



# wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 02:23 AM JST

PDB ID : 8J2M  
EMDB ID : EMD-35950  
Title : The truncated rice Na<sup>+</sup>/H<sup>+</sup> antiporter SOS1 (1-976) in a constitutively active state  
Authors : Zhang, X.Y.; Tang, L.H.; Zhang, C.R.; Nie, J.W.; Chen, Y.H.  
Deposited on : 2023-04-14  
Resolution : 3.40 Å(reported)  
Based on initial model : 8IWO

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

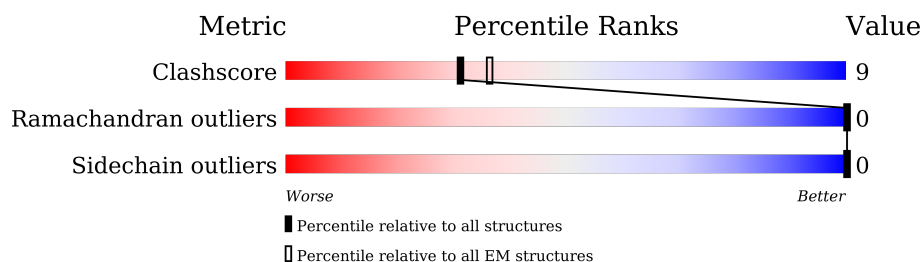
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1038	 33% 8% 59%
1	B	1038	 33% 8% 59%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6574 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 Na<sup>+</sup>/H<sup>+</sup> antiporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	424	Total	C	N	O	S	0	0
			3244	2155	518	560	11		
1	B	424	Total	C	N	O	S	0	0
			3244	2155	518	560	11		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	977	ALA	-	expression tag	UNP Q5ICN3
A	978	ALA	-	expression tag	UNP Q5ICN3
A	979	ALA	-	expression tag	UNP Q5ICN3
A	980	GLU	-	expression tag	UNP Q5ICN3
A	981	ASN	-	expression tag	UNP Q5ICN3
A	982	LEU	-	expression tag	UNP Q5ICN3
A	983	TYR	-	expression tag	UNP Q5ICN3
A	984	PHE	-	expression tag	UNP Q5ICN3
A	985	GLN	-	expression tag	UNP Q5ICN3
A	986	GLY	-	expression tag	UNP Q5ICN3
A	987	LEU	-	expression tag	UNP Q5ICN3
A	988	GLU	-	expression tag	UNP Q5ICN3
A	989	TRP	-	expression tag	UNP Q5ICN3
A	990	SER	-	expression tag	UNP Q5ICN3
A	991	HIS	-	expression tag	UNP Q5ICN3
A	992	PRO	-	expression tag	UNP Q5ICN3
A	993	GLN	-	expression tag	UNP Q5ICN3
A	994	PHE	-	expression tag	UNP Q5ICN3
A	995	GLU	-	expression tag	UNP Q5ICN3
A	996	LYS	-	expression tag	UNP Q5ICN3
A	997	GLY	-	expression tag	UNP Q5ICN3
A	998	SER	-	expression tag	UNP Q5ICN3
A	999	GLY	-	expression tag	UNP Q5ICN3
A	1000	ASP	-	expression tag	UNP Q5ICN3
A	1001	TYR	-	expression tag	UNP Q5ICN3
A	1002	LYS	-	expression tag	UNP Q5ICN3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1003	ASP	-	expression tag	UNP Q5ICN3
A	1004	ASP	-	expression tag	UNP Q5ICN3
A	1005	ASP	-	expression tag	UNP Q5ICN3
A	1006	ASP	-	expression tag	UNP Q5ICN3
A	1007	LYS	-	expression tag	UNP Q5ICN3
A	1008	GLY	-	expression tag	UNP Q5ICN3
A	1009	SER	-	expression tag	UNP Q5ICN3
A	1010	GLY	-	expression tag	UNP Q5ICN3
A	1011	TRP	-	expression tag	UNP Q5ICN3
A	1012	SER	-	expression tag	UNP Q5ICN3
A	1013	HIS	-	expression tag	UNP Q5ICN3
A	1014	PRO	-	expression tag	UNP Q5ICN3
A	1015	GLN	-	expression tag	UNP Q5ICN3
A	1016	PHE	-	expression tag	UNP Q5ICN3
A	1017	GLU	-	expression tag	UNP Q5ICN3
A	1018	LYS	-	expression tag	UNP Q5ICN3
A	1019	LEU	-	expression tag	UNP Q5ICN3
A	1020	GLU	-	expression tag	UNP Q5ICN3
A	1021	ASP	-	expression tag	UNP Q5ICN3
A	1022	TYR	-	expression tag	UNP Q5ICN3
A	1023	LYS	-	expression tag	UNP Q5ICN3
A	1024	ASP	-	expression tag	UNP Q5ICN3
A	1025	ASP	-	expression tag	UNP Q5ICN3
A	1026	ASP	-	expression tag	UNP Q5ICN3
A	1027	ASP	-	expression tag	UNP Q5ICN3
A	1028	LYS	-	expression tag	UNP Q5ICN3
A	1029	HIS	-	expression tag	UNP Q5ICN3
A	1030	HIS	-	expression tag	UNP Q5ICN3
A	1031	HIS	-	expression tag	UNP Q5ICN3
A	1032	HIS	-	expression tag	UNP Q5ICN3
A	1033	HIS	-	expression tag	UNP Q5ICN3
A	1034	HIS	-	expression tag	UNP Q5ICN3
A	1035	HIS	-	expression tag	UNP Q5ICN3
A	1036	HIS	-	expression tag	UNP Q5ICN3
A	1037	HIS	-	expression tag	UNP Q5ICN3
A	1038	HIS	-	expression tag	UNP Q5ICN3
B	977	ALA	-	expression tag	UNP Q5ICN3
B	978	ALA	-	expression tag	UNP Q5ICN3
B	979	ALA	-	expression tag	UNP Q5ICN3
B	980	GLU	-	expression tag	UNP Q5ICN3
B	981	ASN	-	expression tag	UNP Q5ICN3
B	982	LEU	-	expression tag	UNP Q5ICN3

