



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 10:39 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.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

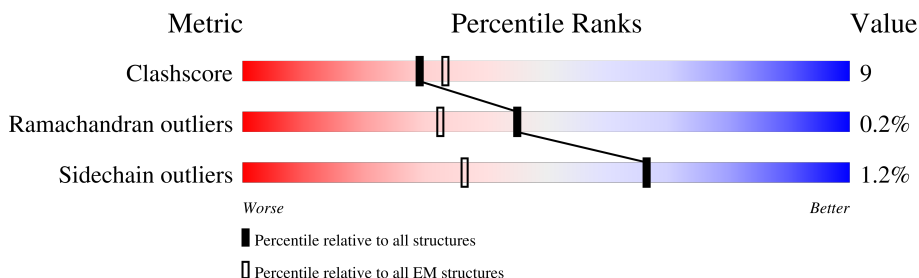
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	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 $\leq 5\%$. 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](#)

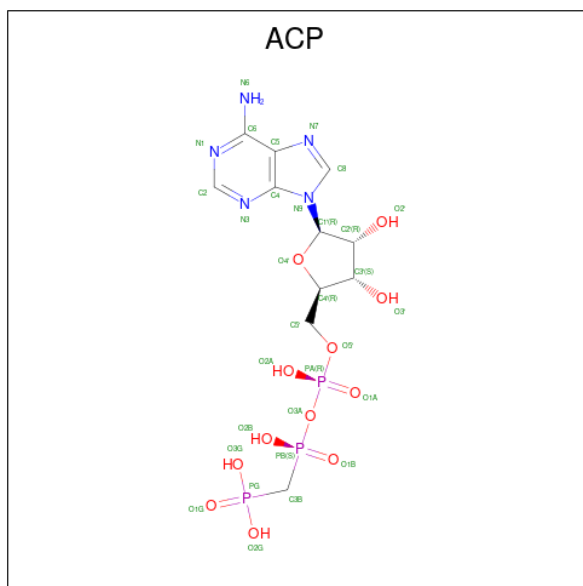
There are 4 unique types of molecules in this entry. The entry contains 115935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	

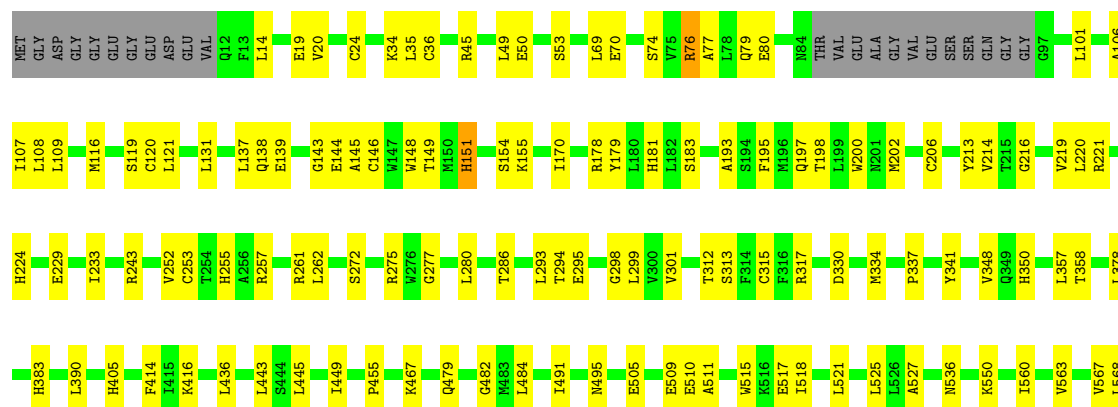
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	

