



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 08:06 AM UTC

PDB ID : 9NWE / pdb_00009nwe
EMDB ID : EMD-49876
Title : E3 ligase UBR4-KCMF1-calmodulin complex
Authors : Yang, Z.; Rape, M.P.
Deposited on : 2025-03-22
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

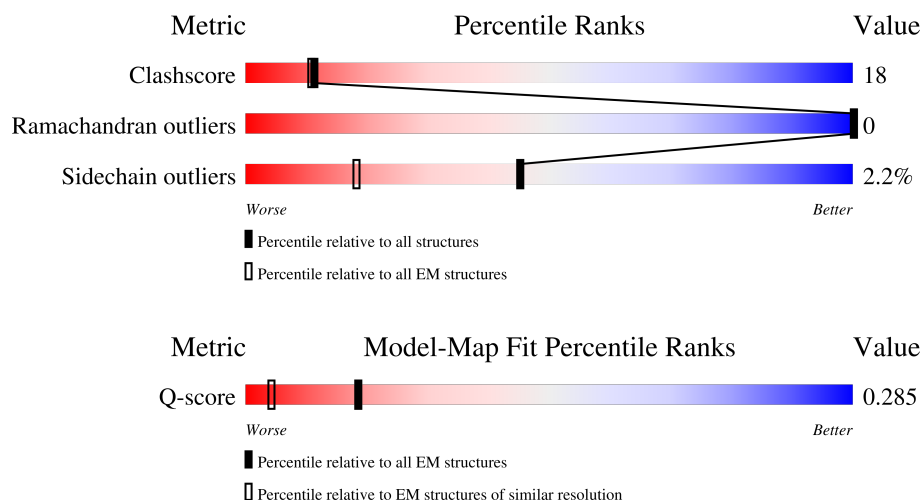
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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

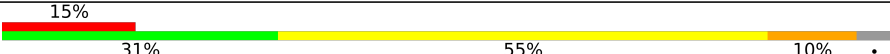
The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5205	
1	B	5205	
2	C	149	
2	D	149	

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Mol	Chain	Length	Quality of chain
3	E	381	
3	F	381	

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
4	ZN	A	5203	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29288 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 E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1660	Total	C	N	O	S	0	0
			13132	8325	2255	2465	87		
1	B	1660	Total	C	N	O	S	0	0
			13134	8325	2255	2467	87		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q5T4S7
A	-20	ASP	-	expression tag	UNP Q5T4S7
A	-19	TYR	-	expression tag	UNP Q5T4S7
A	-18	LYS	-	expression tag	UNP Q5T4S7
A	-17	ASP	-	expression tag	UNP Q5T4S7
A	-16	HIS	-	expression tag	UNP Q5T4S7
A	-15	ASP	-	expression tag	UNP Q5T4S7
A	-14	GLY	-	expression tag	UNP Q5T4S7
A	-13	ASP	-	expression tag	UNP Q5T4S7
A	-12	TYR	-	expression tag	UNP Q5T4S7
A	-11	LYS	-	expression tag	UNP Q5T4S7
A	-10	ASP	-	expression tag	UNP Q5T4S7
A	-9	HIS	-	expression tag	UNP Q5T4S7
A	-8	ASP	-	expression tag	UNP Q5T4S7
A	-7	ILE	-	expression tag	UNP Q5T4S7
A	-6	ASP	-	expression tag	UNP Q5T4S7
A	-5	TYR	-	expression tag	UNP Q5T4S7
A	-4	LYS	-	expression tag	UNP Q5T4S7
A	-3	ASP	-	expression tag	UNP Q5T4S7
A	-2	ASP	-	expression tag	UNP Q5T4S7
A	-1	ASP	-	expression tag	UNP Q5T4S7
A	0	ASP	-	expression tag	UNP Q5T4S7
A	1	LYS	-	expression tag	UNP Q5T4S7
B	-21	MET	-	initiating methionine	UNP Q5T4S7
B	-20	ASP	-	expression tag	UNP Q5T4S7
B	-19	TYR	-	expression tag	UNP Q5T4S7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	LYS	-	expression tag	UNP Q5T4S7
B	-17	ASP	-	expression tag	UNP Q5T4S7
B	-16	HIS	-	expression tag	UNP Q5T4S7
B	-15	ASP	-	expression tag	UNP Q5T4S7
B	-14	GLY	-	expression tag	UNP Q5T4S7
B	-13	ASP	-	expression tag	UNP Q5T4S7
B	-12	TYR	-	expression tag	UNP Q5T4S7
B	-11	LYS	-	expression tag	UNP Q5T4S7
B	-10	ASP	-	expression tag	UNP Q5T4S7
B	-9	HIS	-	expression tag	UNP Q5T4S7
B	-8	ASP	-	expression tag	UNP Q5T4S7
B	-7	ILE	-	expression tag	UNP Q5T4S7
B	-6	ASP	-	expression tag	UNP Q5T4S7
B	-5	TYR	-	expression tag	UNP Q5T4S7
B	-4	LYS	-	expression tag	UNP Q5T4S7
B	-3	ASP	-	expression tag	UNP Q5T4S7
B	-2	ASP	-	expression tag	UNP Q5T4S7
B	-1	ASP	-	expression tag	UNP Q5T4S7
B	0	ASP	-	expression tag	UNP Q5T4S7
B	1	LYS	-	expression tag	UNP Q5T4S7

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	144	Total	C	N	O	S	0	0
			1134	696	182	247	9		
2	D	143	Total	C	N	O	S	0	0
			1127	692	181	245	9		

- Molecule 3 is a protein called E3 ubiquitin-protein ligase KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	46	Total	C	N	O	S	0	0
			380	231	68	79	2		
3	F	45	Total	C	N	O	S	0	0
			371	226	67	76	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	Zn	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
4	B	3	Total	Zn	0
			3	3	

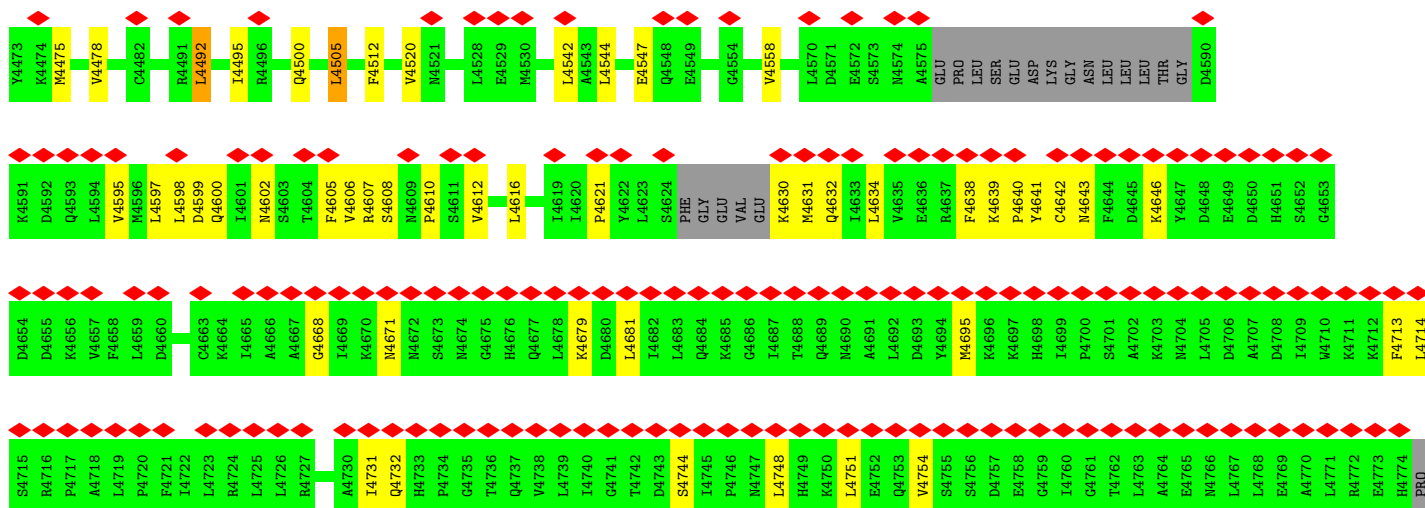
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Ca	0
			2	2	
5	D	2	Total	Ca	0
			2	2	



