



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 05:31 PM JST

PDB ID : 6JGZ
EMDB ID : EMD-9824
Title : Structure of RyR2 (F/P/Ca²⁺ dataset)
Authors : Chi, X.M.; Gong, D.S.; Ren, K.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Zhou, Q.; Yan, N.
Deposited on : 2019-02-16
Resolution : 4.60 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
MolProbity : 4.02b-467
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

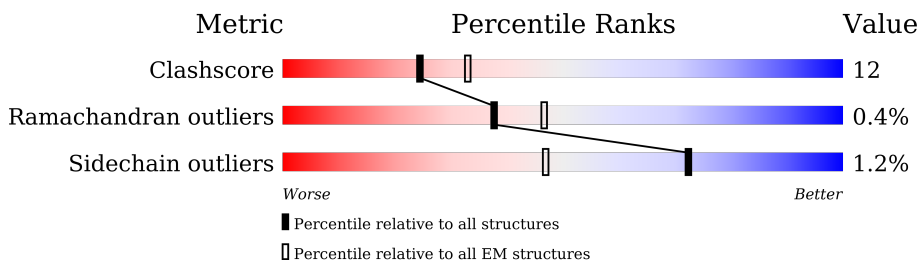
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	108	
1	C	108	
1	E	108	
1	G	108	
2	B	4968	
2	D	4968	
2	F	4968	
2	H	4968	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 109824 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	C	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	D	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	F	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	H	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		

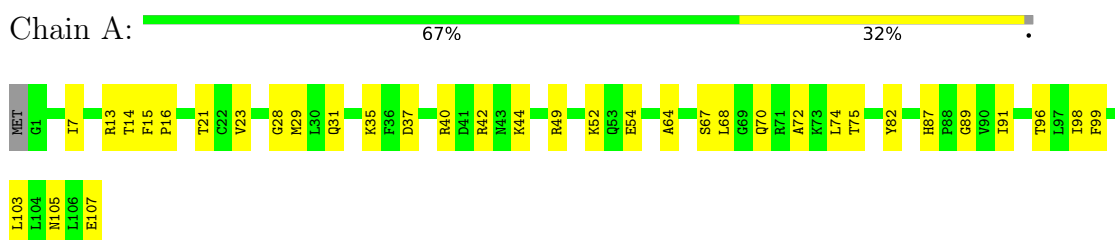
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	H	1	Total	Zn	0
			1	1	

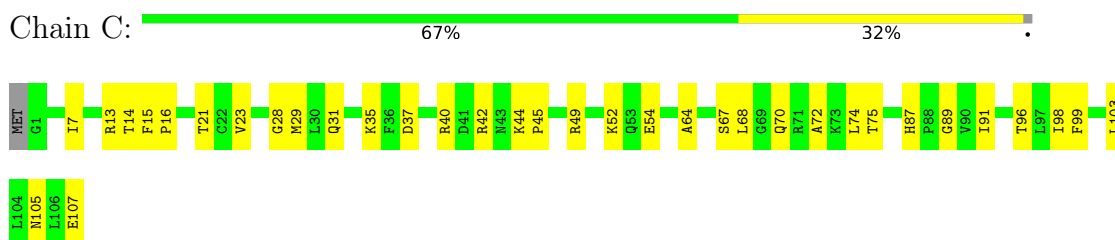
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

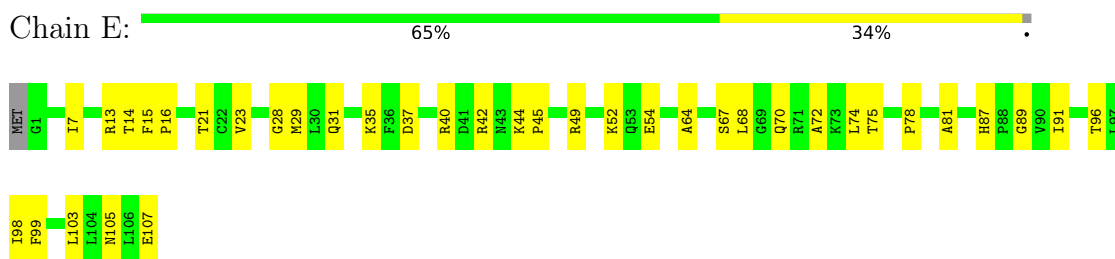
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



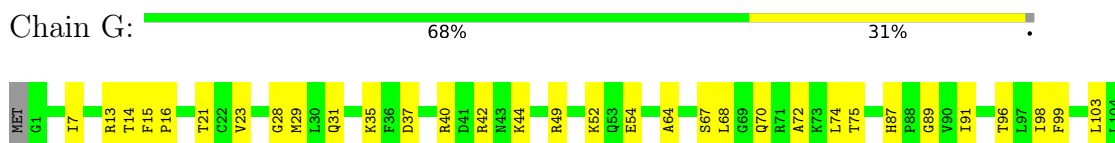
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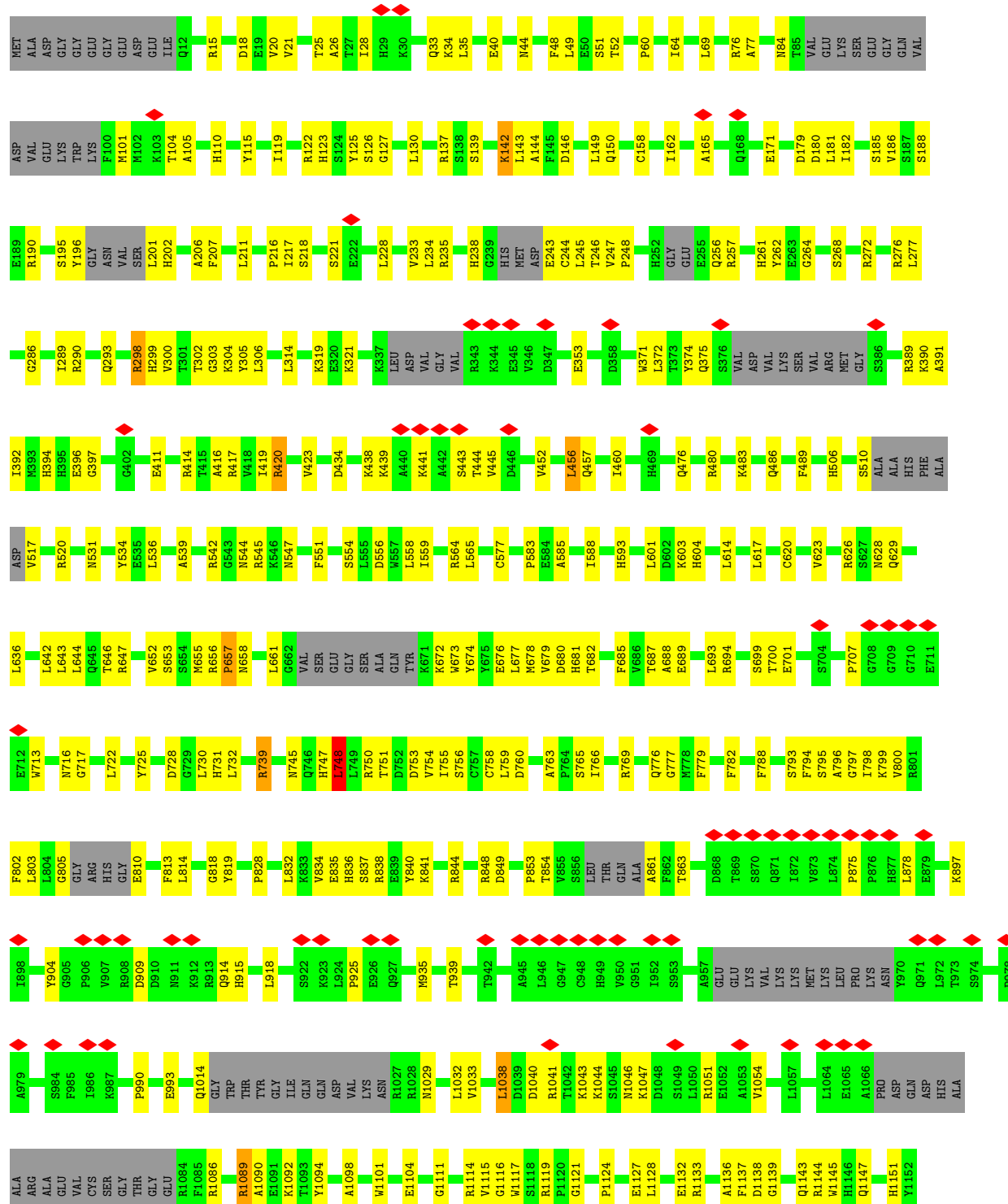