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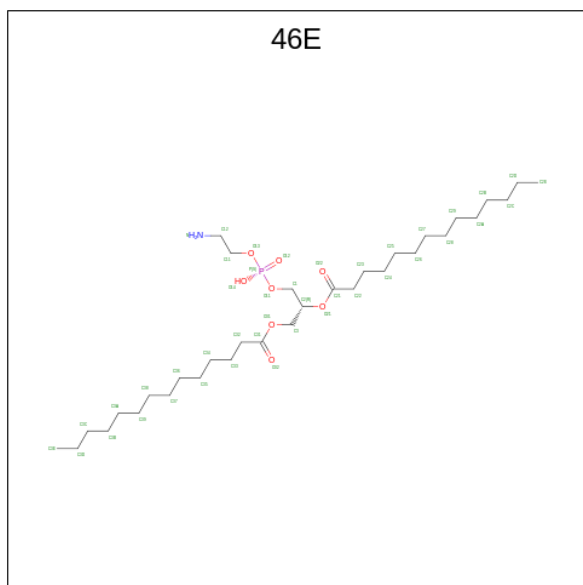
Chain	Residue	Modelled	Actual	Comment	Reference
B	983	TYR	-	expression tag	UNP Q5ICN3
B	984	PHE	-	expression tag	UNP Q5ICN3
B	985	GLN	-	expression tag	UNP Q5ICN3
B	986	GLY	-	expression tag	UNP Q5ICN3
B	987	LEU	-	expression tag	UNP Q5ICN3
B	988	GLU	-	expression tag	UNP Q5ICN3
B	989	TRP	-	expression tag	UNP Q5ICN3
B	990	SER	-	expression tag	UNP Q5ICN3
B	991	HIS	-	expression tag	UNP Q5ICN3
B	992	PRO	-	expression tag	UNP Q5ICN3
B	993	GLN	-	expression tag	UNP Q5ICN3
B	994	PHE	-	expression tag	UNP Q5ICN3
B	995	GLU	-	expression tag	UNP Q5ICN3
B	996	LYS	-	expression tag	UNP Q5ICN3
B	997	GLY	-	expression tag	UNP Q5ICN3
B	998	SER	-	expression tag	UNP Q5ICN3
B	999	GLY	-	expression tag	UNP Q5ICN3
B	1000	ASP	-	expression tag	UNP Q5ICN3
B	1001	TYR	-	expression tag	UNP Q5ICN3
B	1002	LYS	-	expression tag	UNP Q5ICN3
B	1003	ASP	-	expression tag	UNP Q5ICN3
B	1004	ASP	-	expression tag	UNP Q5ICN3
B	1005	ASP	-	expression tag	UNP Q5ICN3
B	1006	ASP	-	expression tag	UNP Q5ICN3
B	1007	LYS	-	expression tag	UNP Q5ICN3
B	1008	GLY	-	expression tag	UNP Q5ICN3
B	1009	SER	-	expression tag	UNP Q5ICN3
B	1010	GLY	-	expression tag	UNP Q5ICN3
B	1011	TRP	-	expression tag	UNP Q5ICN3
B	1012	SER	-	expression tag	UNP Q5ICN3
B	1013	HIS	-	expression tag	UNP Q5ICN3
B	1014	PRO	-	expression tag	UNP Q5ICN3
B	1015	GLN	-	expression tag	UNP Q5ICN3
B	1016	PHE	-	expression tag	UNP Q5ICN3
B	1017	GLU	-	expression tag	UNP Q5ICN3
B	1018	LYS	-	expression tag	UNP Q5ICN3
B	1019	LEU	-	expression tag	UNP Q5ICN3
B	1020	GLU	-	expression tag	UNP Q5ICN3
B	1021	ASP	-	expression tag	UNP Q5ICN3
B	1022	TYR	-	expression tag	UNP Q5ICN3
B	1023	LYS	-	expression tag	UNP Q5ICN3
B	1024	ASP	-	expression tag	UNP Q5ICN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1025	ASP	-	expression tag	UNP Q5ICN3
B	1026	ASP	-	expression tag	UNP Q5ICN3
B	1027	ASP	-	expression tag	UNP Q5ICN3
B	1028	LYS	-	expression tag	UNP Q5ICN3
B	1029	HIS	-	expression tag	UNP Q5ICN3
B	1030	HIS	-	expression tag	UNP Q5ICN3
B	1031	HIS	-	expression tag	UNP Q5ICN3
B	1032	HIS	-	expression tag	UNP Q5ICN3
B	1033	HIS	-	expression tag	UNP Q5ICN3
B	1034	HIS	-	expression tag	UNP Q5ICN3
B	1035	HIS	-	expression tag	UNP Q5ICN3
B	1036	HIS	-	expression tag	UNP Q5ICN3
B	1037	HIS	-	expression tag	UNP Q5ICN3
B	1038	HIS	-	expression tag	UNP Q5ICN3

- Molecule 2 is (2R)-3-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-(tetradecanoyloxy)propyl tetradecanoate (three-letter code: 46E) (formula: C<sub>33</sub>H<sub>66</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
2	B	1	Total	C	N	O	P	0
			43	33	1	8	1	



LEU	GLN	ARG	SER	ALA	LEU	SER	LEU	ILE	SER	GLN	THR	LEU	GLU	LEU	PRO	ARG	THR	GLN	SER	ALA	ALA	ALA	GLU	ASN	LEU	TYR	PHE	GLN	GLY	LEU	GLU	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	SER	TYR	ASP	ASP	LYS		
LYS	LEU	GLU	ASP	TYR	LYS	ASP	ASP	ASP	ASP	ASP	LYS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLU	ASP	GLY	ASP	GLY	GLY	GLY	ASP	ASP	LYS	GLY	SER	TRP	HIS	PRO	GLN	PHE	GLU	LYS	ASP	ASP	ASP	ASP	ASP	ASP

● Molecule 1: Na<sup>+</sup>/H<sup>+</sup> antiporter



TRP	PRO	GLY	GLU	GLN	ARG	GLY	GLU	GLN	ARG	VAL	VAL	ARG	THR	ASP	V398	F249	MET	ASP	ASN	PRO	GLU	ALA	E7	P8	D9	L13	L19	I23	R26	R30	G31	T32	R33	V38	V42	S49	L50	T54	K55	H56	G59	K60	G64	I67	L75	V79	F86	E87	M92	F93	I94	I97	G109	L113	F118								
SER	GLU	LEU	PHE	THR	LEU	THR	THR	THR	LEU	ARG	THR	GLY	THR	TRP	M402	L255	N132	THR	VAL	THR	VAL	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
PRO	ILE	LYS	THR	ASN	GLN	THR	ALA	THR	PRO	THR	VAL	THR	THR	THR	F405	L266	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLN	ARG	THR	THR	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F411	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V391	Q392	T393	H394	L395	K396	P397
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F412	Y270	F249	THR	LYS	THR	THR	LYS	T146	D147	P148	V151	V152	E157	L158	T166	E169	G170	E171	N175	Y183	R188	R193	T194	F195	D196	A197	G198	F203	L204	S205	E206	V207	A211	L216	G219	L220	N231	S387	S388	D389	A390	V						



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	43851	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.598	Depositor
Minimum map value	-0.351	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.158	Depositor
Map size ( $\text{\AA}$ )	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 46E

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	0.48	0/3317	0.66	0/4510
1	B	0.48	0/3317	0.66	0/4510
All	All	0.48	0/6634	0.66	0/9020

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	3244	0	3374	62	0
1	B	3244	0	3374	61	0
2	A	43	0	0	0	0
2	B	43	0	0	0	0
All	All	6574	0	6748	114	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 114 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)
1:A:292:MET:SD	1:B:234:ILE:HG23	2.29	0.73
1:A:234:ILE:HG23	1:B:292:MET:SD	2.32	0.70
1:A:203:PHE:HD2	1:A:204:LEU:HD12	1.58	0.69
1:B:203:PHE:HD2	1:B:204:LEU:HD12	1.58	0.68
1:B:146:THR:O	1:B:147:ASP:OD1	2.12	0.67

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	422/1038 (41%)	408 (97%)	14 (3%)	0	100	100
1	B	422/1038 (41%)	408 (97%)	14 (3%)	0	100	100
All	All	844/2076 (41%)	816 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	344/891 (39%)	344 (100%)	0	100	100
1	B	344/891 (39%)	344 (100%)	0	100	100
All	All	688/1782 (39%)	688 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

2 ligands 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	$\# Z  > 2$
2	46E	B	1101	-	42,42,42	0.32	0	45,47,47	0.35	0
2	46E	A	1101	-	42,42,42	0.31	0	45,47,47	0.35	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
2	46E	B	1101	-	-	30/46/46/46	-
2	46E	A	1101	-	-	30/46/46/46	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