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N4412	T4352	L4273	R4134	VAL	S3966	V3879	S3791	C3677	Q3443	SER	D3298	K3199
K4413	L4353	R4274	T4135	GLU	S3967	V3880	V3792	G3678	L3447	LYS	S3299	I3200
L4414	E4354	L4276	C4146	ALA	L3968	E3881	R3793	E3679	SER	SER	V3300	Q3201
T4415	K4355	V4277	V4149	LEU	Q3969	H3882	R3794	N3680	L3450	THR	L3301	Q3202
S4416	D4356	V4278	V4155	THR	E3970	C3883	L3799	V3681	L3453	LYS	F3302	R3207
L4417	P4357	Q4279	T4155	P4047	K3972	L3884	A3800	Y3682	S3453	LYS	F3304	R3211
D4418	Q4358	T4280	L4158	L4281	L3973	L3887	Q3801	D3580	I3454	SER	L3305	K3212
L4419	Q4359	L4282	R4158	W4059	L3974	R3888	E3802	Y3683	W3455	LYS	Q3306	L3213
P4420	E4360	L4283	K4159	W4059	L3975	A3889	Y3803	R3688	E3457	GLU	S3307	L3214
D4421	D4361	L4284	L4165	W4071	L3979	R3890	C3807	R3583	L3458	GLU	F3309	L3215
A4422	E4362	D4285	L4165	W4071	S3980	S3893	C3807	R3588	P3459	LYS	L3310	F3216
E4423	L4363	T4287	K3981	L4075	K3981	P3894	I3818	N3595	A3460	GLU	V3311	
V4424	Q4364	P4076	Y4169	P4076	S3985	A3895	Q3819	R3595	Y3461	GLU	D3312	Q3226
V4425	G4365	L4077	L4170	L4077	C3985	L3896	K3820	L3605	K3464	LYS	V3315	L3227
K4426	E4366	R4078	E4171	R4078	Q3986	R3897	V3821	K3605	A3465	LYS	V3318	R3228
L4427	R4367	G4079	E4172	G4079	E3987	H3898	F3822	R3697	K3465	GLY	L3319	H3231
V4428	R4368	L4173	L4173	L4080	L3988	L3899	L3699	F3688	V3469	GLU	L3320	L3233
W4429	Q4369	L4186	Y4187	D4081	K3989	L3900	R3825	E3826	D3470	THR	L3323	D3234
C4430	G4369	Y4187	Y4187	G4082	L3990	V3901	K3826	Y3827	K3478	SER	L3324	S3235
T4431	M4370	L4191	L4191	N4083	R3991	Q3903	L3828	K3628	L3478	GLY	C3325	H3236
T4432	E4372	E4303	A4201	G4084	L3994	G3904	L3833	I3629	S3490	GLU	A3326	V3237
N4433	S4373	A4305	W4195	K4085	F3997	L3905	L3836	D3630	V3494	GLU	C3327	R3238
E4434	S4374	T4306	W4196	A4086	L3998	I3906	R3836	L3631	E3495	GLU	L3328	I3240
O4435	S4375	K4307	Y4199	K4089	M3999	L3909	A3839	L3633	E3496	GLU	C3329	K3241
E4436	E4376	L4200	A4201	L4092	V4001	F3910	T3840	I3642	L3497	GLU	S3330	L3244
P4437	P4377	M4311	A4202	L4093	W4002	N3913	S3843	I3726	I3512	THR	K3331	E3245
M4438	G4378	A4312	P4006	K4093	L4003	M3921	V3847	D3646	I3513	GLU	A3337	
R4439	I4379	C4313	V4007	A4094	I4003	R3922	Q3848	F3647	N3514	LYS	ALA	I3249
L4440	G4380	R4319	W4008	L4096	L4008	V3925	P3849	Y3648	L3516	GLY	SER	F3250
V4441	A4381	ASN	L4228	Y4096	V4008	V3926	F3851	E3649	G3517	GLY	SER	L3251
Y4442	L4382	LEU	S4229	Y4096	V4008	R3929	T3850	I3650	C3518	GLY	GLY	A3258
R4443	M4383	ASP	T4230	L4097	V4008	M3929	T3852	Y3651	I3409	GLY	SER	
M4444	R4384	D4324	D4231	L4098	W4011	L3932	A3853	Q3652	F3410	GLY	SER	
R4445	D4385	T4327	L4232	Q4104	M4015	L3932	Q3854	I3652	I3411	GLY	SER	
G4446	I4386	L4331	L4238	Q4106	C4016	L4017	Q3855	S3654	L3412	GLY	SER	
E4447	K4387	L4331	L4244	Q4108	L4018	E3938	T3856	T3655	F3522	GLY	ALA	L3269
L4448	M4388	R4334	L4245	F4108	L4019	A3939	R3857	E3656	Y3525	GLY	SER	I3270
Q4449	M4389	L4335	F4248	R4111	T4024	T3940	ALA	T3657	L3526	GLY	SER	E3274
D4450	I4390	I4338	W4251	R4112	P4027	K3950	LEU	L3658	L3527	GLY	SER	H3275
A4451	Q4391	E4338	E4252	R4115	A4028	V3951	VAL	I3659	C3532	GLY	PRO	
T4452	Q4392	E4343	S4253	L4119	P4029	S3952	LEU	R3662	L3533	GLY	VAL	Q3285
E4453	D4393	N4344	L4254	L4119	T4030	A3953	GLY	C3663	V3534	GLY	ALA	R3286
E4454	C4394	E4345	K4255	L4123	S4031	A3954	CYS	S3664	C3535	GLY	ALA	N3289
D4455	L4395	E4346	R4256	L4123	K4032	K3955	GLY	A3665	N3537	GLY	SER	Q3291
E4456	L4396	T4347	W4263	N4127	K4033	K3957	R3866	S3666	P3538	GLY	GLN	K3292
L4457	D4397	E4348	D4036	W4128	H4034	H3958	T3967	V3667	H3434	GLY	GLN	F3293
S4458	A4398	L4271	P4037	L4129	D4036	D3963	ALA	P3668	I3545	GLY	ALA	K3294
L4459	L4399	C4272	P4038	R4130	W4037	A3965	LEU	A3669	K3546	THR	THR	I3295
D4460	L4400			Q4131	P4038		SER	N3670	S3440	THR	THR	K3296
S4461	E4401			W4132			LEU	P3671		GLN	GLN	
T4462	D4402			L4133			VAL	G3672		ALA	ALA	
T4463	D4403						GLY	V3673		ALA	ALA	
D4464	S4404						GLY	C3674		ALA	ALA	
E4465	D4405						GLY	G3675		ALA	ALA	
E4466	M4406						GLY	N3676		ALA	ALA	
E4467	E4407						GLY	S3787		ALA	ALA	
D4468	L4408						GLY			ALA	ALA	
E4471	V4410						GLY			ALA	ALA	
V4472							GLY			ALA	ALA	

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- Molecule 1: E3 ubiquitin-protein ligase UBR4



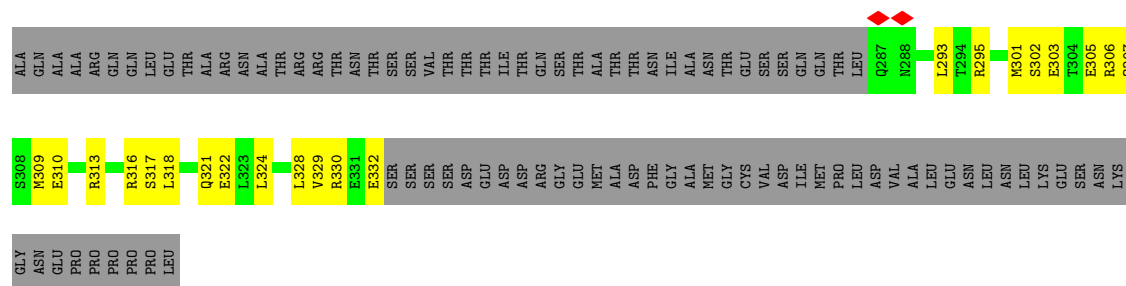
ALA	ASN	ASN	GLU	GLY	LYS	SER	ALA	ASP	MET
ASN	SER	ASN	PRO	GLY	LEU	VAL	SER	THR	ASP
PHE	ASP	ASN	GLN	ASN	GLN	ALA	ALA	TYR	LYS
ILE	GLU	THR	VAL	THR	VAL	CYS	PHE	ASP	HIS
MET	SER	ILE	LYS	SER	LYS	LYS	GLU	ASP	ASP
PRO	PRO	THR	THR	THR	LEU	VAL	MET	GLY	GLY
ALA	ALA	ALA	THR	ALA	LEU	ILE	GLY	ASP	TYR
VAL	VAL	GLN	ASP	ASP	GLU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



