



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 10:55 PM UTC

PDB ID : 8DVV / pdb_00008dvv
EMDB ID : EMD-27746
Title : Recombinant mouse RyR2 triple phosphomimetic mutant
S2807D/S2813D/S2030D in complex with FKBP12.6 and nanodisc un-
der open-state conditions
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samsó, M.
Deposited on : 2022-07-29
Resolution : 3.68 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:

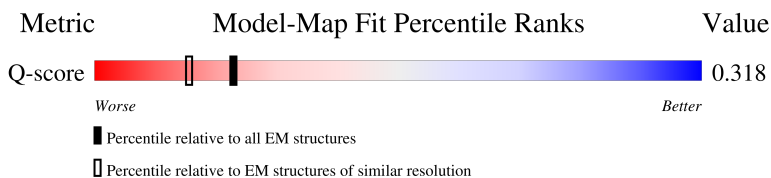
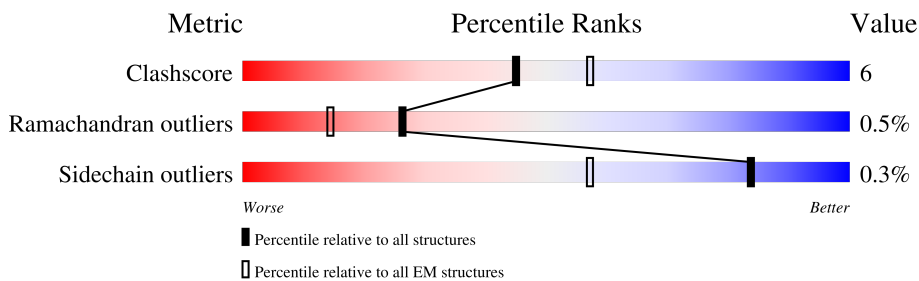
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.68 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	11376 (3.18 - 4.18)

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	<p>12% 66% 12% 22%</p>
1	B	4966	<p>12% 66% 12% 22%</p>
1	C	4966	<p>12% 66% 12% 22%</p>
1	D	4966	<p>12% 66% 12% 22%</p>

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Mol	Chain	Length	Quality of chain	
2	E	107		17%
2	F	107		15%
2	G	107		14%
2	H	107		16%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 119280 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	3886	29055	18436	4944	5507	168	0	0
1	B	3886	29055	18436	4944	5507	168	0	0
1	C	3886	29055	18436	4944	5507	168	0	0
1	D	3886	29055	18436	4944	5507	168	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2030	ASP	SER	engineered mutation	UNP E9Q401
A	2807	ASP	SER	engineered mutation	UNP E9Q401
A	2813	ASP	SER	engineered mutation	UNP E9Q401
B	2030	ASP	SER	engineered mutation	UNP E9Q401
B	2807	ASP	SER	engineered mutation	UNP E9Q401
B	2813	ASP	SER	engineered mutation	UNP E9Q401
C	2030	ASP	SER	engineered mutation	UNP E9Q401
C	2807	ASP	SER	engineered mutation	UNP E9Q401
C	2813	ASP	SER	engineered mutation	UNP E9Q401
D	2030	ASP	SER	engineered mutation	UNP E9Q401
D	2807	ASP	SER	engineered mutation	UNP E9Q401
D	2813	ASP	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	763	480	129	151	3	0	0
2	F	107	763	480	129	151	3	0	0
2	G	107	763	480	129	151	3	0	0

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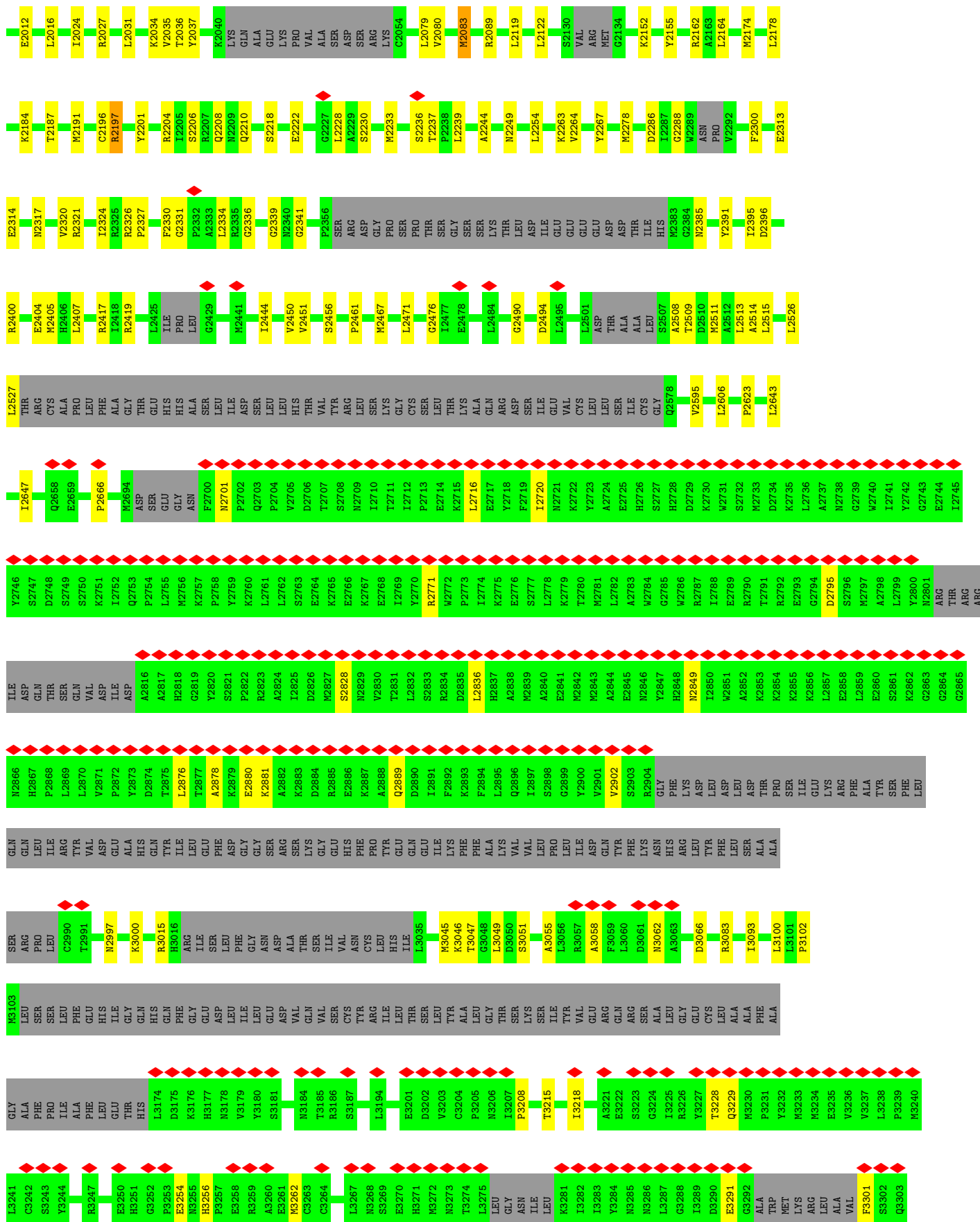
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	107	763	480	129	151	3	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

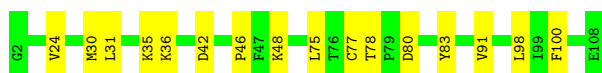
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0