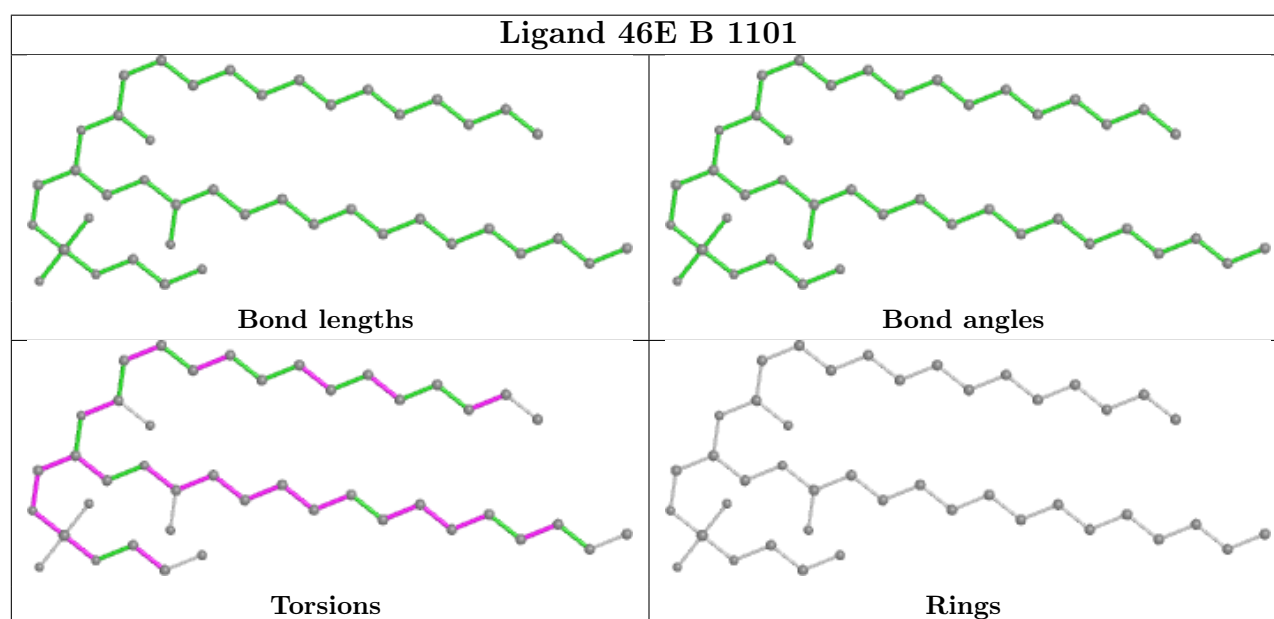
5 of 60 torsion outliers are listed below:

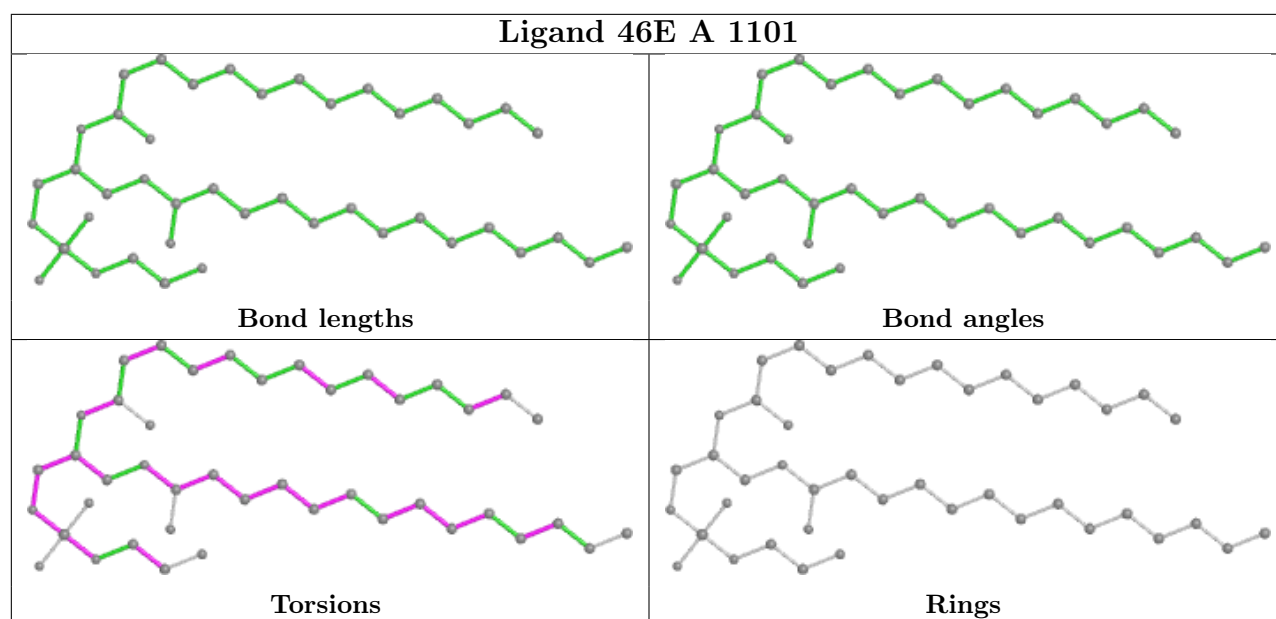
Mol	Chain	Res	Type	Atoms
2	A	1101	46E	C1-O11-P-O12
2	A	1101	46E	C1-O11-P-O13
2	A	1101	46E	C1-O11-P-O14
2	A	1101	46E	C11-O13-P-O11
2	A	1101	46E	C11-O13-P-O12

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.

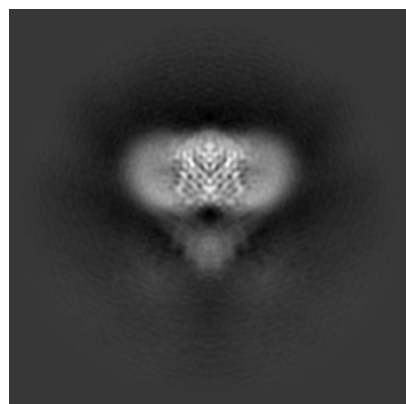
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35950. These allow visual inspection of the internal detail of the map and identification of artifacts.

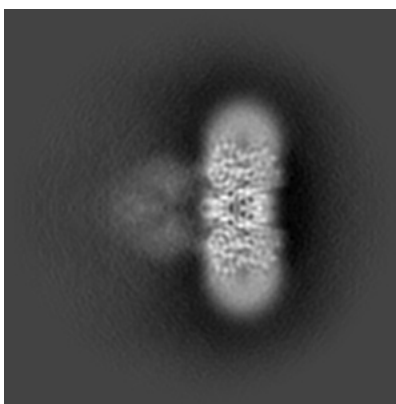
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