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



M105
L106
E107

• Molecule 2: RyR2







V4855	I4856	V4857	A4861	I4862	I4863	Q4864	G4865	I4866	I4867	I4868	D4869	A4870	F4871	L4874	R4875	Q4876	K4766	T4762	S4769	Y4658											P4622	S4623	I4627	K4628	Q4629	Q4630	W4631	S4640	F4641	P4642	N4643	K4648	F4649	V4650	K4651	R4652	K4653	V4654	M4655	D4656	K4657											F4596	V4713	T4716	D4717	F4720	L4721	Y4722	L4723	Q4733	E4833	D4834	D4838	E4841	R4844	I4845	I4846	F4847	D4848	F4851											F4894	I4891	C4892	G4893	K4888	C4889	F4890	D4799	E4798	S4797	N4796	Y4794	F4793	K4792	L4374	R4375	Q4378	D4388	C4389	F4390	I4391	G4389	V4389	D4380	T4301	V4302	P4303	F4306	Q4912	E4913	H4914	N4915	E4931	W4942	F4959	E4964	ASP	GLN	LEU	ASN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
S4769	T4762	K4766	Q4767	L4770	L4774	V4778	V4779	Y4780	L4781	Y4782	ASP	PHE	SER	ASP	ALA	GLU	LYS	LYS	PRO	LYS	LYS	PRO	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS