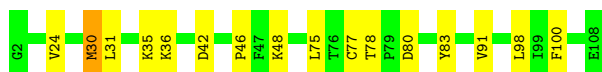
MET	ALA	ASP	ALA	GLY	GLY	ASP	E10	I11	D18	E19	Q33	K34	L35	E40	N57	S63	T66	V67	V68	L69	L73	M81	S200	L82	A83	M84	THR	VAL	GLU	LYS	SER	GLU	GLN	VAL	ASP	VAL	GLU	LYS	TRP	LYS	PHE	MET	M102	L114	Y115	G116	H117	A118	
L121	S124	M128	S139	T140	D141	D146	L149	T153	T161	G172	V175	V184	S185	V186	E189	L192	N198	S199	W201	F207	W212	I217	S218	G226	Y227	L228	V233	L234	R235	H240	T246	V247	P248	H261	R272														
S273	L274	R275	G276	S285	G286	I289	V300	T301	K312	N313	L314	A322	T327	K335	L338	ASP	VAL	GLY	VAL	R343	K344	E345	V346	D347	K355	C361	H365	L370	W371	L372	T373	A376	VAL	ASP	VAL	VAL	M494	I495	N496	L497	V498	L499	E500	C501	I502	D503	R504		
H394	H395	E396	G397	H398	L403	S406	S408	E411	E412	S413	R414	I419	F426	I430	L433	S437	V440	LEU	PRO	THR	I445	L459	D474	R478	L482	K483	Q486	N487	L488	E492	G493	M494	I495	N496	L497	V498	L499	E500	C501	I502	D503	R504							
L505	Y508	S509	S510	A511	A512	H513	F514	V517	L533	L536	A539	L540	I541	R542	G543	N544	R545	K546	N547	C548	A549	Q550	S554	L555	D556	W557	L558	L579	V580	E581	S582	L586	I589	L617	C618	V619	A624	S627	Q628	I632	N650	S654							
P657	M658	Q669	V679	V686	V695	G696	M697	E701	Y706	PRO	GLY	GLY	GLY	GLU	TRP	GLY	GLY	W716	G719	L722	F723	S724	Y725	F727	G728	W727	D728	L732	W733	C736	I737	A738	R739	I740	V741	S742	N745	D753	V754	I755	Q629	I632	N650	S654					
N771	M778	L787	F788	F789	V791	V800	R801	F802	L803	F811	E835	T854	VAL	SER	LEU	THR	THR	GLN	ALA	ALA	PHE	THR	PRO	PRO	VAL	VAL	VAL	PRO	PRO	PRO	HIS	L878	E879	R880	E883	R884	L885	E891	V894	M895	K896	K897	I898	W902					
Q903	Y904	G905	F906	V907	R908	D909	D910	N911	K912	R913	Q914	H915	L918	F921	C922	P925	E926	Q927	N930	Y931	M935	S936	L937	E938	T939	L940	A945	H949	V950	G951	I952	A953	D954	E955	H956	E959	K960	V961	K963	M964	K965	K968	N969	Y970	Q971	L972	T973	S974	
A979	P980	L983	S984	F985	I986	K987	L988	T989	P990	E993	A994	M995	T1017	I1020	Q1021	Q1022	D1023	V1024	K1025	N1026	L1032	L1037	R1041	S1045	N1046	R1047	D1048	R1051	E1052	A1053	V1054	R1055	L1058	G1059	G1061	TYR	HIS	LEU	GLU	ALA	PRO	GLN	ASP	ASP	HIS	ALA	SER	ARG	
ALA	GLU	VAL	CYS	SER	GLY	THR	G1082	R1089	R1100	F1103	V1108	D1112	W1117	P1124	G1129	F1135	A1136	F1137	Q1143	R1144	W1145	Y1152	D1160	C1164	M1165	V1166	D1167	E1170	H1171	T1172	M1173	T1176	L1177	M1178	G1179	E1180	L1190	K1193	D1194	F1195	D1199								
C1205	S1206	Q1211	R1214	M1215	N1216	F1217	T1223	L1224	K1225	F1239	T1243	N1244	R1245	D1246	W1250	L1251	V1261	P1262	E1268	I1269	L1273	P1281	Q1287	F1290	N1294	N1295	N1296	I1299	Y1302	P1307	I1308	GLU	CYS	ALA	GLU	VAL	PHE	SER	LYS	TYR	ALA	VAL	ALA						
GLY	GLY	LEU	PRO	GLY	ALA	GLY	PHE	TYR	LEU	PRO	LYS	ASN	THR	LYS	LEU	GLU	ASP	THR	ALA	HIS	ASP	GLY	LEU	VAL	PRO	ASP	TYR	GLU	ARG	ILE	ASP	LYS	LYS	THR	PRO	LYS	PRO	GLU	PHE	ASN	ASN	HIS	VAL	ASP	TYR	LYS	ALA	VAL	ALA
LYS	PRO	SER	ARG	LEU	LYS	GLN	ARG	PHE	LEU	LEU	ARG	THR	LYS	PRO	PRO	ASP	TYR	THR	VAL	ALA	ALA	ASP	ASP	TYR	GLU	ARG	TYR	ILE	ASP	LEU	MET	GLN	THR	PRO	LYS	PRO	GLU	PHE	ASN	ASN	HIS	VAL	ASP	TYR	LYS	ALA	VAL	ALA	
S1424	T1425	Y1426	P1434	G1444	W1445	I1446	F1450	V1462	R1463	T1464	V1465																																						

