



wwPDB EM Validation Summary Report ⓘ

Jan 25, 2024 – 01:41 PM EST

PDB ID : 8DTZ
EMDB ID : EMD-27712
Title : Recombinant mouse RyR2 triple phosphonull mutant
S2807A/S2813A/S2030A in complex with FKBP12.6 and nanodisc un-
der closed-state conditions
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samsó, M.
Deposited on : 2022-07-26
Resolution : 3.60 Å (reported)
Based on initial model : 6WOU

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:

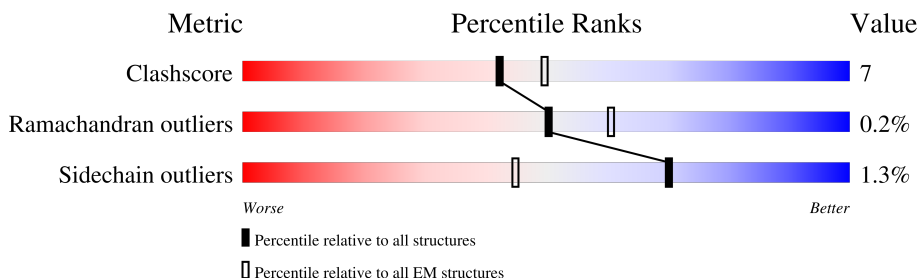
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	4966	
1	B	4966	
1	C	4966	
1	D	4966	
2	E	107	
2	F	107	
2	G	107	
2	H	107	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 129524 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4061	31562	20044	5390	5931	197	0	0
1	B	4061	31562	20044	5390	5931	197	0	0
1	C	4061	31562	20044	5390	5931	197	0	0
1	D	4061	31562	20044	5390	5931	197	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2030	ALA	SER	engineered mutation	UNP E9Q401
A	2807	ALA	SER	engineered mutation	UNP E9Q401
A	2813	ALA	SER	engineered mutation	UNP E9Q401
B	2030	ALA	SER	engineered mutation	UNP E9Q401
B	2807	ALA	SER	engineered mutation	UNP E9Q401
B	2813	ALA	SER	engineered mutation	UNP E9Q401
C	2030	ALA	SER	engineered mutation	UNP E9Q401
C	2807	ALA	SER	engineered mutation	UNP E9Q401
C	2813	ALA	SER	engineered mutation	UNP E9Q401
D	2030	ALA	SER	engineered mutation	UNP E9Q401
D	2807	ALA	SER	engineered mutation	UNP E9Q401
D	2813	ALA	SER	engineered mutation	UNP E9Q401

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	107	818	516	144	154	4	0	0
2	F	107	818	516	144	154	4	0	0
2	G	107	818	516	144	154	4	0	0

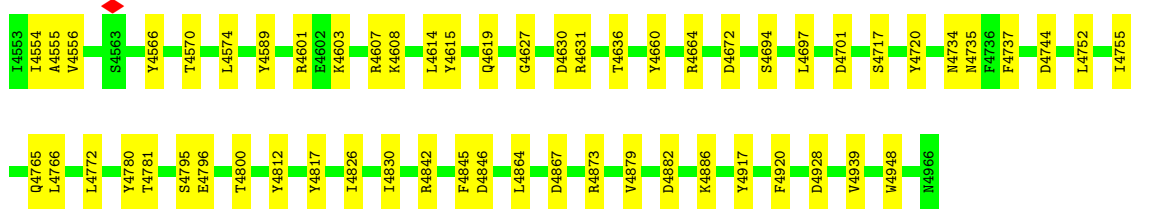
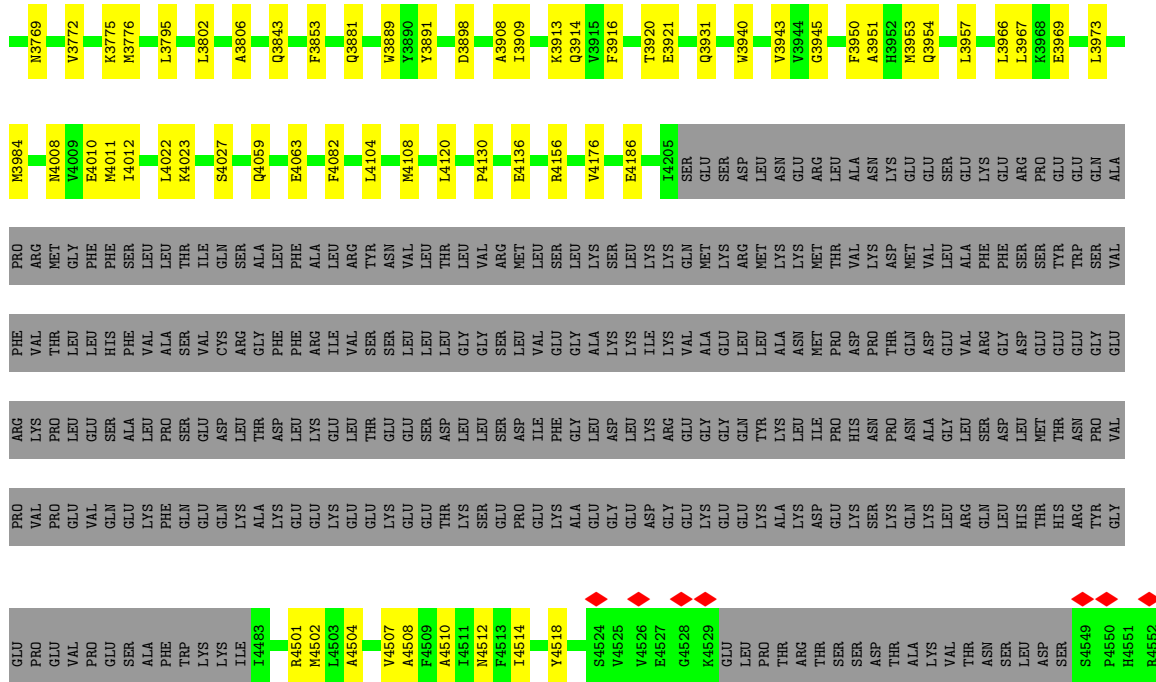
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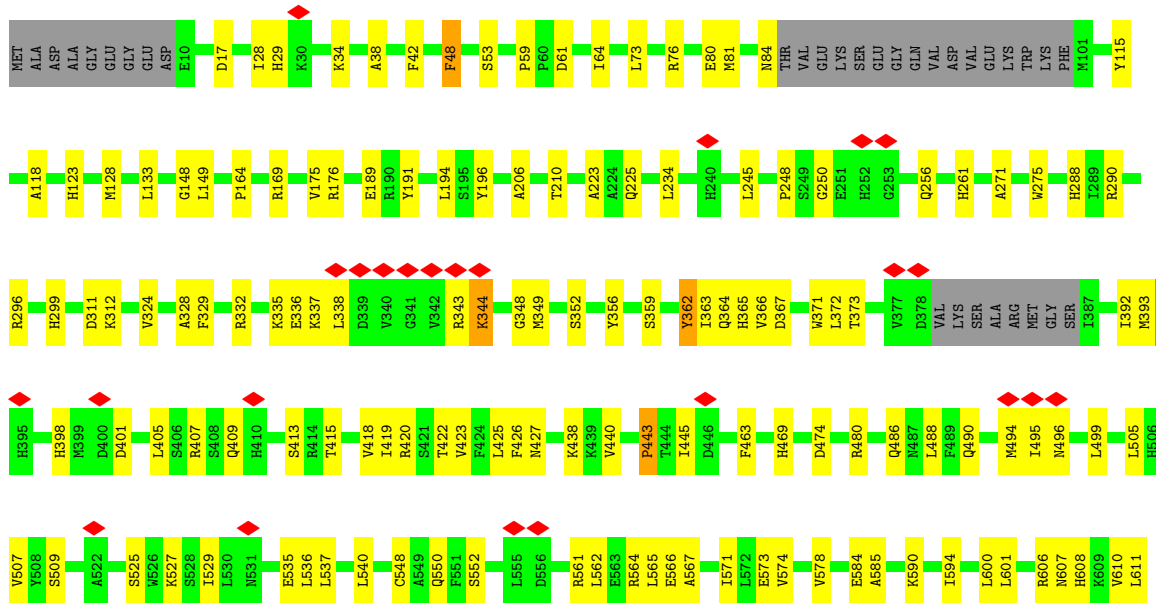
Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