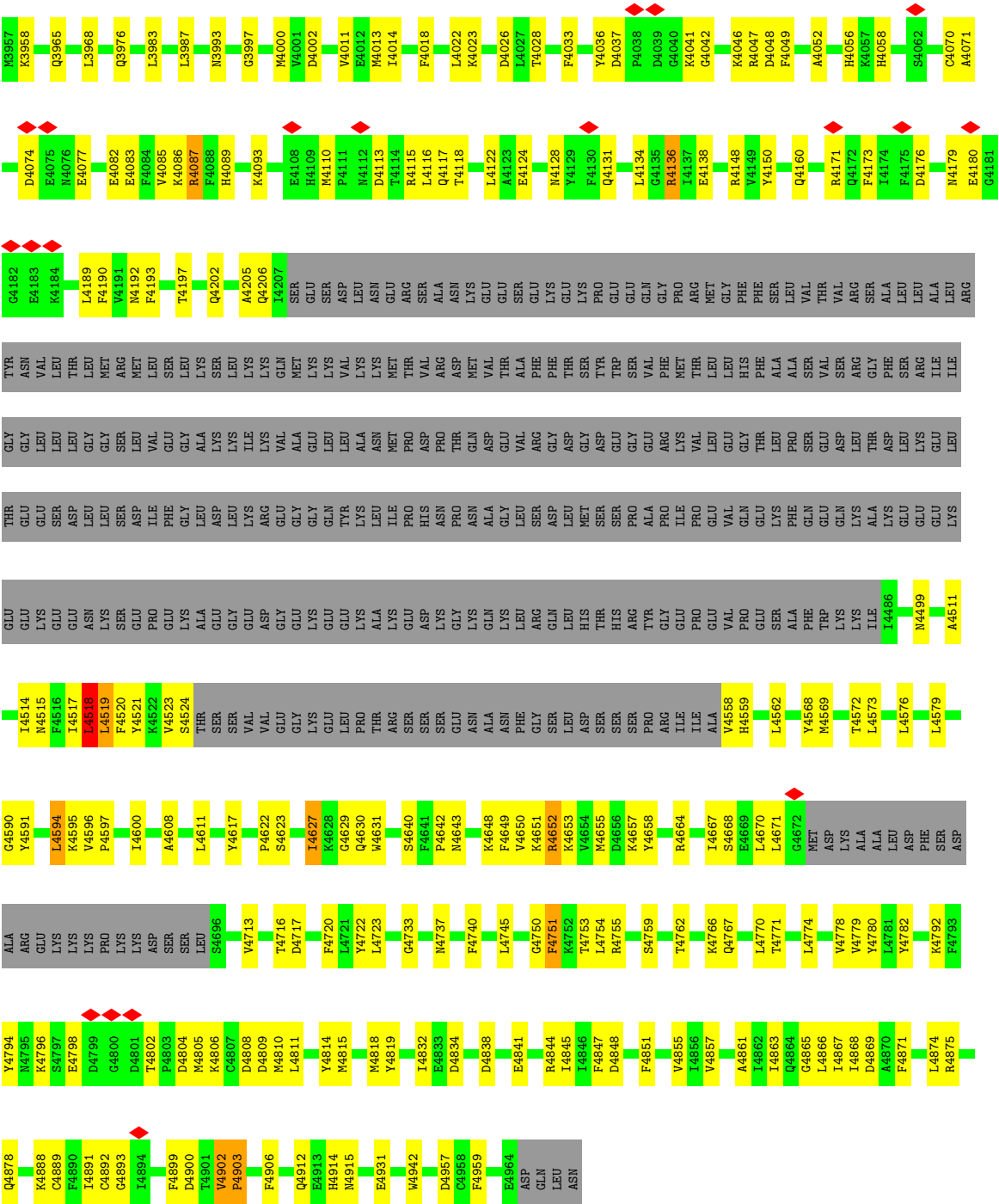
• Molecule 2: RyR2



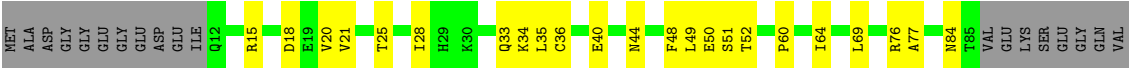








• Molecule 2: RyR2









- Molecule 2: RyR2





M2783	L2784	A2785	M2786	G2787	M2788	A2789	R2790	L2790	E2791	R2792	T2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TTR	ASN	ARG	THR	THR	ARG	ARG	ILE	SER	GLN	THR	SER	VAL	S2752	K2753	Y2754	Q2755	P2756	N2757	K2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	E2770	I2771	V2772	K2773	D2774	P2775	I2776	E2777	A2778	S2779	L2780	K2781	T2782
Y2720	F2721	I2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	K2730	D2731	M2735	L2738	A2739	M2740	G2741	M2742	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	Y2754	Q2755	P2756	N2757	K2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	E2770	I2771	V2772	K2773	D2774	P2775	I2776	E2777	A2778	S2779	L2780	K2781	T2782							
ALA	R2605	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	L2653	SER	GLN	LYS	Y2658	P2679	TYR	MET	GLU	SER	ASN	ARG	TYR	VAL	SER	MET	MET	MET	GLU	GLU	LYS	GLN	SER	SER	SER	ASP	SER	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717	L2718	E2719							
L2473	Y2476	Y2477	GLY	ILE	GLU	V2481	L2488	L2489	GLU	VAL	G2492	L2503	ASP	THR	ALA	ALA	ALA	LYS	GLY	E2416	R2421	S2422	I2423	S2426	LEU	ILE	PRO	GLU	G2431	Q2442	MET	PRO	THR	ILE	ALA	ASP	PRO	VAL	GLN	VAL	GLU	PRO	ASP	MET	ASP	GLY	ALA	GLY	F2461	C2462	P2463	D2464	V2470										
GLY	TRP	ASN	P2293	G2296	R2297	K2298	Y2299	D2301	R2304	I2326	R2327	K2328	P2329	P2330	CYS	PHE	GLY	PRO	SER	ALA	LEU	ARG	GLY	GLY	ASN	G2343	L2344	M2348	T2354	ALA	GLU	ASP	PRO	GLY	PRO	GLY	PRO	VAL	GLN	SER	GLN	MET	LEU	VAL	SER	LYS	MET	PRO	ASP	THR	GLU	GLY											
V2177	G2181	GLY	GLY	GLY	SER	LYS	GLU	ILE	F2190	M2193	N2196	G2197	C2198	R2199	F2200	L2201	C2202	Y2203	F2204	C2205	R2206	I2207	G2208	N2211	Y2221	L2222	N2225	S2226	S2232	P2233	D2250	L2256	G2274	LEU	GLN	SER	GLN	MET	LEU	VAL	SER	LYS	PRO	GLY	THR	PRO	ASP	ILE															
L2059	Q2060	L2063	L2067	A2071	Q2072	V2075	L2076	L2081	V2082	R2083	L2088	R2091	Q2092	I2096	V2100	R2101	A2102	L2103	T2106	D2116	T2117	I2118	L2121	A2122	S2123	Q2126	I2127	L2135	G2136	L2142	M2143	L2144	R2145	G2148	N2152	N2153	K2154	Y2157	P2160																								
GLU	CYS	PRO	CYS	PRO	GLU	ILE	R1994	Q1995	Q1996	L1997	L1998	D1999	D2003	E2011	L2012	D2013	GLU	ASP	GLY	SER	LEU	ASP	GLY	S2022	L2024	T2025	L2026	R2027	L2030	V2034	T2038	Y2039	L2040	LYS	LYS	GLN	ALA	GLU	GLN	ILE	ASN	MET	LEU	SER	ASP	SER	LYS	SER	T2058														
H1835	L1843	I1846	Y1847	E1848	S1849	PHE	GLY	LYS	GLU	ALA	ALA	Q1938	D1939	N1940	G1941	R1942	F1943	R1944	V1948	GLN	ALA	LEU	ASN	CYS	MET	ALA	SER	ASP	THR	GLY	GLY	GLY	PRO	ALA	E1797	A1798	V1799	S1803	R1807	D1808	P1809	F1816	L1817	P1820	L1821	T1827	L1905	Q1906	L1907	I1833	F1834												
F1627	M1628	S1629	L1630	H1631	I1632	P1633	E1634	E1635	S1638	V1639	D1640	I1641	L1642	E1643	E1648	L1651	H1654	S1666	L1667	G1668	M1669	H1670	R1671	A1675	L1676	H1679	E1682	P1683	Q1684	L1685	L1686	Y1687	A1688	I1689	K1692	G1696	R1699	Y1703	T1716	L1719	L1726	I1736	T1737																				
LEU	GLY	ARG	ILE	LYS	ASN	VAL	MET	PRO	SER	CYS	L1570	F1571	S1572	S1573	E1574	H1575	V1579	P1580	P1584	H1587	V1588	Q1589	F1590	L1591	S1592	H1593	V1596	S1597	R1598	P1599	N1601	Q1602	F1603	L1604	K1605	V1606	D1607	V1608	S1609	R1610	I1611	S1612	E1613	R1614	Q1615	G1616	V1617	Q1620	C1621	L1622													



R4844	G4750	V4850	PHE	LEU	LEU	VAL	ALA	GLU	L4122
I4845	K4751	K4651	GLY	ARG	SER	ARG	PHE	LVS	E4123
I4846	F4751	R4652	SER	GLN	ASP	GLY	PHE	GLU	A4124
F4847	K4752	K4653	LEU	LEU	LEU	ASP	THR	LVS	S4125
D4848	T4753	V4654	ASP	HIS	MET	GLY	THR	PRO	
F4851	L4754	M4655	SER	THR	SER	ASP	TYR	GLU	M4128
R4755	R4755	D4656	SER	HIS	SER	SER	TRP	GLU	F4129
S4759	K4657	K4657	SER	ARG	PRO	GLY	SER	GLN	F4130
	Y4658	Y4658	PRO	TYR	ALA	GLU	VAL	GLY	Q4131
			ARG	GLY	PRO	ARG	PHE	PRO	
T4762	R4664	R4664	ILE	GLU	ILE	LVS	MET	ARG	L4134
			ILE	PRO	PRO	VAL	THR	MET	Q4135
K4766	T4667	T4667	ALA	GLU	GLU	LEU	LEU	GLY	R4136
Q4767	S4668	S4668	V4558	VAL	VAL	GLU	LEU	PHE	I4137
	E4669	E4669	H4559	PRO	GLN	GLY	HIS	PHE	E4138
L4770	L4670	L4670	GLU	GLU	THR	THR	PHE	SER	
L4774	L4671	L4671	L4562	SER	LVS	LEU	ALA	LEU	R4148
	G4672	G4672	ALA	ALA	PHE	PRO	ALA	VAL	V4149
	MET	MET	Y4568	PHE	GLN	SER	SER	THR	Y4150
V4778	ASP	ASP	M4569	THR	GLU	GLU	VAL	THR	
I4868	LVS	LVS	LVS	LVS	GLN	ASP	ARG	ARG	Q4160
Y4780	ALA	ALA	T4572	LVS	LEU	LEU	SER	SER	
L4781	ALA	ALA	L4573	ILE	ALA	THR	GLY	ALA	R4171
Y4782	LEU	LEU	L4576		LVS	ASP	PHE	LEU	Q4172
K4792	ASP	ASP	L4579	M4499	GLU	GLU	SER	ALA	F4173
F4793	SER	SER			GLU	GLU	ILE	LEU	
Y4794	ASP	ASP	G4590	A4511	LVS	THR	GLY	ARG	D4176
N4795	ALA	ALA	Y4591		GLU	GLU	GLY	ASN	M4179
K4796	ARG	ARG			LVS	GLU	LEU	VAL	E4180
S4797	GLU	GLU	L4514	L4515	LVS	VAL	LEU	VAL	Q4181
E4798	LVS	LVS	L4516	F4516	GLU	SER	LEU	LEU	Q4182
D4799	K4595	K4595	K4594	L4517	GLU	ASP	LEU	THR	E4183
G4800	V4596	V4596	V4596	L4518	ASN	LEU	GLY	LEU	E4183
D4801	LVS	LVS	P4597	L4519	LVS	LEU	GLY	MET	K4184
T4802	LVS	LVS	F4520	F4521	SER	SER	SER	ARG	
F4803	ASP	ASP	Y4521	Y4521	GLU	ASP	LEU	MET	L4189
D4804	SER	SER	K4522	K4522	PRO	ILE	VAL	SER	F4190
M4805	SER	SER	A4608		GLU	PHE	GLU	SER	V4191
K4806	SER	SER	L4611	S4524	LVS	GLY	GLY	LEU	M4192
C4807	LEU	LEU		THR	ALA	LEU	LVS	SER	
D4808	S4696	S4696	Y4617	SER	GLU	ASP	LVS	THR	Q4202
D4809	V4713	V4713		SER	GLY	LEU	LVS	LEU	
M4810	L4811	L4811	P4622	VAL	GLU	LVS	ILE	LVS	A4205
	T4716	T4716	S4623	VAL	ASP	ARG	LVS	LVS	Q4206
D4717	D4717	D4717	GLY	GLU	GLY	GLU	VAL	MET	I4207
F4720	F4720	F4720	L4627	LVS	LVS	GLY	ALA	GLU	SER
L4721	Y4722	Y4722	K4628	GLU	GLU	GLN	LEU	LVS	GLU
L4723	L4723	L4723	G4629	LEU	GLU	TYR	VAL	LVS	SER
	Y4814	Y4814	Q4630	PRO	LVS	LVS	ALA	LVS	ASP
	M4818	M4818	W4631	THR	ALA	ASN	ASN	LEU	LEU
Y4819	Y4819	Y4819		ARG	LVS	ILE	MET	MET	ASN
	T4832	T4832	S4640	SER	GLU	PRO	PRO	THR	GLU
E4833	E4833	E4833	F4641	SER	ASP	HIS	THR	ARG	GLU
D4834	N4737	N4737	P4642	SER	LVS	ASN	ASP	VAL	SER
	F4740	F4740	N4643	GLU	GLY	PRO	THR	ASP	ALA
				ASN	LVS	ASN	GLN	MET	ASN
D4838			K4648	ALA	GLN	ALA	ASP	VAL	LVS
E4841			F4649	ASN	LVS	GLY	GLU	THR	GLU
									SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	60287	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 ($e^-/\text{\AA}^2$)	48.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	522.616, 522.616, 522.616	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/835	0.58	0/1123
1	C	0.35	0/835	0.58	0/1123
1	E	0.35	0/835	0.58	0/1123
1	G	0.35	0/835	0.58	0/1123
2	B	0.38	0/27132	0.62	12/36687 (0.0%)
2	D	0.38	0/27132	0.62	12/36687 (0.0%)
2	F	0.38	0/27132	0.62	12/36687 (0.0%)
2	H	0.38	0/27132	0.62	12/36687 (0.0%)
All	All	0.38	0/111868	0.61	48/151240 (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
2	B	0	29
2	D	0	29
2	F	0	29
2	H	0	29
All	All	0	116