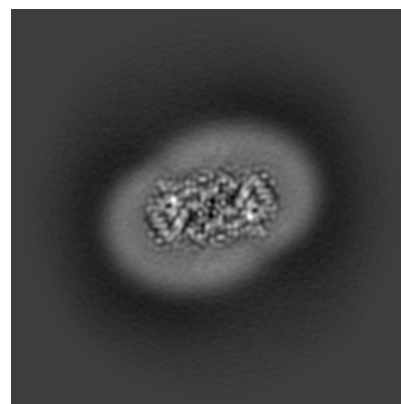
#### 6.1.1 Primary map



X

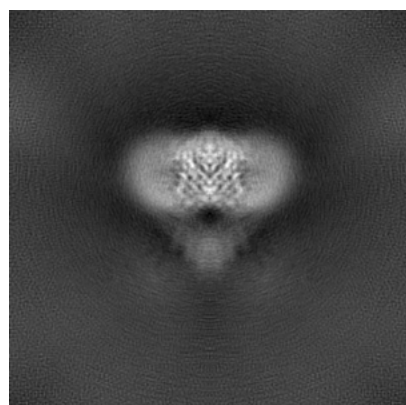


Y

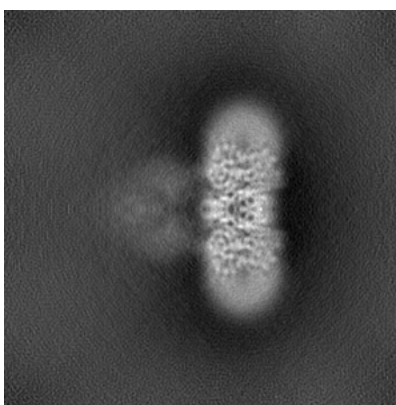


Z

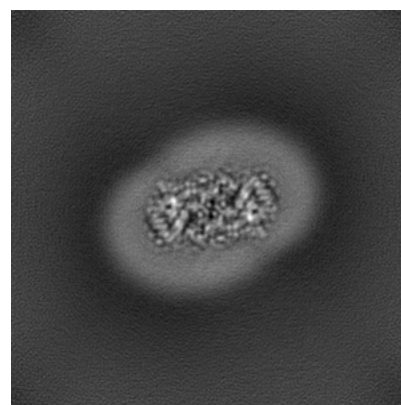
#### 6.1.2 Raw map



X



Y

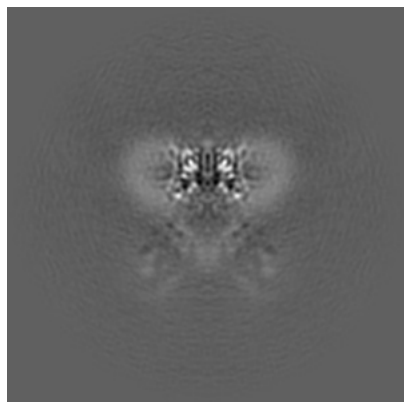


Z

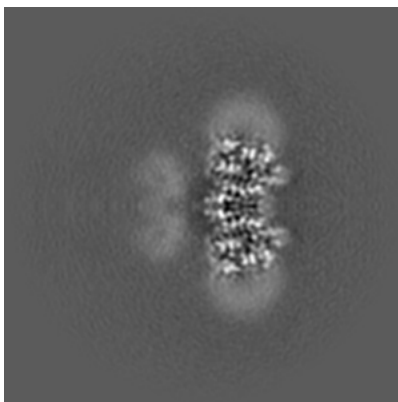
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

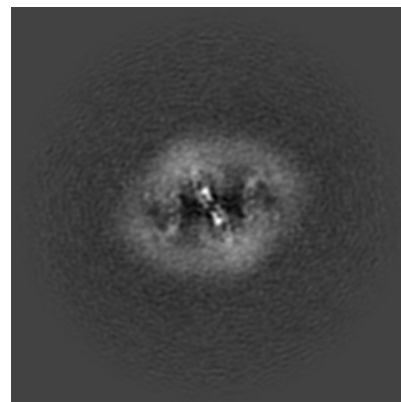
### 6.2.1 Primary map



X Index: 128

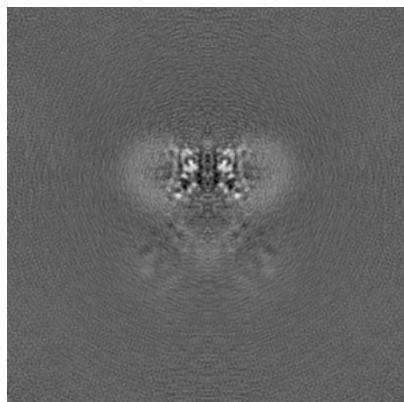


Y Index: 128

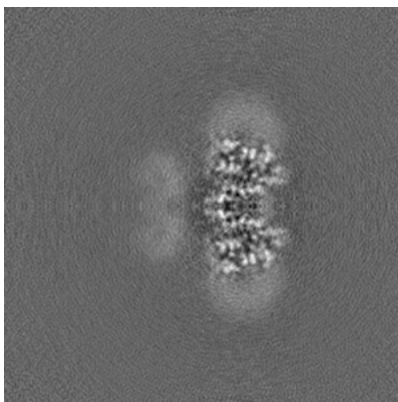


Z Index: 128

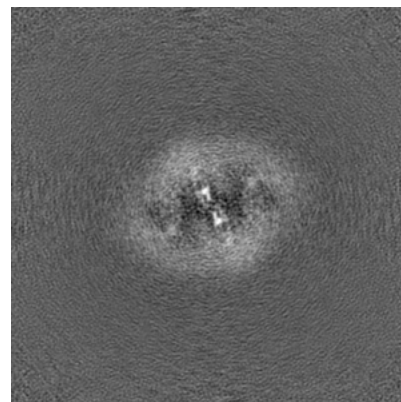
### 6.2.2 Raw map



X Index: 128



Y Index: 128



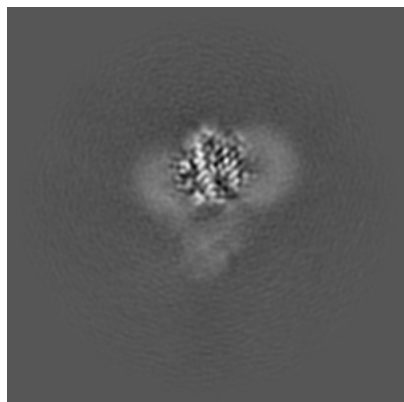
Z Index: 128

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

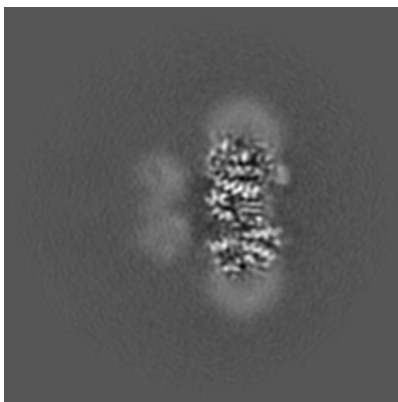


## 6.3 Largest variance slices [i](#)

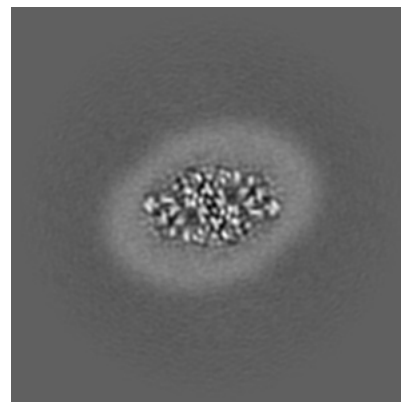
### 6.3.1 Primary map



X Index: 152

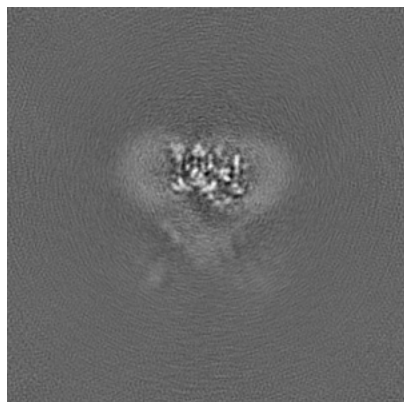


Y Index: 126

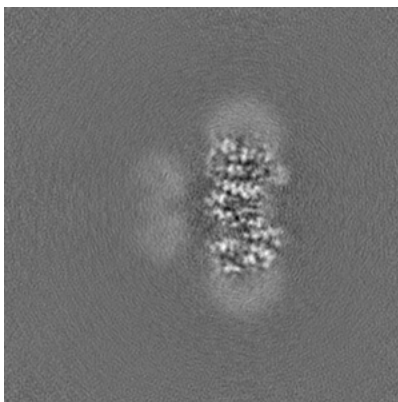


Z Index: 142

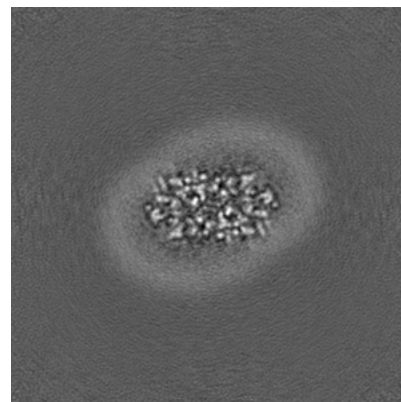
### 6.3.2 Raw map



X Index: 121



Y Index: 127

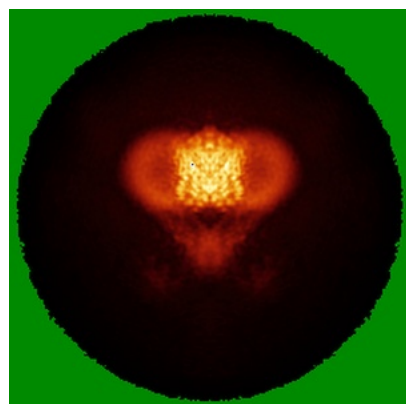


Z Index: 150

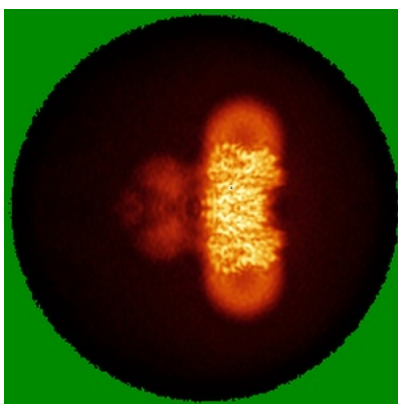
The images above show the largest variance slices of the map in three orthogonal directions.