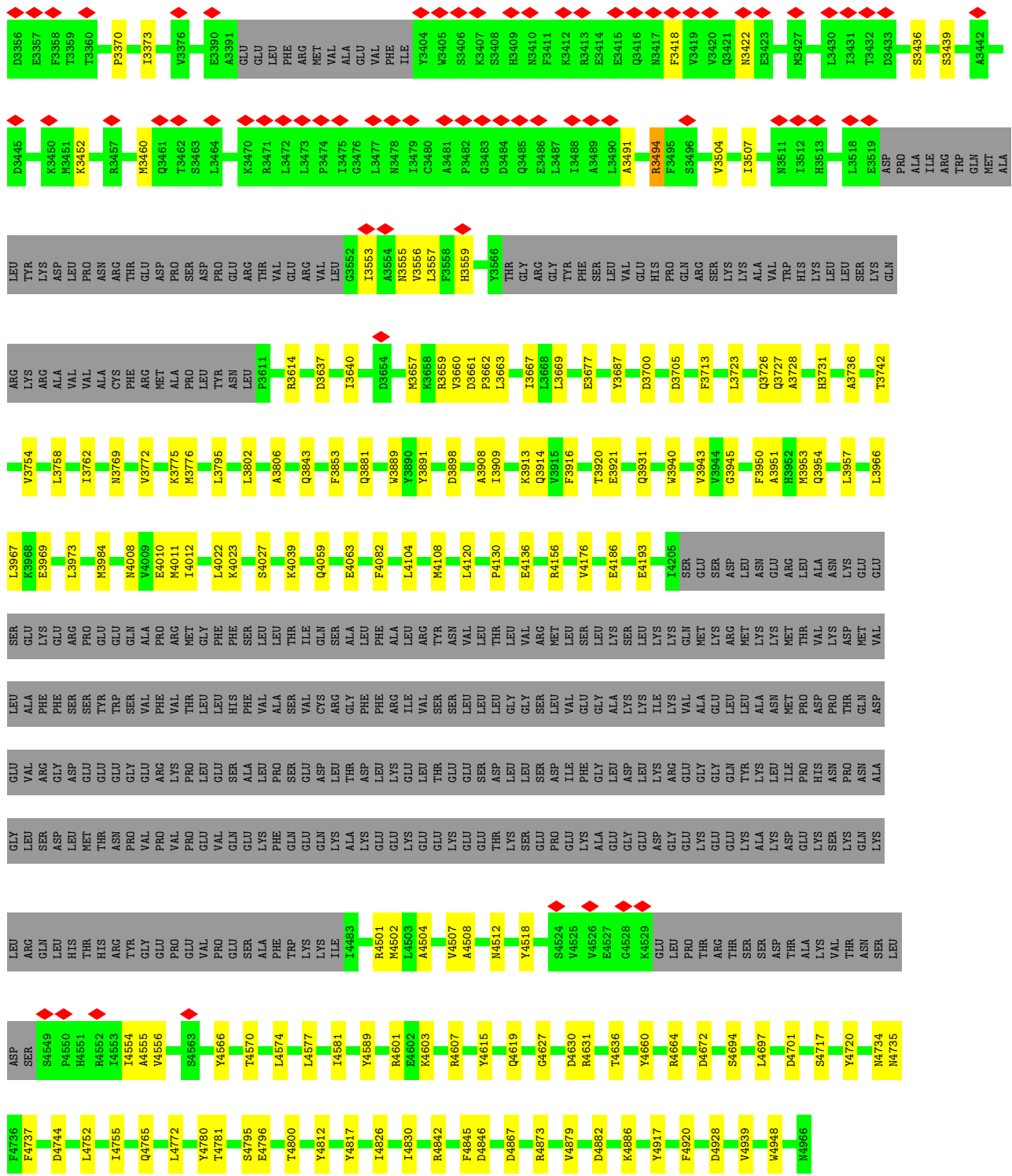
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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



● Molecule 1: Ryanodine receptor 2



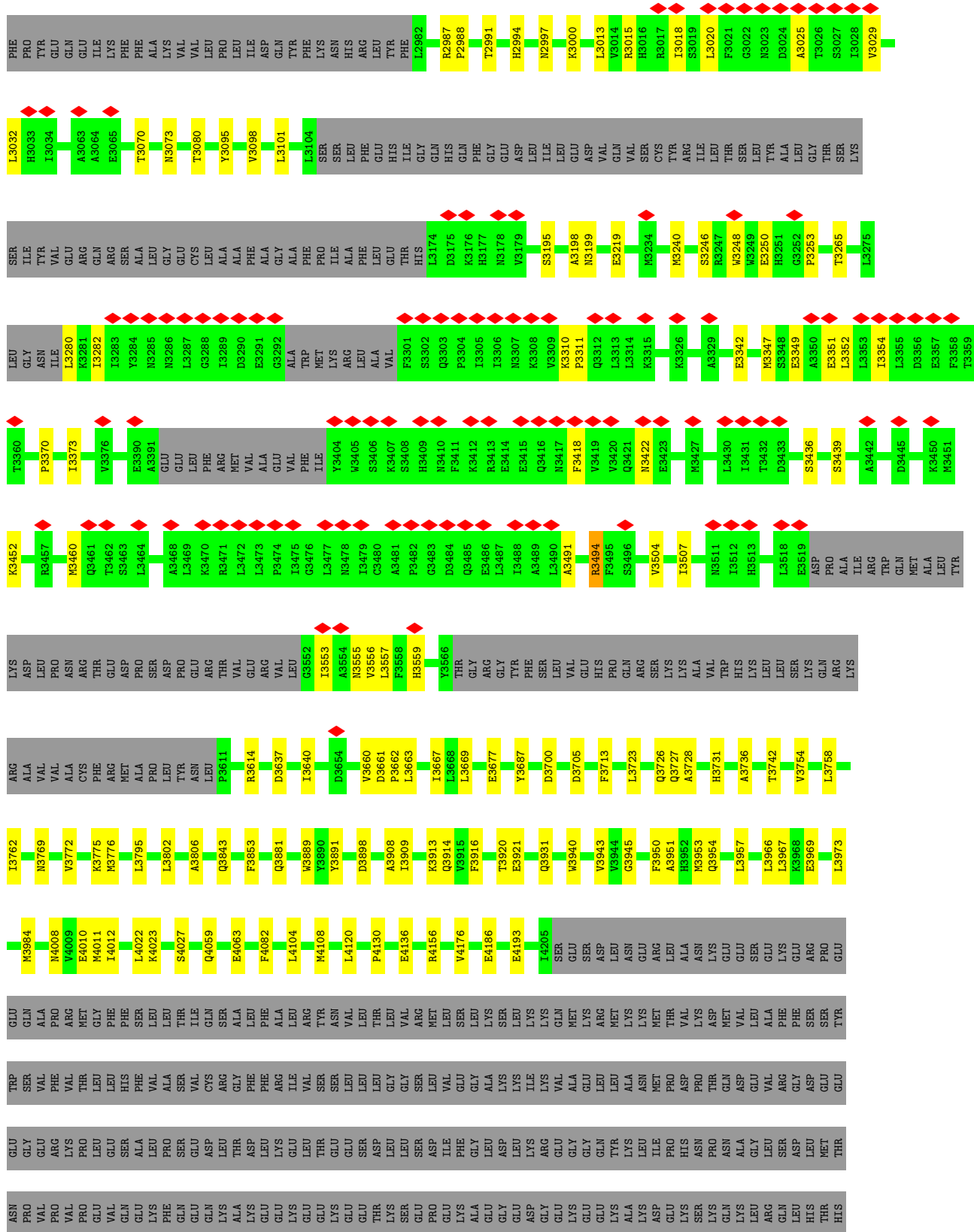


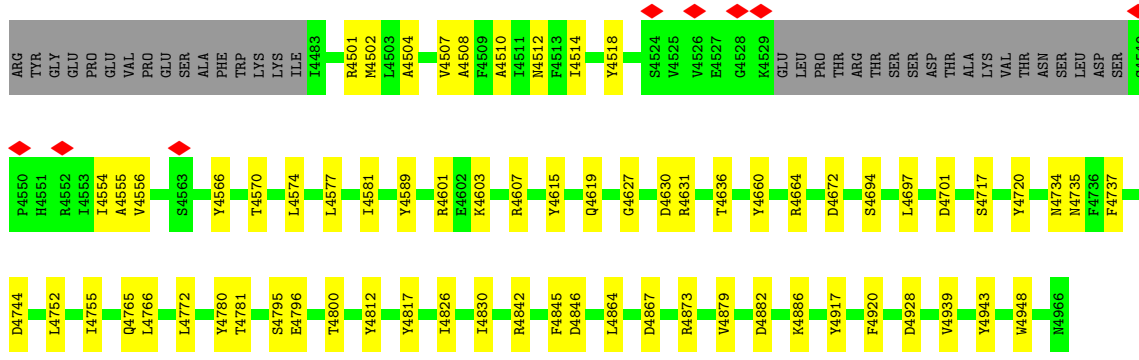
• Molecule 1: Ryanodine receptor 2



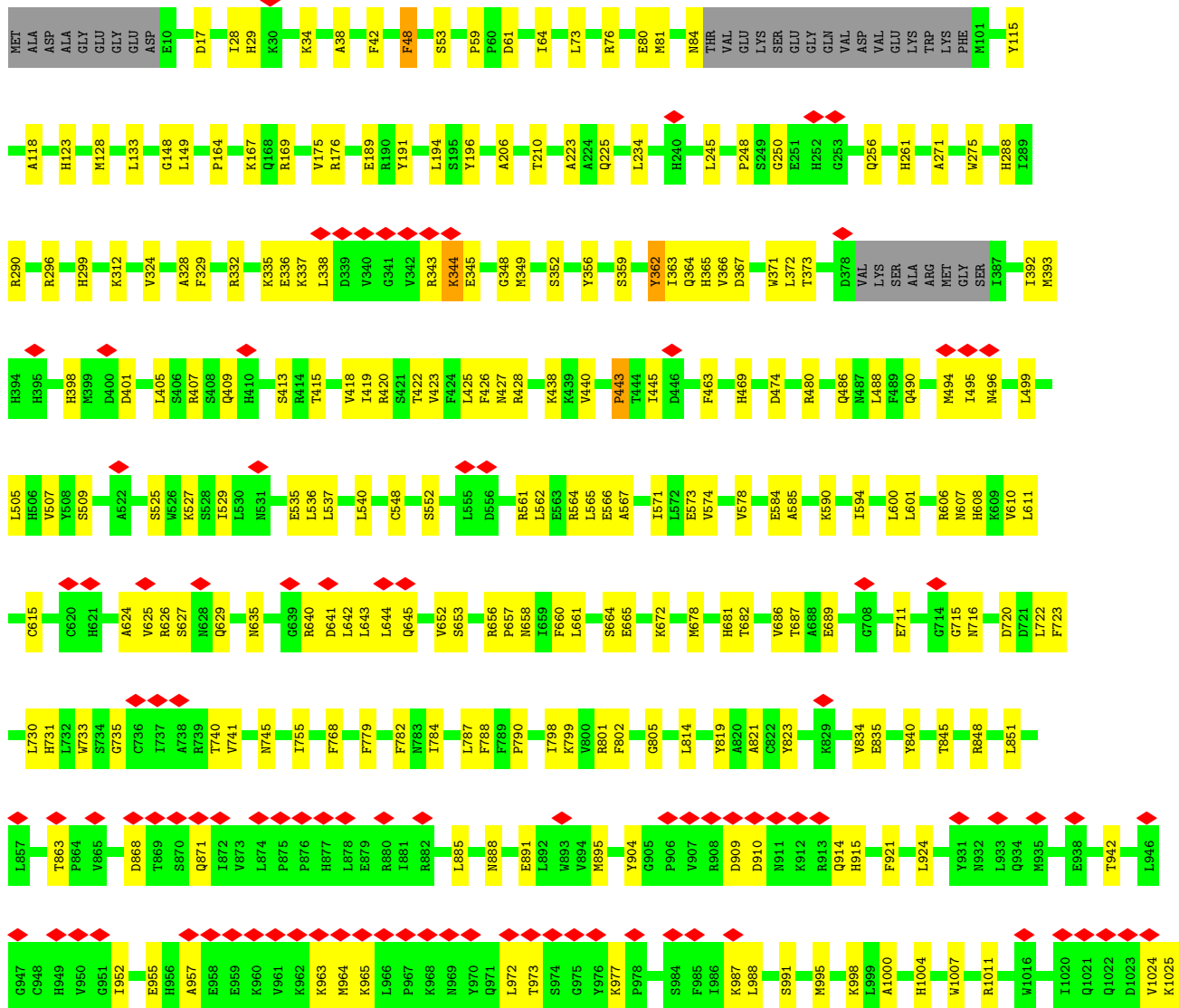
Chain C:





