



wwPDB EM Validation Summary Report

Jan 25, 2024 – 01:35 PM EST


PDB ID : 8DVV
EMDB ID : EMD-27746
Title : Recombinant mouse RyR2 triple phosphomimetic mutant S2807D/S2813D/S2030D in complex with FKBP12.6 and nanodisc under 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:

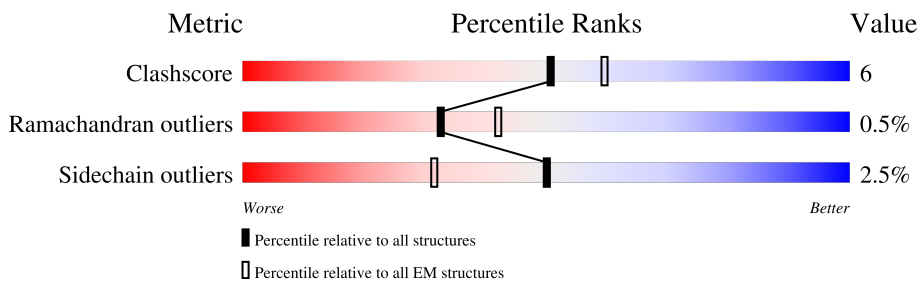
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.68 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)
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 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 (three-letter code: 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

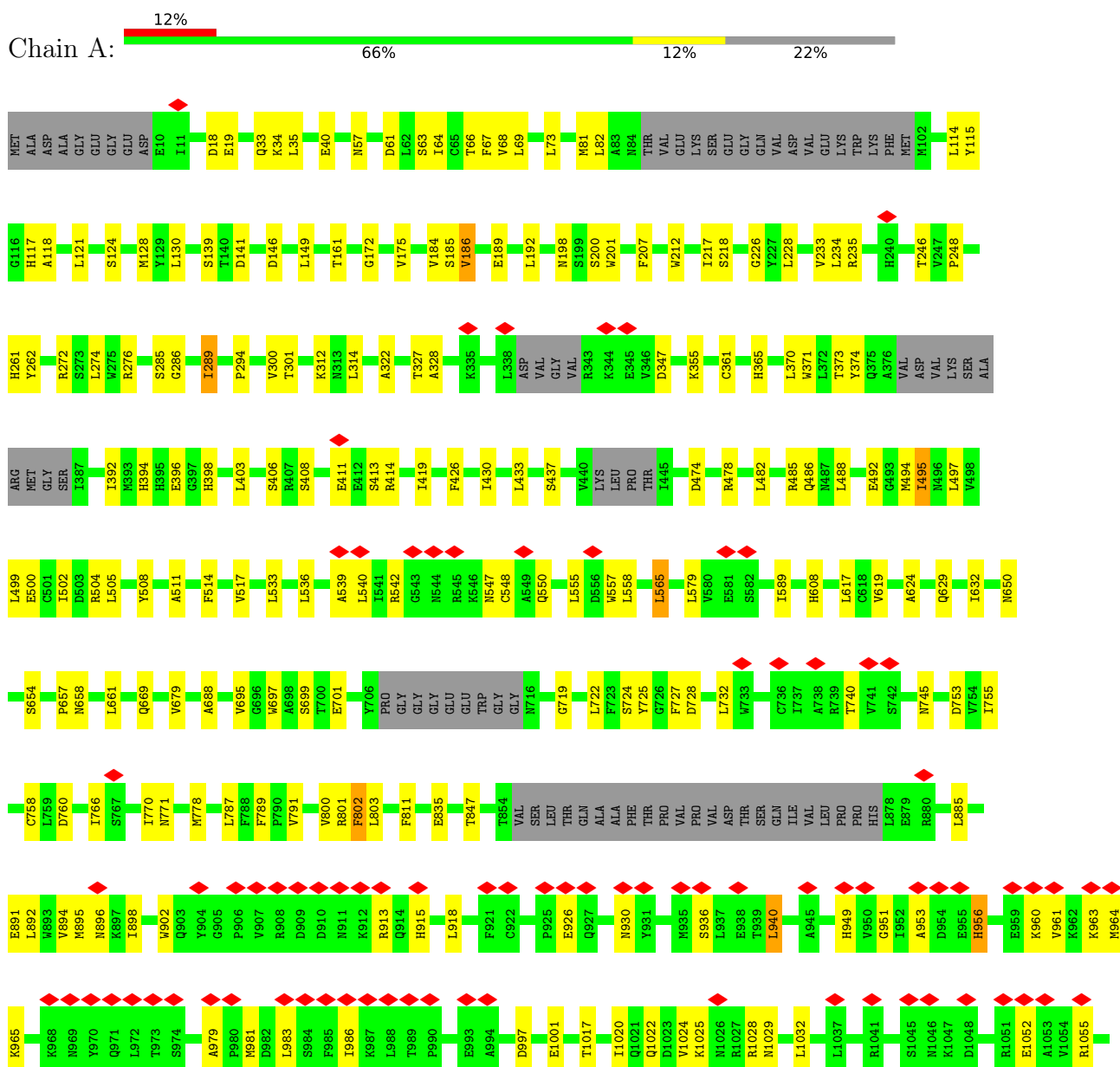
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

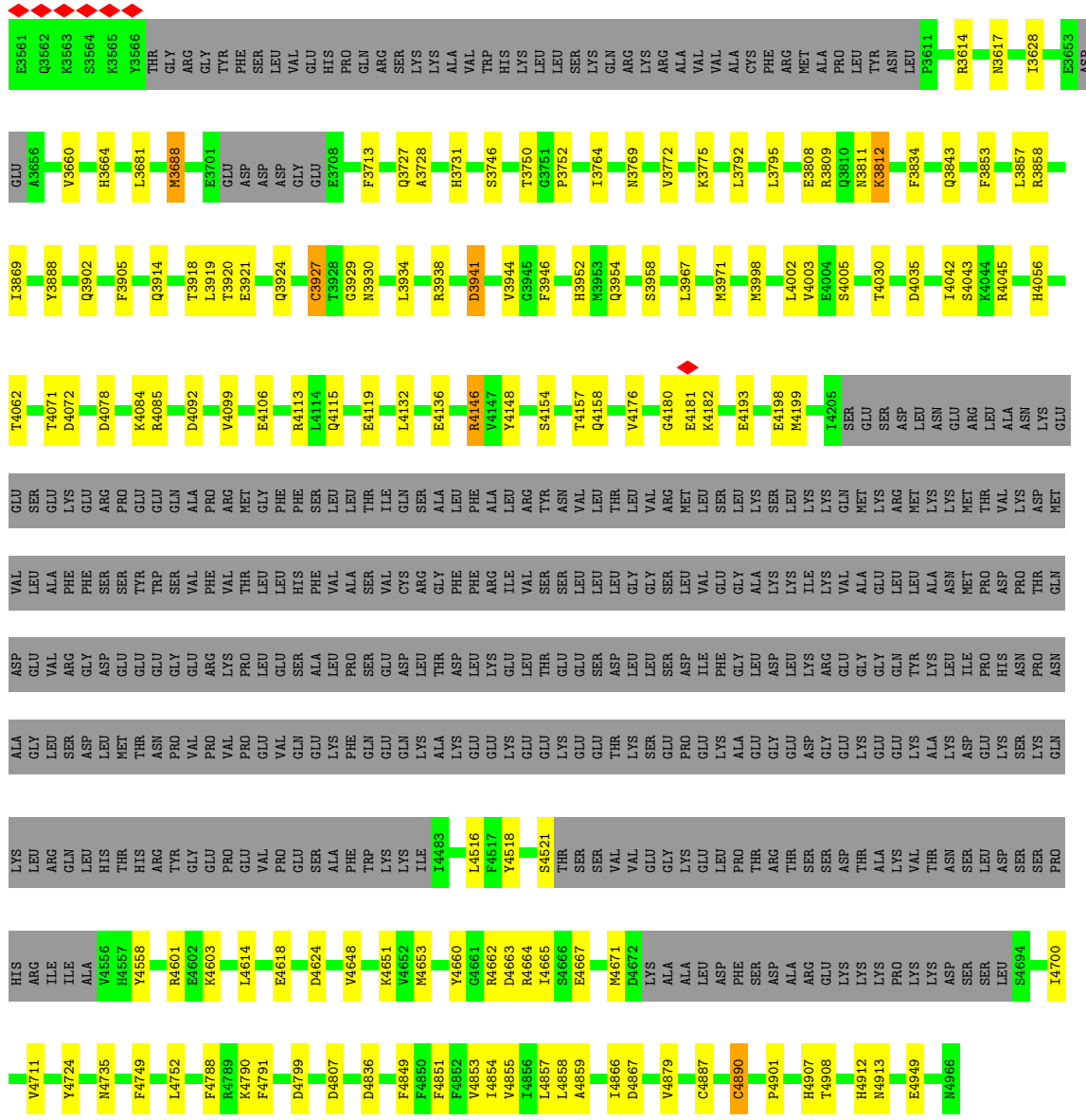
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

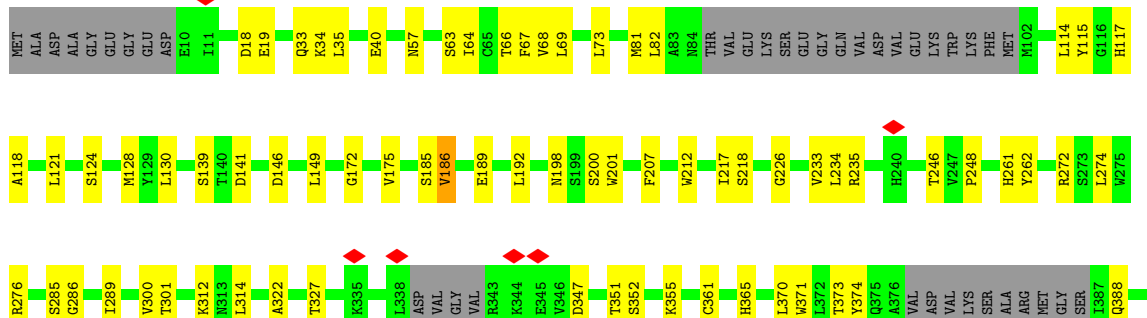
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

