



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 06:39 AM EST

PDB ID : 7K0S
EMDB ID : EMD-22615
Title : Cryo-EM structure of rabbit RyR1 in the presence of Mg²⁺ and AMP-PCP in nanodisc
Authors : Nayak, A.R.; Samso, M.
Deposited on : 2020-09-05
Resolution : 4.50 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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

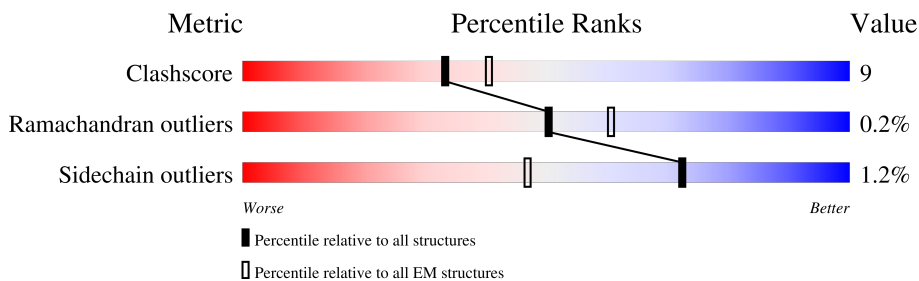
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	5037	
1	B	5037	
1	C	5037	
1	D	5037	

2 Entry composition [i](#)

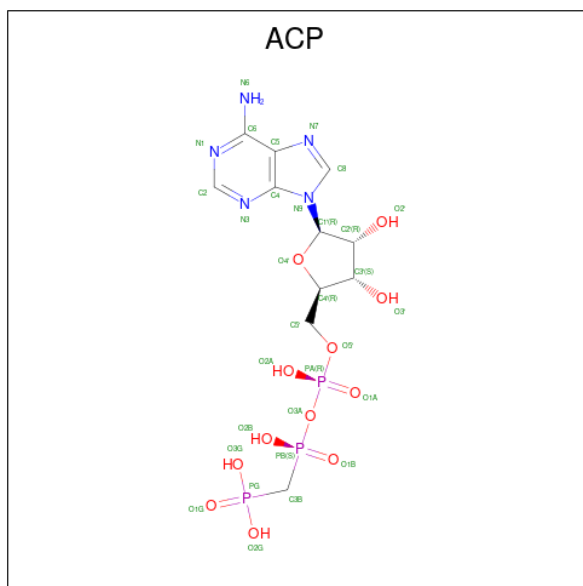
There are 4 unique types of molecules in this entry. The entry contains 115935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4110	Total	C	N	O	S	0	0
			28941	18335	5131	5318	157		
1	B	4110	Total	C	N	O	S	0	0
			28940	18334	5135	5315	156		
1	D	4110	Total	C	N	O	S	0	0
			28963	18348	5134	5324	157		
1	C	4110	Total	C	N	O	S	0	0
			28958	18354	5132	5317	155		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	B	1	Total	C	N	O	P	0
			31	11	5	12	3	

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Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	C	1	Total	C	N	O	P	0
			31	11	5	12	3	

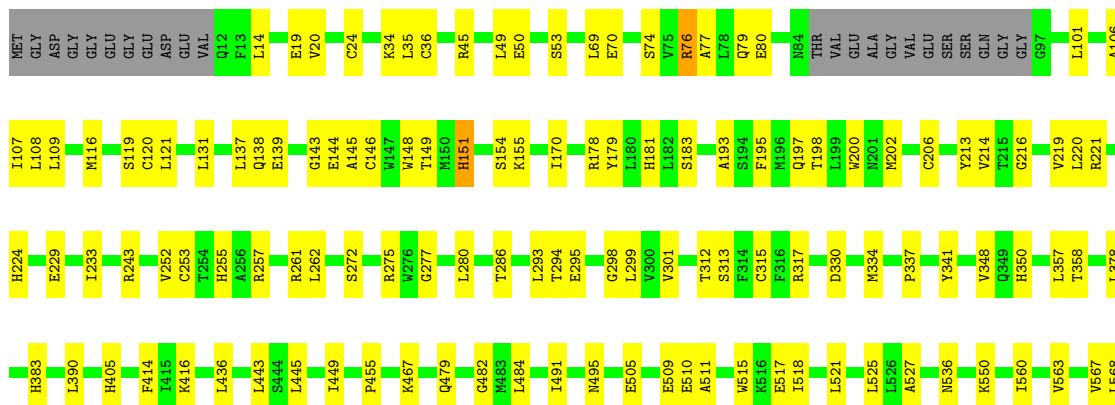
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	2	Total	Mg	0
			2	2	
4	D	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	

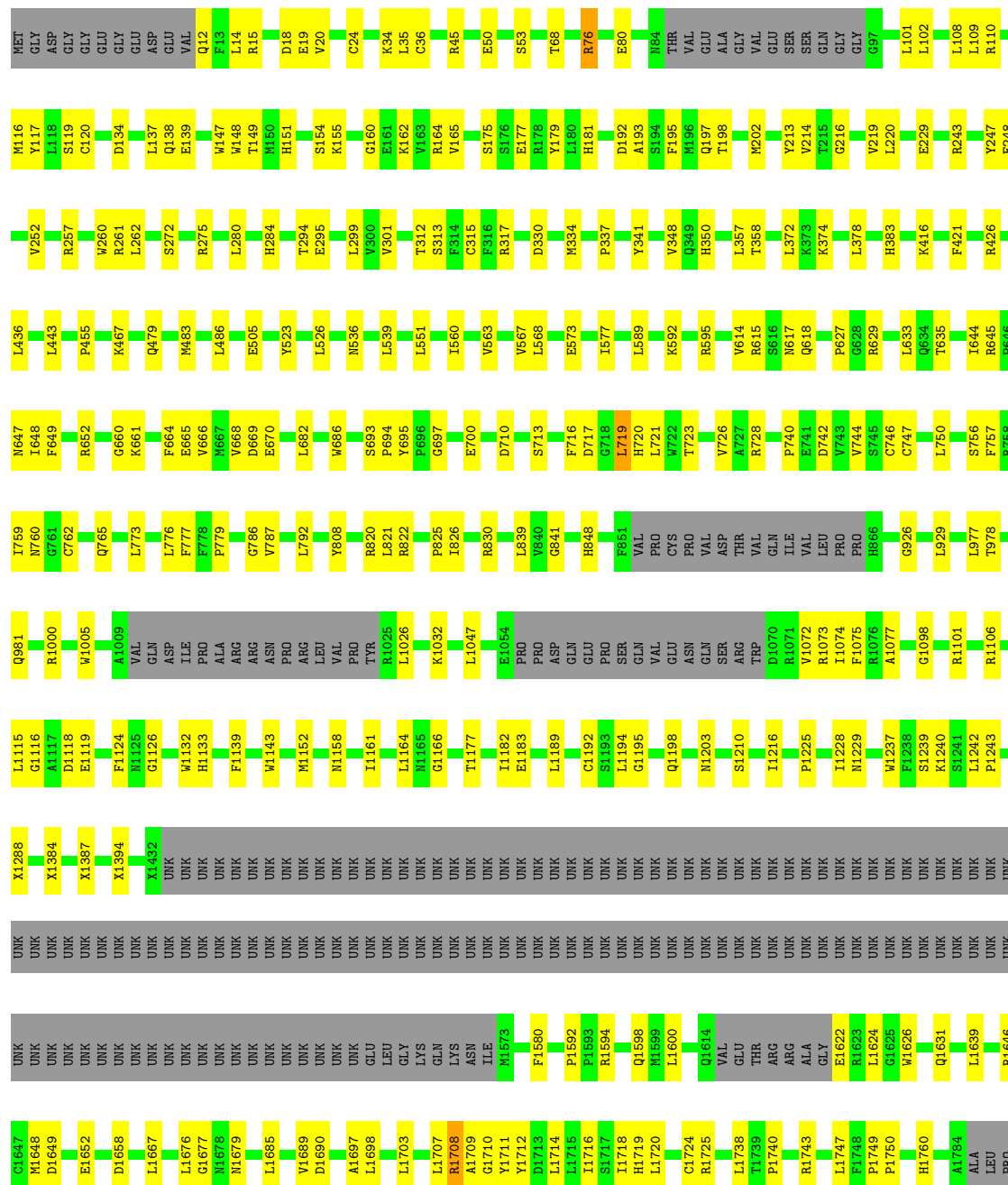
K3821	E3670	X3406	UNK	UNK	L2904	GLU	LYS	ALA	THR	LYS	PRO	L2257	GLU	E1956	E1874	GLU	C1724	L1600
K3824	V3702	X3410	UNK	UNK	T2912	LYS	THR	VAL	ASP	UNK	GLU	T2271	LEU	F1961	GLU	R1725	M1508	
L3835	D3719	X3490	UNK	UNK	L2926	UNK	UNK	UNK	UNK	UNK	GLU	L2273	PRO	E1962	GLU	R1727	P1609	
S3840	Y3722	X3491	UNK	UNK	E2939	GLY	GLY	GLY	GLY	GLY	GLU	A2276	ALA	E1963	GLU	I1735	I1614	
N3845	N3729	X3492	UNK	UNK	GLY	UNK	UNK	UNK	UNK	UNK	GLU	L2286	GLU	A1992	GLU	V1736	VAL	
R3849	N3741	X3493	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	GLU	A2287	THR	R1996	GLU	P1737	GLU	
A3853	GLY	X3535	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	GLY	L2479	UNK	Q2095	GLU	L1738	THR	
V3865	ALA	X3536	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	LYS	L2479	UNK	Q2003	GLU	P1740	ARG	
I3866	GLU	X3537	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ASP	L2479	UNK	Q2007	GLU	R1743	ALA	
D3877	GLU	X3544	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	GLY	V2299	UNK	N2007	GLU	L1747	GLY	
F3880	S3752	X3549	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	LYS	C2310	UNK	F2012	GLU	H1760	R1623	
R3886	E3754	X3551	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ASP	L2314	UNK	G2021	GLU	L1771	G1625	
L3888	K3755	X3554	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	VAL	R2330	UNK	P2022	GLU	L1772	W1626	
Q3889	K3756	X3561	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	F2337	UNK	L2023	GLU	A1627	A1631	
L3890	E3757	X3562	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2487	P2142	UNK	P2024	GLU	ALA	L1639	
L3891	R3758	X3562	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2606	C2158	UNK	H2041	GLU	PRO	R1646	
C3892	K3760	X3601	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2488	L2356	UNK	G2048	GLU	ALA	C1647	
E3893	Q3761	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2607	L2357	UNK	GLU	GLU	V1791	D1649	
F3899	R3762	X3613	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2607	L2358	UNK	GLU	GLU	R1797	E1652	
Q3906	L3763	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2608	L2359	UNK	GLU	GLU	LYS		
R3907	L3764	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2608	F2364	UNK	PRO	GLU	I1802	R1661	
I3913	Q3765	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2688	A2367	UNK	GLU	GLU	K1810	L1667	
L3924	R3766	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2691	L2368	UNK	THR	LYS	A1826	L1676	
Q3927	Q3767	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	X2703	L2376	UNK	SER	GLU	V1839	N1679	
I3930	R3768	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	CYS	A2379	UNK	LEU	GLU	P1840	V1689	
W3935	L3770	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ALA	A2379	UNK	SER	GLU	V1841	D1690	
Y3936	H3771	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ALA	R2392	UNK	ARG	ALA	L1842		
Y3937	T3772	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	GLY	ASP	UNK	LEU	PRO	K1843	A1697	
D3941	R3773	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ALA	GLY	UNK	ARG	GLU	T1847	L1698	
E3944	Q3774	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	LEU	PRO	UNK	SER	GLY	V1850	L1703	
G3947	S3775	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	PRO	VAL	UNK	LEU	GLU	M1851		
M3955	R3776	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ASP	ARG	UNK	THR	THR	G1852	L1707	
V3957	A3776	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	VAL	ASP	UNK	VAL	VAL	I1853	R1708	
F3961	E3777	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ASP	ARG	UNK	ARG	ARG	E1857	A1709	
N3963	M3778	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ASP	ARG	UNK	LEU	VAL	G1710		
S3964	V3779	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	LYS	GLU	UNK	LYS	LYS	Y1711		
	M3793	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	THR	GLU	UNK	LYS	LYS	K1860		
	T3797	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	VAL	ASP	UNK	LYS	LYS	I1866		
	L3804	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ASP	ARG	UNK	LYS	LYS	E1867		
	G3808	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ALA	ARG	UNK	GLU	GLU	M1939		
	N3809	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	SER	ARG	UNK	THR	VAL	L1931		
	K3815	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	TYR	ASP	UNK	LYS	LYS	K1860		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	VAL	ASP	UNK	LYS	VAL	I1931		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ASP	ARG	UNK	THR	ARG	L1922		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ASP	ARG	UNK	ARG	ARG	M1929		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ALA	ARG	UNK	LEU	VAL	K1930		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	SER	ARG	UNK	VAL	VAL	Y1711		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	TYR	GLU	UNK	LYS	LYS	Y1712		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	SER	HIS	UNK	LYS	LYS	I1716		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	SER	PHE	UNK	LYS	LYS	I1866		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	LYS	GLY	UNK	GLU	GLU	E1867		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	ALA	GLU	UNK	LYS	GLU	M1939		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	GLU	PRO	UNK	LYS	LYS	V1870		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	LYS	GLU	UNK	PRO	PRO	F1871		
		UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	E1950		







