



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 01:25 AM UTC

PDB ID : 8HPO / pdb_00008hpo
EMDB ID : EMD-34935
Title : Cryo-EM structure of a SIN3/HDAC complex from budding yeast
Authors : Guo, Z.; Zhan, X.; Wang, C.
Deposited on : 2022-12-12
Resolution : 2.60 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
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

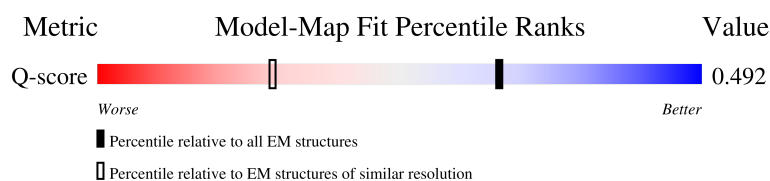
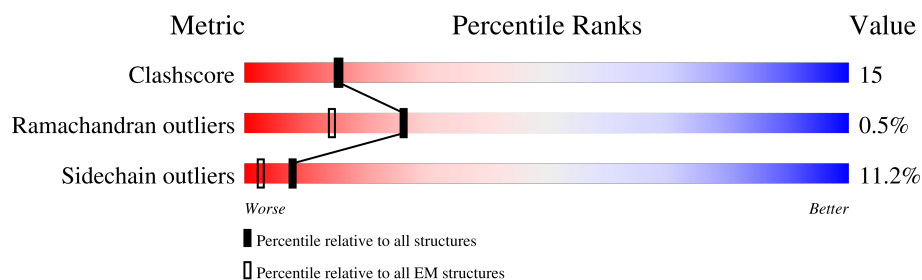
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.



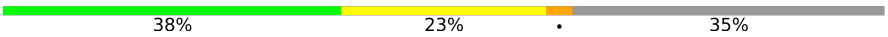
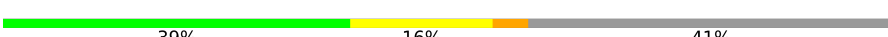
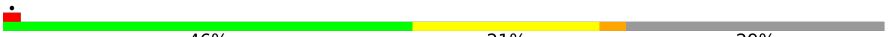
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	K	460	
2	D	327	
3	F	433	
4	G	433	

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Mol	Chain	Length	Quality of chain
5	I	201	
6	A	1536	
6	B	1536	
7	H	405	
8	C	330	
9	E	430	
10	J	294	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SEP	F	265	-	-	X	-
3	TPO	F	365	-	-	X	-
9	TPO	E	167	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 27950 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 Transcriptional regulatory protein UME1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	K	413	Total	C	N	O	0	0
			2038	1212	413	413		

- Molecule 2 is a protein called Transcriptional regulatory protein SDS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	165	Total	C	N	O	P	S	0	0
			1385	863	248	271	1	2		

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	393	Total	C	N	O	P	S	0	0
			3143	1986	525	601	6	25		

- Molecule 4 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	385	Total	C	N	O	S	0	0
			3057	1948	513	571	25		

- Molecule 5 is a protein called Transcriptional regulatory protein SAP30.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	130	Total	C	N	O	P	S	0	0
			1104	696	203	201	1	3		

- Molecule 6 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	637	Total	C	N	O	S	0	0
			5283	3392	887	987	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	613	Total	C	N	O	S	0	0
			5129	3295	862	955	17		

- Molecule 7 is a protein called Transcriptional regulatory protein DEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	233	Total	C	N	O	S	0	0
			1936	1218	340	368	10		

- Molecule 8 is a protein called Transcriptional regulatory protein PHO23.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	138	Total	C	N	O	S	0	0
			1116	703	195	211	7		

- Molecule 9 is a protein called Transcriptional regulatory protein RXT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	E	255	Total	C	N	O	P	S	0	0
			2077	1306	375	391	2	3		

- Molecule 10 is a protein called Transcriptional regulatory protein RXT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	209	Total	C	N	O	S	0	0
			1676	1069	284	321	2		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	F	1	Total	Zn	0
			1	1	
11	G	1	Total	Zn	0
			1	1	

- Molecule 12 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
12	F	2	Total	K	0
			2	2	

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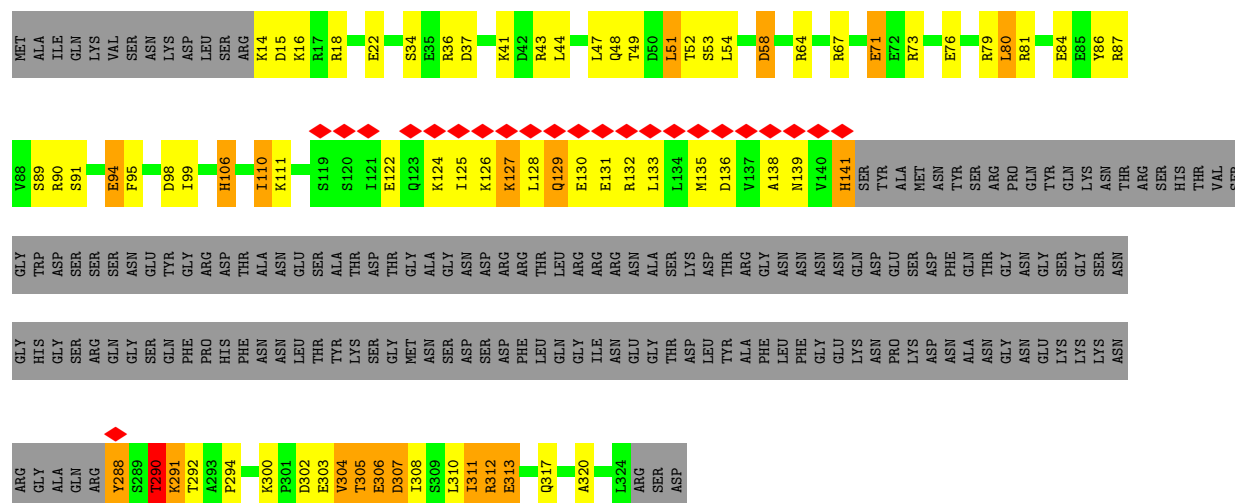
Mol	Chain	Residues	Atoms		AltConf
12	G	2	Total	K	0
			2	2	

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.

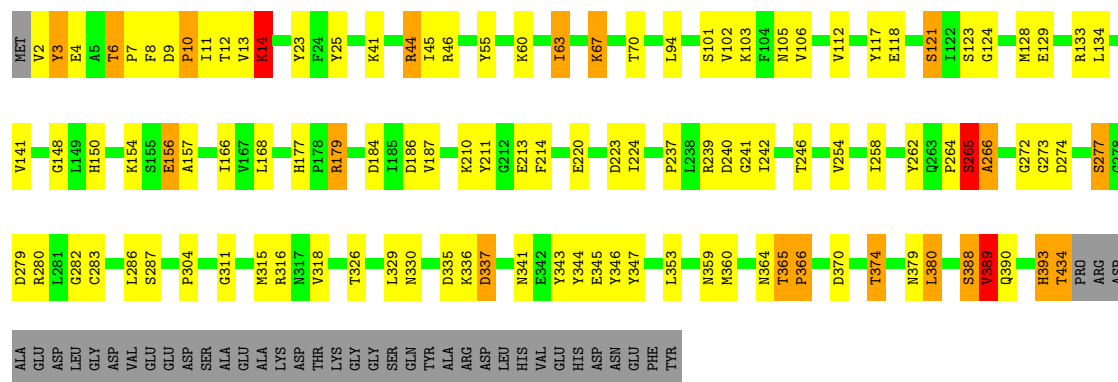
- Molecule 1: Transcriptional regulatory protein UME1