L3472	K3412	L3352	G3288	I3226	I3225	VAL	ASP	I2850	R2790	K2730	CYS
L3473	R3413	L3353	I3289	R3226	R3227	GLU	ASP	W2851	T2791	W2731	LEU
P3474	E3414	I3354	D3290	Y3227	T3228	ARG	ASP	W2852	R2792	S2732	SER
L3475	E3415	L3355	E3291	T3228	Q3229	GLN	THR	K2853	E2793	M2733	ILE
G3476	Q3416	L3356	G3292	Q3229	M3230	ARG	PRO	K2854	E2794	D2734	CYS
L3477	N3417	E3357	ALA	ALA	D3066	ALA	ILE	K2855	G2795	K2735	GLY
N3478	F3418	F3358	TRP	P3231	M3230	GLY	LYS	K2856	S2796	L2736	Q2578
V3479	V3419	T3359	NET	Y3232	Y3232	GLU	LEU	K2857	M2797	A2737	V2595
C3480	V3420	L3360	LYS	M3233	M3233	CYS	PHE	E2858	L2798	N2738	L2606
A3481	Q3421	L3361	ARG	M3234	M3234	ALA	ALA	L2859	L2799	G2739	L2606
P3482	N3422	A3362	LEU	E3235	E3235	ALA	TYR	E2860	Y2800	W2740	P2623
G3483	E3423	R3363	VAL	V3236	V3236	PHE	SER	S2861	M2801	I2741	L2643
D3484	I3424	L3365	F3301	V3237	V3237	ALA	ALA	S2862	ARG	Y2742	L2643
N3425	N3425	L3365	S3302	L3238	L3238	GLY	GLN	Q2863	THR	G2743	I2647
E3486	N3426	Y3366	Q3303	L3238	L3238	ALA	ARG	G2864	ARG	E2744	I2647
L3487	M3427	P3304	P3304	PHE	PHE	PRO	PRO	G2865	ILE	I2745	Q2658
S3428	M3428	I3305	I3305	ALA	ALA	ALA	ASP	G2866	ASP	Y2746	E2659
F3429	F3429	M3307	I3306	PHE	PHE	VAL	VAL	H2867	THR	S2747	P2666
L3430	L3430	K3308	I3308	GLU	GLU	GLU	ASP	P2868	SER	D2748	W0694
I3431	I3431	V3309	V3309	THR	THR	ALA	ALA	L2869	GLN	S2749	W0694
F3432	F3432	K3310	K3310	HIS	HIS	HIS	HIS	L2870	ASP	K2750	ASP
D3433	D3433	P3311	P3311	L3174	L3174	TYR	TYR	L2871	GLN	K2751	GLU
F3434	F3434	I3373	I3373	D3175	D3175	ILE	ILE	P2872	ASP	I2752	GLY
K3435	K3435	L3312	Q3312	K3176	K3176	GLU	GLU	Y2873	A2816	Q2753	ASN
F3495	F3495	F3375	L3313	H3177	H3177	PHE	PHE	D2874	A2817	P2754	F2700
S3496	S3496	V3376	L3314	G3252	G3252	GLY	GLY	H2875	H2818	L2755	N2701
L3497	K3437	D3377	L3314	N3178	N3178	LEU	LEU	T2876	G2819	M2756	F2702
K3498	K3438	Y3378	K3315	V3179	V3179	ASP	PHE	L2877	S2820	K2757	F2703
D3499	N3439	M3256	T3316	F3180	F3180	GLY	GLY	T2877	Y2821	P2758	F2704
F3500	N3440	H3256	H3317	S3181	S3181	ILE	ASN	A2879	S2822	Y2759	F2705
A3501	K3441	P3257	F3318	GLU	GLU	ALA	ALA	E2880	R2823	K2760	D2706
E3502	A3442	E3258	L3319	N3184	N3184	ASP	THR	K2881	R2824	L2761	T2707
E3503	K3443	R3259	P3320	F3185	F3185	SER	SER	E2882	A2824	L2762	S2708
V3504	S3444	A3260	L3321	R3186	R3186	ILE	ILE	K2882	E2824	S2763	L2710
R3505	I3445	F3261	M3322	S3187	S3187	VAL	VAL	A2882	D2826	K2765	T2711
D3506	Q3446	M3262	E3323	L3194	L3194	HIS	HIS	D2884	D2826	E2766	L2712
F3507	Q3447	C3264	K3324	E3201	E3201	CYS	CYS	R2885	M2827	K2767	L2713
L3508	R3448	C3264	L3325	L3194	L3194	ARG	HIS	E2886	S2829	E2768	E2714
R3509	K3449	L3267	K3326	E3201	E3201	THR	ILE	K2887	W2830	I2769	K2715
S3510	K3450	N3268	E3323	D3202	D3202	LEU	ILE	T2887	T2831	R2770	L2716
N3511	M3451	S3269	K3328	V3203	V3203	SER	LYS	A2888	L2833	R2771	E2717
K3452	K3452	E3270	K3328	C3204	C3204	LEU	PHE	Q2889	L2833	W2772	Y2718
R3453	R3453	H3271	L3329	F3205	F3205	TYR	PHE	D2890	R2834	P2773	F2719
L3454	K3454	H3271	A3329	N3206	N3206	ALA	ALA	E2890	E2834	I2774	L2720
G3455	G3455	M3272	V3333	M3207	M3207	LEU	ALA	F2892	D2835	K2775	M2721
Q3456	D3456	N3273	S3334	T3207	T3207	GLY	LYS	F2892	D2835	L2776	K2722
F3457	F3457	E3335	E3334	P3208	P3208	THR	VAL	K2893	H2836	S2777	Y2723
L3458	Y3458	E3336	E3336	T3215	T3215	SER	VAL	F2894	L2837	I2778	A2724
S3459	Q3459	L3275	L3339	L3218	L3218	LEU	PRO	Q2896	A2838	E2776	E2725
ASP	M3460	GLY	K3340	I3218	I3218	ASN	LEU	T2897	M2839	K2777	H2726
PRO	Q3461	ILE	A3343	A3221	A3221	ILE	LEU	S2898	E2840	L2778	H2727
ALA	W3405	LEU	R3344	E3222	E3222	ILE	LEU	Q2899	E2841	L2779	S2727
ILE	S3406	ARG	G3345	S3223	S3223	THR	LEU	S2899	E2841	K2779	E2728
ARG	S3463	THR	D3346	G3224	G3224	THR	VAL	Y2900	M2843	T2780	H2728
TRP	K3407	GLN	M3347	Y3284	Y3284	THR	VAL	V2901	E2844	M2781	S2727
GLN	S3408	MET	S3347	N3285	N3285	SER	VAL	V2902	E2844	L2782	H2729
MET	I3465	ALA	M3348	N3286	N3286	LYS	VAL	S2903	M2846	A2783	D2729
ALA	V3466	LEU	E3349	N3287	N3287	LEU	PRO	S2904	E2847	W2784	
LEU	A3467	TYR	A3350	L3287	L3287	LEU	LEU	R2904	H2848	G2785	
TYR	A3468	LYS	E3351			TYR	LEU	GLY	PHE	W2786	
LYS	L3469					ASP	LEU	ASP	LYS	R2787	
	K3470					LEU	LEU	ASP	ASP	I2788	
	R3471									E2789	



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

Chain G: 85% 14%



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

Chain H: 84% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	73782	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.311	Depositor
Minimum map value	-0.628	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	496.80002, 496.80002, 496.80002	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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: CA, 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	0.13	0/29611	0.37	3/40214 (0.0%)
1	B	0.13	0/29611	0.37	3/40214 (0.0%)
1	C	0.13	0/29611	0.37	3/40214 (0.0%)
1	D	0.13	0/29611	0.37	3/40214 (0.0%)
2	E	0.09	0/778	0.31	0/1060
2	F	0.10	0/778	0.31	0/1060
2	G	0.09	0/778	0.31	0/1060
2	H	0.10	0/778	0.31	0/1060
All	All	0.13	0/121556	0.37	12/165096 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1124	PRO	N-CA-CB	7.41	110.24	103.20
1	D	1124	PRO	N-CA-CB	7.41	110.24	103.20
1	C	1124	PRO	N-CA-CB	7.39	110.22	103.20
1	B	1124	PRO	N-CA-CB	7.36	110.19	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	SER	CB-CA-C	-6.74	108.79	116.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4181	GLU	Peptide
1	B	4181	GLU	Peptide
1	C	4181	GLU	Peptide
1	D	4181	GLU	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	29055	0	27182	364	0
1	B	29055	0	27182	358	0
1	C	29055	0	27182	364	0
1	D	29055	0	27182	375	0
2	E	763	0	709	12	0
2	F	763	0	709	11	0
2	G	763	0	709	11	0
2	H	763	0	709	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	119280	0	111564	1458	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 6.

The worst 5 of 1458 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE1	1:B:2417:ARG:NH1	2.24	0.71
1:D:1205:CYS:SG	1:D:1206:SER:N	2.64	0.71
1:A:1205:CYS:SG	1:A:1206:SER:N	2.64	0.71
1:C:1205:CYS:SG	1:C:1206:SER:N	2.64	0.71
1:B:1205:CYS:SG	1:B:1206:SER:N	2.64	0.70

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	3818/4966 (77%)	3361 (88%)	436 (11%)	21 (1%)	21	52
1	B	3818/4966 (77%)	3361 (88%)	436 (11%)	21 (1%)	21	52
1	C	3818/4966 (77%)	3363 (88%)	435 (11%)	20 (0%)	24	56
1	D	3818/4966 (77%)	3362 (88%)	436 (11%)	20 (0%)	24	56
2	E	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	F	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	G	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	H	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
All	All	15692/20292 (77%)	13831 (88%)	1779 (11%)	82 (0%)	26	56

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1462	VAL
1	B	1462	VAL
1	C	1462	VAL
1	D	1462	VAL
1	A	411	GLU

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	2915/4355 (67%)	2906 (100%)	9 (0%)	86	83
1	B	2915/4355 (67%)	2907 (100%)	8 (0%)	86	83
1	C	2915/4355 (67%)	2907 (100%)	8 (0%)	86	83
1	D	2915/4355 (67%)	2906 (100%)	9 (0%)	86	83
2	E	76/88 (86%)	76 (100%)	0	100	100
2	F	76/88 (86%)	76 (100%)	0	100	100
2	G	76/88 (86%)	75 (99%)	1 (1%)	61	70
2	H	76/88 (86%)	76 (100%)	0	100	100
All	All	11964/17772 (67%)	11929 (100%)	35 (0%)	84	83

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	686	VAL
1	D	1195	PHE
1	D	2477	ILE
1	B	686	VAL
1	B	459	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	608	HIS
2	E	88	HIS
1	D	969	ASN
1	D	3317	HIS
2	H	95	ASN

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 [i](#)

Of 8 ligands modelled in this entry, 8 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.

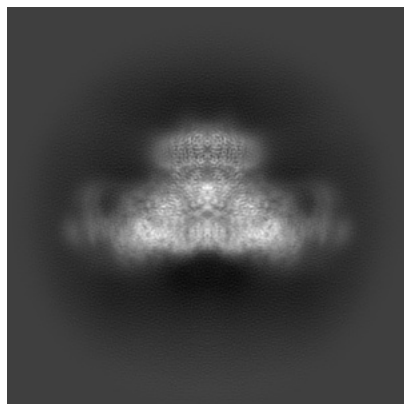
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27746. These allow visual inspection of the internal detail of the map and identification of artifacts.