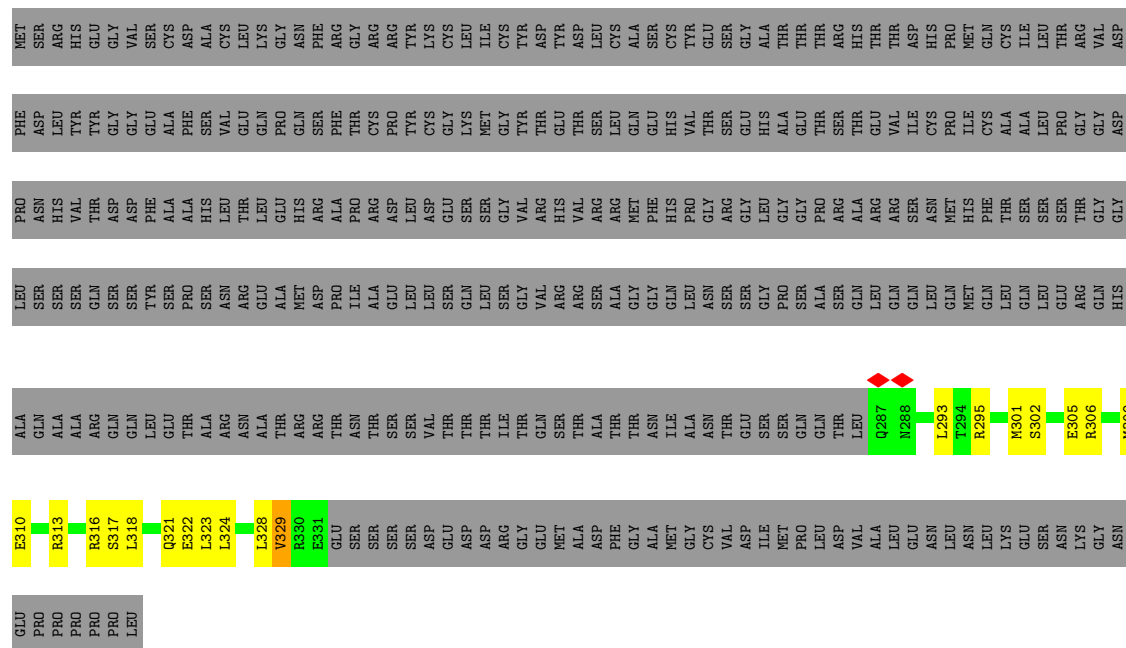




GLN	ASP	GLU	E4769	D4708	Y4647	ASN	E4467	E4407	T4347	L4271	Q4131	K4046
ARG	CYS	LEU	D4648	I4709	D4648	LEU	D4468	L4408	F4348	C4272	V4132	L3968
PRO	LEU	GLU	E4649	W4710	E4649	LEU	E4471	L4409	F4349	L4273	T4135	Q3969
THR	ALA	GLU	D4650	K4711	D4650	THR	E4471	V4410	F4350	K4274	R4142	Y3970
GLN	VAL	GLY	H4651	S4652	H4651	GLY	K4474	M4411	V4351	L4275	C4146	L3973
LEU	ARG	LEU	G4653	G4653	G4653	D4590	M4475	M4412	T4352	L4276	W4071	I3979
THR	ASP	THR	D4654	D4654	D4654	K4591	M4475	K4413	L4353	V4277	V4059	C3985
CYS	VAL	CYS	D4655	D4655	D4655	D4592	M4478	I4414	F4354	V4278	K4061	L4060
ILE	ASN	ILE	K4656	K4656	K4656	Q4593	M4479	I4415	I4155	R4062	R4062	L3987
ARG	LYS	ARG	V4657	V4657	V4657	L4594	C4482	S4416	R4158	W4071	W4071	L3988
GLY	LYS	GLY	L4658	L4658	L4658	G4483	G4484	L4417	K4159	L4075	L4075	L3994
ASP	ASP	ASP	L4659	L4659	L4659	G4484	G4484	D4418	Q4358	L4165	L4165	S3995
ALA	ALA	ALA	D4660	D4660	D4660	R4491	R4492	L4419	Q4359	L4166	L4166	L3997
ARG	ARG	ARG	C4663	C4663	C4663	L4598	L4598	P4420	D4361	D4081	D4081	L3997
GLU	GLU	GLU	K4664	K4664	K4664	D4599	D4599	V4421	F4362	G4082	G4082	L3998
THR	THR	THR	I4665	I4665	I4665	Q4600	Q4600	A4422	L4363	N4083	N4083	L3999
PRO	PRO	PRO	A4666	A4666	A4666	I4601	I4601	E4423	L4364	A4000	A4000	V4001
VAL	VAL	VAL	A4667	A4667	A4667	N4602	N4602	V4424	Q4365	G4084	G4084	N4002
LEU	LEU	LEU	A4668	A4668	A4668	T4604	T4604	Y4425	G4366	K4085	K4085	I4003
LYS	LYS	LYS	I4669	I4669	I4669	F4605	F4605	K4426	R4366	A4086	A4086	V4007
ARG	ARG	ARG	K4670	K4670	K4670	V4606	V4606	W4427	M4367	K4089	K4089	V4008
THR	THR	THR	M4671	M4671	M4671	R4607	R4607	V4428	P4368	L4092	L4092	N4011
MET	MET	MET	N4672	N4672	N4672	S4608	S4608	W4429	G4369	R4093	R4093	N4012
LEU	LEU	LEU	S4673	S4673	S4673	M4609	M4609	C4430	M4370	T4013	T4013	T4013
ARG	ARG	ARG	M4674	M4674	M4674	P4610	P4610	T4431	P4371	L4095	L4095	L4014
GLN	GLN	GLN	H4675	H4675	H4675	S4611	S4611	T4432	Y4372	Y4096	Y4096	N4015
ALA	ALA	ALA	H4676	H4676	H4676	R4622	R4622	M4433	S4373	C4016	C4016	L4017
LEU	LEU	LEU	Q4677	Q4677	Q4677	L4620	L4620	E4434	S4374	L4018	L4018	R4018
GLY	GLY	GLY	L4678	L4678	L4678	M4630	M4630	G4435	M4375	S4229	S4229	L4019
THR	THR	THR	D4679	D4679	D4679	L4542	L4542	P4437	E4376	R4104	R4104	L4020
LEU	LEU	LEU	D4680	D4680	D4680	E4547	E4547	M4438	P4377	W4105	W4105	Q4021
ASN	ASN	ASN	L4681	L4681	L4681	Q4548	Q4548	R4439	Q4378	R4106	R4106	R4022
PRO	PRO	PRO	I4682	I4682	I4682	E4549	E4549	I4440	I4379	Q4107	Q4107	L4023
LYS	LYS	LYS	Q4683	Q4683	Q4683	E4549	E4549	V4441	G4380	F4108	F4108	L4024
GLN	GLN	GLN	Q4684	Q4684	Q4684	G4554	G4554	W4442	P4381	L4109	L4109	K4025
LYS	LYS	LYS	K4685	K4685	K4685	V4554	V4554	R4443	L4382	S4110	S4110	P4026
THR	THR	THR	G4686	G4686	G4686	V4556	V4556	M4444	M4383	R4111	R4111	P4027
VAL	VAL	VAL	T4687	T4687	T4687	L4570	L4570	R4445	F4248	R4112	R4112	A4028
THR	THR	THR	H4748	H4748	H4748	D4571	D4571	G4446	V4251	G4113	G4113	S4031
ASN	ASN	ASN	Q4689	Q4689	Q4689	E4571	E4571	L4447	E4252	K4114	K4114	K4035
LYS	LYS	LYS	M4690	M4690	M4690	S4572	S4572	L4448	S4253	R4115	R4115	D4036
THR	THR	THR	A4691	A4691	A4691	S4573	S4573	G4449	I4254	P4118	P4118	VAL
ALA	ALA	ALA	L4692	L4692	L4692	M4574	M4574	D4450	R4255	L4119	L4119	PRO
LEU	LEU	LEU	D4693	D4693	D4693	A4575	A4575	I4338	R4256	GLU	GLU	VAL
LEU	LEU	LEU	Y4694	Y4694	Y4694	E4576	E4576	E4343	H4257	L4123	L4123	GLU
LYS	LYS	LYS	M4695	M4695	M4695	P4577	P4577	N4344	F4258	G4124	G4124	ALA
GLN	GLN	GLN	K4696	K4696	K4696	LEU	LEU	E4345	V4263	N4126	N4126	LEU
TYR	TYR	TYR	D4757	D4757	D4757	SER	SER	V4346	L4267	N4127	N4127	THR
THR	THR	THR	H4698	H4698	H4698	GLU	GLU	E4401	R4130	L4128	L4128	Y4045
ASP	ASP	ASP	I4699	I4699	I4699	GLU	GLU	D4402				
GLU	GLU	GLU	P4700	P4700	P4700	ASP	ASP	D4403				
ALA	ALA	ALA	S4701	S4701	S4701	LYS	LYS	S4404				
THR	THR	THR	A4702	A4702	A4702	GLY	GLY	G4405				
LEU	LEU	LEU	K4703	K4703	K4703			M4406				
THR	THR	THR	M4704	M4704	M4704							
ARG	ARG	ARG	L4705	L4705	L4705							
GLY	GLY	GLY	M4706	M4706	M4706							
THR	THR	THR	L4768	L4768	L4768							



- Molecule 3: E3 ubiquitin-protein ligase KCMF1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.493	Depositor
Minimum map value	-0.698	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.146	Depositor
Map size ($\text{\AA}$)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	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: CA, 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	A	0.61	1/13355 (0.0%)	0.90	24/18055 (0.1%)
1	B	0.64	6/13357 (0.0%)	0.91	24/18057 (0.1%)
2	C	1.06	2/1146 (0.2%)	1.31	5/1539 (0.3%)
2	D	1.14	2/1138 (0.2%)	1.34	8/1526 (0.5%)
3	E	0.36	0/382	0.68	0/511
3	F	0.35	0/373	0.77	1/499 (0.2%)
All	All	0.66	11/29751 (0.0%)	0.94	62/40187 (0.2%)

