



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 01:48 AM UTC

PDB ID : 5GOA / pdb_00005goa
EMDB ID : EMD-9529
Title : Cryo-EM structure of RyR2 in open state
Authors : Peng, W.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-26
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

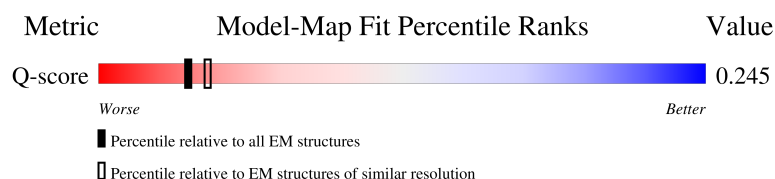
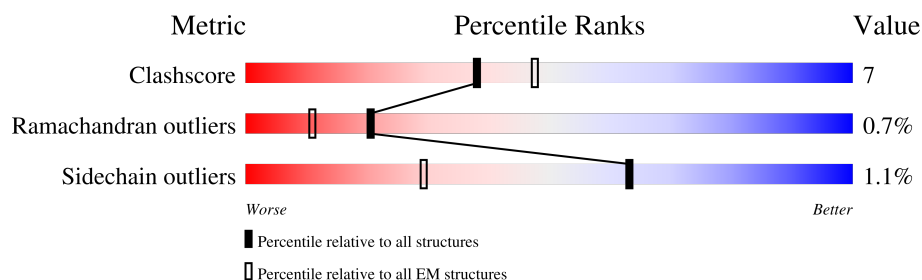
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

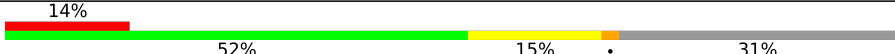
The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	A	4968	
1	B	4968	
1	C	4968	
1	D	4968	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105072 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	B	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	C	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	D	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		

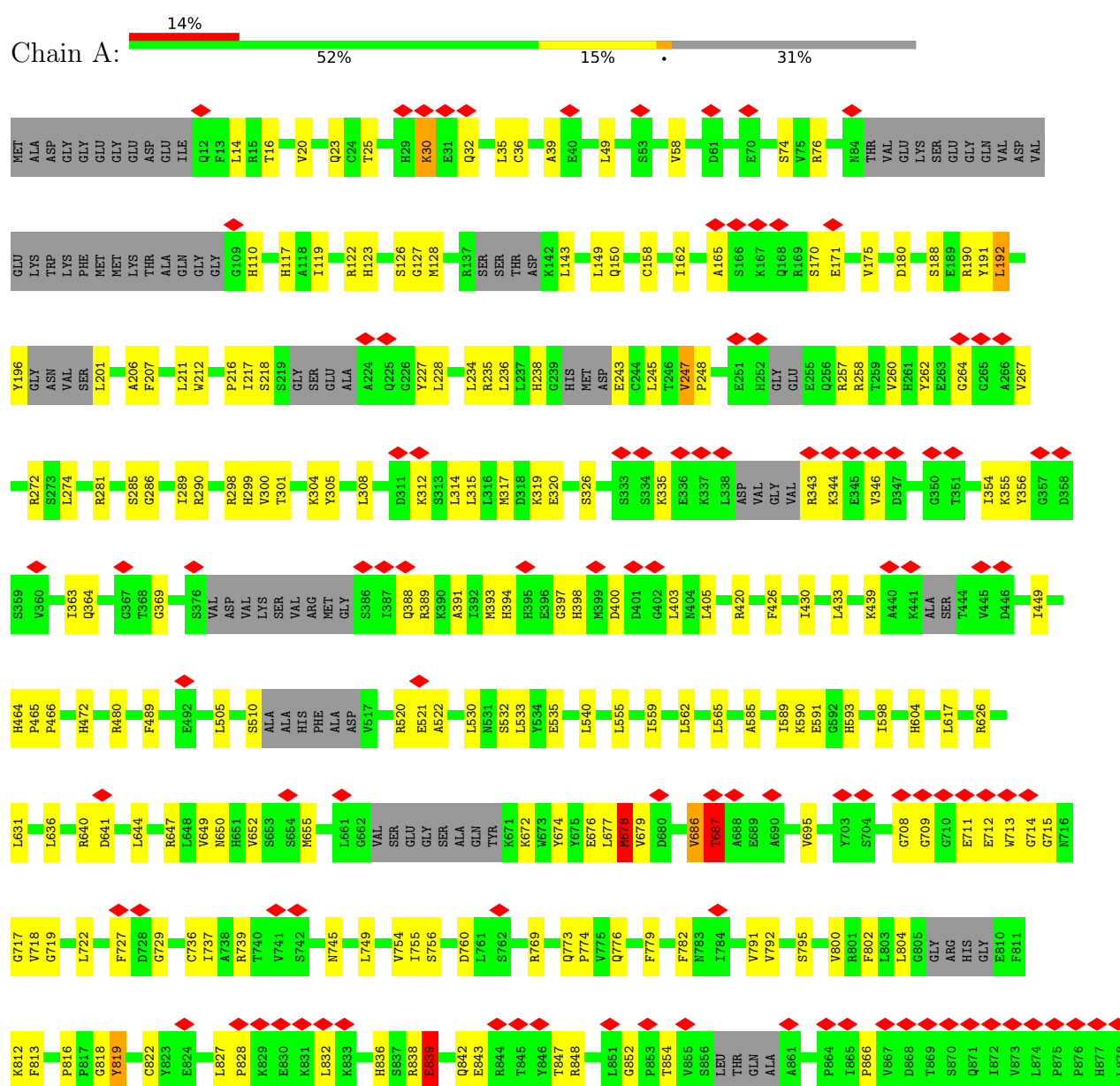
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots [i](#)

