



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 04:19 AM EDT

PDB ID : 5TAQ
EMDB ID : EMD-8382
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 3&4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

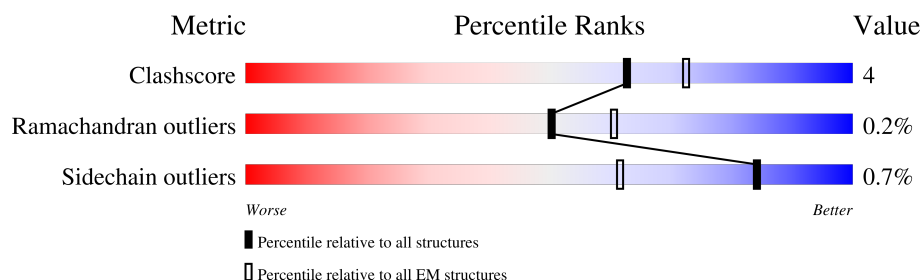
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

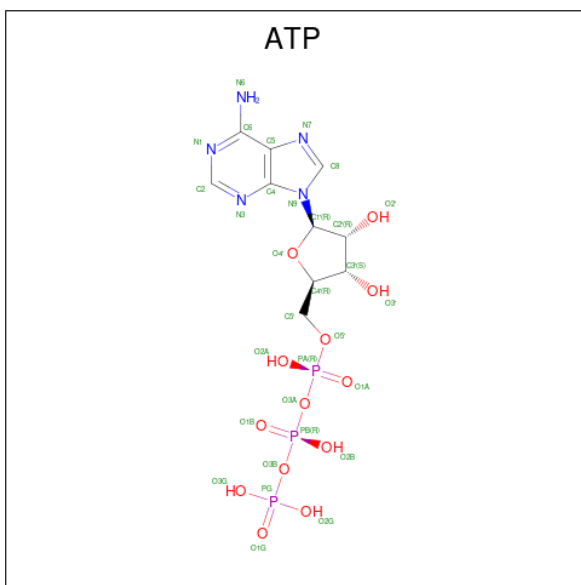
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

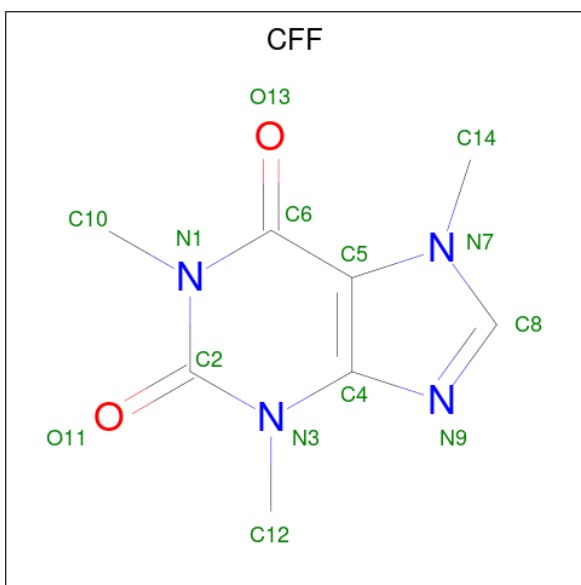
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	

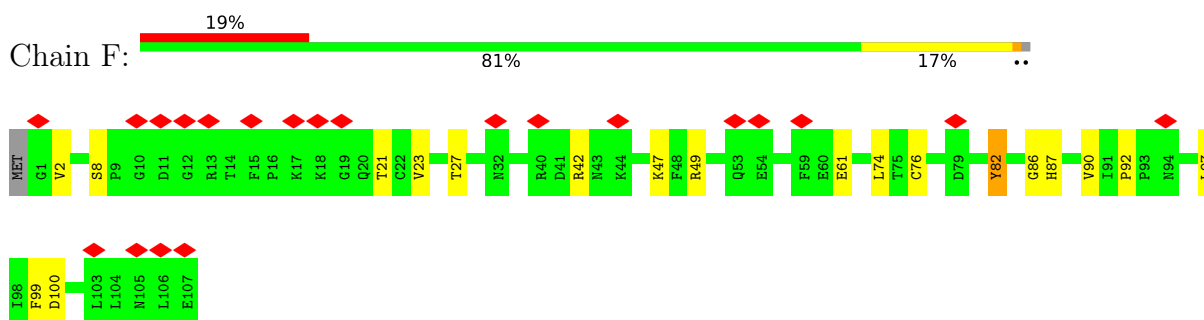
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	

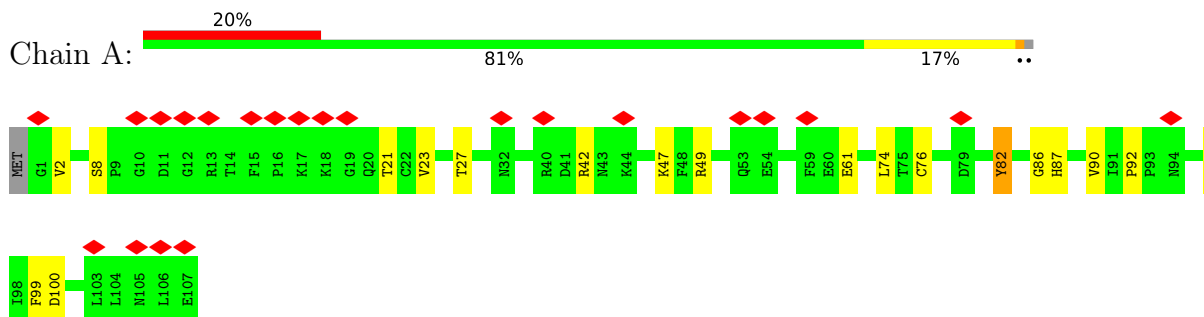
3 Residue-property plots [i](#)

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

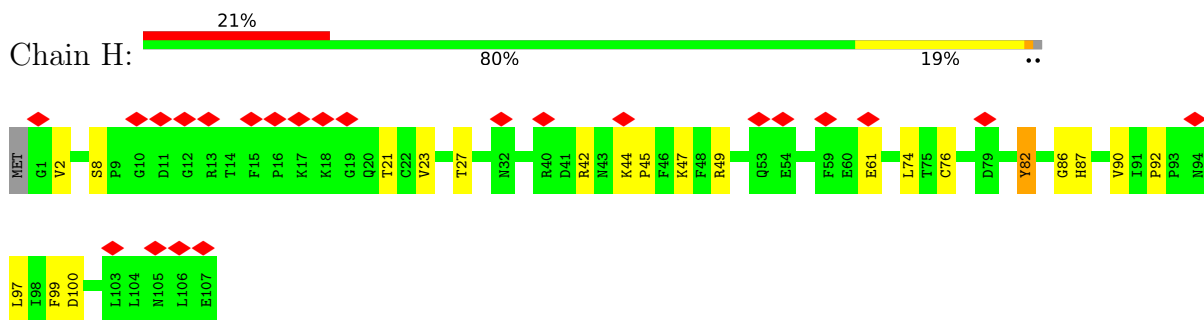
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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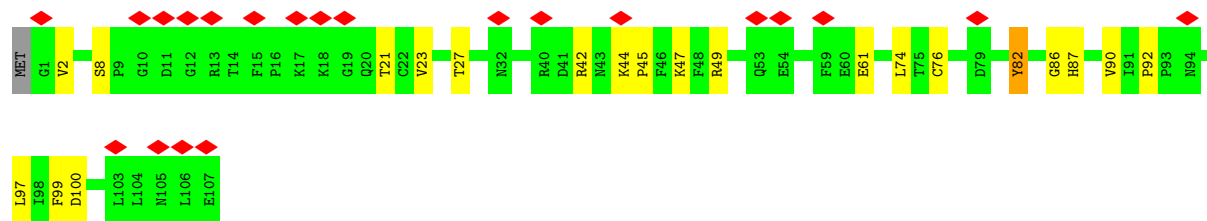


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

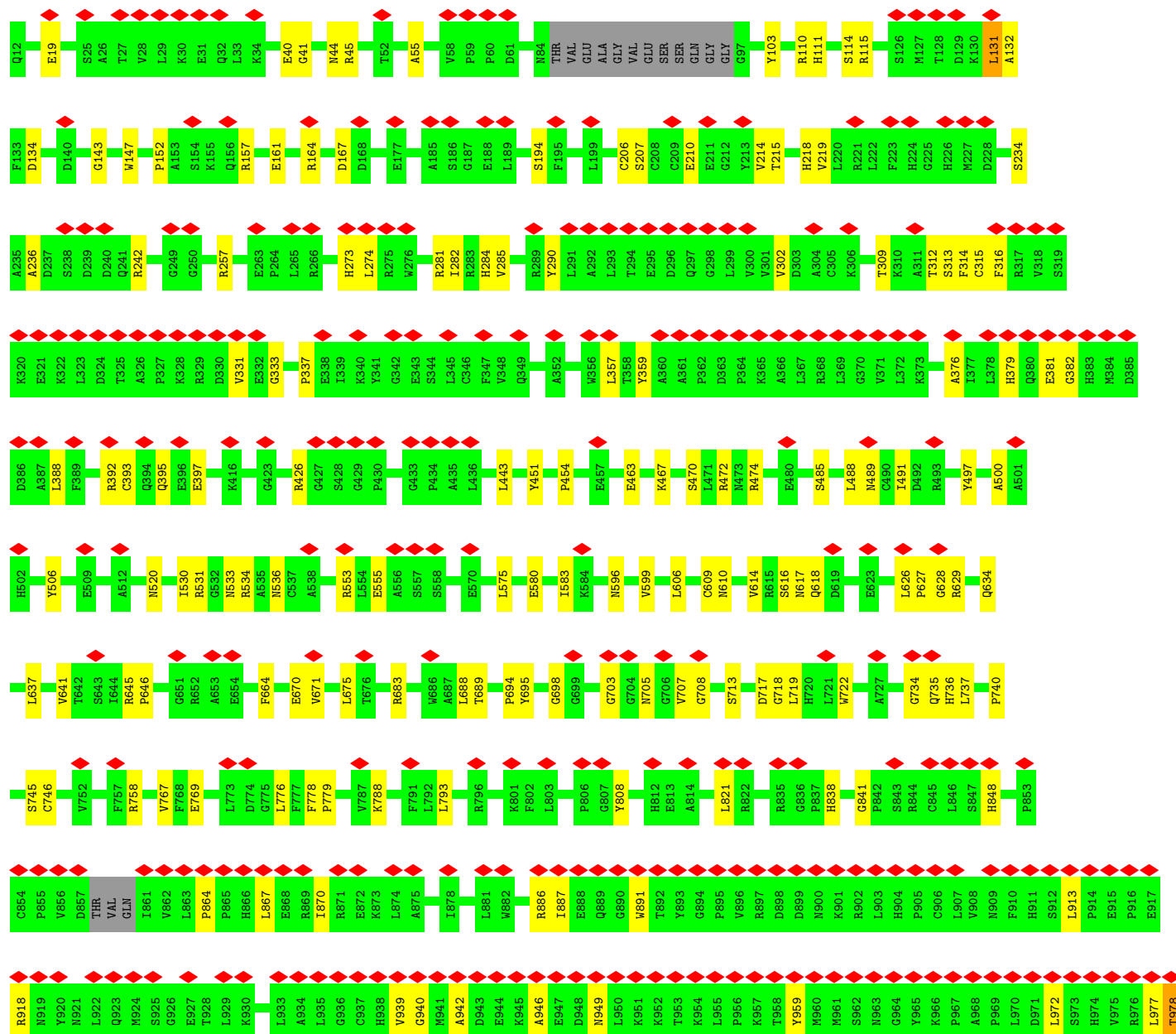
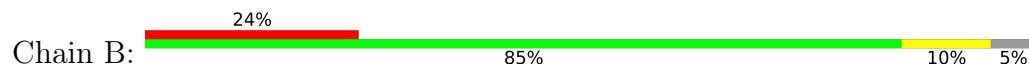