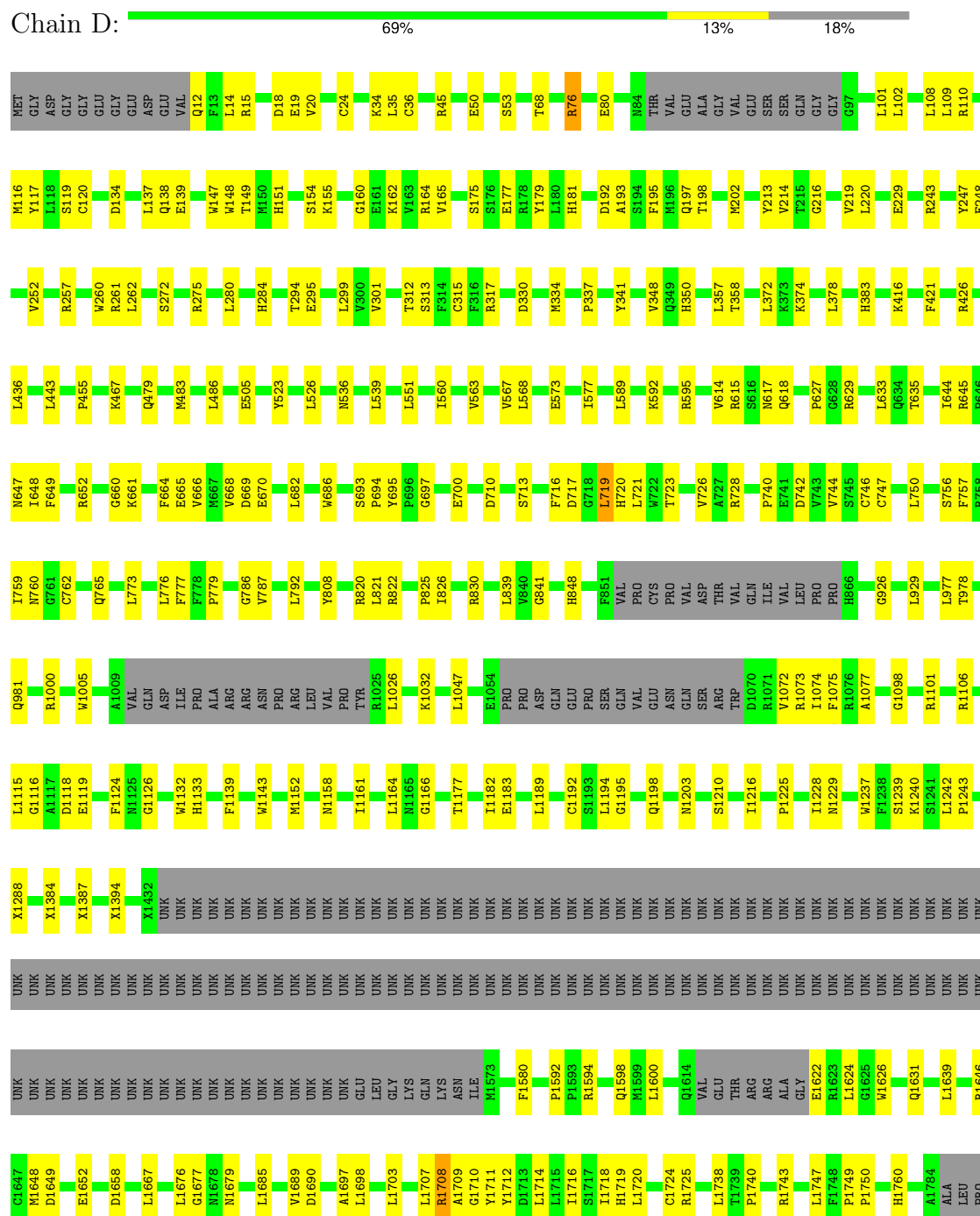
K3821	E3870	X3406	UNK	UNK	L2904	GLU	LYS	ALA	THR	LYS	PRO	L2257	GLU	E1956	E1874	G1724	L1600
K3824	V3702	X3410	UNK	UNK	T2912	LYS	THR	VAL	ASP	UNK	GLU	T2271	GLU	F1961	GLU	R1725	M1608
L3835	D3719	X3490	UNK	UNK	L2926	UNK	UNK	UNK	UNK	UNK	GLU	L2273	PRO	E1963	GLU	R1727	P1609
S3840	Y3722	X3491	UNK	UNK	E2939	GLY	GLU	GLU	GLU	GLU	L2474	A2276	ALA	R1964	GLU	I1735	I1614
N3845	N3729	X3492	UNK	UNK	GLY	N2734	GLU	F2735	GLY	N2414	L2477	L2286	K2089	A1992	GLU	V1736	VAL
R3849	N3741	X3493	UNK	UNK	UNK	F2736	THR	D2737	UNK	P2477	L2479	L2288	Q2095	R1996	GLU	P1737	GLU
A3853	GLY	X3495	UNK	UNK	UNK	P2737	GLU	UNK	UNK	GLY	L2479	V2299	S2099	Q2003	GLU	T1739	THR
V3865	GLU	X3535	UNK	UNK	UNK	T2742	LYS	T2747	UNK	LYS	UNK	C2310	V2103	N2007	GLU	P1740	ARG
I3866	ALA	X3536	UNK	UNK	UNK	I2747	UNK	I2747	UNK	ASP	UNK	L2314	S2113	F2012	GLU	L1743	ALA
D3877	GLU	X3544	UNK	UNK	UNK	H2763	UNK	H2763	UNK	ALA	UNK	L2314	P2114	G2041	GLU	R1760	GLY
F3880	E3747	X3549	UNK	UNK	UNK	W2766	UNK	W2766	UNK	VAL	X2487	R2330	E2115	C2021	ASP	L1771	ARG
R3886	S3752	X3550	UNK	UNK	UNK	D2769	UNK	D2769	UNK	X2488	X2606	F2337	Q2127	P2022	GLU	R1772	ARG
R3887	F3753	X3551	UNK	UNK	UNK	N2773	UNK	N2773	UNK	X2607	X2608	F2340	Y2128	P2024	GLU	A1784	ALA
L3888	E3754	X3554	UNK	UNK	UNK	W2774	UNK	W2774	UNK	X2608	X2609	F2340	Y2128	D2030	LYS	A1784	LEU
Q3889	K3756	X3561	UNK	UNK	UNK	S2776	UNK	S2776	UNK	X2641	X2642	E2348	C2158	H2041	GLU	PRO	ALA
L3890	N3757	X3562	UNK	UNK	UNK	Y2777	UNK	Y2777	UNK	X2642	X2643	N2349	M2158	GLU	GLU	ALA	C1646
L3891	K3760	X3601	UNK	UNK	UNK	Q2778	UNK	Q2778	UNK	X2643	X2644	L2356	C2158	GLU	GLU	GLY	C1647
E3893	R3761	X3613	UNK	UNK	UNK	Q2779	UNK	Q2779	UNK	X2644	X2645	L2357	M2158	GLU	GLU	D1649	D1649
F3899	L3763	LYS	UNK	UNK	UNK	E2779	UNK	E2779	UNK	X2645	X2646	L2358	I2162	GLU	GLU	E1652	E1652
Q3906	L3764	SER	UNK	UNK	UNK	W2780	UNK	W2780	UNK	X2646	X2647	L2359	I2167	GLU	GLU	R1797	R1797
I3913	F3765	LYS	UNK	UNK	UNK	N2781	UNK	N2781	UNK	X2647	X2648	F2364	V2168	PRO	GLU	I1802	I1802
L3924	Q3766	ALA	UNK	UNK	UNK	E2782	UNK	E2782	UNK	X2648	X2649	A2367	E2175	GLU	GLU	K1810	K1810
Q3927	Q3767	VAL	UNK	UNK	UNK	E2783	UNK	E2783	UNK	X2649	X2650	L2368	I2179	GLU	GLU	A1826	A1826
I3930	S3768	TRP	UNK	UNK	UNK	E2784	UNK	E2784	UNK	X2650	X2651	L2376	I2182	THR	GLU	V1839	V1839
W3935	L3770	HIS	UNK	UNK	UNK	L2785	UNK	L2785	UNK	X2651	X2652	A2379	I2185	LEU	GLU	P1840	P1840
Y3937	H3771	LYS	UNK	UNK	UNK	K2786	UNK	K2786	UNK	X2652	X2653	R2392	I2185	SER	GLU	V1841	V1841
D3941	T3772	LEU	UNK	UNK	UNK	H2788	UNK	H2788	UNK	X2653	X2654	GLY	I2188	ARG	ALA	L1842	L1842
E3944	R3773	LEU	UNK	UNK	UNK	P2789	UNK	P2789	UNK	X2654	X2655	PRO	N2188	LEU	PRO	K1843	K1843
M3955	Q3774	SER	UNK	UNK	UNK	R2792	UNK	R2792	UNK	X2655	X2656	GLY	F2191	SER	GLY	T1847	T1847
V3957	G3775	GLN	UNK	UNK	UNK	Y2794	UNK	Y2794	UNK	X2656	X2657	LEU	N2196	LEU	GLU	V1850	V1850
V3961	A3776	ARG	UNK	UNK	UNK	K2795	UNK	K2795	UNK	X2657	X2658	VAL	R2199	THR	ASP	M1851	M1851
F3962	E3777	ARG	UNK	UNK	UNK	T2796	UNK	T2796	UNK	X2658	X2659	ARG	V2207	VAL	VAL	G1852	G1852
N3963	M3778	ALA	UNK	UNK	UNK	F2797	UNK	F2797	UNK	X2659	X2660	ARG	M1929	ARG	ARG	I1853	I1853
S3964	V3779	VAL	UNK	UNK	UNK	K2800	UNK	K2800	UNK	X2660	X2661	THR	M1929	LEU	LEU	E1857	E1857
	M3793	ALA	UNK	UNK	UNK	K2810	UNK	K2810	UNK	X2661	X2662	GLY	K1930	VAL	VAL	G1710	G1710
G3947	T3797	CYS	UNK	UNK	UNK	S2812	UNK	S2812	UNK	X2662	X2663	ARG	L1931	THR	THR	Y1711	Y1711
M3955	I3804	PHE	UNK	UNK	UNK	K2813	UNK	K2813	UNK	X2663	X2664	GLY	V1935	LYS	LYS	K1860	K1860
S3956	L3805	ARG	UNK	UNK	UNK	E2896	UNK	E2896	UNK	X2664	X2665	THR	M1939	GLU	GLU	I1866	I1866
V3957	G3808	MET	UNK	UNK	UNK	K2897	UNK	K2897	UNK	X2665	X2666	ASP	M1939	LEU	LEU	E1867	E1867
V3961	N3809	T3839	UNK	UNK	UNK	G2898	UNK	G2898	UNK	X2666	X2667	VAL	K1931	VAL	VAL	K1860	K1860
F3962	K3815	K3658	UNK	UNK	UNK	G2899	UNK	G2899	UNK	X2667	X2668	ARG	V1935	LYS	LYS	I1866	I1866
S3964		W3661	UNK	UNK	UNK	G2900	UNK	G2900	UNK	X2668	X2669	THR	M1939	GLU	GLU	E1867	E1867
			UNK	UNK	UNK	E2820	UNK	E2820	UNK	X2669	X2670	GLY	M1939	LEU	LEU	V1870	V1870
			UNK	UNK	UNK	TRP	UNK	TRP	UNK	X2670	X2671	PRO	K1931	GLU	GLU	F1871	F1871
			UNK	UNK	UNK	ILE	UNK	ILE	UNK	X2671	X2672	GLY	M1939	LEU	LEU	L1716	L1716
			UNK	UNK	UNK		UNK		UNK	X2672	X2673	GLY	M1939	GLU	GLU	H1719	H1719
			UNK	UNK	UNK		UNK		UNK	X2673	X2674	GLY	M1939	GLU	GLU	L1720	L1720
			UNK	UNK	UNK		UNK		UNK	X2674	X2675	GLY	M1939	GLU	GLU	F1871	F1871
			UNK	UNK	UNK		UNK		UNK	X2675	X2676	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2676	X2677	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2677	X2678	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2678	X2679	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2679	X2680	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2680	X2681	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2681	X2682	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2682	X2683	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2683	X2684	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2684	X2685	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2685	X2686	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2686	X2687	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2687	X2688	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2688	X2689	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2689	X2690	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2690	X2691	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2691	X2692	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2692	X2693	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2693	X2694	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2694	X2695	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2695	X2696	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2696	X2697	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2697	X2698	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2698	X2699	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2699	X2700	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2700	X2701	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2701	X2702	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2702	X2703	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2703	X2704	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2704	X2705	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2705	X2706	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2706	X2707	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2707	X2708	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2708	X2709	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2709	X2710	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2710	X2711	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2711	X2712	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2712	X2713	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2713	X2714	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2714	X2715	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2715	X2716	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2716	X2717	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2717	X2718	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2718	X2719	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2719	X2720	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2720	X2721	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2721	X2722	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2722	X2723	GLY	M1939	GLU	GLU		
			UNK	UNK	UNK		UNK		UNK	X2723	X2724	GLY	M1939	GLU	GLU		



WORLDWIDE
PDB
PROTEIN DATA BANK



- Molecule 1: RyR1



WORLDWIDE
PDB
PROTEIN DATA BANK



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PDB
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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: ACP, MG, 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	0.26	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%)	44	78
1	B	3191/5037 (63%)	2934 (92%)	247 (8%)	10 (0%)	37	72
1	C	3191/5037 (63%)	2929 (92%)	254 (8%)	8 (0%)	37	72
1	D	3191/5037 (63%)	2932 (92%)	253 (8%)	6 (0%)	44	78
All	All	12764/20148 (63%)	11738 (92%)	997 (8%)	29 (0%)	45	78