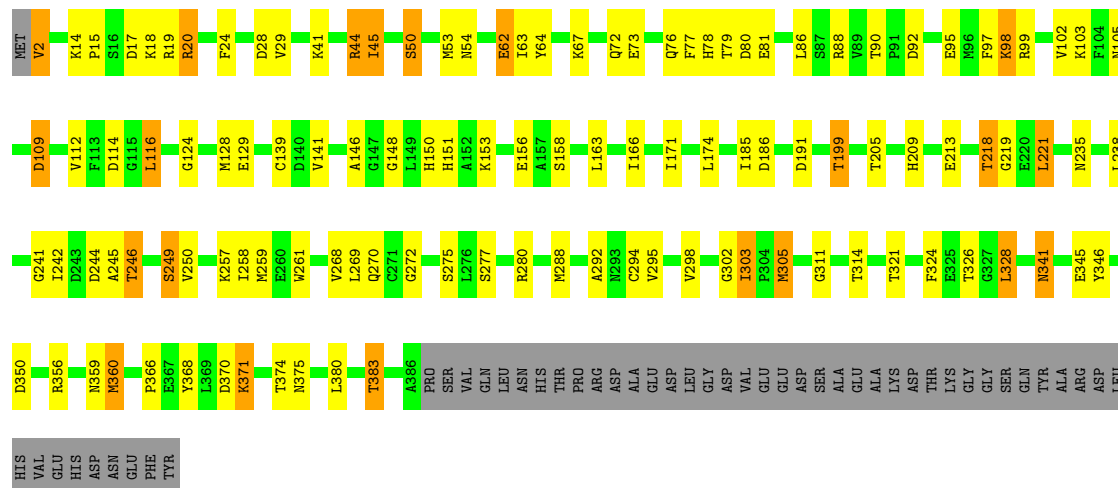
• Molecule 3: Histone deacetylase RPD3

Chain F: 65% 21% 9%



• Molecule 4: Histone deacetylase RPD3

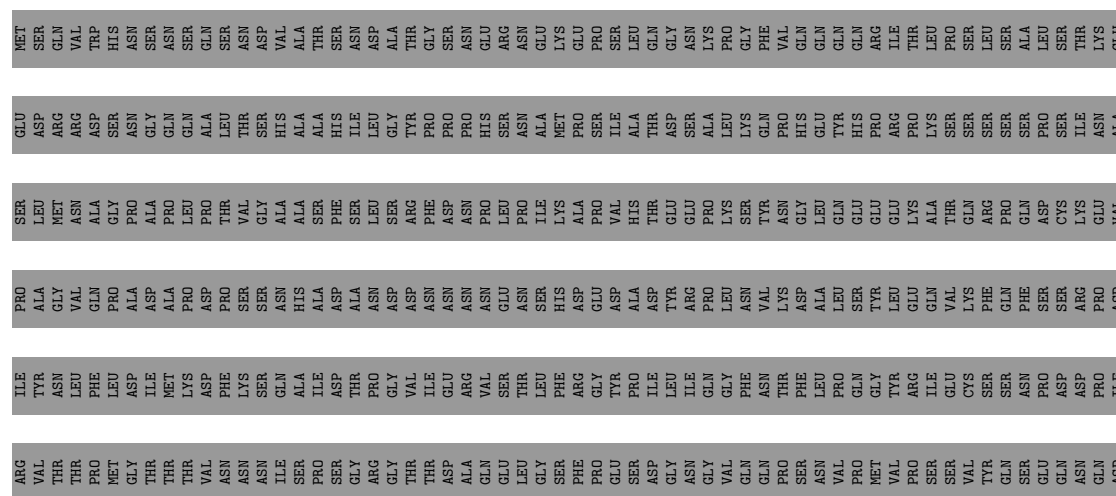
Chain G: 62% 22% 5% 11%



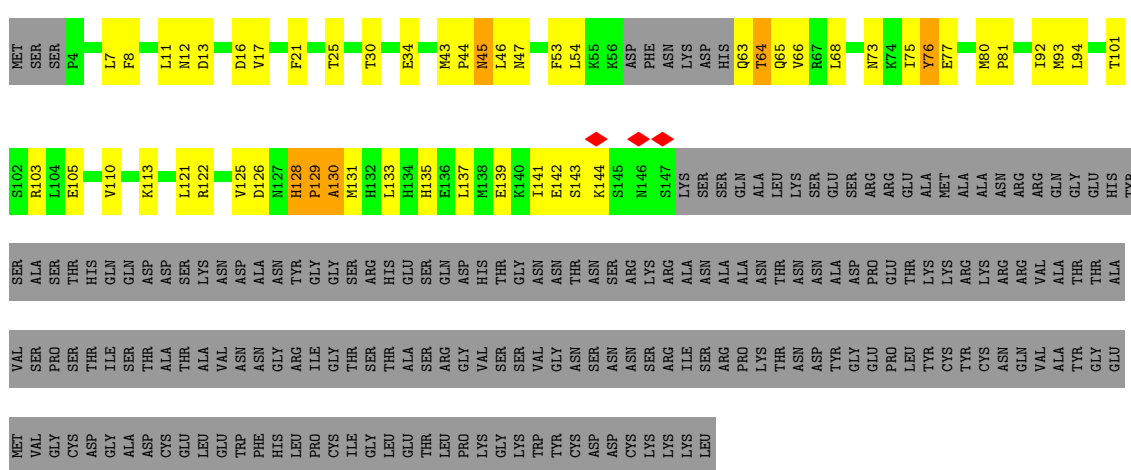
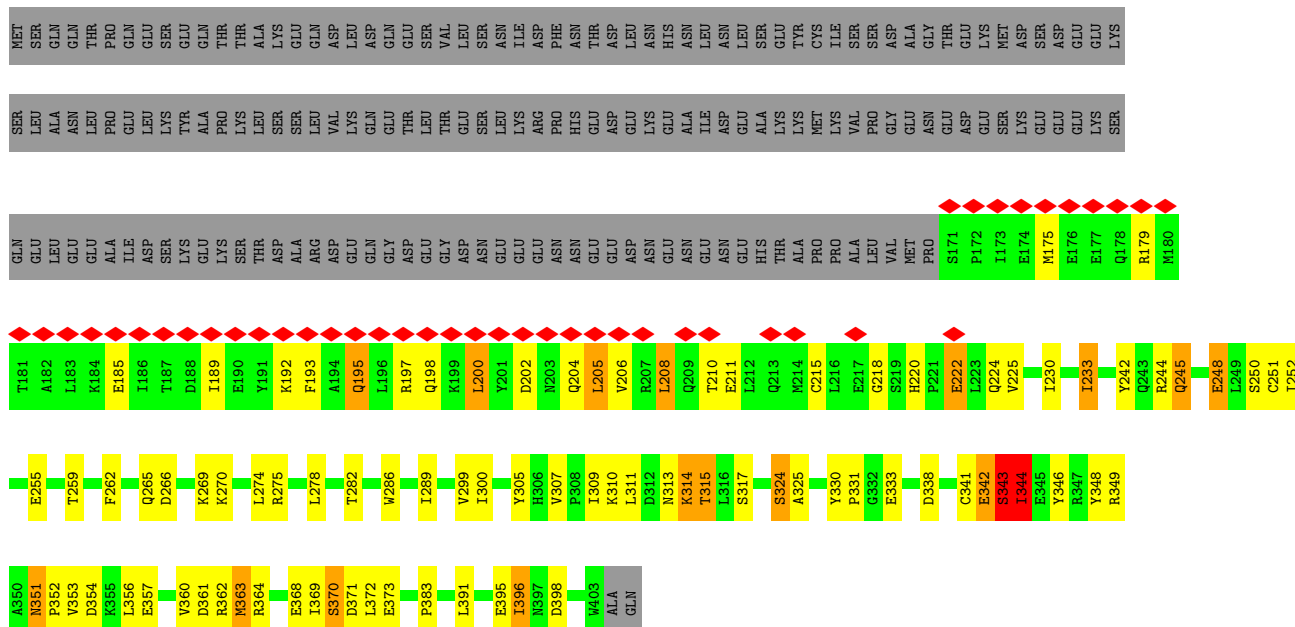
[illegible]