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

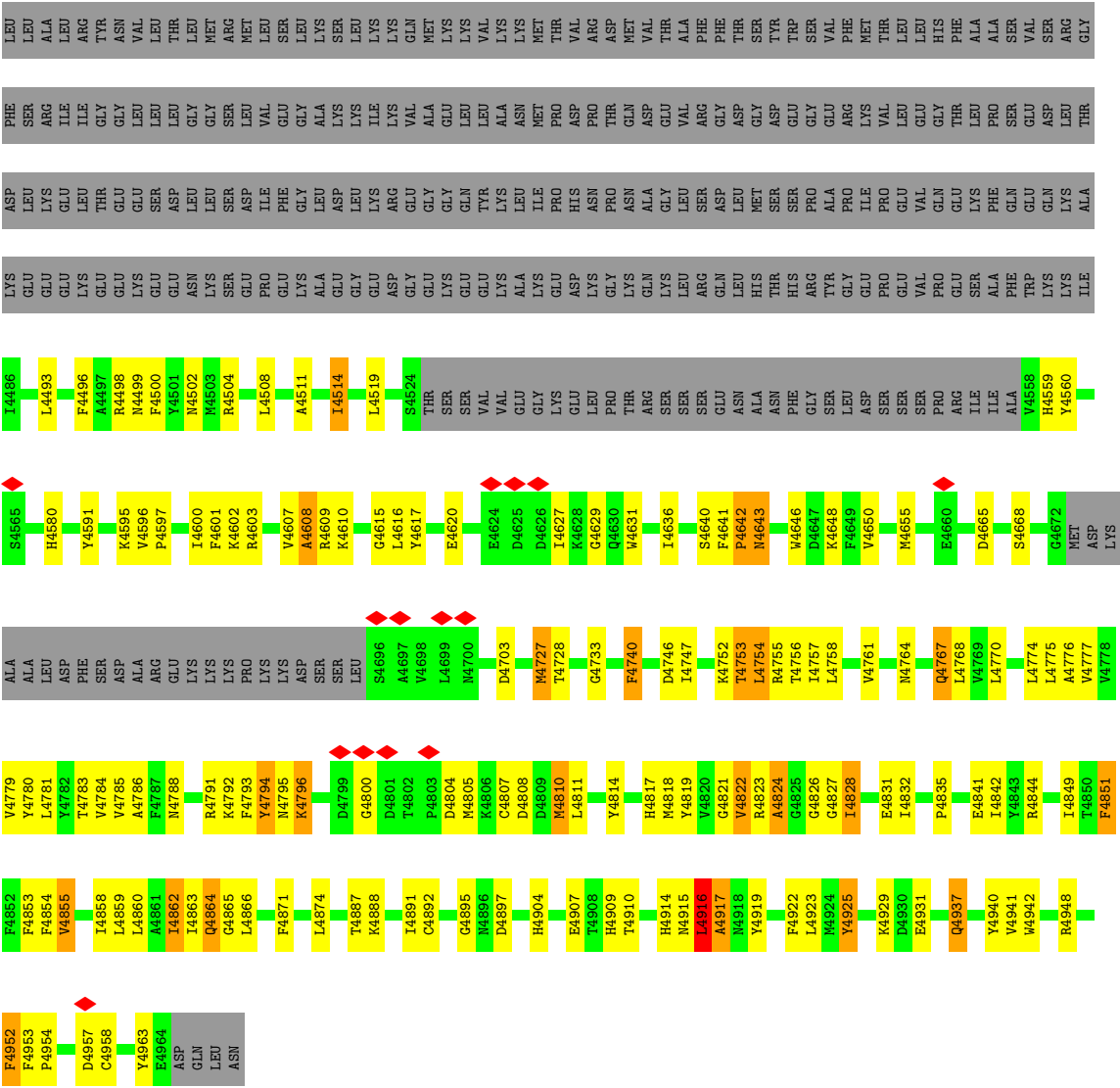
• Molecule 1: RyR2



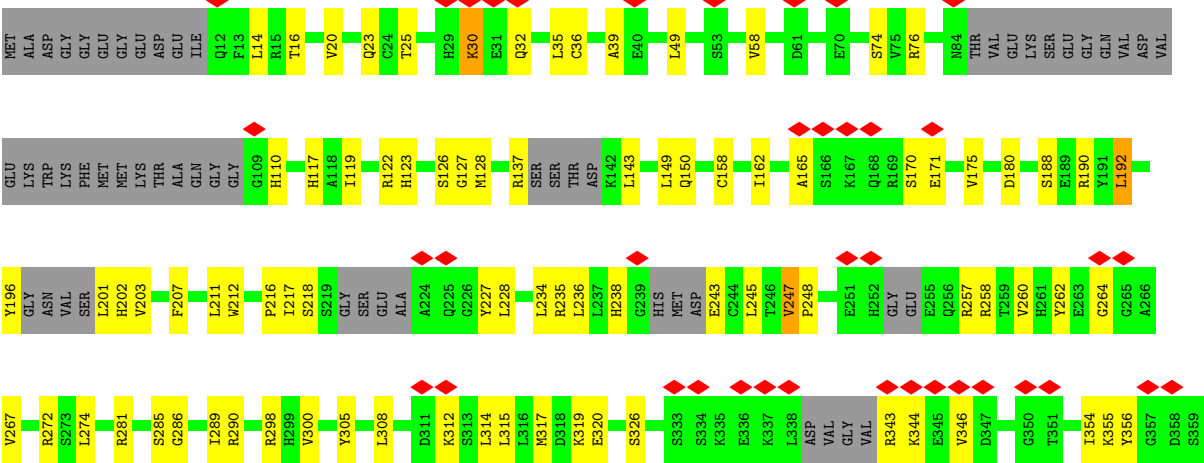
ALA	THR	E1763	V1664	Q1581	M1487	ASP	GLY	SER	S1186	GLU	GLY	E879
ALA	LEU	S1764	A1666	P1584	V1488	ASP	HIS	PRO	G1187	R1084	ILE	R880
THR	LYS	S1767	A1665	ARG	C1489	ARG	LEU	CYS	S1188	F1085	GLN	I381
ALA	GLU	F1768	GLY	ASP	A1490	ASP	VAL	LEU	E1189	R1086	GLN	R882
ARG	PRO	V1769	GLU	TYR	L1586	TYR	PRO	LYS	L1190	F1088	VAL	I389
CYS	CYS	S1770	SER	ASP	H1587	ASP	ARG	VAL	E1193	R1089	LYS	L292
THR	ALA	I1770	MET	TYR	V1588	TYR	VAL	T1286	L1193	A1090	ASN	W893
LYS	SER	I1771	SER	ASP	Q1589	ASP	ASP	Q1293	D1194	E1091	R1027	W894
GLU	ASP	D1681	GLY	LEU	F1590	LEU	LYS	N1294	F1196	Y1094	L1032	M895
ASP	SER	I1689	GLN	THR	H1593	THR	LYS	M1300	D1197	A1098	V1033	M896
ARG	ARG	N1690	GLY	SER	T1425	SER	ALA	R1303	E1104	E1095	E957	K897
LEU	LEU	N1691	GLY	THR	R1431	THR	THR	L1197	F1105	H956	GLU	I898
GLU	GLU	K1692	GLY	THR	I1432	THR	THR	E1106	E1105	E955	LYS	E999
GLN	GLN	Y1693	GLY	PRO	F1433	PRO	PRO	G1121	E1106	D954	VAL	L900
GLU	PRO	M1694	GLU	PHE	F1434	PHE	PHE	E1132	E1132	E956	LYS	G901
ALA	ALA	P1695	ASN	ASN	C1310	ASN	ASN	R1133	E1132	E957	LYS	W902
GLU	GLU	R1699	GLY	ALA	E1309	ALA	GLY	E1133	E1132	E957	ASN	Q903
GLU	GLU	Y1703	GLY	GLN	E1310	GLN	GLY	E1133	E1132	E957	ASN	Y904
LYS	SER	V1709	GLY	HIS	E1311	HIS	VAL	E1133	E1132	E957	ASN	G905
GLY	GLY	Q1800	ASP	ASP	V1511	ASP	PHE	E1133	E1132	E957	ASN	P906
LYS	LYS	E1801	ALA	ALA	W1440	ALA	TYR	E1133	E1132	E957	ASN	V907
ARG	ARG	G1802	SER	SER	W1441	SER	ALA	E1133	E1132	E957	ASN	R908
PRO	PRO	S1803	GLN	GLN	W1442	GLN	GLY	E1133	E1132	E957	ASN	D909
LYS	LYS	L1804	GLN	GLN	W1443	GLN	ILE	E1133	E1132	E957	ASN	D910
GLY	GLY	D1808	GLY	GLY	W1444	GLY	GLY	E1133	E1132	E957	ASN	N911
CYS	CYS	V1810	GLY	GLY	W1445	GLY	GLY	E1133	E1132	E957	ASN	K912
CYS	CYS	F1816	GLY	GLY	D1449	GLY	GLY	E1133	E1132	E957	ASN	R913
GLU	GLU	L1817	GLY	GLY	A1456	GLY	GLY	E1133	E1132	E957	ASN	Q914
GLU	GLU	F1818	GLY	GLY	L1459	GLY	GLY	E1133	E1132	E957	ASN	H915
ILE	ILE	V1819	GLY	GLY	ASP	GLY	GLY	E1133	E1132	E957	ASN	L318
ARG	ARG	L1821	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	V919
ASP	ASP	I1823	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	E920
GLN	GLN	H1833	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	F921
LEU	LEU	F1834	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	S922
LEU	LEU	H1835	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	K923
LEU	LEU	N1836	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	L924
LEU	LEU	E1847	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	P925
THR	THR	P1848	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	E926
ASN	ASN	S1849	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	Q927
LEU	LEU	VAL	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	N930
LEU	LEU	PHE	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	Y931
GLU	GLU	LYS	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	N932
VAL	VAL	GLY	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	L933
ASN	ASN	GLY	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	Q934
GLN	GLN	ALA	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	M935
LEU	LEU	PRO	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	S936
ASN	ASN	GLY	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	L937
GLU	GLU	GLY	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	E938
GLU	GLU	GLY	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	T939
SER	SER	ASP	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	K941
LEU	LEU	L2024	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	T942
LEU	LEU	Y2039	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	L943
LEU	LEU	GLY	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	L944
LEU	LEU	GLY	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	A945
LEU	LEU	GLY	GLY	GLY	ARG	GLY	GLY	E1133	E1132	E957	ASN	L946