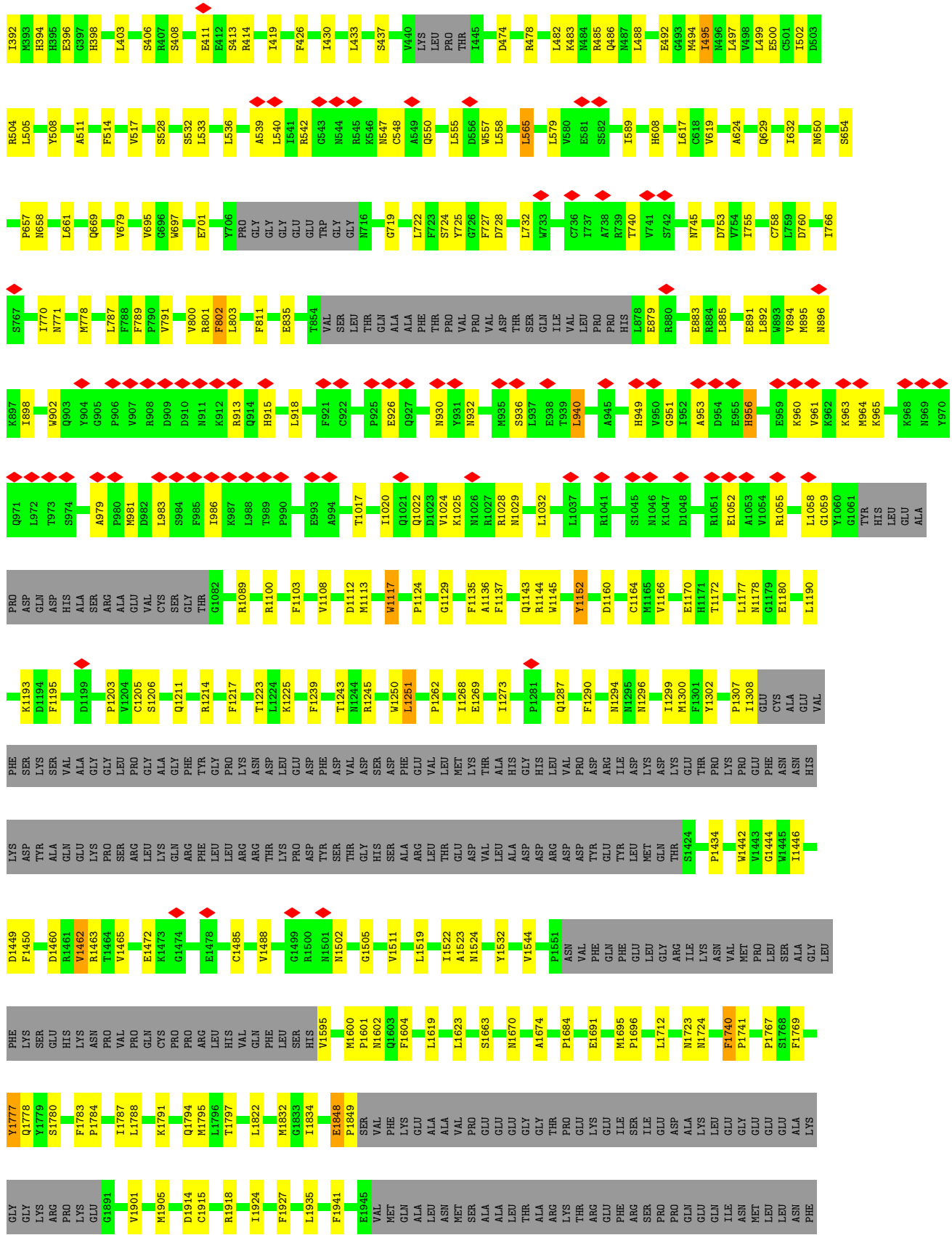
• Molecule 1: Ryanodine receptor 2

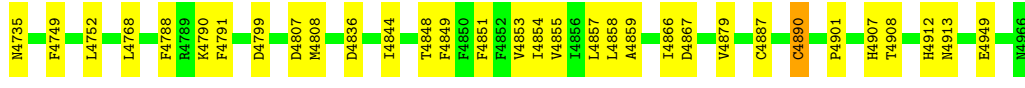
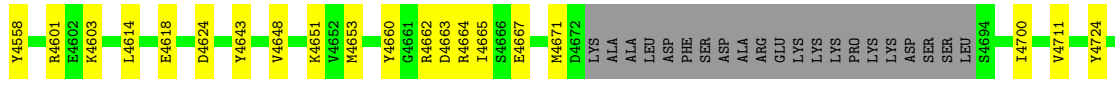




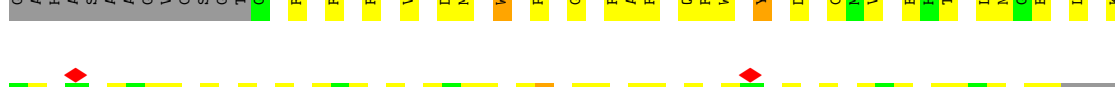
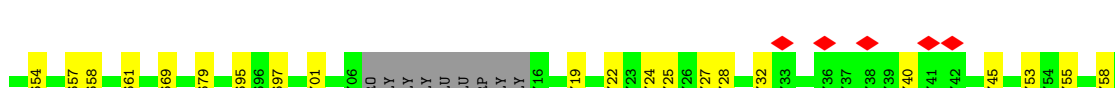
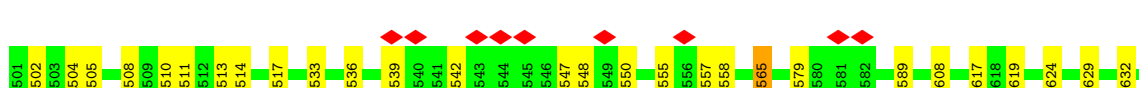
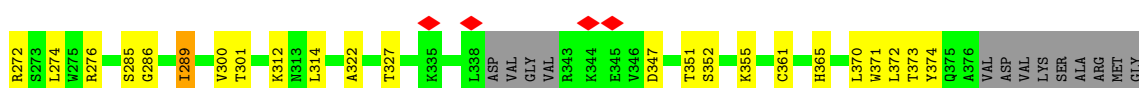
● Molecule 1: Ryanodine receptor 2