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1753	LEU	CA-CB-CG	6.30	129.80	115.30
2	B	1753	LEU	CA-CB-CG	6.30	129.79	115.30
2	D	1753	LEU	CA-CB-CG	6.30	129.78	115.30
2	F	1753	LEU	CA-CB-CG	6.29	129.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	814	LEU	CA-CB-CG	5.94	128.97	115.30

There are no chirality outliers.

5 of 116 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	105	ALA	Peptide
2	B	142	LYS	Peptide
2	B	221	SER	Peptide
2	B	321	LYS	Peptide
2	B	657	PRO	Peptide

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	819	0	824	25	0
1	C	819	0	824	25	0
1	E	819	0	824	26	0
1	G	819	0	824	24	0
2	B	26636	0	25174	673	0
2	D	26636	0	25174	667	0
2	F	26636	0	25174	671	0
2	H	26636	0	25174	682	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	109824	0	103992	2512	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 12.

The worst 5 of 2512 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4520:PHE:CD1	2:F:4562:LEU:HD21	1.50	1.47
2:B:4520:PHE:CD1	2:B:4562:LEU:HD21	1.50	1.47
2:D:4520:PHE:CD1	2:D:4562:LEU:HD21	1.50	1.46
2:H:4520:PHE:CD1	2:H:4562:LEU:HD21	1.50	1.44
2:B:4808:ASP:HB3	2:D:4523:VAL:CG2	1.55	1.36

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	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	C	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	E	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	G	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3365/4968 (68%)	2969 (88%)	382 (11%)	14 (0%)	34	72
2	D	3365/4968 (68%)	2969 (88%)	382 (11%)	14 (0%)	34	72
2	F	3365/4968 (68%)	2968 (88%)	383 (11%)	14 (0%)	34	72
2	H	3365/4968 (68%)	2968 (88%)	383 (11%)	14 (0%)	34	72
All	All	13880/20304 (68%)	12254 (88%)	1570 (11%)	56 (0%)	38	72

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	143	LEU
2	B	4595	LYS
2	D	143	LEU
2	D	4595	LYS
2	F	143	LEU

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	88/89 (99%)	87 (99%)	1 (1%)	73	85
1	C	88/89 (99%)	87 (99%)	1 (1%)	73	85
1	E	88/89 (99%)	87 (99%)	1 (1%)	73	85
1	G	88/89 (99%)	87 (99%)	1 (1%)	73	85
2	B	2688/4355 (62%)	2655 (99%)	33 (1%)	71	84
2	D	2688/4355 (62%)	2655 (99%)	33 (1%)	71	84
2	F	2688/4355 (62%)	2655 (99%)	33 (1%)	71	84
2	H	2689/4355 (62%)	2655 (99%)	34 (1%)	69	82
All	All	11105/17776 (62%)	10968 (99%)	137 (1%)	72	84

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	1054	VAL
2	H	2206	ARG
2	H	4518	LEU
2	D	2027	ARG
2	D	1089	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	681	HIS
2	F	4160	GLN
2	F	1265	HIS
2	F	3813	ASN
2	H	23	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 4 ligands modelled in this entry, 4 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.

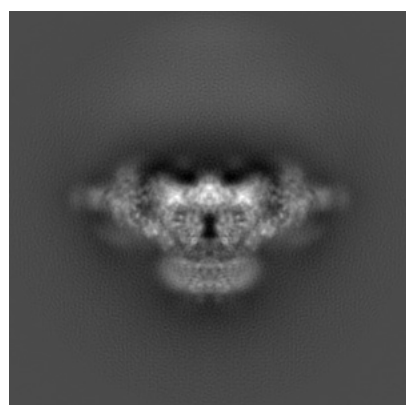
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9824. These allow visual inspection of the internal detail of the map and identification of artifacts.