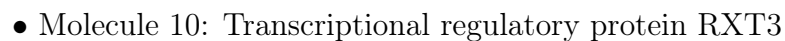
Chain A: 26% 14% 59%

Chain A	Chain B	Chain C	Chain D	Chain E	Chain F	Chain G	Chain H	Chain I	Chain J	Chain K	Chain L	Chain M	Chain N	Chain O	Chain P	Chain Q	Chain R	Chain S	Chain T	Chain U	Chain V	Chain W	Chain X	Chain Y	Chain Z
C767	K671	LEU	THR	THR	GLN	ARG	GLN	ARG	TLE	PRO	SER	PRO	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
R770	A672	PRO	LEU	THR	GLN	ALA	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
C774	K673	ILE	GLU	THR	ALA	GLN	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
L778	L676	SER	GLN	GLN	GLN	PRO	PRO	MET	GLY	ASP	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
N779	G677	PHE	THR	ALA	GLN	ASP	LEU	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
D780	N678	SER	ALA	ALA	GLN	ILE	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
A789	K679	PRO	SER	PRO	GLN	GLN	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
D792	H680	SER	SER	SER	GLN	GLN	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
D792	L681	ASN	ILE	ILE	GLN	PHE	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
D792	Y682	THR	GLN	GLN	GLN	LEU	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
D792	T683	GLY	GLN	GLN	GLN	ILE	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
N801	L686	THR	GLN	GLN	GLN	ILE	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
N802	M690	VAL	GLN	GLN	GLN	GLN	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
T806	L691	HIS	GLN	HIS	GLN	MET	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
L807	Y692	GLU	HIS	GLN	GLN	ALA	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
F808	S693	THR	GLN	GLN	GLN	ALA	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
K809	Q694	SER	SER	SER	GLN	GLN	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
K810	I695	ILE	ILE	ILE	GLN	ASP	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
E811	L699	SER	SER	SER	GLN	GLN	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
D818	D700	PRO	PRO	PRO	GLN	GLN	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
D818	D701	ILE	ILE	ILE	GLN	HIS	GLN	THR	ASN	ALA	LEU	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
E822	L702	ALA	ALA	ALA	GLN	MET	GLN	THR	ASN	ALA	LEU	THR													

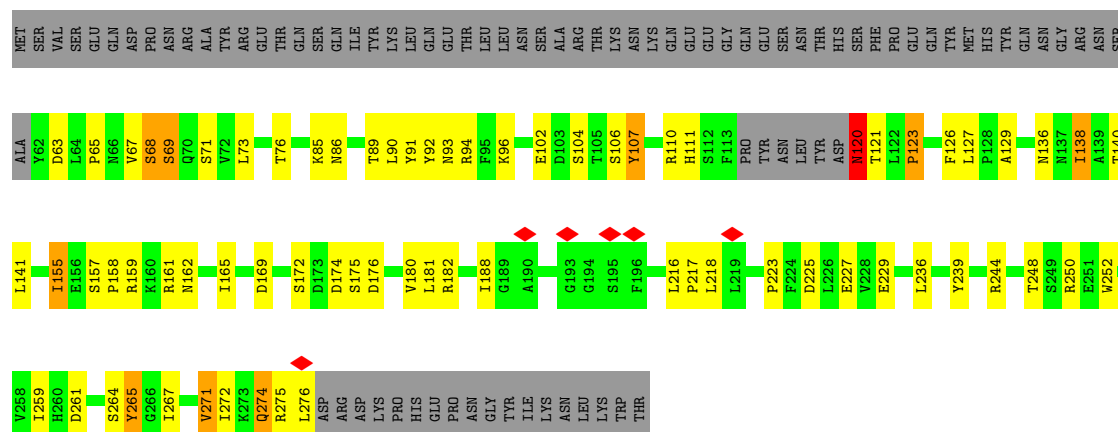








Chain J:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	665105	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.442	Depositor
Minimum map value	-2.664	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, K, SEP, ZN

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	K	0.12	0/2033	0.37	0/2822
2	D	0.60	1/1393 (0.1%)	0.93	7/1866 (0.4%)
3	F	0.65	3/3156 (0.1%)	0.81	14/4262 (0.3%)
4	G	0.24	0/3137	0.45	0/4246
5	I	0.34	0/1119	0.66	1/1500 (0.1%)
6	A	0.24	0/5400	0.48	0/7289
6	B	0.21	0/5245	0.53	1/7077 (0.0%)
7	H	0.26	0/1976	0.52	0/2674
8	C	0.23	0/1134	0.50	0/1529
9	E	0.42	1/2082 (0.0%)	0.67	5/2799 (0.2%)
10	J	0.44	2/1718 (0.1%)	0.69	5/2335 (0.2%)
All	All	0.36	7/28393 (0.0%)	0.59	33/38399 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1
5	I	0	1
6	A	0	1
6	B	0	2
7	H	0	4
9	E	0	2
All	All	0	11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	10	PRO	N-CA	19.07	1.69	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	14	LYS	C-N	18.50	1.50	1.33
10	J	123	PRO	C-N	13.41	1.49	1.33
2	D	294	PRO	C-N	12.91	1.50	1.33
3	F	9	ASP	C-N	10.66	1.46	1.33

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	9	ASP	CA-C-N	17.51	138.67	119.93
3	F	9	ASP	C-N-CA	17.51	138.67	119.93
2	D	307	ASP	CB-CA-C	-13.79	87.91	110.79
10	J	123	PRO	CA-C-N	13.09	133.87	120.38
10	J	123	PRO	C-N-CA	13.09	133.87	120.38

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	891	ALA	Peptide
3	F	265	SEP	Mainchain
7	H	314	LYS	Peptide
7	H	342	GLU	Peptide
5	I	174	SEP	Mainchain

5.2 Too-close contacts [i](#)

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	K	2038	0	890	9	0
2	D	1385	0	1388	87	0
3	F	3143	0	2983	91	0
4	G	3057	0	2932	74	0
5	I	1104	0	1087	47	0
6	A	5283	0	5216	167	0
6	B	5129	0	5096	204	0
7	H	1936	0	1896	66	0
8	C	1116	0	1133	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	2077	0	2136	76	0
10	J	1676	0	1637	45	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
12	F	2	0	0	0	0
12	G	2	0	0	0	0
All	All	27950	0	26394	794	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 15.

The worst 5 of 794 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)
3:F:10:PRO:N	3:F:10:PRO:CA	1.69	1.36
3:F:6:TPO:CG2	3:F:7:PRO:HD2	1.68	1.23
9:E:176:ILE:CD1	9:E:374:LEU:HD12	1.77	1.15
9:E:167:TPO:CG2	9:E:168:PRO:HD2	1.81	1.10
5:I:177:GLU:O	5:I:179:ASP:N	1.82	1.09

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	K	403/460 (88%)	396 (98%)	7 (2%)	0	100	100
2	D	160/327 (49%)	157 (98%)	3 (2%)	0	100	100
3	F	386/433 (89%)	357 (92%)	26 (7%)	3 (1%)	16	34
4	G	383/433 (88%)	360 (94%)	23 (6%)	0	100	100
5	I	127/201 (63%)	110 (87%)	14 (11%)	3 (2%)	4	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	627/1536 (41%)	593 (95%)	32 (5%)	2 (0%)	36	58
6	B	605/1536 (39%)	551 (91%)	54 (9%)	0	100	100
7	H	231/405 (57%)	208 (90%)	20 (9%)	3 (1%)	9	21
8	C	134/330 (41%)	128 (96%)	3 (2%)	3 (2%)	5	10
9	E	245/430 (57%)	217 (89%)	24 (10%)	4 (2%)	7	16
10	J	205/294 (70%)	188 (92%)	17 (8%)	0	100	100
All	All	3506/6385 (55%)	3265 (93%)	223 (6%)	18 (0%)	26	46

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	177	GLU
5	I	178	THR
7	H	344	ILE
9	E	42	GLN
9	E	71	ARG

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	
2	D	153/289 (53%)	125 (82%)	28 (18%)	2	3
3	F	328/361 (91%)	300 (92%)	28 (8%)	10	22
4	G	326/367 (89%)	288 (88%)	38 (12%)	5	11
5	I	119/178 (67%)	107 (90%)	12 (10%)	7	15
6	A	585/1391 (42%)	524 (90%)	61 (10%)	7	14
6	B	574/1391 (41%)	515 (90%)	59 (10%)	7	15
7	H	213/371 (57%)	186 (87%)	27 (13%)	4	9
8	C	129/290 (44%)	120 (93%)	9 (7%)	14	31
9	E	234/391 (60%)	201 (86%)	33 (14%)	3	6
10	J	190/269 (71%)	165 (87%)	25 (13%)	4	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2851/5298 (54%)	2531 (89%)	320 (11%)	8 12