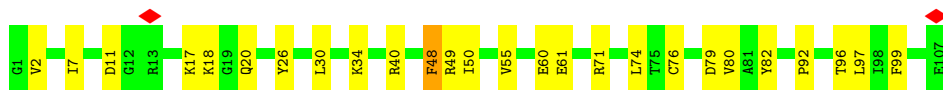


● Molecule 1: Ryanodine receptor 2



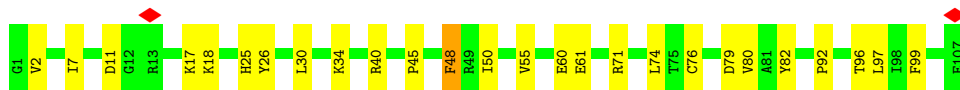
L1082	E1127	L1283	I1432	N1552	R1638	P1784	V1901	M2166	L2287	F2439
L1128	L1128	K1284	F1433	V1553	D1641	I1787	M1905	H2167	G2288	Q2440
S1130	G1129	V1285	P1434	F1554	L1643	L1796	L1908	E2168	W2289	M2441
D1131	D1131	S1292	G1435	E1557	E1644	P1810	R1920	T2169	M2307	P2442
R1041	R1144	T1297	Y1441	LEU	L1645	T1814	V1925	E2172	C2307	THR
K1044	W1145	D1298	G1444	GLY	L1646	T1815	V1926	E2173	W2308	ILE
S1045	W1153	I1299	W1446	ARG	E1647	E1816	F1927	M2174	R2321	ALA
D1048	G1163	Y1302	W1449	ILE	L1651	Y1827	S1928	N2175	P2332	ALA
S1049	V1166	R1303	F1450	LYS	F1654	Y1827	D1929	N2176	A2333	ASP
L11050	L1182	S1317	F1450	ASN	H1655	P1849	K1934	G2180	L2334	GLY
R1051	L1183	A1319	F1457	LEU	H1655	SER	M1938	G2181	R2335	VAL
E1052	E1189	GLY	V1465	ALA	L1661	VAL	N1938	E2185	E2337	VAL
A1053	L1190	GLY	Y1472	GLY	S1679	PHE	F1941	I2186	G2341	ASP
V1054	A1191	LEU	LYS	LEU	H1680	GLY	R1942	I2186	S2357	ASP
D1062	F1192	PRO	E1472	PHE	L1686	ALA	M1944	P2189	R2358	ALA
H1063	K1193	ARG	LYS	LYS	I1690	ALA	F1943	K2190	S2357	ASP
H1063	F1195	GLY	GLY	GLU	E1691	VAL	Y1943	M2191	R2358	ASP
L1064	D1196	ALA	V1476	GLU	M1692	VAL	M1944	V2192	E2337	ASP
E1065	T1204	PRO	R1482	HIS	M1695	GLU	Q1948	C2196	E2337	ASP
A1066	C1205	LEU	S1483	ASN	M1695	GLU	A1949	R2197	I2186	ASP
P1067	ARG	LEU	N1484	PRO	L1699	GLY	L1950	H2216	I2186	ASP
D1068	S1206	PRO	C1485	VAL	M1699	GLY	M1951	L2216	R2189	ASP
Q1069	L1207	ASN	Y1486	PRO	L1706	THR	S1953	S2218	K2190	ASP
D1070	L1224	LEU	M1487	CYS	I1710	PRO	A1954	L2209	M2191	ASP
H1071	E1237	GLU	V1488	PRO	I1710	GLU	A1955	L2220	Y2219	ASP
A1072	V1241	ASP	A1490	ARG	L1720	GLU	T1957	M2083	L2220	ASP
S1073	VAL	SER	M1502	ARG	M1721	GLU	A1958	L2223	S2224	ASP
R1074	GLY	ASP	S1503	HIS	M1722	ILE	R1959	S2225	S2225	ASP
A1075	HIS	SER	M1504	VAL	M1728	ILE	K1960	L2228	L2228	ASP
E1076	ASP	ASP	G1505	GLN	T1731	GLU	THR	L2231	L2228	ASP
V1077	SER	ASP	L1506	PHE	K1735	GLU	ARG	P2231	L2228	ASP
Q1078	LEU	LEU	E1507	LEU	T1734	GLU	ARG	M2233	A2232	ASP
S1079	VAL	VAL	G1509	HIS	K1735	GLY	SER	R2234	M2233	ASP
G1080	THR	ASP	V1511	V1595	F1764	GLY	PRO	T2237	R2234	ASP
T1081	VAL	VAL	G1517	L1605	S1765	GLU	PRO	R2257	E2262	ASP
E1083	ALA	ALA	L1518	D1608	F1766	GLU	GLN	E2262	R2266	ASP
R1084	HIS	HIS	L1519	F1628	S1766	GLU	GLN	R2266	M2278	ASP
F1085	ASP	ASP	T1520	M1629	F1767	LYS	ILE	L2279	L2279	ASP
R1086	LEU	LEU	Y1532	A1546	S1768	GLY	ASN	H2157	L2279	ASP
R1089	VAL	VAL	Q1533	F1628	F1769	LYS	LEU	P2158	L2279	ASP
A1090	ARG	ARG	Y1533	F1628	M1774	ARG	LEU	N2159	S2281	ASP
E1091	TYR	TYR	Q1533	M1629	M1774	ARG	LEU	L2159	K2282	ASP
K1092	ASP	ASP	A1547	A1547	Y1777	PRO	ASN	L2160	G2283	ASP
E1104	ILE	ILE	A1548	P1634	Y1779	GLU	PHE	M2161	Y2284	ASP
H1113	THR	THR	S1550	E1636	P1781	GLU	ASN	R2162	P2285	ASP
W1117	LYS	LYS	P1551	N1637	L1897	GLU	LEU	G2165	D2286	ASP
S1118	ASP	ASP	Y1426	E1636	L1897	GLU	LEU	G2165	D2286	ASP
R1119	ASP	ASP	Y1427	E1636	L1897	GLU	LEU	G2165	D2286	ASP
C1122	ASP	ASP	Y1428	E1636	L1897	GLU	LEU	G2165	D2286	ASP
L1126	LYS	LYS	S1429	N1637	L1897	GLU	LEU	G2165	D2286	ASP

