Full wwPDB EM Validation Report ⓘ

May 15, 2025 – 10:21 am BST

PDB ID	:	9GRY / pdb_00009gry
EMDB ID	:	EMD-51528
Title	:	Cryo-EM structure of human SLC35B1-Q113F variant with AMP-PNP
Authors	:	Gulati, A.; Ahn, D.; Suades, A.; Drew, D.
Deposited on	:	2024-09-13
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Validation 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:

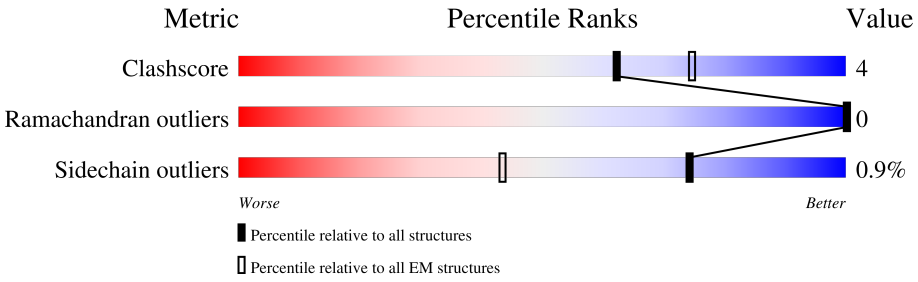
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

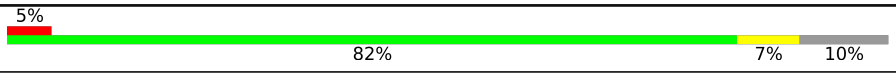
The reported resolution of this entry is 3.00 Å.

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 >=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 <=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	329	
2	B	612	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8482 atoms, of which 4226 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 human SLC35B1-Q113F.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	295	4730	1555	2410	359	390	16	0	0

- Molecule 2 is a protein called Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	241	3708	1208	1803	308	381	8	0	0