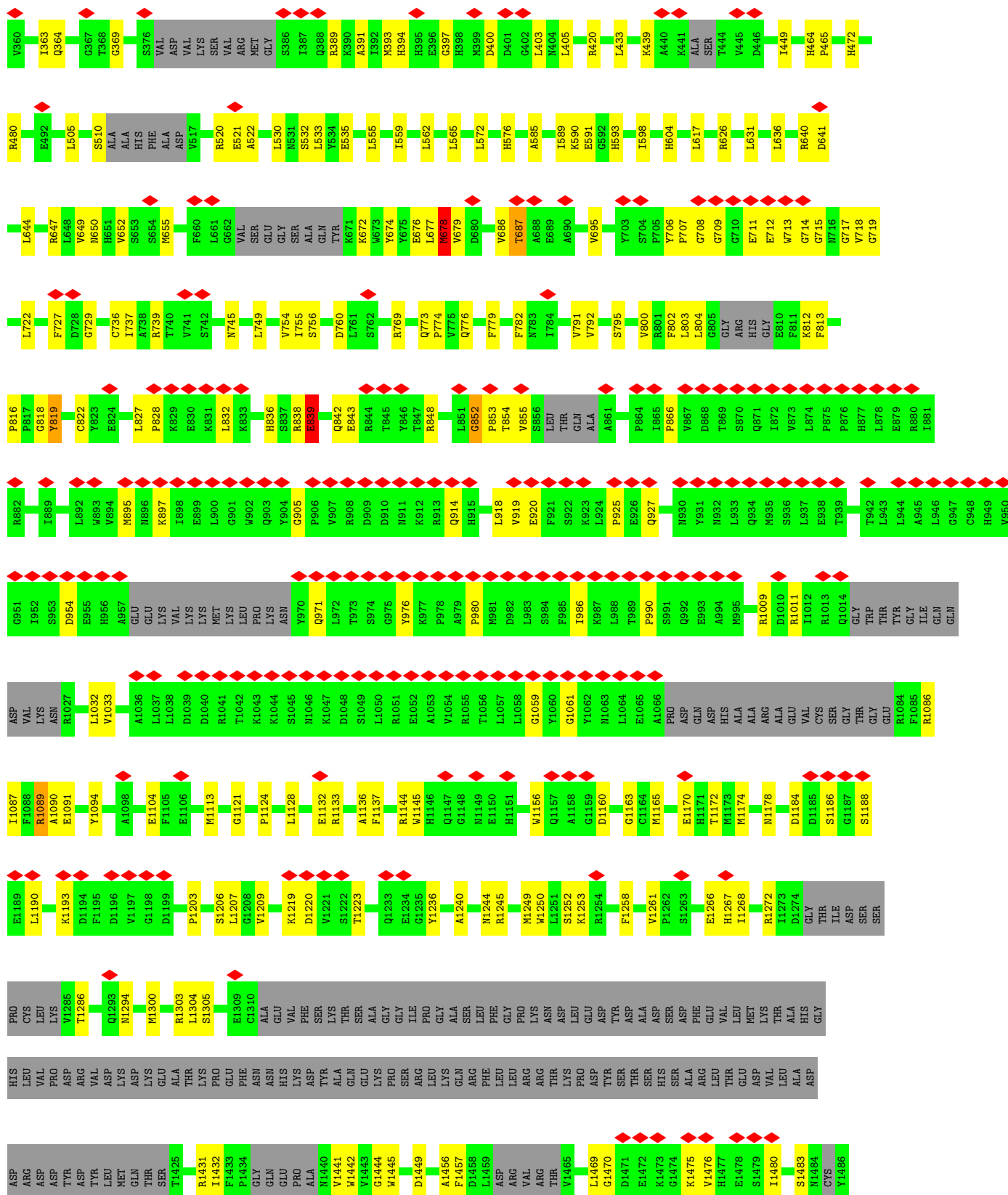


E4077	T4078	V3980	W3891	M3798	ASP	ARG	PRO	GLY	ASP	GLY	ARG	GLU	ASP	TYR	GLN	SER	TYR	ASN	THR	E3125
G4181	V3982	V3981	Y3892	Q3799	ASP	MET	GLU	ASP	ASP	ILE	ASP	ILE	ASN	TYR	PRO	MET	TYR	ASN	THR	D3126
G4182	W3885	M3982	Y3893	S3800	GLY	ALA	VAL	LYS	ASP	ILE	ALA	ASN	ASP	SER	TYR	MET	SER	GLY	THR	E3067
E4183	V4086	L3983	K3896	S3802	GLU	LEU	THR	VAL	GLU	LEU	LEU	MET	ASN	SER	ALA	ARG	SER	LYS	THR	Q3128
E4184	E3888	E3889	T3899	L3804	GLU	TYR	ARG	GLU	GLU	ILE	TYR	SER	PHE	TRP	PHE	TRP	SER	SER	SER	V3129
E4185	G3989	G3990	Y3900	D3805	VAL	ASN	ARG	VAL	VAL	ALA	ASN	PHE	VAL	TRP	PRO	TRP	ARG	GLU	GLU	S3130
E4186	Q3904	E4090	Q3904	R3811	GLY	LEU	ASP	ASP	ASP	ILE	R3613	THR	ILE	GLY	LEU	HIS	ARG	ALA	ALA	C3131
E4187	N3906	N3905	R3905	R3812	GLY	GLY	ASP	ILE	ASP	ASN	R3614	THR	ASN	PRO	ILE	GLY	PRO	ALA	ALA	C3132
E4188	F3907	F3907	K3814	K3813	VAL	GLY	Q3729	ALA	Q3729	THR	Y3625	THR	ARG	GLU	ARG	PRO	GLU	LEU	LEU	R3133
E4189	A3910	A3910	A3914	A3914	ALA	VAL	A3730	VAL	A3730	LYS	Y3625	THR	ARG	ASN	PHE	ASN	ASN	LEU	LEU	T3134
E4190	D4002	D4002	D4002	GLU	GLY	GLY	R3732	VAL	R3732	SER	H3635	THR	VAL	ASN	THR	ASN	ASN	LEU	LEU	T3135
E4191	M4003	M4003	M4003	GLY	GLY	GLY	H3733	PHE	H3733	LYS	H3635	THR	VAL	PRO	ASP	PRO	PRO	PRO	THR	T3136
E4192	E4006	E4006	E4006	LEU	LEU	LEU	D3734	THR	D3734	ARG	I3642	THR	ASN	ARG	LEU	ARG	ASN	ASN	THR	S3137
E4193	F4017	F4017	F4017	GLY	GLY	GLY	Q3743	THR	Q3743	ARG	I3642	THR	ASN	ARG	LEU	ARG	ASN	ASN	THR	S3137
E4194	D4019	D4019	D4019	LYS	VAL	VAL	I3745	THR	I3745	ARG	I3642	THR	ASN	ARG	LEU	ARG	ASN	ASN	THR	S3137
E4195	F4021	F4021	F4021	LEU	LEU	LEU	S3748	THR	S3748	ARG	I3642	THR	ASN	ARG	LEU	ARG	ASN	ASN	THR	S3137
E4196	L4022	L4022	L4022	GLN	GLN	GLN	E3751	SER	E3751	LEU	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4200	V4011	V4011	V4011	VAL	VAL	VAL	M3755	GLY	M3755	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4201	T4014	T4014	T4014	GLU	GLU	GLU	T3759	GLY	T3759	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4202	L4015	L4015	L4015	GLU	GLU	GLU	L3760	GLY	L3760	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4203	K4016	K4016	K4016	GLY	GLY	GLY	G3763	GLY	G3763	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4204	F4018	F4018	F4018	GLY	GLY	GLY	L3766	GLY	L3766	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4205	M4020	M4020	M4020	LYS	VAL	VAL	L3767	GLY	L3767	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4206	F4021	F4021	F4021	LEU	LEU	LEU	N3768	GLY	N3768	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4207	L4134	L4134	L4134	GLN	GLN	GLN	G3770	GLY	G3770	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3144
E4208	G4135	G4135	G4135	VAL	VAL	VAL	N3771	GLY	N3771	GLY	I3665	THR	THR	THR	GLY	THR	ASN	ASN	THR	S3