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	E	367	LEU
6	B	1226	GLU
6	B	657	GLU
6	B	881	ASP
10	J	106	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	694	GLN
10	J	120	ASN
6	B	801	ASN
6	B	1206	GLN
6	A	836	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
3	TPO	F	365	3	8,10,11	0.91	0	10,14,16	1.28	2 (20%)
3	TPO	F	12	3	8,10,11	0.84	0	10,14,16	1.17	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPO	F	6	3	8,10,11	1.06	1 (12%)	10,14,16	1.37	1 (10%)
2	SEP	D	309	2	8,9,10	0.97	0	7,12,14	0.83	0
9	SEP	E	171	9	8,9,10	0.71	0	7,12,14	1.52	2 (28%)
3	SEP	F	265	3	8,9,10	2.07	1 (12%)	7,12,14	2.39	3 (42%)
3	TPO	F	434	3	8,10,11	0.65	0	10,14,16	1.46	2 (20%)
5	SEP	I	174	5	8,9,10	1.00	0	7,12,14	0.82	0
9	TPO	E	167	9	8,10,11	3.24	1 (12%)	10,14,16	1.70	2 (20%)
3	SEP	F	388	3	8,9,10	0.75	0	7,12,14	1.11	1 (14%)

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
3	TPO	F	365	3	-	7/9/11/13	-
3	TPO	F	12	3	-	1/9/11/13	-
3	TPO	F	6	3	-	1/9/11/13	-
2	SEP	D	309	2	-	3/6/8/10	-
9	SEP	E	171	9	-	3/6/8/10	-
3	SEP	F	265	3	-	5/6/8/10	-
3	TPO	F	434	3	-	3/9/11/13	-
5	SEP	I	174	5	-	2/6/8/10	-
9	TPO	E	167	9	-	5/9/11/13	-
3	SEP	F	388	3	-	4/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	167	TPO	P-OG1	-8.69	1.44	1.59
3	F	265	SEP	O-C	-4.82	1.01	1.20
3	F	6	TPO	P-O3P	-2.03	1.47	1.54

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	265	SEP	O2P-P-OG	-4.57	94.74	106.67
9	E	167	TPO	P-OG1-CB	-3.99	112.48	123.33
3	F	434	TPO	O-C-CA	-3.01	117.03	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	265	SEP	OG-P-O1P	2.84	114.11	106.44
3	F	365	TPO	P-OG1-CB	-2.82	115.66	123.33

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	309	SEP	C-CA-CB-OG
3	F	12	TPO	O-C-CA-CB
3	F	265	SEP	N-CA-CB-OG
3	F	265	SEP	C-CA-CB-OG
3	F	265	SEP	CB-OG-P-O2P

There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	365	TPO	8	0
3	F	6	TPO	5	0
3	F	265	SEP	6	0
3	F	434	TPO	3	0
9	E	167	TPO	8	0
3	F	388	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

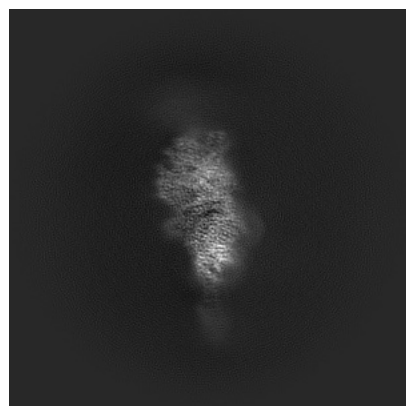
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34935. These allow visual inspection of the internal detail of the map and identification of artifacts.

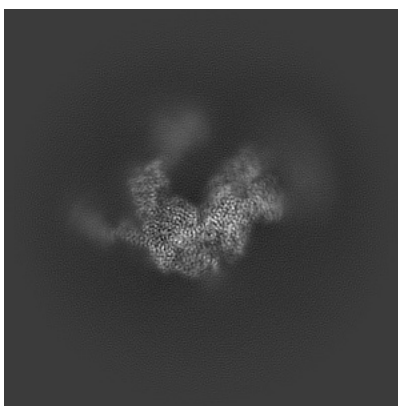
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

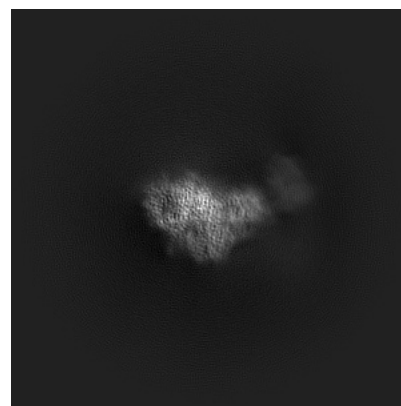
6.1.1 Primary map



X

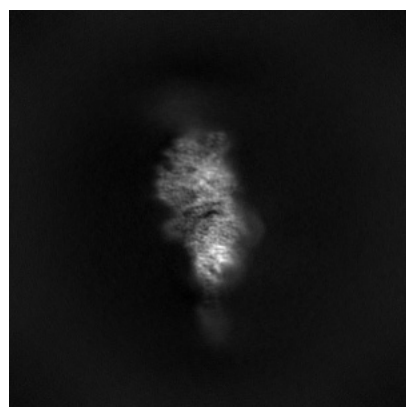


Y

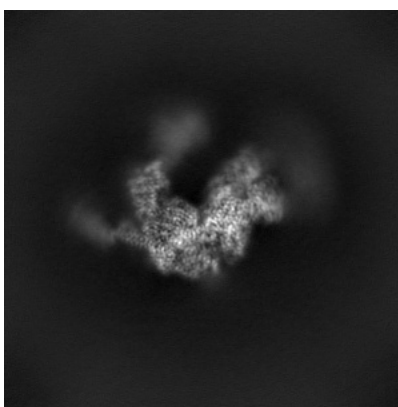


Z

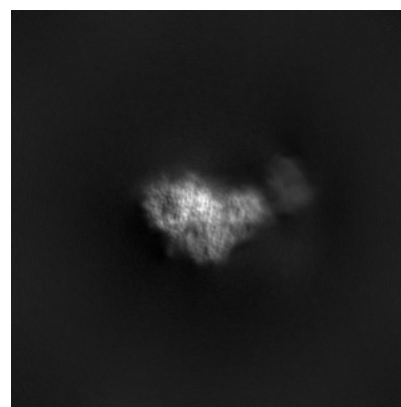
6.1.2 Raw map



X



Y

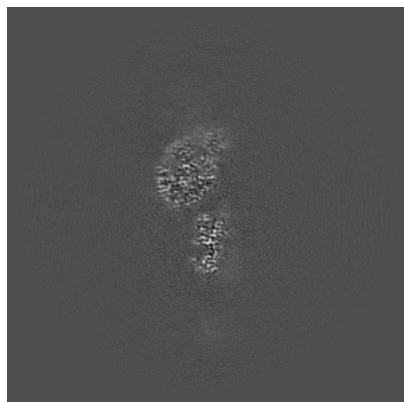


Z

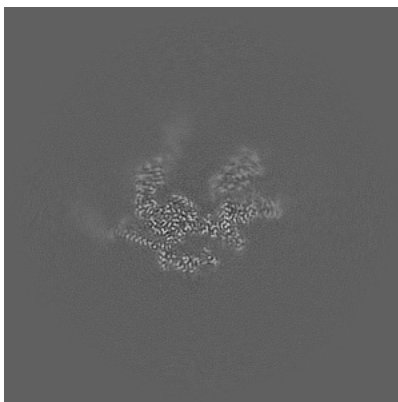
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

