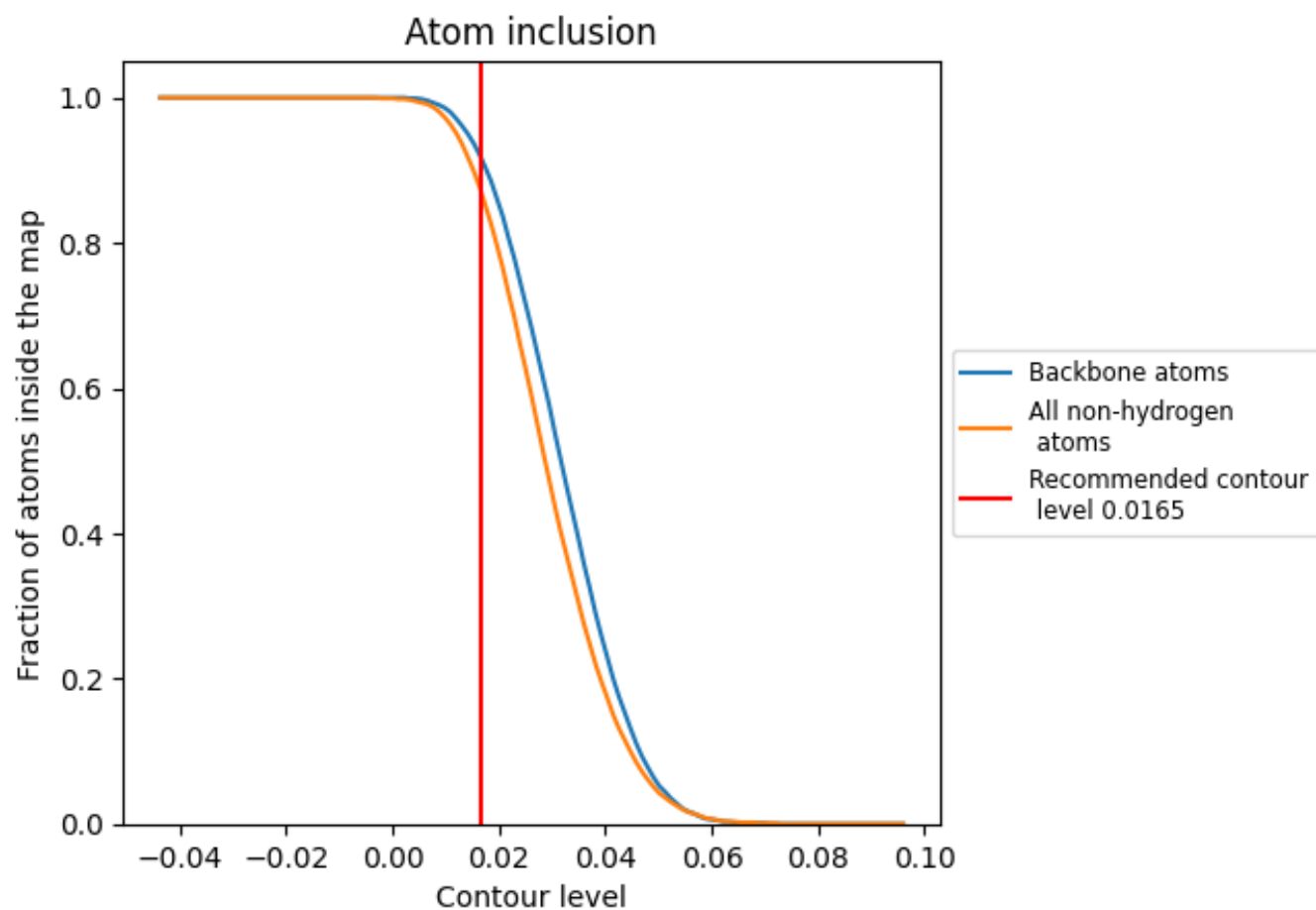
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.3650
4	 0.7590	 0.2470
5	 0.9560	 0.3240
6	 0.7370	 0.2920
7	 0.8780	 0.4000
A	 0.8620	 0.3820
B	 0.7770	 0.3570
C	 0.9500	 0.3930
D	 0.8950	 0.4320
G	 0.8130	 0.3570
L	 0.6570	 0.3490
N	 0.9380	 0.3830
R	 0.9110	 0.3380
S	 0.7060	 0.3240
U	 0.9150	 0.3240
X	 0.7540	 0.4020
z	 0.9620	 0.3970