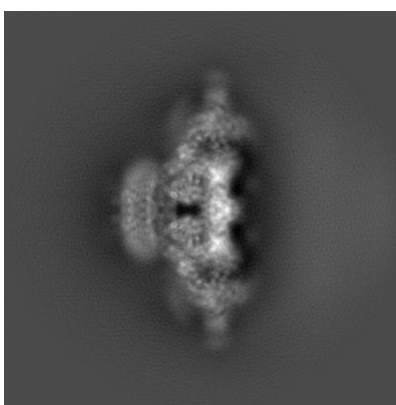
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

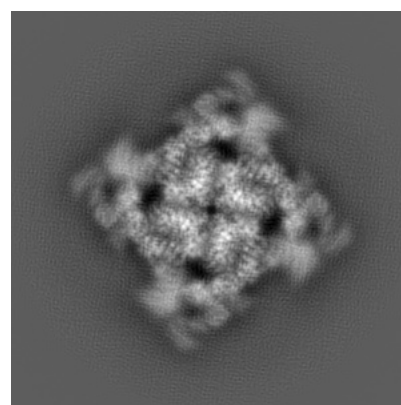
6.1.1 Primary map



X



Y

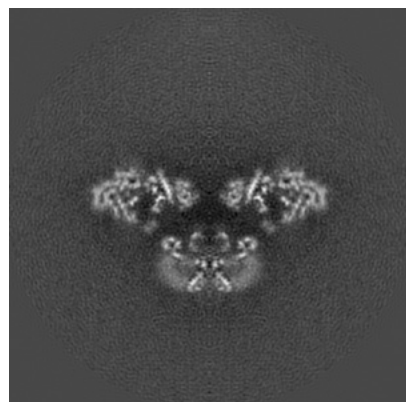


Z

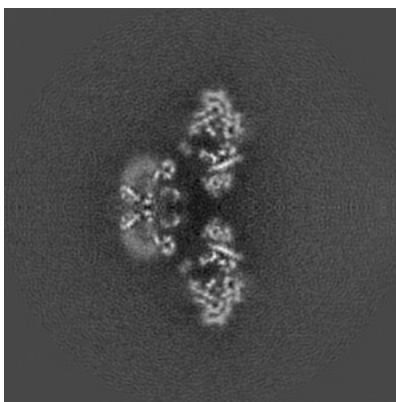
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

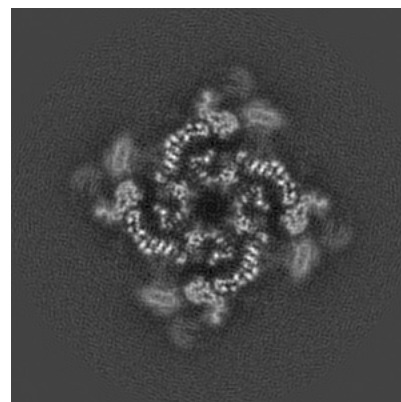
6.2.1 Primary map



X Index: 200



Y Index: 200

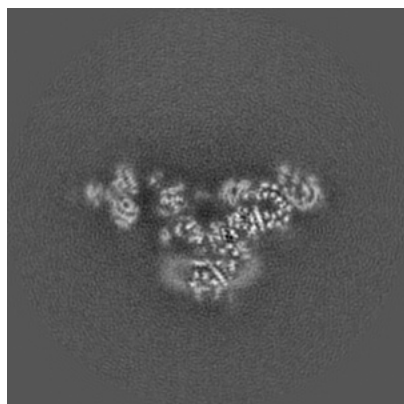


Z Index: 200

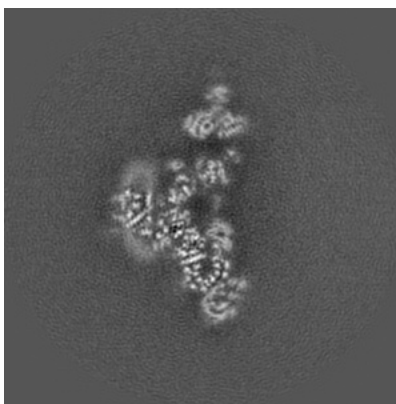
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

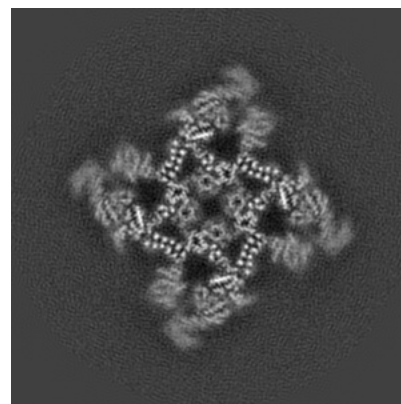
6.3.1 Primary map



X Index: 189



Y Index: 189

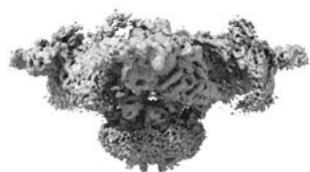


Z Index: 209

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

6.4 Orthogonal surface views [i](#)

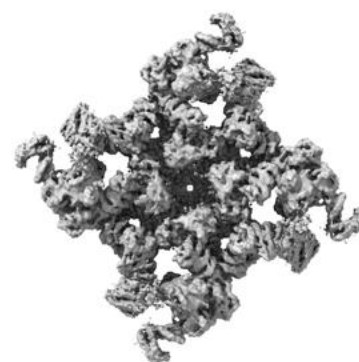
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