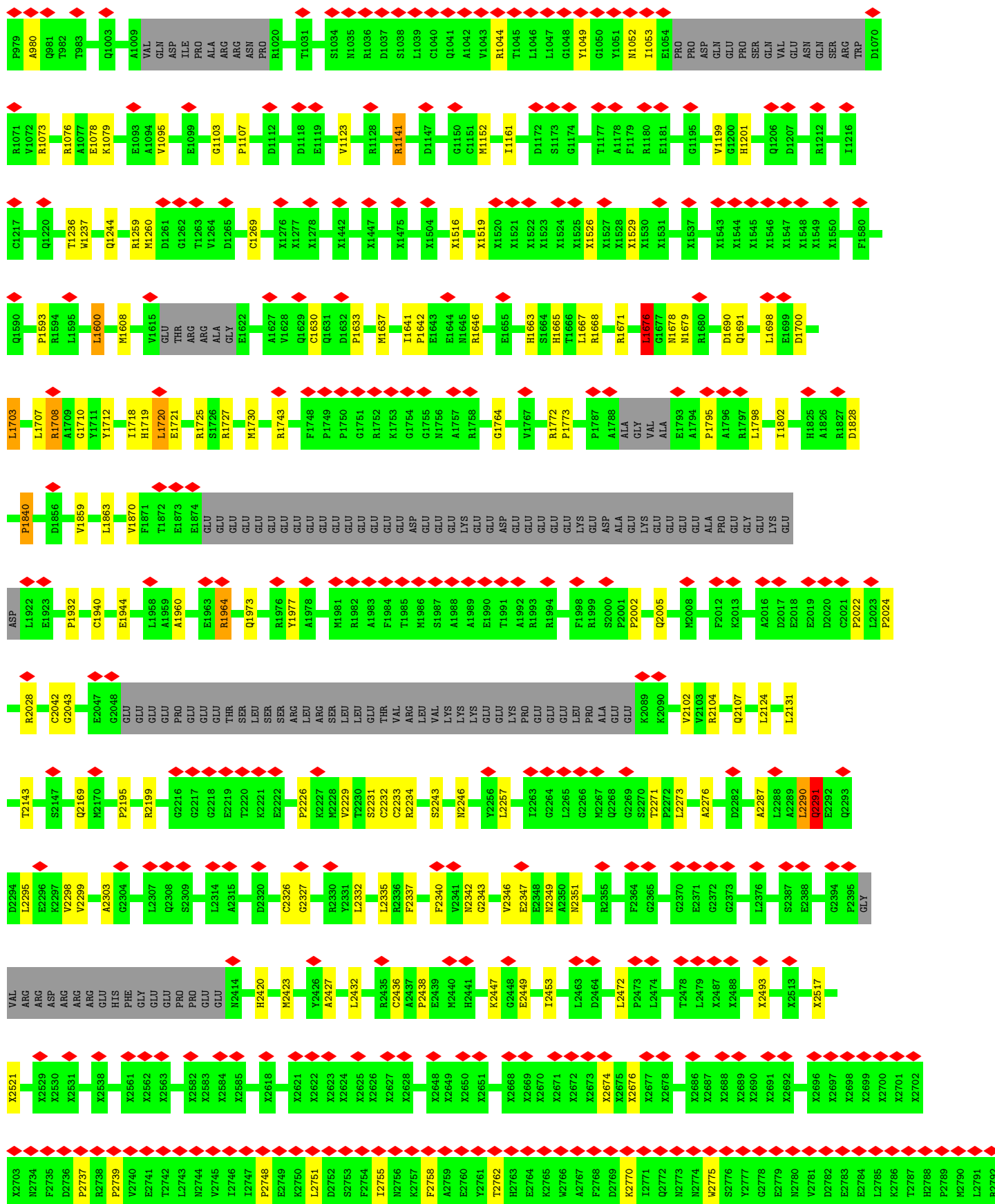
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



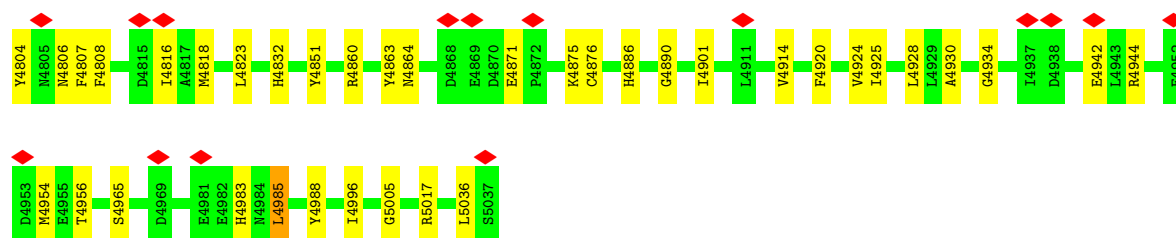


• Molecule 2: Ryanodine receptor 1

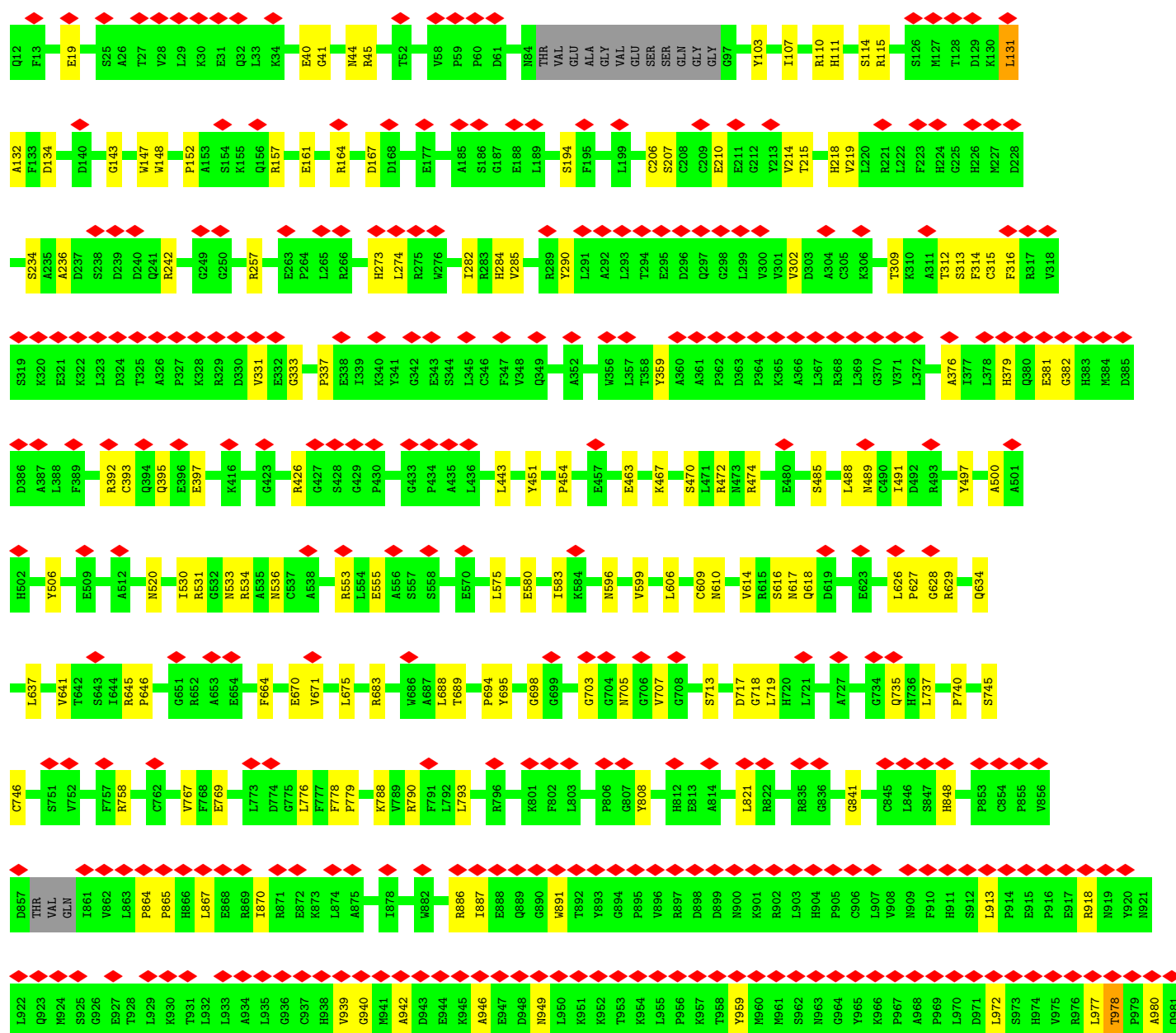
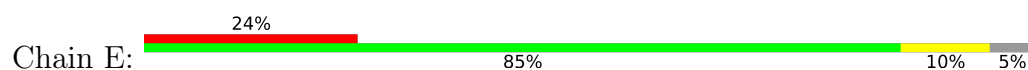