There are 244 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ASP	-	expression tag	UNP A0A4P1LXE0
B	2	ILE	-	expression tag	UNP A0A4P1LXE0
B	3	VAL	-	expression tag	UNP A0A4P1LXE0
B	4	MET	-	expression tag	UNP A0A4P1LXE0
B	5	THR	-	expression tag	UNP A0A4P1LXE0
B	6	GLN	-	expression tag	UNP A0A4P1LXE0
B	7	SER	-	expression tag	UNP A0A4P1LXE0
B	8	PRO	-	expression tag	UNP A0A4P1LXE0
B	9	ALA	-	expression tag	UNP A0A4P1LXE0
B	10	SER	-	expression tag	UNP A0A4P1LXE0
B	11	LEU	-	expression tag	UNP A0A4P1LXE0
B	12	THR	-	expression tag	UNP A0A4P1LXE0
B	13	VAL	-	expression tag	UNP A0A4P1LXE0
B	14	SER	-	expression tag	UNP A0A4P1LXE0
B	15	LEU	-	expression tag	UNP A0A4P1LXE0
B	16	GLY	-	expression tag	UNP A0A4P1LXE0
B	17	GLN	-	expression tag	UNP A0A4P1LXE0
B	18	SER	-	expression tag	UNP A0A4P1LXE0
B	19	VAL	-	expression tag	UNP A0A4P1LXE0
B	20	THR	-	expression tag	UNP A0A4P1LXE0
B	21	ILE	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	22	SER	-	expression tag	UNP A0A4P1LXE0
B	23	CYS	-	expression tag	UNP A0A4P1LXE0
B	24	ARG	-	expression tag	UNP A0A4P1LXE0
B	25	ALA	-	expression tag	UNP A0A4P1LXE0
B	26	SER	-	expression tag	UNP A0A4P1LXE0
B	27	GLU	-	expression tag	UNP A0A4P1LXE0
B	28	ASN	-	expression tag	UNP A0A4P1LXE0
B	29	VAL	-	expression tag	UNP A0A4P1LXE0
B	30	GLU	-	expression tag	UNP A0A4P1LXE0
B	31	TYR	-	expression tag	UNP A0A4P1LXE0
B	32	TYR	-	expression tag	UNP A0A4P1LXE0
B	33	GLY	-	expression tag	UNP A0A4P1LXE0
B	34	THR	-	expression tag	UNP A0A4P1LXE0
B	35	SER	-	expression tag	UNP A0A4P1LXE0
B	36	LEU	-	expression tag	UNP A0A4P1LXE0
B	37	MET	-	expression tag	UNP A0A4P1LXE0
B	38	GLN	-	expression tag	UNP A0A4P1LXE0
B	39	TRP	-	expression tag	UNP A0A4P1LXE0
B	40	TYR	-	expression tag	UNP A0A4P1LXE0
B	41	GLN	-	expression tag	UNP A0A4P1LXE0
B	42	GLN	-	expression tag	UNP A0A4P1LXE0
B	43	LYS	-	expression tag	UNP A0A4P1LXE0
B	44	PRO	-	expression tag	UNP A0A4P1LXE0
B	45	GLY	-	expression tag	UNP A0A4P1LXE0
B	46	GLN	-	expression tag	UNP A0A4P1LXE0
B	47	PRO	-	expression tag	UNP A0A4P1LXE0
B	48	PRO	-	expression tag	UNP A0A4P1LXE0
B	49	LYS	-	expression tag	UNP A0A4P1LXE0
B	50	PHE	-	expression tag	UNP A0A4P1LXE0
B	51	LEU	-	expression tag	UNP A0A4P1LXE0
B	52	ILE	-	expression tag	UNP A0A4P1LXE0
B	53	TYR	-	expression tag	UNP A0A4P1LXE0
B	54	GLY	-	expression tag	UNP A0A4P1LXE0
B	55	ALA	-	expression tag	UNP A0A4P1LXE0
B	56	SER	-	expression tag	UNP A0A4P1LXE0
B	57	ASN	-	expression tag	UNP A0A4P1LXE0
B	58	ILE	-	expression tag	UNP A0A4P1LXE0
B	59	GLU	-	expression tag	UNP A0A4P1LXE0
B	60	SER	-	expression tag	UNP A0A4P1LXE0
B	61	GLY	-	expression tag	UNP A0A4P1LXE0
B	62	VAL	-	expression tag	UNP A0A4P1LXE0
B	63	PRO	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	64	ALA	-	expression tag	UNP A0A4P1LXE0
B	65	ARG	-	expression tag	UNP A0A4P1LXE0
B	66	PHE	-	expression tag	UNP A0A4P1LXE0
B	67	SER	-	expression tag	UNP A0A4P1LXE0
B	68	GLY	-	expression tag	UNP A0A4P1LXE0
B	69	SER	-	expression tag	UNP A0A4P1LXE0
B	70	GLY	-	expression tag	UNP A0A4P1LXE0
B	71	SER	-	expression tag	UNP A0A4P1LXE0
B	72	GLY	-	expression tag	UNP A0A4P1LXE0
B	73	THR	-	expression tag	UNP A0A4P1LXE0
B	74	ASP	-	expression tag	UNP A0A4P1LXE0
B	75	PHE	-	expression tag	UNP A0A4P1LXE0
B	76	SER	-	expression tag	UNP A0A4P1LXE0
B	77	LEU	-	expression tag	UNP A0A4P1LXE0
B	78	ASN	-	expression tag	UNP A0A4P1LXE0
B	79	ILE	-	expression tag	UNP A0A4P1LXE0
B	80	HIS	-	expression tag	UNP A0A4P1LXE0
B	81	PRO	-	expression tag	UNP A0A4P1LXE0
B	82	VAL	-	expression tag	UNP A0A4P1LXE0
B	83	GLU	-	expression tag	UNP A0A4P1LXE0
B	84	GLU	-	expression tag	UNP A0A4P1LXE0
B	85	ASP	-	expression tag	UNP A0A4P1LXE0
B	86	ASP	-	expression tag	UNP A0A4P1LXE0
B	87	ILE	-	expression tag	UNP A0A4P1LXE0
B	88	ALA	-	expression tag	UNP A0A4P1LXE0
B	89	MET	-	expression tag	UNP A0A4P1LXE0
B	90	TYR	-	expression tag	UNP A0A4P1LXE0
B	91	PHE	-	expression tag	UNP A0A4P1LXE0
B	92	CYS	-	expression tag	UNP A0A4P1LXE0
B	93	GLN	-	expression tag	UNP A0A4P1LXE0
B	94	GLN	-	expression tag	UNP A0A4P1LXE0
B	95	SER	-	expression tag	UNP A0A4P1LXE0
B	96	ARG	-	expression tag	UNP A0A4P1LXE0
B	97	LYS	-	expression tag	UNP A0A4P1LXE0
B	98	VAL	-	expression tag	UNP A0A4P1LXE0
B	99	PRO	-	expression tag	UNP A0A4P1LXE0
B	100	TYR	-	expression tag	UNP A0A4P1LXE0
B	101	THR	-	expression tag	UNP A0A4P1LXE0
B	102	PHE	-	expression tag	UNP A0A4P1LXE0
B	103	GLY	-	expression tag	UNP A0A4P1LXE0
B	104	SER	-	expression tag	UNP A0A4P1LXE0
B	105	GLY	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	106	THR	-	expression tag	UNP A0A4P1LXE0
B	107	LYS	-	expression tag	UNP A0A4P1LXE0
B	108	LEU	-	expression tag	UNP A0A4P1LXE0
B	109	GLU	-	expression tag	UNP A0A4P1LXE0
B	110	ILE	-	expression tag	UNP A0A4P1LXE0
B	111	LYS	-	expression tag	UNP A0A4P1LXE0
B	112	GLY	-	expression tag	UNP A0A4P1LXE0
B	113	SER	-	expression tag	UNP A0A4P1LXE0
B	426	VAL	ALA	conflict	UNP A0A4P1LXE0
B	483	LEU	-	expression tag	UNP A0A4P1LXE0
B	484	GLY	-	expression tag	UNP A0A4P1LXE0
B	485	SER	-	expression tag	UNP A0A4P1LXE0
B	486	GLY	-	expression tag	UNP A0A4P1LXE0
B	487	GLU	-	expression tag	UNP A0A4P1LXE0
B	488	VAL	-	expression tag	UNP A0A4P1LXE0
B	489	GLN	-	expression tag	UNP A0A4P1LXE0
B	490	LEU	-	expression tag	UNP A0A4P1LXE0
B	491	GLN	-	expression tag	UNP A0A4P1LXE0
B	492	GLU	-	expression tag	UNP A0A4P1LXE0
B	493	SER	-	expression tag	UNP A0A4P1LXE0
B	494	GLY	-	expression tag	UNP A0A4P1LXE0
B	495	PRO	-	expression tag	UNP A0A4P1LXE0
B	496	GLY	-	expression tag	UNP A0A4P1LXE0
B	497	LEU	-	expression tag	UNP A0A4P1LXE0
B	498	VAL	-	expression tag	UNP A0A4P1LXE0
B	499	LYS	-	expression tag	UNP A0A4P1LXE0
B	500	PRO	-	expression tag	UNP A0A4P1LXE0
B	501	SER	-	expression tag	UNP A0A4P1LXE0
B	502	GLN	-	expression tag	UNP A0A4P1LXE0
B	503	SER	-	expression tag	UNP A0A4P1LXE0
B	504	LEU	-	expression tag	UNP A0A4P1LXE0
B	505	SER	-	expression tag	UNP A0A4P1LXE0
B	506	LEU	-	expression tag	UNP A0A4P1LXE0
B	507	THR	-	expression tag	UNP A0A4P1LXE0
B	508	CYS	-	expression tag	UNP A0A4P1LXE0
B	509	SER	-	expression tag	UNP A0A4P1LXE0
B	510	VAL	-	expression tag	UNP A0A4P1LXE0
B	511	THR	-	expression tag	UNP A0A4P1LXE0
B	512	GLY	-	expression tag	UNP A0A4P1LXE0
B	513	TYR	-	expression tag	UNP A0A4P1LXE0
B	514	SER	-	expression tag	UNP A0A4P1LXE0
B	515	ILE	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	516	THR	-	expression tag	UNP A0A4P1LXE0
B	517	SER	-	expression tag	UNP A0A4P1LXE0
B	518	ASP	-	expression tag	UNP A0A4P1LXE0
B	519	TYR	-	expression tag	UNP A0A4P1LXE0
B	520	TYR	-	expression tag	UNP A0A4P1LXE0
B	521	TRP	-	expression tag	UNP A0A4P1LXE0
B	522	ASN	-	expression tag	UNP A0A4P1LXE0
B	523	TRP	-	expression tag	UNP A0A4P1LXE0
B	524	ILE	-	expression tag	UNP A0A4P1LXE0
B	525	ARG	-	expression tag	UNP A0A4P1LXE0
B	526	GLN	-	expression tag	UNP A0A4P1LXE0
B	527	PHE	-	expression tag	UNP A0A4P1LXE0
B	528	PRO	-	expression tag	UNP A0A4P1LXE0
B	529	GLY	-	expression tag	UNP A0A4P1LXE0
B	530	ASN	-	expression tag	UNP A0A4P1LXE0
B	531	LYS	-	expression tag	UNP A0A4P1LXE0
B	532	LEU	-	expression tag	UNP A0A4P1LXE0
B	533	GLU	-	expression tag	UNP A0A4P1LXE0
B	534	TRP	-	expression tag	UNP A0A4P1LXE0
B	535	MET	-	expression tag	UNP A0A4P1LXE0
B	536	ALA	-	expression tag	UNP A0A4P1LXE0
B	537	TYR	-	expression tag	UNP A0A4P1LXE0
B	538	ILE	-	expression tag	UNP A0A4P1LXE0
B	539	ARG	-	expression tag	UNP A0A4P1LXE0
B	540	TYR	-	expression tag	UNP A0A4P1LXE0
B	541	ASP	-	expression tag	UNP A0A4P1LXE0
B	542	GLY	-	expression tag	UNP A0A4P1LXE0
B	543	THR	-	expression tag	UNP A0A4P1LXE0
B	544	SER	-	expression tag	UNP A0A4P1LXE0
B	545	ASP	-	expression tag	UNP A0A4P1LXE0
B	546	TYR	-	expression tag	UNP A0A4P1LXE0
B	547	ASN	-	expression tag	UNP A0A4P1LXE0
B	548	PRO	-	expression tag	UNP A0A4P1LXE0
B	549	SER	-	expression tag	UNP A0A4P1LXE0
B	550	LEU	-	expression tag	UNP A0A4P1LXE0
B	551	LYS	-	expression tag	UNP A0A4P1LXE0
B	552	ASN	-	expression tag	UNP A0A4P1LXE0
B	553	ARG	-	expression tag	UNP A0A4P1LXE0
B	554	ILE	-	expression tag	UNP A0A4P1LXE0
B	555	SER	-	expression tag	UNP A0A4P1LXE0
B	556	ILE	-	expression tag	UNP A0A4P1LXE0
B	557	THR	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	558	ARG	-	expression tag	UNP A0A4P1LXE0
B	559	ASP	-	expression tag	UNP A0A4P1LXE0
B	560	THR	-	expression tag	UNP A0A4P1LXE0
B	561	SER	-	expression tag	UNP A0A4P1LXE0
B	562	LYS	-	expression tag	UNP A0A4P1LXE0
B	563	ASN	-	expression tag	UNP A0A4P1LXE0
B	564	GLN	-	expression tag	UNP A0A4P1LXE0
B	565	PHE	-	expression tag	UNP A0A4P1LXE0
B	566	PHE	-	expression tag	UNP A0A4P1LXE0
B	567	LEU	-	expression tag	UNP A0A4P1LXE0
B	568	LYS	-	expression tag	UNP A0A4P1LXE0
B	569	LEU	-	expression tag	UNP A0A4P1LXE0
B	570	ASN	-	expression tag	UNP A0A4P1LXE0
B	571	SER	-	expression tag	UNP A0A4P1LXE0
B	572	VAL	-	expression tag	UNP A0A4P1LXE0
B	573	ALA	-	expression tag	UNP A0A4P1LXE0
B	574	THR	-	expression tag	UNP A0A4P1LXE0
B	575	GLU	-	expression tag	UNP A0A4P1LXE0
B	576	ASP	-	expression tag	UNP A0A4P1LXE0
B	577	THR	-	expression tag	UNP A0A4P1LXE0
B	578	ALA	-	expression tag	UNP A0A4P1LXE0
B	579	THR	-	expression tag	UNP A0A4P1LXE0
B	580	TYR	-	expression tag	UNP A0A4P1LXE0
B	581	TYR	-	expression tag	UNP A0A4P1LXE0
B	582	CYS	-	expression tag	UNP A0A4P1LXE0
B	583	ALA	-	expression tag	UNP A0A4P1LXE0
B	584	ARG	-	expression tag	UNP A0A4P1LXE0
B	585	ALA	-	expression tag	UNP A0A4P1LXE0
B	586	TYR	-	expression tag	UNP A0A4P1LXE0
B	587	TYR	-	expression tag	UNP A0A4P1LXE0
B	588	TYR	-	expression tag	UNP A0A4P1LXE0
B	589	ASP	-	expression tag	UNP A0A4P1LXE0
B	590	GLY	-	expression tag	UNP A0A4P1LXE0
B	591	ILE	-	expression tag	UNP A0A4P1LXE0
B	592	ASN	-	expression tag	UNP A0A4P1LXE0
B	593	PHE	-	expression tag	UNP A0A4P1LXE0
B	594	ASP	-	expression tag	UNP A0A4P1LXE0
B	595	TYR	-	expression tag	UNP A0A4P1LXE0
B	596	TRP	-	expression tag	UNP A0A4P1LXE0
B	597	GLY	-	expression tag	UNP A0A4P1LXE0
B	598	GLN	-	expression tag	UNP A0A4P1LXE0
B	599	GLY	-	expression tag	UNP A0A4P1LXE0