- Molecule 1: RyR1







S5037	F4921	I4783	GLY	PRO	THR	GLY	GLY	VAL	M4097	L3965	Q3830	M3729	VAL	UNK
F4922	F4784	F4785	TRP	LYS	THR	TRP	GLY	ALA	K4101	Y3988	Q3833	H3732	TRP	UNK
F4923	V4924	T4785	GLY	LYS	PRO	GLY	ASP	ARG	Q4102	Y3988	Q3833	S3732	HIS	UNK
I4925	V4924	T4785	GLY	LYS	PRO	GLY	ASP	ALA	F4103	N3976	L3835	C3733	LYS	UNK
L4928	M4798	M4798	ALA	PRO	PRO	ALA	GLY	ALA	T4104	N3976	L3835	C3733	LEU	UNK
L4929	H4812	H4812	GLY	SER	PRO	GLY	ALA	ALA	E4107	R3984	S3840	E3737	SER	UNK
L4930	H4812	H4812	GLY	PRO	PRO	GLY	ALA	ALA	E4107	R3984	S3840	E3737	LYS	UNK
L4931	I4816	I4816	ALA	PRO	PRO	GLY	GLY	THR	F4132	W3986	L3842	N3741	GLN	UNK
L4932	V4820	V4820	GLY	LYS	GLY	GLY	GLY	VAL	F4132	W3986	L3842	N3741	ARG	UNK
L4933	V4820	V4820	SER	LYS	SER	ALA	GLY	ALA	P4158	V3989	N3845	ALA	ARG	UNK
L4934	V4820	V4820	GLY	LYS	PRO	GLY	GLY	ALA	P4158	V3989	N3845	ALA	ARG	UNK
L4935	L4823	L4823	ASP	GLY	ILE	GLY	GLY	GLY	R4161	F3996	A3846	GLY	ALA	UNK
L4936	V4838	V4838	GLY	ALA	LEU	ALA	ASP	ALA	R4161	F3996	A3846	GLY	VAL	UNK
L4937	M4839	M4839	GLY	GLY	LYS	GLY	ASP	ALA	Y4173	M3999	A3853	V3751	ALA	UNK
L4938	T4840	T4840	GLY	GLY	ARG	ALA	ALA	ARG	R4180	K4002	V3865	V3751	CYS	UNK
L4939	V4841	V4841	GLY	ALA	LEU	LEU	GLY	LEU	R4180	K4002	V3865	V3751	PHE	UNK
L4940	V4841	V4841	GLY	ALA	LEU	TRP	ASP	ALA	M4184	L4003	I3866	E3755	ARG	UNK
R4944	L4844	L4844	GLY	GLY	VAL	GLY	ASP	ALA	M4184	L4003	I3866	E3755	MET	UNK
D4945	Y4851	Y4851	GLY	GLY	ASP	GLY	GLY	GLY	I4010	E4011	D3877	T3639	UNK	
Q4946	V4666	V4666	GLY	GLY	GLY	GLY	GLY	GLY	E4011	E4011	D3877	T3639	UNK	
Q4949	V4666	V4666	GLY	GLY	GLY	GLY	GLY	GLY	L4012	L4012	D3877	T3639	UNK	
C4958	F4859	F4859	GLY	GLY	GLY	GLY	GLY	GLY	L4013	L4013	R3886	K3760	UNK	
F4959	R4860	R4860	GLY	GLY	GLY	GLY	GLY	GLY	L4017	L4017	R3887	Q3761	UNK	
D4966	F4862	F4862	GLY	GLY	GLY	GLY	GLY	GLY	D4018	D4018	R3888	R3762	UNK	
D4966	R4863	R4863	GLY	GLY	GLY	GLY	GLY	GLY	L4019	L4019	Q3889	L3763	UNK	
H4978	N4864	N4864	GLY	GLY	PRO	GLY	GLY	GLY	Q4020	Q4020	L3891	Y3765	UNK	
H4978	K4865	K4865	GLY	GLY	PRO	GLY	GLY	GLY	K4021	K4021	Q3766	Q3766	UNK	
E4982	S4866	S4866	GLY	GLY	GLY	GLY	GLY	GLY	D4022	D4022	N3896	Q3767	UNK	
E4982	D4868	D4868	GLY	GLY	GLY	GLY	GLY	GLY	F4025	F4025	F3899	S3768	UNK	
L4985	E4869	E4869	GLY	GLY	GLY	GLY	GLY	GLY	M4026	M4026	Q3900	R3769	UNK	
M4989	K4870	K4870	GLY	GLY	GLY	GLY	GLY	GLY	L4027	L4027	N3901	H3771	UNK	
L4995	M4874	M4874	GLY	GLY	GLY	GLY	GLY	GLY	PRO	PRO	Y3902	T3772	UNK	
L4996	C4875	C4875	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L3903	R3773	UNK	
L4997	L4704	L4704	VAL	VAL	PRO	VAL	VAL	VAL	GLY	GLY	R3904	G3774	UNK	
K4998	V4705	V4705	ALA	ALA	LYS	ALA	ALA	ALA	M4034	M4034	T3905	A3775	UNK	
D4999	F4711	F4711	GLY	GLY	ASP	GLY	GLY	GLY	V4035	V4035	Q3906	M3778	UNK	
E5000	F4711	F4711	GLY	GLY	ASP	GLY	GLY	GLY	Q4043	Q4043	L3913	V3779	UNK	
H5003	V4716	V4716	GLY	GLY	GLY	GLY	GLY	GLY	V4055	V4055	L3924	Q3781	UNK	
V5011	F4719	F4719	ALA	ALA	ASN	PHE	ALA	ALA	L4059	L4059	Q3927	K3787	UNK	
R5017	G4895	G4895	GLY	GLY	GLY	GLY	GLY	GLY	D4063	D4063	E3928	X3406	UNK	
C5018	I4897	I4897	GLY	GLY	GLY	GLY	GLY	GLY	M4064	M4064	S3931	X3410	UNK	
W5019	G4898	G4898	GLY	GLY	LYS	ASP	GLY	GLY	F4065	F4065	D3941	T3797	UNK	
R5029	P4904	P4904	ALA	ALA	GLY	GLY	GLY	GLY	L4066	L4066	E3885	X3535	UNK	
W5030	Y4912	Y4912	ALA	ALA	VAL	GLY	GLY	GLY	K4067	K4067	E3886	X3536	UNK	
Q5031	R4913	R4913	GLY	GLY	PRO	GLY	GLY	GLY	I4071	I4071	E3944	X3537	UNK	
W5032	Y4919	Y4919	GLY	GLY	GLY	GLY	GLY	GLY	G3947	G3947	P3697	X3613	UNK	
E5033	D4917	D4917	GLY	GLY	ALA	GLY	GLY	GLY	S3803	S3803	E3712	LYS	UNK	
	I4918	I4918	GLY	GLY	PRO	GLY	GLY	GLY	T3804	T3804	L3805	SER	UNK	
	F4920	F4920	GLY	GLY	PRO	GLY	GLY	GLY	F4093	F4093	A3954	LYS	UNK	
			GLY	GLY	PRO	GLY	GLY	GLY	Q4094	Q4094	M3955	LYS	UNK	
			GLY	GLY	PRO	GLY	GLY	GLY	K4095	K4095	A3724	LYS	UNK	
			GLY	GLY	PRO	GLY	GLY	GLY	A4096	A4096	Y3725	ALA	UNK	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	68155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	478.72, 478.72, 478.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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: MG, ZN, ACP