• Molecule 1: RyR2

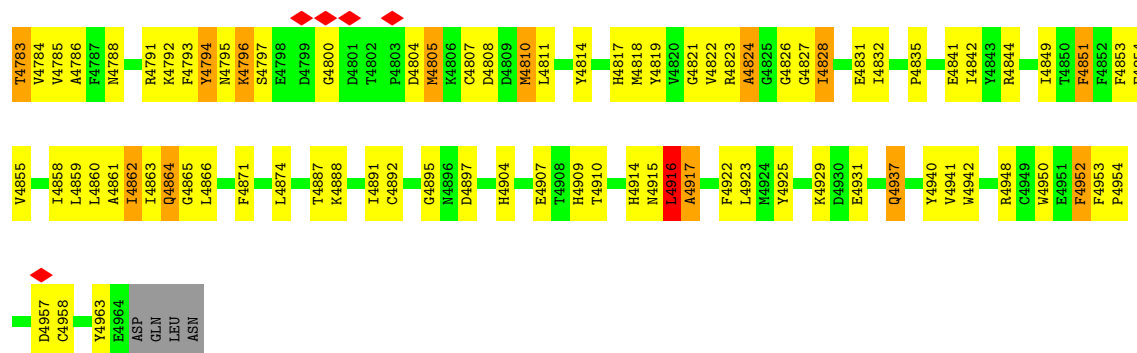




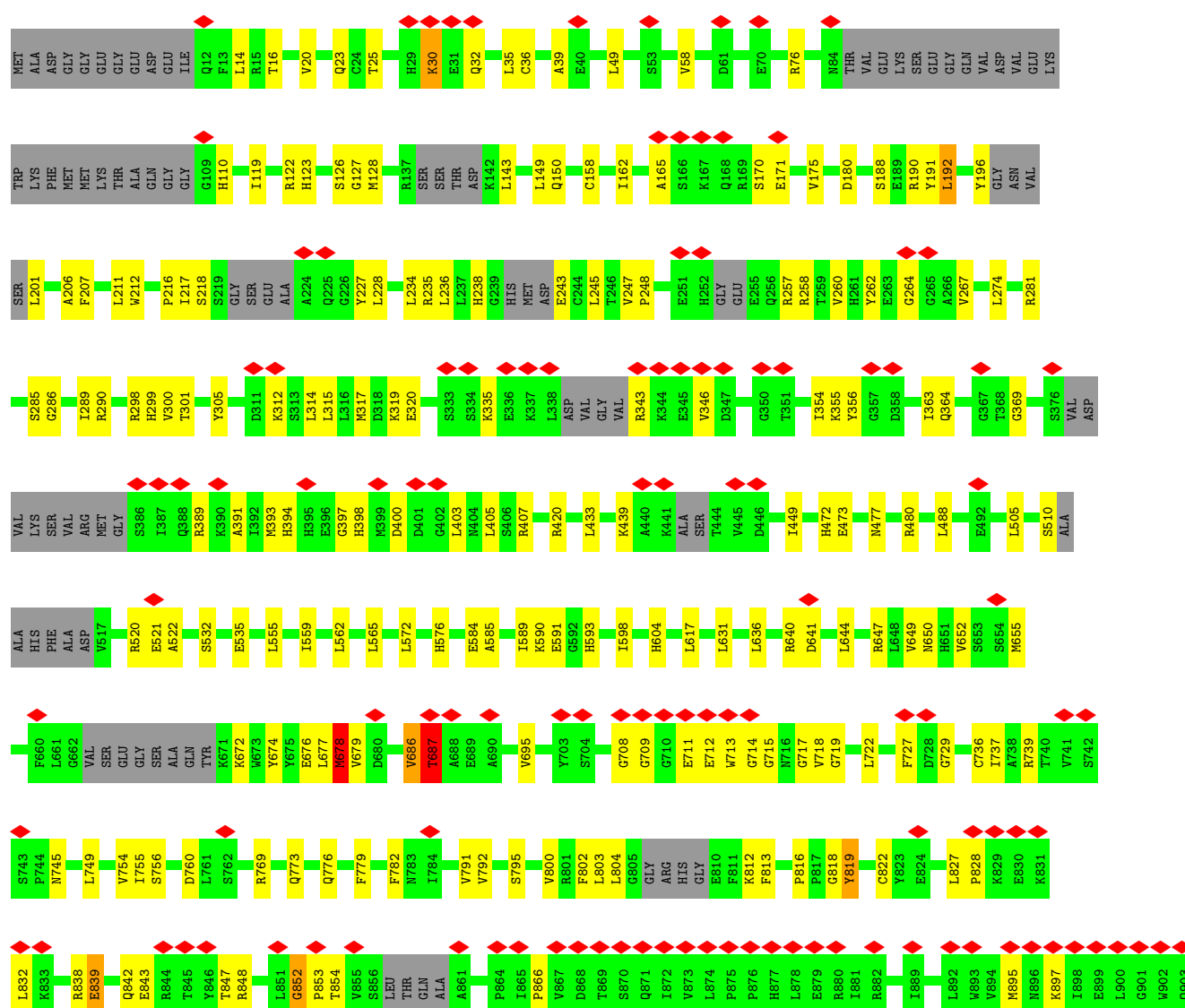








• Molecule 1: RyR2





LEU	ASN	PHE	LYS	ASP	LYS	SER	CYS	PRO	CYS	PRO	GLU	GLU	ILE	ARG	ASP	GLN	LEU	D1999	T2239	D2013	GLU	ASP	SER	LEU	ASP	GLY	ASN	SER	ASP	L2024	V2039	LEU	LYS	LYS	GLN	ALA	GLU	LYS	VAL	GLU	SER	ASP	SER	LYS	THR	LYS	THR	PHE	SER	T2058	A2071	Q2072	F2073						
S2074	V2075	I2076	E2077	D2078	P2079	E2080	L2081	R2083	A2084	M2085	L2103	I2109	L2121	A2122	S2123	L2130	V2133	ARG	MET	GLY	E2138	M2143	D2149	F2156	M2163	L2166	M2173	E2174	V2175	G2181	GLY	GLY	GLU	SER	LYS	GLN	ALA	GLU	LYS	LEU	VAL	GLU	SER	ASP	SER	LYS	THR	LYS	THR	PHE	SER	L2191	K2192	M2193	V2194	F2204			
M2211	K2212	K2213	D2217	L2222	S2226	S2227	V2228	GLY	ALA	SER	PRO	ALA	ALA	PRO	ARG	GLY	SER	T2239	P2240	L2241	D2242	V2243	L2254	A2255	L2256	L2258	E2259	E2260	P2261	D2262	L2263	E2264	R2268	C2273	G2274	L2275	GLN	SER	CYS	GLN	LYS	MET	LEU	VAL	SER	LYS	THR	LYS	TYR	PRO	ASP	ILE	GLY						
TRP	ASN	P2293	D2301	R2304	F2305	A2306	L2326	R2327	R2328	E2330	CYS	PHE	GLY	PRO	ALA	ALA	LEU	ARG	SER	GLY	GLU	GLY	G2343	M2348	E2349	L2354	ALA	GLU	ASP	PRO	ARG	ASP	GLY	PRO	THR	SER	GLY	SER	LYS	MET	PRO	ASP	PRO	THR	GLU	GLY	GLU	ASP	ASP										
THR	ILE	HIS	MET	G2386	M2390	C2403	A2404	PRO	GLU	MET	HIS	ILE	ALA	ALA	LYS	GLY	E2416	S2426	L2427	ILE	PRO	LEU	G2431	G2435	V2436	L2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	ALA	F2461	C2462	P2463	D2464								
H2465	M2469	R2475	V2476	Y2477	GLY	ILE	GLU	V2481	Q2482	D2483	L2489	VAL	G2492	P2495	D2496	L2503	ASP	THR	ALA	LEU	SER	ALA	T2511	R2519	Y2520	L2521	C2522	T2523	L2528	L2529	THR	ARG	CYS	ALA	F2534	L2535	F2536	T2552	V2553	TYR	ARG	LEU	SER	K2558	A2565	D2568	S2569												
I2570	E2571	V2572	C2573	L2574	L2575	S2576	ILE	CYS	GLY	GLN	LEU	P2583	S2584	Q2587	R2591	V2597	P2598	L2599	L2600	N2601	HIS	ALA	K2605	M2606	P2607	H2614	C2618	C2623	L2624	P2625	G2626	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635	E2636	E2637	K2644	I2649	F2650	D2651	A2652	L2653	SER										
GLN	LYS	LYS	Y2658	E2659	Q2660	E2661	L2662	L2665	A2666	L2667	P2668	C2669	V2673	A2674	G2675	A2676	L2677	P2678	P2679	ASP	TYR	MET	GLU	SER	ASN	VAL	THR	ARG	ILE	SER	GLN	THR	SER	GLN	SER	VAL	SER	LYS	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717				
L2718	E2719	Y2720	F2721	L2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	D2730	H2731	K2732	W2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	G2741	W2742	I2743	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	M2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	E2768	E2769	K2770	I2771	Y2772	R2773	W2774	P2775	I2776	K2777	
E2778	S2779	L2780	K2781	T2782	M2783	L2784	A2785	G2786	G2787	W2788	R2789	I2790	E2791	L2792	T2793	A2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	V2816	D2817	A2818	H2820	G2821	Y2822	S2823	F2824	R2825	A2826	L2827	D2828	M2829	S2830	N2831	V2832	T2833	L2834	S2835	D2836	D2837		
L2838	H2839	A2840	M2841	A2842	E2843	M2844	M2845	A2846	E2847	M2848	Y2849	H2850	N2851	L2852	W2853	K2854	A2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	M2868	H2869	P2870	L2871	L2872	V2873	P2874	D2875	D2876	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897	
Q2898	I2899	N2900	G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	GLU	LEU	THR	ASN	HIS	ARG	ILE	GLU	LYS	ARG	L2982	F2983	L2984	S2985	A2986	A2987	S2988	P2989	F2990	L2991	C2992	S2993	G2994	G2995	H2996	A2997	S2998	N2999	K3000	E3001	K3002	E3003	K3004	V3005	THR	SER	LEU	F3009	C3010	K3011	L3012	G3013	V3014	L3015	V3016	K3017

E4006	A3914	R3731	H5635	VAL	SER	SER	VAL	THR	ASN	LEU	L3138	Q3078	H3018
V4011	V3917	L3732	I3642	LEU	LEU	LEU	PHE	THR	PRO	PRO	Y3139	G3079	R3019
T4014	N3919	H3733	I3645	HIS	ASP	ASP	HIS	LEU	ARG	THR	A3140	Q3080	I3020
L4015	T3920	D3734	L3648	LEU	THR	THR	LEU	PRO	ALA	VAL	L3141	F3081	S3021
F4017	T3921	R3735	P3648	GLN	ASP	ASP	GLU	LEU	MET	GLU	T3143	HIS	I3022
F4018	T3922	A3736	GLY	LYS	VAL	VAL	VAL	MET	CYS	VAL	S3144	ARG	F3023
D4019	E3923	A3737	ALA	THR	ASP	ASP	GLN	LEU	ALA	PRO	LYS	ASN	G3024
M4020	Y3924	M3740	VAL	THR	ASP	ASP	GLN	LEU	ALA	THR	ILE	ASN	H3025
F4021	I3925	V3741	PRO	MET	ILE	ILE	GLU	LEU	ASN	PRO	TYR	PRO	D3026
L4022	Q3926	L3742	ARG	ARG	ARG	ARG	ARG	LYS	ASN	PRO	GLY	GLY	A3027
S4030	T3930	T3744	GLU	GLN	GLY	GLY	GLY	LEU	SER	SER	E3149	VAL	T3028
D4031	G3931	I3745	ASP	THR	SER	SER	ASP	GLU	HIS	LEU	E3150	THR	ILE
T4032	N3932	S3748	GLY	THR	ILE	ILE	LYS	VAL	MET	LYS	R3151	GLN	VAL
D4039	Q3933	E3751	LYS	LEU	LEU	LEU	SER	THR	THR	MET	Q3152	ILE	ASN
S4045	L3936	L3755	R3661	VAL	GLN	GLN	VAL	GLU	LEU	GLU	S3154	TYR	CYS
K4046	S3939	M3755	L3665	GLU	GLY	GLY	ASP	GLU	LEU	GLU	A3155	T3098	H3035
A4052	R3940	T3759	L3670	HIS	LEU	LEU	THR	ASP	GLY	ILE	L3156	T3099	I3036
H4056	L3941	L3760	L3668	GLN	GLU	GLU	ASP	LEU	ILE	VAL	G3157	T3100	L3037
T4060	V3945	G3763	L3671	SER	PRO	PRO	ASP	LYS	LYS	ALA	E3158	A3101	G3038
Q4061	V3951	T3766	R3674	LYS	ALA	ALA	THR	PHE	ILE	THR	L3160	L3102	Q3039
S4062	F3952	N3768	T3675	ALA	LEU	LEU	ARG	VAL	ILE	SER	A3161	L3103	T3040
E4063	A3953	G3769	A3676	TRP	GLN	GLN	TRP	SER	ASN	GLY	A3162	M3105	L3041
L4067	H3954	Q3770	L3677	HIS	MET	MET	ALA	LYS	LEU	ARG	F3163	L3106	D3042
L4068	M3955	S3772	E3684	LYS	ALA	LEU	LEU	THR	ILE	THR	A3164	S3107	A3043
A4071	L3959	V3774	E3685	SER	LYS	LYS	ARG	PHE	GLU	PRO	G3165	S3108	T3045
E4072	Q3965	L3779	L3688	GLN	LEU	LEU	LEU	ARG	GLY	HIS	A3166	L3109	V3046
T4073	L3968	E3780	Y3689	ARG	PRO	PRO	ILE	GLU	TRP	VAL	PHE	F3110	H3047
E4075	E3971	Y3781	K3696	LYS	ASN	ASN	GLU	GLN	LYS	VAL	A3170	E3111	K3048
N4076	L3972	L3782	S3699	ALA	THR	THR	LEU	ASN	ARG	VAL	F3171	H3112	T3049
E4077	D3974	K3783	S3700	VAL	GLU	GLU	ASP	PHE	LEU	LEU	L3172	I3113	G3050
T4078	L3975	E3784	HIS	VAL	ASP	ASP	ILE	VAL	ALA	PRO	E3173	G3114	L3051
V4085	M3982	L3794	ASP	ALA	THR	THR	CYS	VAL	VAL	MEI	T3174	Q3115	E3052
R4086	L3983	L3797	GLU	CYS	SER	SER	ALA	GLN	PHE	LEU	H3175	H3116	S3053
R4087	Y3892	M3798	ASP	PHE	ASP	ASP	PRO	GLU	SER	CYS	L3176	Q3117	V3054
HIS	E3988	Q3799	ASP	ARG	PRO	PRO	GLY	ASP	GLN	TRP	L3177	F3118	K3055
E4090	G3989	C3801	ASP	ALA	GLU	GLU	ILE	ILE	ILE	TYR	D3177	GLY	SER
T4095	N3990	S3802	GLY	PRO	LYS	LYS	GLN	THR	THR	VAL	K3178	ALA	LEU
V4101	V3991	V3803	VAL	ASN	VAL	VAL	ILE	ALA	ASN	TRP	H3179	ASP	ARG
L4102	Q3992	L3804	GLU	THR	ARG	ARG	ALA	PHE	LYS	VAL	N3180	LEU	ALA
M4110	K3998	D3805	VAL	ASN	VAL	VAL	ALA	LEU	LYS	GLU	I3181	ILE	F3061
N4112	D4002	R3811	L3806	LYS	ASP	ASP	LEU	ILE	PRO	HIS	T3182	E3124	L3062
D4113	M4003	Q3812	S3714	ASP	ILE	ILE	THR	THR	GLN	GLY	Y3183	D3126	D3063
		K3814	Q3729	ALA	ASN	ASN	THR	ARG	LEU	PRO	ILE	V3127	N3064
			A3730	ASN				LEU	LYS	GLU	ASN	Q3128	A3065
									THR	THR	ASN	Q3129	A3066
									LYS	LYS	LYS	V3129	E3067
									SER	SER	SER	C3131	D3068
									ARG	ARG	ARG	Y3132	E3070
									GLU	GLU	GLU	R3133	T3072
									ALA	ALA	ALA	I3134	K3073
									LEU	LEU	LEU	L3135	E3074
									ASN	ASN	ASN	T3136	K3075
												S3137	K3077