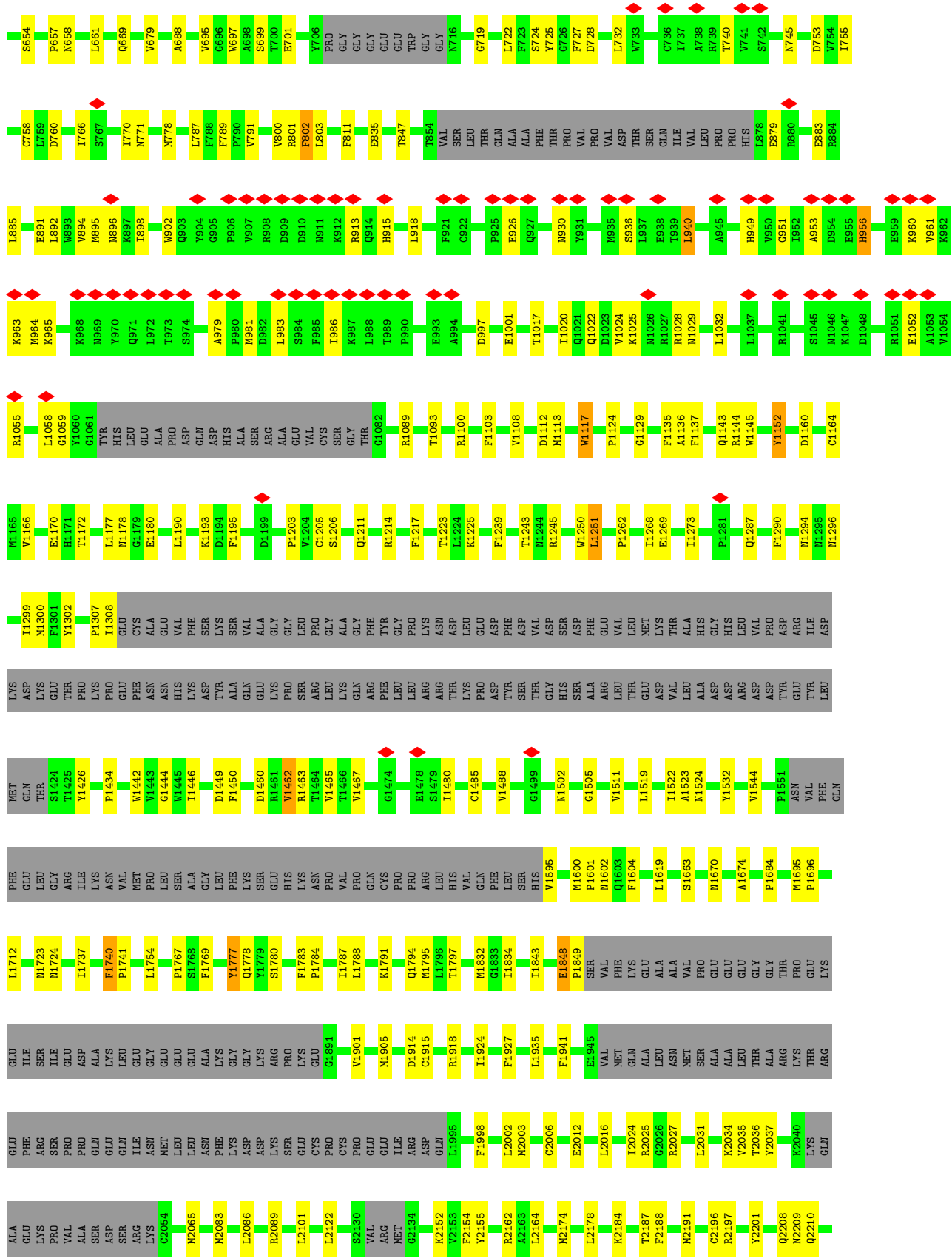


● Molecule 1: Ryanodine receptor 2



E2768	M2467	THR	S2236	LYS	ASN	S1768	SER	HIS	VAL	PHE
L2769	L2471	GLY	T2237	C2054	MET	F1769	ALA	LYS	ALA	ASP
Y2770	G2476	LYS	P2238	M2065	LEU	F1777	GLY	ASP	GLY	GLY
R2771	L2477	SER	L2239	M2083	LEU	Y1778	LEU	TYR	TYR	LYS
M2772	E2478	SER	M2244	L2086	PHE	Q1778	PHE	ALA	ALA	GLN
P2773	F2482	LEU	M2249	R2089	ASP	Y1779	LYS	VAL	VAL	VAL
E2774	L2483	ASP	L2254	L2122	ASP	S1780	GLY	GLY	ALA	GLY
K2775	L2484	ILE	K2263	L2130	LYS	F1783	LYS	PRO	GLY	PRO
L2776	L2484	LYS	V2264	S2130	ARG	P1784	ARG	LEU	LEU	LEU
E2777	G2490	GLU	V2267	VAL	CYS	I1787	ASN	GLY	LEU	GLY
Y2778	D2494	GLU	Y2278	ARG	PRO	L1788	PRO	VAL	ALA	GLY
K2779	L2495	GLU	M2278	MET	GLU	K1791	GLN	GLN	ARG	ARG
T2780	L2501	THR	D2286	G2134	GLU	T1792	CYS	THR	PHE	THR
M2781	ASP	ILE	G2287	K2152	ILE	I1793	PRO	LEU	LEU	GLY
K2782	THR	HIS	G2288	V2153	ASP	Q1794	PRO	LEU	LEU	PRO
Y2783	ALA	ASP	G2289	F2154	ARG	M1795	ARG	ARG	ARG	LYS
A2784	ALA	N2385	ASN	Y2155	GLN	L1796	LEU	THR	THR	ASN
G2785	LEU	Y2391	PRO	R2162	CYS	T1797	HIS	LYS	LYS	ASP
H2786	S2507	PRO	V2292	R2163	PRO	L1822	GLN	PRO	GLN	ASP
S2787	A2508	GLY	V2292	A2163	ASP	M1832	PHE	TYR	ASP	PHE
I2788	T2509	GLY	F2300	L2164	ASP	G1833	LEU	ASP	ASP	ASP
E2789	P2510	ILE	R2301	L2164	ARG	I1834	LEU	VAL	VAL	VAL
R2790	M2511	HIS	R2302	M2174	GLU	I1843	HIS	GLY	GLY	ASP
T2791	A2512	ASP	E2314	L2178	ILE	E1848	SER	ASP	ASP	ASP
A2792	L2513	THR	V2320	L2178	ASP	P1849	ALA	ALA	ALA	PHE
S2793	A2514	ALA	R2321	K2184	GLN	SER	LEU	LEU	LEU	GLY
M2794	L2515	LEU	R2321	T2187	ASP	VAL	VAL	VAL	VAL	VAL
K2795	L2526	LEU	T2324	F2188	MET	VAL	PHE	PHE	VAL	VAL
S2796	THR	THR	R2325	R2188	GLN	VAL	LYS	LYS	GLN	GLY
M2797	ARG	ARG	R2326	M2191	ALA	GLY	GLY	GLY	PHE	ASP
A2798	CYS	CYS	P2327	C2196	LEU	ALA	PRO	PRO	PHE	ASP
L2799	PRO	PRO	F2330	R2197	LEU	ALA	GLU	GLU	GLN	LEU
G2799	LEU	LEU	G2331	Y2201	ALA	ALA	VAL	VAL	GLY	GLY
M2800	ALA	LEU	A2332	R2204	LEU	LEU	GLY	GLY	GLY	GLY
R2792	THR	LEU	L2334	I2205	THR	THR	THR	THR	THR	THR
E2793	GLU	GLU	R2335	R2207	ARG	ARG	ARG	ARG	ARG	ARG
G2794	THR	THR	G2336	Q2208	LYS	LYS	LYS	LYS	LYS	LYS
D2795	HIS	HIS	G2339	N2209	ARG	ARG	ARG	ARG	ARG	ARG
S2796	HIS	ILE	M2340	Q2210	GLU	GLU	GLU	GLU	GLU	GLU
L2797	ALA	ALA	G2341	S2218	PHE	PHE	PHE	PHE	PHE	PHE
M2798	SER	SER	P2356	E2222	SER	SER	SER	SER	SER	SER
A2799	LEU	LEU	G2359	A2222	PRO	PRO	PRO	PRO	PRO	PRO
L2799	LEU	LEU	M2340	L2228	VAL	VAL	VAL	VAL	VAL	VAL
Y2800	LEU	LEU	G2341	A2229	ALA	ALA	ALA	ALA	ALA	ALA
M2801	LEU	LEU	P2356	S2230	SER	SER	SER	SER	SER	SER
ARG	THR	THR	SER	P2356	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	P2356	PRO	PRO	PRO	PRO	PRO	PRO
ILE	ILE	ILE	ILE	P2356	VAL	VAL	VAL	VAL	VAL	VAL
ASP	ASP	ASP	ASP	P2356	ALA	ALA	ALA	ALA	ALA	ALA
GLN	GLN	GLN	GLN	P2356	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	P2356	ILE	ILE	ILE	ILE	ILE	ILE
GLN	GLN	GLN	GLN	P2356	PRO	PRO	PRO	PRO	PRO	PRO
VAL	VAL	VAL	VAL	P2356	GLN	GLN	GLN	GLN	GLN	GLN
ASP	ASP	ASP	ASP	P2356	ALA	ALA	ALA	ALA	ALA	ALA
A2816	A2816	A2816	A2816	P2356	GLY	GLY	GLY	GLY	GLY	GLY
A2817	A2817	A2817	A2817	P2356	ILE	ILE	ILE	ILE	ILE	ILE
H2818	H2818	H2818	H2818	P2356	PRO	PRO	PRO	PRO	PRO	PRO
G2819	G2819	G2819	G2819	P2356	VAL	VAL	VAL	VAL	VAL	VAL
Y2820	Y2820	Y2820	Y2820	P2356	ASP	ASP	ASP	ASP	ASP	ASP
S2821	S2821	S2821	S2821	P2356	PRO	PRO	PRO	PRO	PRO	PRO
P2822	P2822	P2822	P2822	P2356	GLN	GLN	GLN	GLN	GLN	GLN
R2823	R2823	R2823	R2823	P2356	ALA	ALA	ALA	ALA	ALA	ALA
A2824	A2824	A2824	A2824	P2356	GLY	GLY	GLY	GLY	GLY	GLY
I2825	I2825	I2825	I2825	P2356	ILE	ILE	ILE	ILE	ILE	ILE
D2826	D2826	D2826	D2826	P2356	PRO	PRO	PRO	PRO	PRO	PRO
M2827	M2827	M2827	M2827	P2356	VAL	VAL	VAL	VAL	VAL	VAL

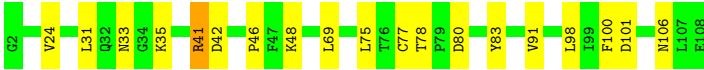
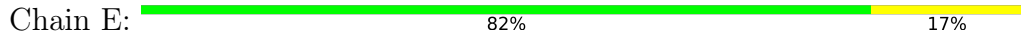
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R3448	K3450	M3451	R3453	K3454	G3455	D3456	R3457	Y3458	S3459	M3460	T3462	S3463	L3464	I3465	V3466	A3467	A3468	K3470	R3471	L3472	L3473	P3474	I3475	G3477	N3478	I3479	C3480	A3481	P3482	G3483	Q3484	L3487	I3488	L3490	A3491	N3492	R3493	A3494	F3495	S3496	K3498	D3499	T3500	E3501	E3502	E3503	V3504	R3505	D3506	I3507							
N3388	P3389	GLU	ALA	GLU	LEU	PHE	ARG	MET	VAL	ALA	GLU	PHE	ILE	Y3404	M3405	S3406	K3407	S3408	H3409	N3410	F3411	K3412	R3413	E3414	E3415	Q3416	N3417	F3418	V3419	V3420	Q3421	N3422	E3423	L3424	N3425	N3426	M3427	S3428	F3429	L3430	I3431	D3433	T3434	K3435	K3437	M3438	S3439	A3441	I3443	S3444	D3445	Q3446	E3447				
R3324	L3325	K3326	K3327	K3328	A3329	V3333	S3334	E3335	E3336	L3339	K3340	A3343	R3344	G3345	D3346	M3347	S3348	E3349	A3350	E3351	E3352	L3353	I3354	L3355	D3356	E3357	F3358	T3359	T3360	L3361	A3362	R3363	D3364	L3365	Y3366	A3367	F3368	L3369	P3370	L3371	L3372	I3373	K3374	F3375	V3376	D3377	Y3378	N3379	R3380	A3381	K3382	W3383	L3384	K3385	E3387		
C3264	L3267	N3268	S3269	E3270	S3195	L3194	L3196	E3201	D3202	V3203	C3204	P3205	N3206	L3207	P3208	T3215	I3218	A3221	E3222	S3223	G3224	I3225	R3226	Y3227	T3228	Q3229	N3230	F3231	Y3232	N3233	N3234	E3235	V3236	V3237	L3238	P3239	N3240	L3241	C3242	S3243	Y3244	R3247	E3250	H3251	P3253	E3254	N3255	H3256	P3257	E3258	R3259	A3260					
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GLU	ASP	VAL	GLN	VAL	SER	CYS	TYR	ARG	ILE	LEU	THR	SER	LYS	SER	ILE	TYR	VAL	GLU	ARG	GLN	ARG	ALA	LEU	GLY	CYS	LEU	ALA	ALA	PHE	ALA	GLY	ALA	PHE	LEU	GLU	THR	HIS	L3174	D3175	K3176	H3177	N3178	V3179	Y3180	S3181												
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A2888	Q2889	D2890	L2891	F2892	K2893	F2894	L2895	Q2896	K3046	S2898	G2899	Y2900	V2901	V2902	S2903	R2904	GLY	PHE	LYS	ASP	LEU	ASP	LEU	THR	PRO	ILE	GLN	ASP	ARG	THR	PRO	ILE	GLN	LEU	GLN	ARG	VAL	VAL	ASP	GLY	ASP	ALA	HIS	GLN	TYR	ILE	GLY	ASP	GLY	SER	ARG						
SER	LYS	GLY	HIS	PHE	PRO	TYR	GLU	GLN	ILE	LYS	PHE	VAL	VAL	LEU	PRO	ILE	GLN	ASP	TYR	GLN	LYS	ASN	HIS	ARG	LEU	TYR	PHE	LEU	ALA	ALA	ARG	PRO	SER	PHE	LEU	SER	LEU	VAL	ILE	ALA	ILE	SER	GLN	PHE	GLY	ASN	ASP	ALA									
THR	SER	ILE	VAL	ASN	CYS	HIS	L3035	M3045	K3046	T3047	G3048	L3049	D3050	S3051	A3055	L3056	R3057	A3058	F3059	L3060	D3061	N3062	A3063	D3066	R3083	K3087	I3093	L3100	L3101	P3102	M3103	LEU	SER	SER	PHE	GLU	HIS	GLY	GLN	ILE	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA							