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	0.26	0/25057	0.50	1/34021 (0.0%)
1	B	0.27	0/25055	0.50	3/34016 (0.0%)
1	C	0.26	0/25076	0.50	2/34047 (0.0%)
1	D	0.26	0/25078	0.50	2/34045 (0.0%)
All	All	0.26	0/100266	0.50	8/136129 (0.0%)

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	C	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3751	VAL	C-N-CA	-5.77	107.27	121.70
1	B	719	LEU	CA-CB-CG	5.62	128.23	115.30
1	D	3751	VAL	C-N-CA	-5.62	107.66	121.70
1	D	719	LEU	CA-CB-CG	5.56	128.08	115.30
1	C	4891	VAL	O-C-N	5.30	131.18	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	4892	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	28941	0	24397	483	0
1	B	28940	0	24404	519	0
1	C	28958	0	24429	510	0
1	D	28963	0	24439	493	0
2	A	31	0	14	7	0
2	B	31	0	14	4	0
2	C	31	0	14	3	0
2	D	31	0	14	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	115935	0	97725	1937	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 1937 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:3773:ARG:CB	1:A:3815:LYS:HE3	1.46	1.45
1:C:3765:TYR:CE1	1:C:4750:ILE:HG23	1.52	1.40
1:A:4921:PHE:O	1:A:4925:ILE:HG22	1.27	1.30
1:A:3767:GLN:O	1:A:3772:THR:HB	1.29	1.28
1:D:3674:ILE:HG12	1:D:3769:ARG:CD	1.64	1.28

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3191/5037 (63%)	2943 (92%)	243 (8%)	5 (0%)	47	81
1	B	3191/5037 (63%)	2934 (92%)	247 (8%)	10 (0%)	41	76
1	C	3191/5037 (63%)	2929 (92%)	254 (8%)	8 (0%)	41	76
1	D	3191/5037 (63%)	2932 (92%)	253 (8%)	6 (0%)	47	81
All	All	12764/20148 (63%)	11738 (92%)	997 (8%)	29 (0%)	50	81

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4866	SER
1	A	4870	ASP
1	B	3662	ILE
1	B	3666	ASP
1	B	4867	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2452/3264 (75%)	2421 (99%)	31 (1%)	69	82
1	B	2452/3264 (75%)	2419 (99%)	33 (1%)	69	82
1	C	2455/3264 (75%)	2425 (99%)	30 (1%)	71	84
1	D	2458/3264 (75%)	2431 (99%)	27 (1%)	73	85
All	All	9817/13056 (75%)	9696 (99%)	121 (1%)	72	84

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4936	ILE
1	C	4875	LYS
1	D	3759	GLU
1	C	4868	ASP
1	C	4944	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	151	HIS
1	C	4946	GLN
1	D	3761	GLN
1	C	4223	ASN
1	D	2180	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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	ACP	C	5101	4	27,33,33	1.33	5 (18%)	32,52,52	1.50	4 (12%)
2	ACP	A	5101	4	27,33,33	1.35	5 (18%)	32,52,52	1.51	5 (15%)
2	ACP	D	5101	4	27,33,33	1.37	5 (18%)	32,52,52	1.46	4 (12%)
2	ACP	B	5101	4	27,33,33	0.89	1 (3%)	32,52,52	0.84	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
2	ACP	C	5101	4	-	7/15/38/38	0/3/3/3
2	ACP	A	5101	4	-	5/15/38/38	0/3/3/3
2	ACP	D	5101	4	-	9/15/38/38	0/3/3/3
2	ACP	B	5101	4	-	8/15/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	PG-O3G	2.87	1.61	1.54
2	C	5101	ACP	PG-O3G	2.86	1.61	1.54
2	C	5101	ACP	PG-O2G	2.85	1.61	1.54
2	D	5101	ACP	PG-O3G	2.83	1.61	1.54
2	D	5101	ACP	PG-O2G	2.83	1.61	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5101	ACP	PB-O3A-PA	-4.14	119.42	132.56
2	A	5101	ACP	PB-O3A-PA	-4.07	119.65	132.56
2	D	5101	ACP	PB-O3A-PA	-3.87	120.27	132.56
2	A	5101	ACP	N3-C2-N1	-3.70	122.90	128.68
2	C	5101	ACP	N3-C2-N1	-3.65	122.98	128.68

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5101	ACP	C5'-O5'-PA-O1A
2	A	5101	ACP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

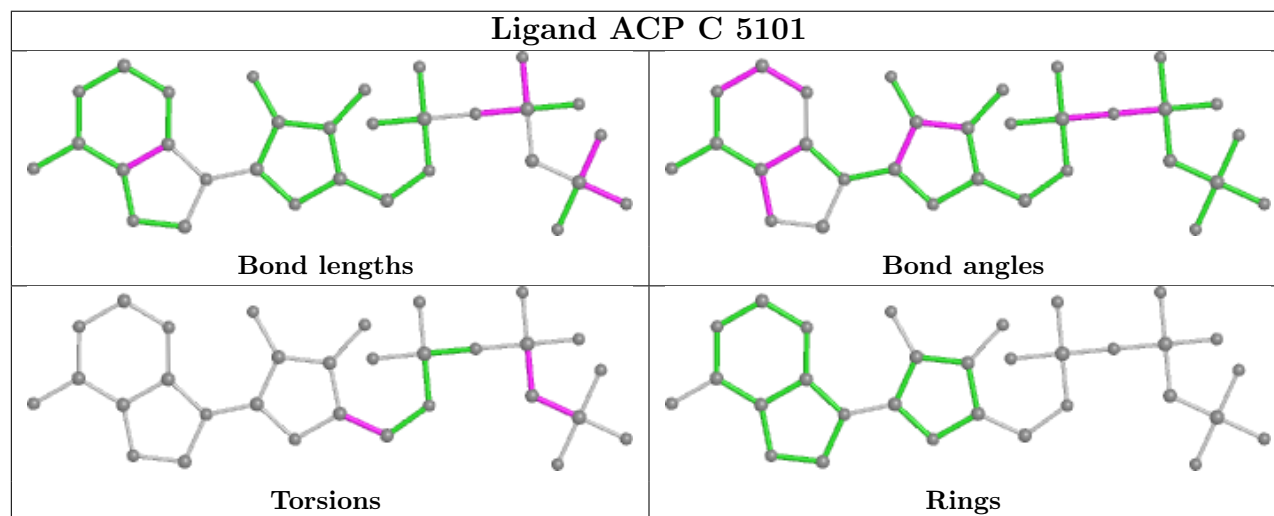
Mol	Chain	Res	Type	Atoms
2	B	5101	ACP	PG-C3B-PB-O1B
2	B	5101	ACP	PG-C3B-PB-O3A
2	B	5101	ACP	C5'-O5'-PA-O2A