PHE	ALA	GLY	THR	GLU	HIS	HIS	ALA	SER	ILE	ASP	SER	LEU	LEU	HIS	THR	VAL	TVR	ARG	LEU	SER	LYS	GLN	ARG	ASP	LEU	LEU	ILE	GLU	VAL	CYS	LEU	SER	ILE	C2576	L2579	R2580	M2584	Q2585	H2586	L2587	L2588	K2603	L2606	K2607	T2610	M2611														
H2612	E2716	E2717	E2718	F2719	I2720	N2721	I2722	Y2723	A2724	E2725	H2726	S2727	D2728	D2729	K2730	W2731	S2732	M2733	D2734	K2735	L2736	A2737	N2738	Q2739	W2740	I2741	Y2742	Q2743	E2744	I2745	Y2746	S2747	D2748	S2749	K2751	F2700	N2701	P2702	Q2703	P2704	V2705	D2706	K2757	P2758	Y2759	K2760	L2761	L2762	S2763	E2764	K2765	E2766	K2767	E2768	I2769	Y2770	W2771	W2772	I2774	K2775
E2776	S2777	L2778	K2779	T2780	M2781	L2782	A2783	W2784	G2785	W2786	R2787	L2788	E2789	R2790	W2791	R2792	E2793	G2794	D2795	S2796	M2797	A2798	L2799	Y2800	N2801	ARG	THR	ARG	ARG	ILE	ALA	GLN	THR	SER	GLN	VAL	ALA	ILE	ASP	A2816	A2817	H2818	G2819	Y2820	S2821	P2822	R2823	A2824	L2825	D2826	M2827	S2828	M2829	V2830	T2831	L2832	S2833	R2834	D2835	
L2836	H2837	A2838	M2839	A2840	E2841	M2842	M2843	A2844	E2845	N2846	Y2847	H2848	N2849	I2850	W2851	A2852	K2853	K2854	K2855	K2856	L2857	E2858	L2859	E2860	S2861	K2862	G2863	G2864	N2865	H2866	H2867	P2868	L2869	L2870	Y2871	P2872	Y2873	D2874	T2875	L2876	T2877	A2878	K2879	E2880	K2881	A2882	K2883	D2884	R2885	E2886	K2887	A2888	Q2889	D2890	I2891	F2892	K2893	D2894	L2895	
Q2896	L2897	S2898	G2899	Y2900	V2901	V2902	S2903	R2904	GLY	PHE	LEU	ASP	LEU	ASP	THR	PRO	SER	ILE	GLU	LYS	ARG	PHE	ALA	TVR	LEU	ILE	LEU	ILE	ARG	TVR	VAL	GLU	ALA	HIS	TYR	LEU	PHE	GLU	PHE	ASP	GLY	GLY	SER	ARG	THR	LYS	GLY	GLU	HIS	PHE	PRO	TYR								
GLU	GLN	GLU	ILE	LYS	PHE	PHE	ALA	VAL	VAL	LEU	PRO	LEU	ILE	ASP	GLN	TYR	PHE	LYS	ASN	HIS	ARG	LEU	TYR	PHE	L2982	R2987	P2988	T2991	H2994	N2997	K3000	L3013	V3014	R3015	H3016	R3017	I3018	S3019	L3020	F3021	G3022	N3023	A3025	T3026	K3027	L3028	V3029	L3032	H3033	I3034										
A3063	A3064	E3065	T3070	N3073	T3080	Y3095	V3098	L3101	L3104	SER	LEU	PHE	ALA	PHE	GLU	HIS	ILE	GLY	GLN	HIS	GLN	PHE	GLY	GLU	LEU	ILE	GLU	ASP	VAL	GLN	VAL	SER	CYS	TYR	ARG	ILE	LEU	THR	THR	SER	LEU	TYR	ALA	LEU	GLY	THR	LYS	ILE	TYR											
VAL	GLU	ARG	GLN	ARG	SER	ALA	GLY	GLU	CYS	LEU	ALA	PHE	ALA	ALA	ALA	ALA	THR	HIS	L3174	D3175	K3176	H3177	N3178	V3179	S3195	A3198	N3199	E3219	Q3312	L3313	L3314	K3315	K3326	R3247	W3248	W3249	E3250	H3251	G3252	P3253	E3254	N3255	T3265	L3275	LEU															
GLY	ASN	ILE	K3281	I3282	I3283	Y3284	N3286	L3287	G3288	I3289	D3290	E3291	G3292	ALA	TRP	LYS	ARG	LEU	ALA	VAL	F3301	S3302	Q3303	P3304	I3305	I3306	N3307	K3308	V3309	K3310	K3311	Q3312	L3313	L3314	K3315	K3326	A3329	E3342	M3347	S3348	E3349	A3350	E3351	L3352	L3353	I3354	L3355	D3356	E3357	F3358	T3359	T3360								
P3370	L3371	L3372	I3373	V3376	E3390	A3391	GLU	GLU	LEU	PHE	ARG	MET	VAL	ALA	GLU	VAL	PHE	ILE	Y3404	W3405	S3406	K3407	S3408	H3409	N3410	F3411	K3412	R3413	E3414	E3415	Q3416	N3417	F3418	V3419	V3420	Q3421	N3422	E3423	M3427	L3430	I3431	T3432	D3433	S3436	S3439	A3442	D3445	K3450	M3451											
K3452	R3457	M3460	Q3461	T3462	S3463	L3464	A3468	L3469	K3470	R3471	L3472	L3473	P3474	I3475	G3476	L3477	N3478	I3479	C3480	A3481	P3482	G3483	D3484	Q3485	E3486	L3487	I3488	A3489	L3490	A3491	R3494	V3504	I3507	N3511	I3512	H3513	L3518	E3519	ASP	PRO	ALA	ILE	ARG	TRP	GLN	MET	ALA	LEU	TYR	LYS	ASP									
LEU	PRO	ASN	ARG	THR	GLU	ASP	PRO	PRO	GLU	ARG	THR	VAL	VAL	LEU	VAL	ILE	Y3555	N3556	L3557	F3558	H3559	V3566	THR	GLY	ARG	GLY	PHE	L3487	I3488	A3489	L3490	A3491	R3494	V3504	I3507	N3511	I3512	H3513	L3518	E3519	ASP	PRO	ALA	ILE	ARG	TRP	GLN	MET	ALA	LEU	TYR	LYS	ASP							



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 76% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	136874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.95	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.288	Depositor
Minimum map value	-1.682	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	496.79996, 496.79996, 496.79996	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0799999, 1.0799999, 1.0799999	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	0.25	0/32214	0.52	8/43602 (0.0%)
1	B	0.25	0/32214	0.52	8/43602 (0.0%)
1	C	0.25	0/32214	0.52	8/43602 (0.0%)
1	D	0.25	0/32214	0.52	8/43602 (0.0%)
2	E	0.27	0/834	0.54	0/1123
2	F	0.27	0/834	0.54	0/1123
2	G	0.27	0/834	0.54	0/1123
2	H	0.27	0/834	0.54	0/1123
All	All	0.25	0/132192	0.52	32/178900 (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	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4022	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	4022	LEU	CA-CB-CG	6.16	129.46	115.30
1	C	4022	LEU	CA-CB-CG	6.16	129.46	115.30
1	D	4022	LEU	CA-CB-CG	6.16	129.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	LEU	CA-CB-CG	6.11	129.35	115.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1777	TYR	Peptide
1	A	4023	LYS	Peptide
1	A	443	PRO	Peptide
1	A	4555	ALA	Peptide
1	B	443	PRO	Peptide

5.2 Too-close contacts [i](#)

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	31562	0	30401	448	0
1	B	31562	0	30401	448	0
1	C	31562	0	30401	452	0
1	D	31562	0	30401	449	0
2	E	818	0	824	19	0
2	F	818	0	824	22	0
2	G	818	0	824	20	0
2	H	818	0	824	20	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
All	All	129524	0	124900	1834	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 1834 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:B:329:PHE:HB3	1:B:363:ILE:HD11	1.67	0.76
1:D:329:PHE:HB3	1:D:363:ILE:HD11	1.67	0.76
1:A:329:PHE:HB3	1:A:363:ILE:HD11	1.67	0.75
1:C:329:PHE:HB3	1:C:363:ILE:HD11	1.67	0.75
1:C:1954:ALA:HA	1:C:1958:ALA:HB3	1.69	0.75

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	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	47	79
1	B	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	47	79
1	C	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	47	79
1	D	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	47	79
2	E	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	F	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	G	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
All	All	16464/20292 (81%)	14804 (90%)	1632 (10%)	28 (0%)	50	79

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	LYS
1	A	1484	ASN
1	A	3253	PRO
1	B	344	LYS
1	B	1484	ASN

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	3319/4352 (76%)	3276 (99%)	43 (1%)	69	86
1	B	3319/4352 (76%)	3276 (99%)	43 (1%)	69	86
1	C	3319/4352 (76%)	3276 (99%)	43 (1%)	69	86
1	D	3319/4352 (76%)	3276 (99%)	43 (1%)	69	86
2	E	88/88 (100%)	87 (99%)	1 (1%)	73	88
2	F	88/88 (100%)	87 (99%)	1 (1%)	73	88
2	G	88/88 (100%)	87 (99%)	1 (1%)	73	88
2	H	88/88 (100%)	87 (99%)	1 (1%)	73	88
All	All	13628/17760 (77%)	13452 (99%)	176 (1%)	70	86

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2219	TYR
1	D	851	LEU
1	C	2667	CYS
1	D	48	PHE
1	D	1641	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2223	ASN
1	D	3930	ASN
1	B	3930	ASN
1	B	2223	ASN
1	D	3948	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

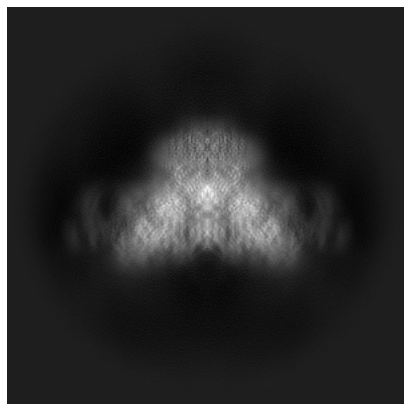
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27712. These allow visual inspection of the internal detail of the map and identification of artifacts.

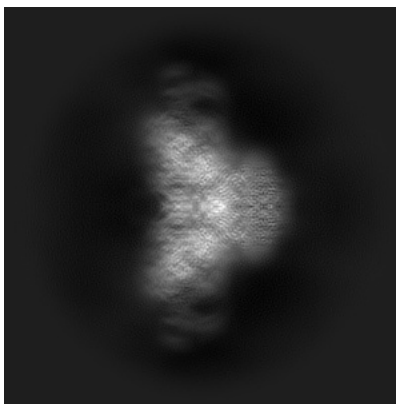
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