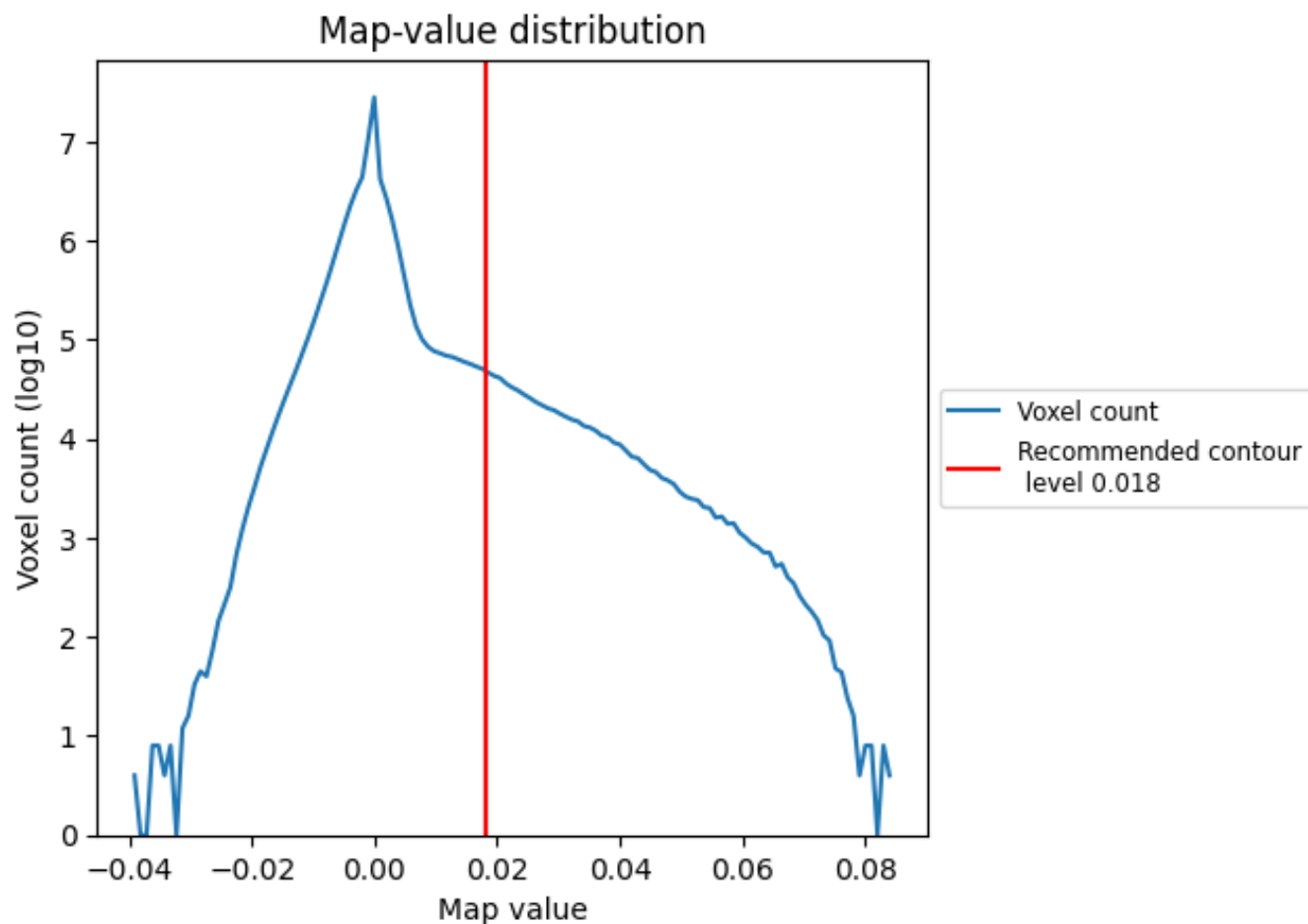
6.5 Mask visualisation

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

7 Map analysis [i](#)

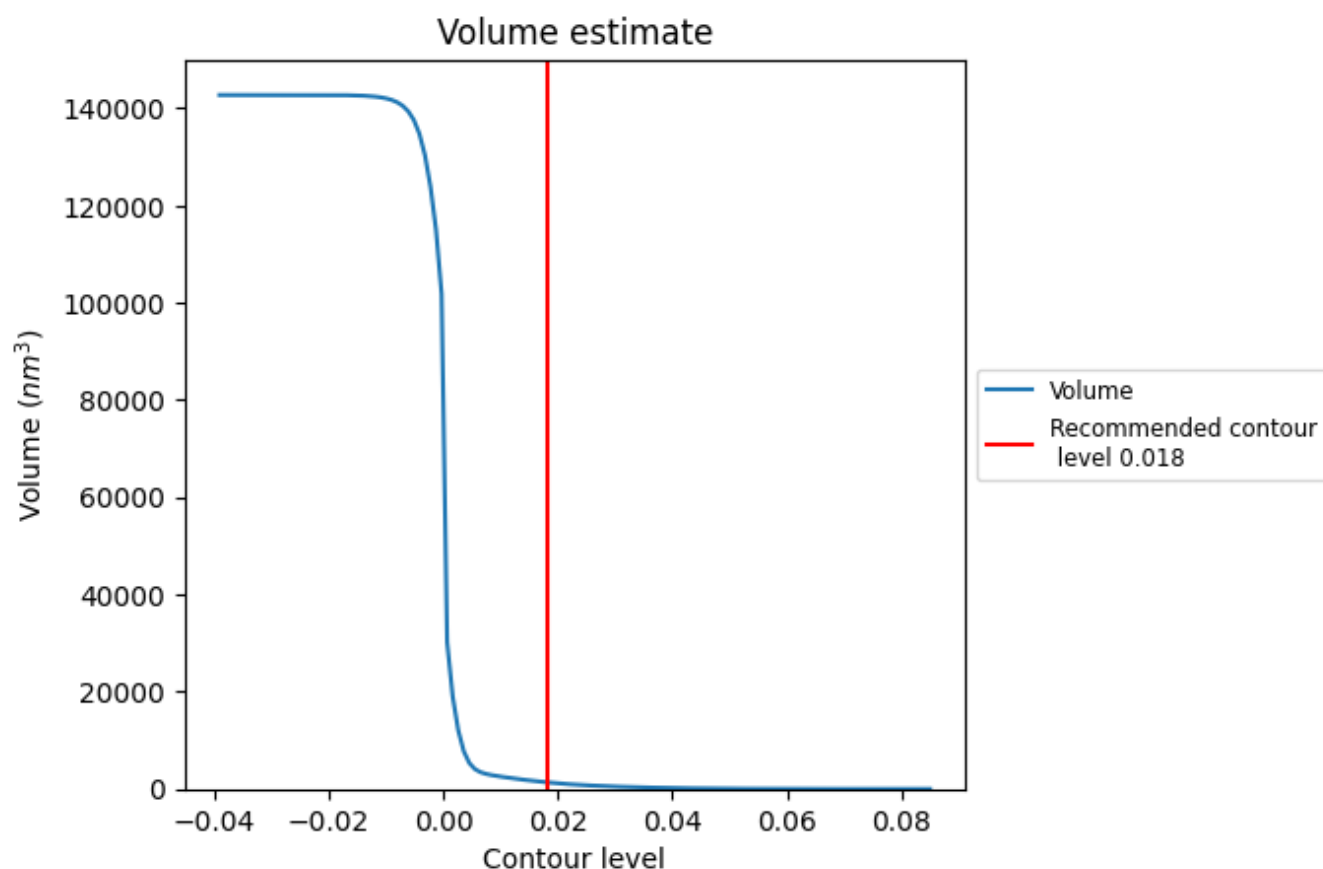
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

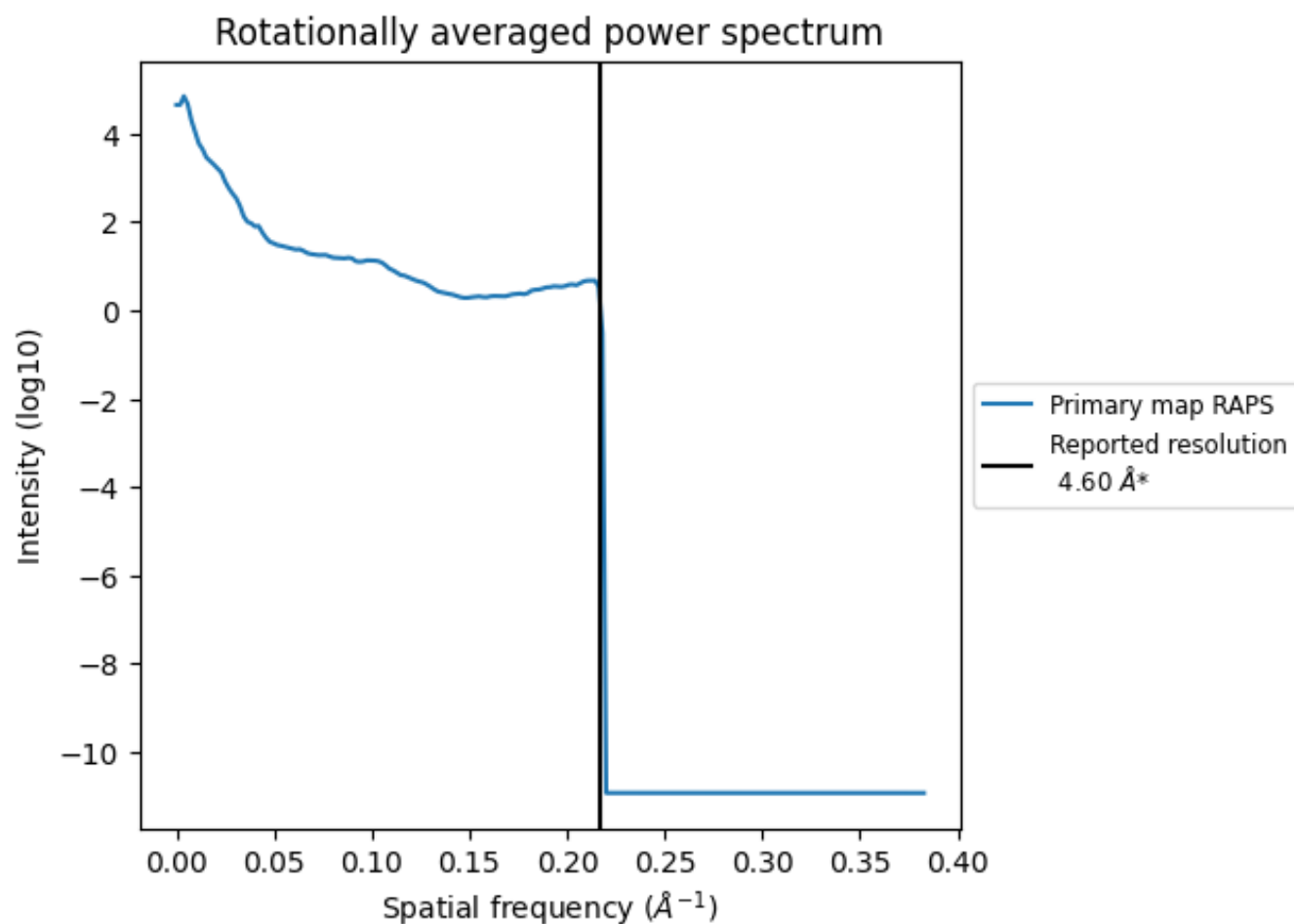
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1373 nm^3 ; this corresponds to an approximate mass of 1240 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 ⓘ