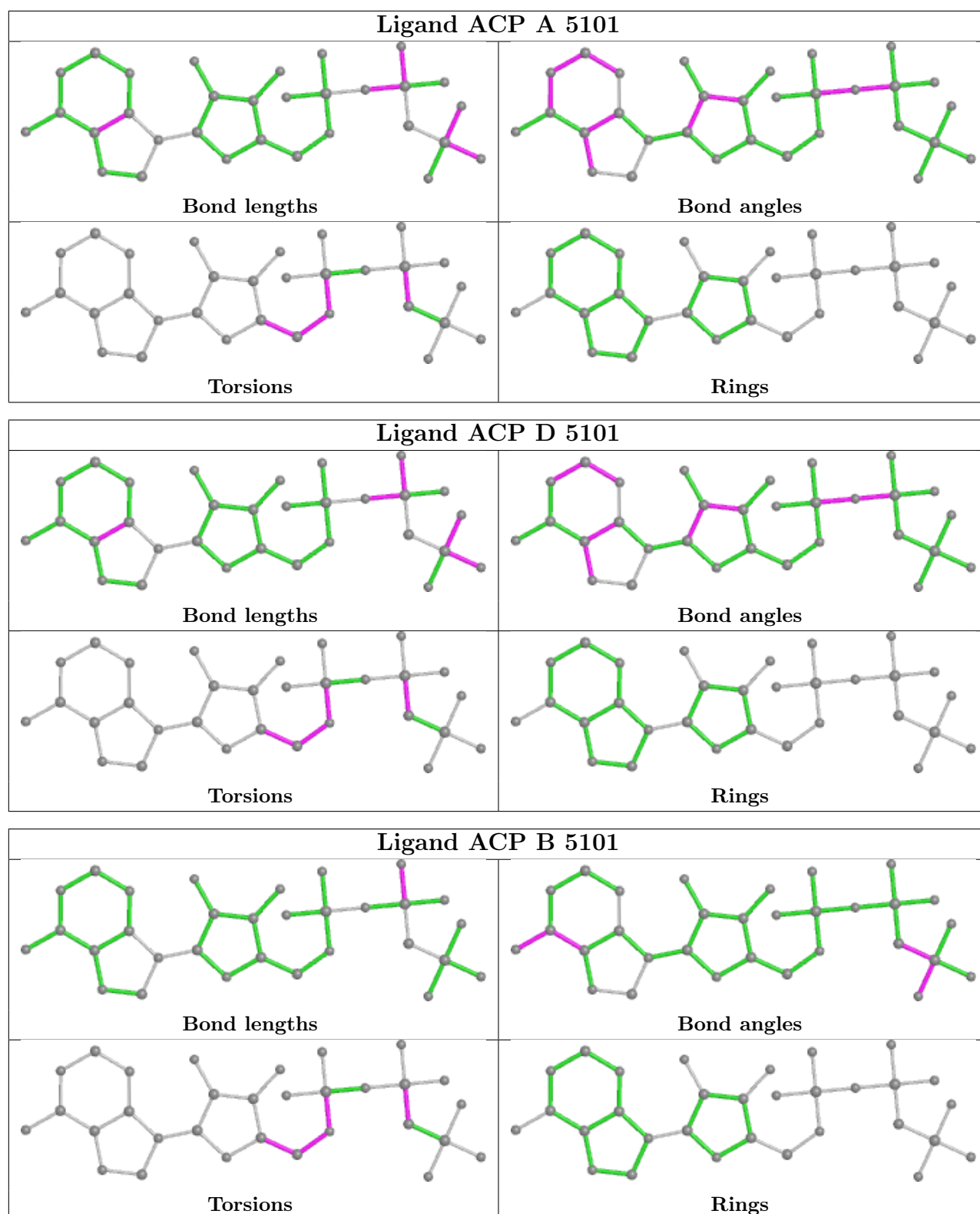
There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5101	ACP	3	0
2	A	5101	ACP	7	0
2	D	5101	ACP	8	0
2	B	5101	ACP	4	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 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	6
1	B	6
1	C	6
1	A	6

The worst 5 of 24 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3302:UNK	C	3303:UNK	N	17.16
1	B	3302:UNK	C	3303:UNK	N	17.15
1	C	3302:UNK	C	3303:UNK	N	17.10
1	A	3302:UNK	C	3303:UNK	N	17.01
1	A	3510:UNK	C	3511:UNK	N	16.97

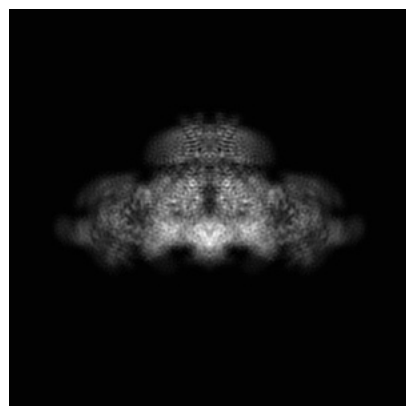
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22615. These allow visual inspection of the internal detail of the map and identification of artifacts.

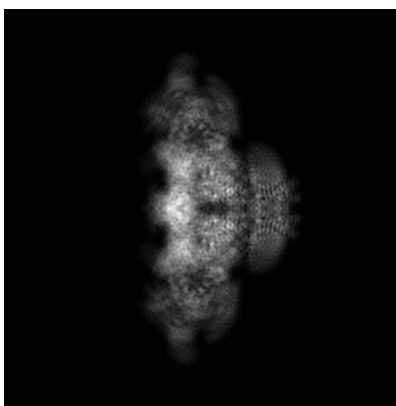
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

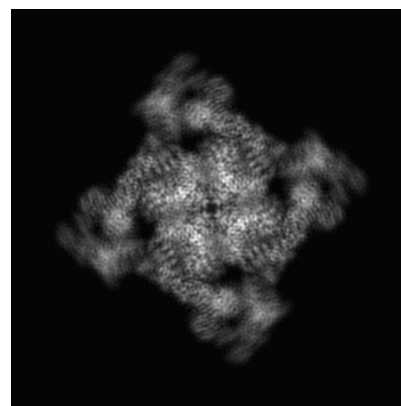
6.1.1 Primary map



X

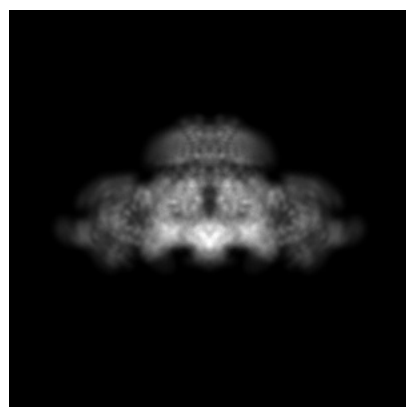


Y

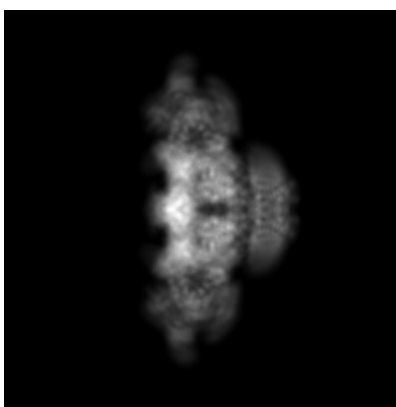


Z

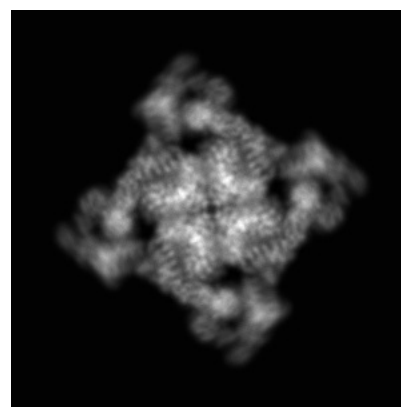
6.1.2 Raw map



X



Y

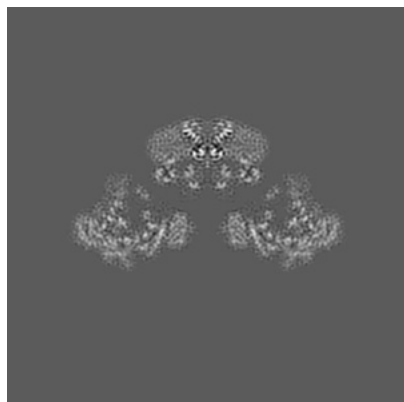


Z

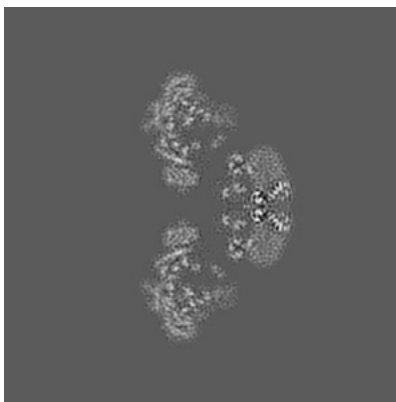
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