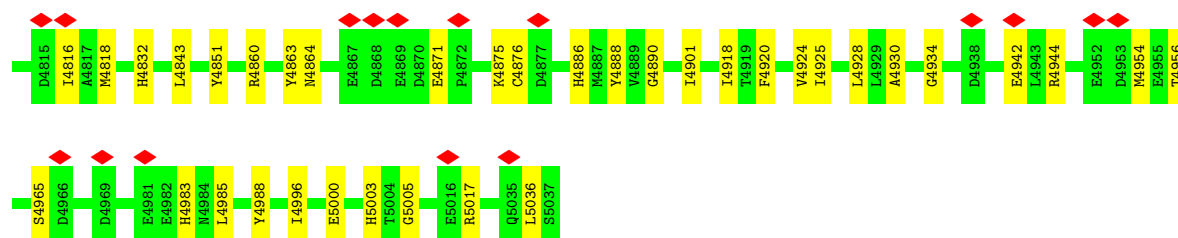


• Molecule 2: Ryanodine receptor 1

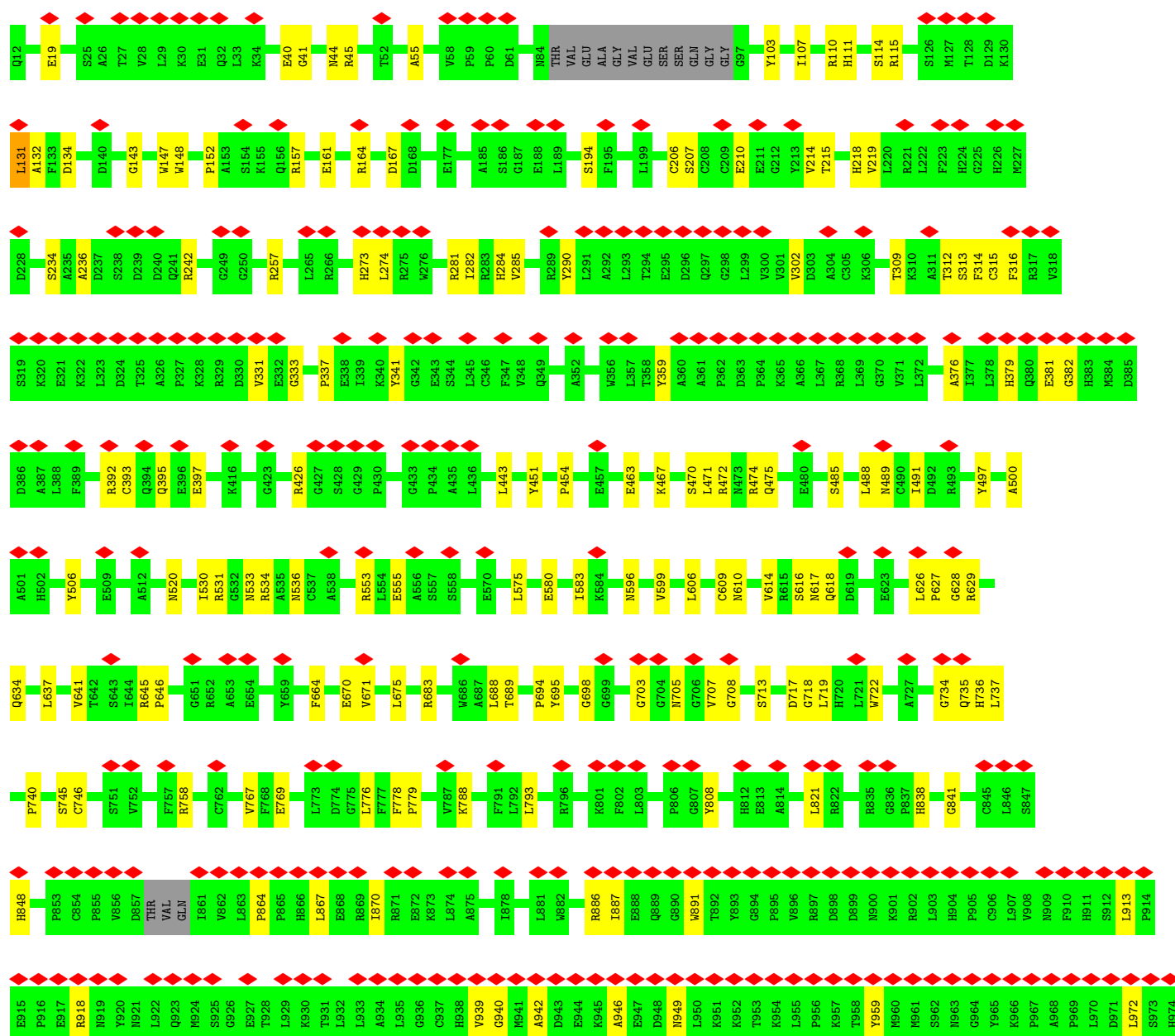
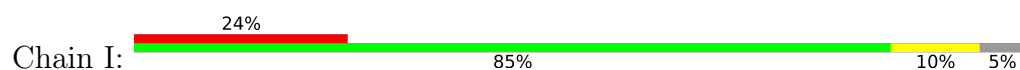


F2735	D2736	P2737	P2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	S2753	L2755	N2756	K2757	F2758	A2759	E2760	V2761	T2762	H2763	E2764	K2765	N2766	A2767	F2768	D2769	K2770	L2771	N2773	N2774	N2775	S2776	V2777	G2778	E2779	N2780	V2781	D2782	E2783	L2784	L2785	K2786	T2787	H2788	F2789	N2790	L2791	F2793	V2794																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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E2292	Q2293	D2294	L2295	E2296	K2297	V2298	V2299	A2303	G2304	L2307	Q2308	S2309	L2314	A2315	D2320	C2326	G2327	R2330	Y2331	L2332	L2335	R2336	F2337	F2340	N2341	V2342	G2343	E2347	N2351	R2355	R2359	F2364	G2365	G2370	E2371	G2372	G2373	L2376	S2387	E2388	F2395	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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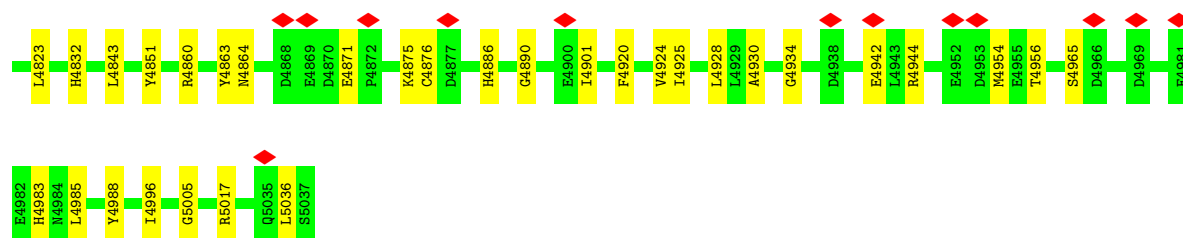


• Molecule 2: Ryanodine receptor 1

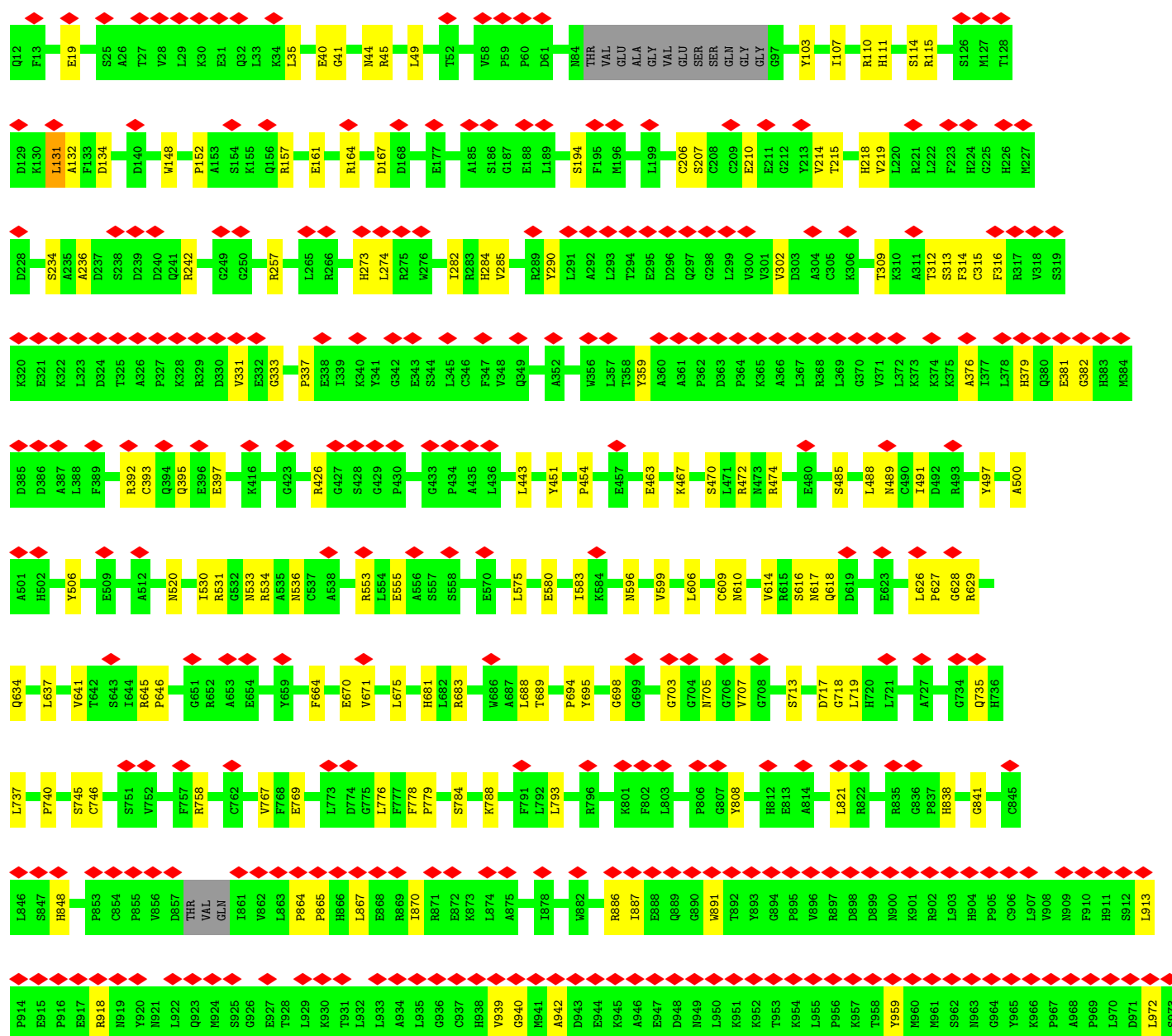
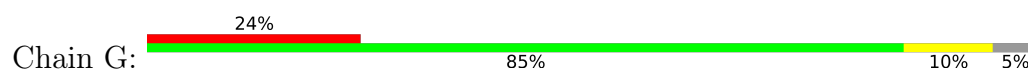