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

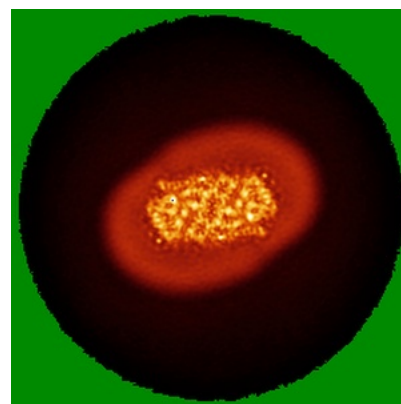
### 6.4.1 Primary map



X

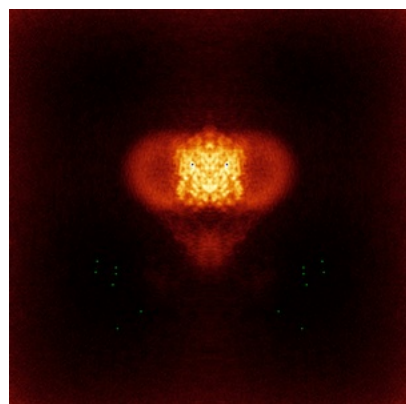


Y

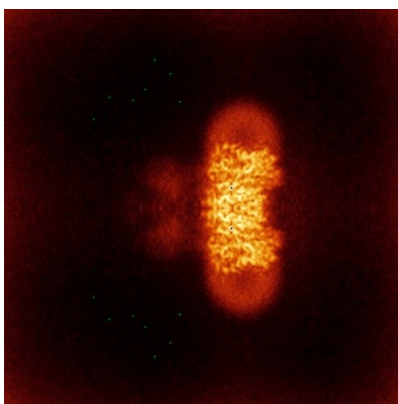


Z

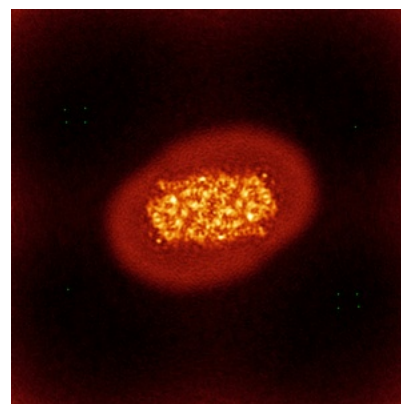
### 6.4.2 Raw map



X



Y

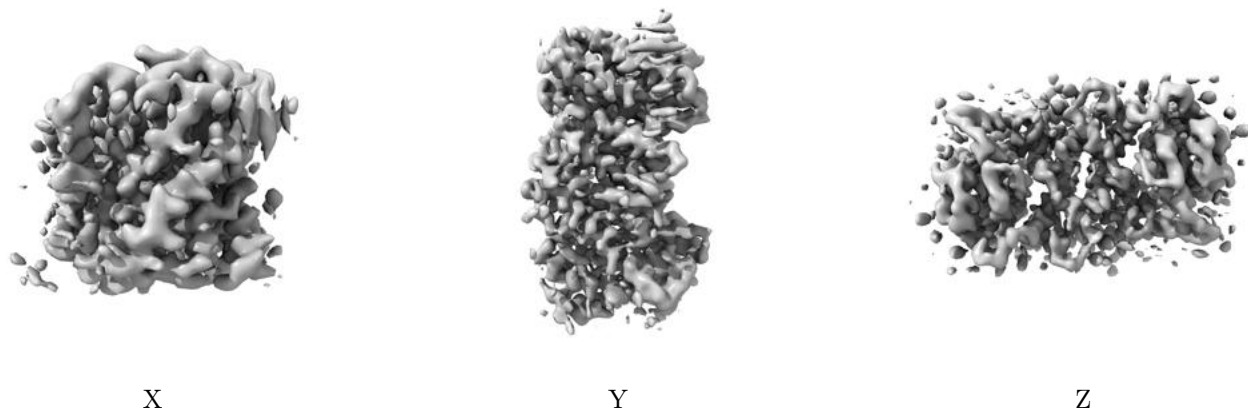


Z

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.

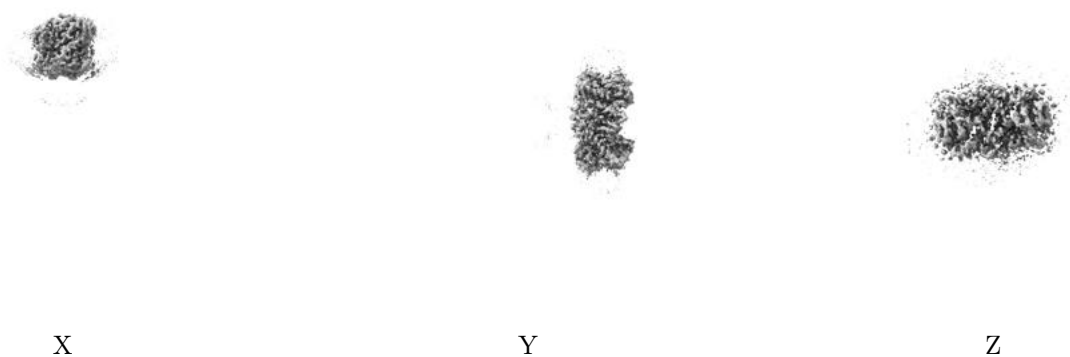
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.158. 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.