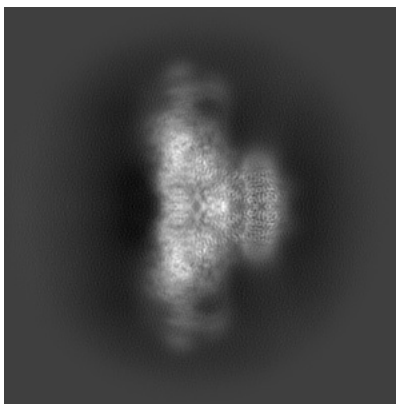
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

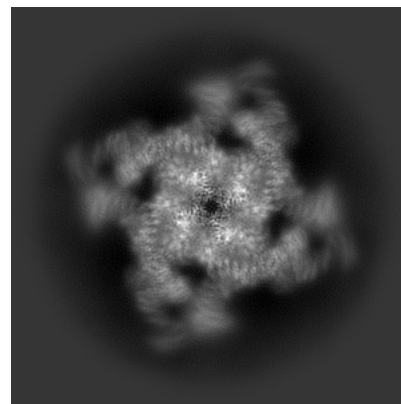
6.1.1 Primary map



X

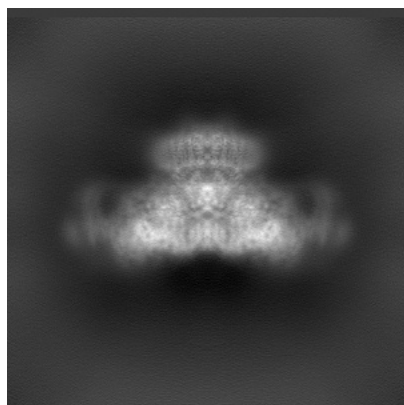


Y

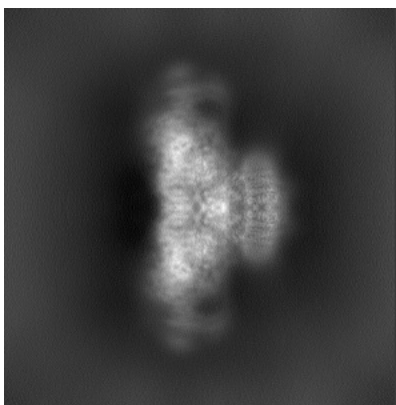


Z

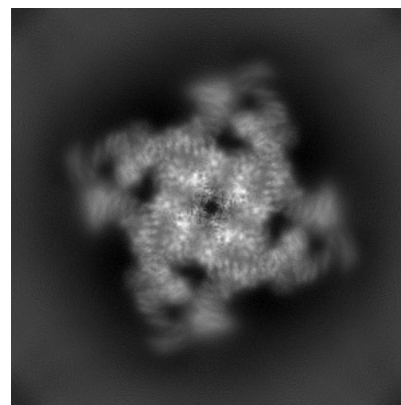
6.1.2 Raw map



X



Y

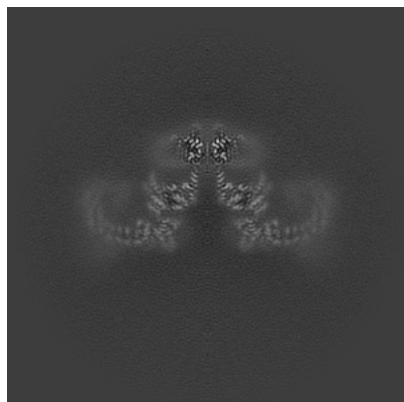


Z

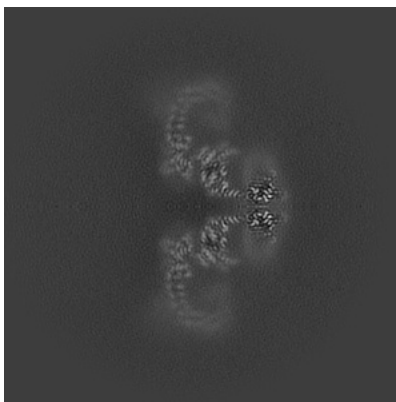
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

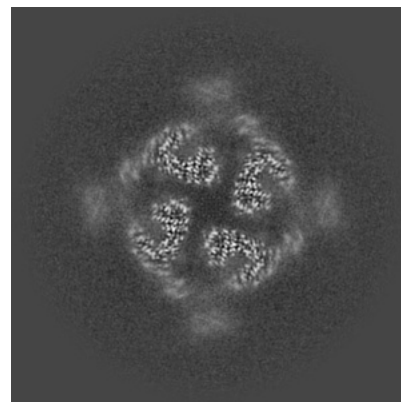
6.2.1 Primary map



X Index: 230

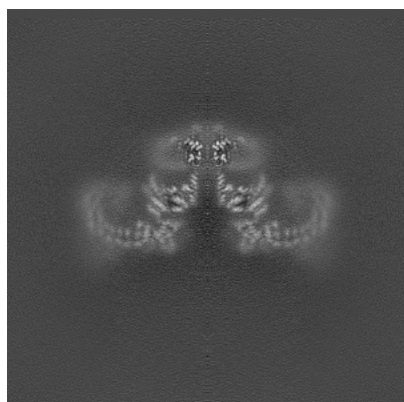


Y Index: 230

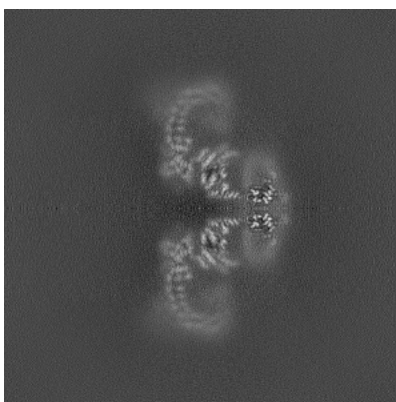


Z Index: 230

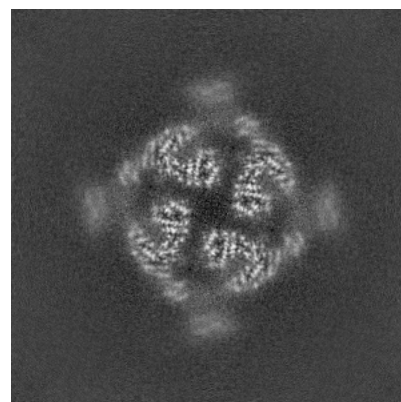
6.2.2 Raw map



X Index: 230



Y Index: 230

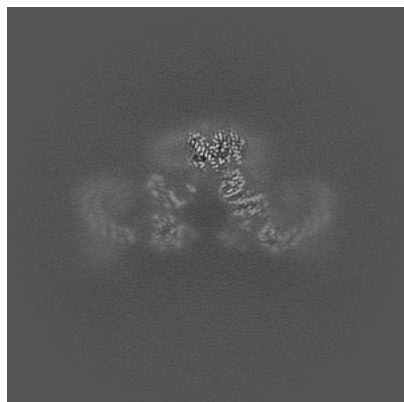


Z Index: 230

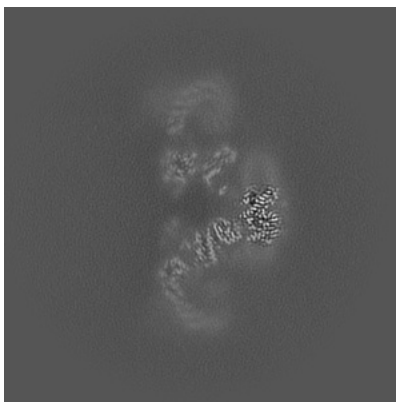
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