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L4831	GLY	E3965	E3733	E3733	X3600	X3438	X3332	X3255	X3094	X2985	L2914	
L4832	GLY	E3966	E3734	E3734	X3601	X3439	X3333	X3256	X3095	X2986		
L4833	GLY	E3967	E3735	E3735	X3602	X3440	X3334	X3257	X3096	X2987		
L4834	GLY	E3968	E3736	E3736	X3603	X3441	X3335	X3258	X3097	X2988		
L4835	GLY	E3969	E3737	E3737	X3604	X3442	X3336	X3259	X3098	X2989		
L4836	GLY	E3970	E3738	E3738	X3605	X3443	X3337	X3260	X3099	X2990		
L4837	GLY	E3971	E3739	E3739	X3606	X3444	X3338	X3261	X3100	X2991		
L4838	GLY	E3972	E3740	E3740	X3607	X3445	X3339	X3262	X3101	X2992		
L4839	GLY	E3973	E3741	E3741	X3608	X3446	X3340	X3263	X3102	X2993		
L4840	GLY	E3974	E3742	E3742	X3609	X3447	X3341	X3264	X3103	X2994		
L4841	GLY	E3975	E3743	E3743	X3610	X3448	X3342	X3265	X3104	X2995		
L4842	GLY	E3976	E3744	E3744	X3611	X3449	X3343	X3266	X3105	X2996		
L4843	GLY	E3977	E3745	E3745	X3612	X3450	X3344	X3267	X3106	X2997		
L4844	GLY	E3978	E3746	E3746	X3613	X3451	X3345	X3268	X3107	X2998		
L4845	GLY	E3979	E3747	E3747	X3614	X3452	X3346	X3269	X3108	X2999		
L4846	GLY	E3980	E3748	E3748	X3615	X3453	X3347	X3270	X3109	X3000		
L4847	GLY	E3981	E3749	E3749	X3616	X3454	X3348	X3271	X3110	X3001		
L4848	GLY	E3982	E3750	E3750	X3617	X3455	X3349	X3272	X3111	X3002		
L4849	GLY	E3983	E3751	E3751	X3618	X3456	X3350	X3273	X3112	X3003		
L4850	GLY	E3984	E3752	E3752	X3619	X3457	X3351	X3274	X3113	X3004		
L4851	GLY	E3985	E3753	E3753	X3620	X3458	X3352	X3275	X3114	X3005		
L4852	GLY	E3986	E3754	E3754	X3621	X3459	X3353	X3276	X3115	X3006		
L4853	GLY	E3987	E3755	E3755	X3622	X3460	X3354	X3277	X3116	X3007		
L4854	GLY	E3988	E3756	E3756	X3623	X3461	X3355	X3278	X3117	X3008		
L4855	GLY	E3989	E3757	E3757	X3624	X3462	X3356	X3279	X3118	X3009		
L4856	GLY	E3990	E3758	E3758	X3625	X3463	X3357	X3280	X3119	X3010		
L4857	GLY	E3991	E3759	E3759	X3626	X3464	X3358	X3281	X3120	X3011		
L4858	GLY	E3992	E3760	E3760	X3627	X3465	X3359	X3282	X3121	X3012		
L4859	GLY	E3993	E3761	E3761	X3628	X3466	X3360	X3283	X3122	X3013		
L4860	GLY	E3994	E3762	E3762	X3629	X3467	X3361	X3284	X3123	X3014		
L4861	GLY	E3995	E3763	E3763	X3630	X3468	X3362	X3285	X3124	X3015		
L4862	GLY	E3996	E3764	E3764	X3631	X3469	X3363	X3286	X3125	X3016		
L4863	GLY	E3997	E3765	E3765	X3632	X3470	X3364	X3287	X3126	X3017		
L4864	GLY	E3998	E3766	E3766	X3633	X3471	X3365	X3288	X3127	X3018		
L4865	GLY	E3999	E3767	E3767	X3634	X3472	X3366	X3289	X3128	X3019		
L4866	GLY	E4000	E3768	E3768	X3635	X3473	X3367	X3290	X3129	X3020		
L4867	GLY	E4001	E3769	E3769	X3636	X3474	X3368	X3291	X3130	X3021		
L4868	GLY	E4002	E3770	E3770	X3637	X3475	X3369	X3292	X3131	X3022		
L4869	GLY	E4003	E3771	E3771	X3638	X3476	X3370	X3293	X3132	X3023		
L4870	GLY	E4004	E3772	E3772	X3639	X3477	X3371	X3294	X3133	X3024		
L4871	GLY	E4005	E3773	E3773	X3640	X3478	X3372	X3295	X3134	X3025		
L4872	GLY	E4006	E3774	E3774	X3641	X3479	X3373	X3296	X3135	X3026		
L4873	GLY	E4007	E3775	E3775	X3642	X3480	X3374	X3297	X3136	X3027		
L4874	GLY	E4008	E3776	E3776	X3643	X3481	X3375	X3298	X3137	X3028		
L4875	GLY	E4009	E3777	E3777	X3644	X3482	X3376	X3299	X3138	X3029		
L4876	GLY	E4010	E3778	E3778	X3645	X3483	X3377	X3300	X3139	X3030		
L4877	GLY	E4011	E3779	E3779	X3646	X3484	X3378	X3301	X3140	X3031		
L4878	GLY	E4012	E3780	E3780	X3647	X3485	X3379	X3302	X3141	X3032		
L4879	GLY	E4013	E3781	E3781	X3648	X3486	X3380	X3303	X3142	X3033		
L4880	GLY	E4014	E3782	E3782	X3649	X3487	X3381	X3304	X3143	X3034		
L4881	GLY	E4015	E3783	E3783								

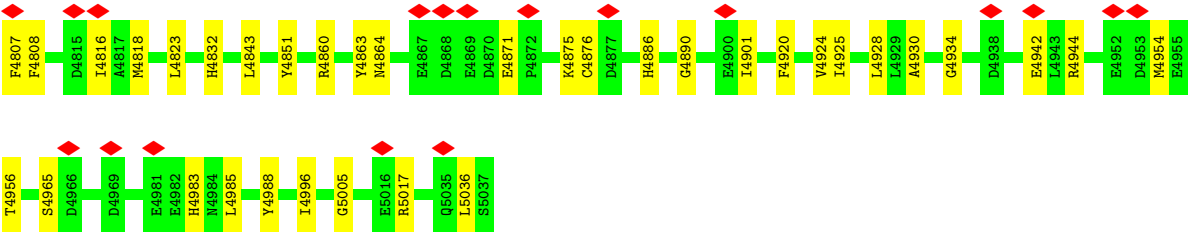


• Molecule 2: Ryanodine receptor 1





C4645	Y4560	D4046	L3805	W3661	X3520	X3373	X3269	X3006	K2914	GLY	Y2855	W2794
Y4666	L4567	L4066	M3809	I3662	X3530	X3374	X3270	X3010	E2915		N2856	K2795
Y4669	A4570	D4070	V3812	E3665	X3533	X3378	X3274	X3019	A2917		P2857	T2796
R4673	M4574	D4079	K3815	H3667	X3534	X3381	X3275	X3020	D2918		Q2858	S2798
E4674	V4582	Y4090	L3842	S3668	X3540	X3386	X3276	X3021	P2859		P2860	E2799
K4680	D3843	Y4083	D3843	G3661	X3543	X3387	X3277	X3022	E2921		D2861	K2800
G4685	Q3850	Y4083	Q3850	E3662	X3544	X3388	X3281	X3023	L2862		L2862	D2801
L4686	G3857	R4084	G3857	Q3663	X3545	X3389	X3284	X3027	S2863		S2863	E2803
I4688	M3858	G4086	M3858	E3664	X3546	X3390	X3285	X3037	G2864		G2864	I2804
D4694	V3859	K4091	V3859	E3665	X3547	X3391	X3286	X3038	E2865		V2865	Y2805
D4695	M3860	A4096	M3860	E3666	X3548	X3392	X3287	X3040	L2926		L2926	W2806
V4697	D3862	N4097	D3862	E3667	X3549	X3393	X3290	X3042	K2928		K2928	W2807
K4698	G3863	N4098	G3863	E3668	X3550	X3394	X3291	X3043	P2868		P2868	F2808
G4699	T3864	D4098	T3864	E3669	X3553	X3395	X3292	X3044	I2869		I2869	T2809
Y4715	T3865	G4105	T3865	E3691	X3554	X3396	X3293	X3045	L2930		L2930	K2810
H4728	I3866	P4106	I3866	E3692	X3558	X3397	X3294	X3046	L2931		L2931	E2811
G4729	M3867	N4120	M3867	E3693	X3559	X3398	X3295	X3047	Q2872		Q2872	S2812
M4743	R3868	E4152	R3868	E3712	X3560	X3399	X3296	X3048	M2932		M2932	L2813
D4744	Q3869	Y4155	Q3869	S3714	X3561	X3400	X3297	X3049	N2933		N2933	K2814
L4745	M3870	P4155	M3870	K3715	X3562	X3401	X3313	X3050	G2934		G2934	L2815
A4746	G3871	H4156	G3871	E3736	X3563	X3402	X3314	X3053	A2936		A2936	F2816
	K3872	Y4173	K3872	E3737	X3564	X3404	X3318	X3054	V2937		V2937	T2817
	D3873	R4180	D3873	G3738	X3565	X3405	X3319	X3055	T2938		T2938	A2818
	Q3889	A4186	Q3889	G3739	X3566	X3409	X3320	X3060	R2889		R2889	W2819
	M3896	S4187	M3896	E3740	X3567	X3410	X3321	X3061	K2890		K2890	E2820
	I3915	R4188	I3915	N3741	X3568	X3412	X3322	X3062	N2881		N2881	W2821
	T3919	E4209	T3919	GLU	X3576	X3413	X3230	X3063	Y2882		Y2882	T2823
	S3929	R4215	S3929	ALA	X3580	X3414	X3231	X3064	N2884		N2884	E2824
	Y3937	G4226	Y3937	GLU	X3581	X3415	X3232	X3065	T2885		T2885	K2825
	M3955	E4227	M3955	ALA	X3582	X3416	X3233	X3134	W2886		W2886	G2826
	Q3960	A4228	Q3960	GLU	X3583	X3417	X3234	X3135	R2888		R2888	E2828
	G3971	E4232	G3971	GLU	X3584	X3418	X3235	X3136	K2889		K2889	G2829
	R3984	L4233	R3984	ALA	X3585	X3419	X3236	X3137	K2891		K2891	E2830
	K4002	S4236	K4002	GLU	X3586	X3421	X3241	X3138	Q2892		Q2892	GLU
	L4019	X4321	L4019	E3747	X3587	X3422	X3242	X3142	ARG		ARG	THR
	E4032	X4322	E4032	E3754	X3588	X3423	X3243	X3143	GLU		GLU	THR
	G4033	F4540	G4033	T3772	X3589	X3441	X3244	X3144	L2894		L2894	GLU
	N4641	R4548	N4641	R3773	X3609	X3452	X3245	X3153	E2895		E2895	LYS
	A4642		A4642	E3777	X3610	X3453	X3246	X3156	A2896		A2896	LYS
				M3778	X3611	X3454	X3247	X3157	K2897		K2897	THR
				L3780	X3612	X3455	X3248	X3158	ARG		ARG	ARG
				Q3781	X3613	X3456	X3249	X3159	LYS		LYS	LYS
				S3784	X3614	X3464	X3250	X3160	ILE		ILE	ILE
				K3787	X3615	X3467	X3251	X3161	SER		SER	GLN
				I3804	X3616	X3468	X3252	X3162	THR		THR	THR
					X3656	X3469	X3253	X3163	ALA		ALA	ALA
					Y3657	X3470	X3254	X3164	GLN		GLN	GLN
					K3658	X3471	X3255	X3165	THR		THR	THR
							X3256	X3166	TYR		TYR	TYR
							X3257	X3167	L2905		L2905	L2904
							X3258	X3168	V2906		V2906	V2904
							X3259	X3169	ASP		ASP	ASP
							X3260	X3170	PRO		PRO	PRO
							X3261	X3171	ARG		ARG	ARG
							X3262	X3172	GLU		GLU	GLU
							X3263	X3173				
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.070	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CFF, ZN, ATP