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
1	A	0	2
1	B	0	1
All	All	0	3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4013	THR	C-O	-6.08	1.17	1.24
1	B	4023	LEU	C-O	-6.06	1.17	1.24
1	A	3968	LEU	C-O	-5.96	1.16	1.24
2	D	14	LYS	CA-C	-5.91	1.45	1.52
2	C	14	LYS	CA-C	-5.89	1.45	1.52

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3792	VAL	CA-C-N	-17.13	96.38	120.71
1	A	3792	VAL	C-N-CA	-17.13	96.38	120.71
1	A	3792	VAL	O-C-N	13.47	136.41	122.54
1	A	3969	GLN	CB-CA-C	-12.40	91.86	110.96
2	C	86	ILE	N-CA-C	-11.11	97.20	111.09

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3286	ARG	Sidechain
1	A	4319	ARG	Sidechain
1	B	4112	ARG	Sidechain

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	13132	0	13358	477	0
1	B	13134	0	13352	460	0
2	C	1134	0	1063	91	0
2	D	1127	0	1055	112	0
3	E	380	0	376	30	0
3	F	371	0	370	17	0
4	A	3	0	0	3	0
4	B	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	29288	0	29574	1056	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 18.

The worst 5 of 1056 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:4032:LYS:CE	3:E:307:GLN:HG3	1.25	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4307:LYS:CG	1:A:4475:MET:HE1	1.45	1.44
1:A:4307:LYS:HG3	1:A:4475:MET:CE	1.47	1.42
1:A:4032:LYS:CE	3:E:307:GLN:CG	2.11	1.28
1:B:4098:THR:OG1	2:D:113:LEU:HD21	1.18	1.26

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	1644/5205 (32%)	1590 (97%)	54 (3%)	0	100	100
1	B	1644/5205 (32%)	1599 (97%)	45 (3%)	0	100	100
2	C	142/149 (95%)	131 (92%)	11 (8%)	0	100	100
2	D	139/149 (93%)	127 (91%)	12 (9%)	0	100	100
3	E	44/381 (12%)	44 (100%)	0	0	100	100
3	F	43/381 (11%)	43 (100%)	0	0	100	100
All	All	3656/11470 (32%)	3534 (97%)	122 (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	1471/4542 (32%)	1439 (98%)	32 (2%)	45	71
1	B	1471/4542 (32%)	1443 (98%)	28 (2%)	50	73
2	C	123/127 (97%)	118 (96%)	5 (4%)	27	60
2	D	122/127 (96%)	114 (93%)	8 (7%)	15	47
3	E	45/330 (14%)	45 (100%)	0	100	100
3	F	44/330 (13%)	44 (100%)	0	100	100
All	All	3276/9998 (33%)	3203 (98%)	73 (2%)	45	71

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4542	LEU
2	D	78	LYS
1	B	4649	GLU
2	D	21	ASP
1	A	4400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4002	ASN
1	B	4651	HIS
1	B	4011	ASN
1	B	4500	GLN
2	C	43	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

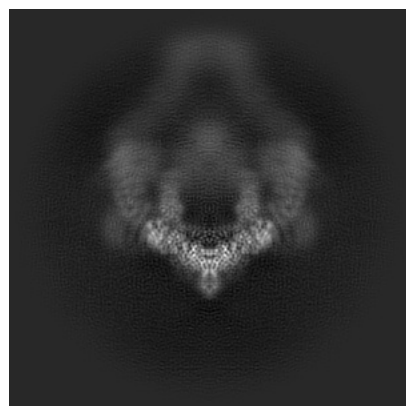
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49876. These allow visual inspection of the internal detail of the map and identification of artifacts.

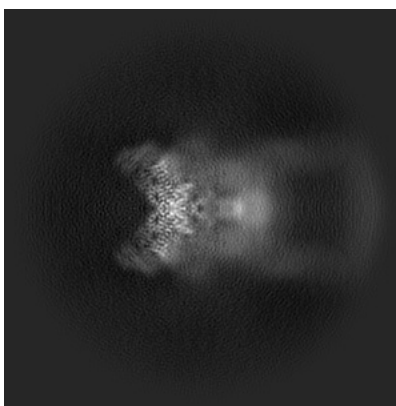
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

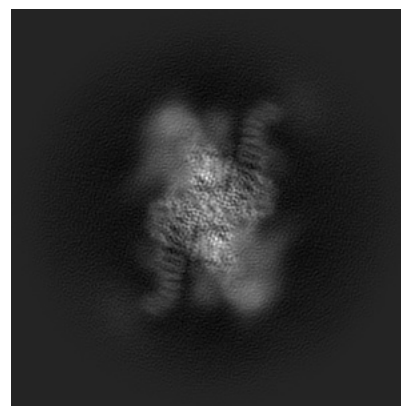
6.1.1 Primary map



X

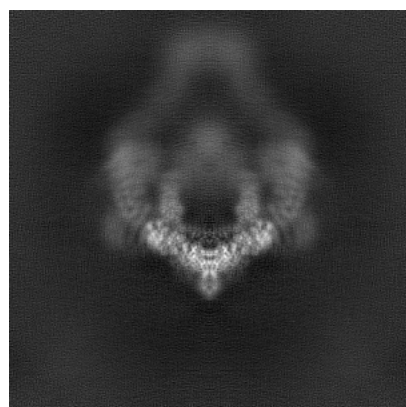


Y

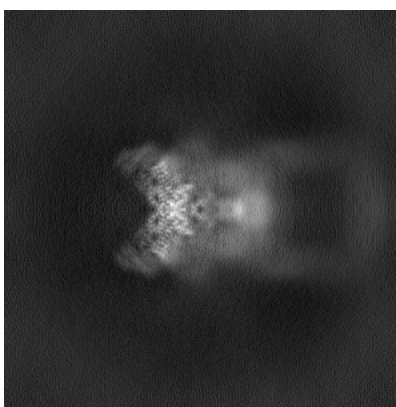


Z

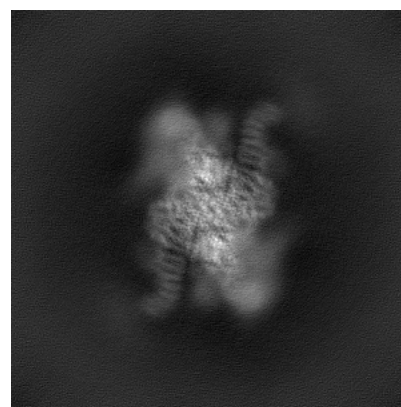
6.1.2 Raw map



X



Y

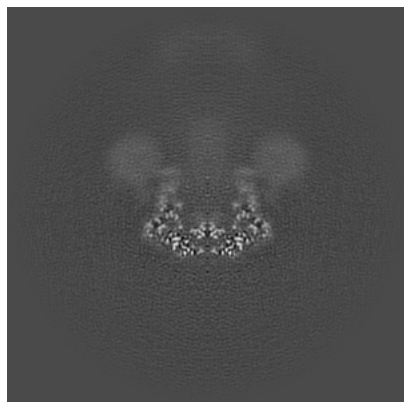


Z

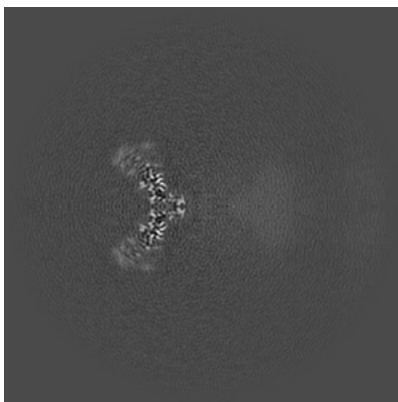
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