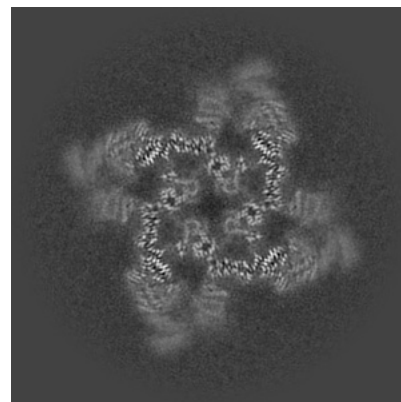
6.3.1 Primary map



X Index: 222

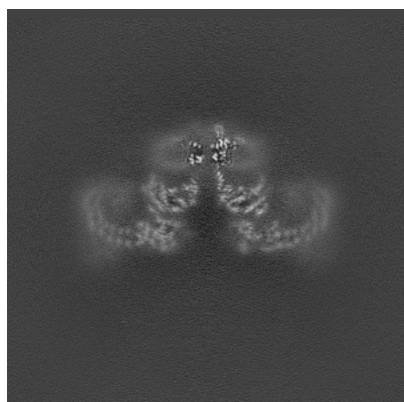


Y Index: 222

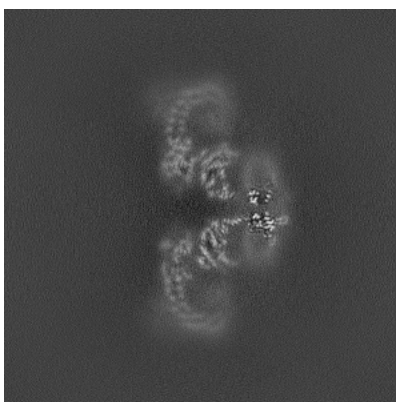


Z Index: 203

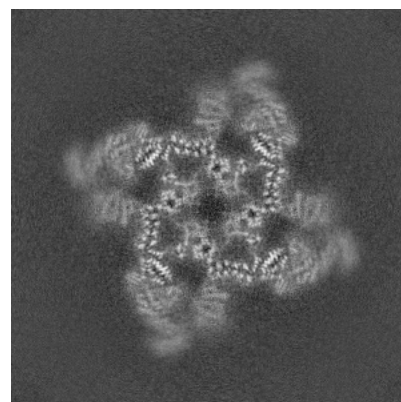
6.3.2 Raw map



X Index: 228



Y Index: 228

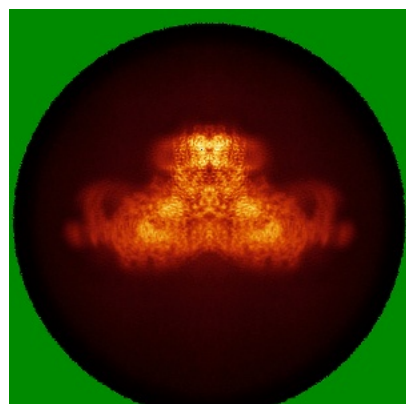


Z Index: 203

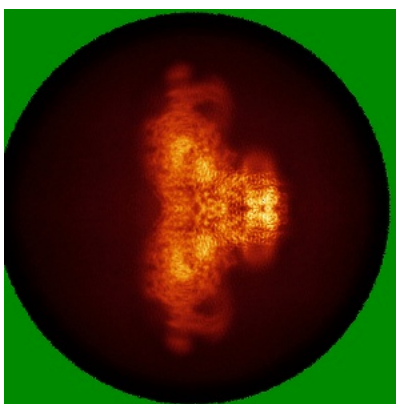
The images above show the largest variance slices of the map in three orthogonal directions.

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

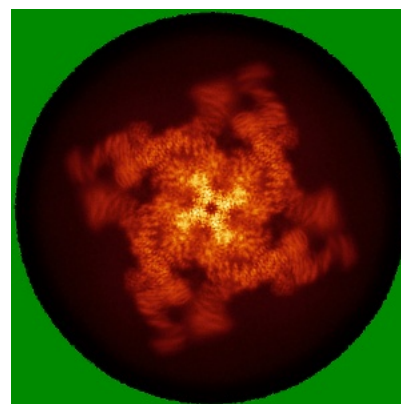
6.4.1 Primary map



X

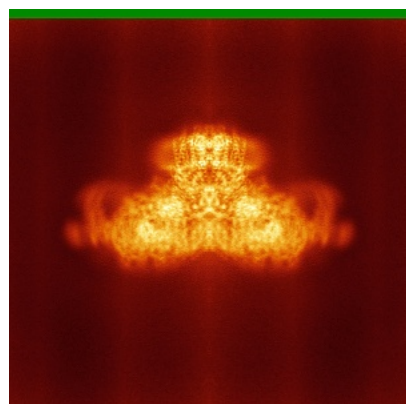


Y

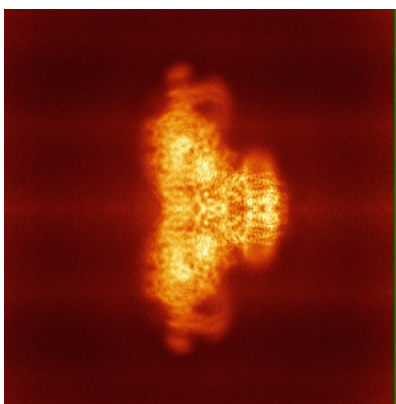


Z

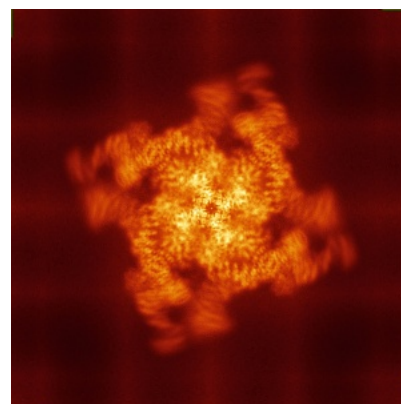
6.4.2 Raw map



X



Y

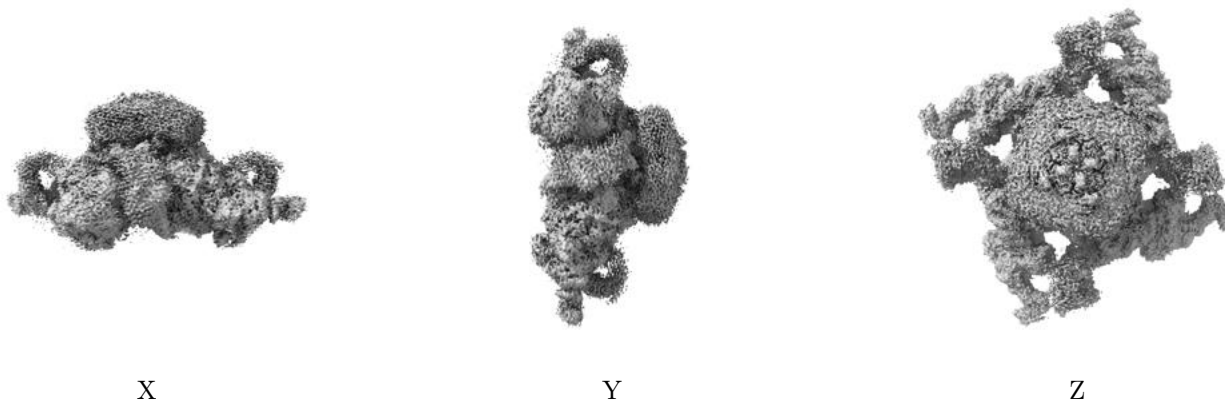


Z

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.