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%)	65	77
1	B	2452/3264 (75%)	2419 (99%)	33 (1%)	65	77
1	C	2455/3264 (75%)	2425 (99%)	30 (1%)	67	79
1	D	2458/3264 (75%)	2431 (99%)	27 (1%)	70	80
All	All	9817/13056 (75%)	9696 (99%)	121 (1%)	66	79

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 oligosaccharides 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	A	5101	4	27,33,33	1.31	4 (14%)	33,52,52	1.41	3 (9%)
2	ACP	C	5101	4	27,33,33	1.29	4 (14%)	33,52,52	1.39	3 (9%)
2	ACP	B	5101	4	27,33,33	0.92	1 (3%)	33,52,52	0.84	2 (6%)
2	ACP	D	5101	4	27,33,33	1.34	4 (14%)	33,52,52	1.35	4 (12%)

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	A	5101	4	-	6/15/38/38	0/3/3/3
2	ACP	C	5101	4	-	7/15/38/38	0/3/3/3
2	ACP	B	5101	4	-	8/15/38/38	0/3/3/3
2	ACP	D	5101	4	-	9/15/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	PG-O3G	2.92	1.61	1.55
2	C	5101	ACP	PG-O3G	2.91	1.61	1.55
2	C	5101	ACP	PG-O2G	2.90	1.61	1.55
2	D	5101	ACP	PG-O3G	2.88	1.61	1.55
2	D	5101	ACP	PG-O2G	2.87	1.61	1.55

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5101	ACP	N3-C2-N1	-4.25	122.90	128.67
2	C	5101	ACP	N3-C2-N1	-4.20	122.98	128.67
2	C	5101	ACP	PB-O3A-PA	-3.97	119.42	132.37
2	A	5101	ACP	PB-O3A-PA	-3.90	119.65	132.37
2	D	5101	ACP	PB-O3A-PA	-3.71	120.27	132.37

There are no chirality outliers.

5 of 30 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...

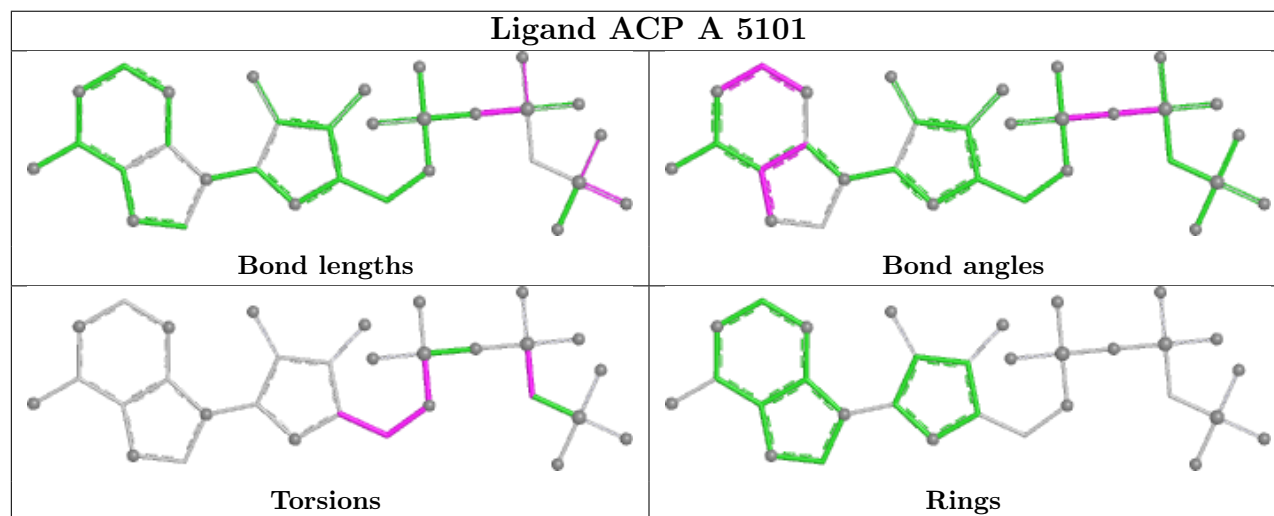
Mol	Chain	Res	Type	Atoms
2	B	5101	ACP	PG-C3B-PB-O1B
2	B	5101	ACP	PG-C3B-PB-O3A
2	B	5101	ACP	C5'-O5'-PA-O2A

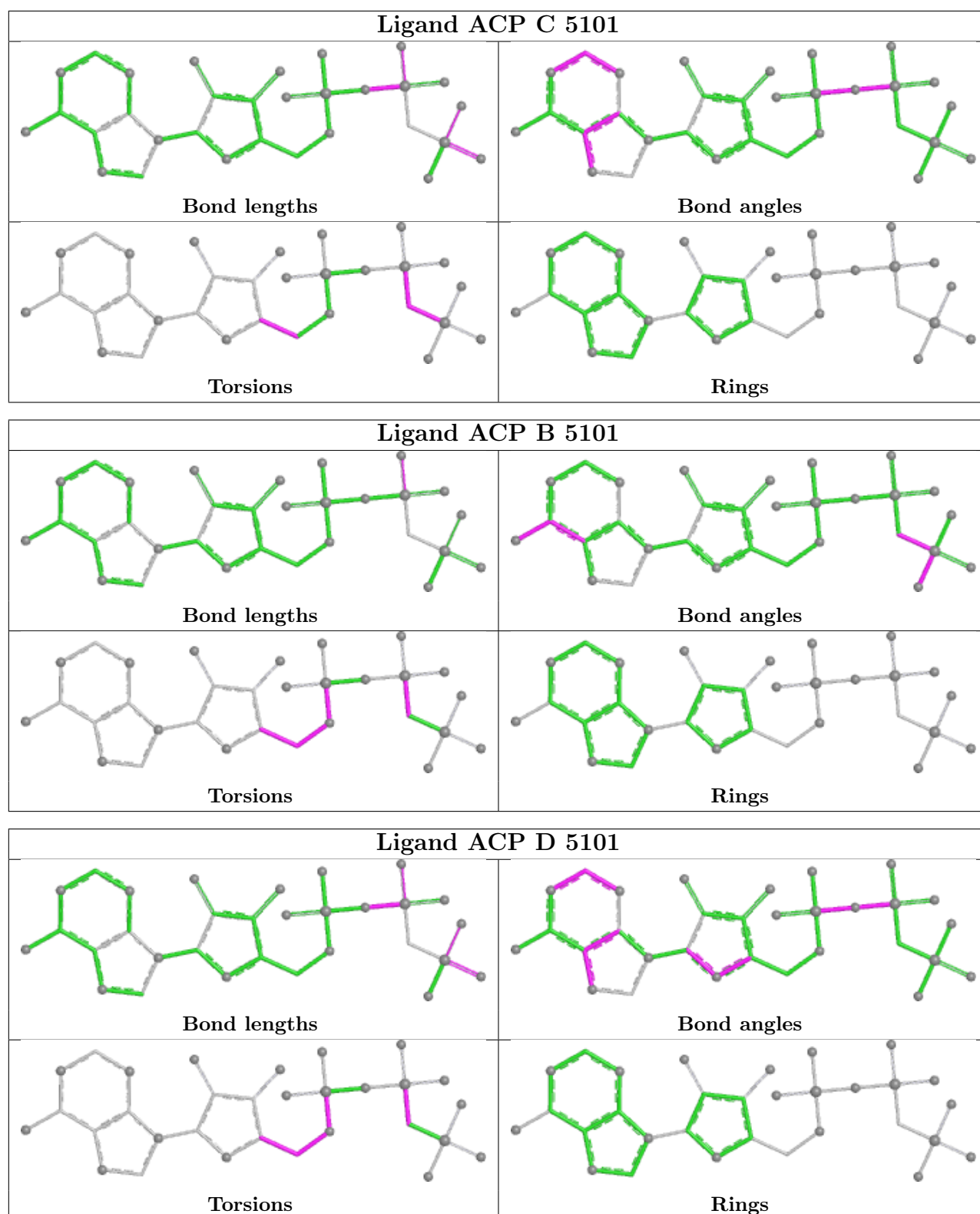
There are no ring outliers.

4 monomers are involved in 22 short contacts:

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

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

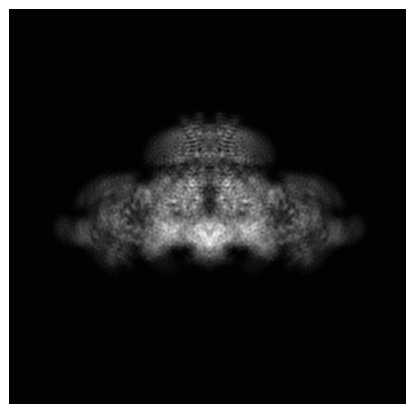
6 Map visualisation [i](#)

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.