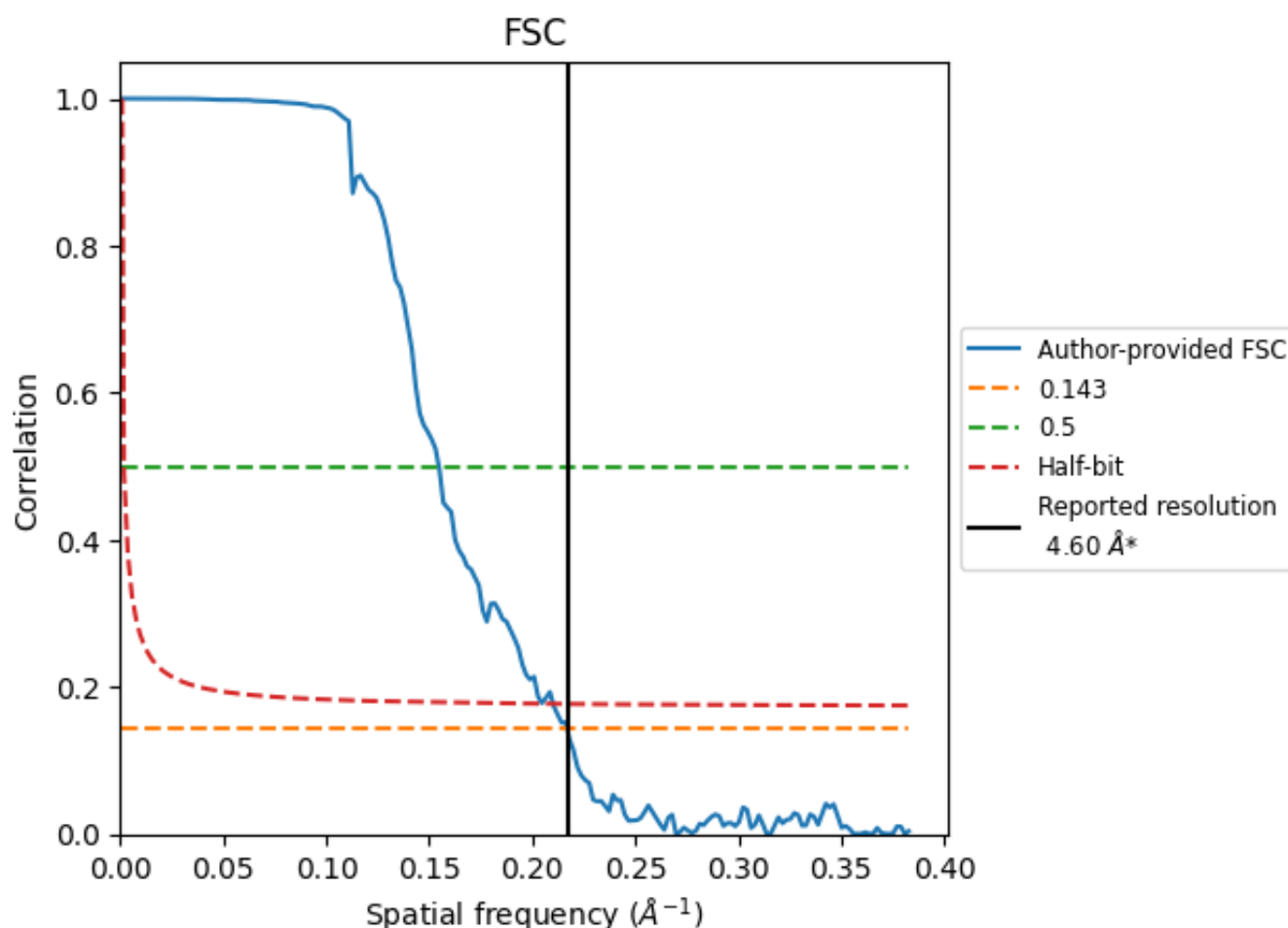


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

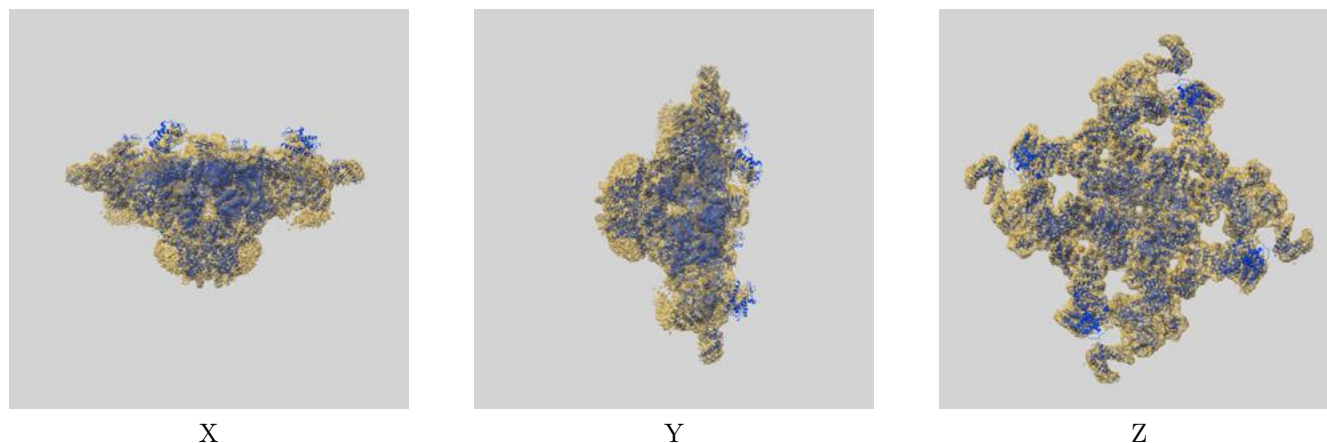
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	6.46	4.76
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