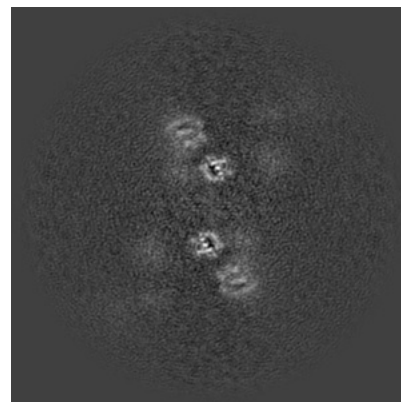
6.2.1 Primary map



X Index: 200

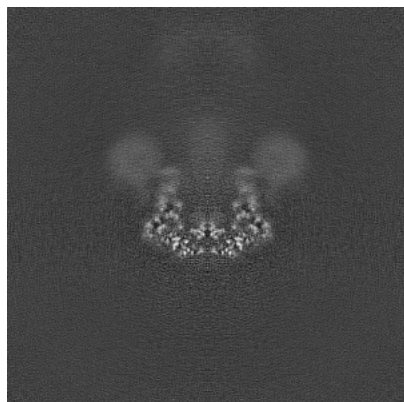


Y Index: 200

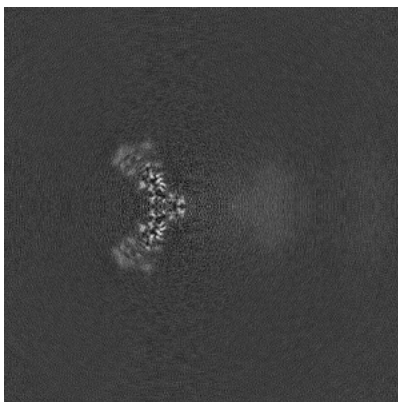


Z Index: 200

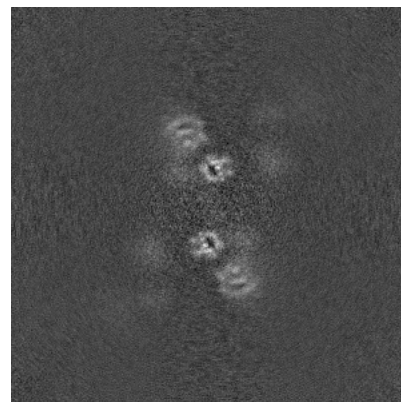
6.2.2 Raw map



X Index: 200



Y Index: 200

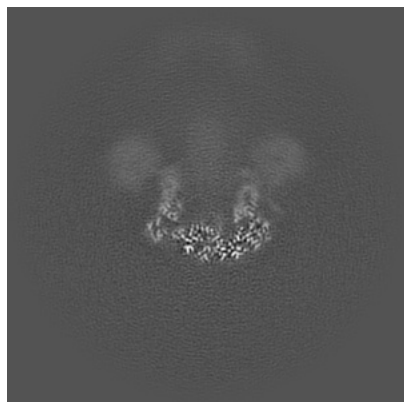


Z Index: 200

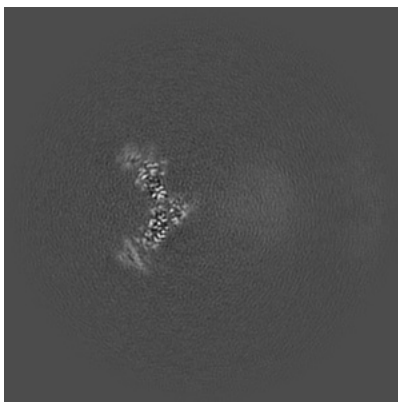
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

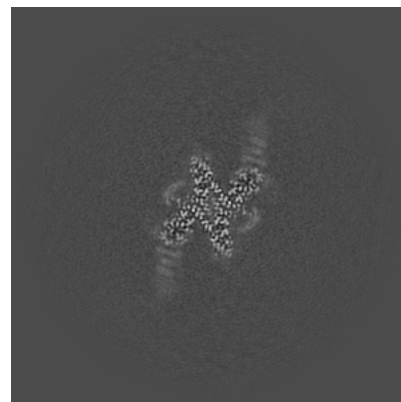
6.3.1 Primary map



X Index: 195



Y Index: 194

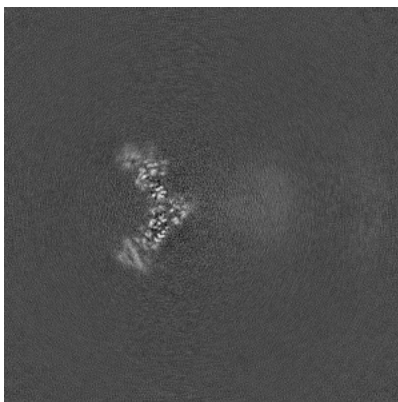


Z Index: 158

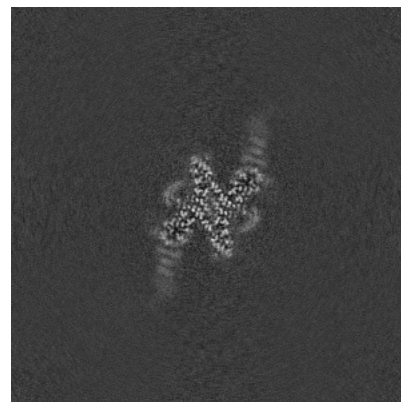
6.3.2 Raw map



X Index: 195



Y Index: 194

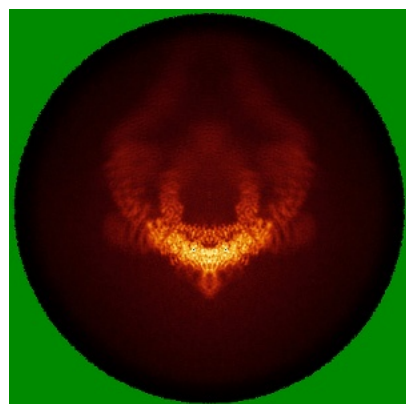


Z Index: 158

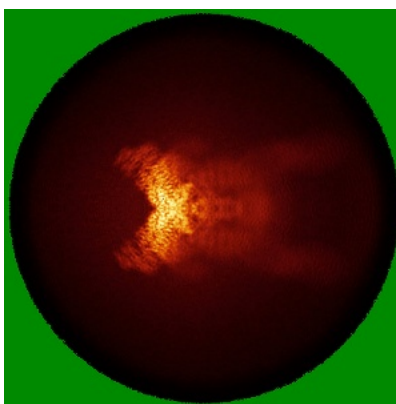
The images above show the largest variance slices of the map in three orthogonal directions.

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

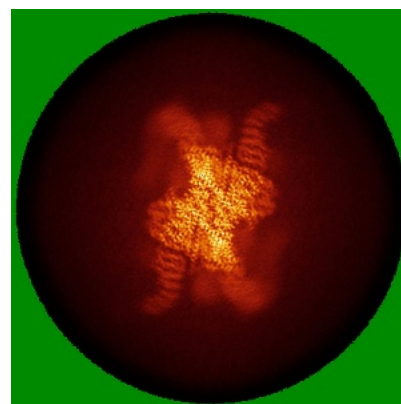
6.4.1 Primary map



X



Y

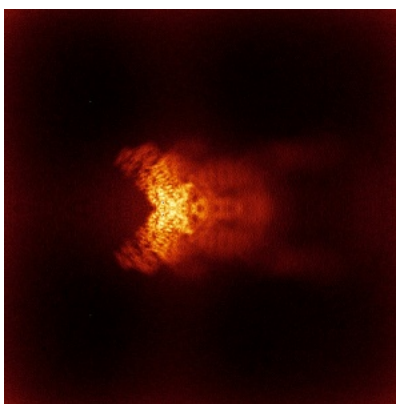


Z

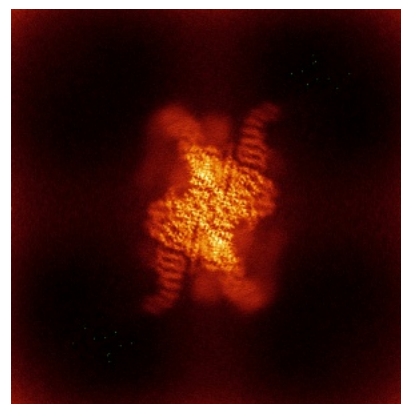
6.4.2 Raw map



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.

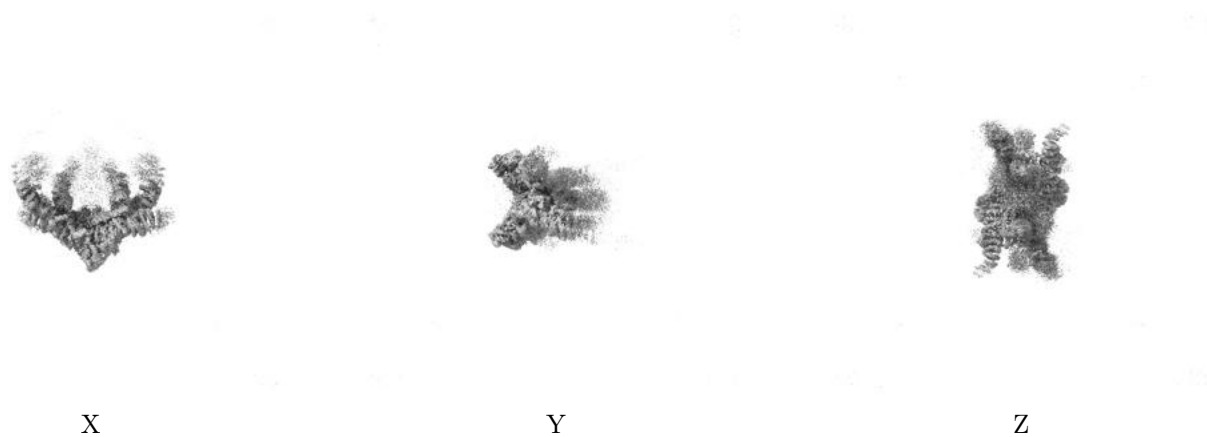
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.146. 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.