Frequency	Percentage
Daily	14%
Often	52%
Sometimes	16%
Never	31%

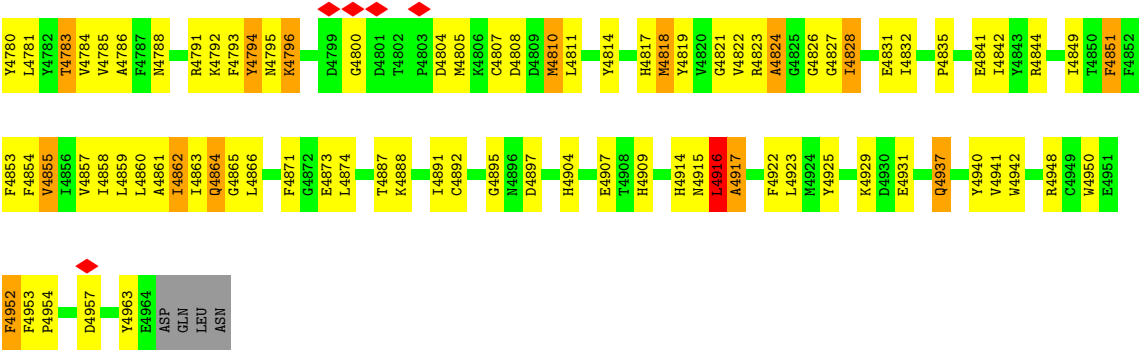












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133196	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: 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	1.41	210/26752 (0.8%)	1.10	88/36151 (0.2%)
1	B	1.41	203/26752 (0.8%)	1.10	89/36151 (0.2%)
1	C	1.41	202/26752 (0.8%)	1.10	88/36151 (0.2%)
1	D	1.41	210/26752 (0.8%)	1.11	93/36151 (0.3%)
All	All	1.41	825/107008 (0.8%)	1.10	358/144604 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23
1	B	0	23
1	C	0	24
1	D	0	23
All	All	0	93

The worst 5 of 825 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4849	ILE	C-O	16.70	1.44	1.24
1	D	4849	ILE	C-O	16.67	1.44	1.24
1	C	4849	ILE	C-O	15.45	1.44	1.24
1	B	4849	ILE	C-O	15.28	1.43	1.24
1	C	4150	TYR	C-O	-10.51	1.11	1.23

The worst 5 of 358 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1847	GLU	CA-C-N	12.00	134.84	119.84
1	B	1847	GLU	C-N-CA	12.00	134.84	119.84
1	A	1847	GLU	CA-C-N	11.99	134.83	119.84
1	A	1847	GLU	C-N-CA	11.99	134.83	119.84
1	D	1847	GLU	CA-C-N	11.96	134.79	119.84

There are no chirality outliers.

5 of 93 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	641	ASP	Peptide
1	A	686	VAL	Peptide
1	A	791	VAL	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	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	26267	0	24896	399	0
1	B	26267	0	24897	389	0
1	C	26267	0	24897	388	0
1	D	26267	0	24896	396	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	105072	0	99586	1519	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 7.

The worst 5 of 1519 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:D:4818:MET:CG	1:D:4818:MET:SD	2.01	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4818:MET:CG	1:C:4818:MET:SD	2.01	1.48
1:C:3700:CYS:CB	1:C:3700:CYS:SG	2.04	1.45
1:B:3700:CYS:CB	1:B:3700:CYS:SG	2.05	1.43
1:D:3700:CYS:SG	1:D:3700:CYS:CB	2.05	1.43

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3289/4968 (66%)	2988 (91%)	279 (8%)	22 (1%)	18	54
1	B	3289/4968 (66%)	2994 (91%)	273 (8%)	22 (1%)	18	54
1	C	3289/4968 (66%)	2988 (91%)	280 (8%)	21 (1%)	21	58
1	D	3289/4968 (66%)	2986 (91%)	282 (9%)	21 (1%)	21	58
All	All	13156/19872 (66%)	11956 (91%)	1114 (8%)	86 (1%)	20	54

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1737	THR
1	A	1756	SER
1	A	4071	ALA
1	B	1737	THR
1	B	1756	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2660/4355 (61%)	2629 (99%)	31 (1%)	63	73
1	B	2657/4355 (61%)	2631 (99%)	26 (1%)	68	75
1	C	2658/4355 (61%)	2629 (99%)	29 (1%)	65	73
1	D	2660/4355 (61%)	2629 (99%)	31 (1%)	63	73
All	All	10635/17420 (61%)	10518 (99%)	117 (1%)	63	73

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	192	LEU
1	D	4122	LEU
1	C	2293	PRO
1	D	4032	THR
1	D	1632	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 264 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1938	GLN
1	D	2387	ASN
1	D	4880	GLN
1	B	2090	HIS
1	B	1620	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

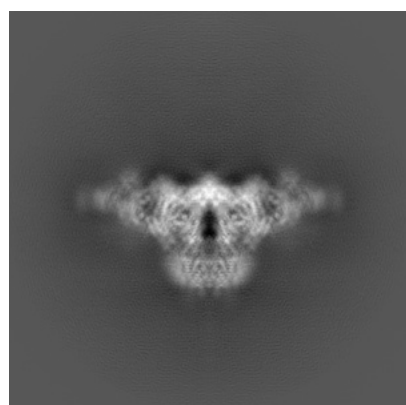
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9529. These allow visual inspection of the internal detail of the map and identification of artifacts.

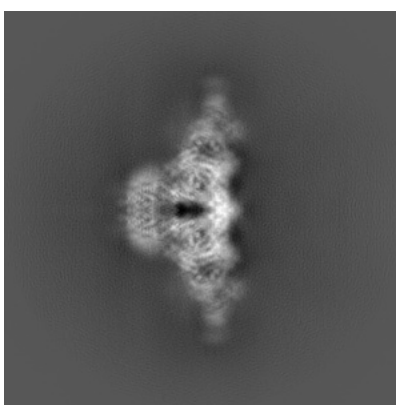
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

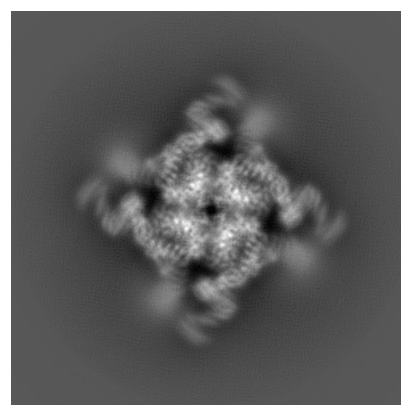
6.1.1 Primary map



X



Y

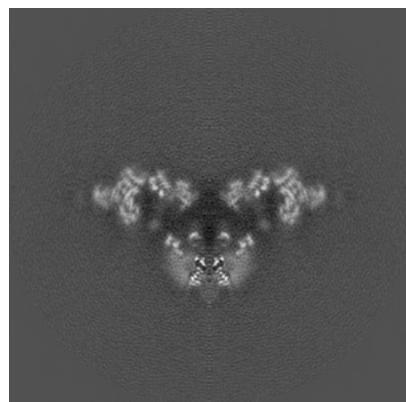


Z

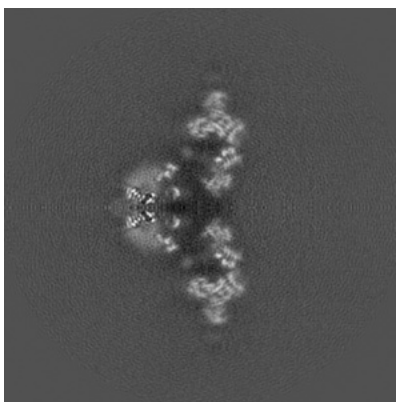
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