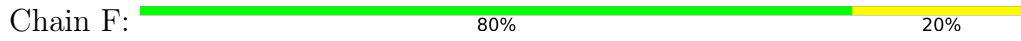
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E2222	ASP	K2765	I2825	R2885	GLY	E3258
L2228	GLY	K2766	D2826	E2886	GLY	R3259
A2229	VAL	E2767	M2827	K2887	ARG	A3260
S2230	PRG	K2768	S2828	Q2888	SER	C3264
S2236	PRG	E2769	N2829	Q2889	GLY	L3267
T2237	THR	Y2770	V2830	Q2890	HIS	N3268
P2238	SER	R2771	T2831	I2891	ASP	S3269
L2239	CYS	W2772	L2832	F2892	PRO	E3270
A2244	LEU	P2773	S2833	C2893	THR	S3195
N2249	LEU	E2714	R2834	F2894	GLU	L3196
L2254	ASP	K2715	D2835	L2895	GLN	E3201
K2263	ILE	L2716	L2836	Q2896	ILE	D3202
Y2264	GLU	E2717	H2837	I2897	PHE	D3203
Y2267	GLU	Y2718	A2838	S2898	PHE	V3203
K2278	GLU	F2719	M2839	Q2899	ALA	C3204
G2288	ASP	N2720	E2840	Y2900	L3049	P3205
W2289	THR	V2721	M2781	V2901	S3051	N3206
ASN	ILE	K2722	L2782	V2902	A3055	I3207
P2292	HIS	K2723	A2783	S2903	L3056	P3208
F2300	GLU	Y2724	E2784	R2904	R3057	T3215
L2301	LEU	E2725	A2844	GLY	A3058	I3218
R2302	ASP	H2726	G2785	PHE	F3059	A3221
E2314	PRO	S2727	W2786	LYS	L3060	E3222
V2320	GLY	R2728	R2787	ASP	D3061	S3223
R2321	ILE	H2729	L2788	LEU	N3062	I3225
I2324	ILE	D2729	E2789	ASP	A3063	R3226
R2325	HIS	K2730	R2790	LEU	D3066	A3227
R2326	ALA	W2731	W2791	LEU	R3083	T3228
P2327	ALA	L2606	T2792	LEU	K3087	Q3229
F2330	ALA	L2515	E2793	GLY	I3093	M3230
G2331	LEU	L2526	R2794	LEU	L3100	P3231
A2333	LEU	L2527	G2794	LEU	L3101	Y3232
L2334	LEU	THR	D2795	ARG	F3102	M3233
R2335	LEU	ARG	D2796	ARG	ALA	M3234
G2336	LEU	CYS	S2796	LEU	ALA	E3235
G2339	LEU	ALA	K2857	LEU	ALA	V3236
M2340	LEU	ALA	L2857	LEU	ALA	L3238
M2341	LEU	LEU	E2858	LEU	ARG	P3239
M2344	LEU	PHE	L2859	LEU	PRO	M3240
V2450	LEU	LEU	L2860	LEU	LEU	L3241
V2451	LEU	ALA	N2800	LEU	LEU	C3242
S2456	LEU	GLY	I2741	LEU	LEU	S3243
ARG	THR	THR	Y2742	GLN	LEU	Y3244
ASP	THR	THR	Y2743	GLN	LEU	R3247
GLY	THR	THR	G2743	LEU	LEU	E3250
HIS	HIS	ASP	E2744	LEU	LEU	H3251
ALA	ALA	SER	I2745	VAL	LEU	G3252
SER	SER	GLU	Y2746	ASP	LEU	P3253
LEU	LEU	GLY	S2747	GLY	LEU	E3254
ILE	ASP	ASN	D2748	ARG	LEU	M3255
ASP	ASP	ASN	L2750	THR	LEU	H3256
LEU	LEU	LEU	K2751	THR	GLY	
LEU	LEU	LEU	I2752	ILE	LEU	
LEU	LEU	LEU	Q2753	LEU	LEU	
LEU	LEU	LEU	P2754	PHE	LEU	
LEU	LEU	LEU	L2755	ASP	LEU	
LEU	LEU	LEU	M2756	ASP	LEU	
LEU	LEU	LEU	K2757	ASP	LEU	
LEU	LEU	LEU	P2758	ASP	LEU	
LEU	LEU	LEU	Y2759	ASP	LEU	
LEU	LEU	LEU	K2760	ASP	LEU	
LEU	LEU	LEU	L2761	ASP	LEU	
LEU	LEU	LEU	L2762	ASP	LEU	
LEU	LEU	LEU	S2763	ASP	LEU	

34966

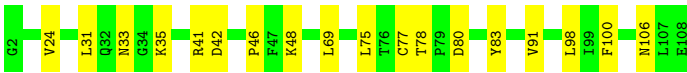
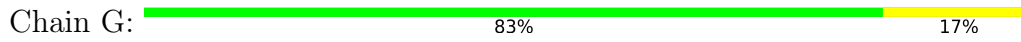
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



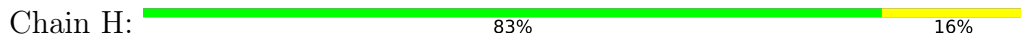
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



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



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	0.25	0/29611	0.50	4/40214 (0.0%)
1	B	0.25	0/29611	0.50	4/40214 (0.0%)
1	C	0.25	0/29611	0.50	4/40214 (0.0%)
1	D	0.25	0/29611	0.50	4/40214 (0.0%)
2	E	0.25	0/778	0.49	0/1060
2	F	0.25	0/778	0.50	0/1060
2	G	0.25	0/778	0.50	0/1060
2	H	0.25	0/778	0.50	0/1060
All	All	0.25	0/121556	0.50	16/165096 (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 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	565	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	565	LEU	CA-CB-CG	6.01	129.12	115.30
1	C	565	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	565	LEU	CA-CB-CG	6.00	129.09	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4002	LEU	CA-CB-CG	5.81	128.67	115.30

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	342	0
1	B	29055	0	27182	341	0
1	C	29055	0	27182	342	0
1	D	29055	0	27182	352	0
2	E	763	0	709	11	0
2	F	763	0	709	12	0
2	G	763	0	709	10	0
2	H	763	0	709	10	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	1372	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 1372 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:C:1205:CYS:SG	1:C:1206:SER:N	2.64	0.71
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: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%)	25	62
1	B	3818/4966 (77%)	3361 (88%)	436 (11%)	21 (1%)	25	62
1	C	3818/4966 (77%)	3363 (88%)	435 (11%)	20 (0%)	29	66
1	D	3818/4966 (77%)	3362 (88%)	436 (11%)	20 (0%)	29	66
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%)	32	66

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%)	2845 (98%)	70 (2%)	49	70
1	B	2915/4355 (67%)	2845 (98%)	70 (2%)	49	70
1	C	2915/4355 (67%)	2845 (98%)	70 (2%)	49	70
1	D	2915/4355 (67%)	2844 (98%)	71 (2%)	49	70
2	E	76/88 (86%)	72 (95%)	4 (5%)	22	54
2	F	76/88 (86%)	72 (95%)	4 (5%)	22	54
2	G	76/88 (86%)	72 (95%)	4 (5%)	22	54
2	H	76/88 (86%)	72 (95%)	4 (5%)	22	54
All	All	11964/17772 (67%)	11667 (98%)	297 (2%)	50	70

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1449	ASP
2	F	41	ARG
1	D	1740	PHE
1	D	3664	HIS
1	B	1740	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2249	ASN
1	C	3811	ASN
1	B	1147	GLN
1	B	2249	ASN
1	B	3811	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 monosaccharides 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.

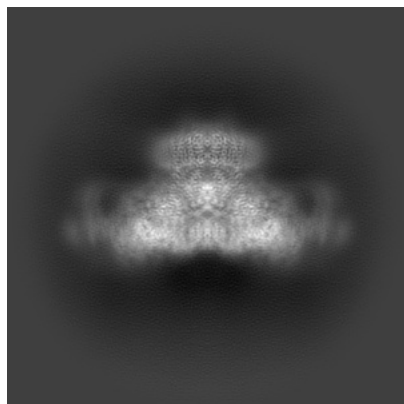
6 Map visualisation [i](#)

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.