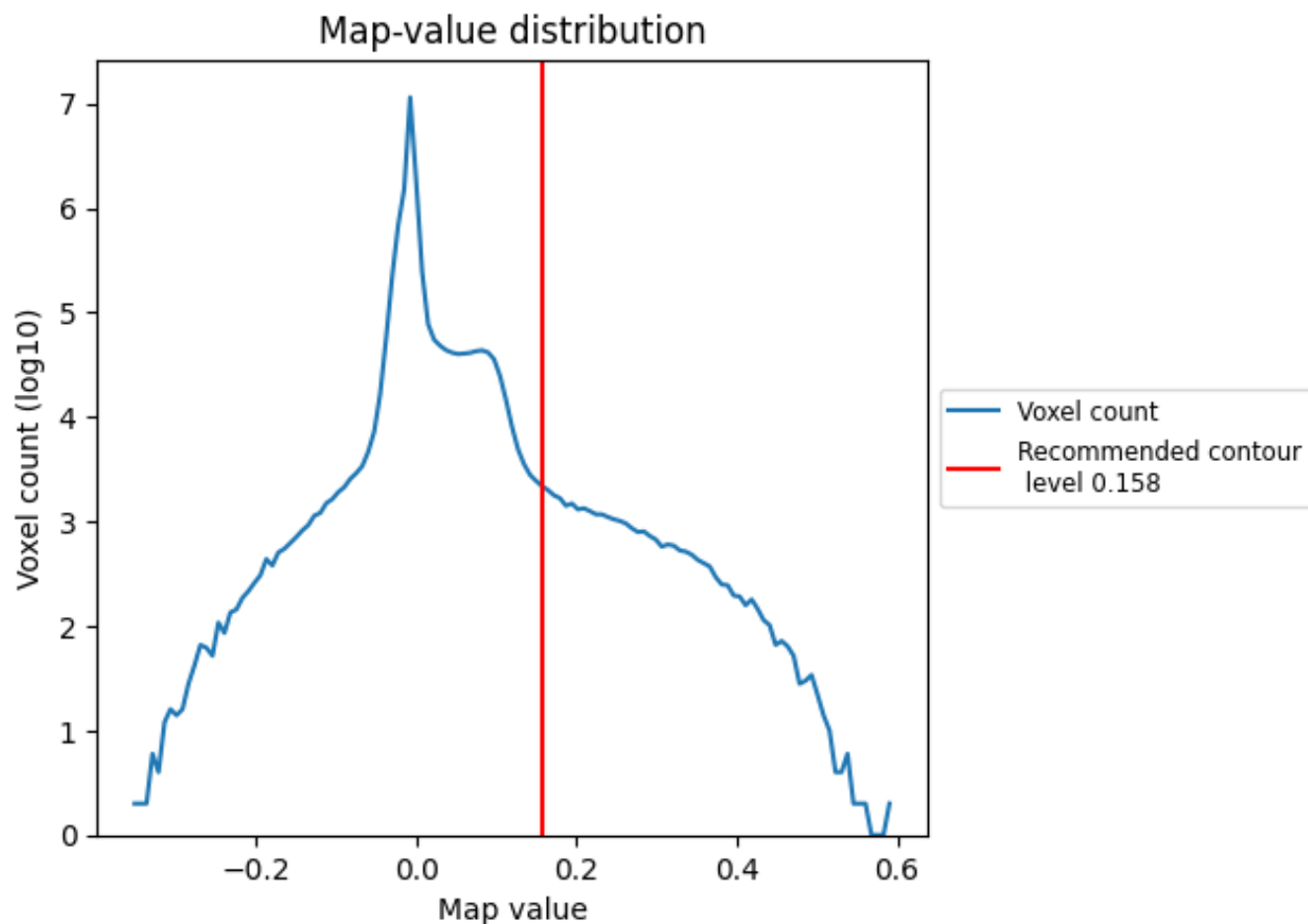
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

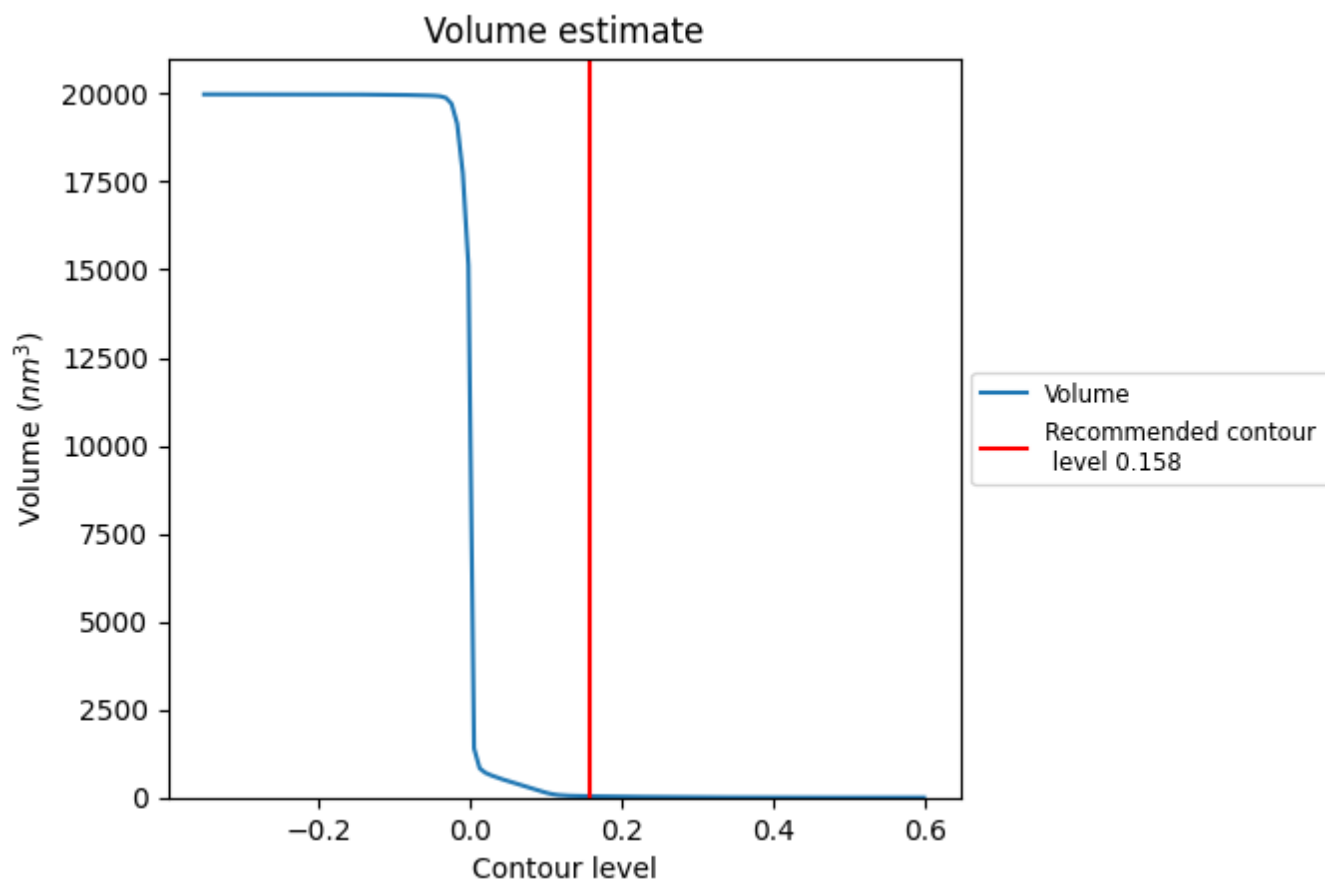
This section contains the results of statistical analysis of the map.