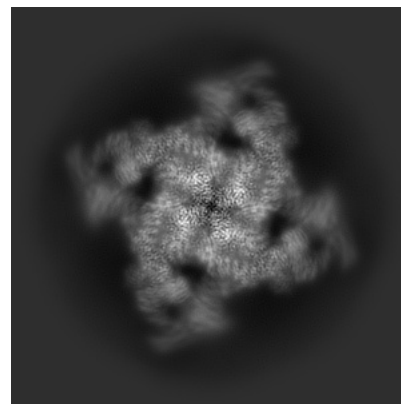
6.1.1 Primary map



X

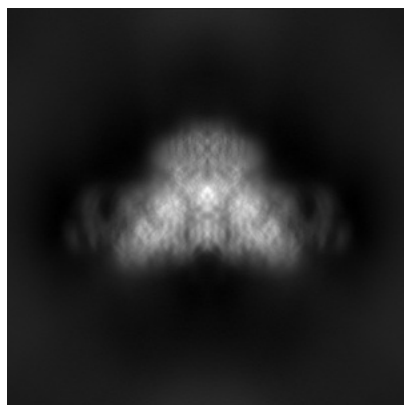


Y

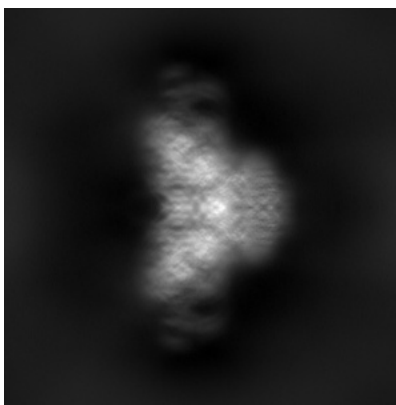


Z

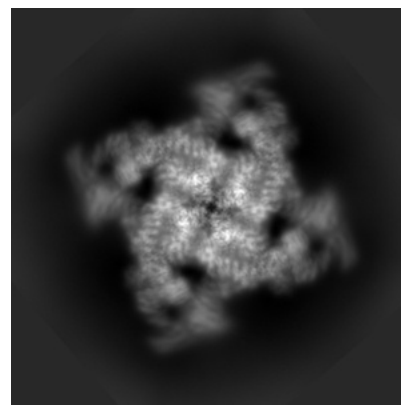
6.1.2 Raw map



X



Y

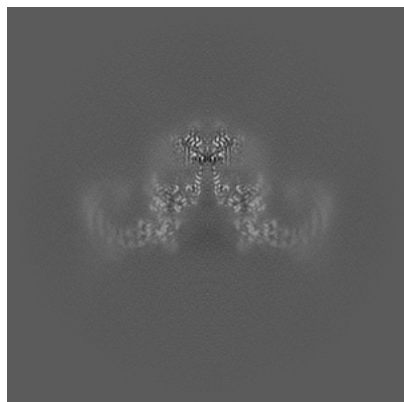


Z

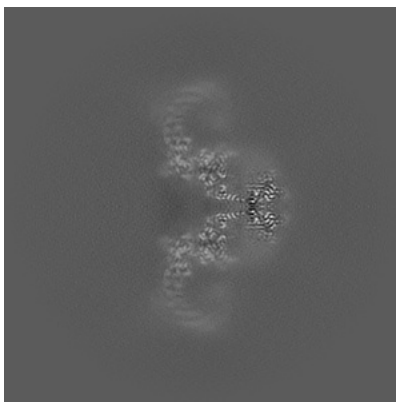
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

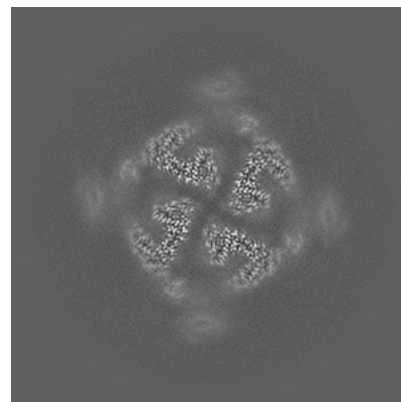
6.2.1 Primary map



X Index: 230

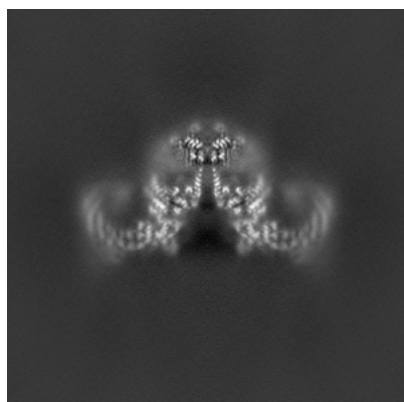


Y Index: 230

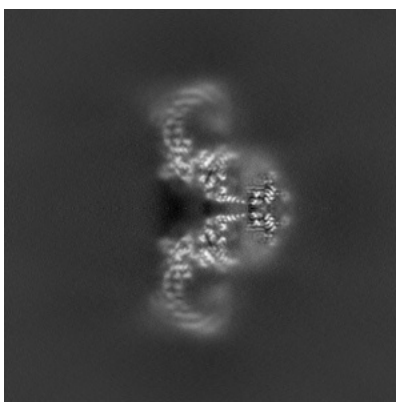


Z Index: 230

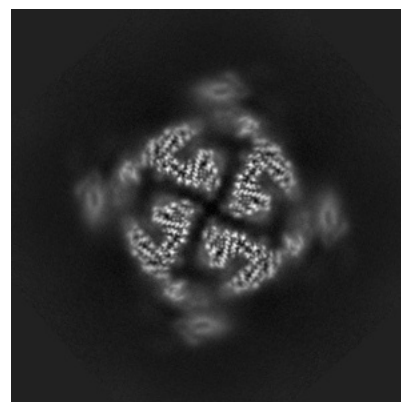
6.2.2 Raw map



X Index: 230



Y Index: 230

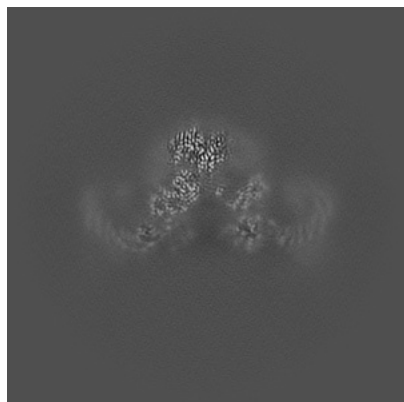


Z Index: 230

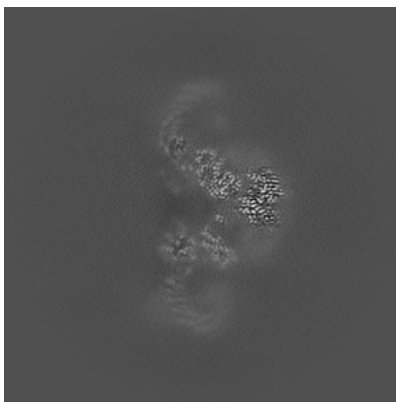
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

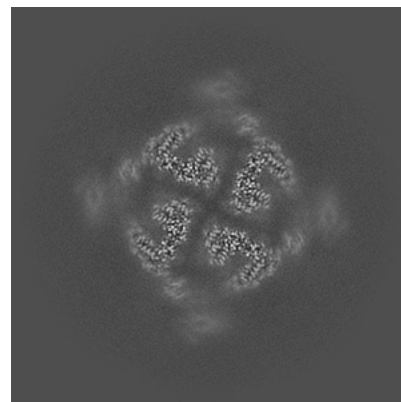
6.3.1 Primary map



X Index: 236

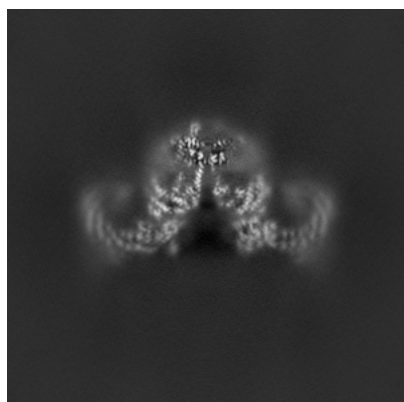


Y Index: 236

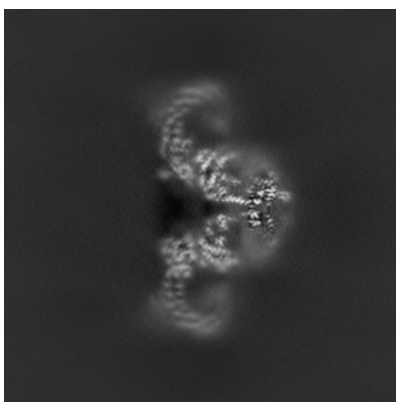


Z Index: 229

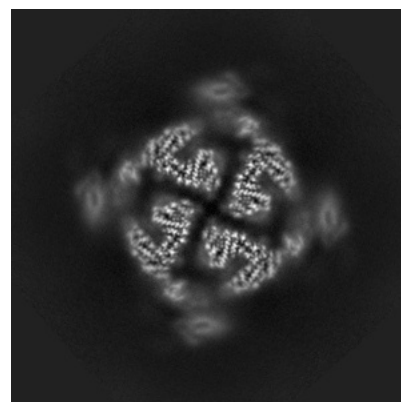
6.3.2 Raw map



X Index: 232



Y Index: 232

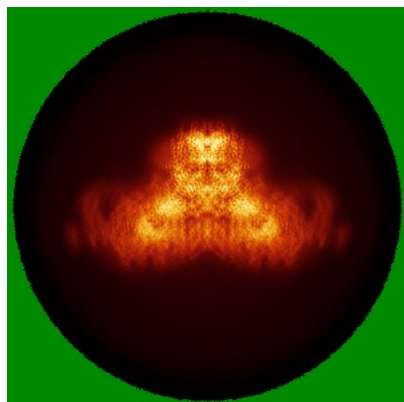


Z Index: 230

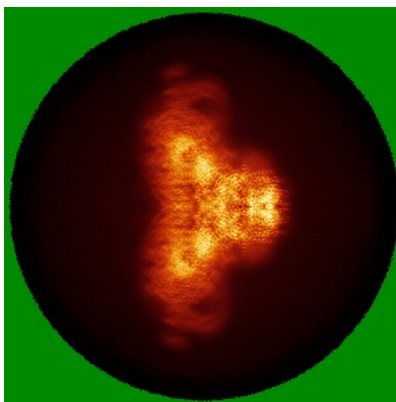
The images above show the largest variance slices of the map in three orthogonal directions.