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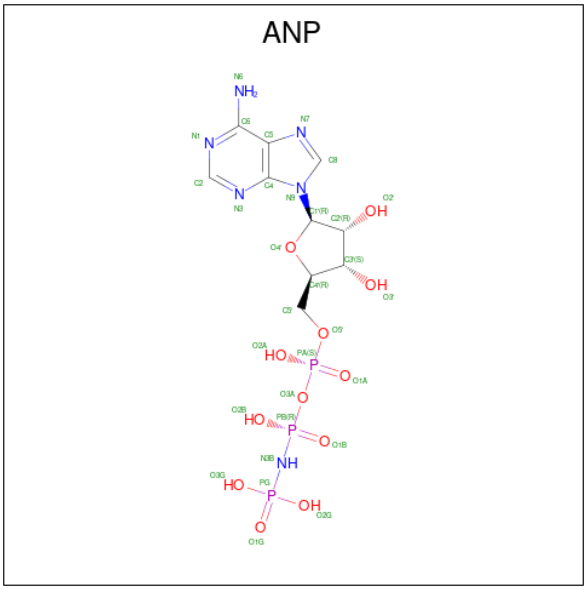
Chain	Residue	Modelled	Actual	Comment	Reference
B	600	THR	-	expression tag	UNP A0A4P1LXE0
B	601	THR	-	expression tag	UNP A0A4P1LXE0
B	602	LEU	-	expression tag	UNP A0A4P1LXE0
B	603	THR	-	expression tag	UNP A0A4P1LXE0
B	604	VAL	-	expression tag	UNP A0A4P1LXE0
B	605	SER	-	expression tag	UNP A0A4P1LXE0
B	606	SER	-	expression tag	UNP A0A4P1LXE0
B	607	GLU	-	expression tag	UNP A0A4P1LXE0
B	608	ASN	-	expression tag	UNP A0A4P1LXE0
B	609	LEU	-	expression tag	UNP A0A4P1LXE0
B	610	TYR	-	expression tag	UNP A0A4P1LXE0
B	611	PHE	-	expression tag	UNP A0A4P1LXE0
B	612	GLN	-	expression tag	UNP A0A4P1LXE0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



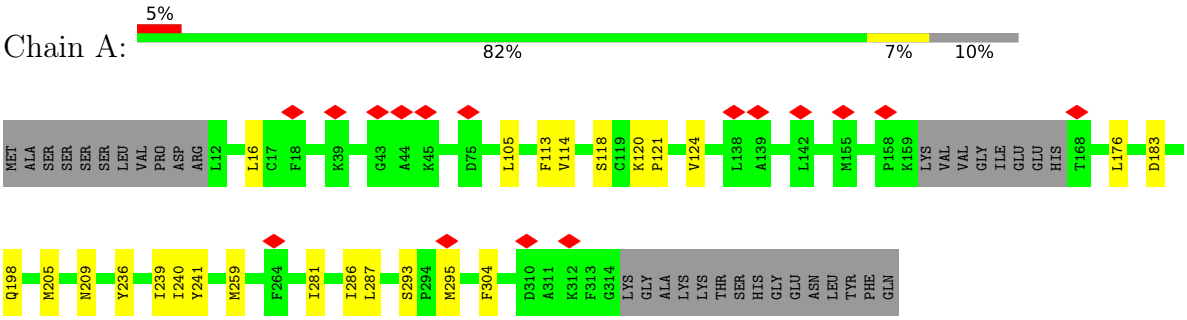
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

3 Residue-property plots (i)

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: human SLC35B1-Q113F

Chain A:



• Molecule 2: Maltodextrin-binding protein

Chain B:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	329709	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 ($e^-/Å^2$)	59.3	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.160	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	269.568, 269.568, 269.568	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.13	0/2379	0.29	0/3230
2	B	0.15	0/1954	0.30	0/2653
All	All	0.14	0/4333	0.30	0/5883

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	2320	2410	2410	16	0
2	B	1905	1803	1803	20	0
3	A	31	13	13	1	0
All	All	4256	4226	4226	35	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 4.

All (35) 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)
2:B:109:GLU:N	2:B:109:GLU:OE1	2.10	0.82
2:B:498:VAL:HG21	2:B:504:LEU:HD12	1.76	0.67
2:B:559:ASP:OD2	2:B:562:LYS:NZ	2.31	0.63
2:B:59:GLU:OE1	2:B:60:SER:N	2.34	0.59
1:A:205:MET:O	1:A:209:ASN:ND2	2.38	0.55
1:A:113:PHE:HA	1:A:176:LEU:HD11	1.90	0.53
1:A:105:LEU:HD23	1:A:105:LEU:O	2.09	0.53
1:A:281:ILE:HD12	1:A:304:PHE:CZ	2.44	0.52
2:B:87:ILE:HD11	2:B:109:GLU:HA	1.91	0.51
1:A:281:ILE:HD12	1:A:304:PHE:HZ	1.77	0.50
2:B:594:ASP:OD2	2:B:595:TYR:N	2.46	0.49
2:B:489:GLN:N	2:B:489:GLN:OE1	2.47	0.48
1:A:198:GLN:NE2	2:B:36:LEU:HD21	2.30	0.47
2:B:522:ASN:N	2:B:522:ASN:OD1	2.47	0.46
1:A:114:VAL:O	1:A:118:SER:OG	2.31	0.46
2:B:492:GLU:OE1	2:B:599:GLY:N	2.49	0.46
1:A:295:MET:HG2	1:A:295:MET:O	2.16	0.45
2:B:67:SER:O	2:B:77:LEU:HD12	2.18	0.44
2:B:52:ILE:HD12	2:B:77:LEU:HD13	2.00	0.44
1:A:183:ASP:OD2	1:A:183:ASP:C	2.61	0.43
1:A:236:TYR:O	1:A:239:ILE:HG22	2.18	0.43
2:B:87:ILE:O	2:B:87:ILE:CG2	2.67	0.43
2:B:4:MET:HE1	2:B:37:MET:HE1	2.01	0.42
2:B:84:GLU:OE1	2:B:84:GLU:C	2.63	0.42
1:A:120:LYS:N	1:A:121:PRO:CD	2.82	0.42
2:B:87:ILE:O	2:B:87:ILE:HG23	2.20	0.42
2:B:498:VAL:HG21	2:B:504:LEU:CD1	2.48	0.41
1:A:286:ILE:HG23	1:A:287:LEU:N	2.35	0.41
1:A:16:LEU:C	1:A:16:LEU:HD12	2.46	0.41
2:B:535:MET:HE1	2:B:569:LEU:HD21	2.03	0.41
1:A:120:LYS:NZ	3:A:401:ANP:O1B	2.39	0.41
2:B:507:THR:HG23	2:B:566:PHE:CD1	2.56	0.41
1:A:240:ILE:O	1:A:241:TYR:C	2.64	0.40
2:B:52:ILE:HG12	2:B:58:ILE:HD13	2.02	0.40
1:A:259:MET:SD	1:A:259:MET:C	3.05	0.40

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	291/329 (88%)	280 (96%)	11 (4%)	0	100	100
2	B	237/612 (39%)	227 (96%)	10 (4%)	0	100	100
All	All	528/941 (56%)	507 (96%)	21 (4%)	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	252/281 (90%)	250 (99%)	2 (1%)	79	90
2	B	211/507 (42%)	209 (99%)	2 (1%)	75	89
All	All	463/788 (59%)	459 (99%)	4 (1%)	74	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	A	293	SER
2	B	104	SER
2	B	522	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	102	ASN
1	A	254	GLN
2	B	530	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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	$\#\|Z\| > 2$
3	ANP	A	401	-	29,33,33	1.08	4 (13%)	31,52,52	1.10	2 (6%)

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	ANP	A	401	-	-	4/14/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ANP	PG-O1G	2.43	1.50	1.46
3	A	401	ANP	PG-N3B	2.41	1.69	1.63
3	A	401	ANP	PB-O3A	-2.38	1.56	1.59
3	A	401	ANP	PB-O1B	2.28	1.49	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ANP	PB-O3A-PA	-3.81	119.21	132.62
3	A	401	ANP	C5-C6-N6	2.28	123.82	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ANP	PG-N3B-PB-O3A
3	A	401	ANP	C5'-O5'-PA-O3A
3	A	401	ANP	O4'-C4'-C5'-O5'
3	A	401	ANP	C5'-O5'-PA-O1A