### 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.

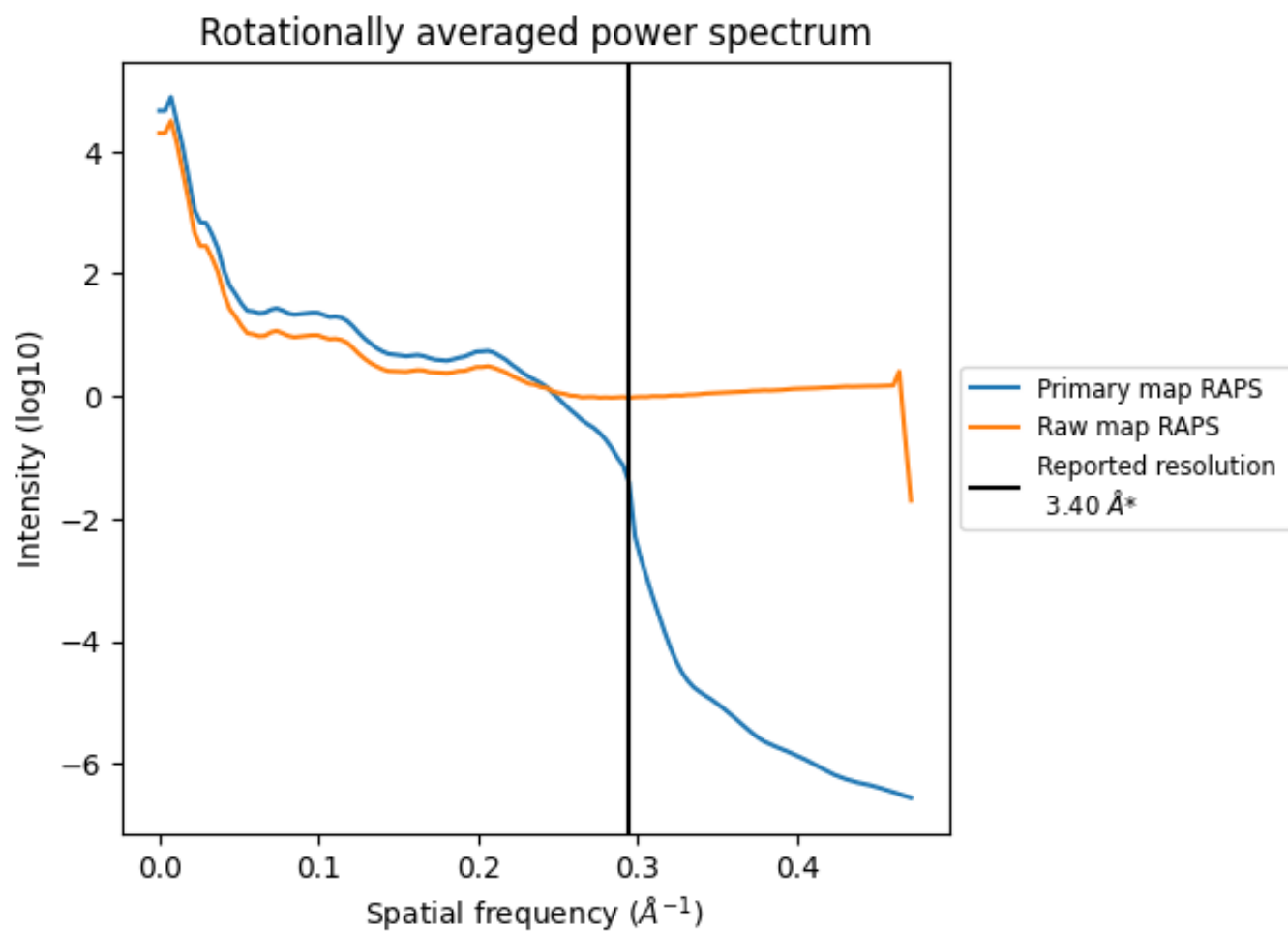
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 37 nm<sup>3</sup>; this corresponds to an approximate mass of 34 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 ⓘ

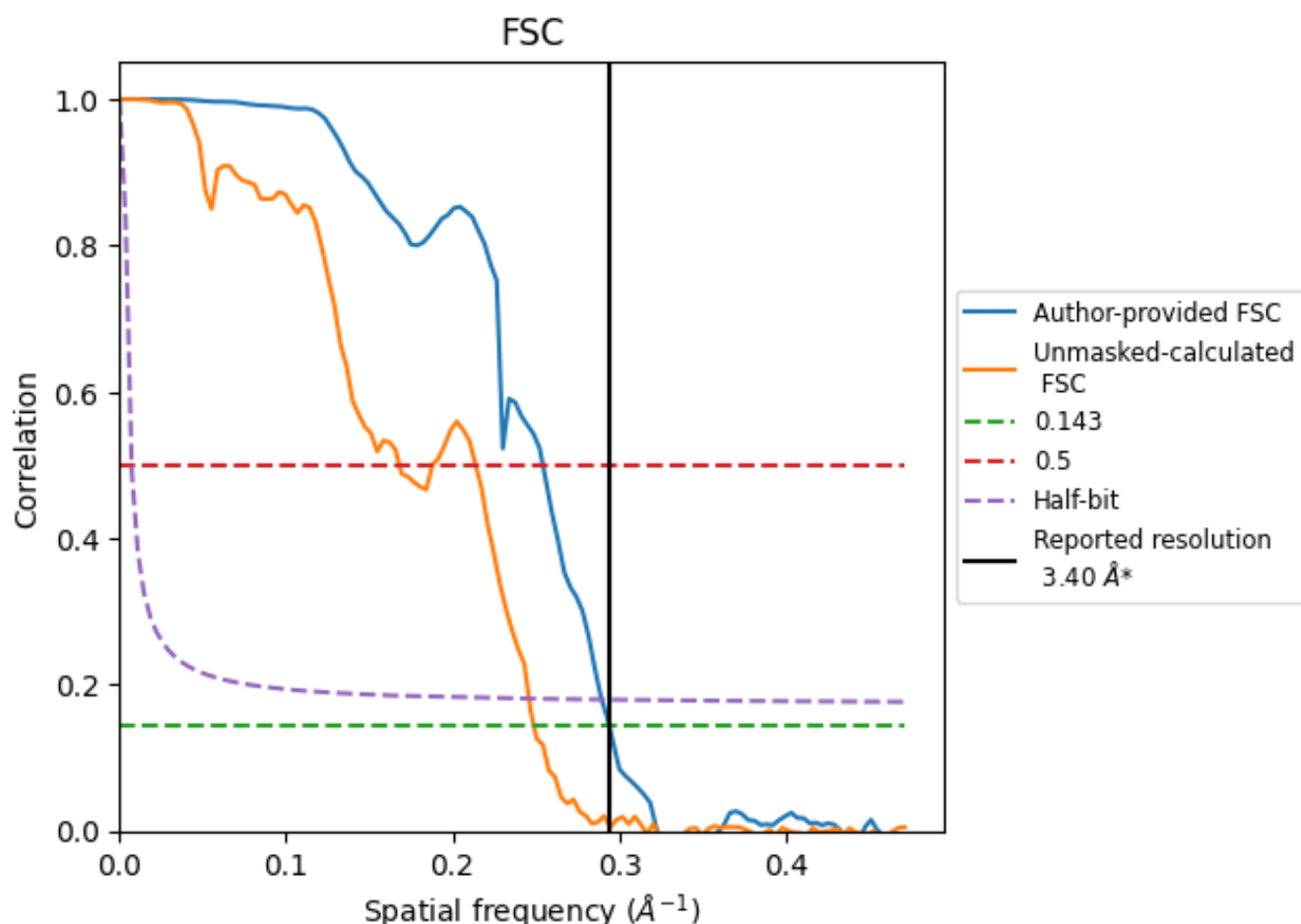


\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 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 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.93	3.45
Unmasked-calculated*	4.02	5.95	4.07

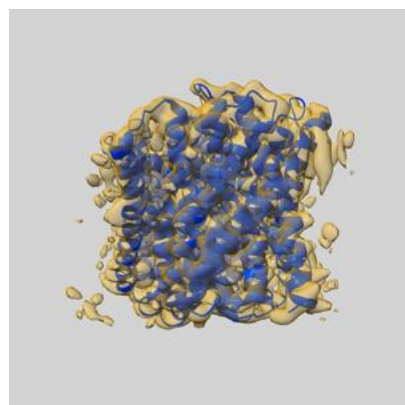
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.4 by more than 10 %



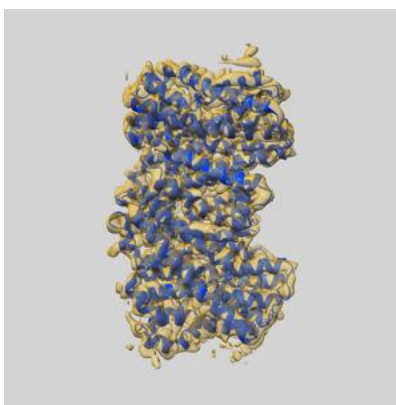
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35950 and PDB model 8J2M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

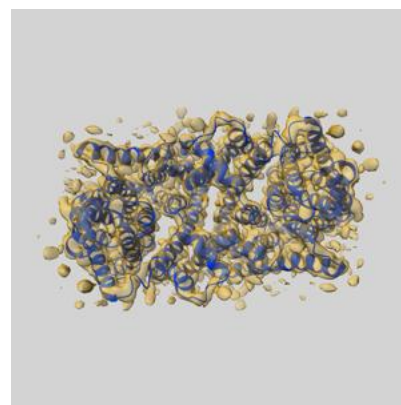
### 9.1 Map-model overlay [i](#)