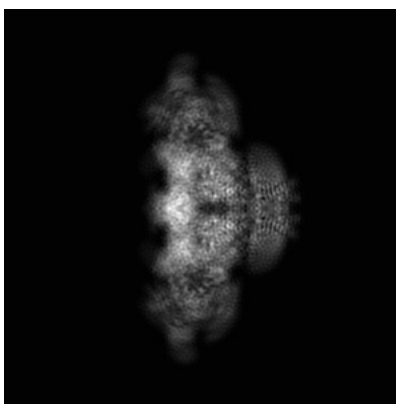
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

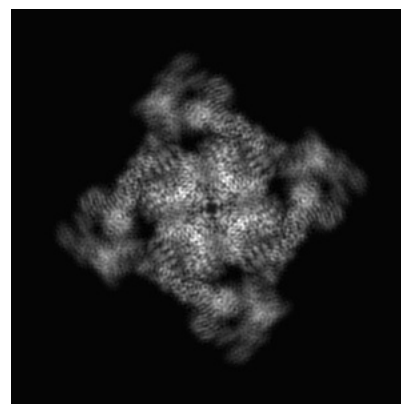
6.1.1 Primary map



X

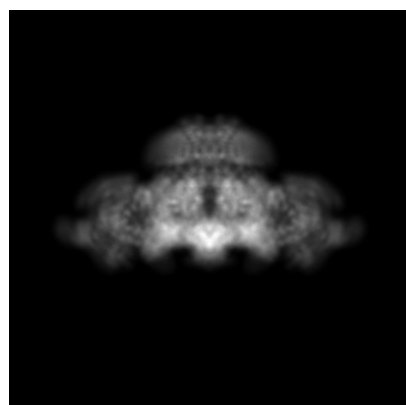


Y

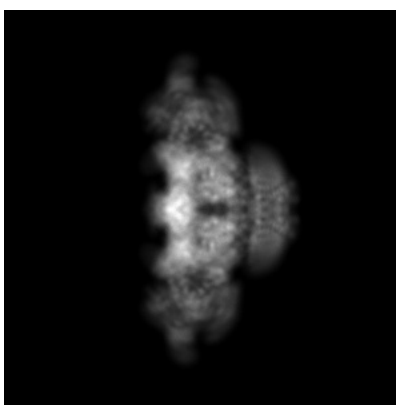


Z

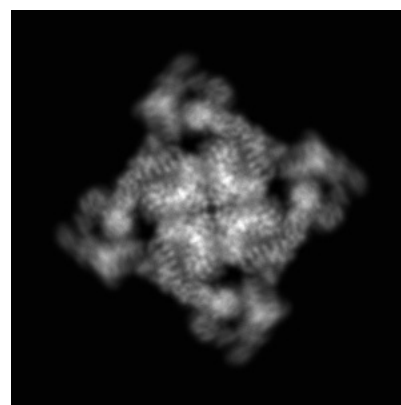
6.1.2 Raw map



X



Y

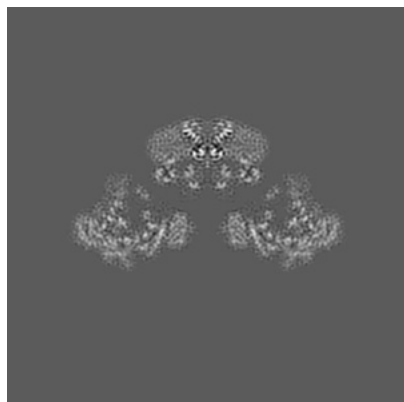


Z

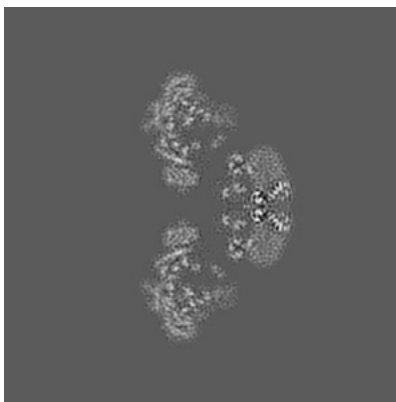
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

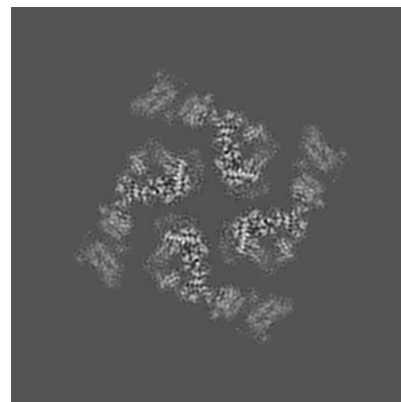
6.2.1 Primary map



X Index: 176

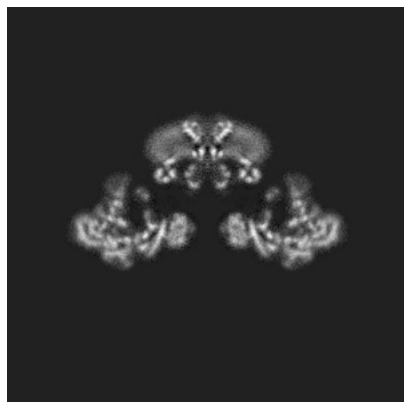


Y Index: 176

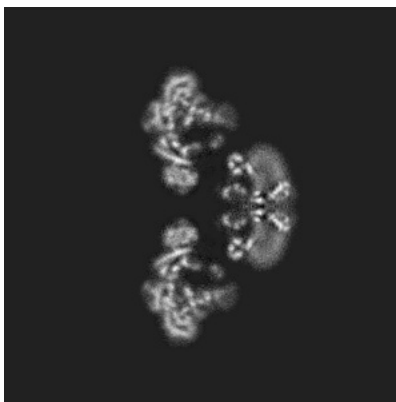


Z Index: 176

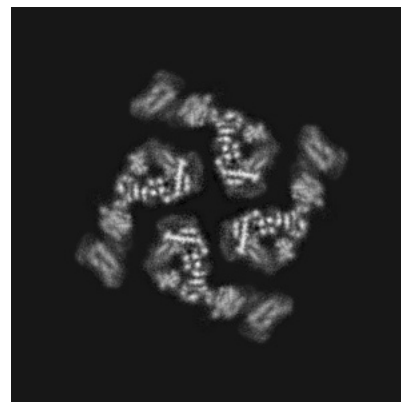
6.2.2 Raw map



X Index: 176



Y Index: 176

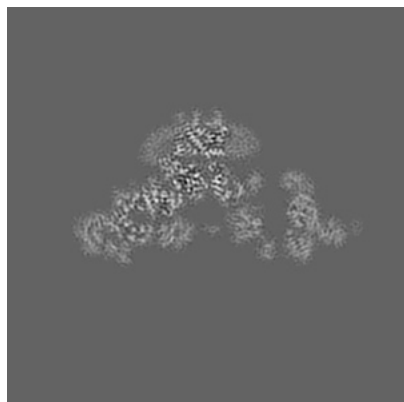


Z Index: 176

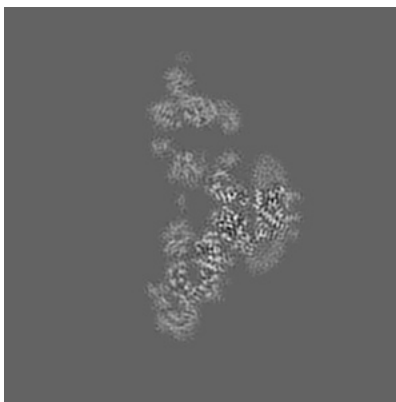
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