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	0.32	0/834	0.54	0/1123
1	F	0.32	0/834	0.54	0/1123
1	H	0.32	0/834	0.54	0/1123
1	J	0.32	0/834	0.54	0/1123
2	B	0.32	0/25428	0.57	13/34534 (0.0%)
2	E	0.32	0/25428	0.57	13/34534 (0.0%)
2	G	0.32	0/25428	0.57	13/34534 (0.0%)
2	I	0.32	0/25428	0.57	13/34534 (0.0%)
All	All	0.32	0/105048	0.57	52/142628 (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	2
1	F	0	2
1	H	0	2
1	J	0	2
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	80

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.14	134.03	115.30
2	B	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	I	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	4639	MET	C-N-CA	6.84	138.79	121.70

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
1	A	82	TYR	Peptide
1	F	8	SER	Peptide
1	F	82	TYR	Peptide
1	H	8	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	10	0
1	F	818	0	824	10	0
1	H	818	0	824	11	0
1	J	818	0	824	11	0
2	B	29499	0	24752	242	0
2	E	29499	0	24752	242	0
2	G	29499	0	24752	241	0
2	I	29499	0	24752	243	0
3	B	31	0	12	1	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102392	986	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 4.

The worst 5 of 986 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.73	0.70
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.69
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.73	0.69
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.75	0.69

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	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	47	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	47	80
2	G	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	47	80
2	I	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	47	80
All	All	13360/18096 (74%)	11884 (89%)	1452 (11%)	24 (0%)	50	80

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1840	PRO
2	B	1932	PRO
2	B	4641	PRO
2	E	1708	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	84	90

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1600	LEU

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Mol	Chain	Res	Type
2	G	1964	ARG
2	G	4120	ASN
2	E	1676	LEU
2	E	1600	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	4691	GLN
2	G	3771	HIS
2	G	111	HIS
2	G	949	ASN
2	G	4120	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	5101	-	26,33,33	0.87	1 (3%)	31,52,52	1.54	5 (16%)
3	ATP	I	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.55	5 (16%)
3	ATP	B	5101	-	26,33,33	0.87	1 (3%)	31,52,52	1.57	5 (16%)
4	CFF	E	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.20	1 (12%)
4	CFF	G	5102	-	8,15,15	2.53	4 (50%)	8,23,23	1.19	1 (12%)
3	ATP	G	5101	-	26,33,33	0.87	1 (3%)	31,52,52	1.54	5 (16%)
4	CFF	I	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.19	1 (12%)
4	CFF	B	5102	-	8,15,15	2.52	3 (37%)	8,23,23	1.19	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	5101	-	-	4/18/38/38	0/3/3/3
3	ATP	I	5101	-	-	4/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C6-N1	-4.46	1.31	1.38
4	I	5102	CFF	C6-N1	-4.46	1.31	1.38
4	G	5102	CFF	C6-N1	-4.44	1.31	1.38
4	B	5102	CFF	C6-N1	-4.43	1.31	1.38
4	E	5102	CFF	C5-C4	-4.41	1.33	1.39

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	PB-O3B-PG	-3.54	120.69	132.83
3	E	5101	ATP	PB-O3B-PG	-3.53	120.71	132.83
3	G	5101	ATP	PB-O3B-PG	-3.51	120.77	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	ATP	PB-O3B-PG	-3.51	120.80	132.83
3	E	5101	ATP	PA-O3A-PB	-3.35	121.34	132.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

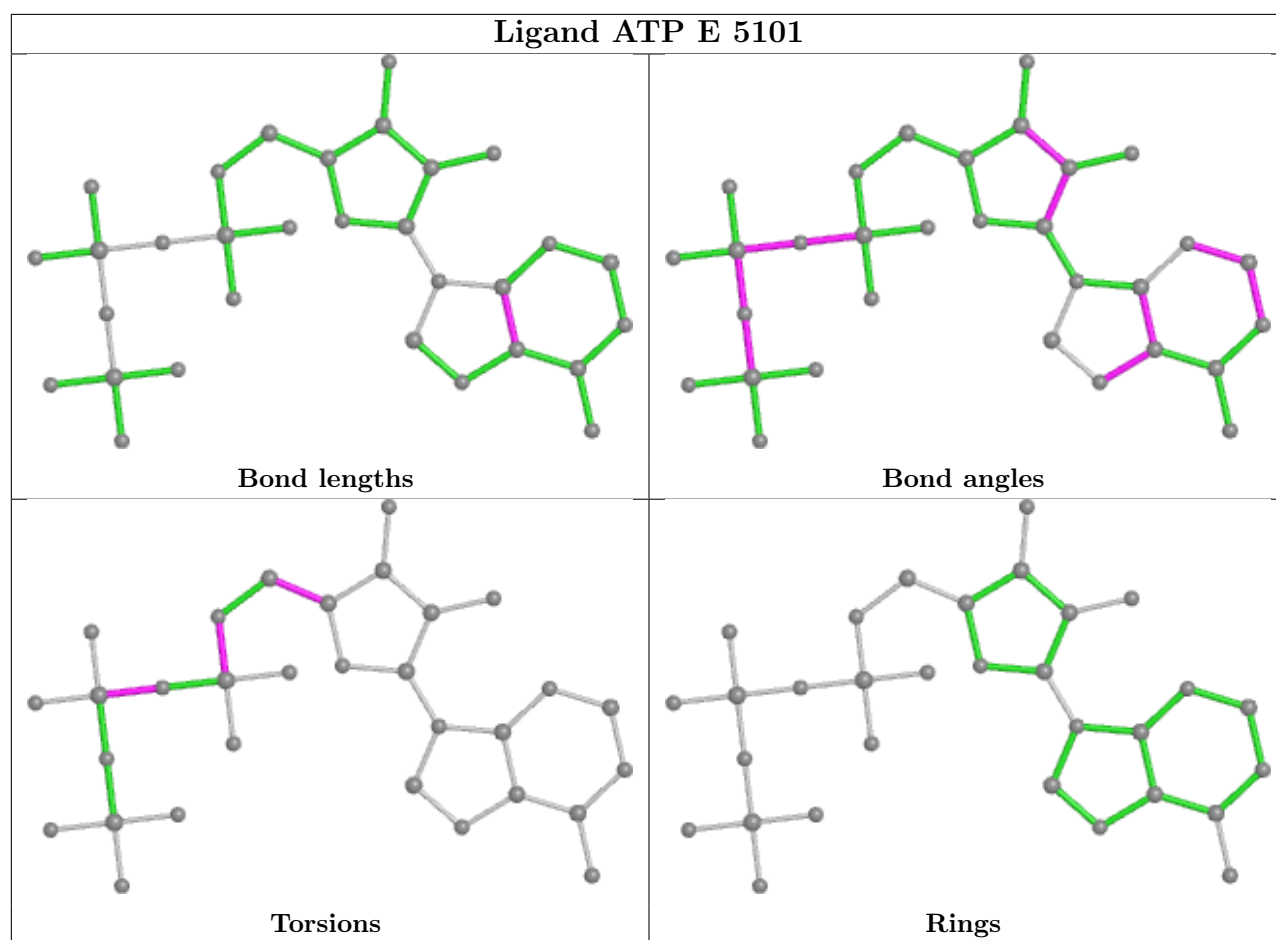
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	PA-O3A-PB-O1B

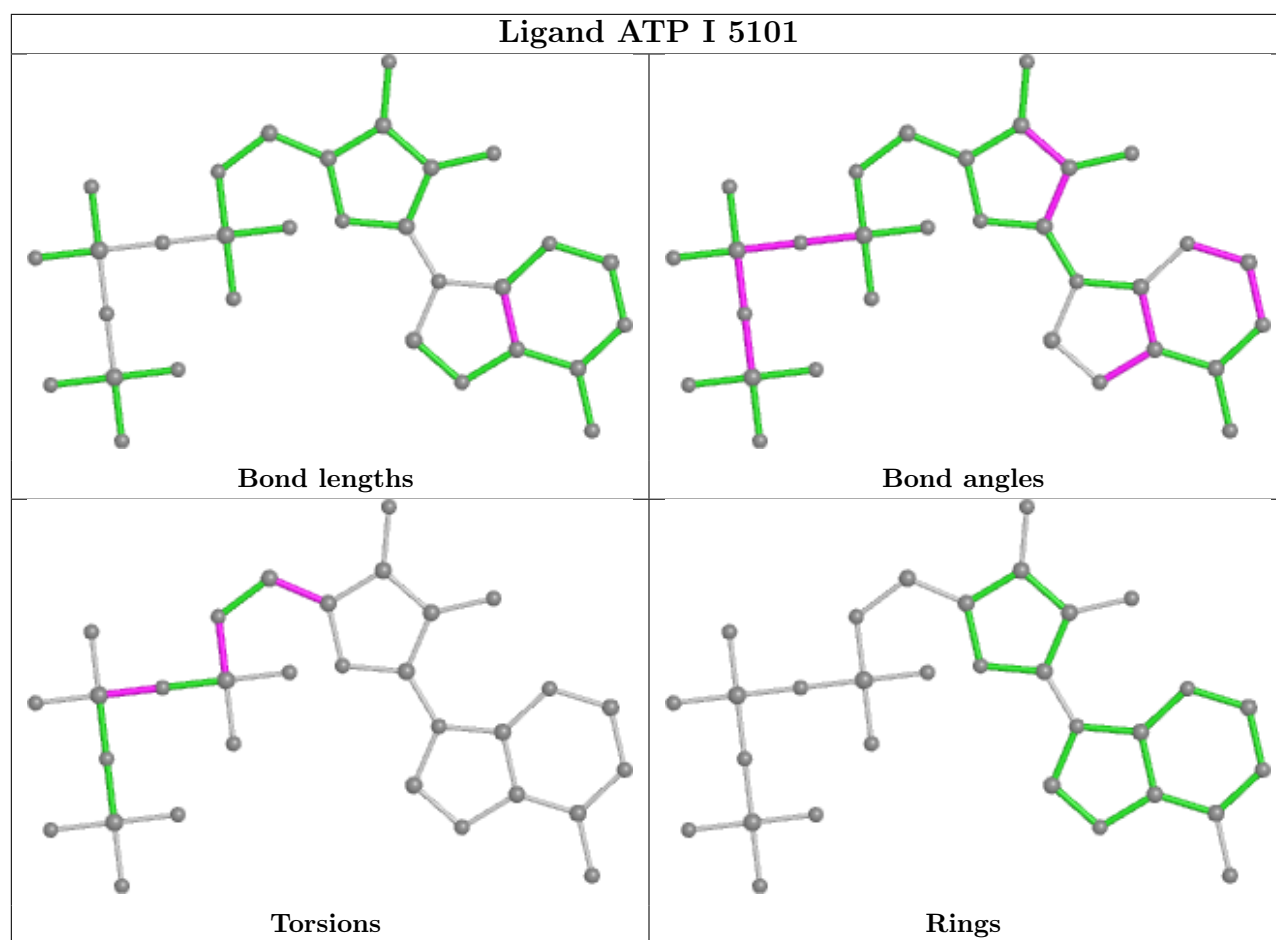
There are no ring outliers.