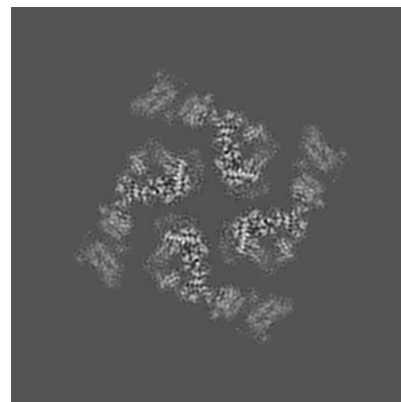
6.2.1 Primary map



X Index: 176

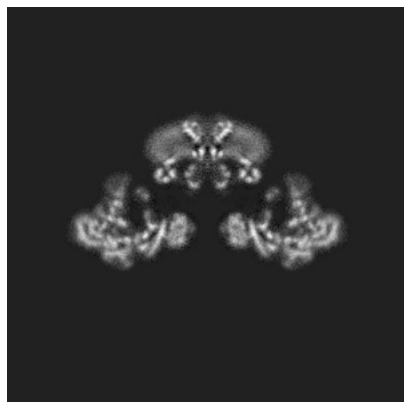


Y Index: 176

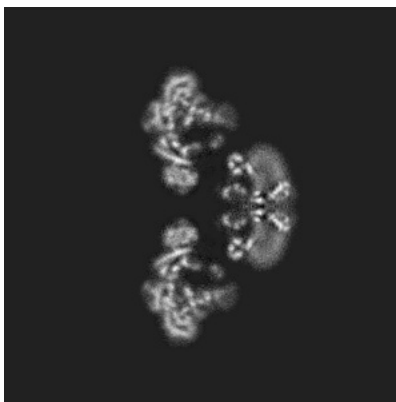


Z Index: 176

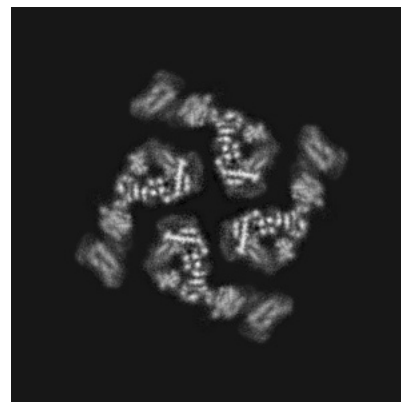
6.2.2 Raw map



X Index: 176



Y Index: 176

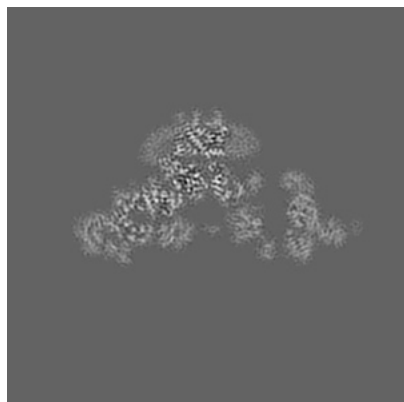


Z Index: 176

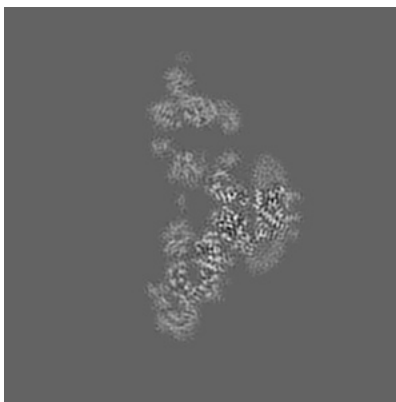
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

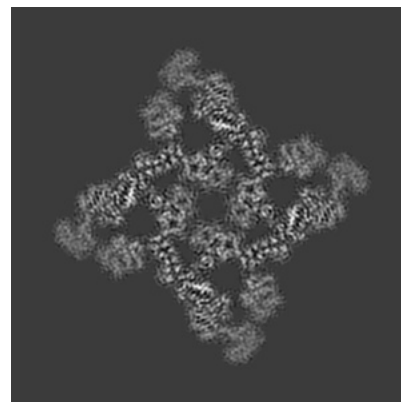
6.3.1 Primary map



X Index: 165

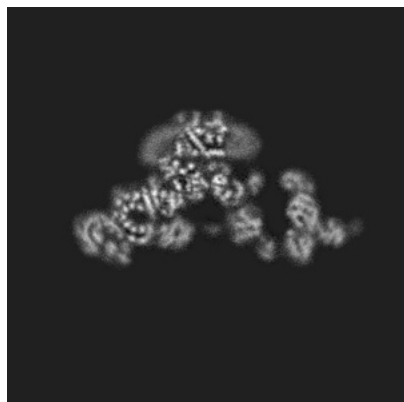


Y Index: 187

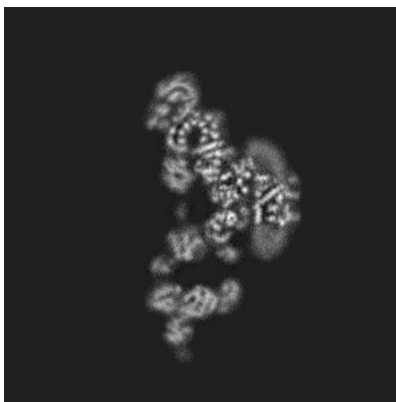


Z Index: 160

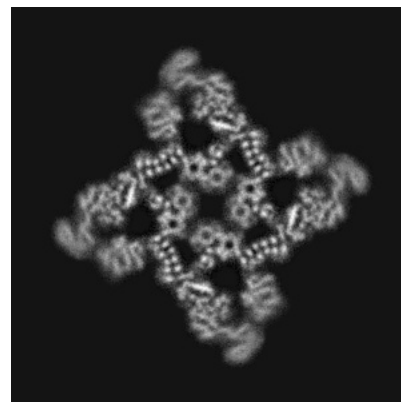
6.3.2 Raw map



X Index: 165



Y Index: 165

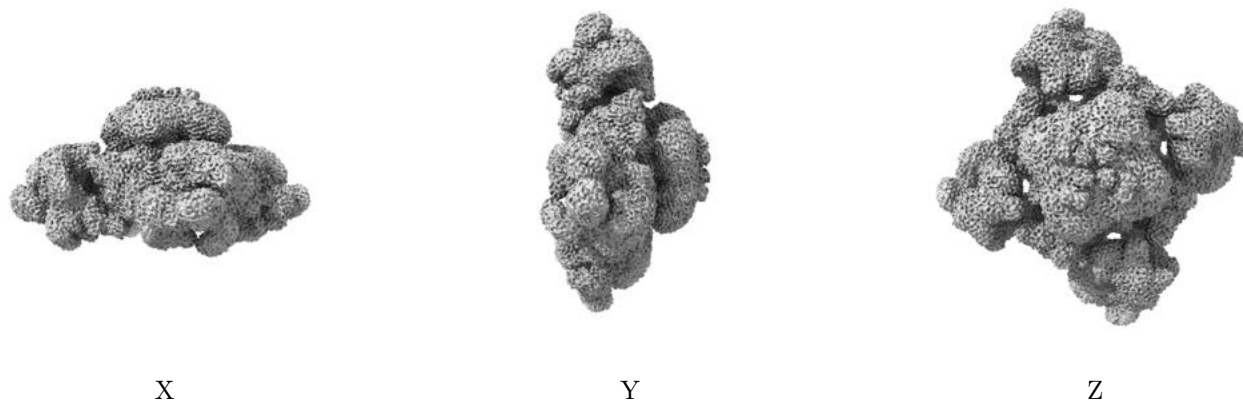


Z Index: 160

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

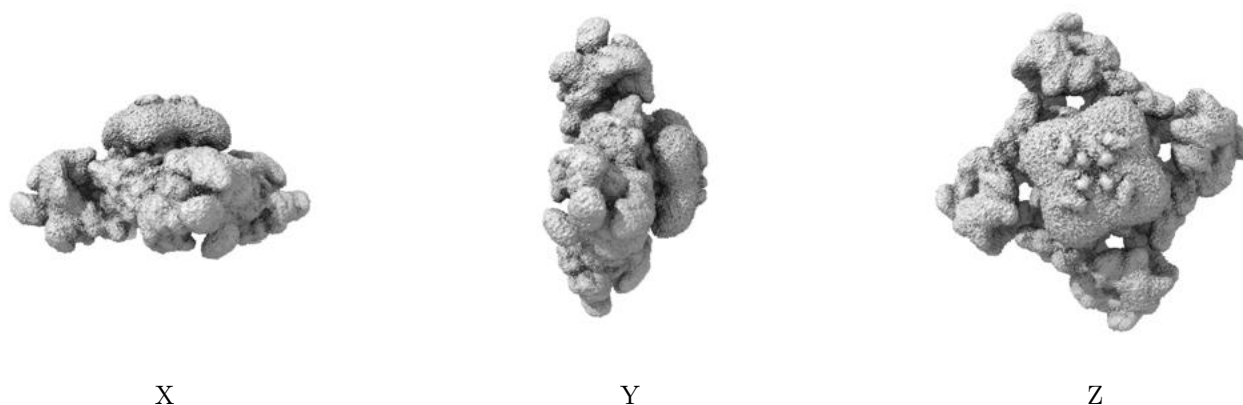
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