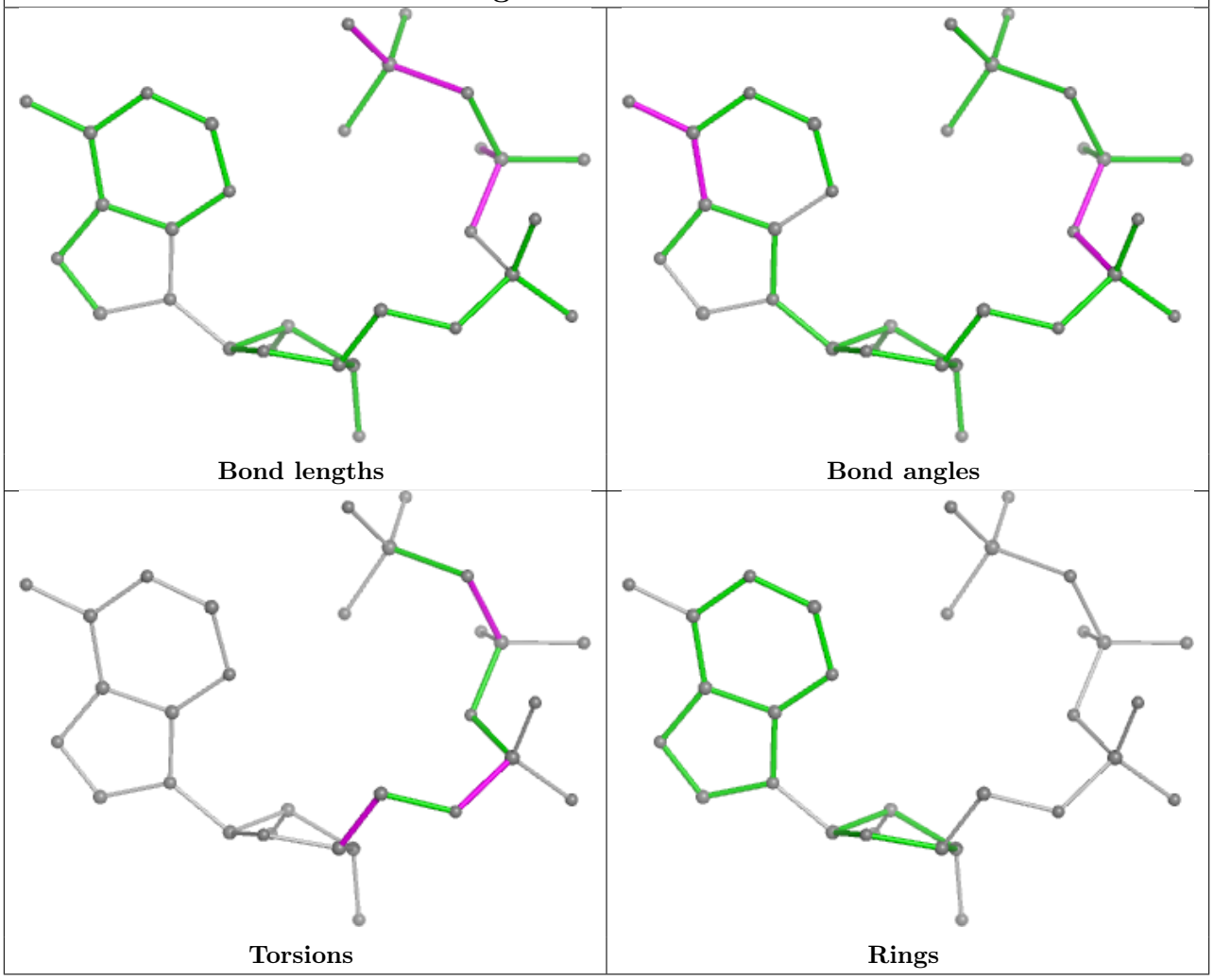
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ANP	1	0

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

Ligand ANP A 401



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.

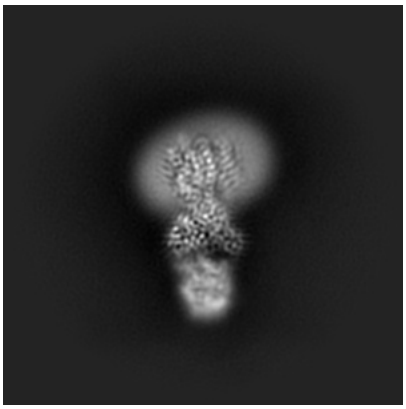
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51528. These allow visual inspection of the internal detail of the map and identification of artifacts.

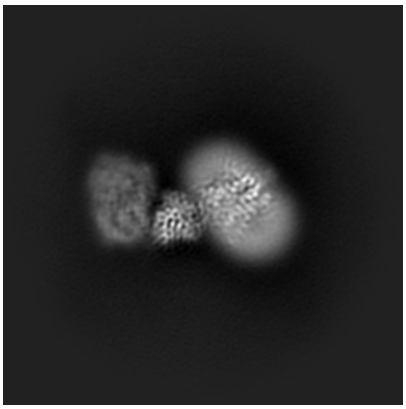
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

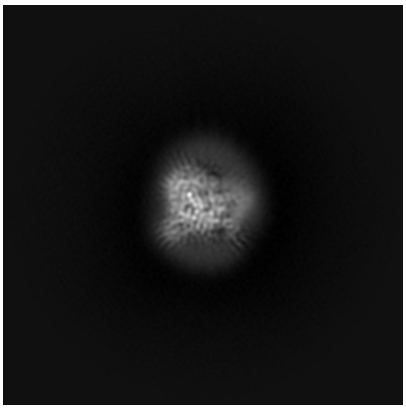
6.1.1 Primary map



X

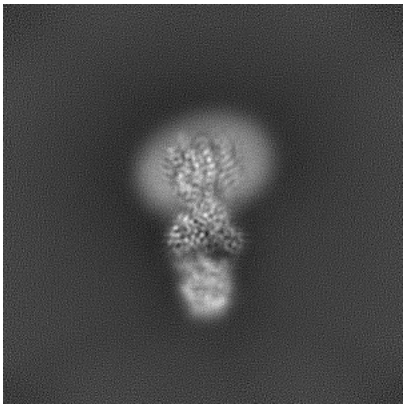


Y

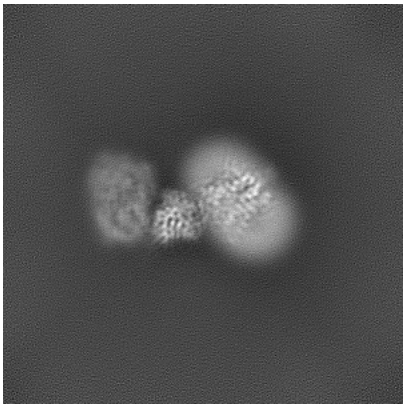


Z

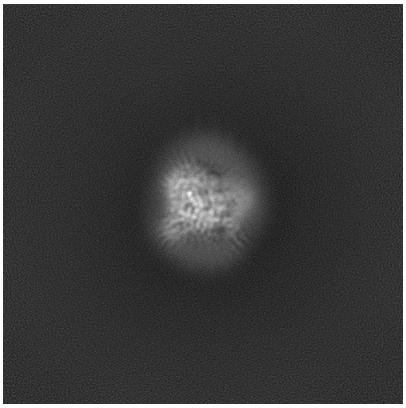
6.1.2 Raw map



X



Y

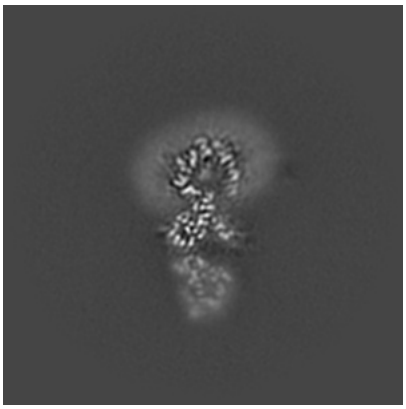


Z

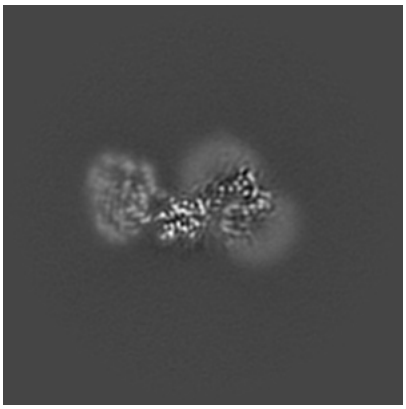
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