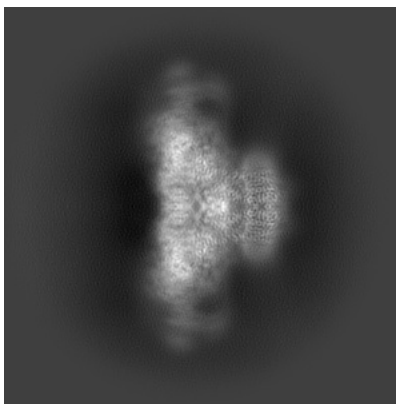
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

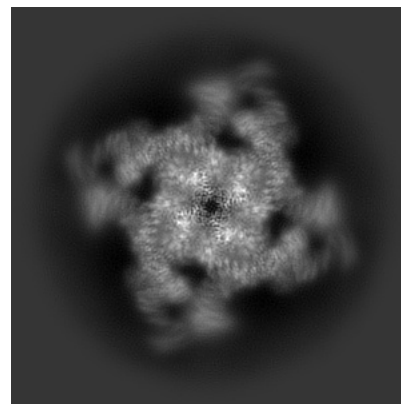
6.1.1 Primary map



X

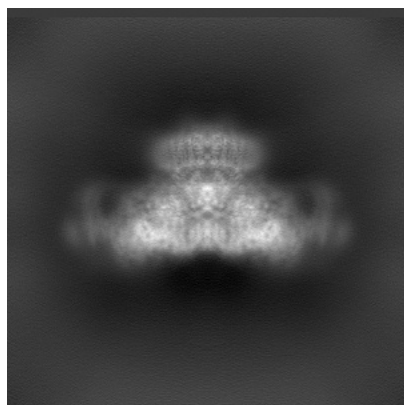


Y

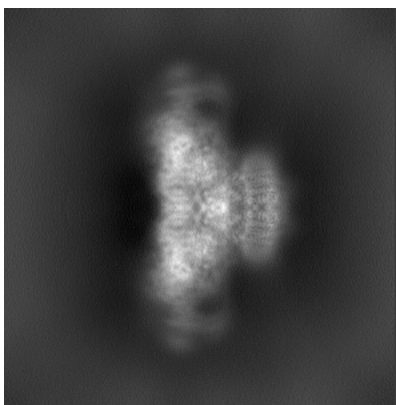


Z

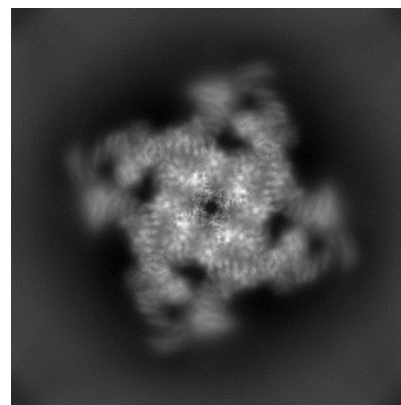
6.1.2 Raw map



X



Y

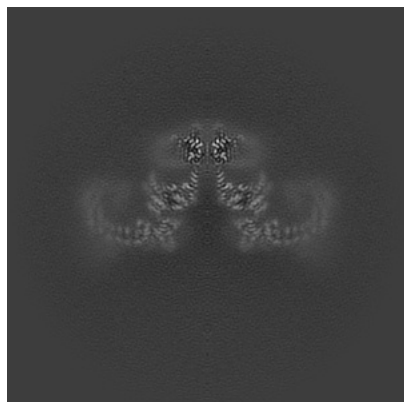


Z

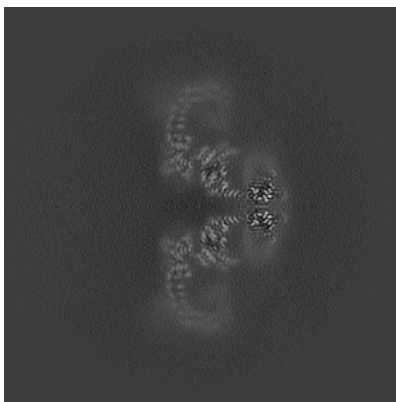
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

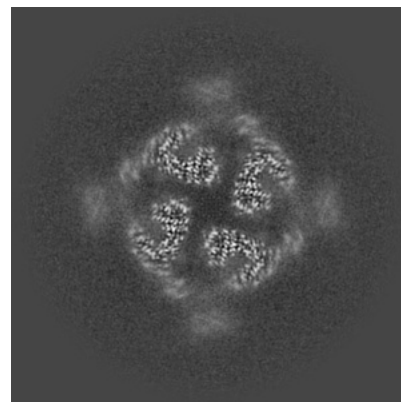
6.2.1 Primary map



X Index: 230

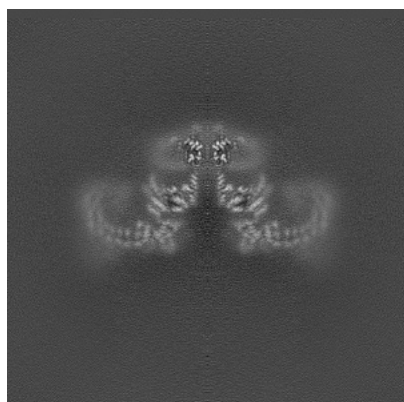


Y Index: 230

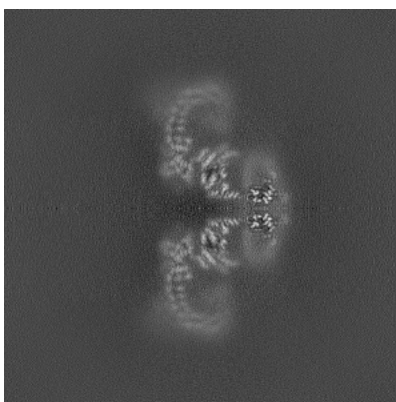


Z Index: 230

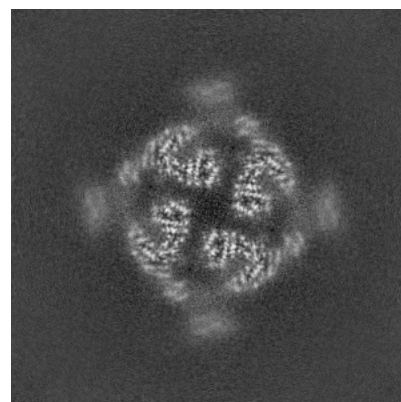
6.2.2 Raw map



X Index: 230



Y Index: 230

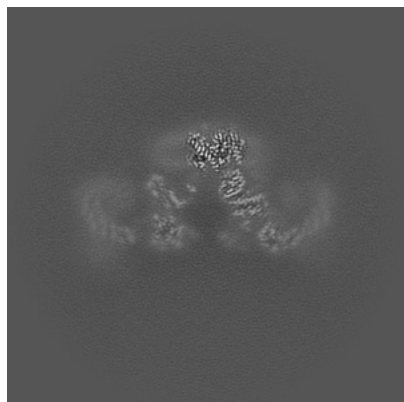


Z Index: 230

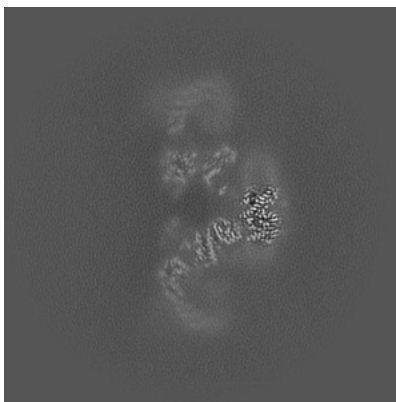
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