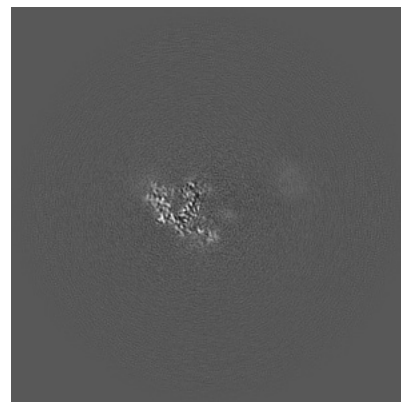
6.2.1 Primary map



X Index: 200

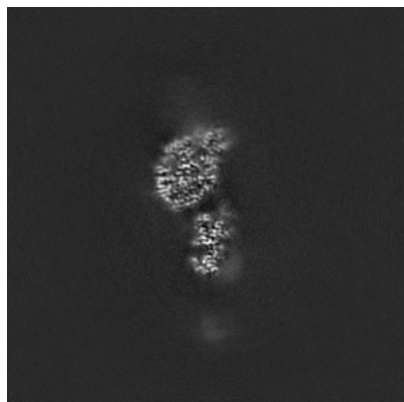


Y Index: 200

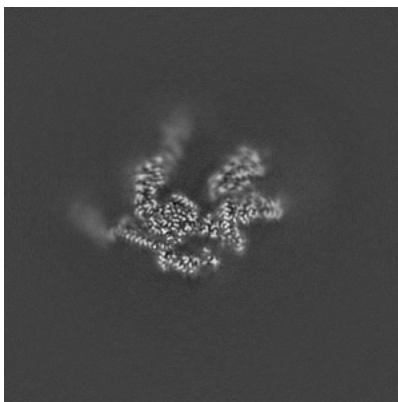


Z Index: 200

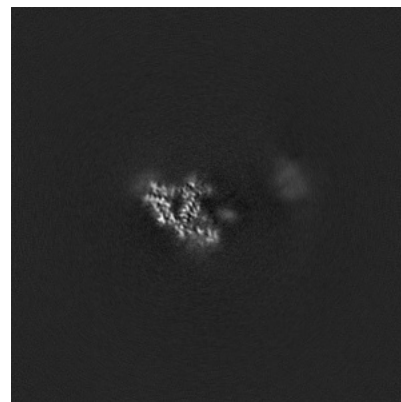
6.2.2 Raw map



X Index: 200



Y Index: 200

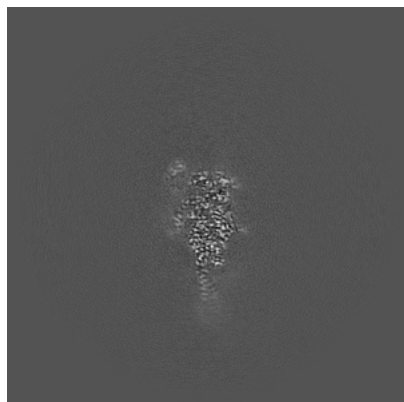


Z Index: 200

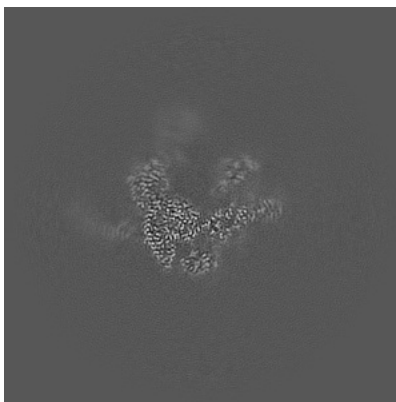
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

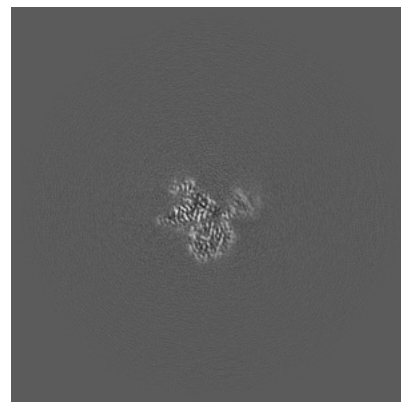
6.3.1 Primary map



X Index: 176

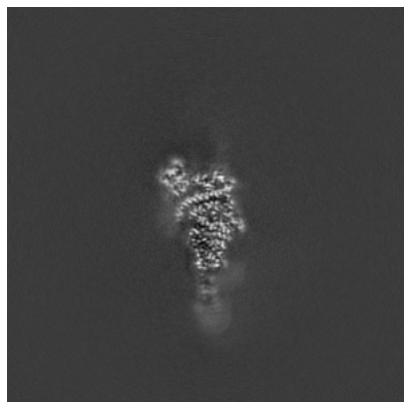


Y Index: 208

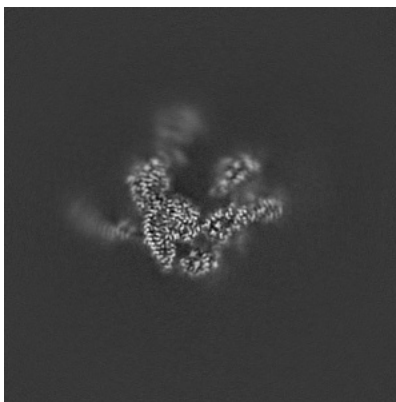


Z Index: 225

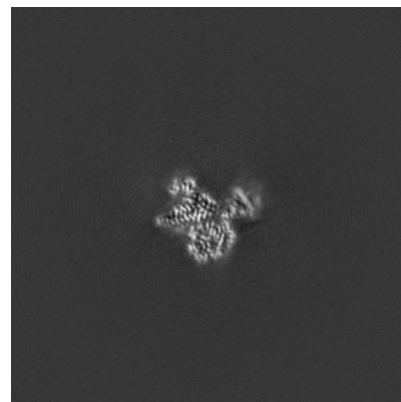
6.3.2 Raw map



X Index: 180



Y Index: 208

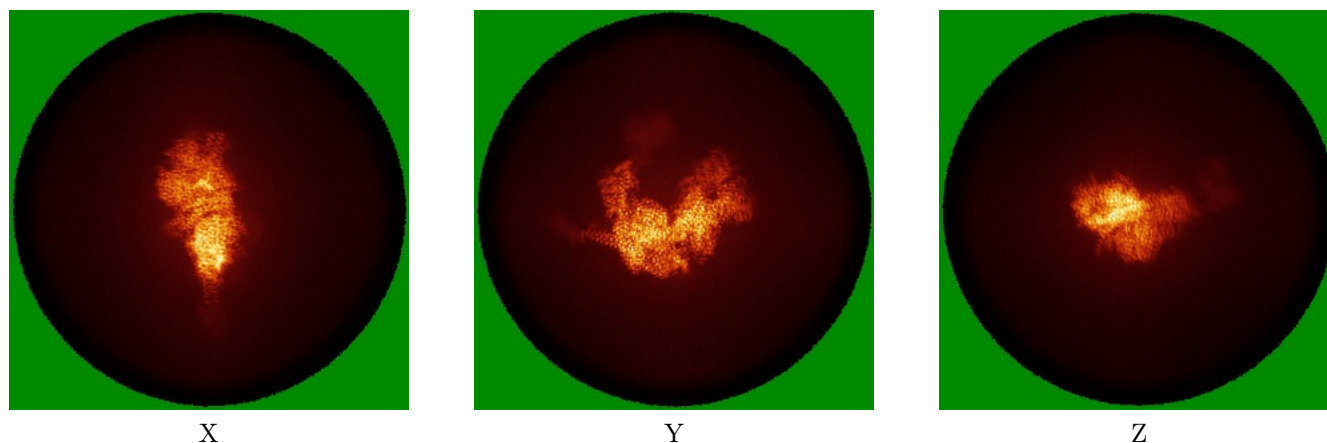


Z Index: 225

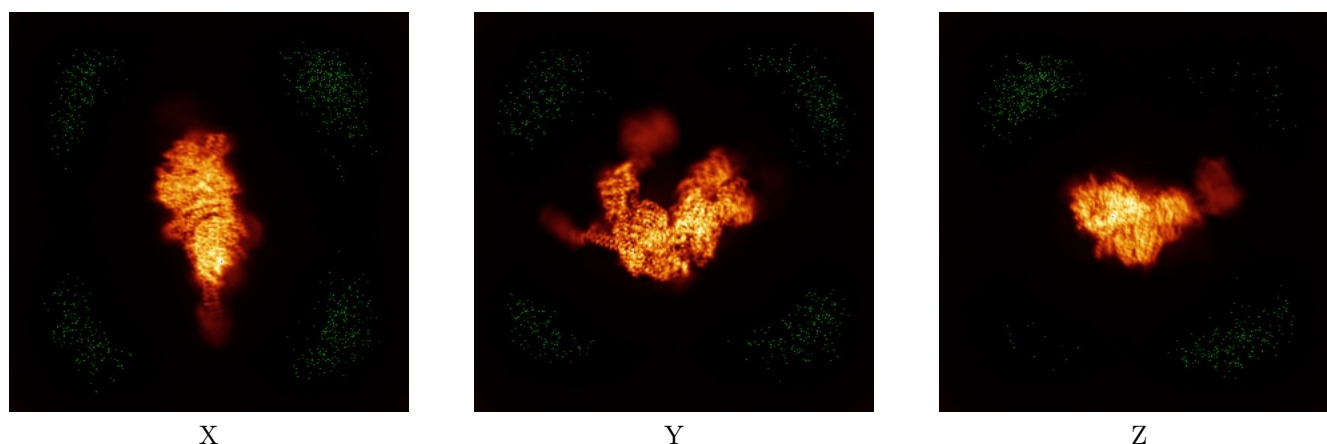
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