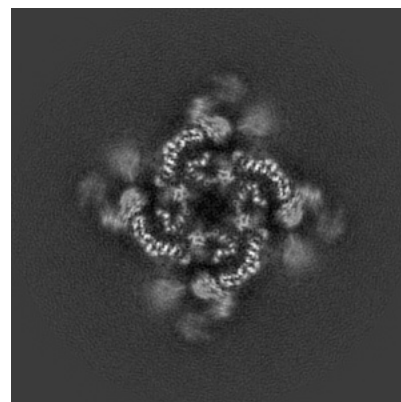
6.2.1 Primary map



X Index: 260



Y Index: 260

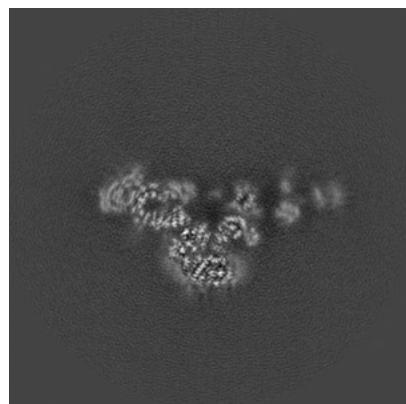


Z Index: 260

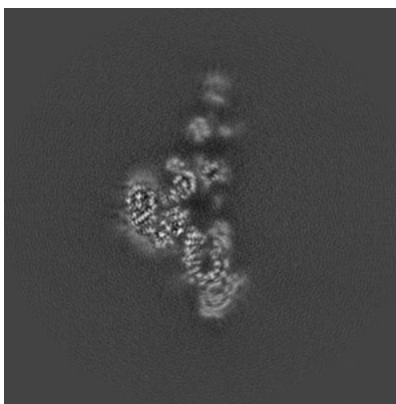
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

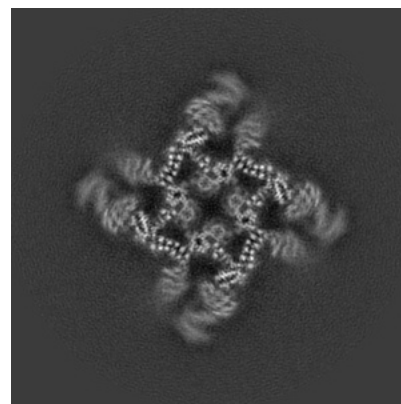
6.3.1 Primary map



X Index: 276



Y Index: 244

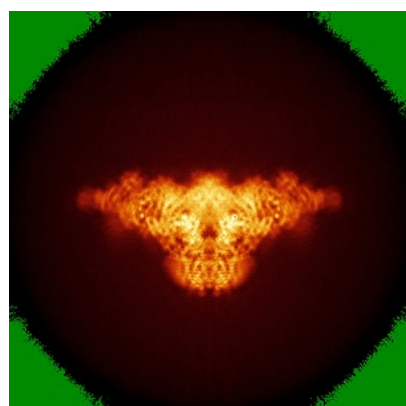


Z Index: 271

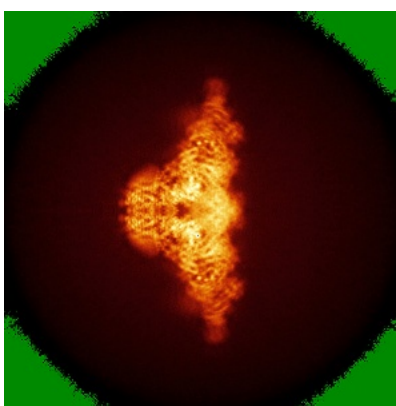
The images above show the largest variance slices of the map in three orthogonal directions.

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

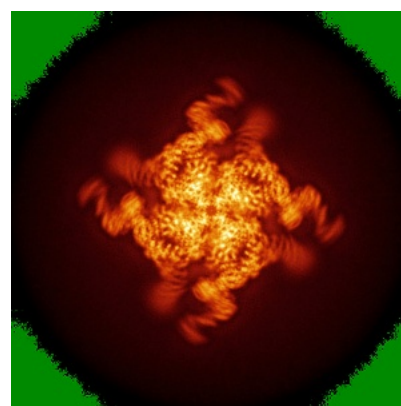
6.4.1 Primary map



X



Y

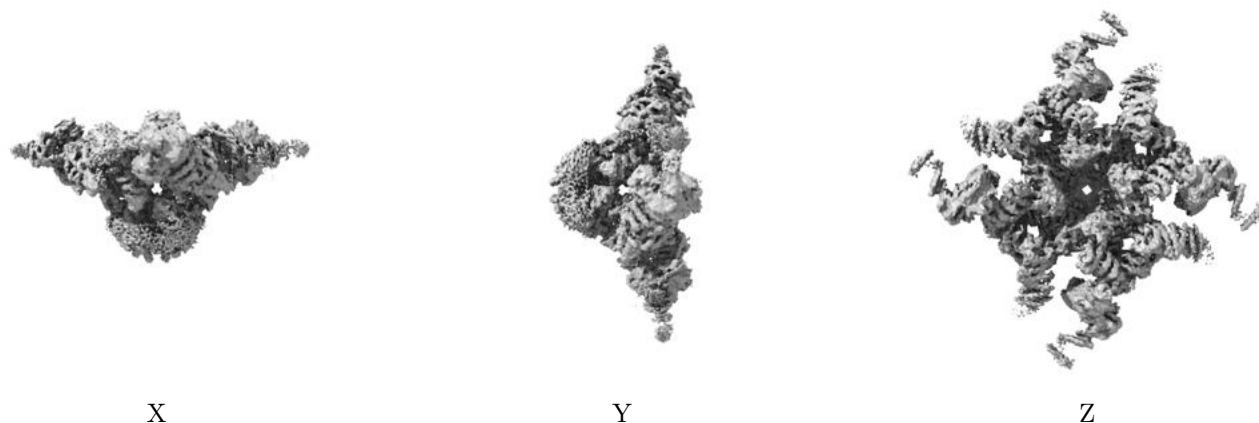


Z

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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

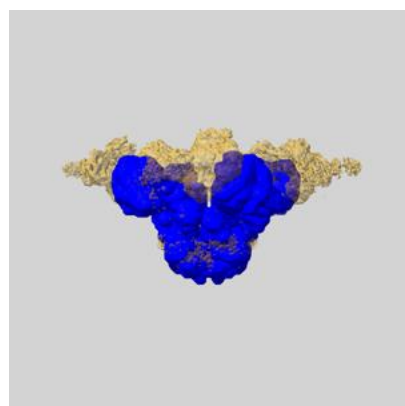
6.6 Mask visualisation [i](#)

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

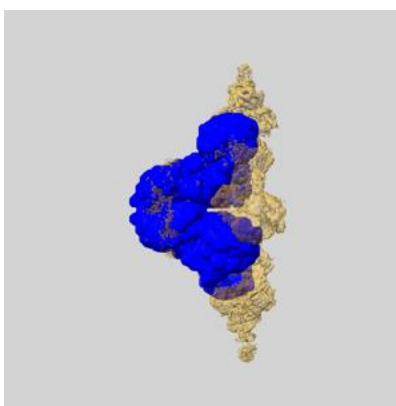
A mask typically either:

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

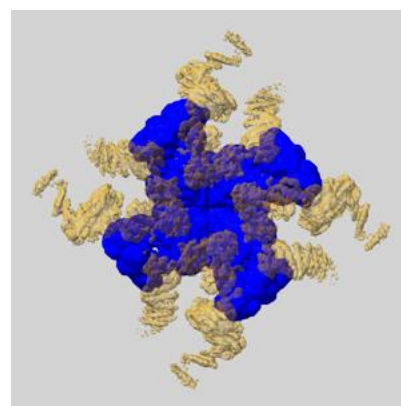
6.6.1 emd_9529_msk_1.map [i](#)