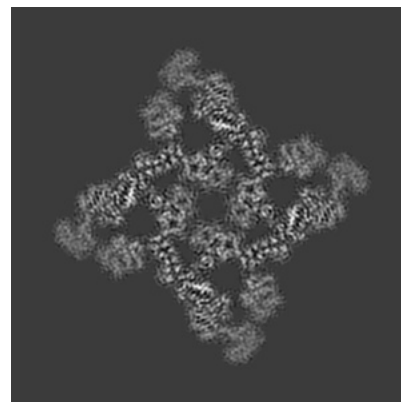
6.3.1 Primary map



X Index: 165

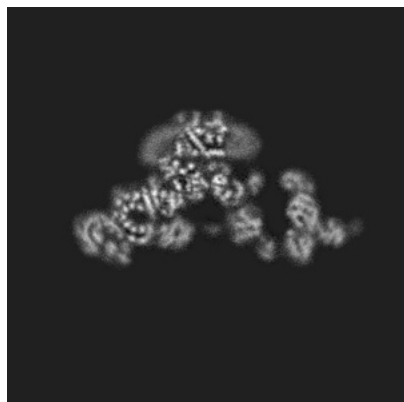


Y Index: 187

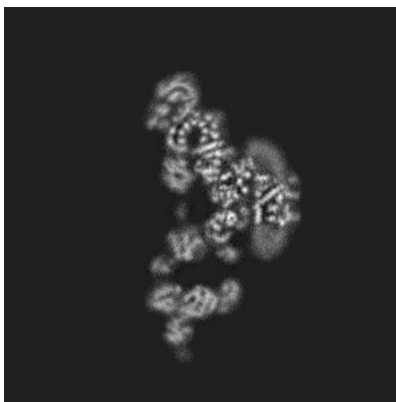


Z Index: 160

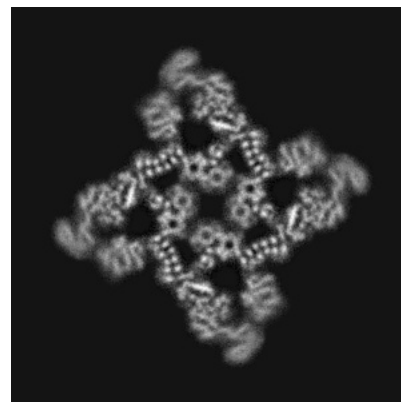
6.3.2 Raw map



X Index: 165



Y Index: 165

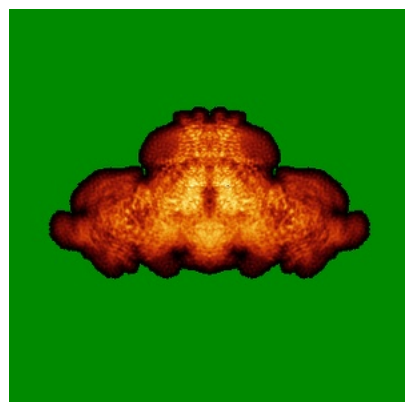


Z Index: 160

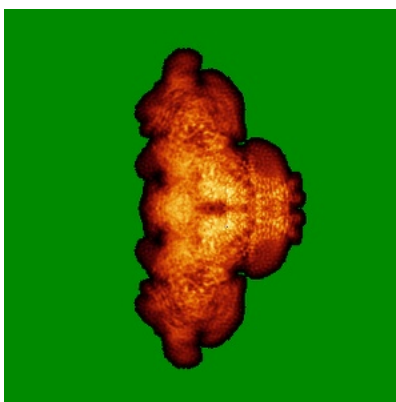
The images above show the largest variance slices of the map in three orthogonal directions.

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

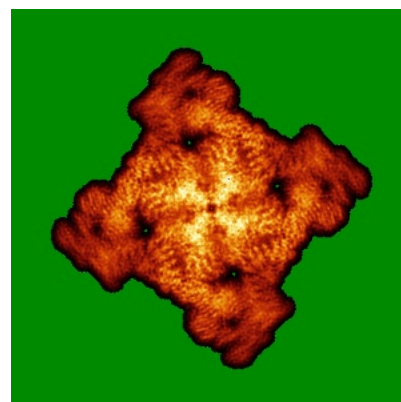
6.4.1 Primary map



X

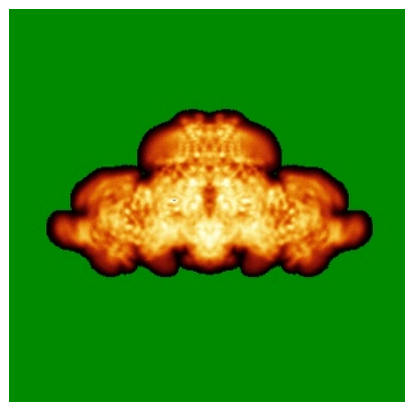


Y

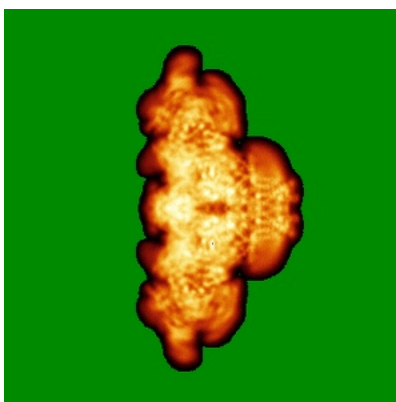


Z

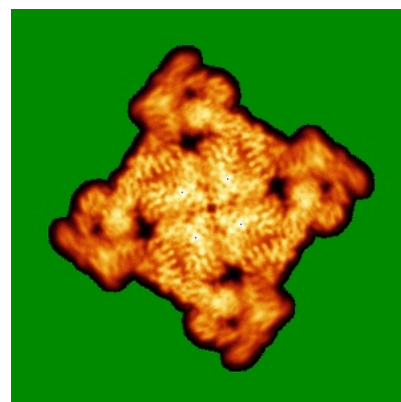
6.4.2 Raw map



X



Y

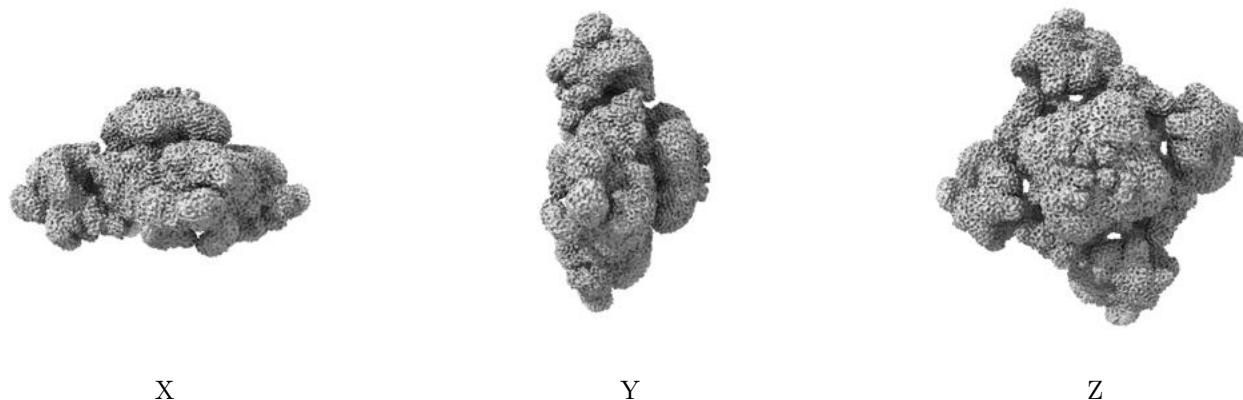


Z

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.

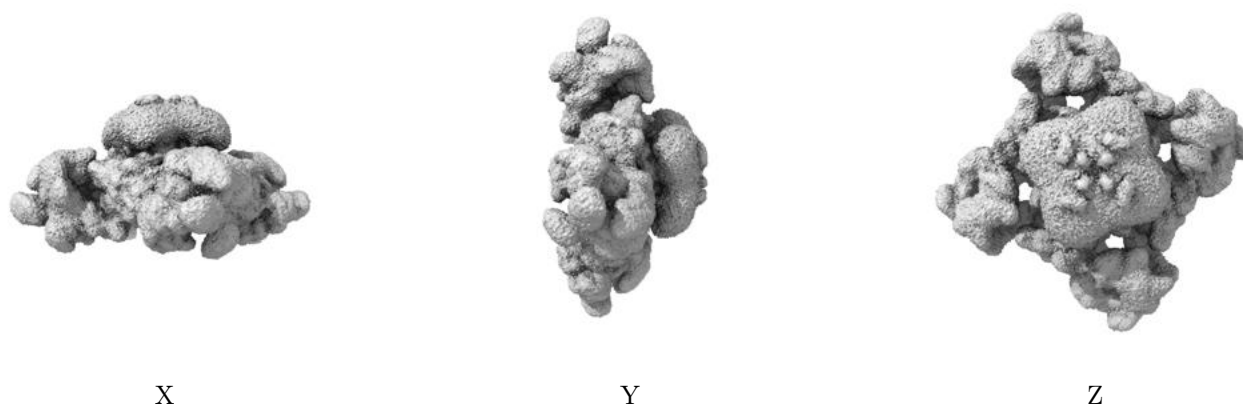
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

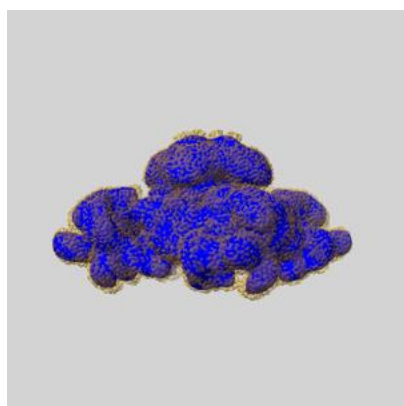
6.6 Mask visualisation [i](#)