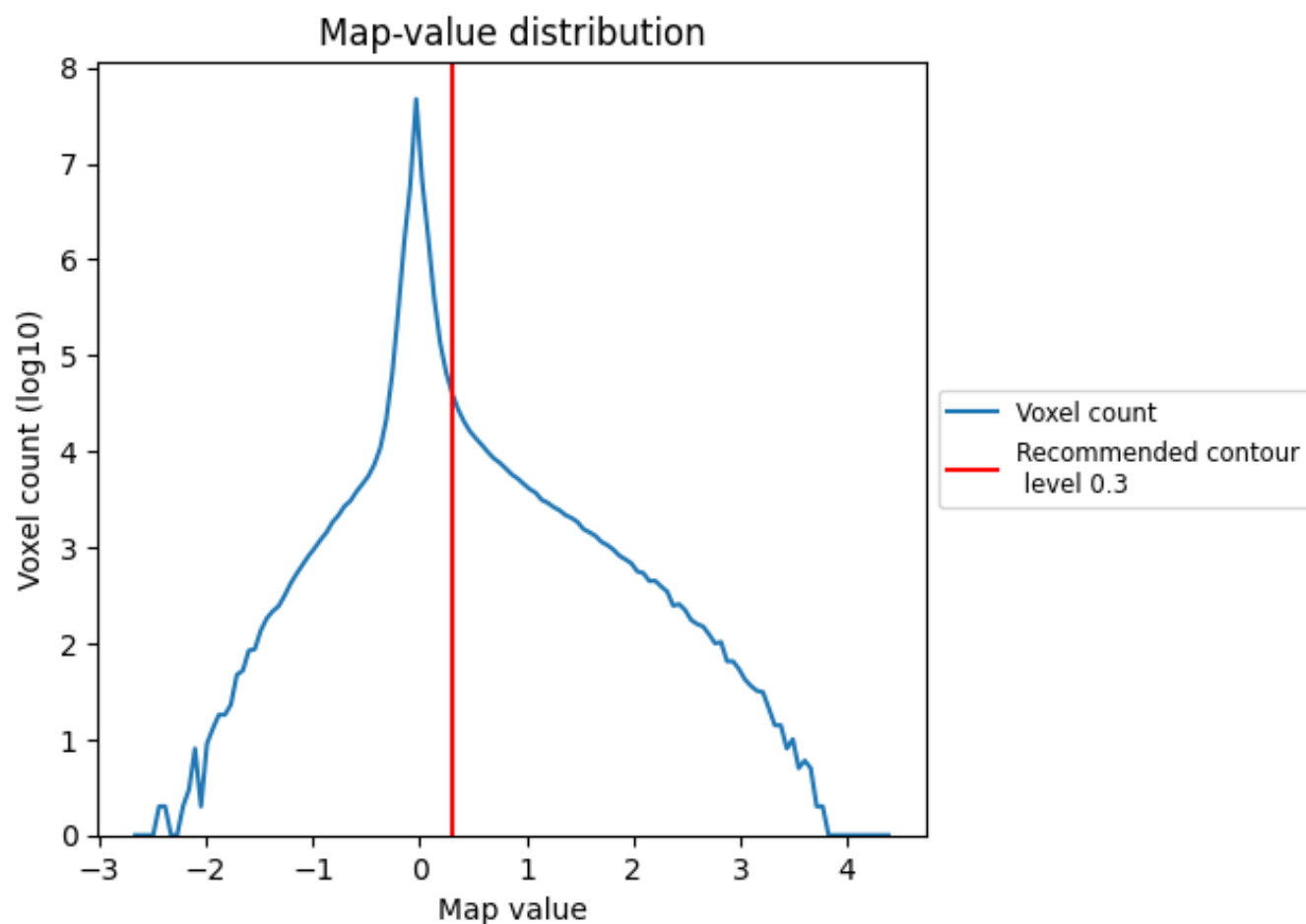
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

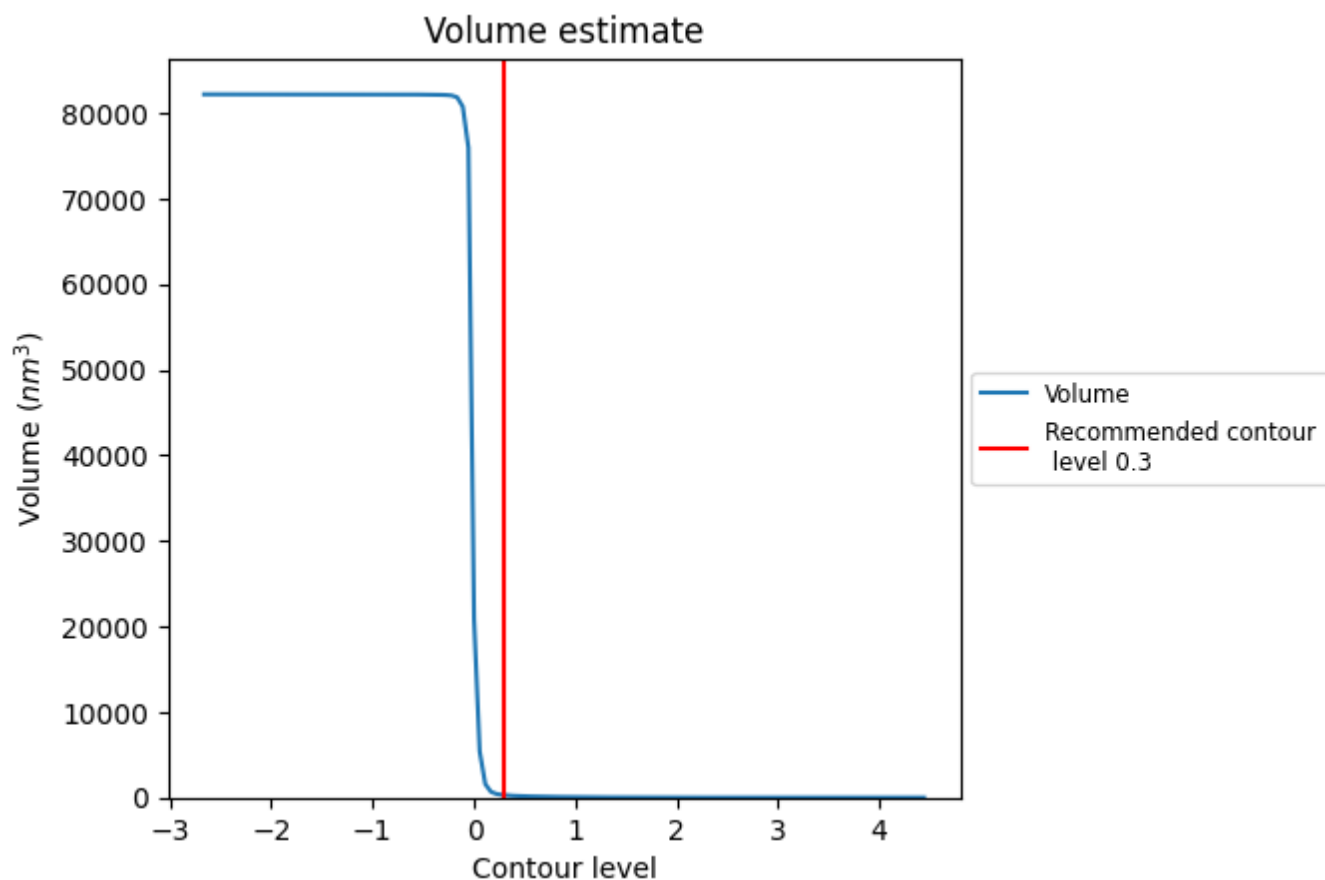
This section contains the results of statistical analysis of the map.

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.