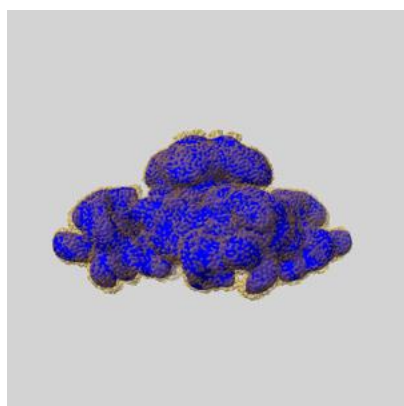
6.5 Mask visualisation [i](#)

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

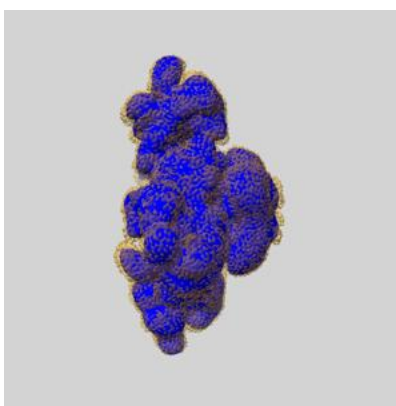
A mask typically either:

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

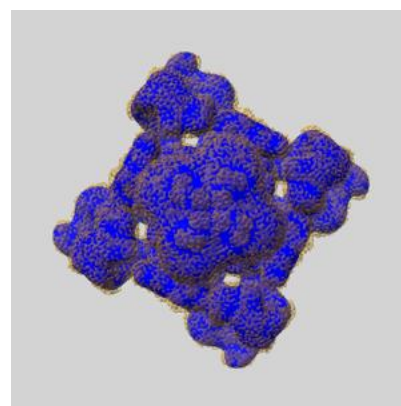
6.5.1 emd_22615_msk_1.map [i](#)



X



Y

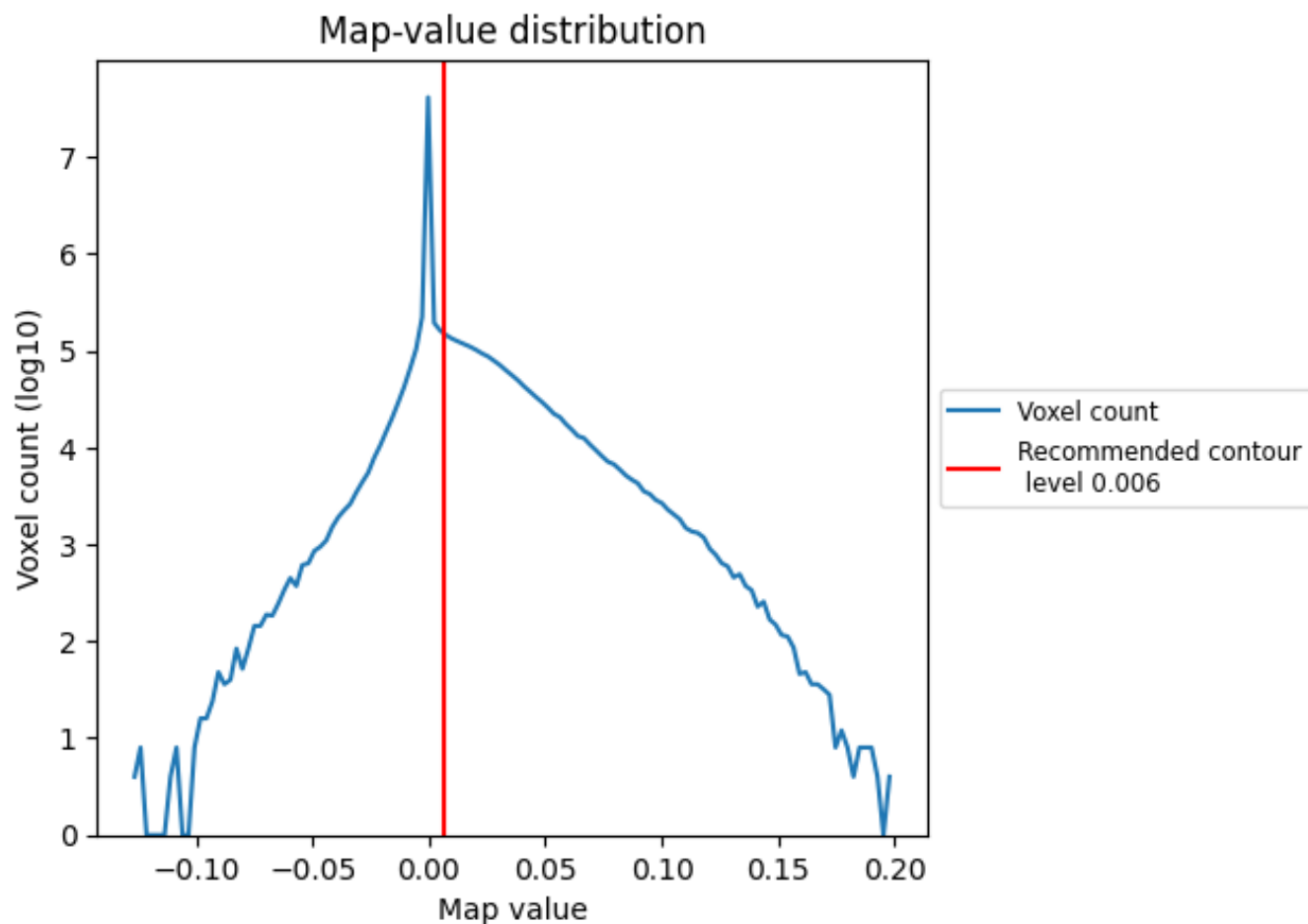


Z

7 Map analysis [i](#)

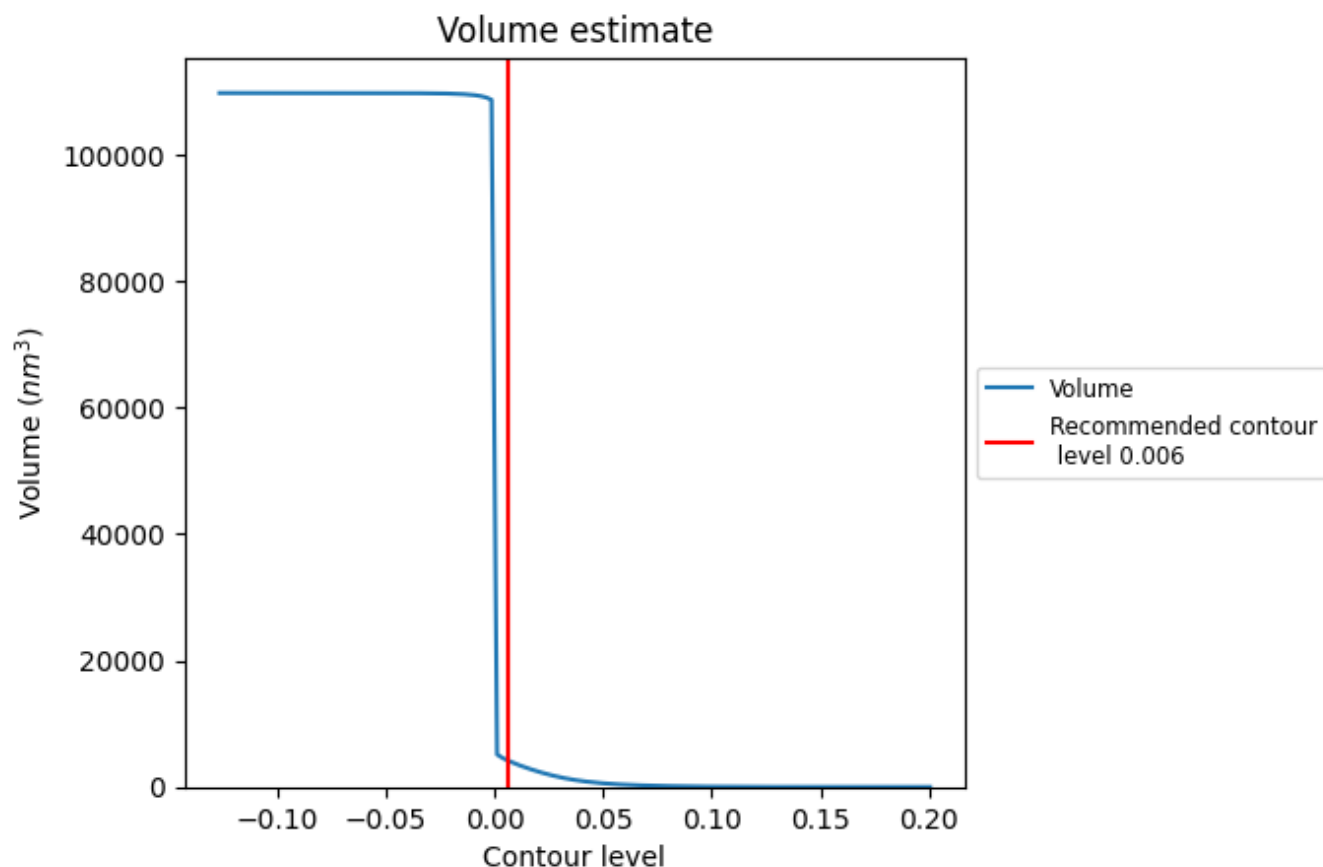
This section contains the results of statistical analysis of the map.