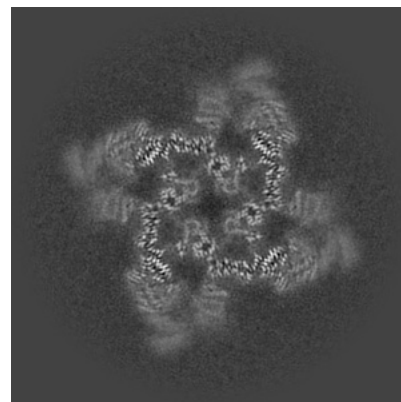
6.3.1 Primary map



X Index: 222

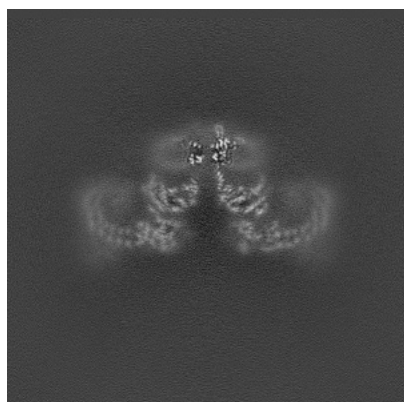


Y Index: 222

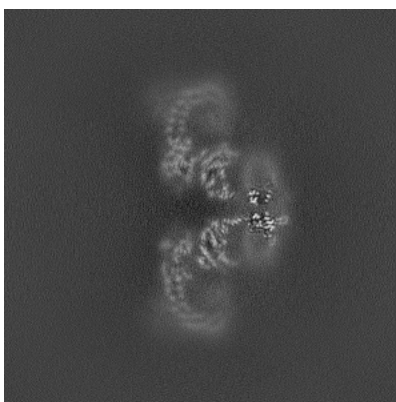


Z Index: 203

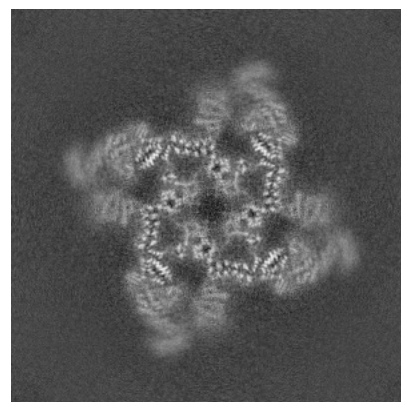
6.3.2 Raw map



X Index: 228



Y Index: 228

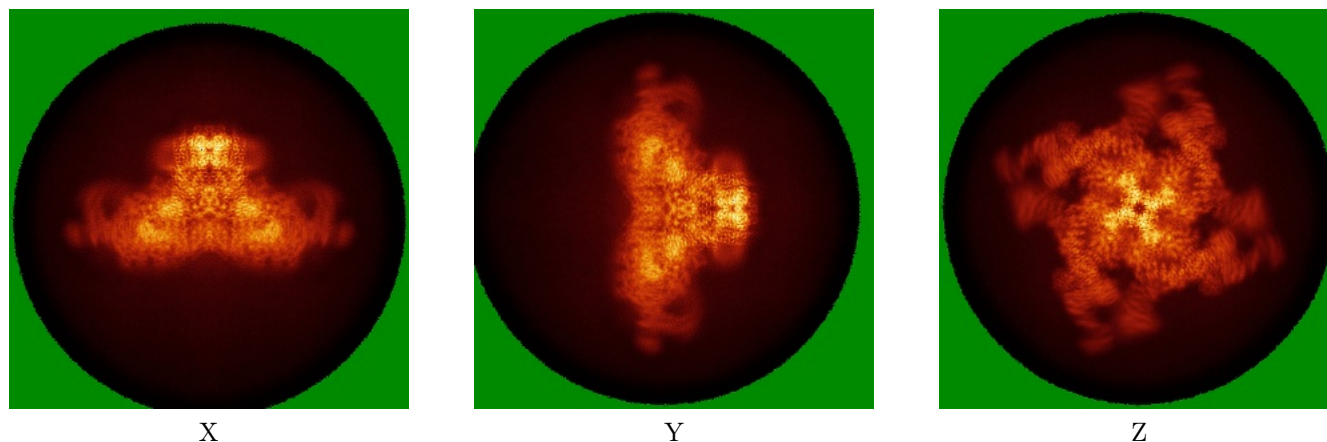


Z Index: 203

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

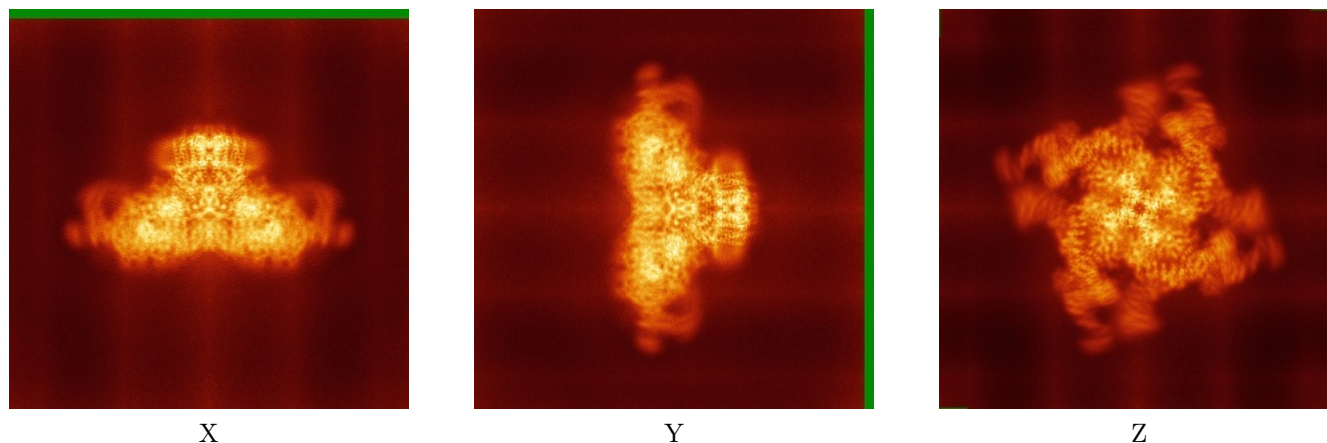


X

Y

Z

6.4.2 Raw map



X

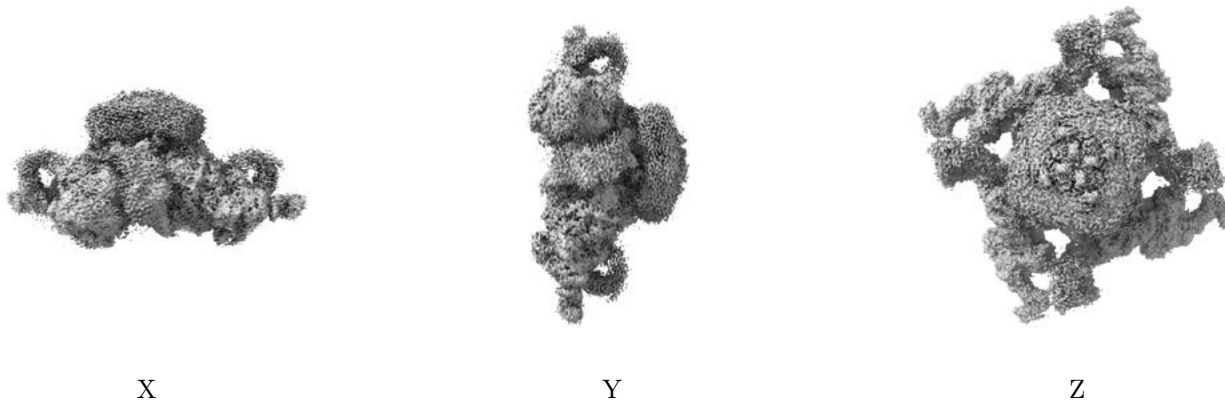
Y

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.

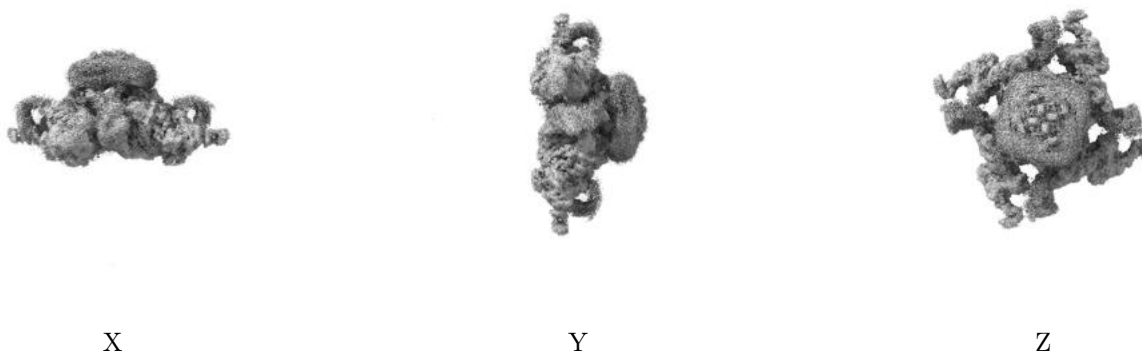
6.5 Orthogonal surface views [i](#)

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.

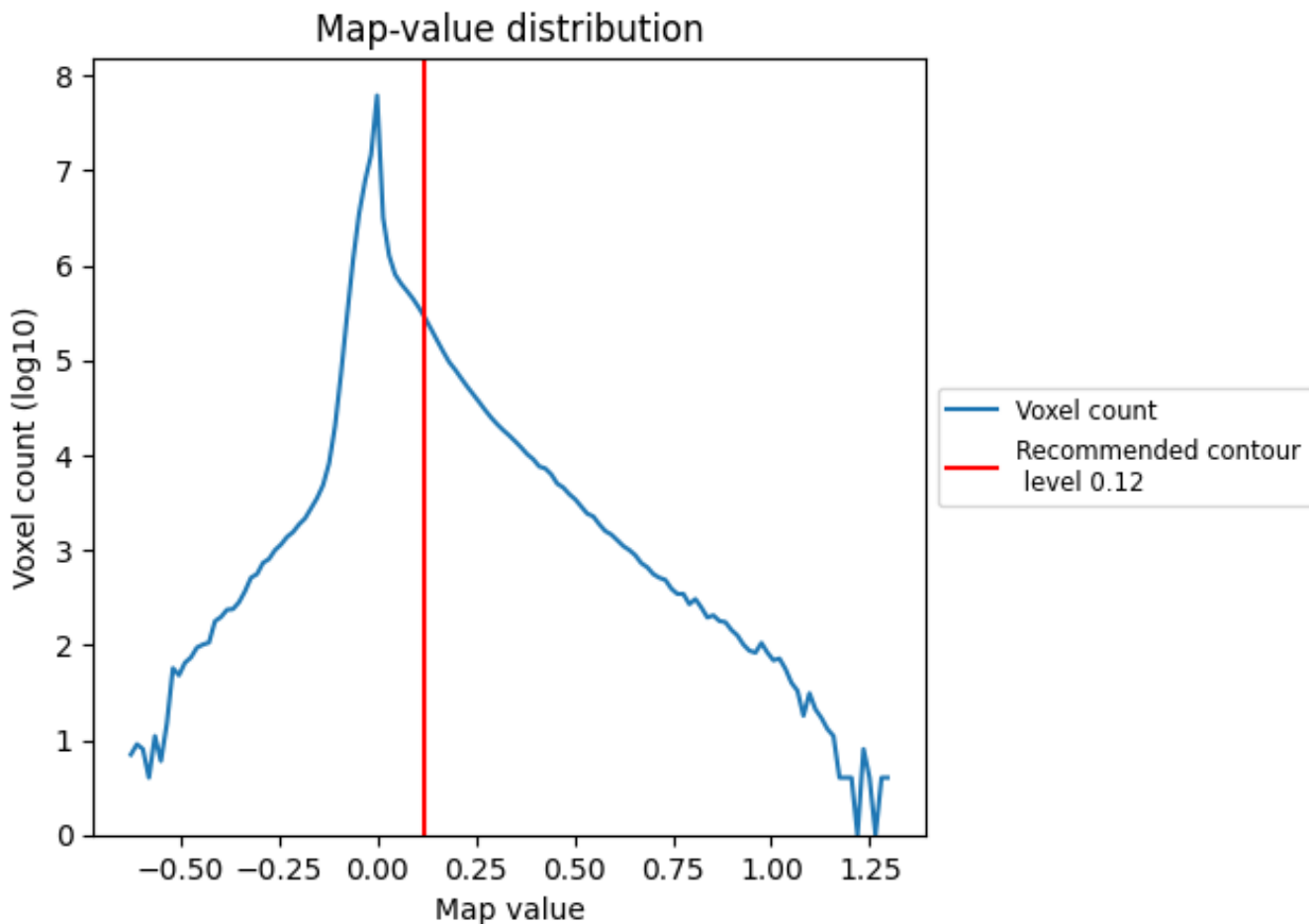
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