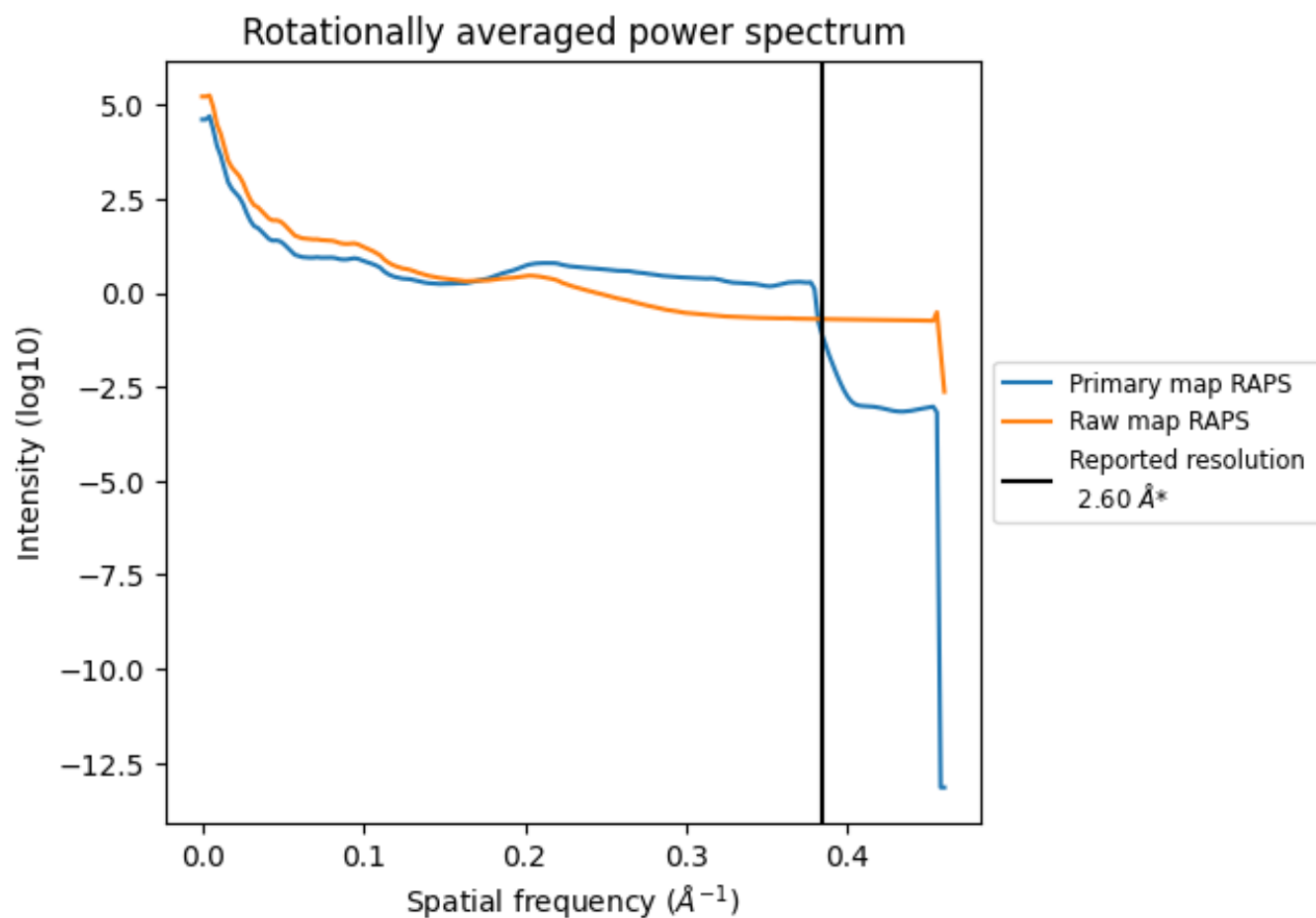
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm^3 ; this corresponds to an approximate mass of 257 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 ⓘ

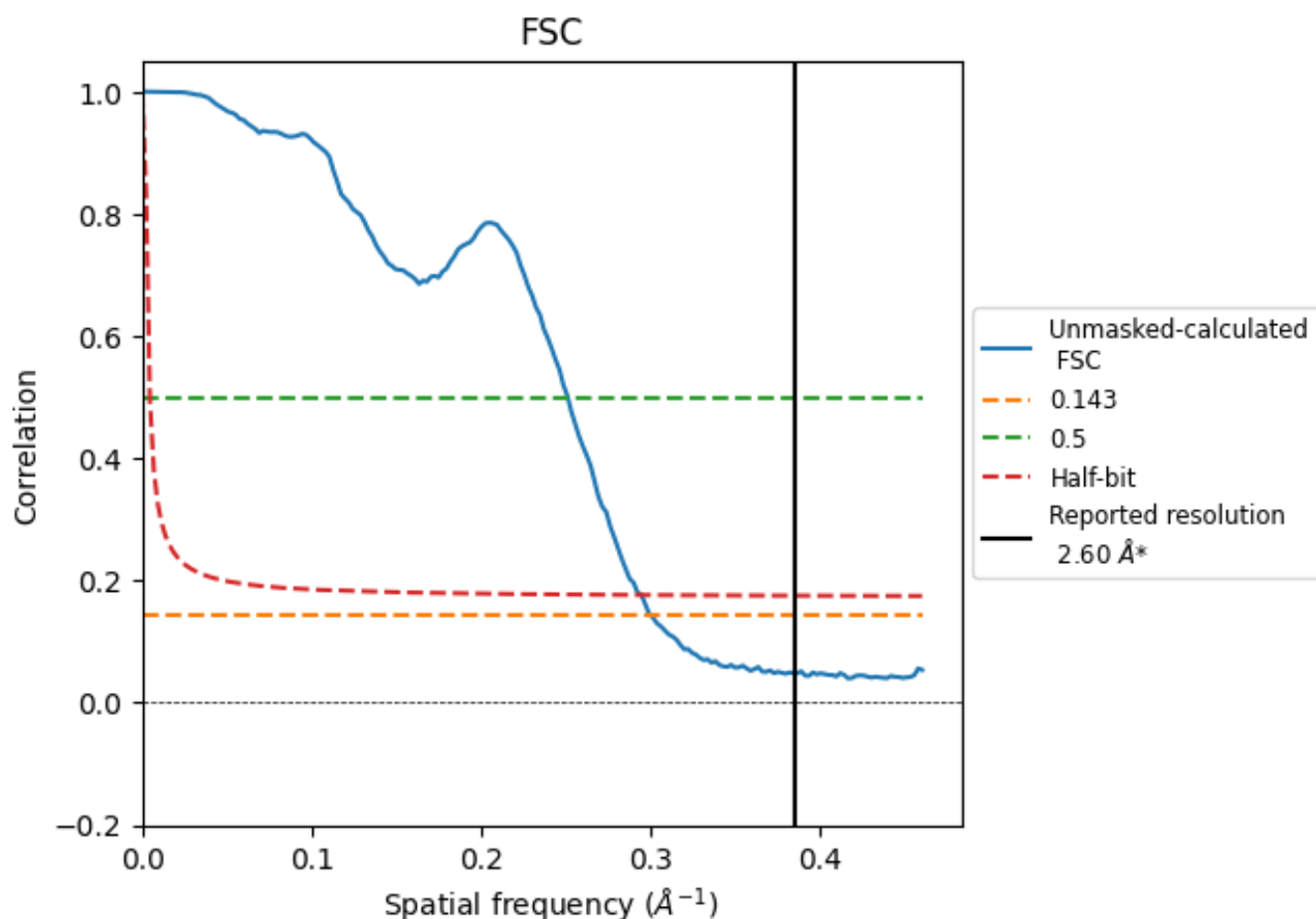


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 $0.385 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

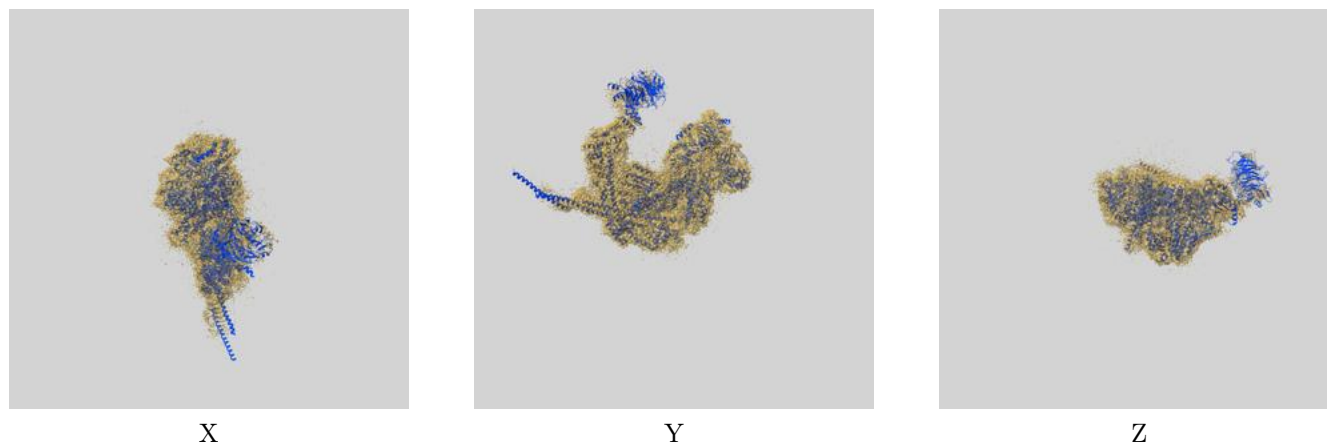
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	3.99	3.40