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

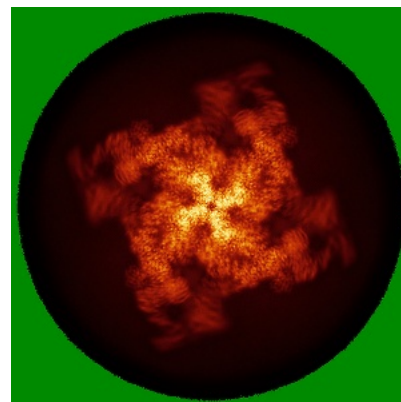
6.4.1 Primary map



X



Y

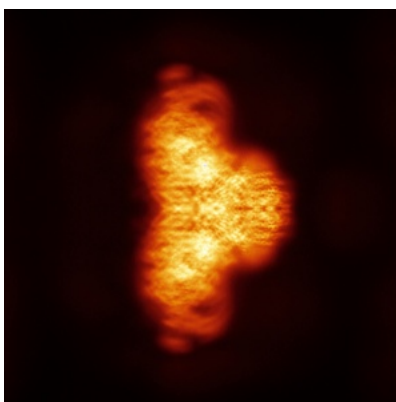


Z

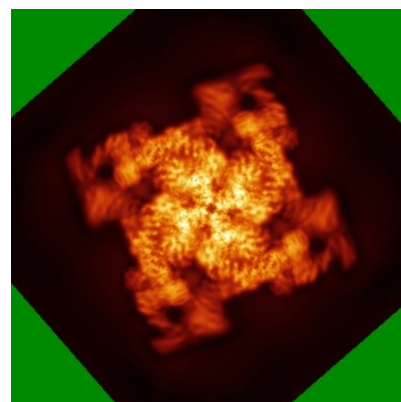
6.4.2 Raw map



X



Y

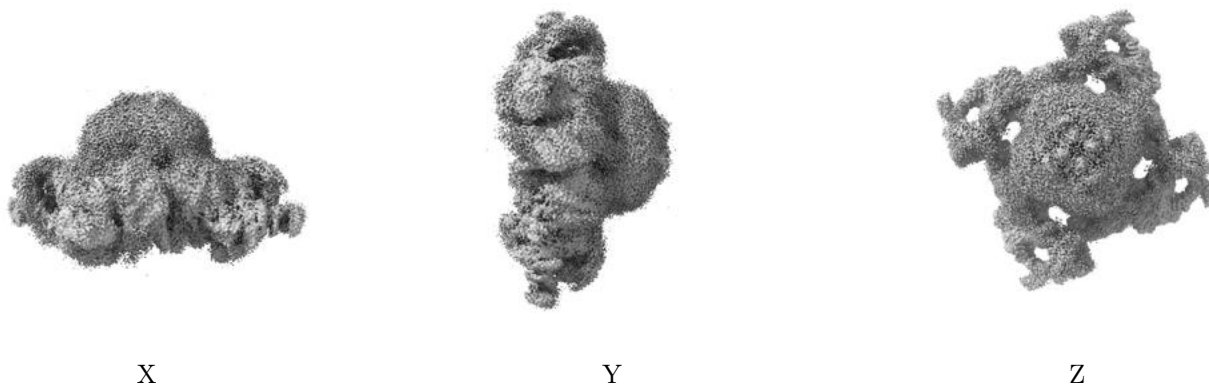


Z

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.

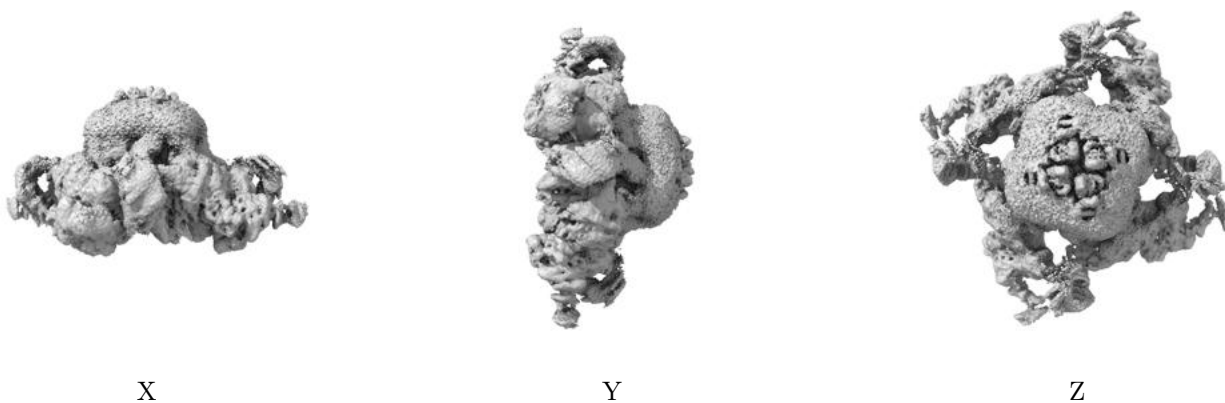
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

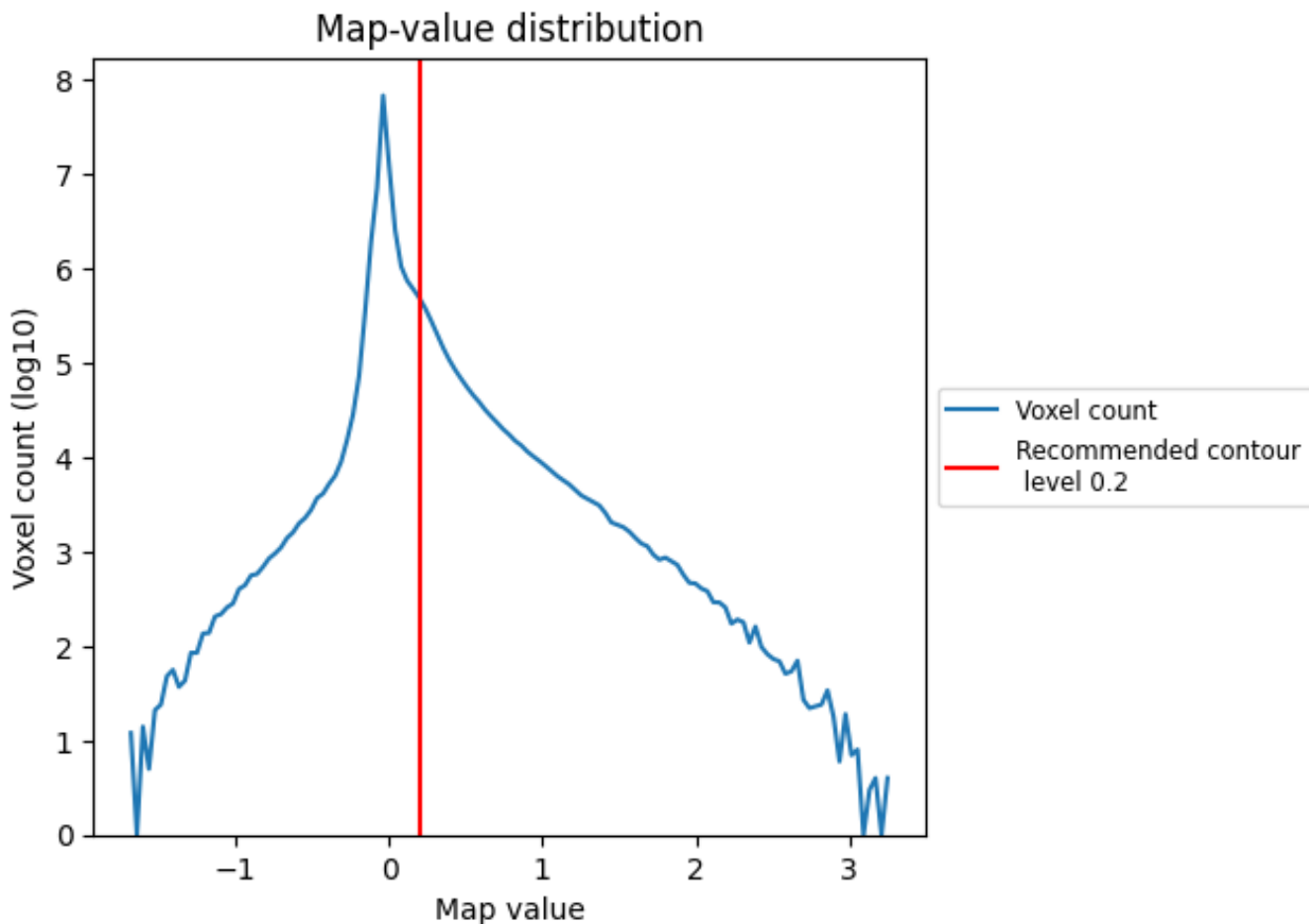
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