X



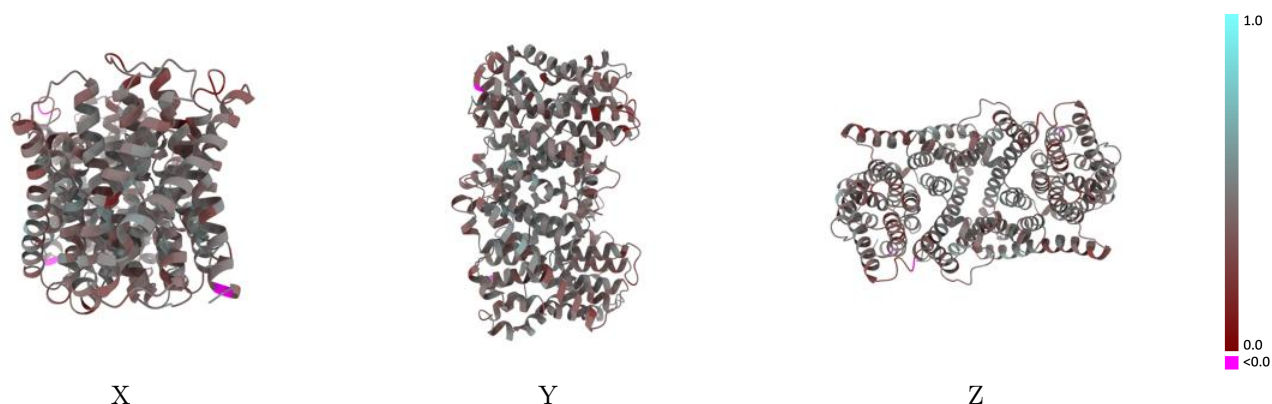
Y



Z

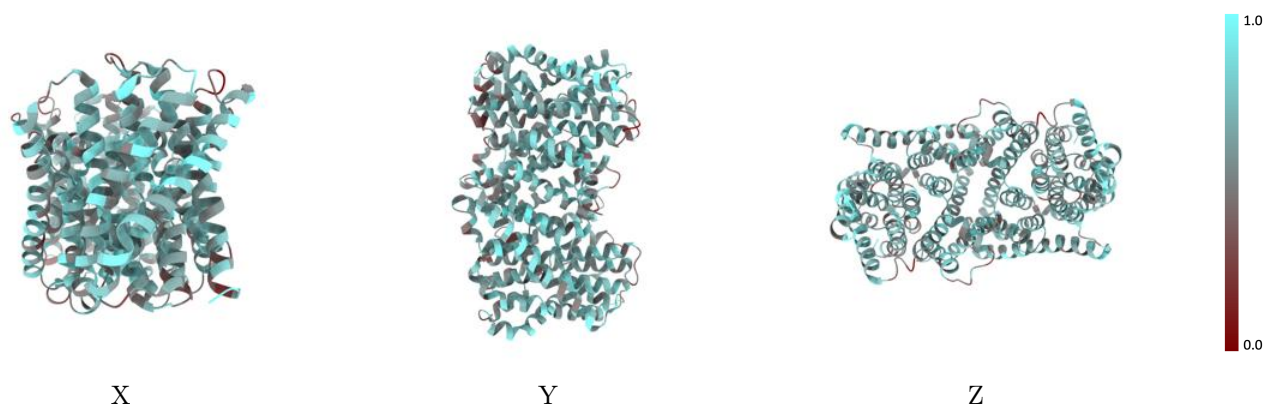
The images above show the 3D surface view of the map at the recommended contour level 0.158 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



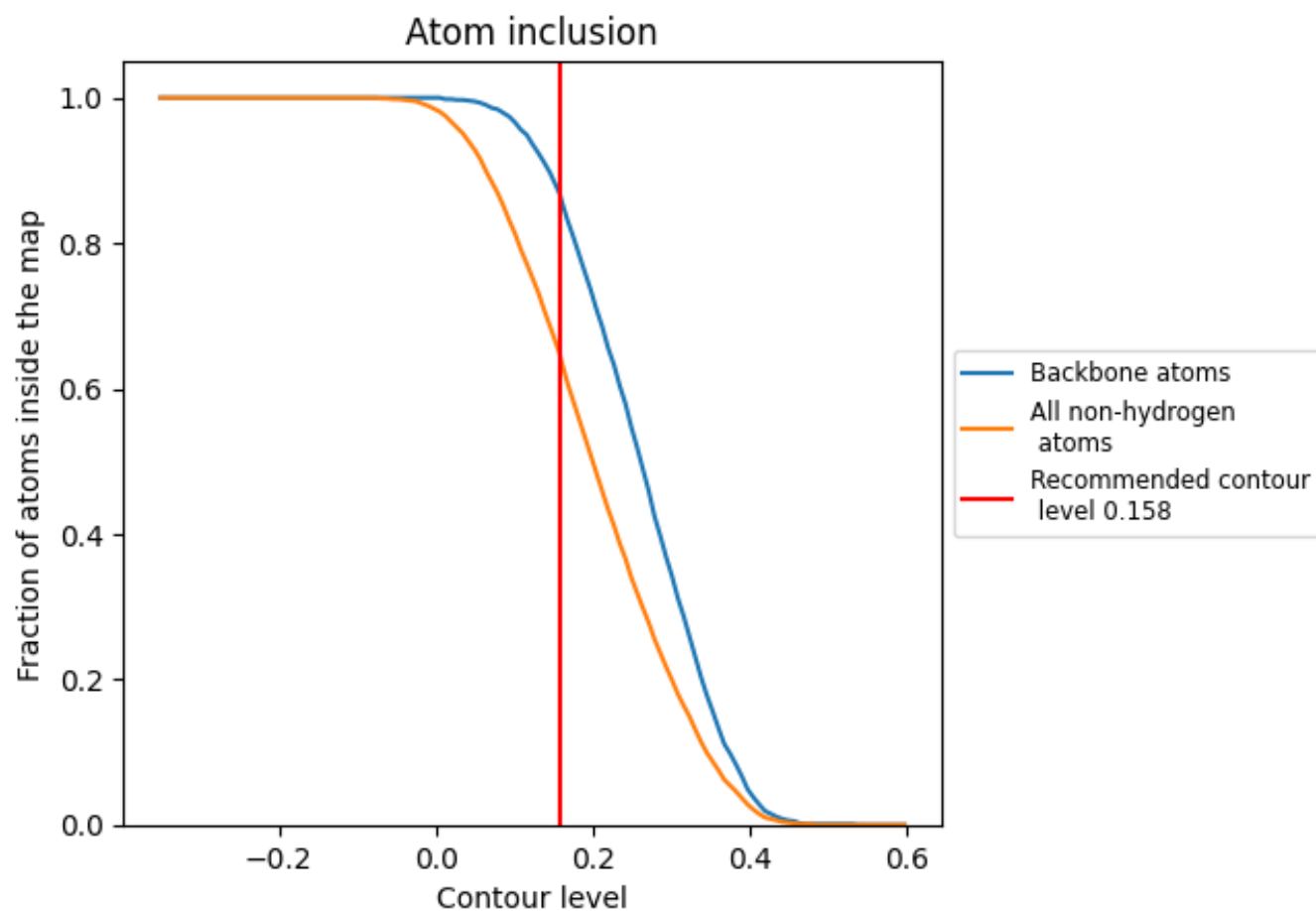
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.158).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 65% 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 (0.158) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6480	<div></div> 0.4190
A	<div></div> 0.6490	<div></div> 0.4180
B	<div></div> 0.6460	<div></div> 0.4200