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.

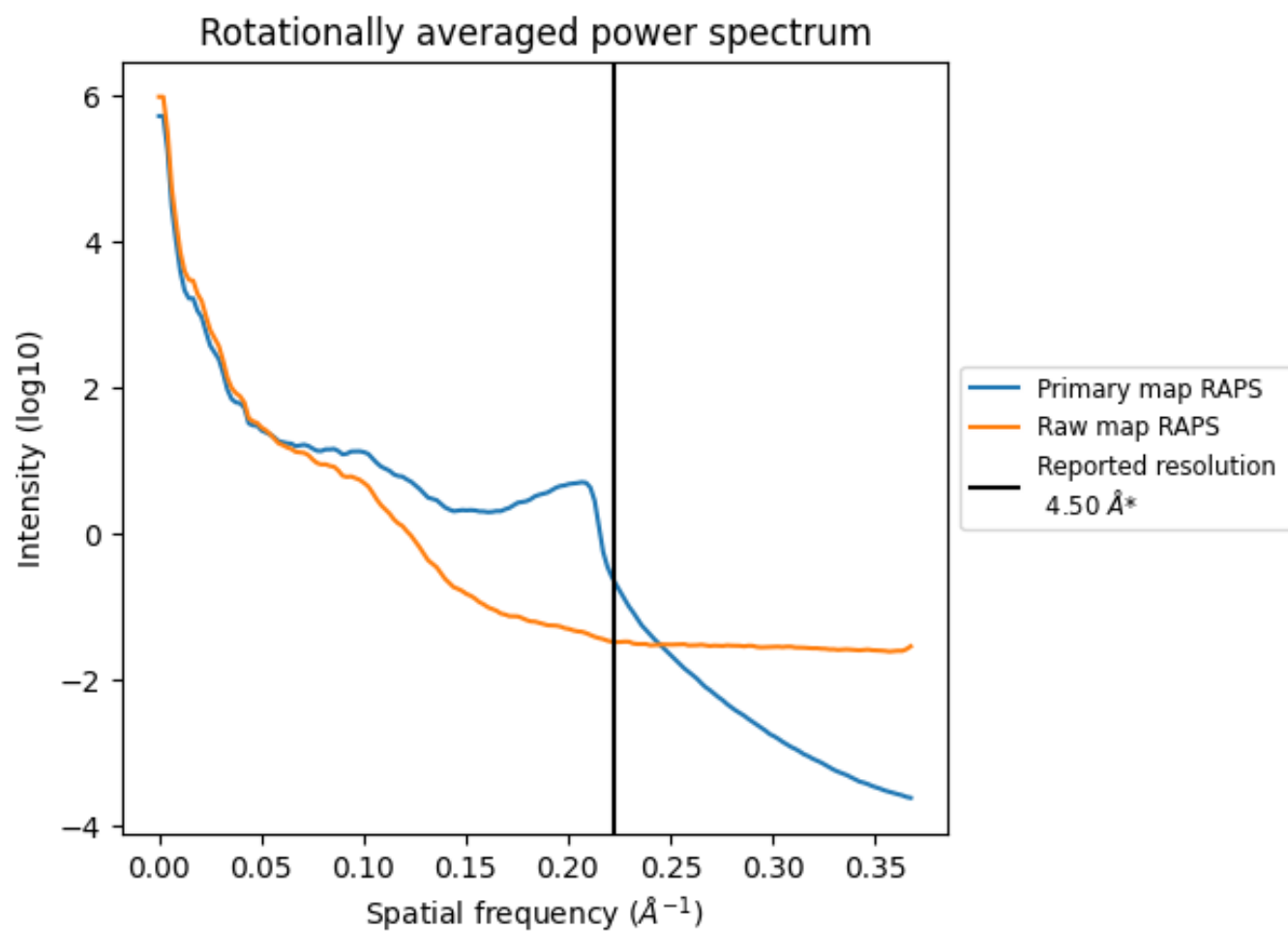
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4210 nm^3 ; this corresponds to an approximate mass of 3803 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 ⓘ