*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 3.34 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

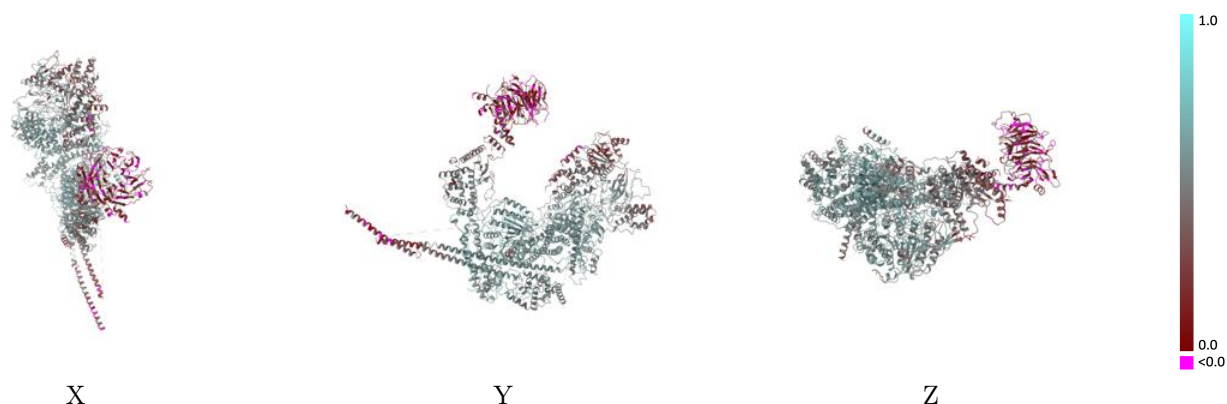
This section contains information regarding the fit between EMDB map EMD-34935 and PDB model 8HPO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



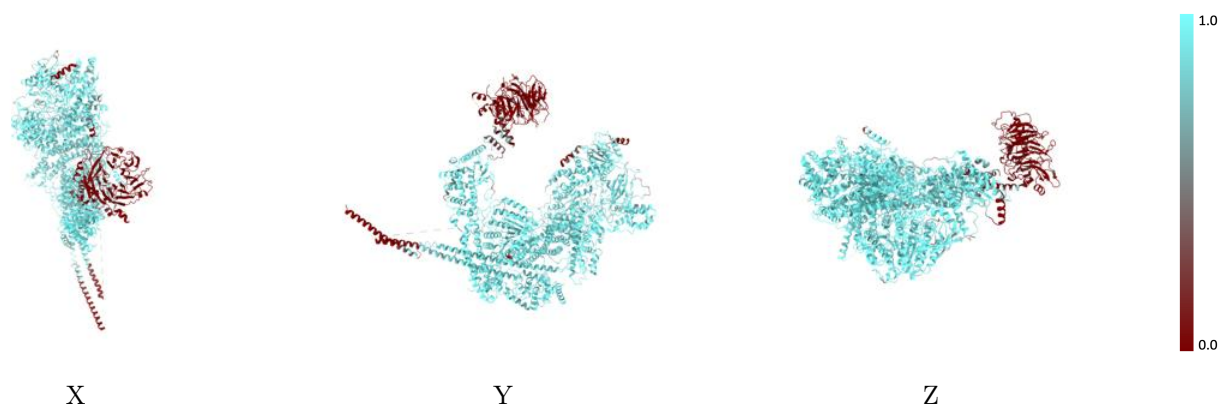
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



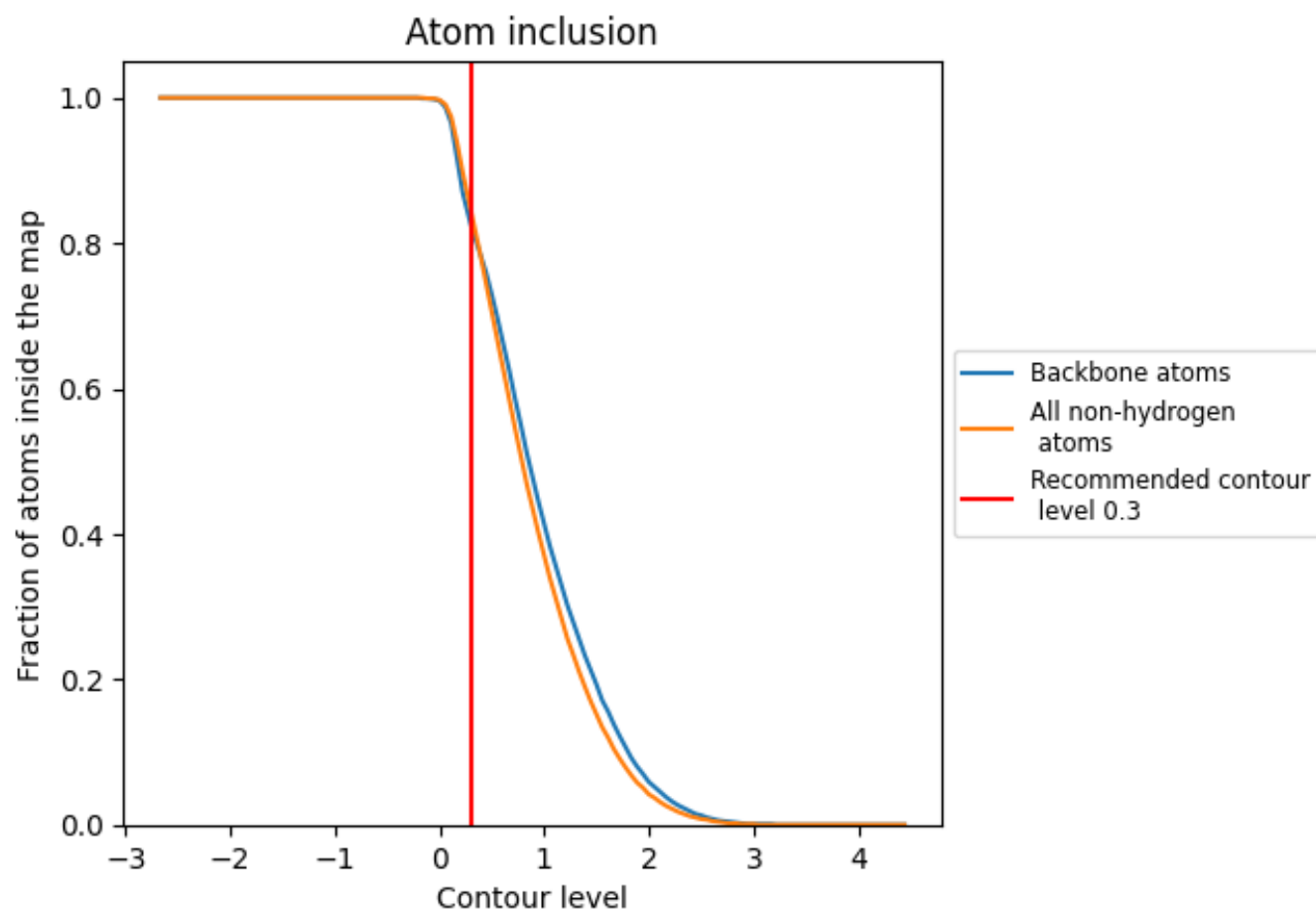
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 84% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.4920
A	0.9060	0.5100
B	0.8730	0.4350
C	0.9450	0.5490
D	0.8150	0.4870
E	0.9620	0.5630
F	0.9820	0.6110
G	0.9760	0.5680
H	0.7740	0.4960
I	0.9440	0.5560
J	0.9110	0.4930
K	0.0340	0.1540