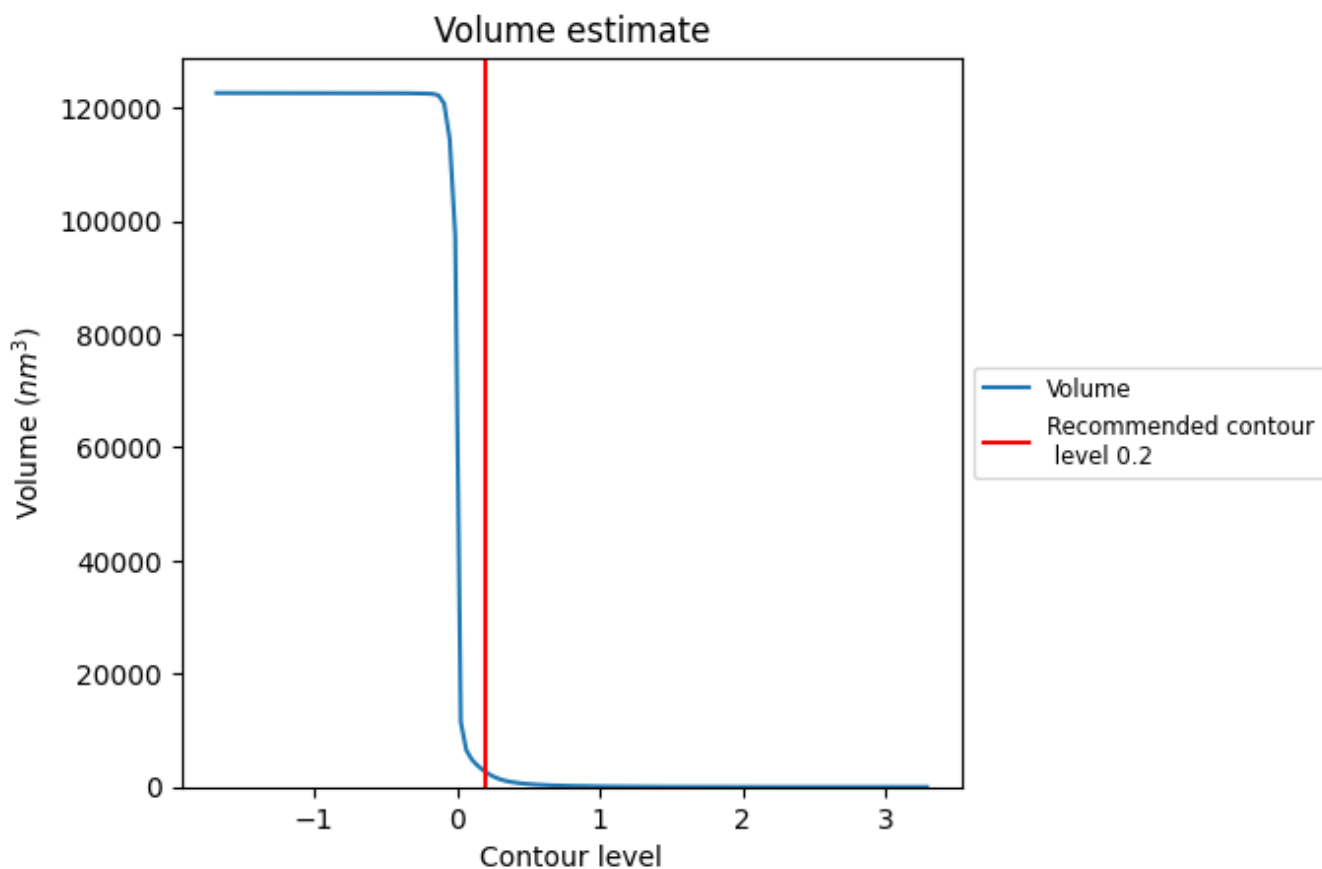
This section contains the results of statistical analysis of the map.

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.

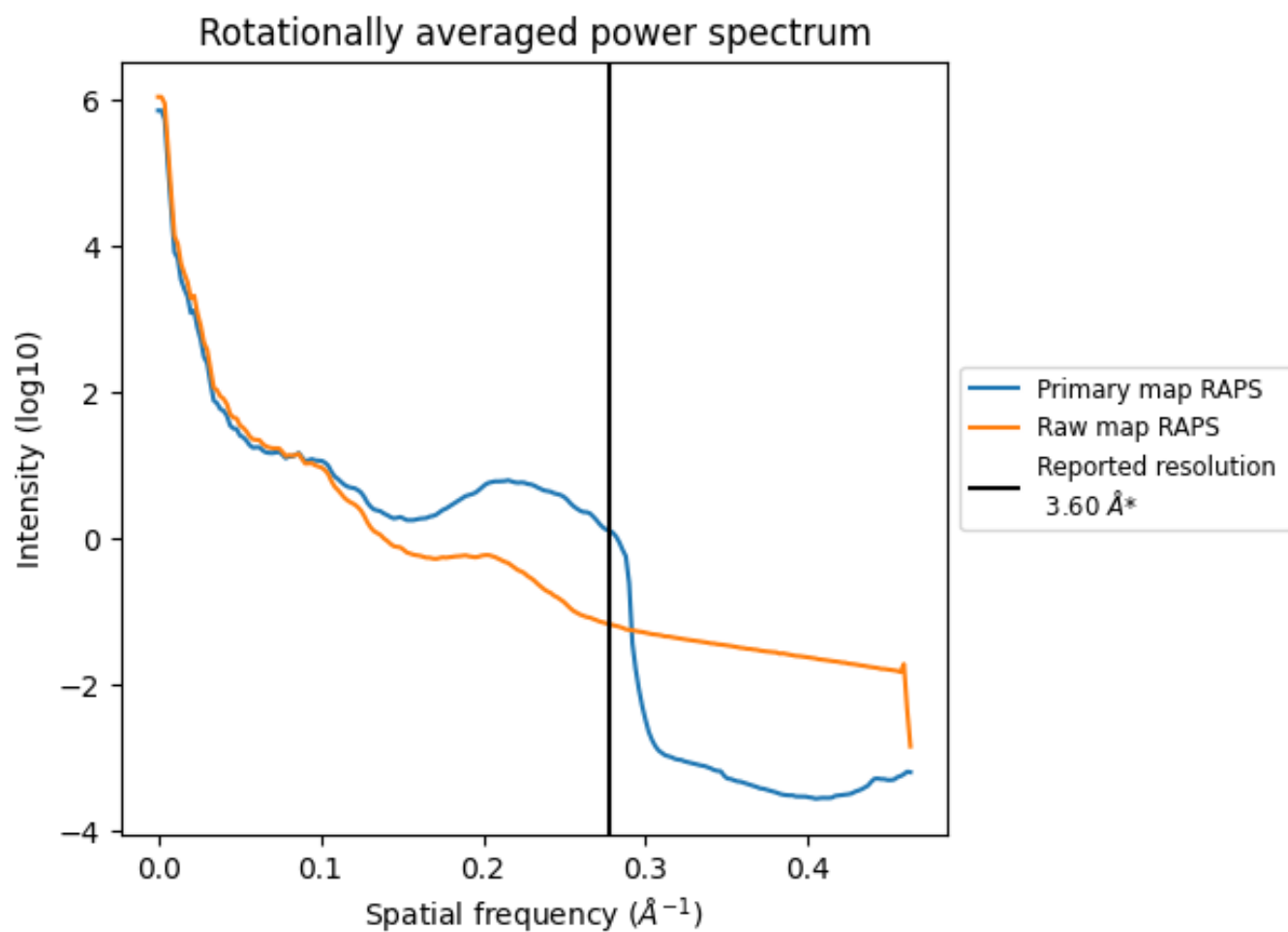
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2673 nm^3 ; this corresponds to an approximate mass of 2415 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 i