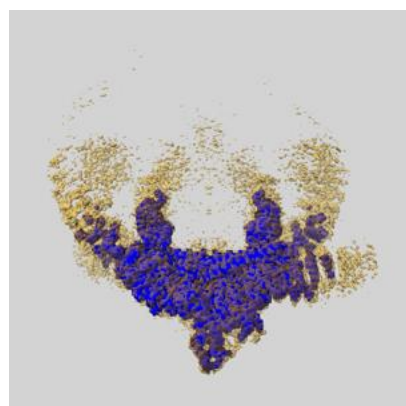
6.6 Mask visualisation [i](#)

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

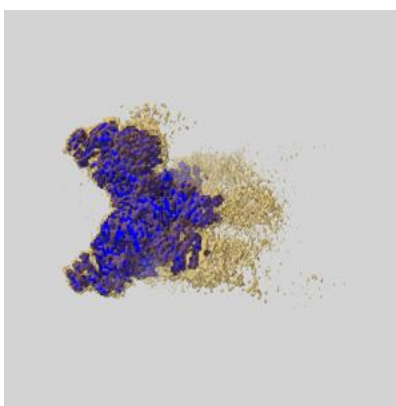
A mask typically either:

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

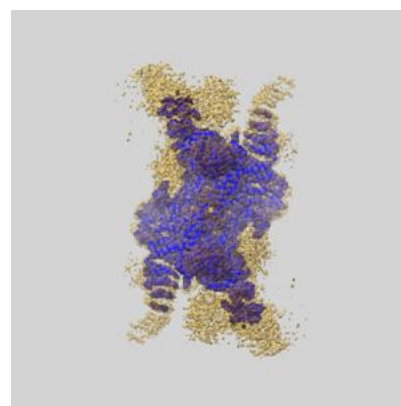
6.6.1 emd_49876_msk_1.map [i](#)



X



Y

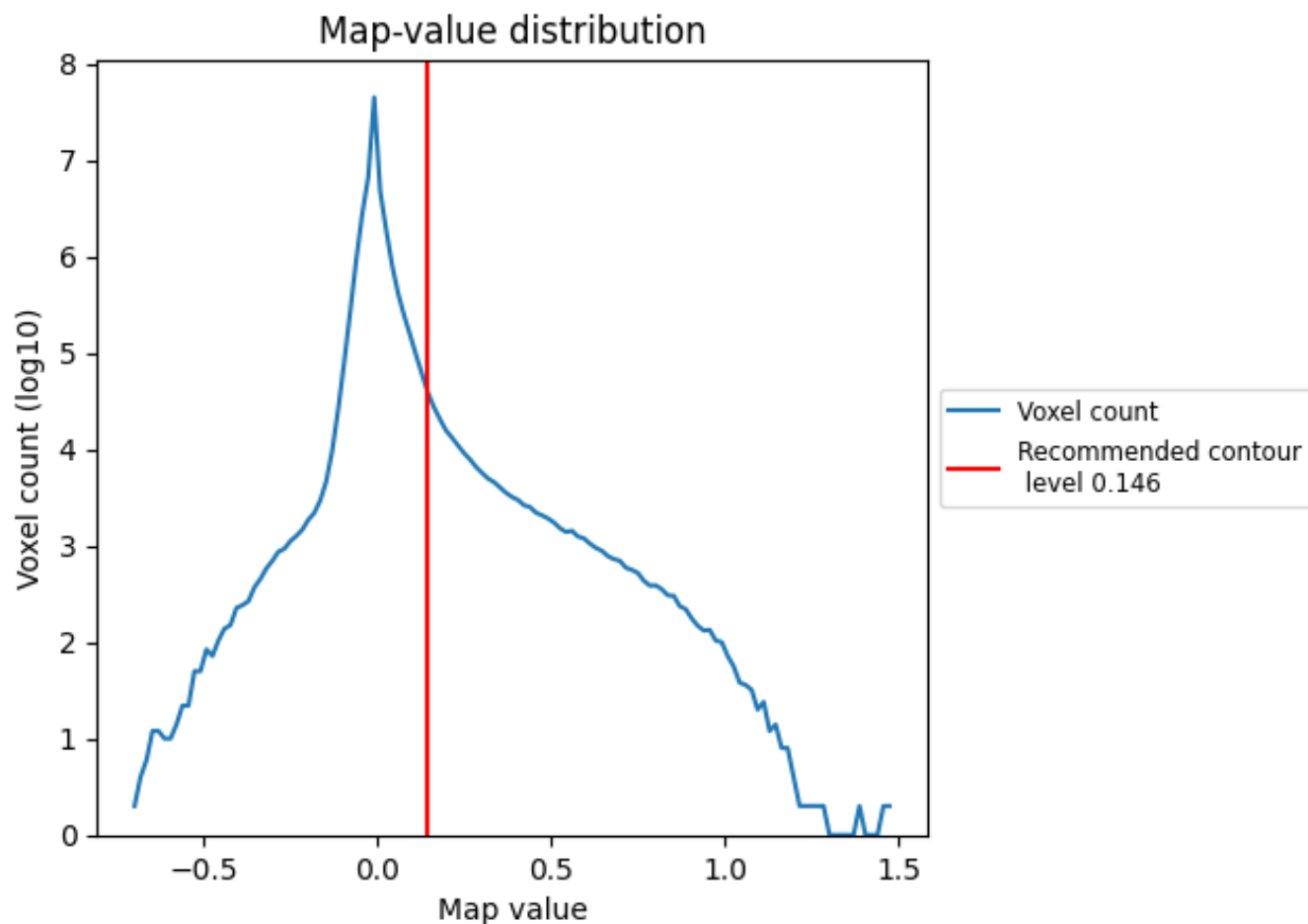


Z

7 Map analysis [i](#)

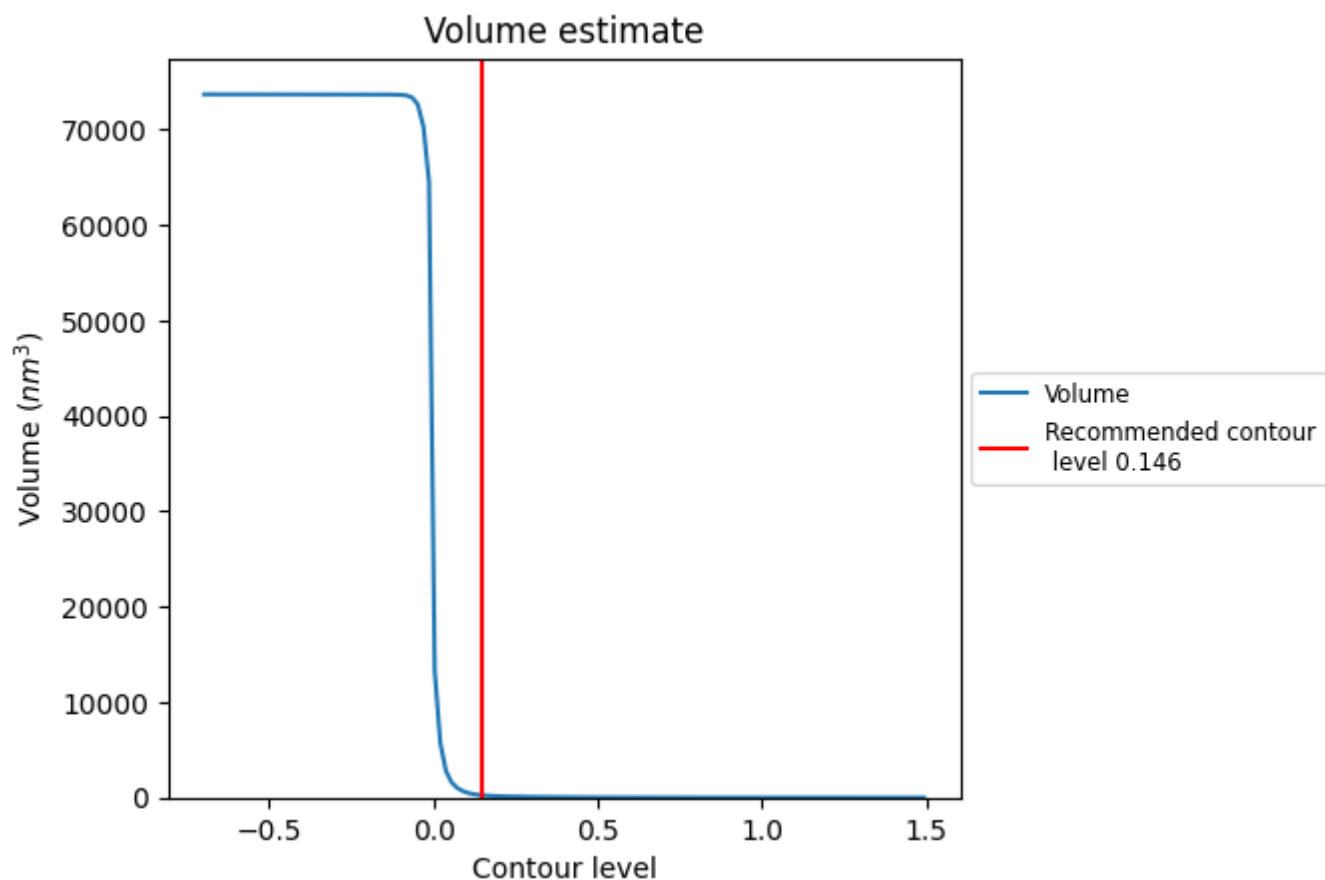
This section contains the results of statistical analysis of the map.