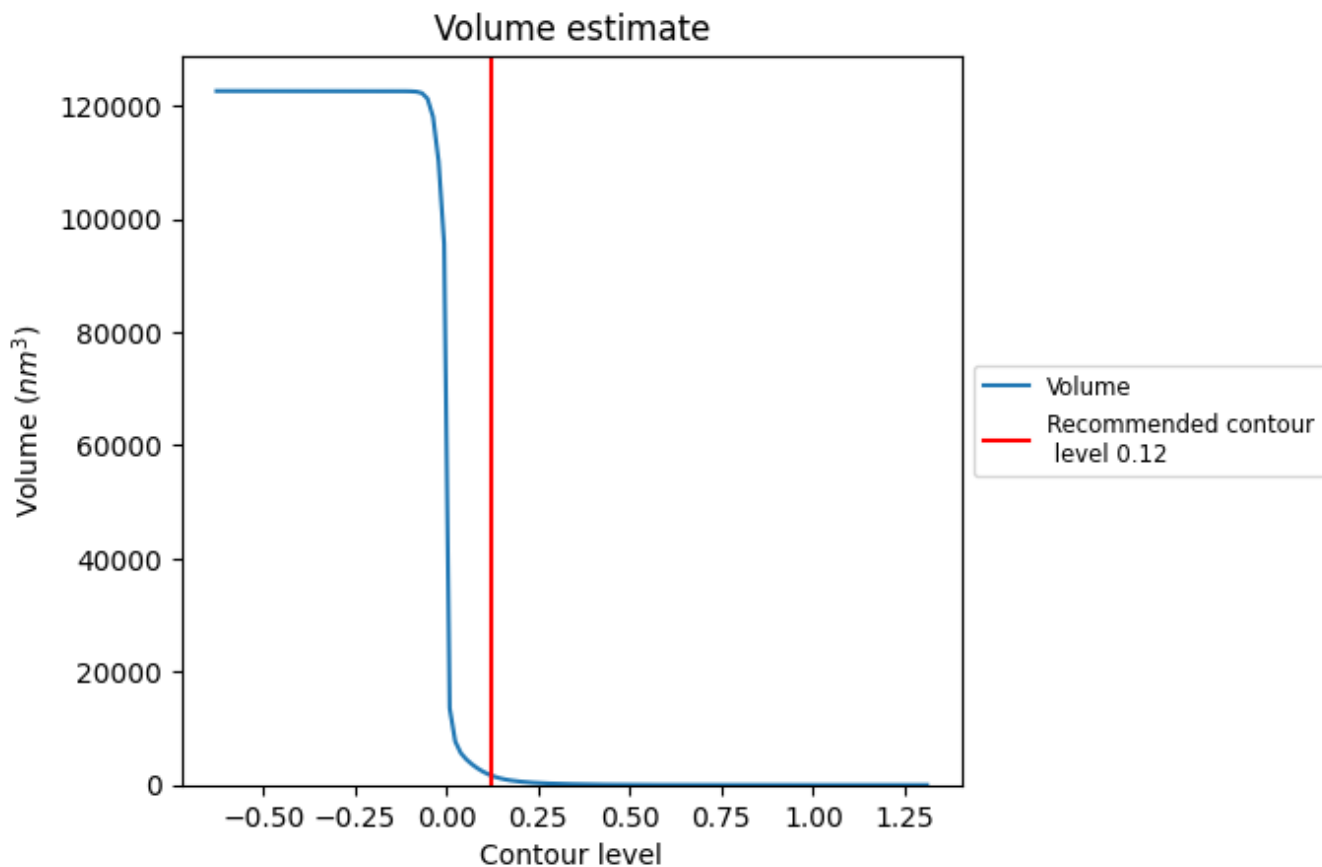
This section contains the results of statistical analysis of the map.

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.

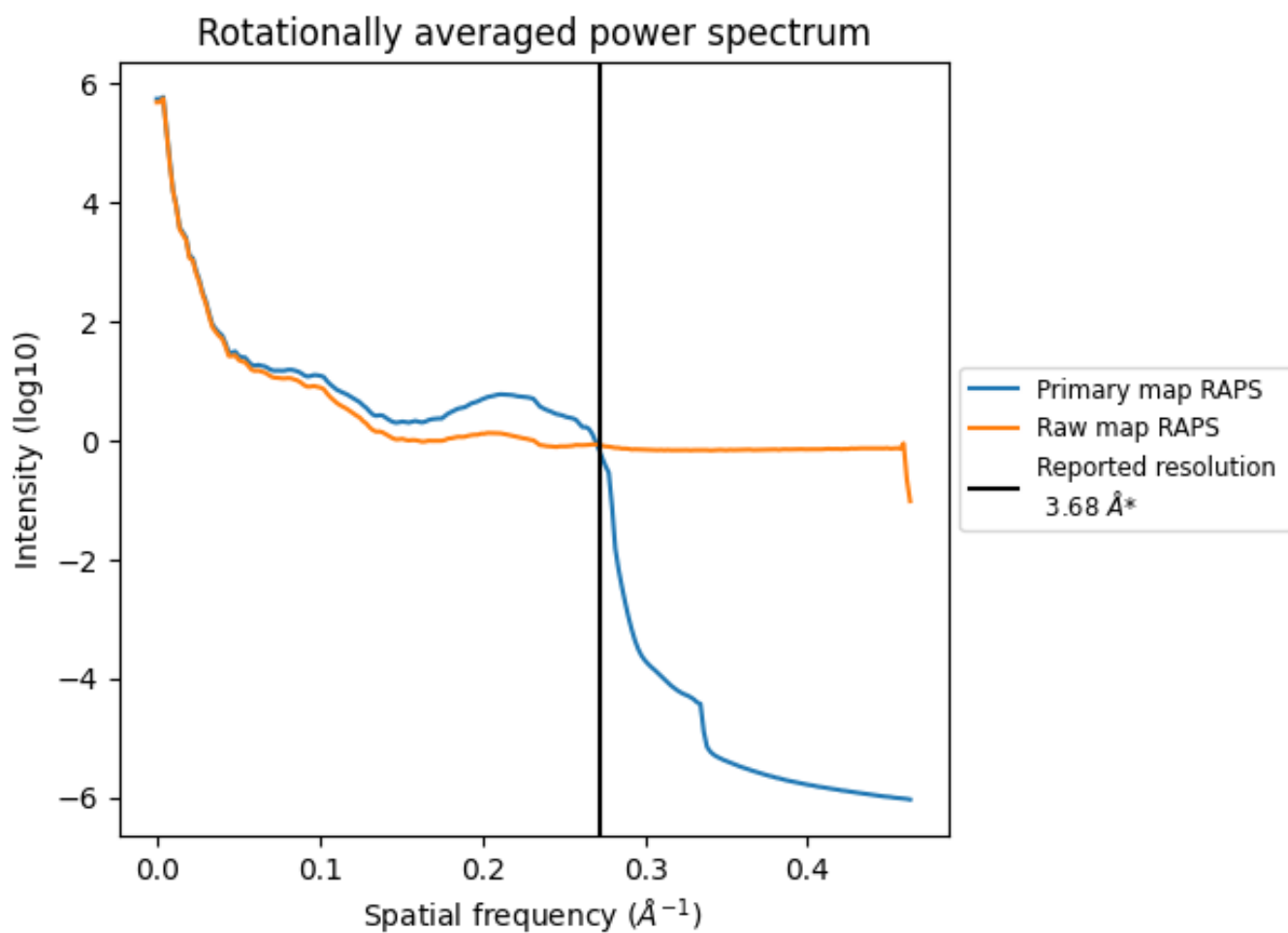
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1734 nm^3 ; 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

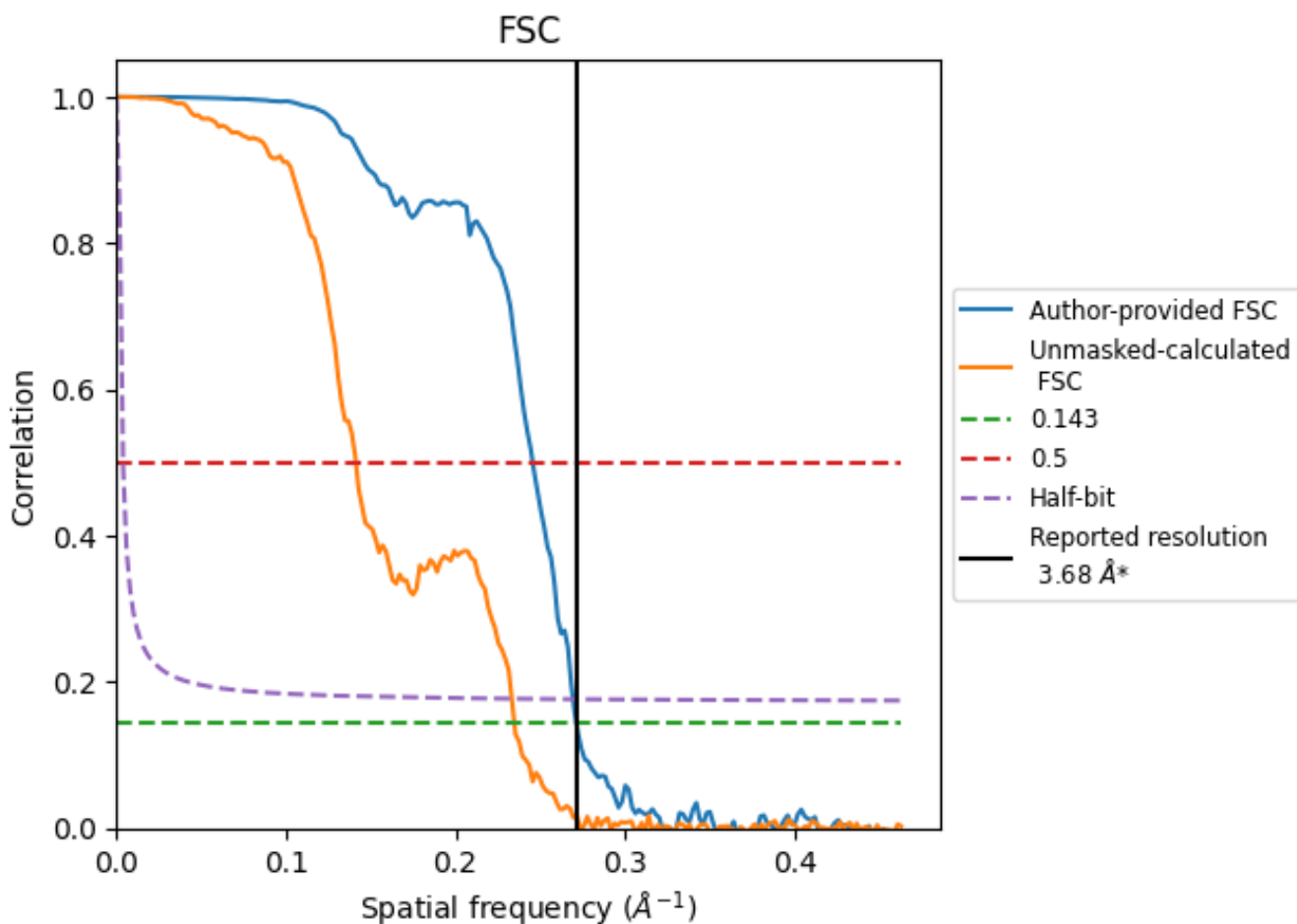


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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](#)