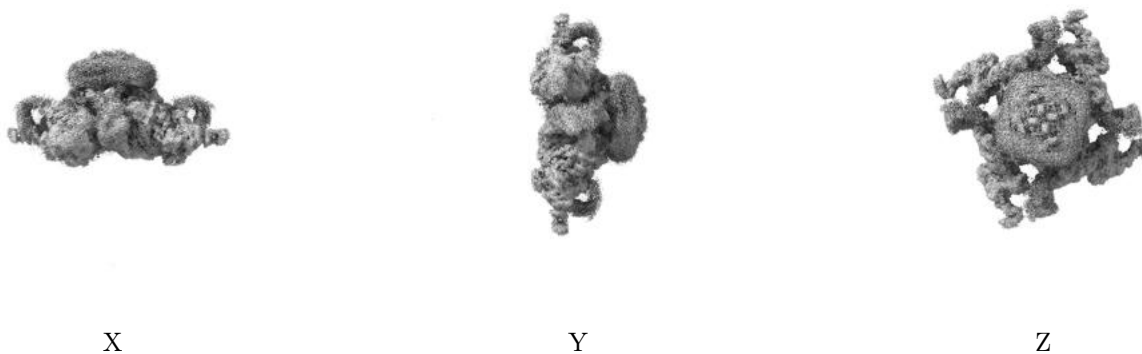
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

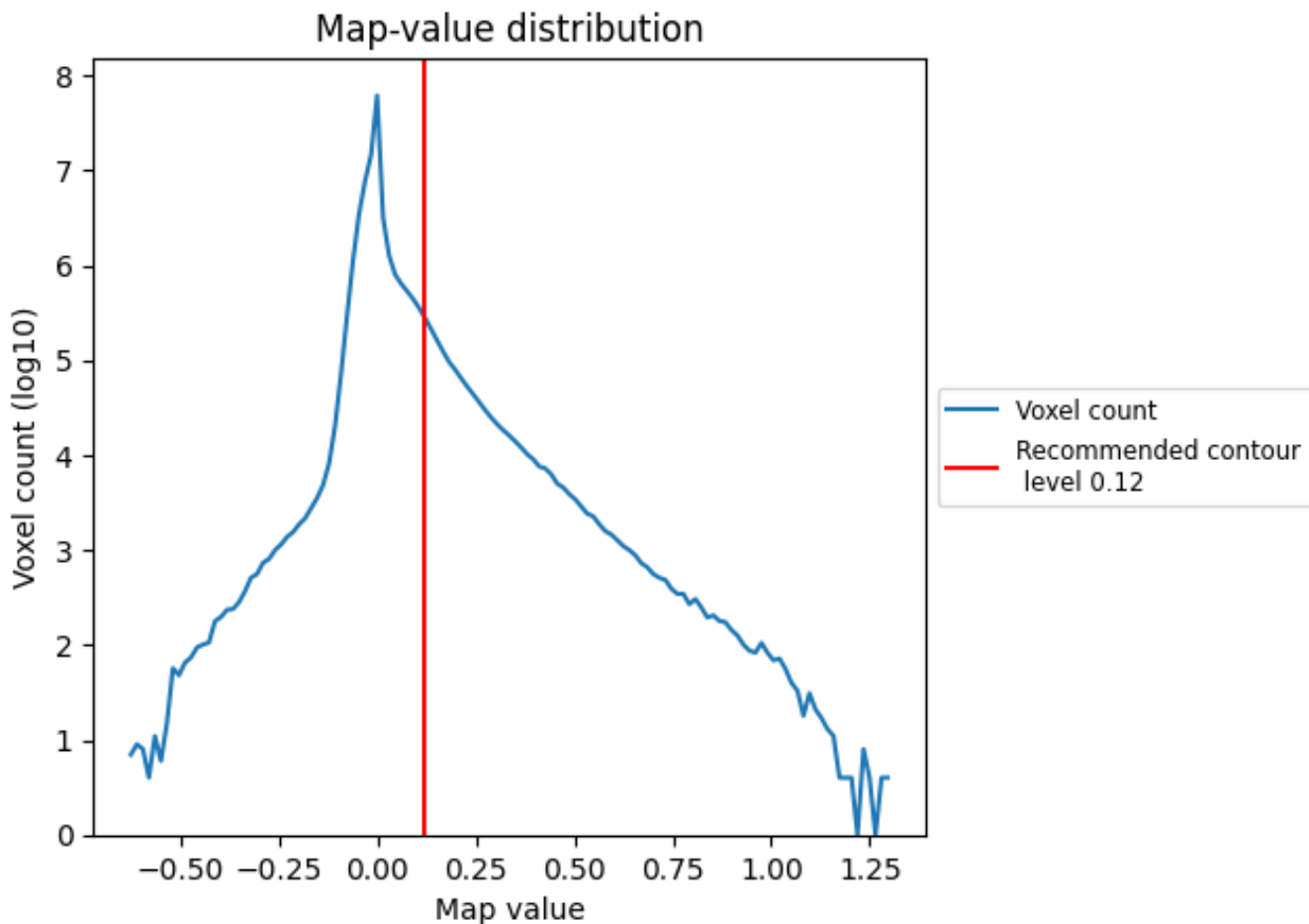
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

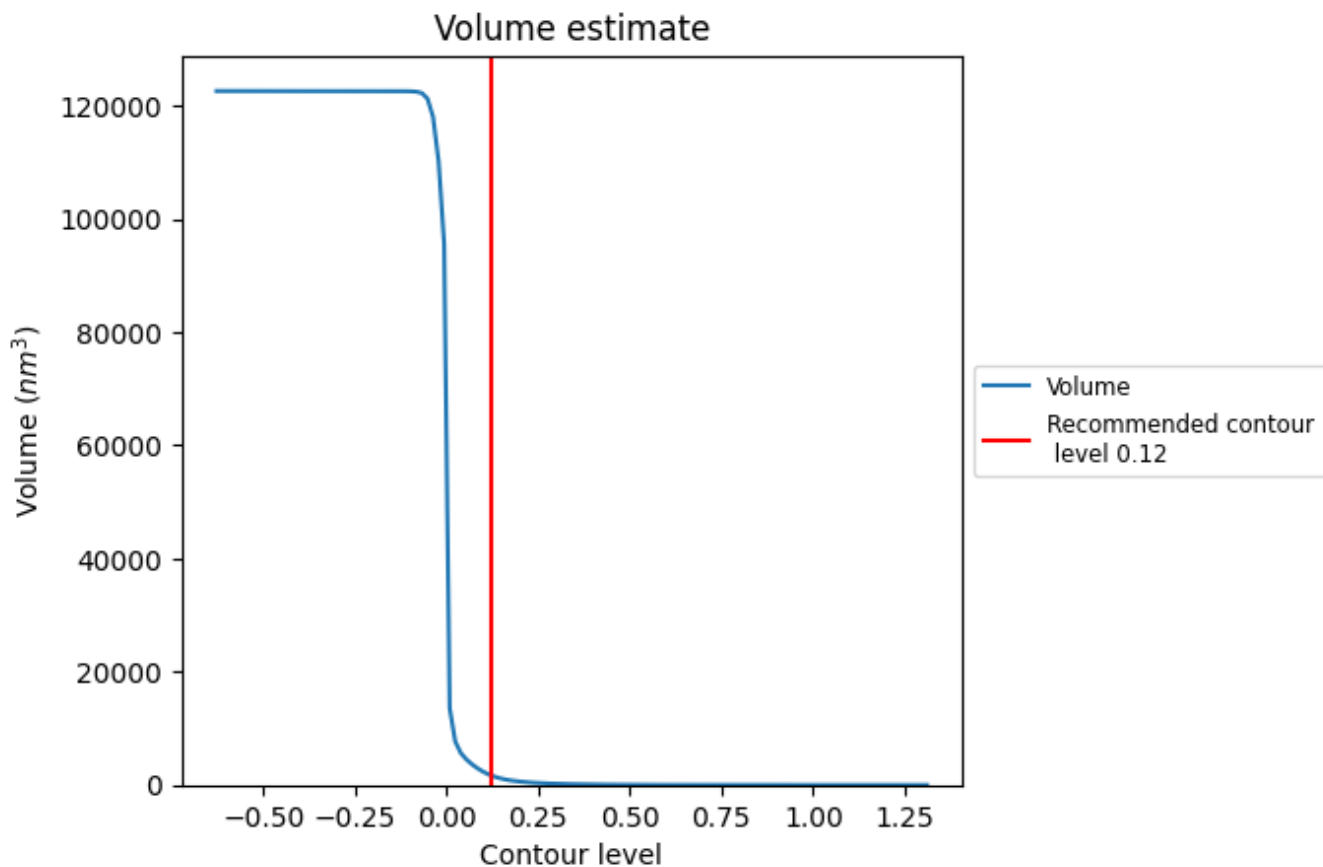
This section contains the results of statistical analysis of the map.