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.

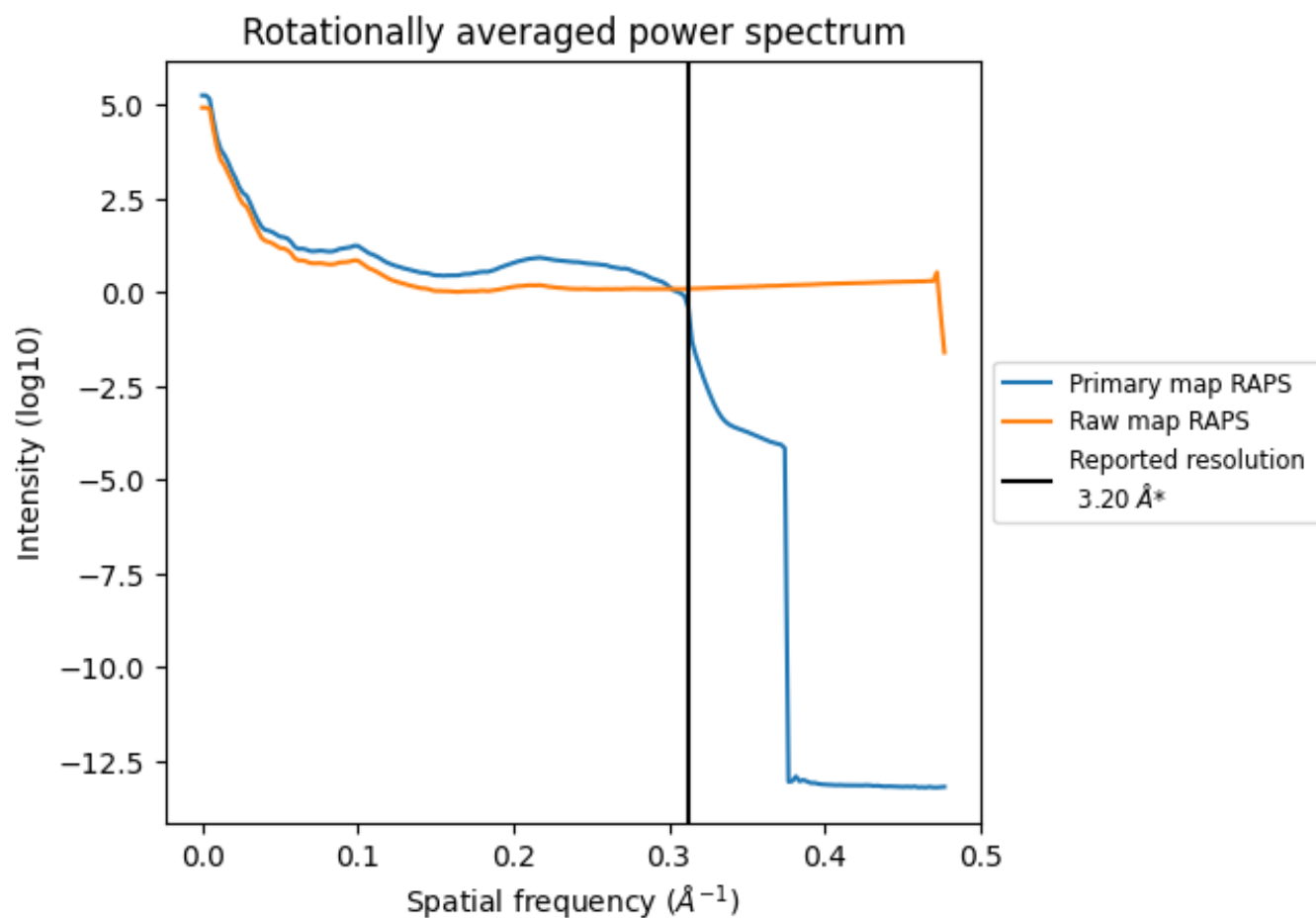
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm^3 ; this corresponds to an approximate mass of 223 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 ⓘ

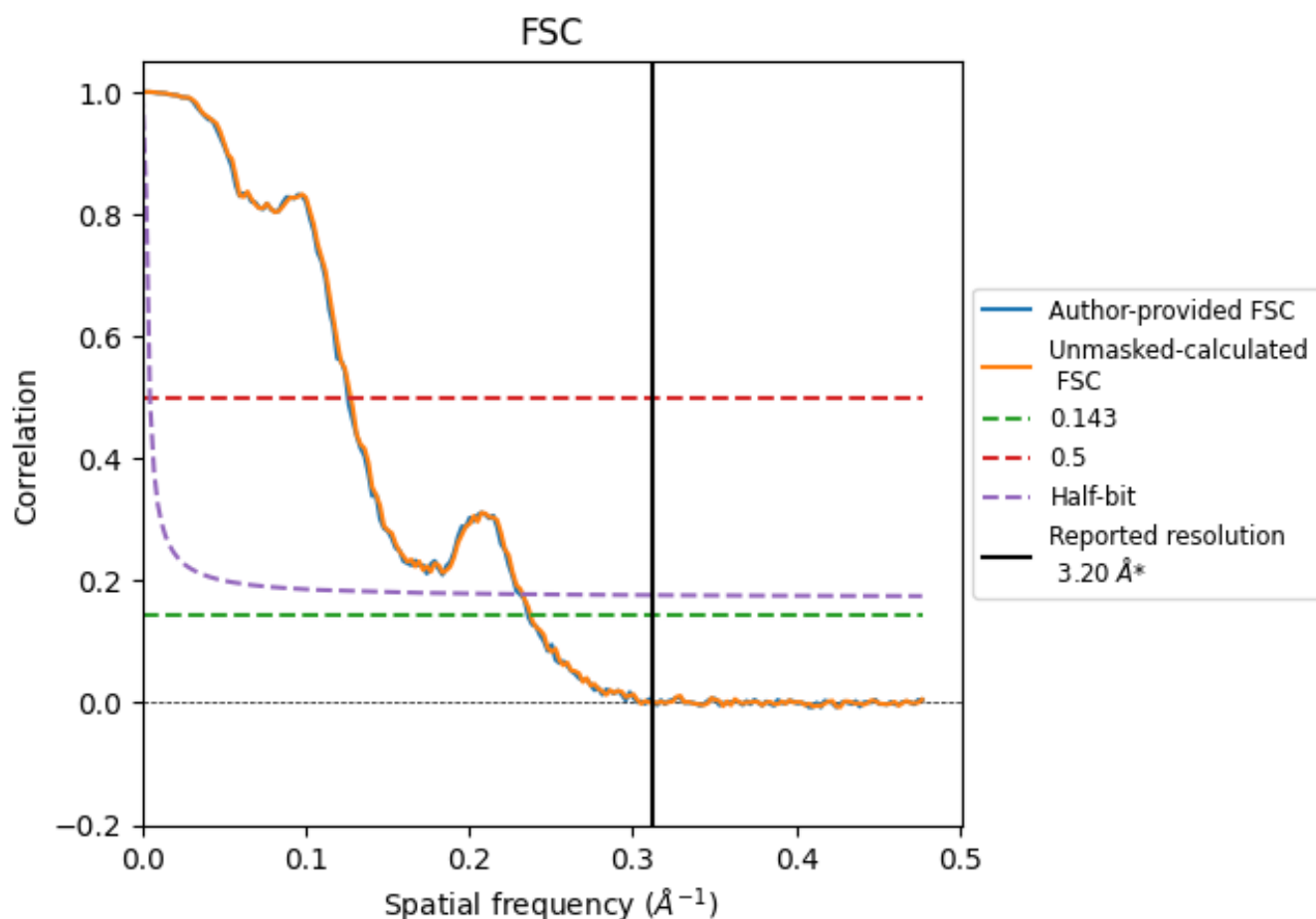


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	4.24	7.94	4.33
Unmasked-calculated*	4.21	7.84	4.30