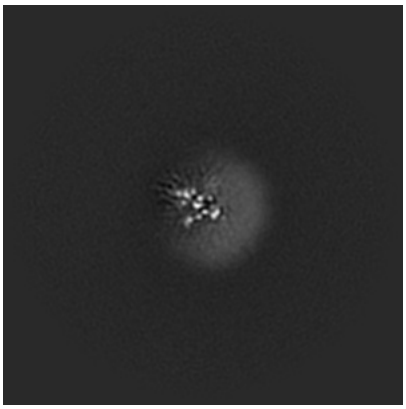
6.2.1 Primary map



X Index: 208

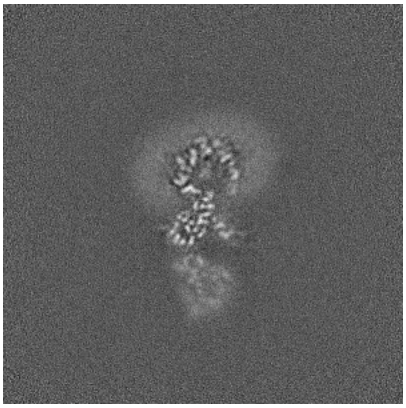


Y Index: 208

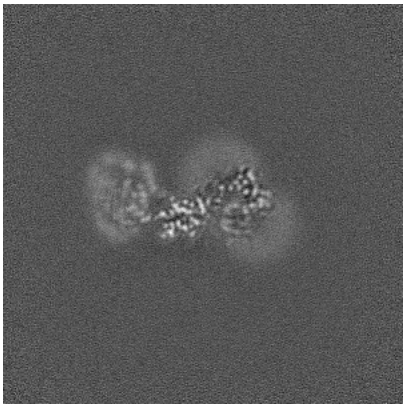


Z Index: 208

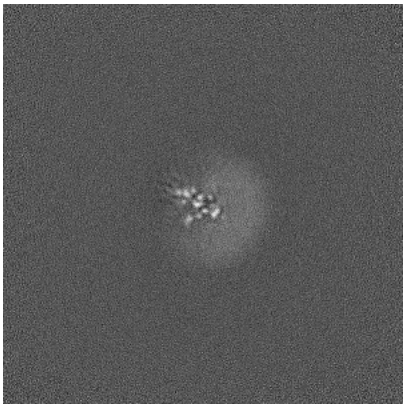
6.2.2 Raw map



X Index: 208



Y Index: 208

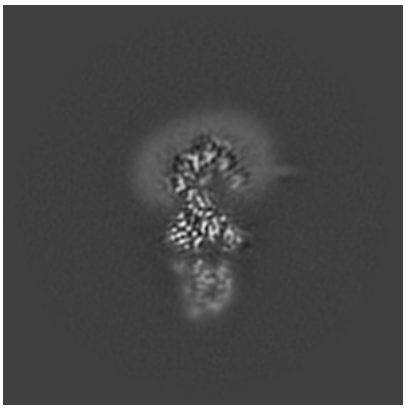


Z Index: 208

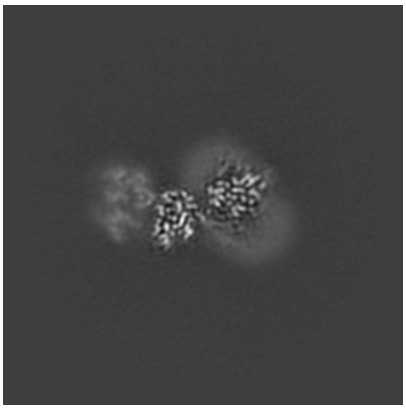
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

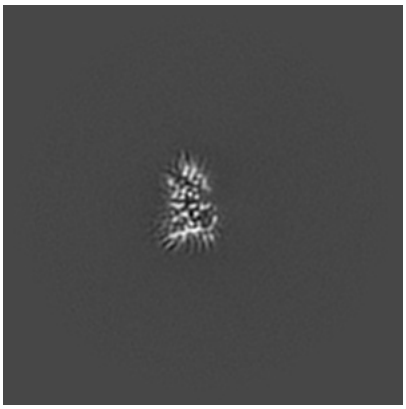
6.3.1 Primary map



X Index: 202

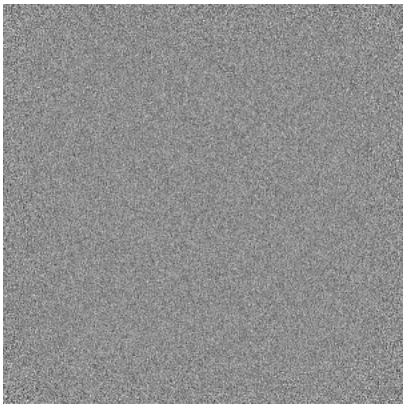


Y Index: 191

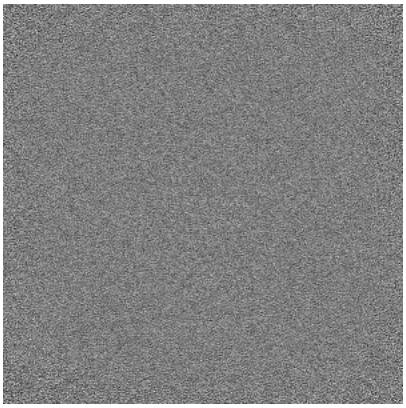


Z Index: 176

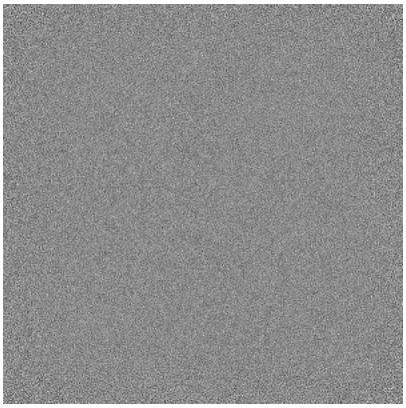
6.3.2 Raw map



X Index: 0



Y Index: 0

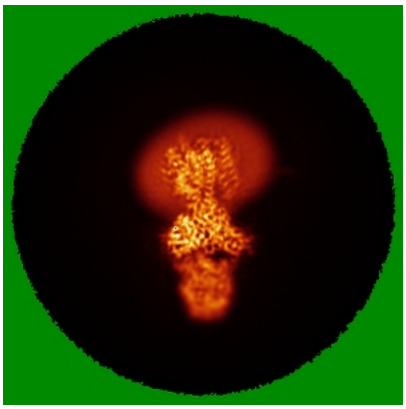


Z Index: 0

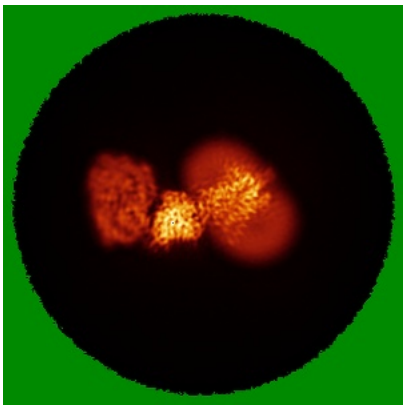
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

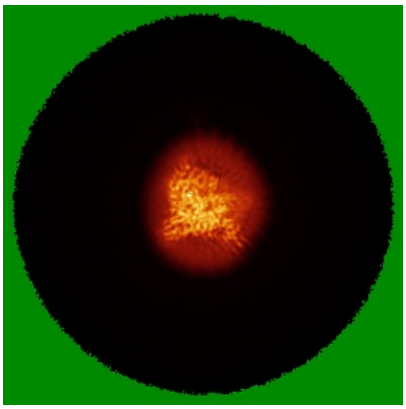
6.4.1 Primary map



X

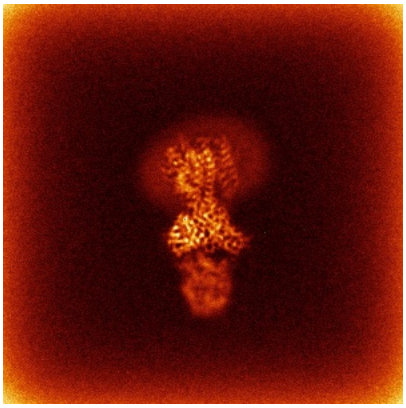


Y

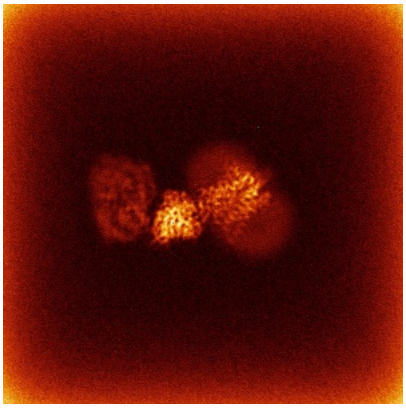


Z

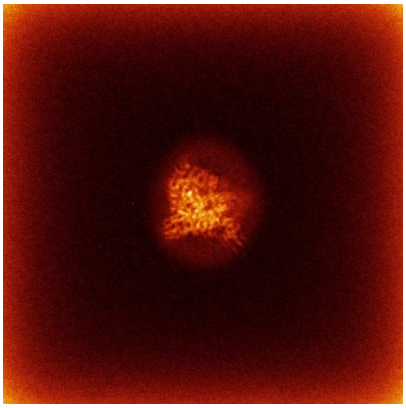
6.4.2 Raw map



X



Y

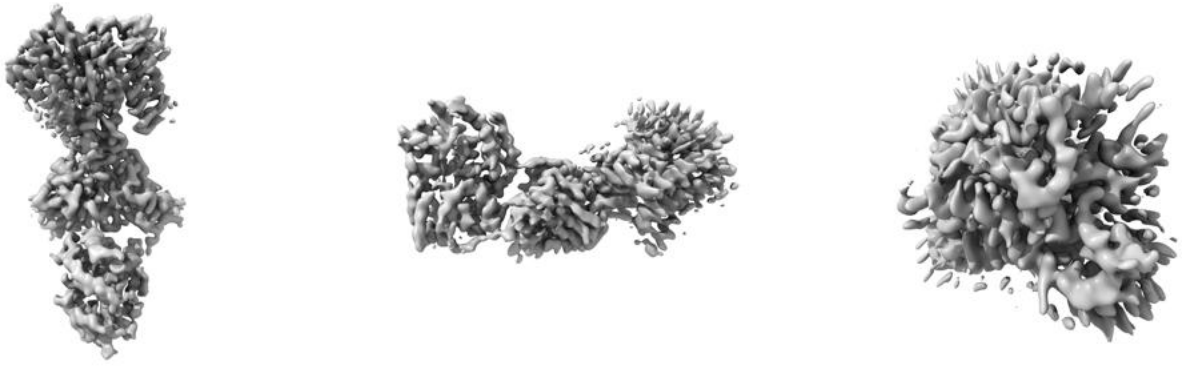


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. 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

X Y Z

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.