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.

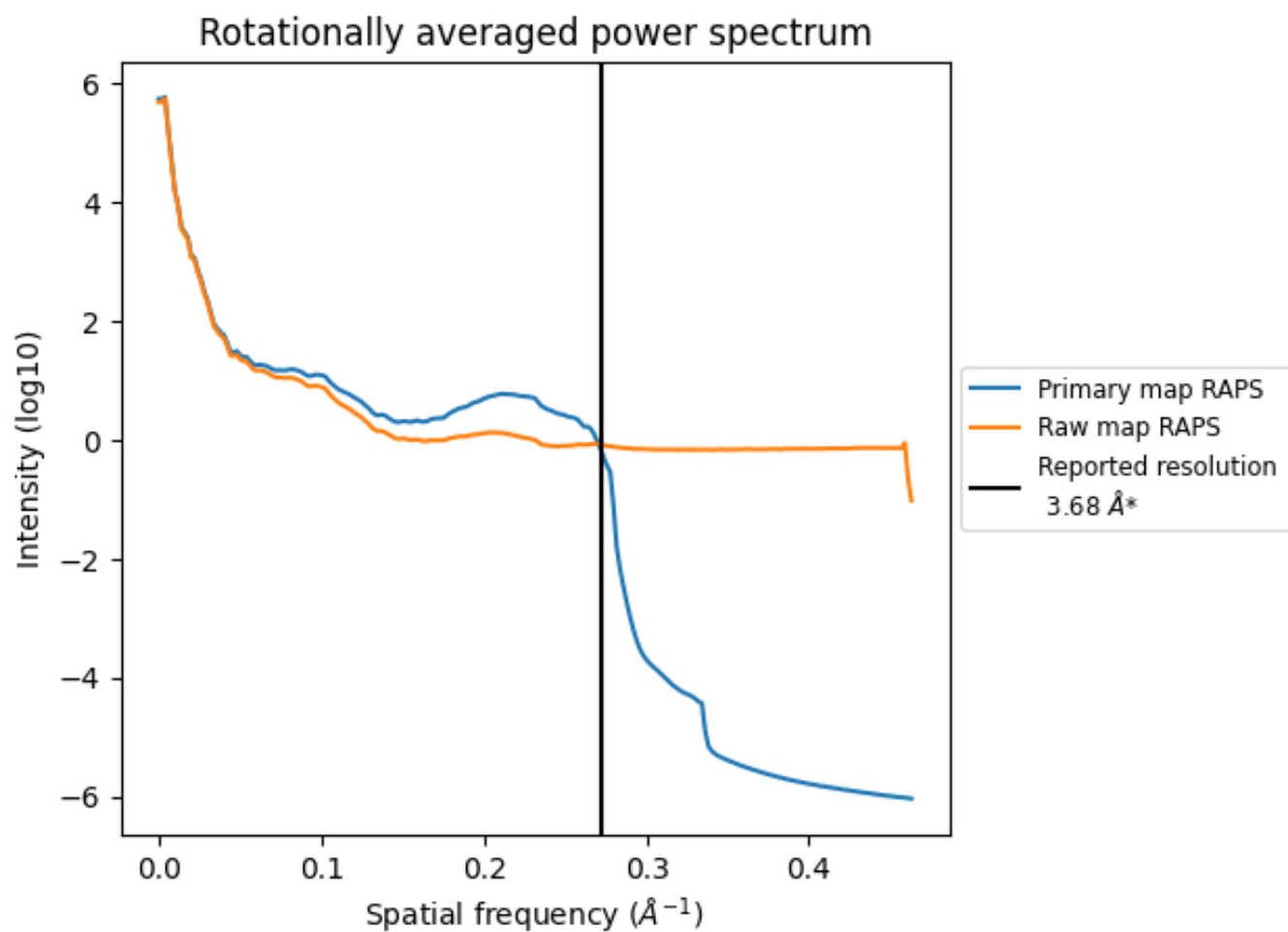
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1734 nm³; this corresponds to an approximate mass of 1567 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