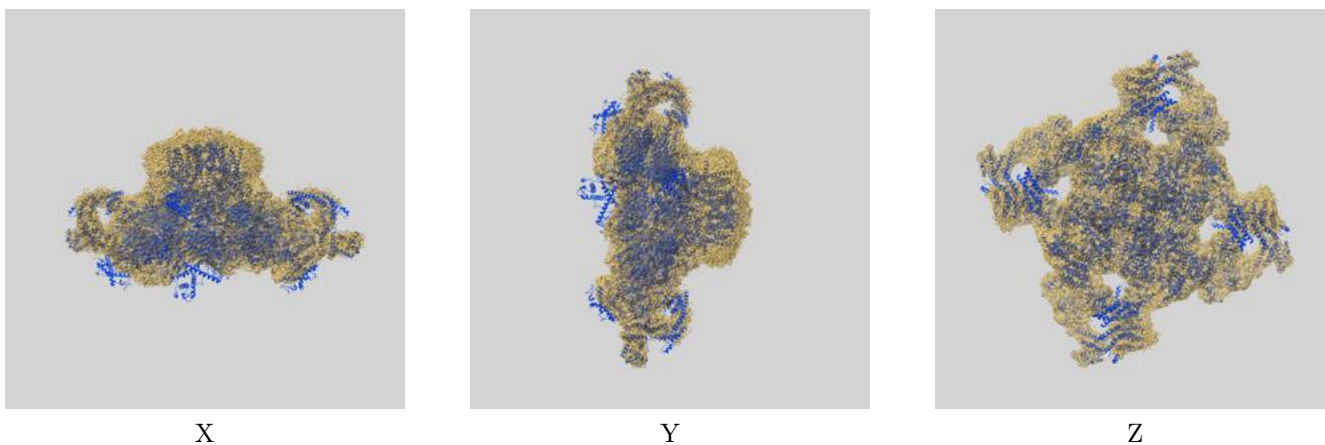
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.07	3.71
Unmasked-calculated*	4.26	7.08	4.29

*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](#)

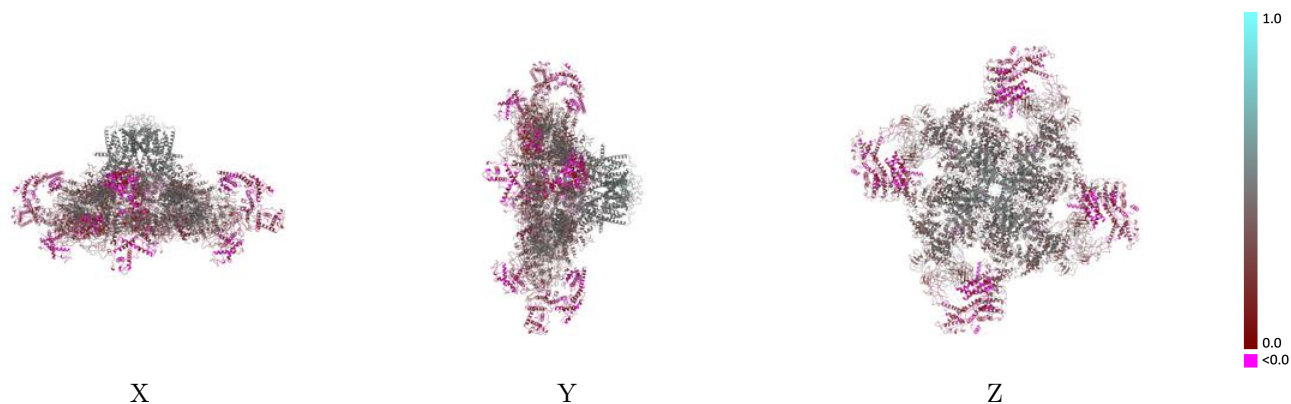
This section contains information regarding the fit between EMDB map EMD-27746 and PDB model 8DVV. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



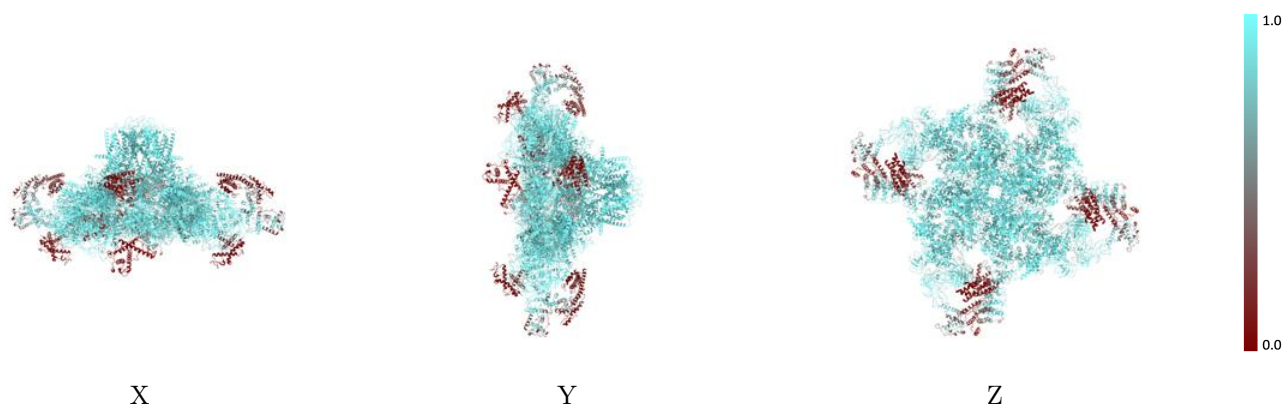
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



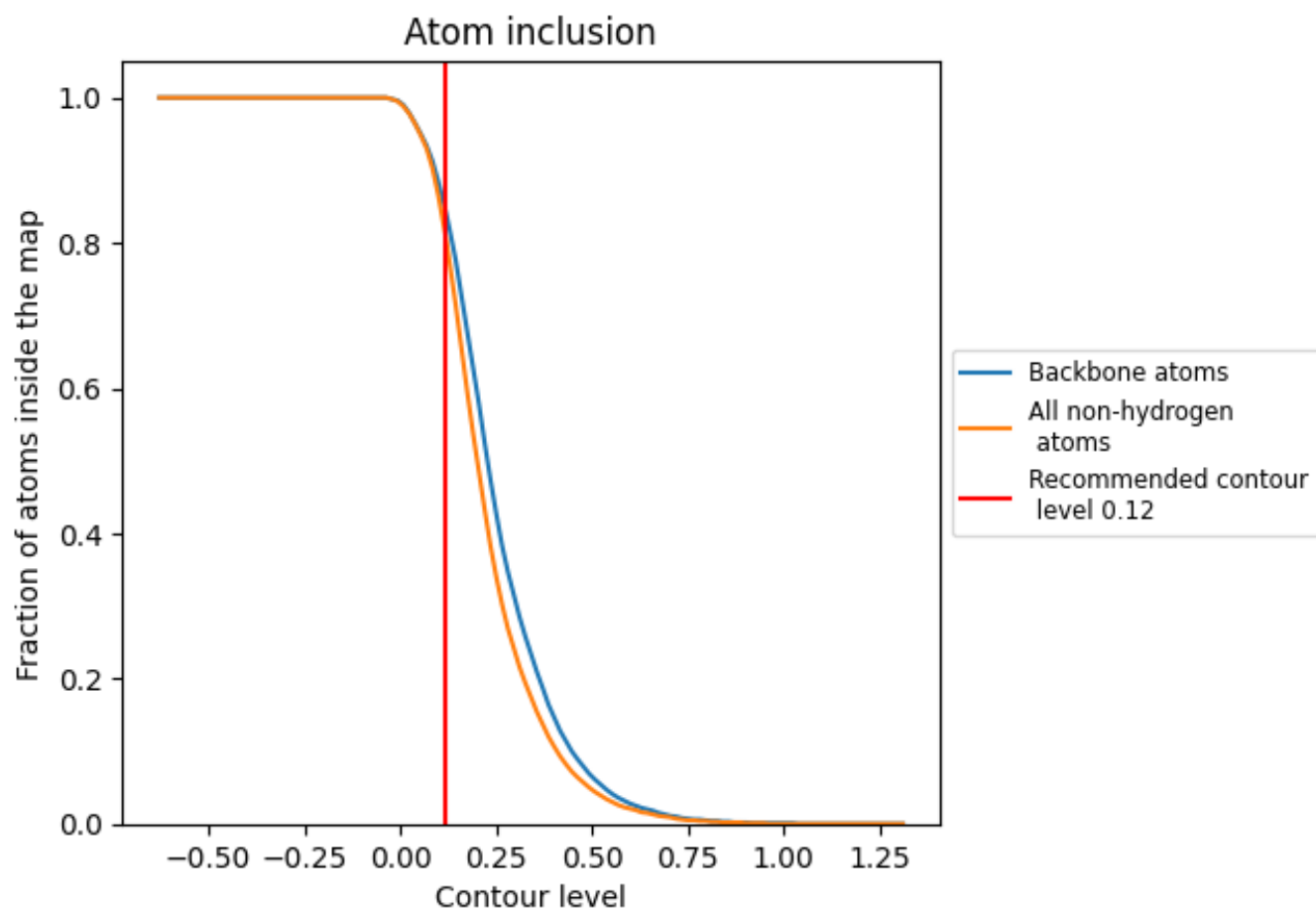
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.12).



















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