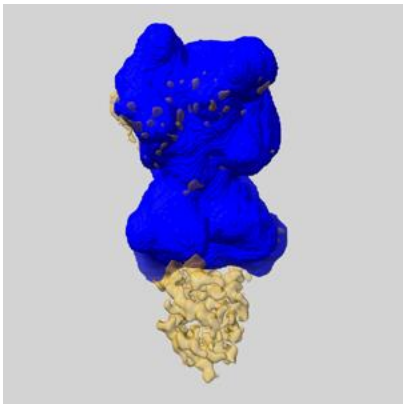
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

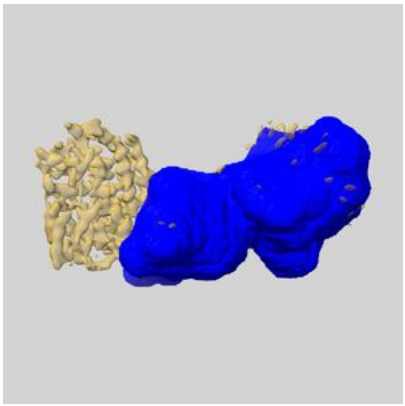
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

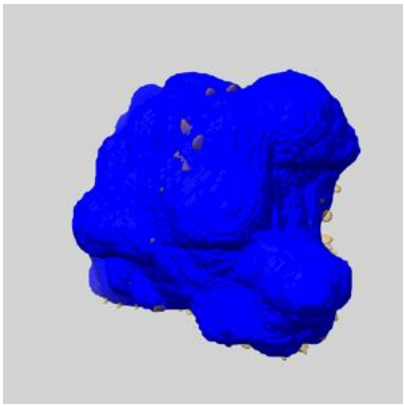
6.6.1 emd_51528_msk_1.map (i)



X



Y

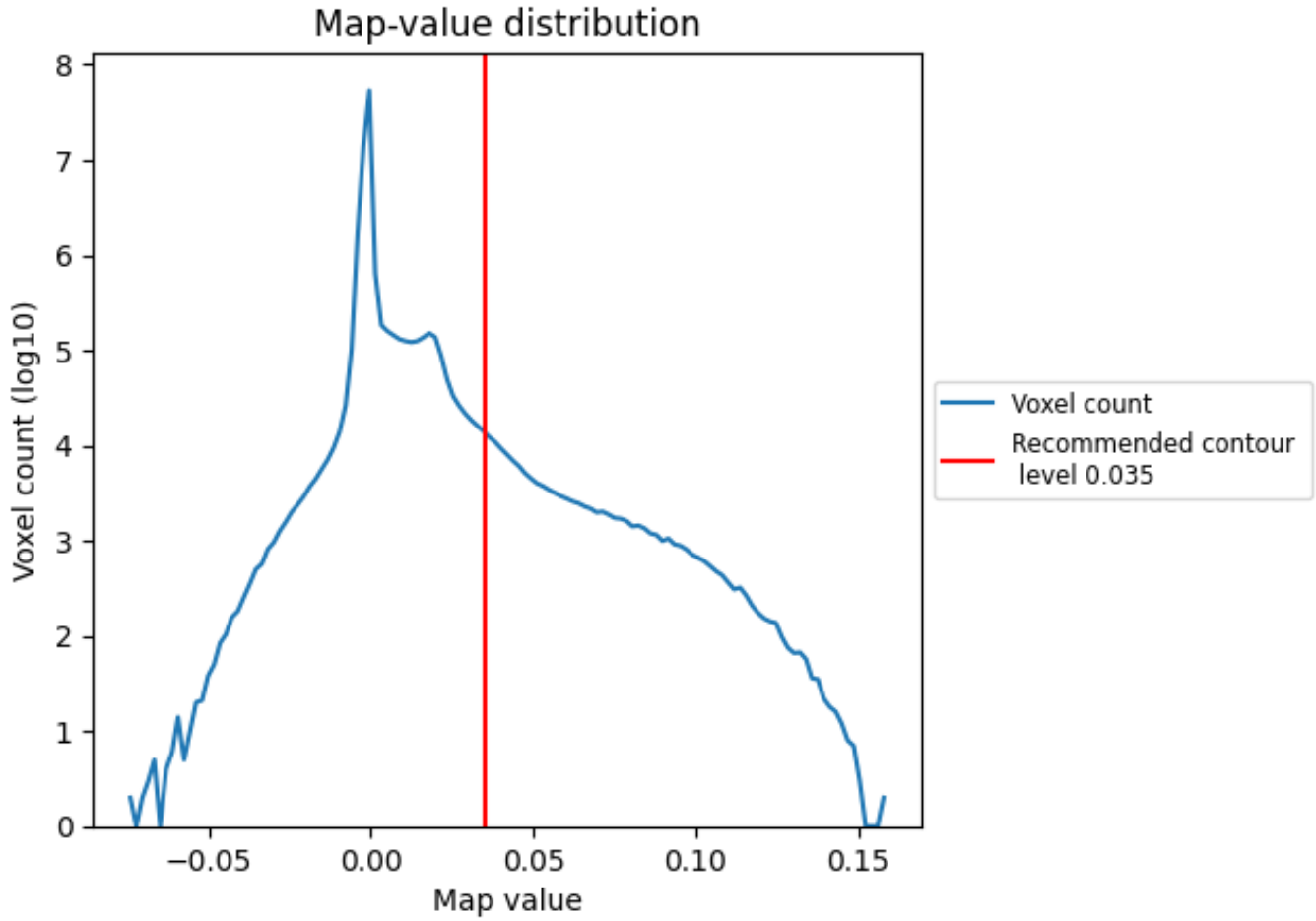


Z

7 Map analysis

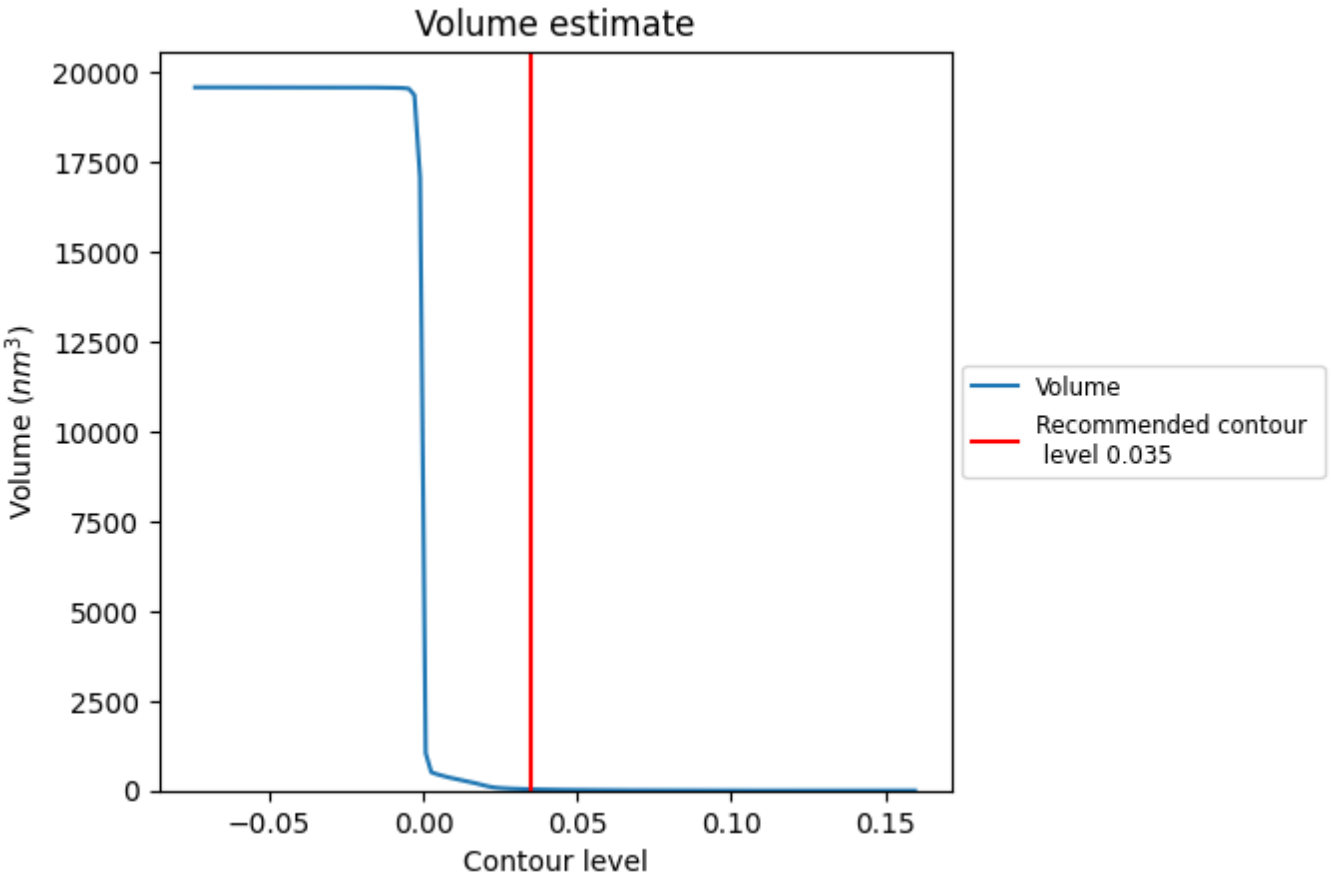
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