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

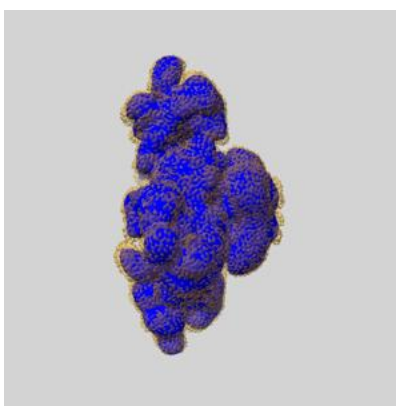
A mask typically either:

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

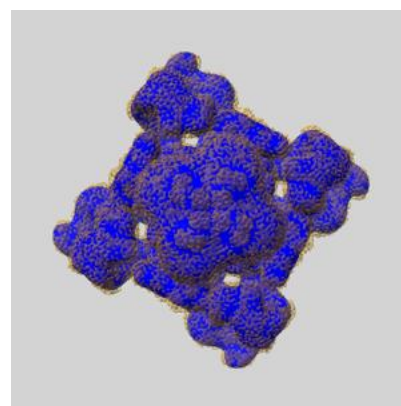
6.6.1 emd_22615_msk_1.map [i](#)



X



Y

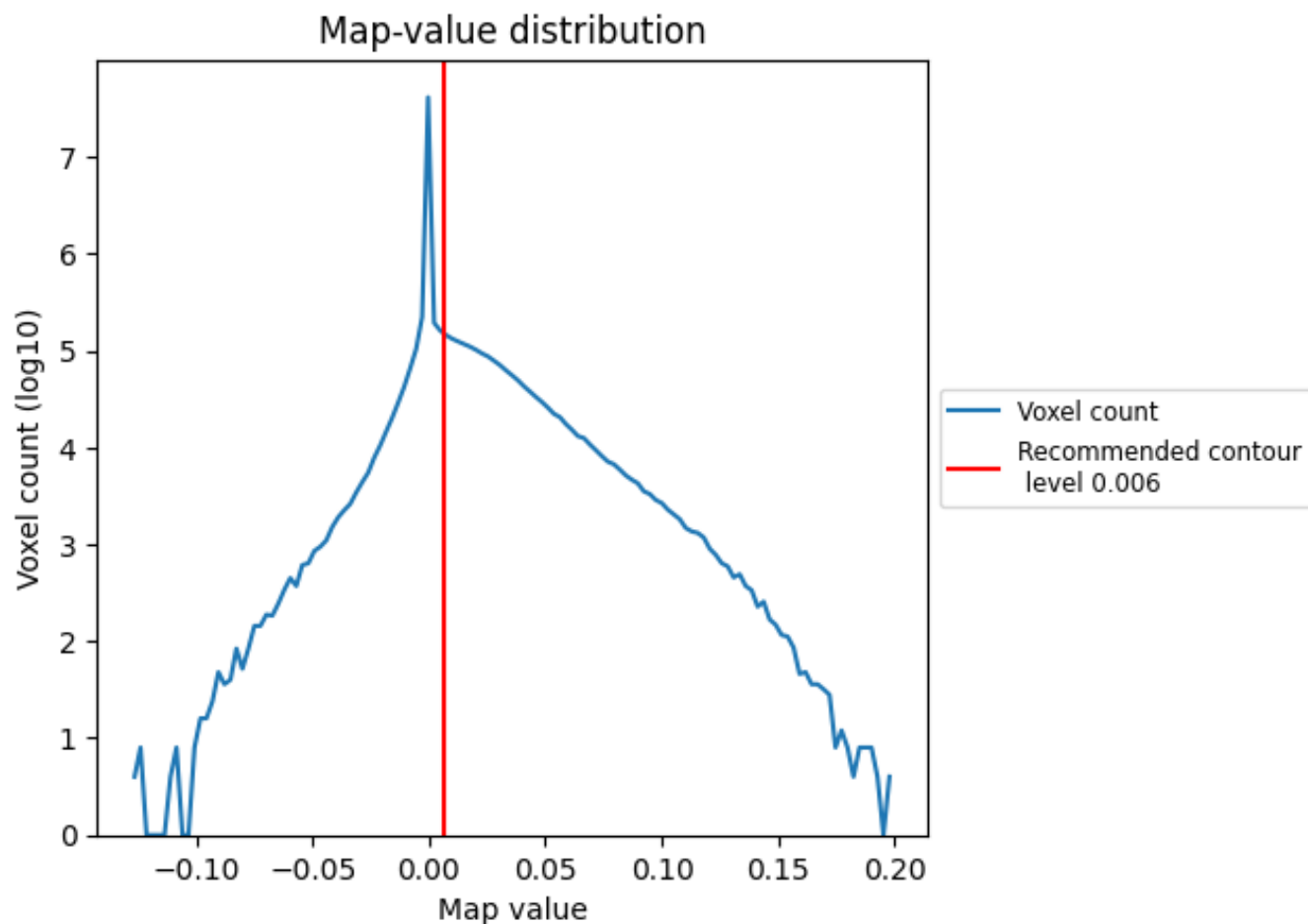


Z

7 Map analysis [i](#)

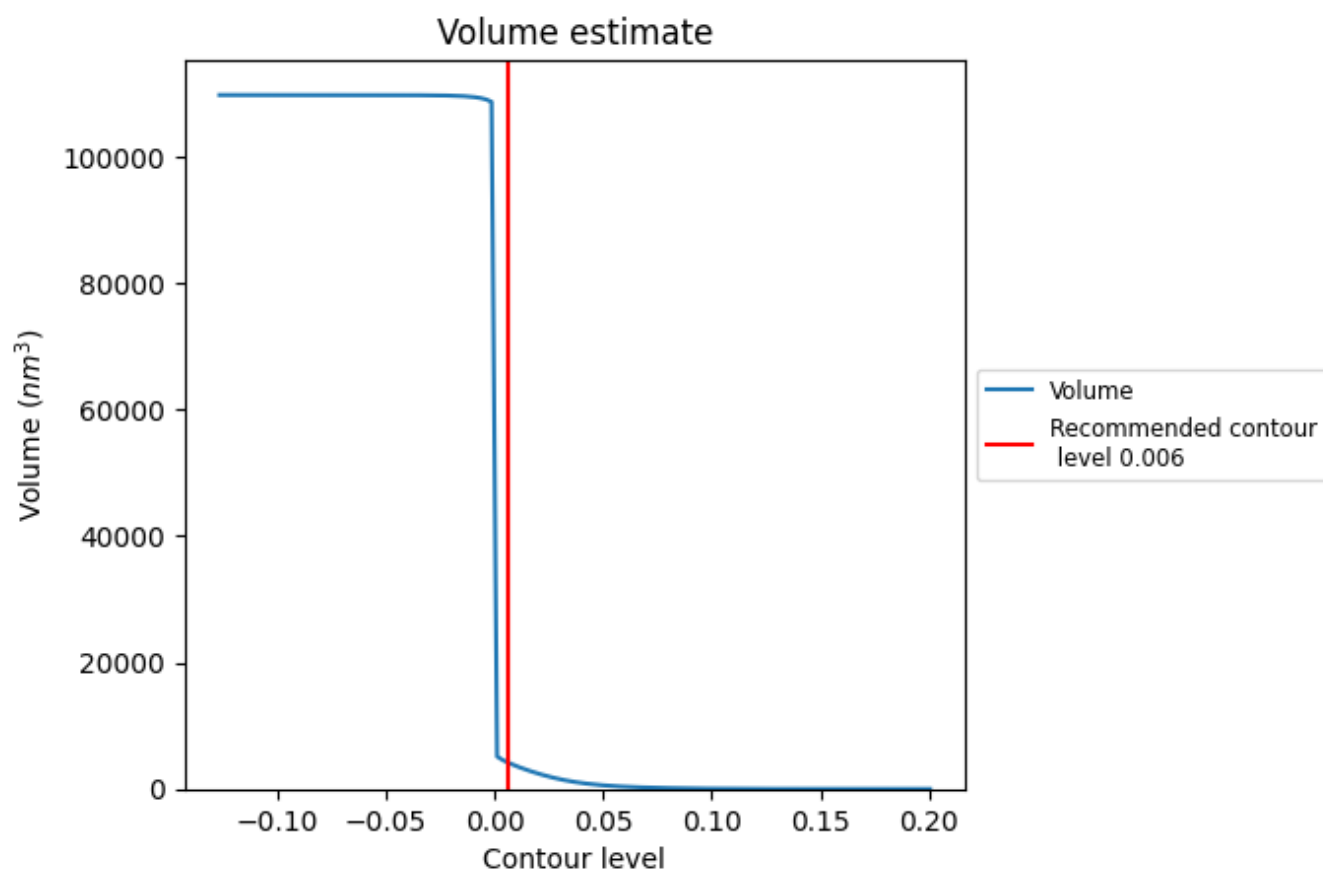
This section contains the results of statistical analysis of the map.