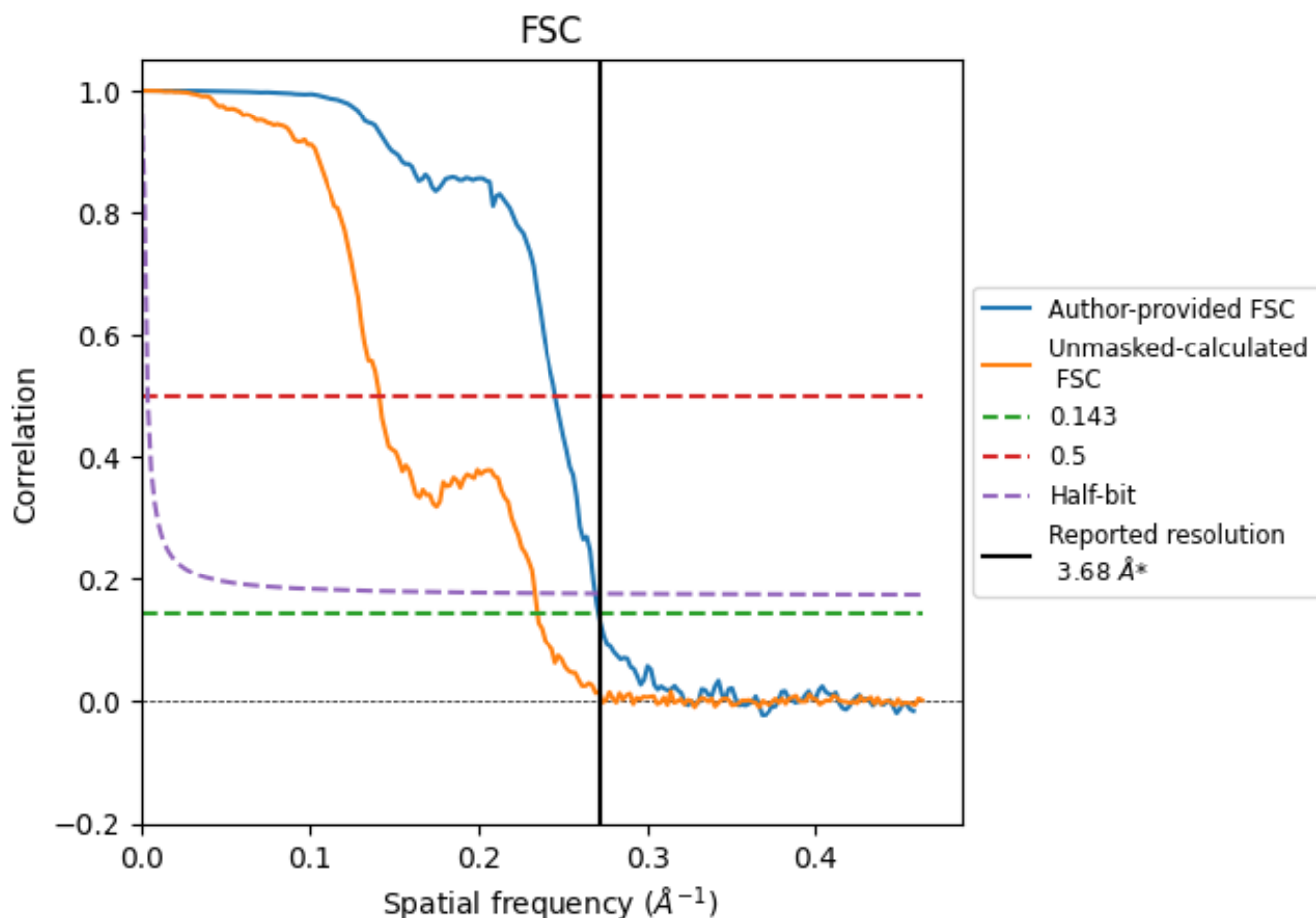


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 Å⁻¹

8.2 Resolution estimates [i](#)

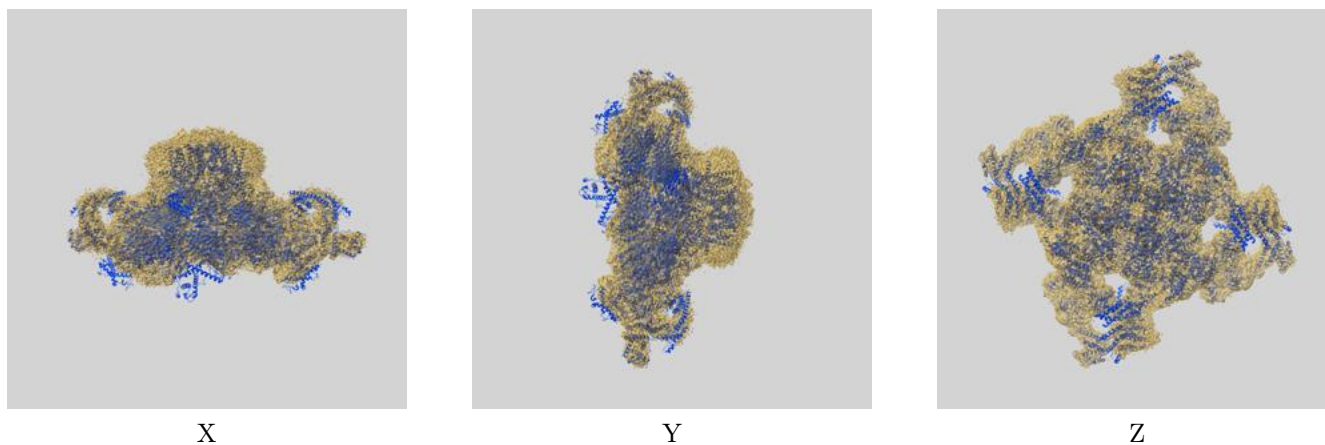
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.07	3.71
Unmasked-calculated*	4.26	7.08	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.68 by more than 10 %

9 Map-model fit [i](#)

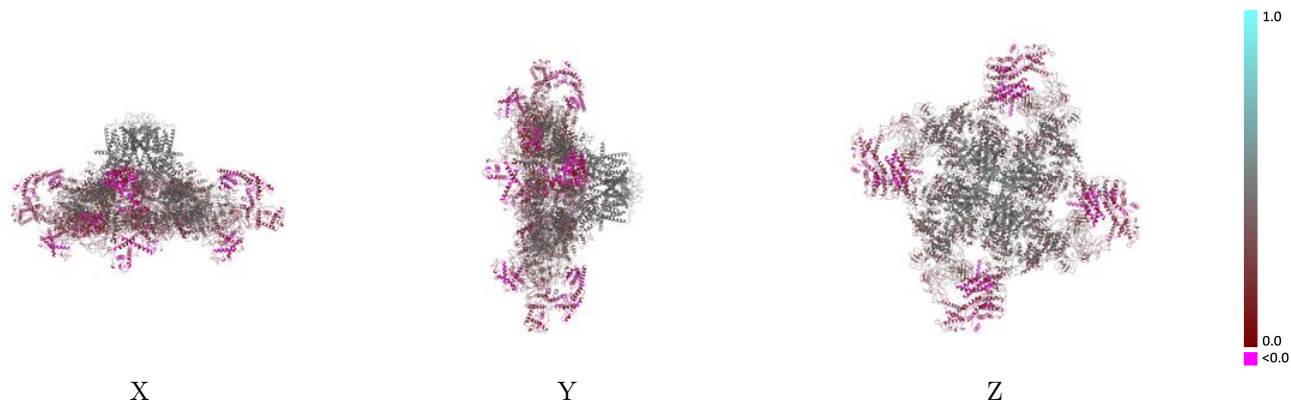
This section contains information regarding the fit between EMDB map EMD-27746 and PDB model 8DVV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.12 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](#)

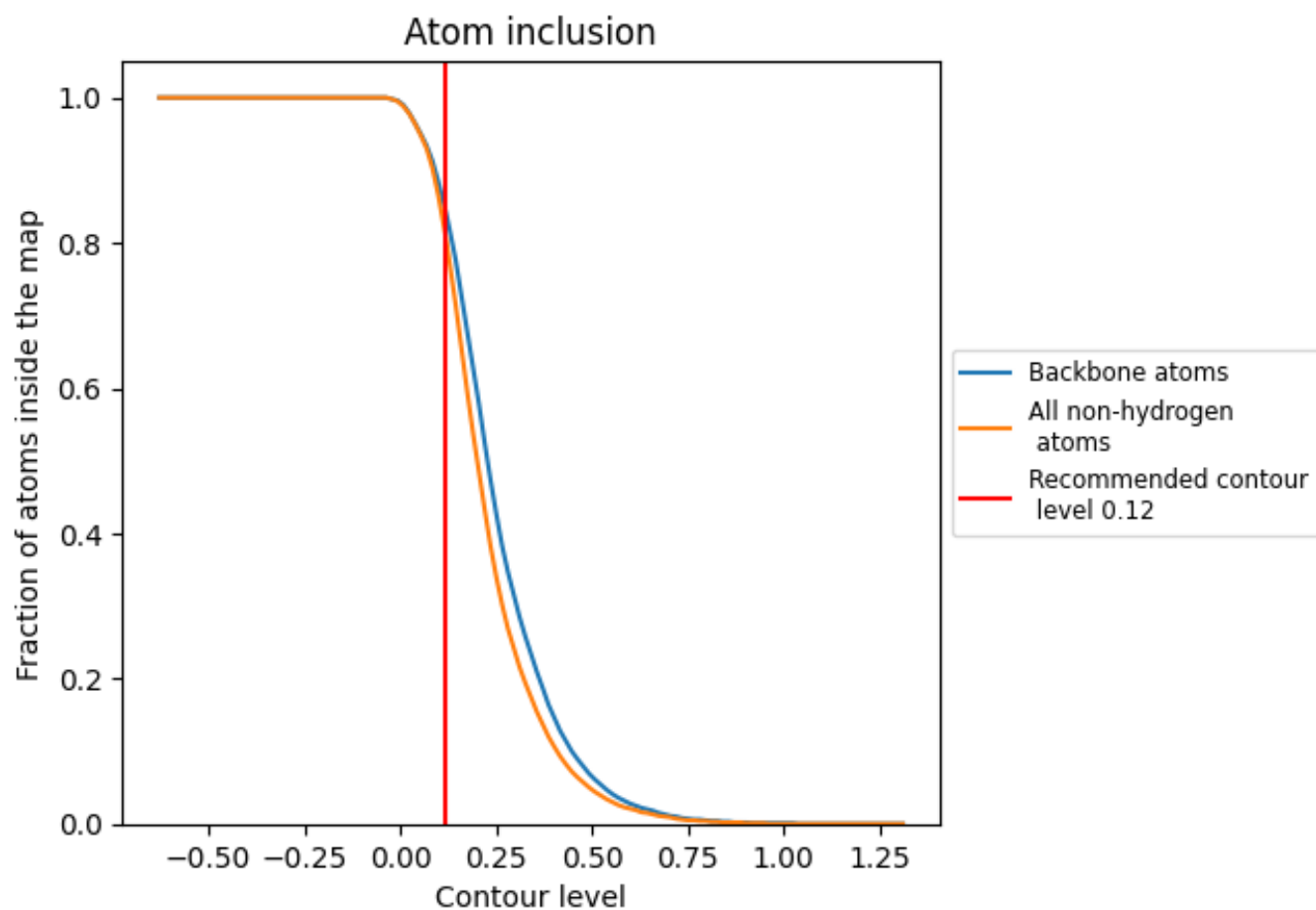


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.



















9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.3180
A	 0.8010	 0.3150
B	 0.8010	 0.3160
C	 0.8010	 0.3160
D	 0.8010	 0.3160
E	 0.9510	 0.3910
F	 0.9510	 0.3940
G	 0.9520	 0.3930
H	 0.9520	 0.3910