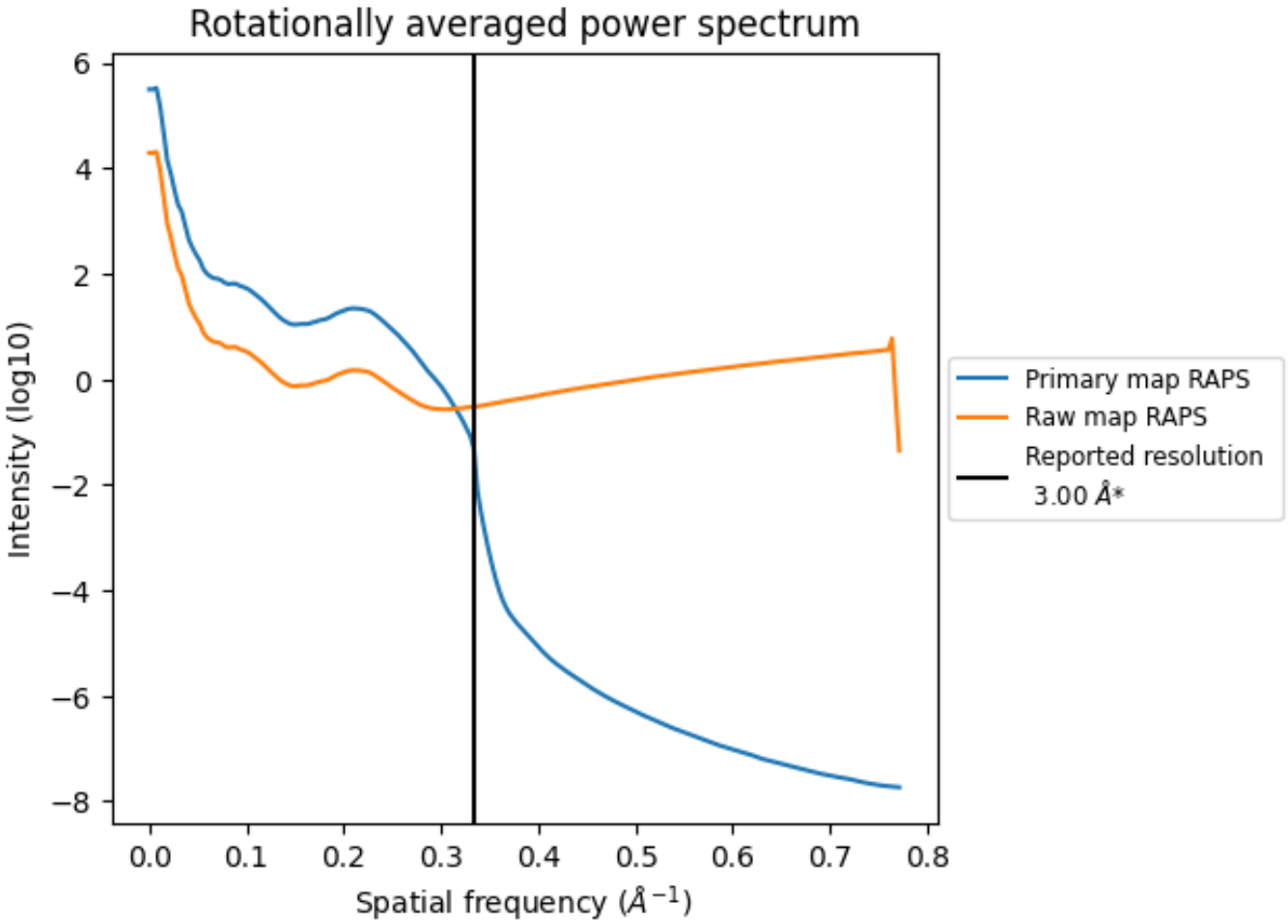
7.2 Volume estimate (i)



The volume at the recommended contour level is 36 nm^3; this corresponds to an approximate mass of 32 kDa.

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

7.3 Rotationally averaged power spectrum (i)

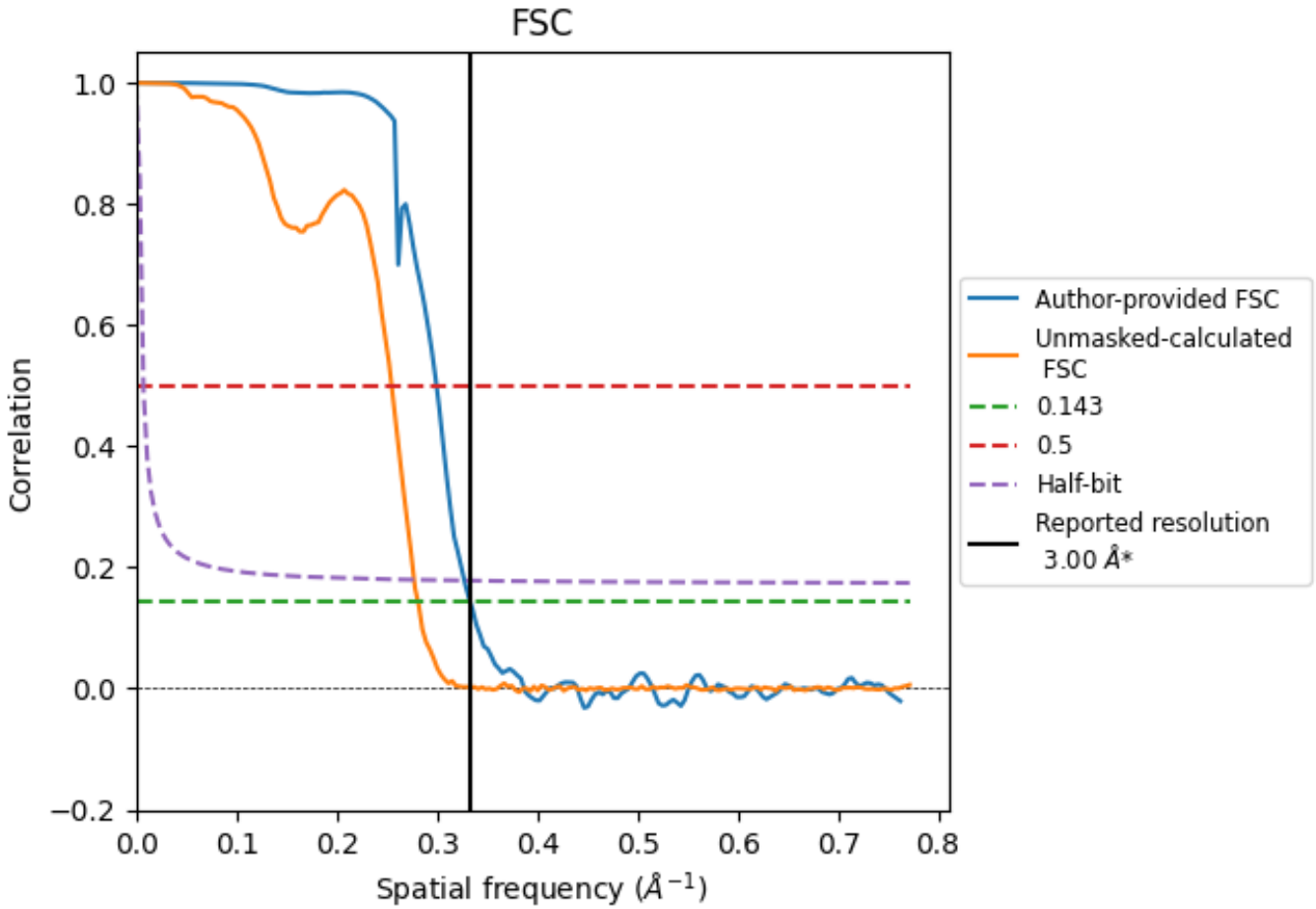


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

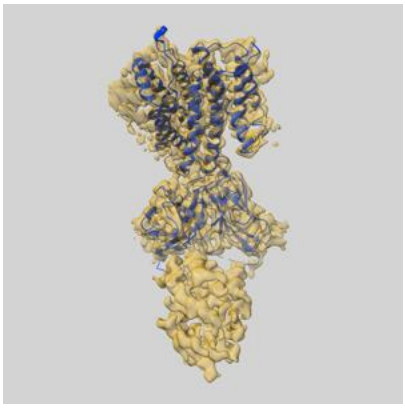
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.34	3.05
Unmasked-calculated*	3.56	3.92	3.61