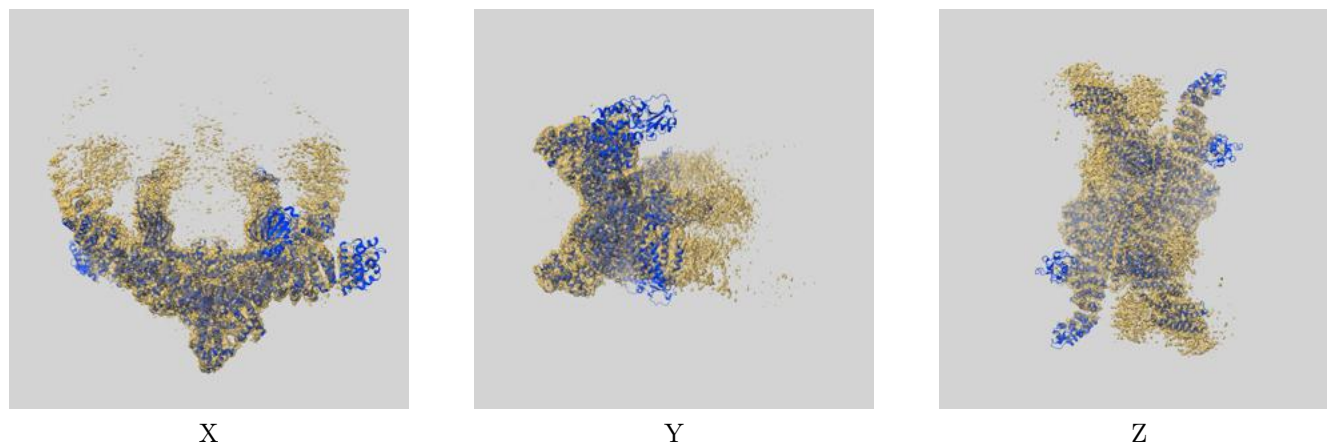
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

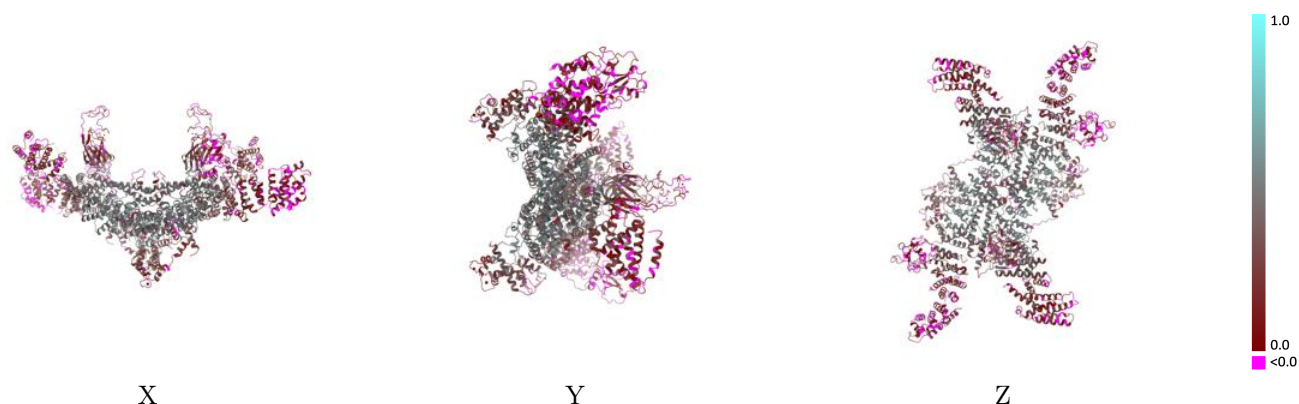
This section contains information regarding the fit between EMDB map EMD-49876 and PDB model 9NWE. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



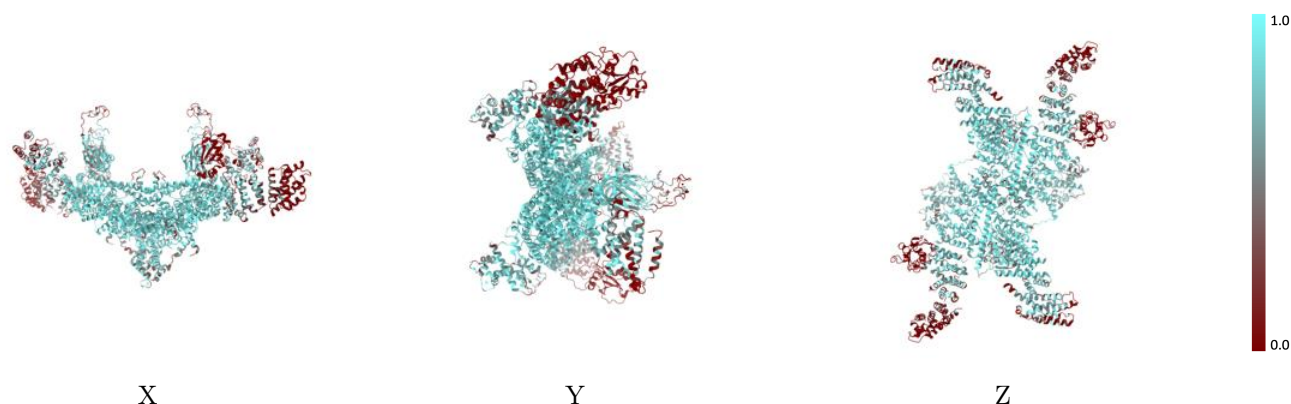
The images above show the 3D surface view of the map at the recommended contour level 0.146 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



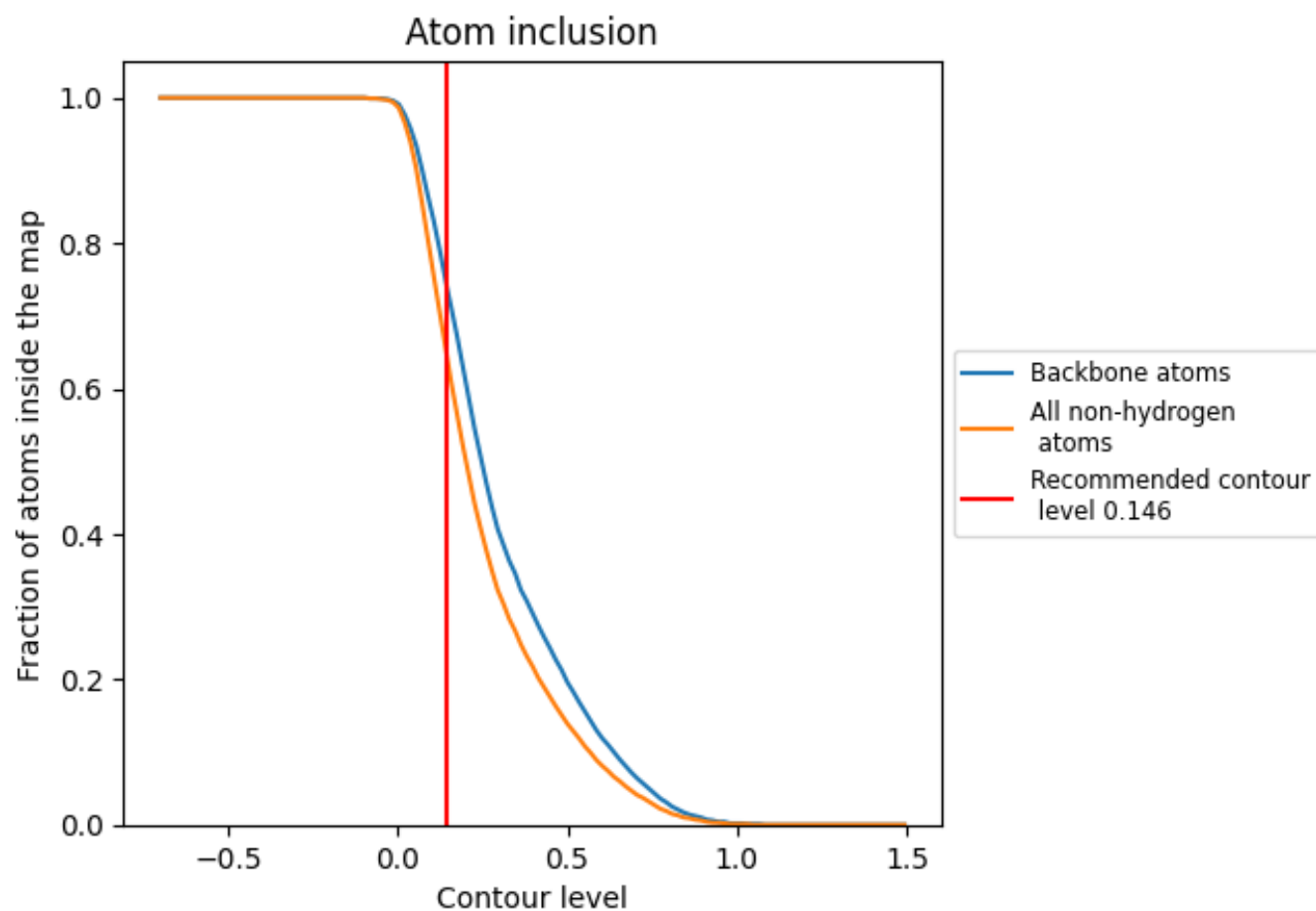
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.146).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.146) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.2850
A	0.6370	0.2880
B	0.6360	0.2870
C	0.6210	0.2260
D	0.6390	0.2360
E	0.8160	0.3900
F	0.8230	0.3850

1.0

0.0

<0.0