X



Y

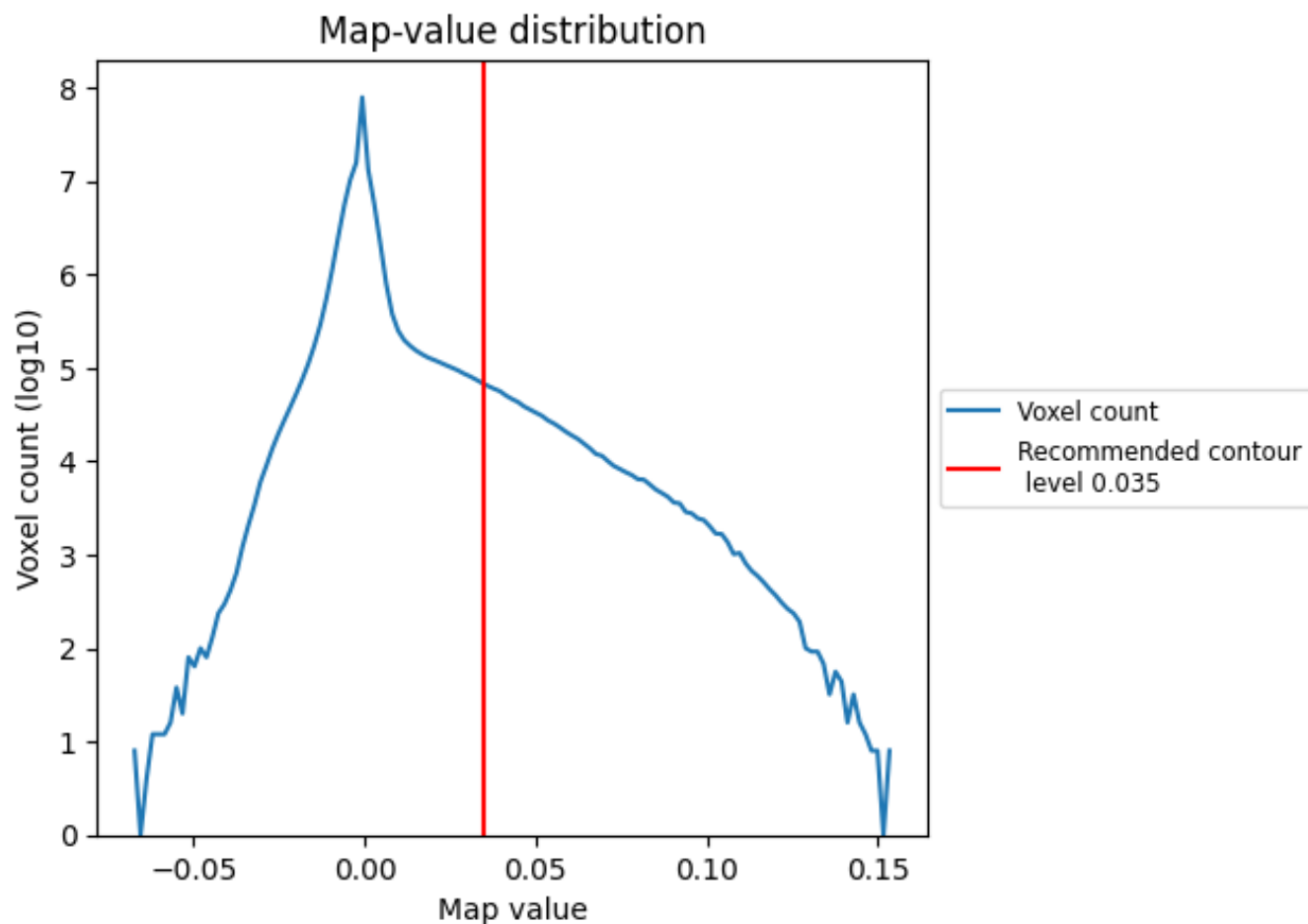


Z

7 Map analysis [i](#)

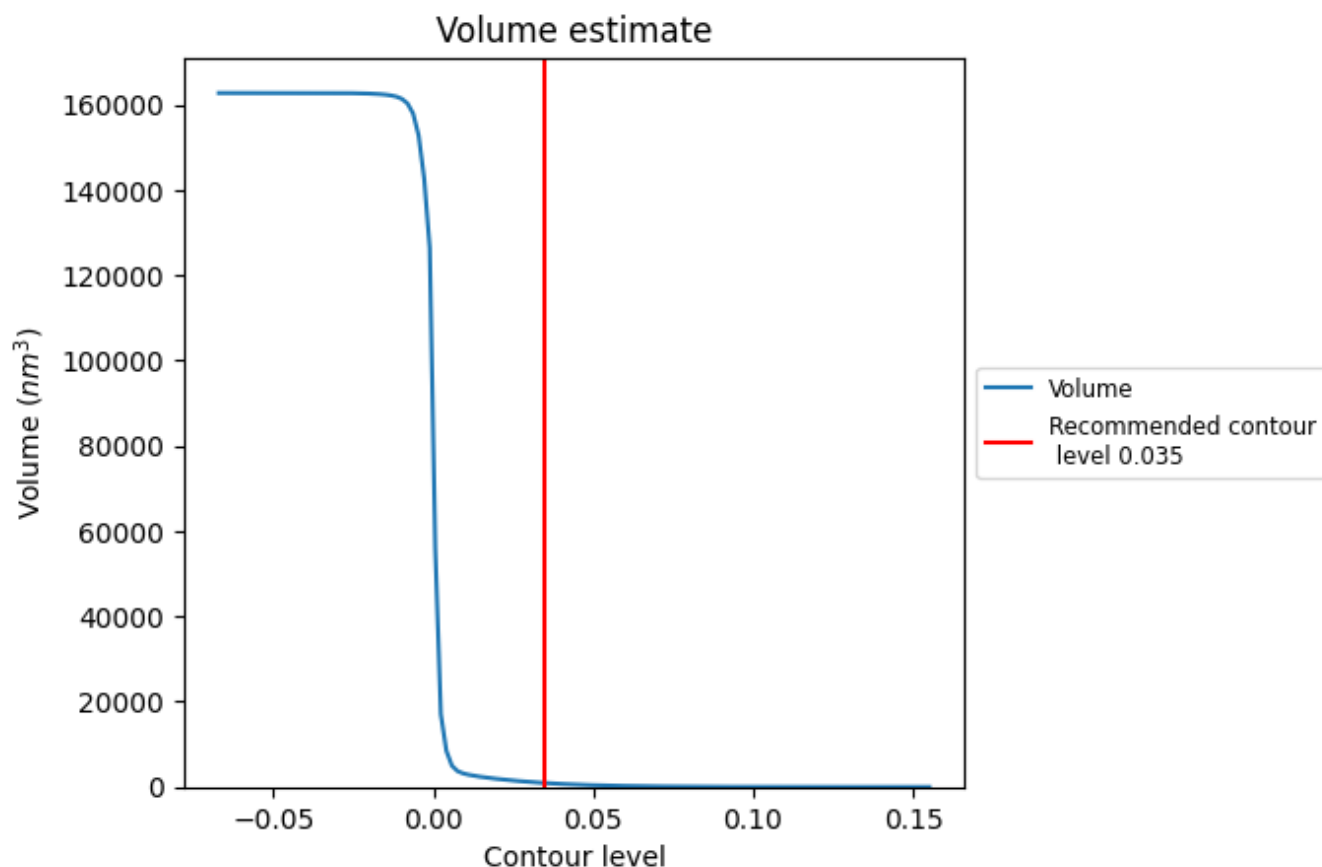
This section contains the results of statistical analysis of the map.

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.

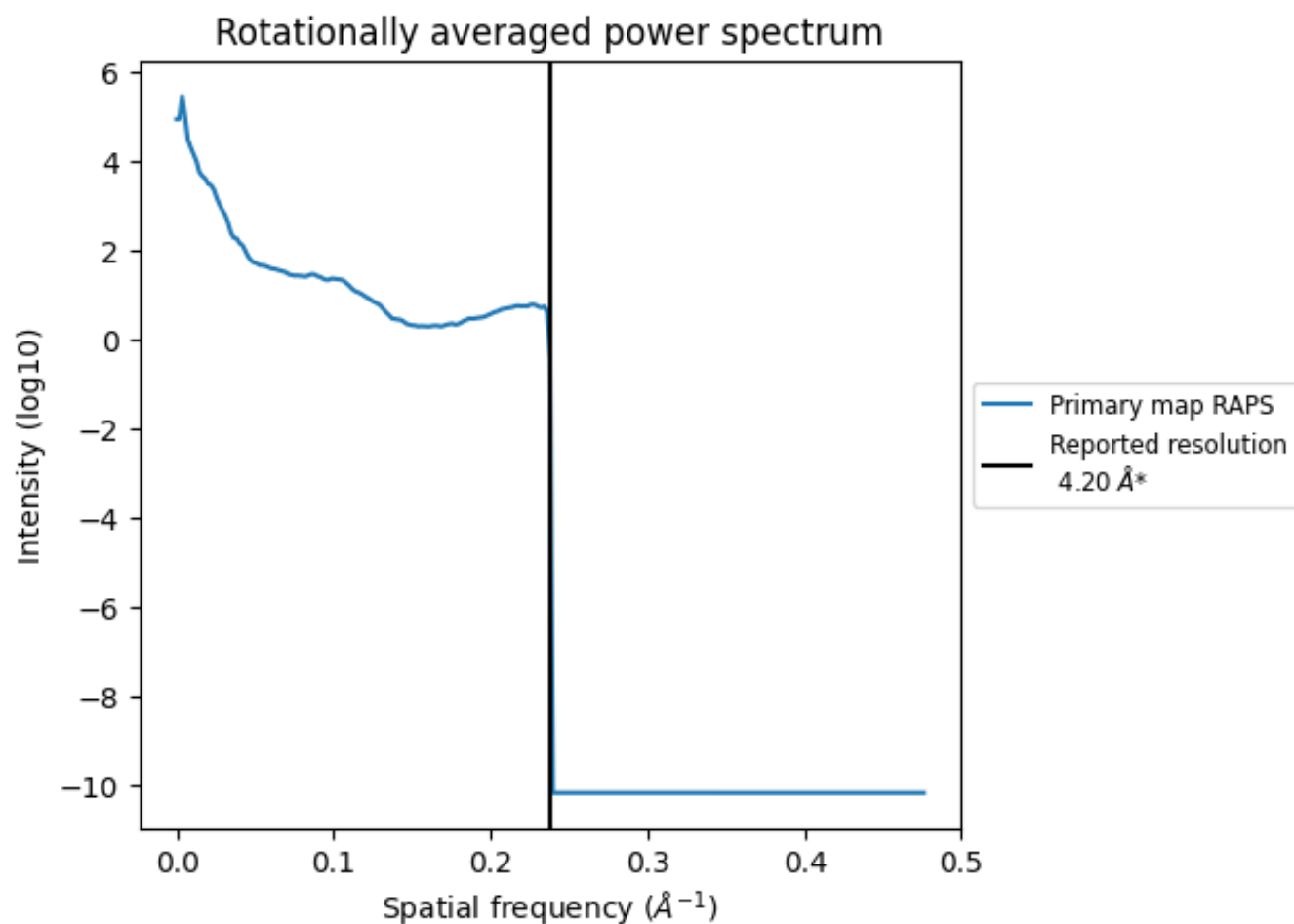
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 919 nm^3 ; this corresponds to an approximate mass of 830 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 0.238 Å⁻¹