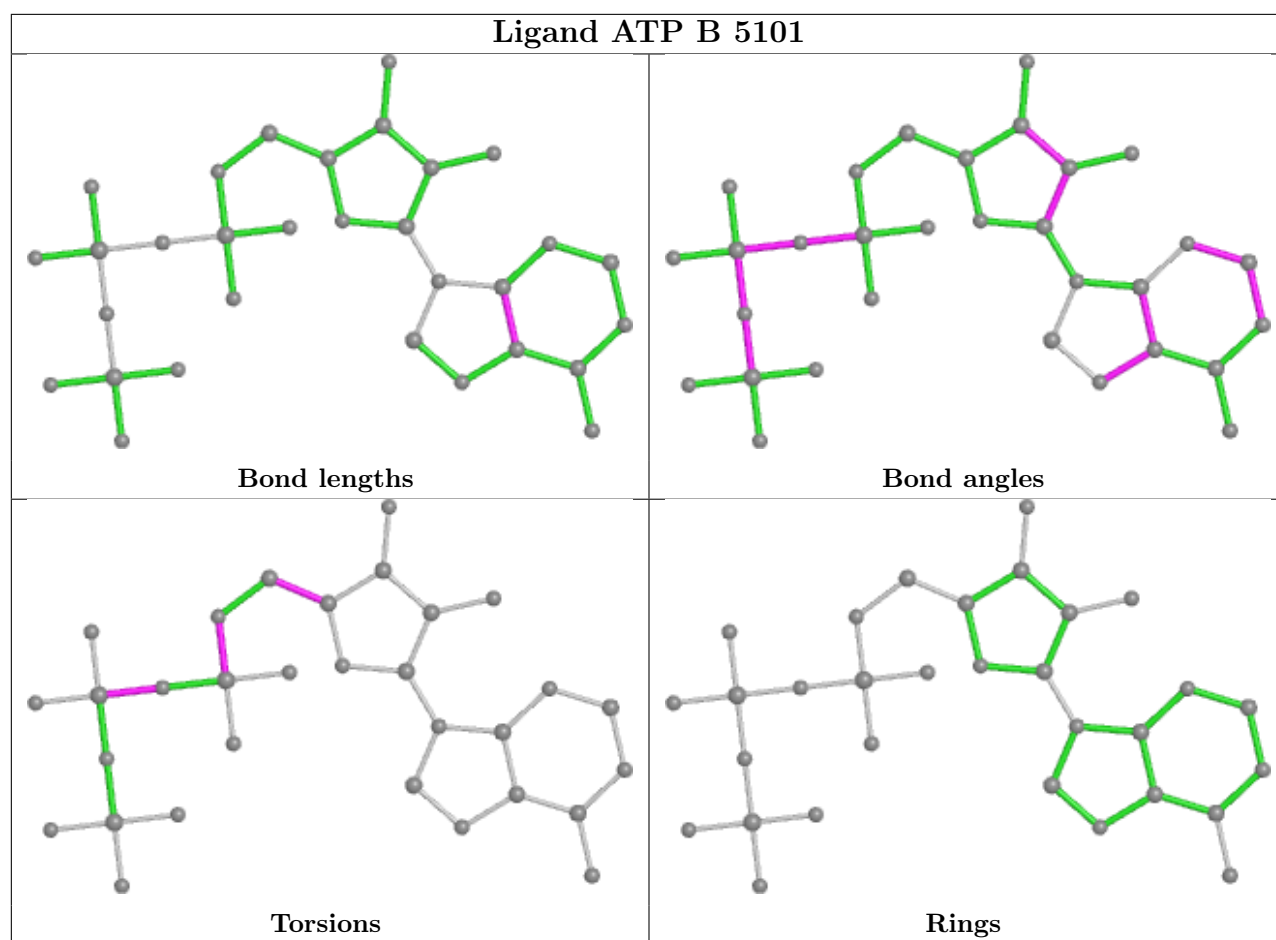
5 monomers are involved in 5 short contacts:

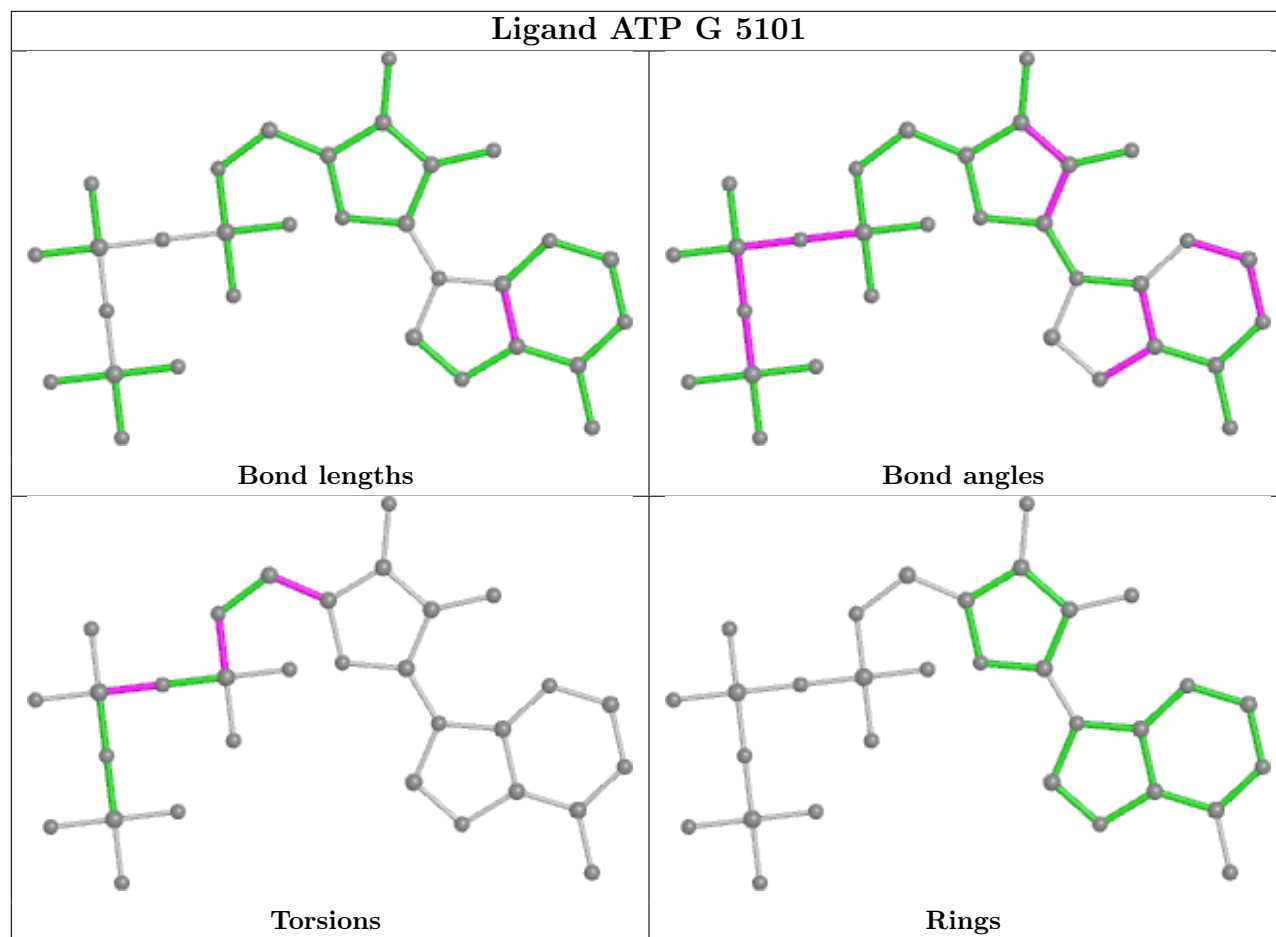
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
4	E	5102	CFF	1	0
4	G	5102	CFF	1	0
4	I	5102	CFF	1	0
4	B	5102	CFF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	14
2	B	14
2	I	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	72.62
1	B	4345:UNK	C	4540:PHE	N	72.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.60
1	G	4345:UNK	C	4540:PHE	N	72.60
1	E	3613:UNK	C	3639:THR	N	43.07

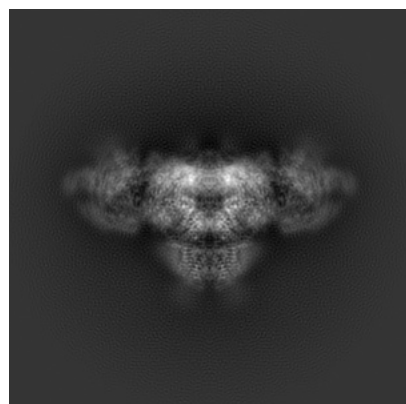
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8382. These allow visual inspection of the internal detail of the map and identification of artifacts.