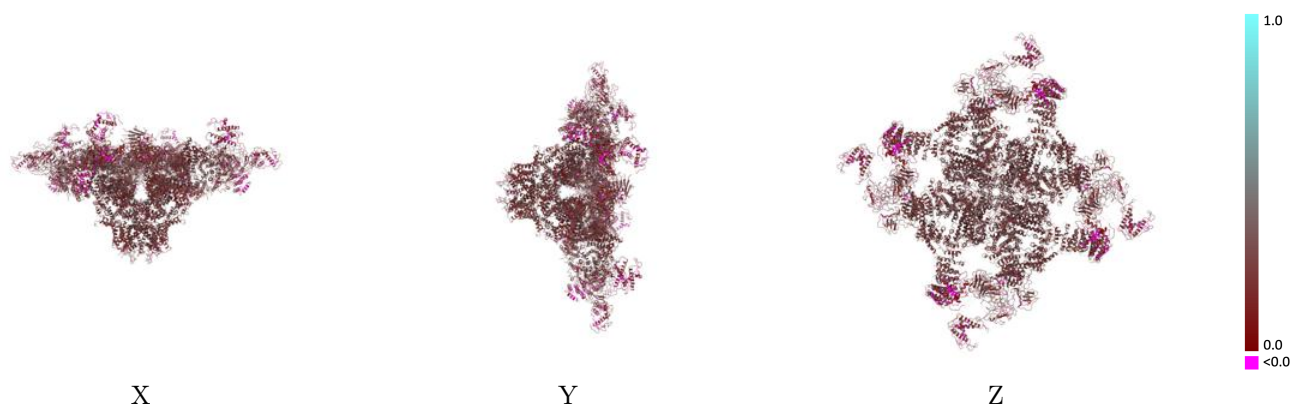
This section contains information regarding the fit between EMDB map EMD-9824 and PDB model 6JGZ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



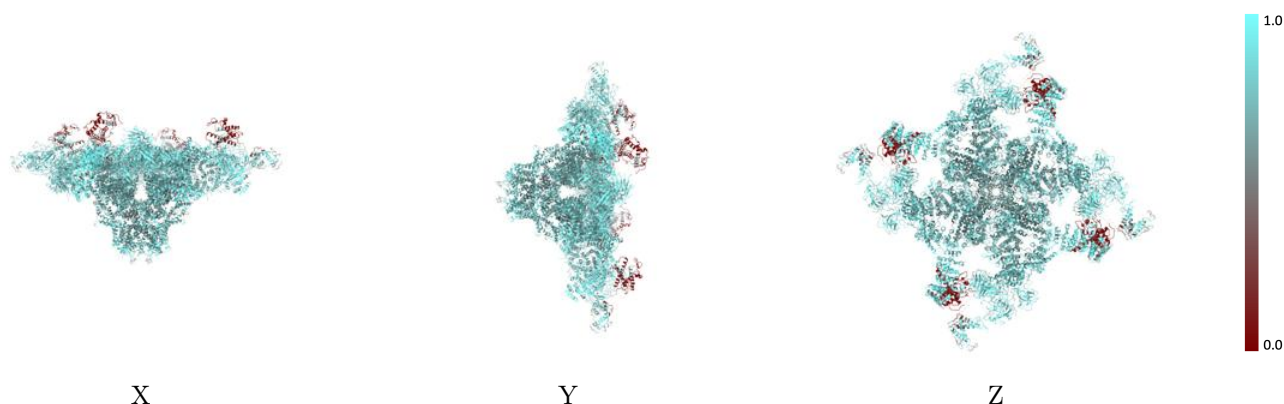
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



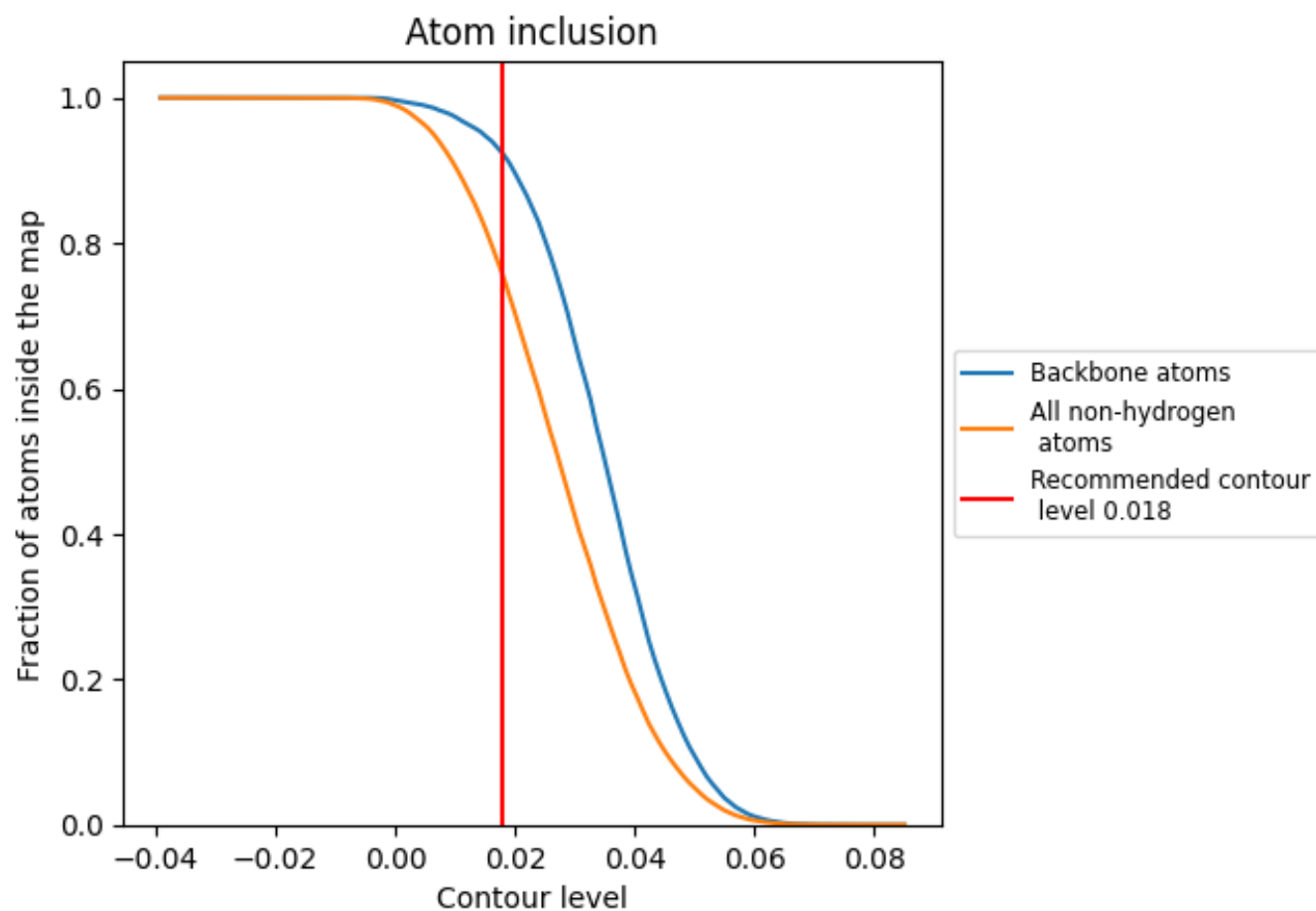
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 76% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7551	<div><div></div></div> 0.2490
A	<div><div></div></div> 0.8166	<div><div></div></div> 0.2650
B	<div><div></div></div> 0.7531	<div><div></div></div> 0.2480
C	<div><div></div></div> 0.8191	<div><div></div></div> 0.2650
D	<div><div></div></div> 0.7533	<div><div></div></div> 0.2490
E	<div><div></div></div> 0.8166	<div><div></div></div> 0.2650
F	<div><div></div></div> 0.7531	<div><div></div></div> 0.2480
G	<div><div></div></div> 0.8141	<div><div></div></div> 0.2650
H	<div><div></div></div> 0.7532	<div><div></div></div> 0.2480

1.0

0.0

<0.0