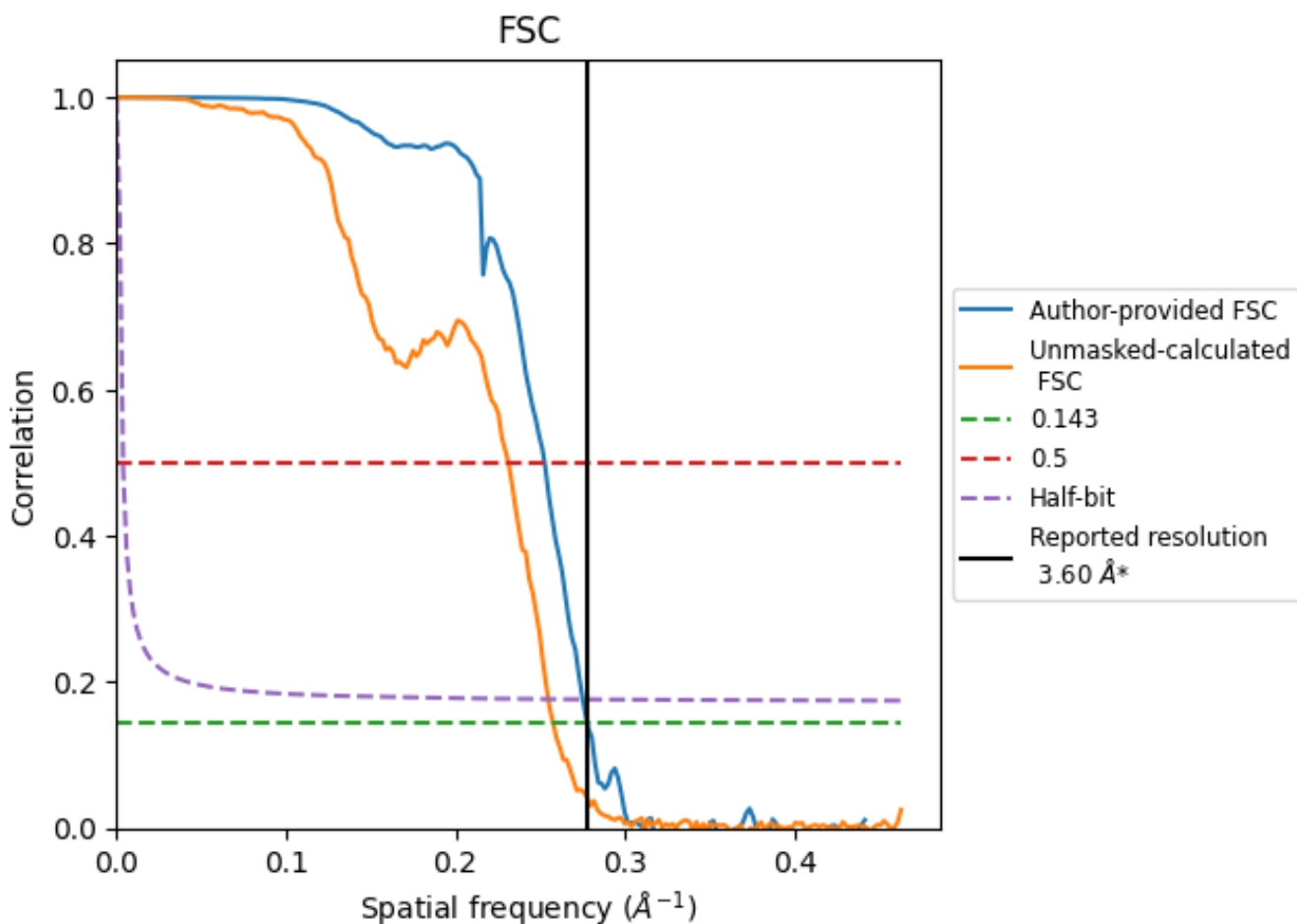


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

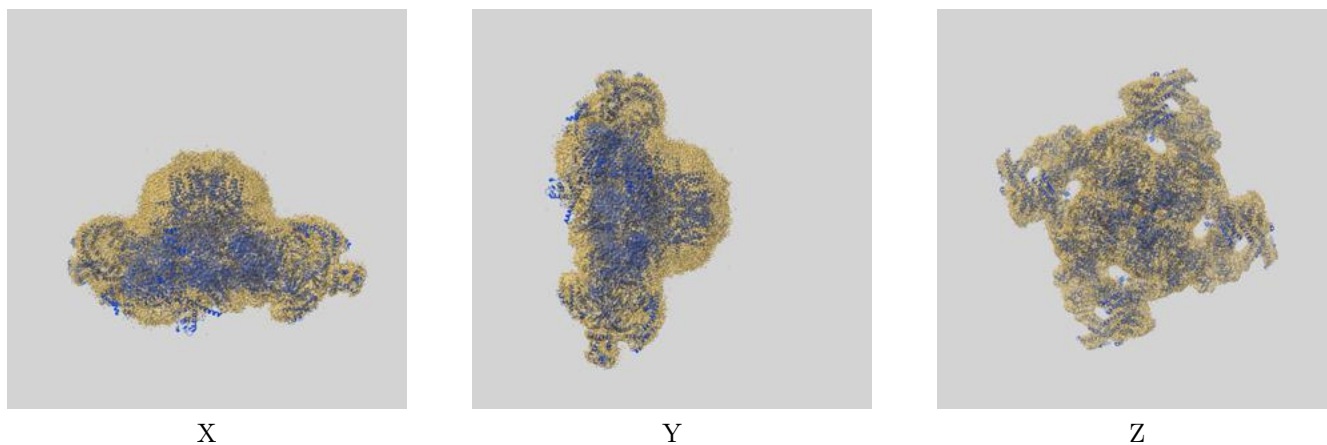
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	3.96	3.64
Unmasked-calculated*	3.88	4.32	3.92

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

9 Map-model fit [i](#)

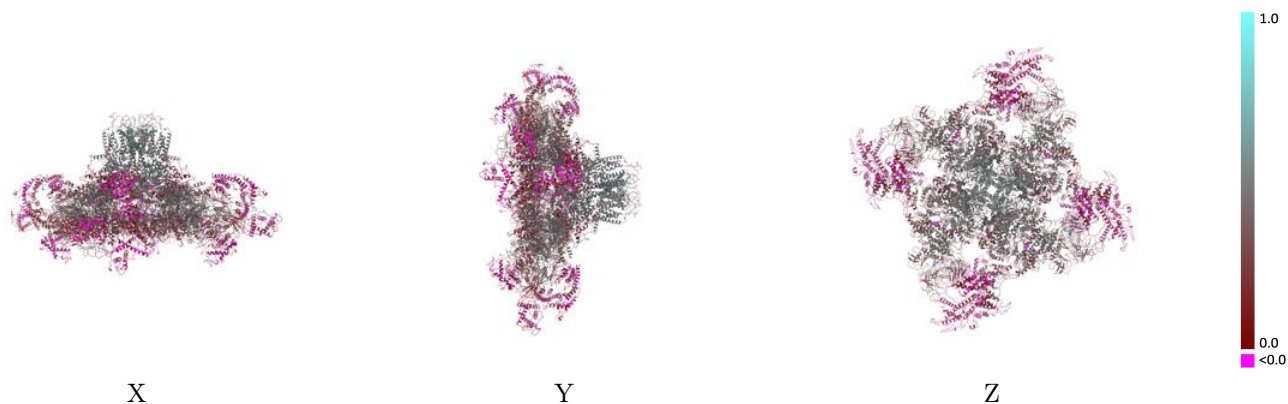
This section contains information regarding the fit between EMDB map EMD-27712 and PDB model 8DTZ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



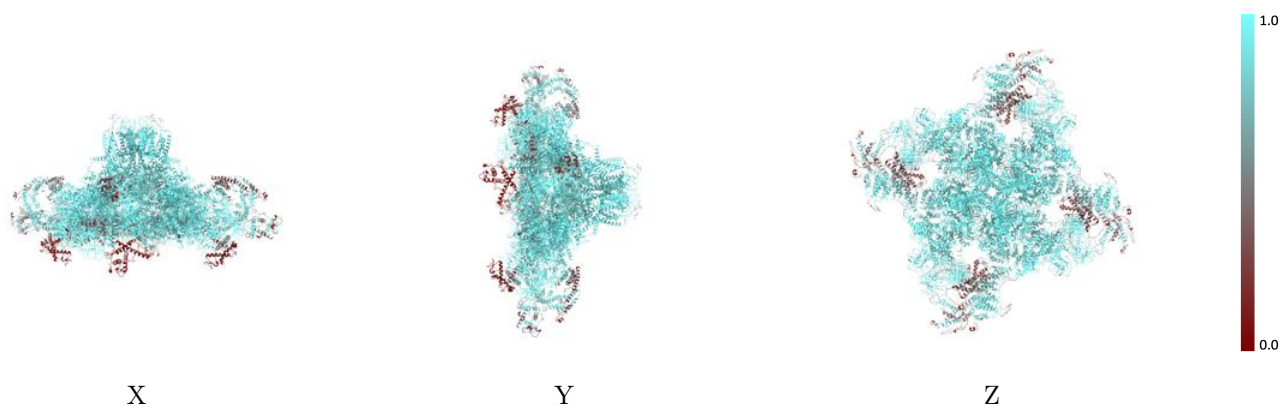
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



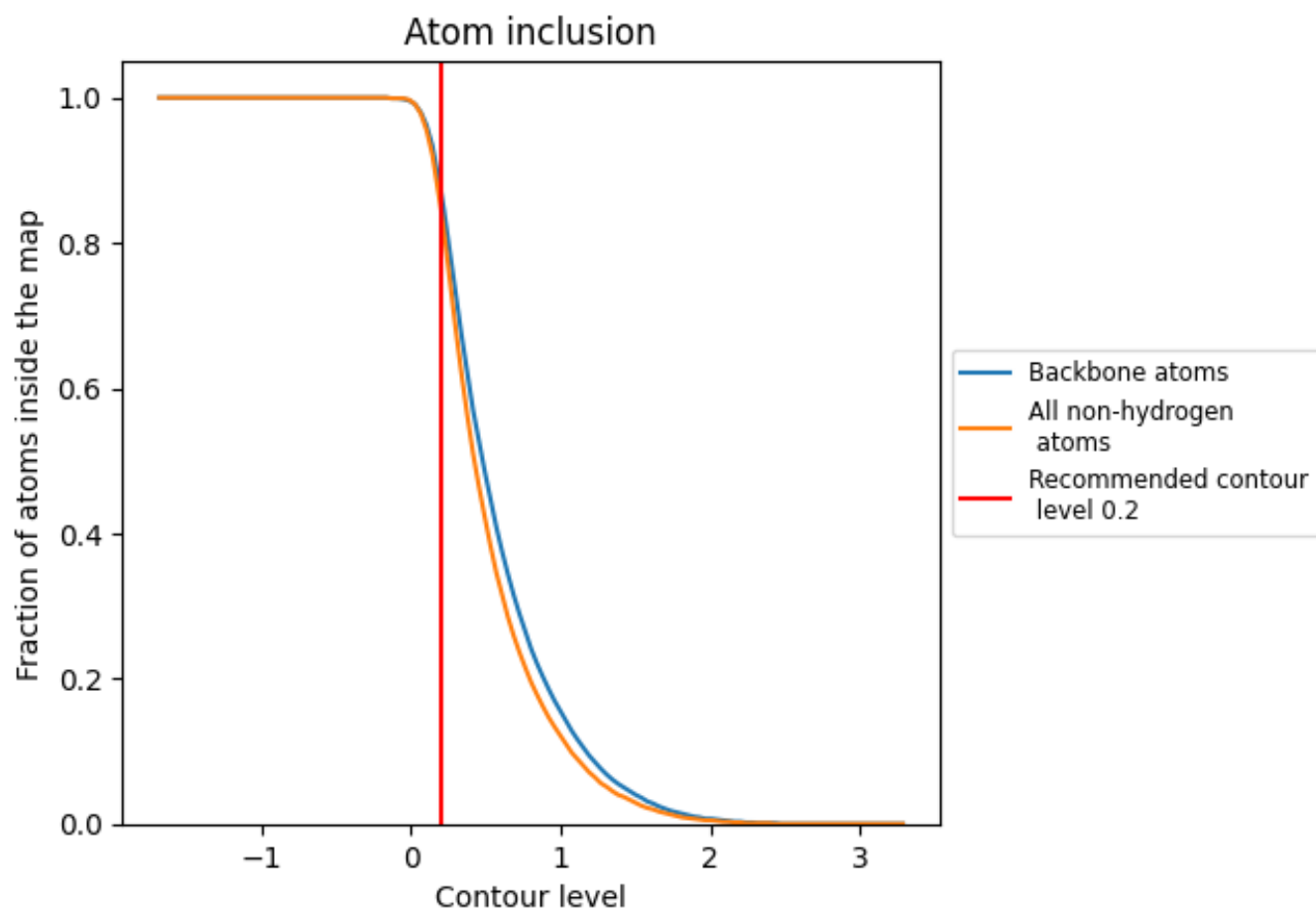
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.3020
A	 0.8450	 0.3010
B	 0.8450	 0.3000
C	 0.8460	 0.3000
D	 0.8450	 0.3010
E	 0.9380	 0.3560
F	 0.9370	 0.3550
G	 0.9340	 0.3570
H	 0.9370	 0.3580