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.

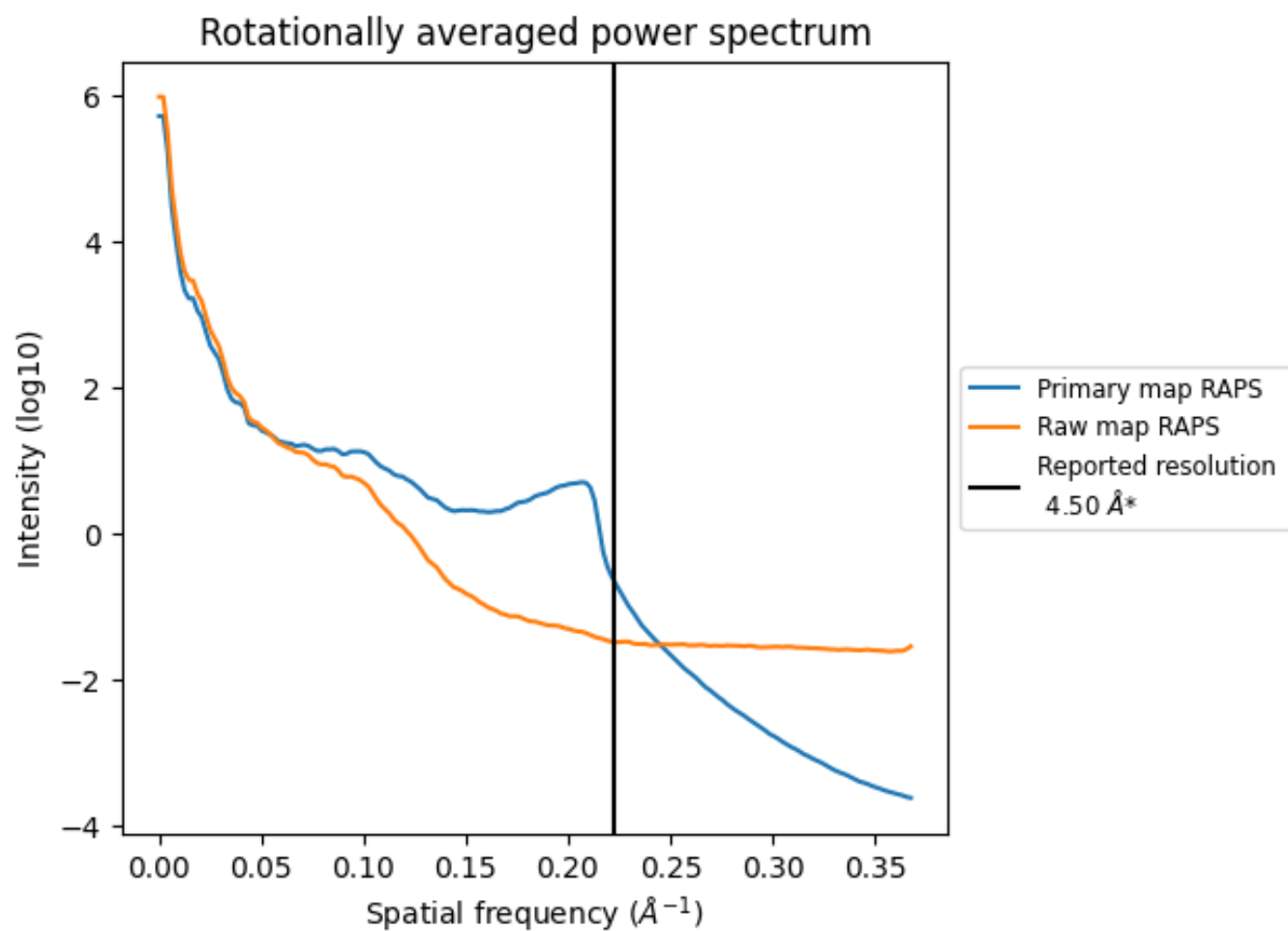
7.2 Volume estimate [i](#)



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 ⓘ

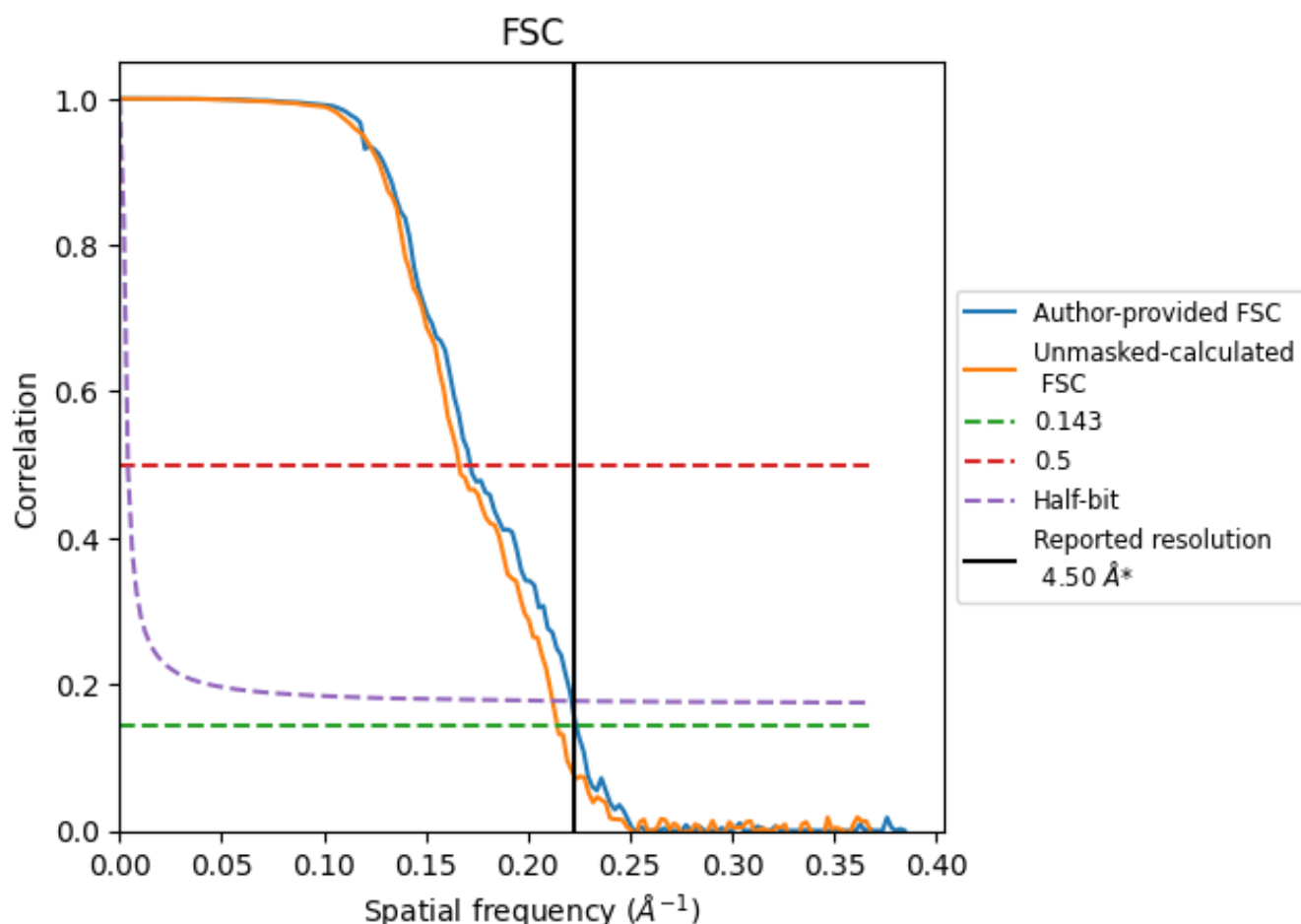


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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](#)