*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 3.56 differs from the reported value 3.0 by more than 10 %

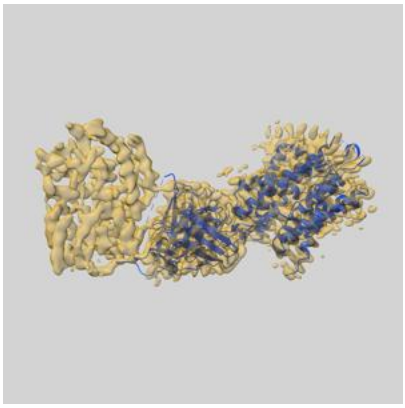
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51528 and PDB model 9GRY. Per-residue inclusion information can be found in section 3 on page 10.

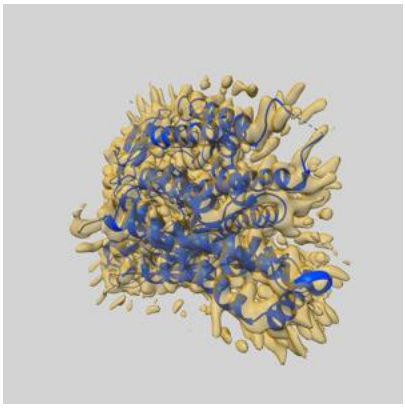
9.1 Map-model overlay



X



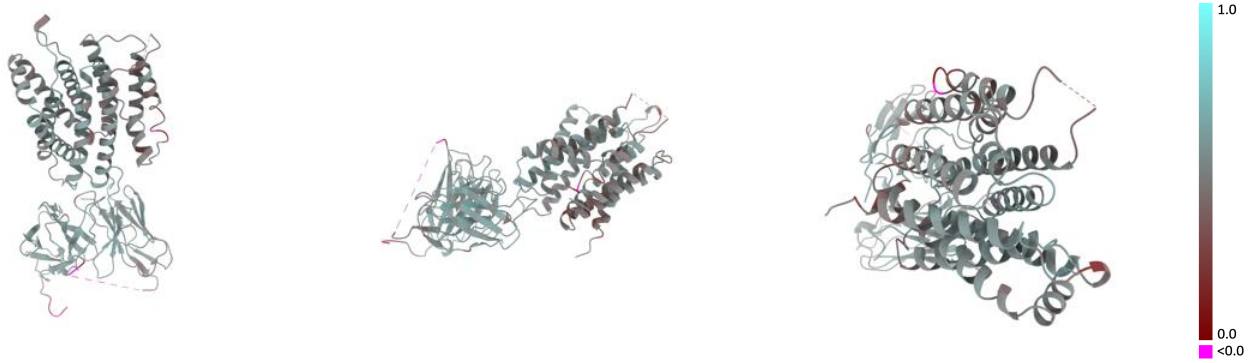
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

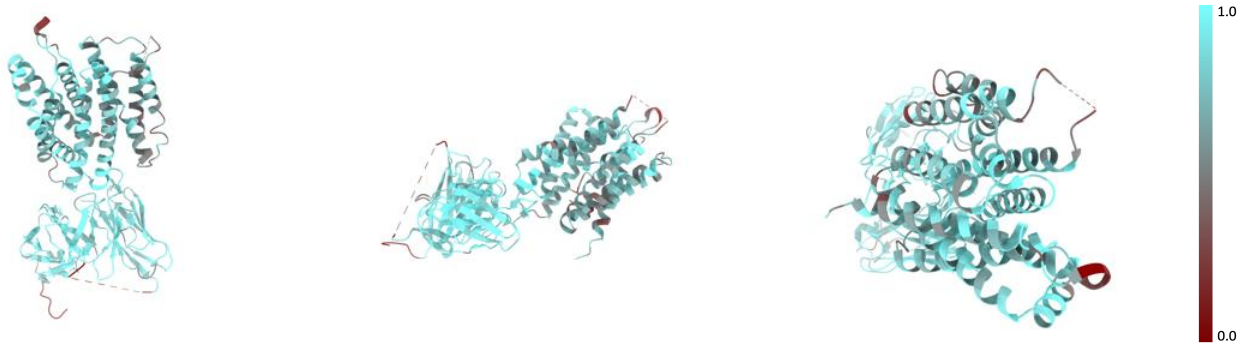
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

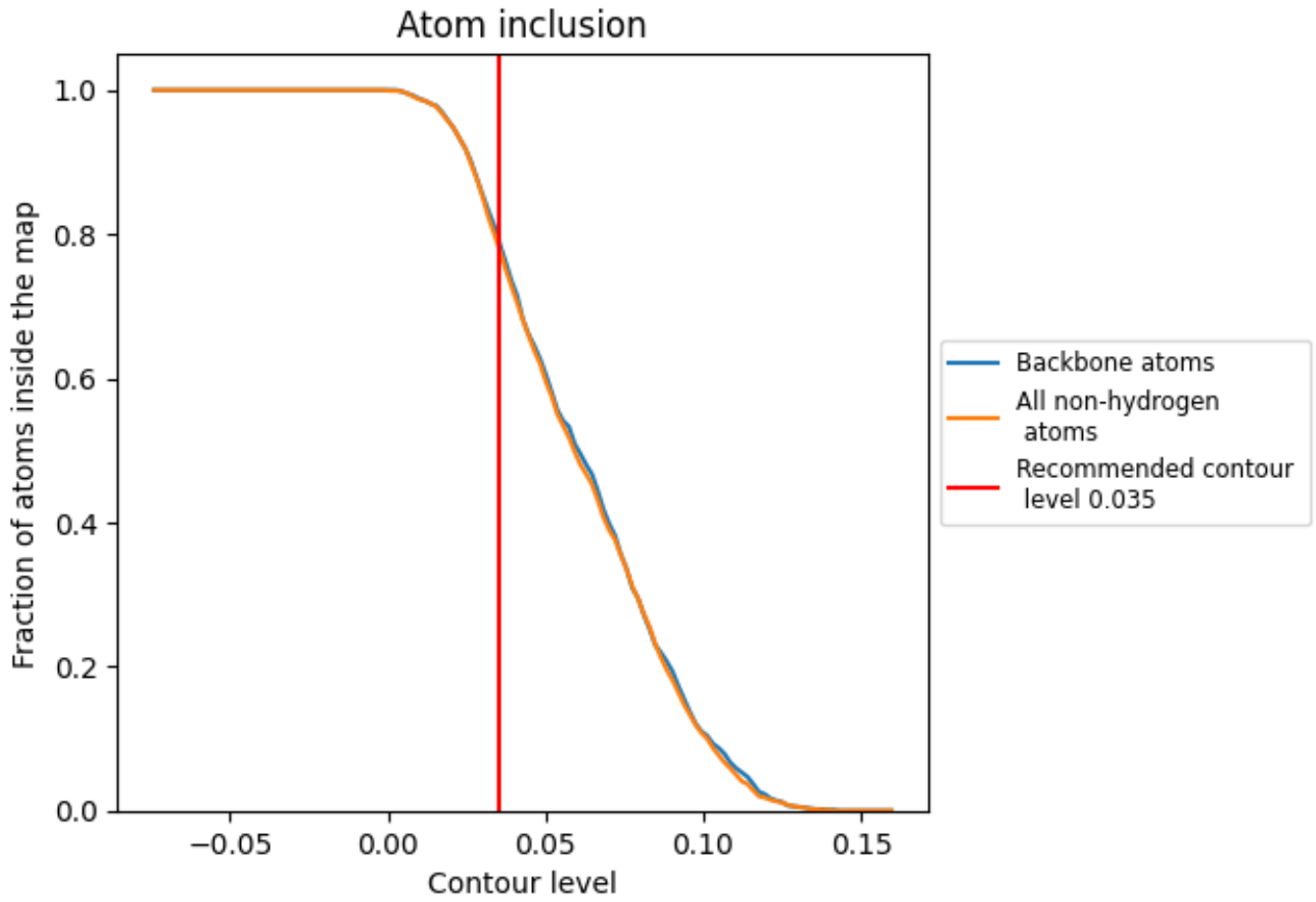
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.5120
A	0.7350	0.4950
B	0.8410	0.5330