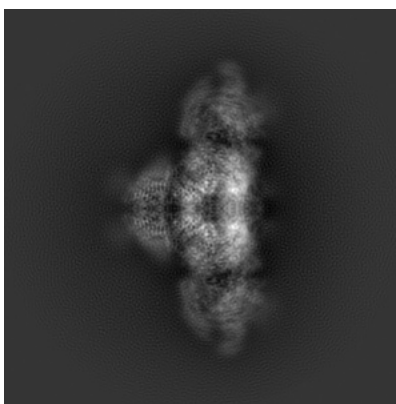
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

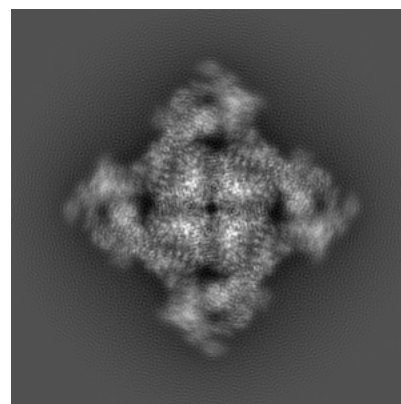
6.1.1 Primary map



X

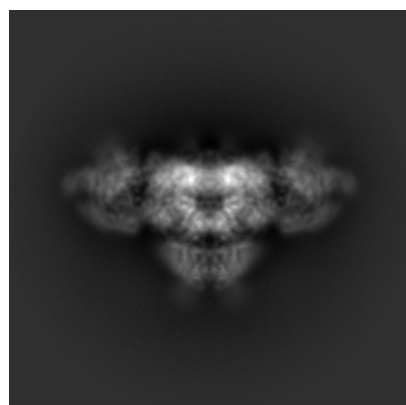


Y

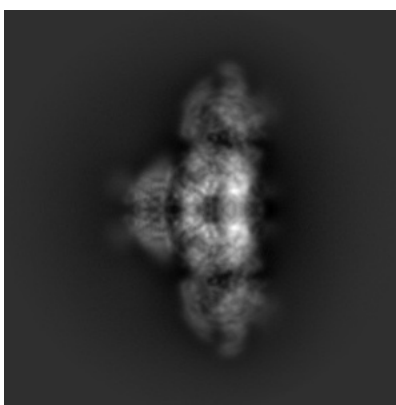


Z

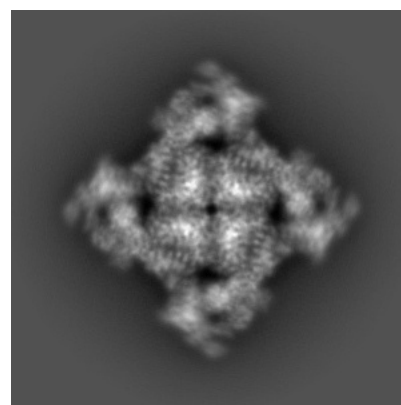
6.1.2 Raw map



X



Y

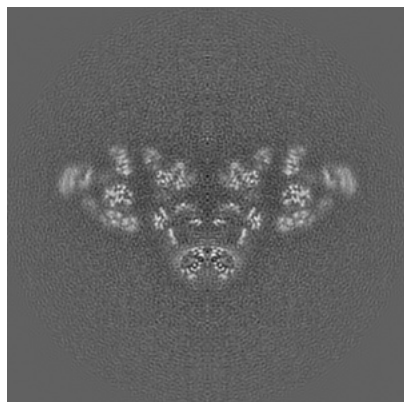


Z

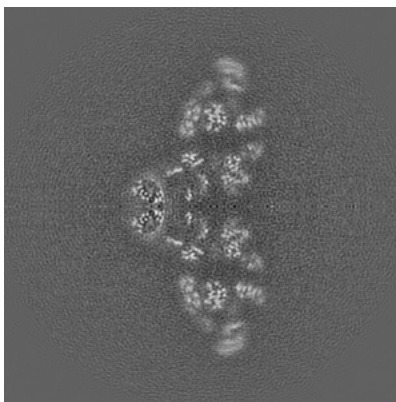
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

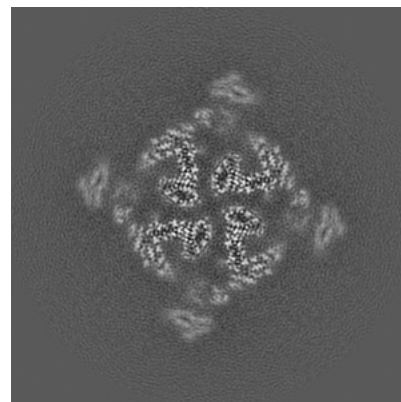
6.2.1 Primary map



X Index: 200

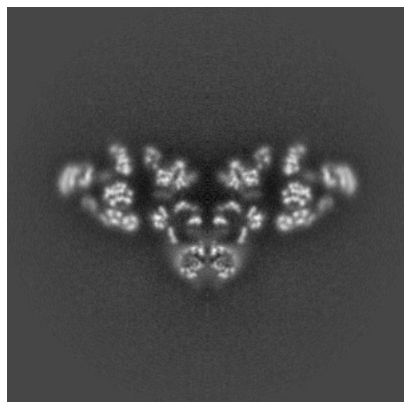


Y Index: 200

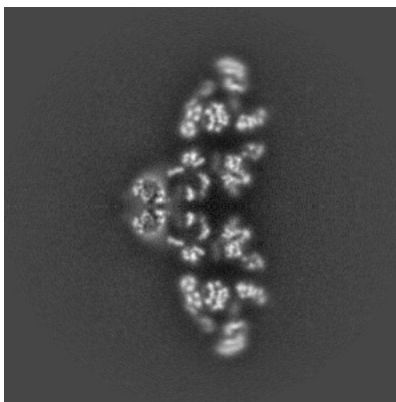


Z Index: 200

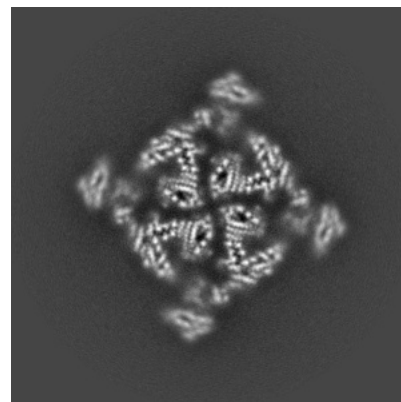
6.2.2 Raw map



X Index: 200



Y Index: 200

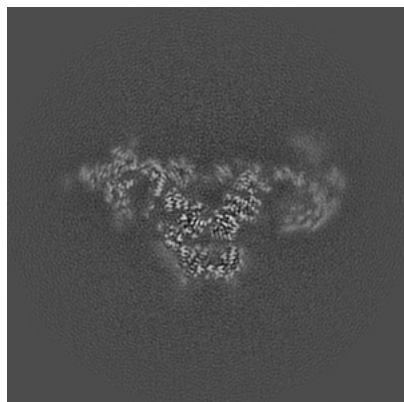


Z Index: 200

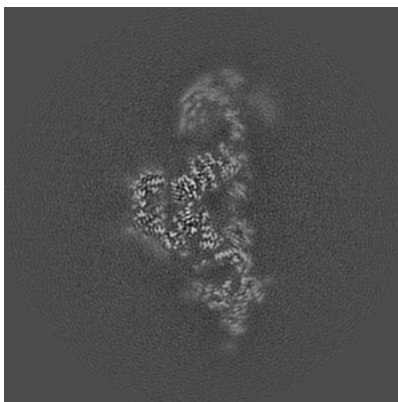
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