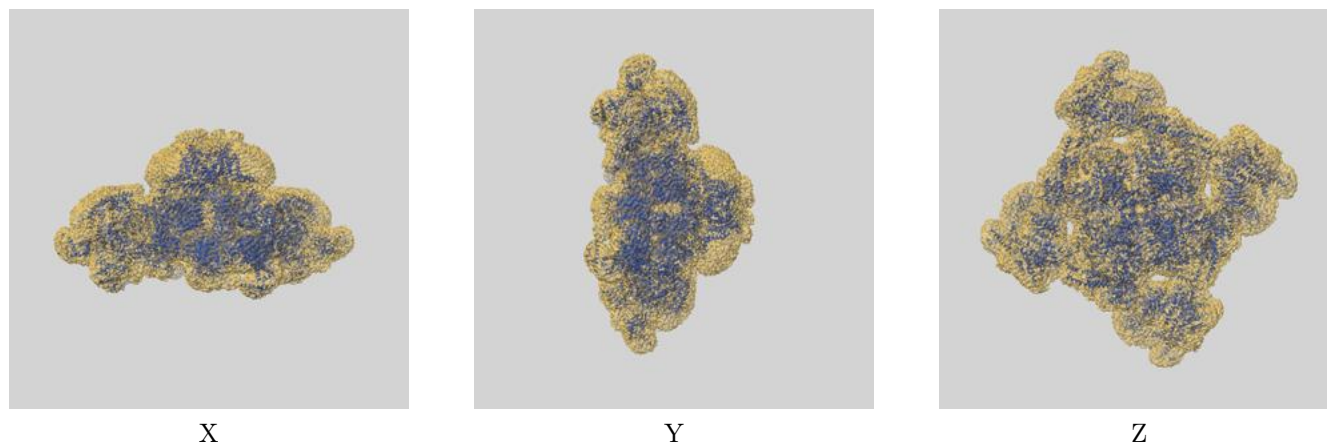
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.47	5.82	4.52
Unmasked-calculated*	4.66	6.01	4.71

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

9 Map-model fit [i](#)

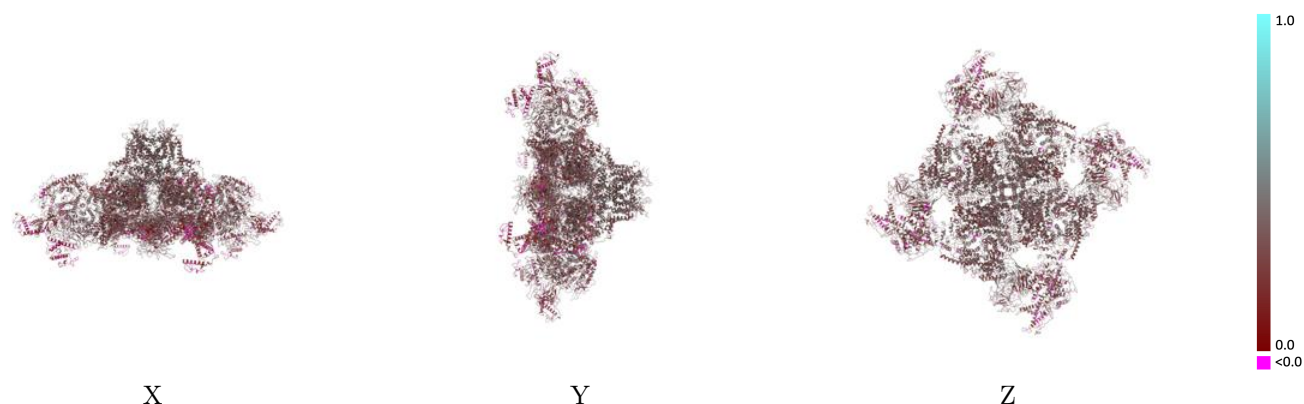
This section contains information regarding the fit between EMDB map EMD-22615 and PDB model 7K0S. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



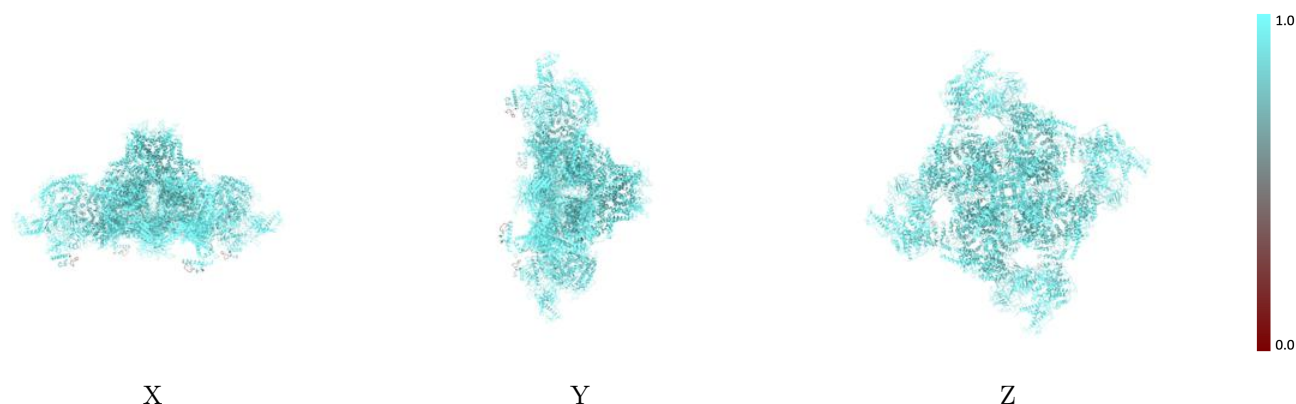
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



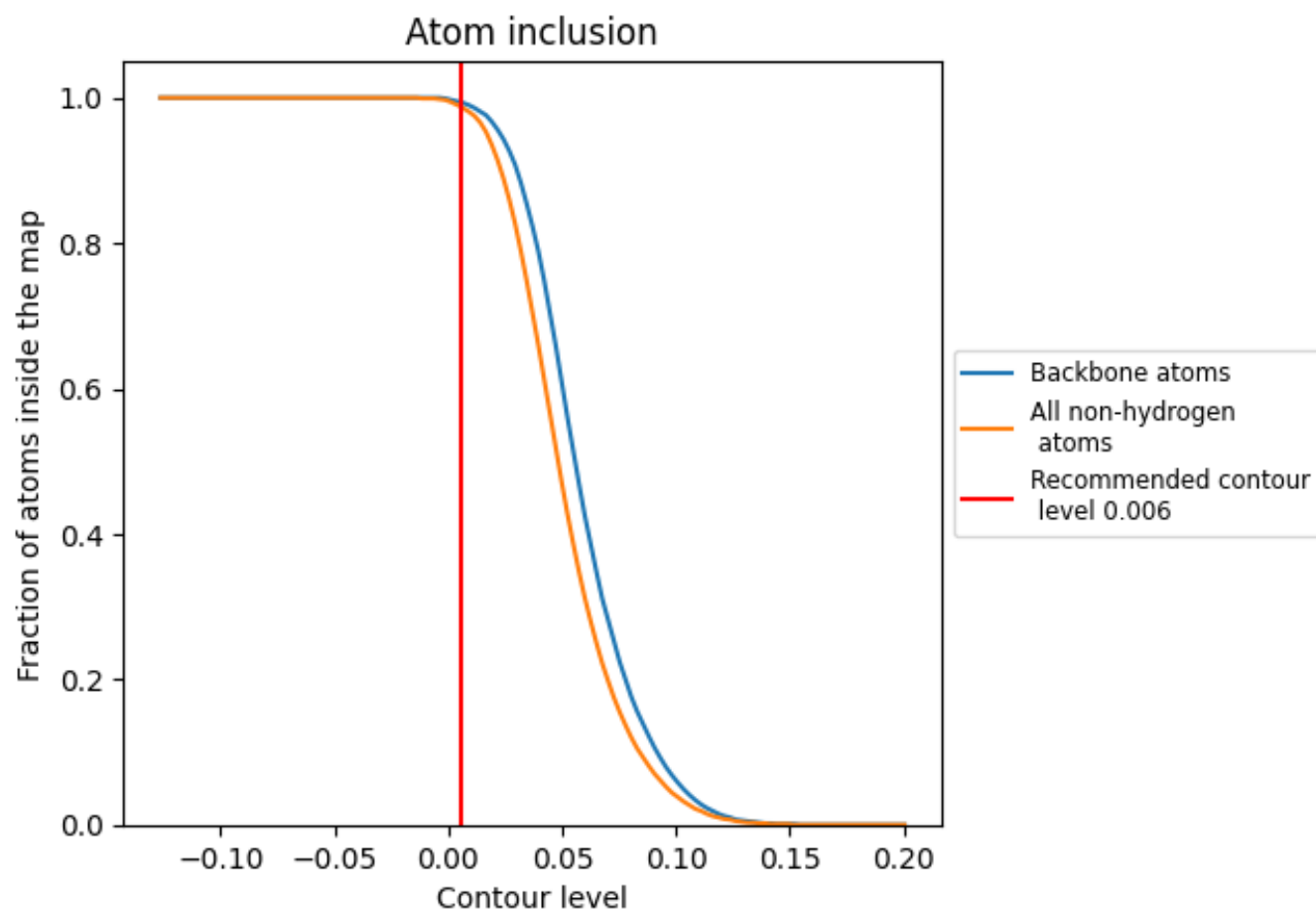
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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> 0.9870	<div></div> 0.3120
A	<div></div> 0.9870	<div></div> 0.3110
B	<div></div> 0.9870	<div></div> 0.3120
C	<div></div> 0.9870	<div></div> 0.3120
D	<div></div> 0.9870	<div></div> 0.3110