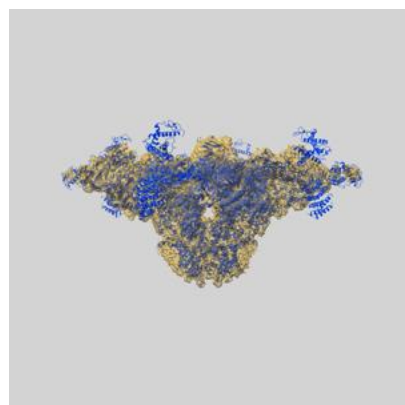
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

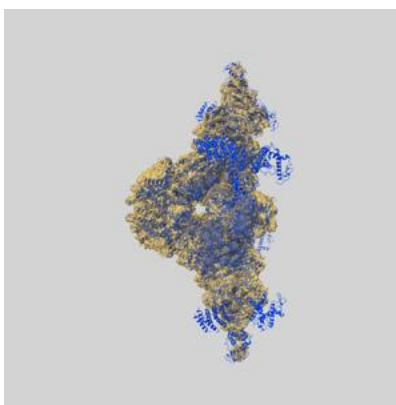
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9529 and PDB model 5GOA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

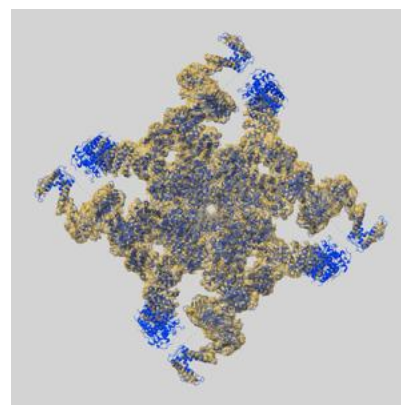
9.1 Map-model overlay [i](#)



X



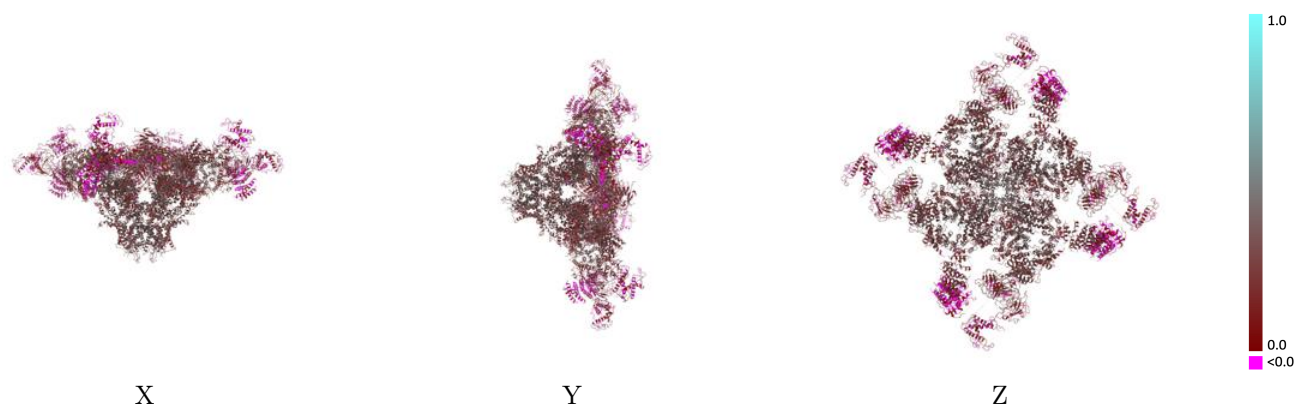
Y



Z

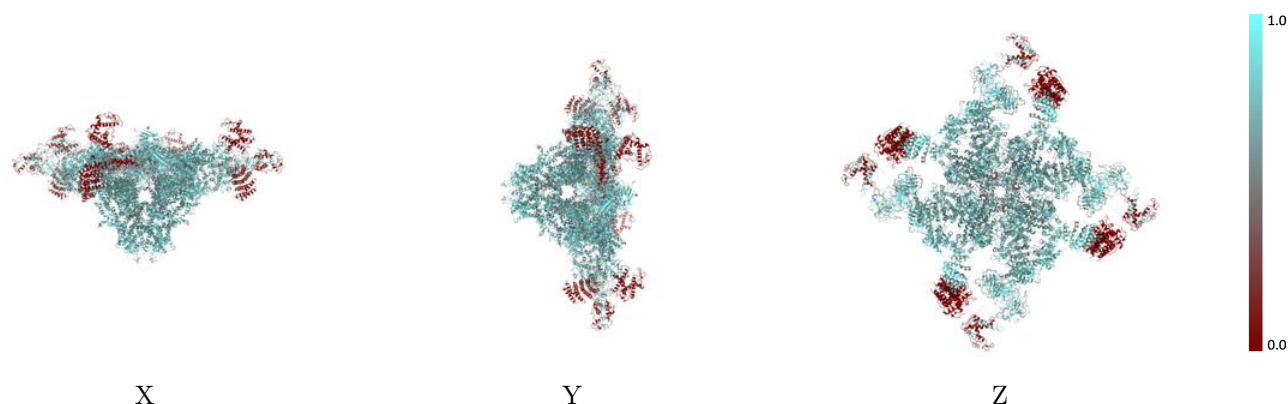
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



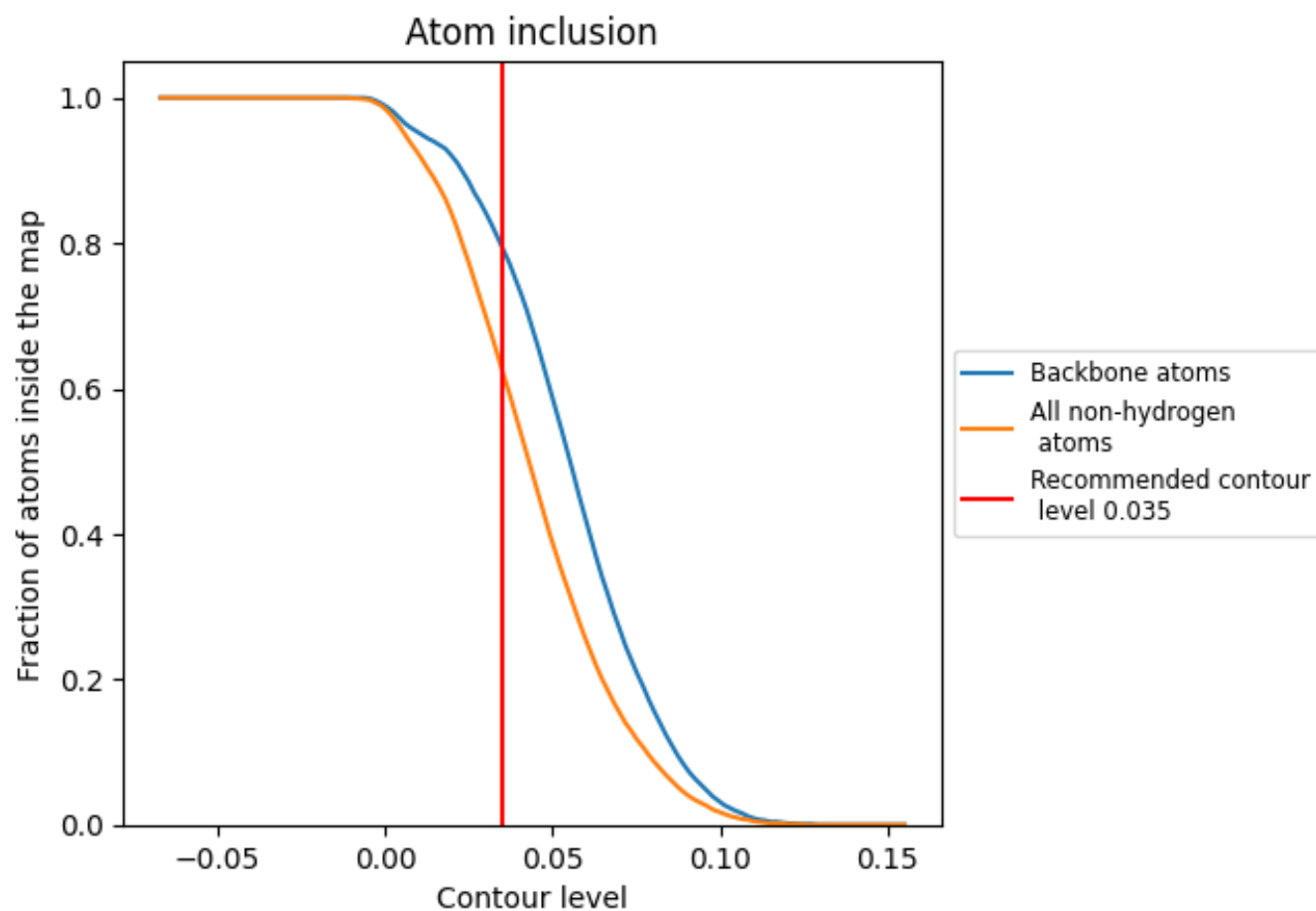
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 62% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6230	0.2450
A	0.6230	0.2450
B	0.6240	0.2440
C	0.6230	0.2440
D	0.6230	0.2440