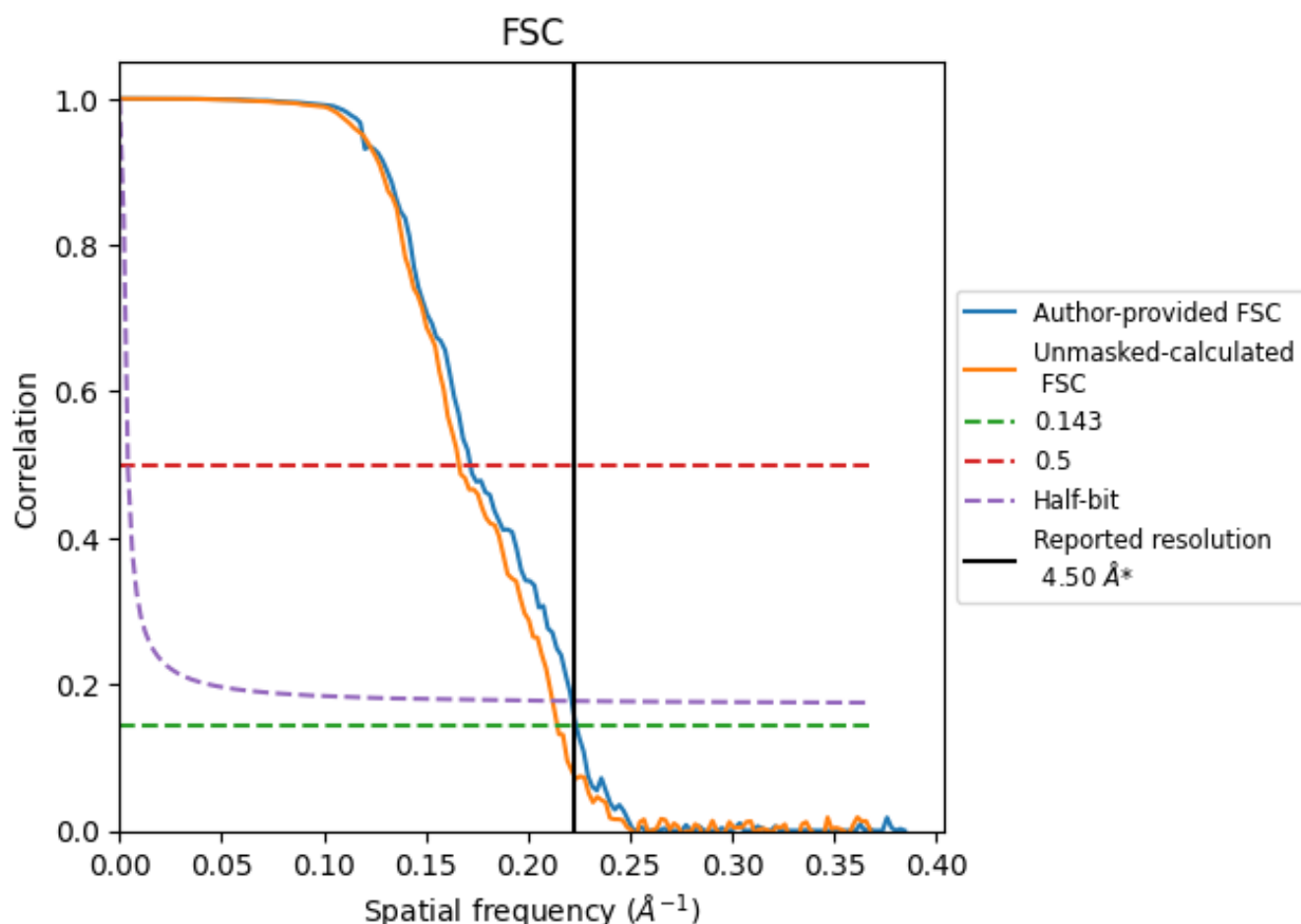


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 \AA^{-1}

8.2 Resolution estimates [i](#)

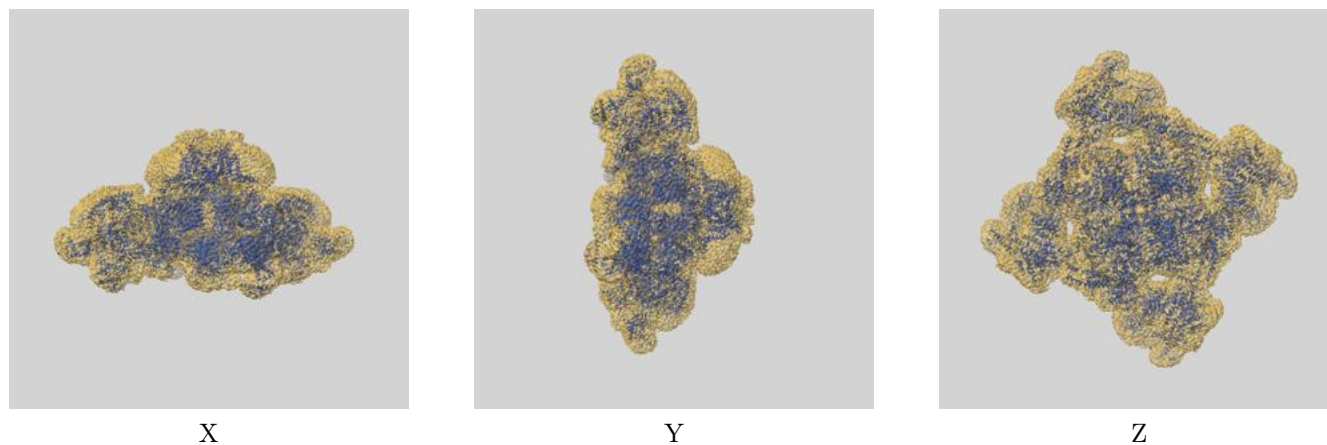
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.47	5.82	4.52
Unmasked-calculated*	4.66	6.01	4.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

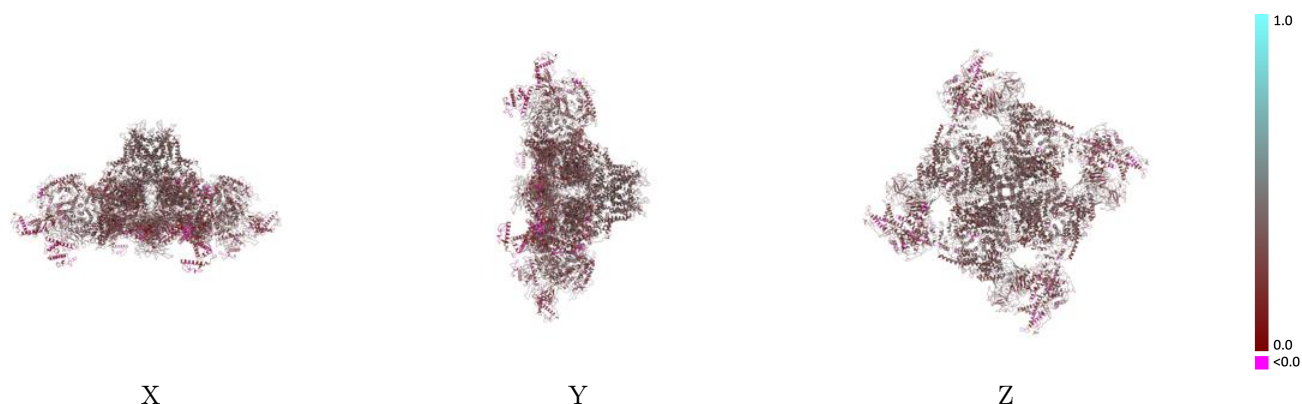
This section contains information regarding the fit between EMDB map EMD-22615 and PDB model 7K0S. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



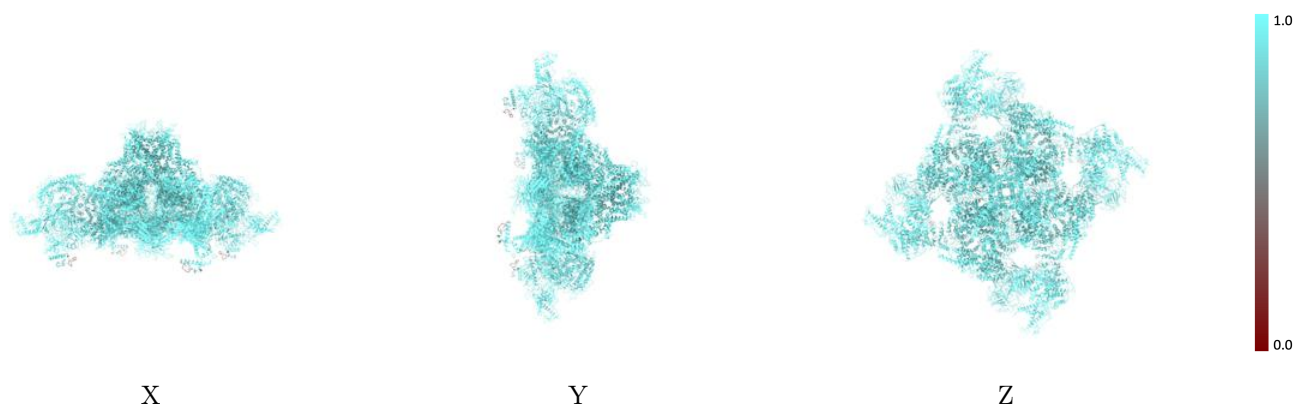
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



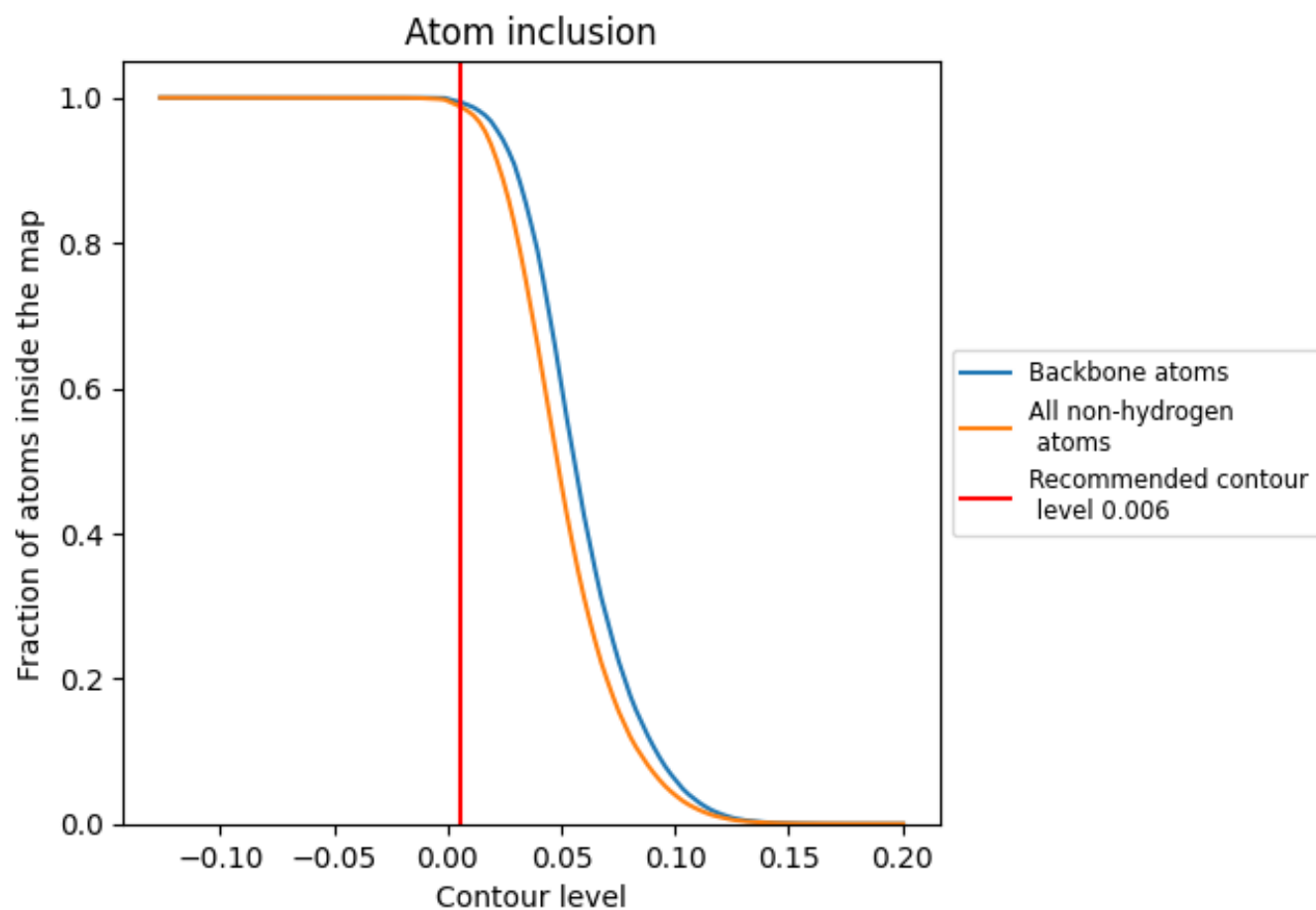
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9871	<div></div> 0.3120
A	<div></div> 0.9872	<div></div> 0.3110
B	<div></div> 0.9873	<div></div> 0.3120
C	<div></div> 0.9873	<div></div> 0.3120
D	<div></div> 0.9865	<div></div> 0.3110