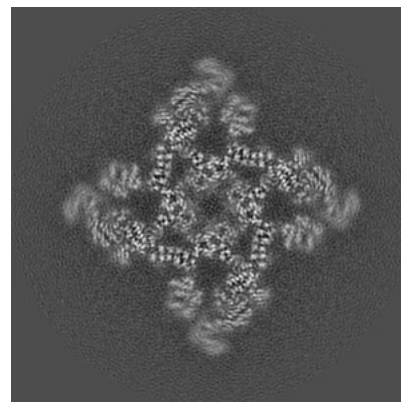
6.3.1 Primary map



X Index: 216

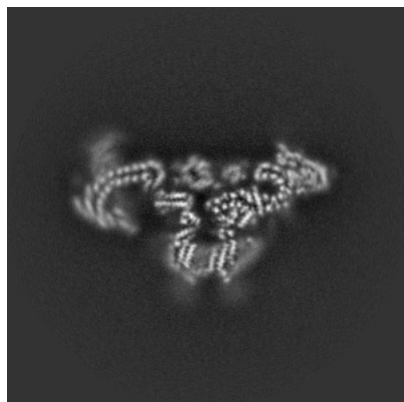


Y Index: 184

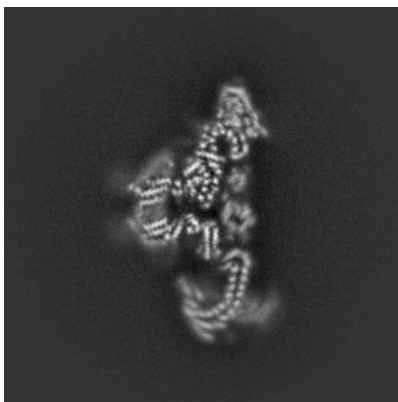


Z Index: 226

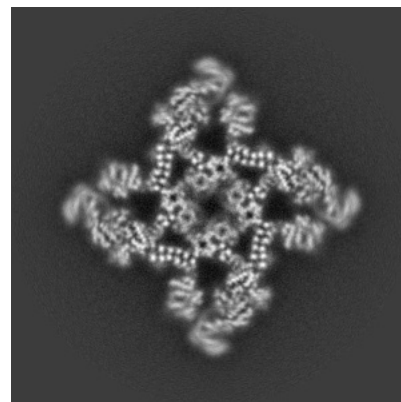
6.3.2 Raw map



X Index: 176



Y Index: 224

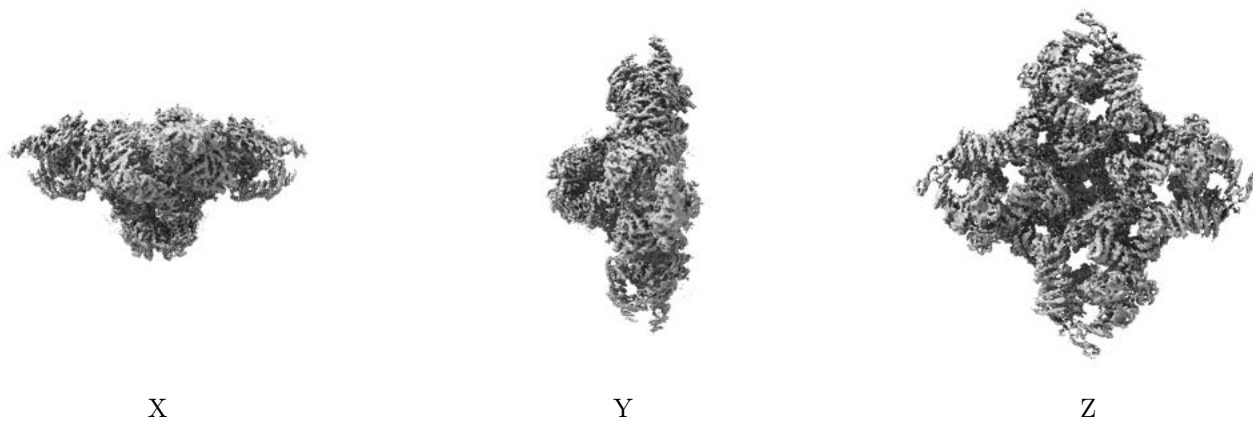


Z Index: 227

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

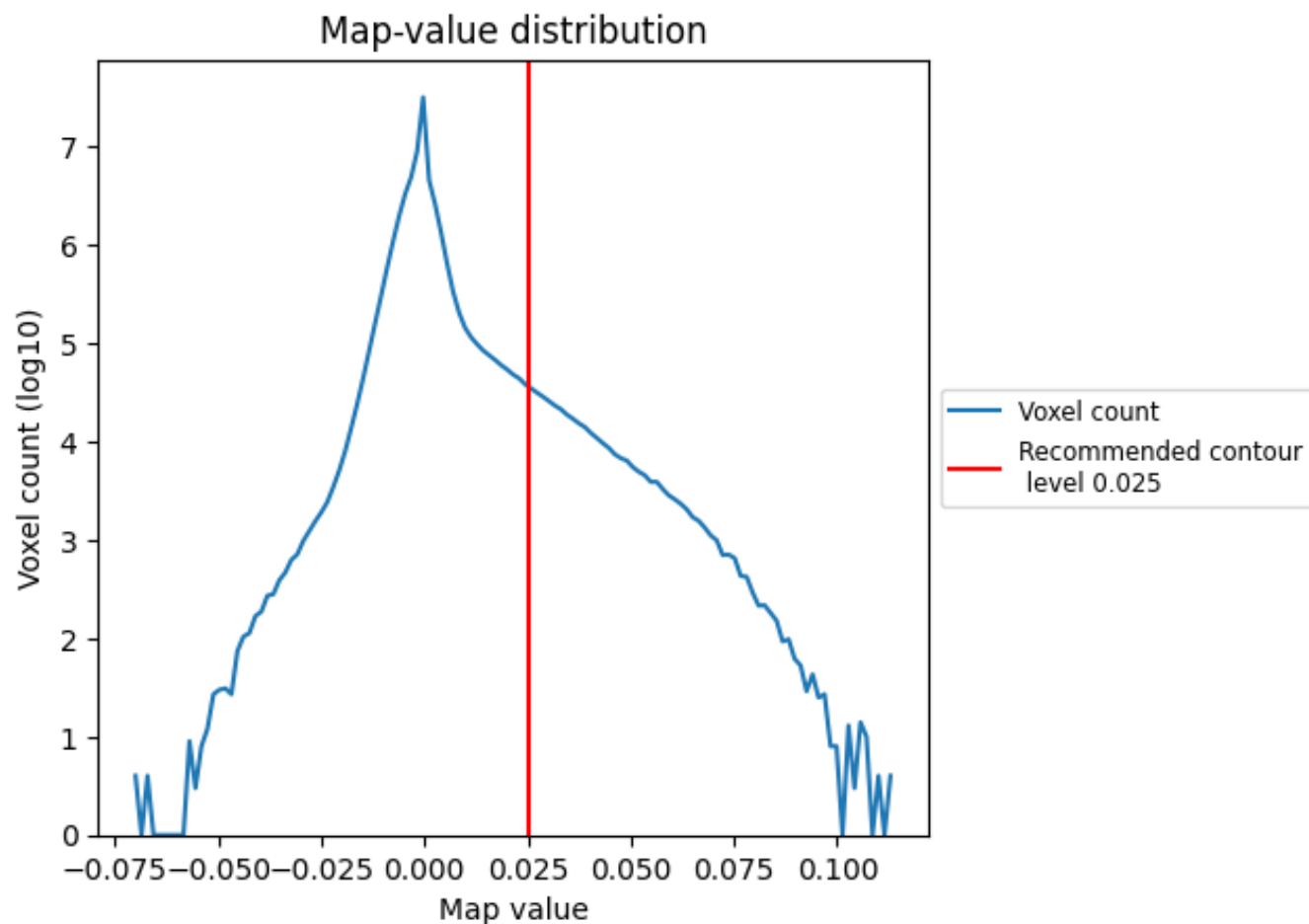
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

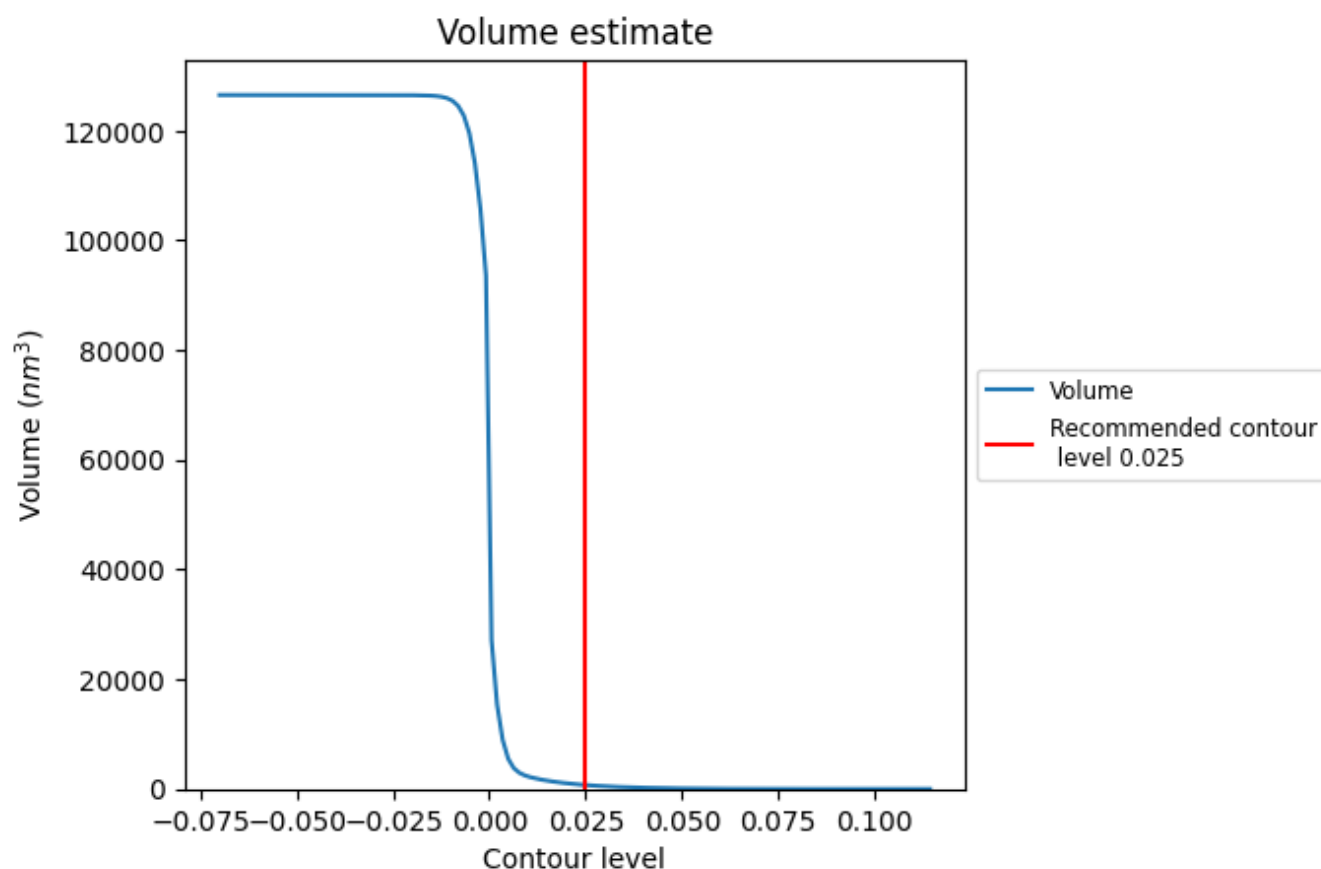
This section contains the results of statistical analysis of the map.

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.

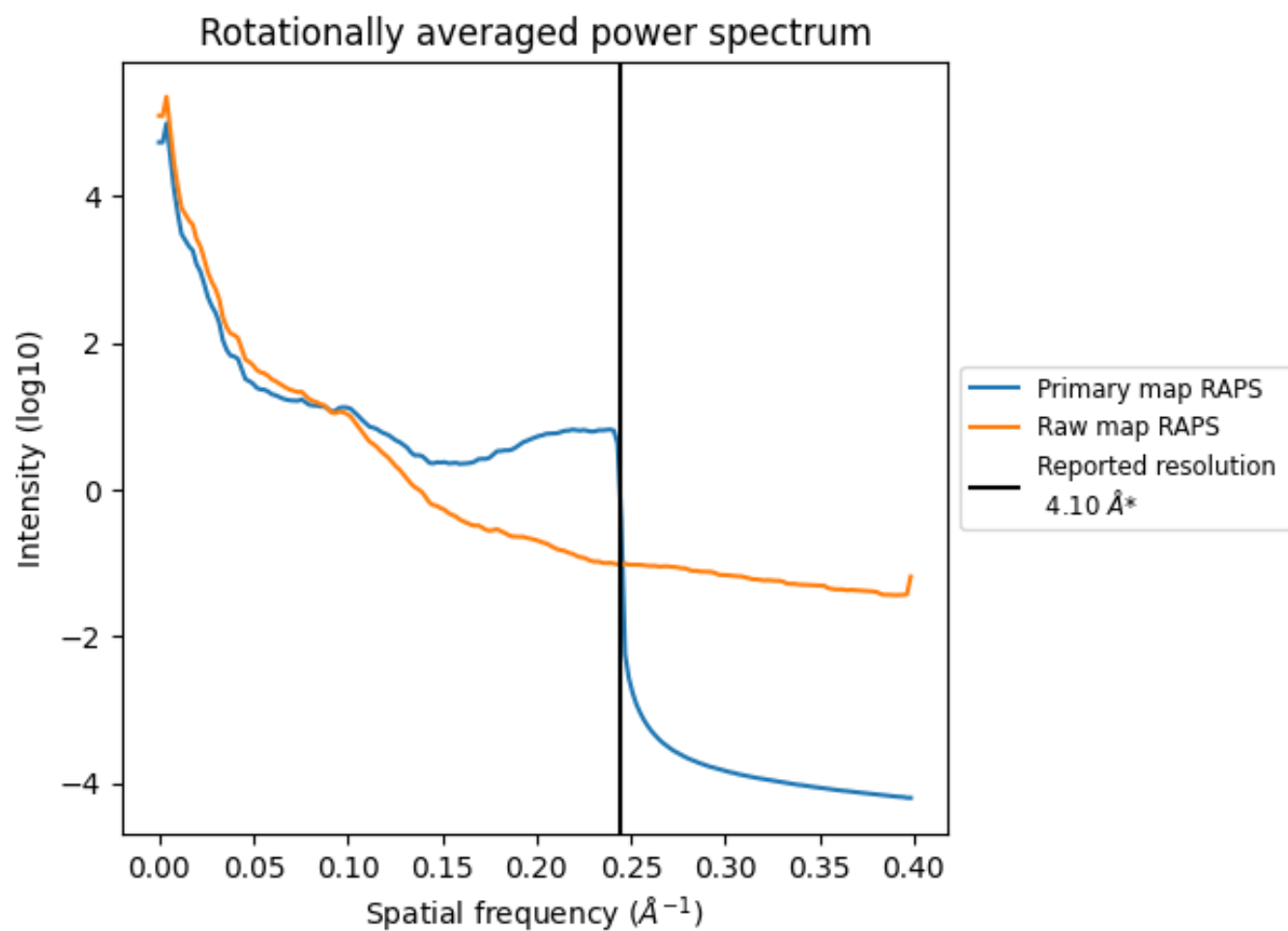
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 713 nm³; this corresponds to an approximate mass of 644 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

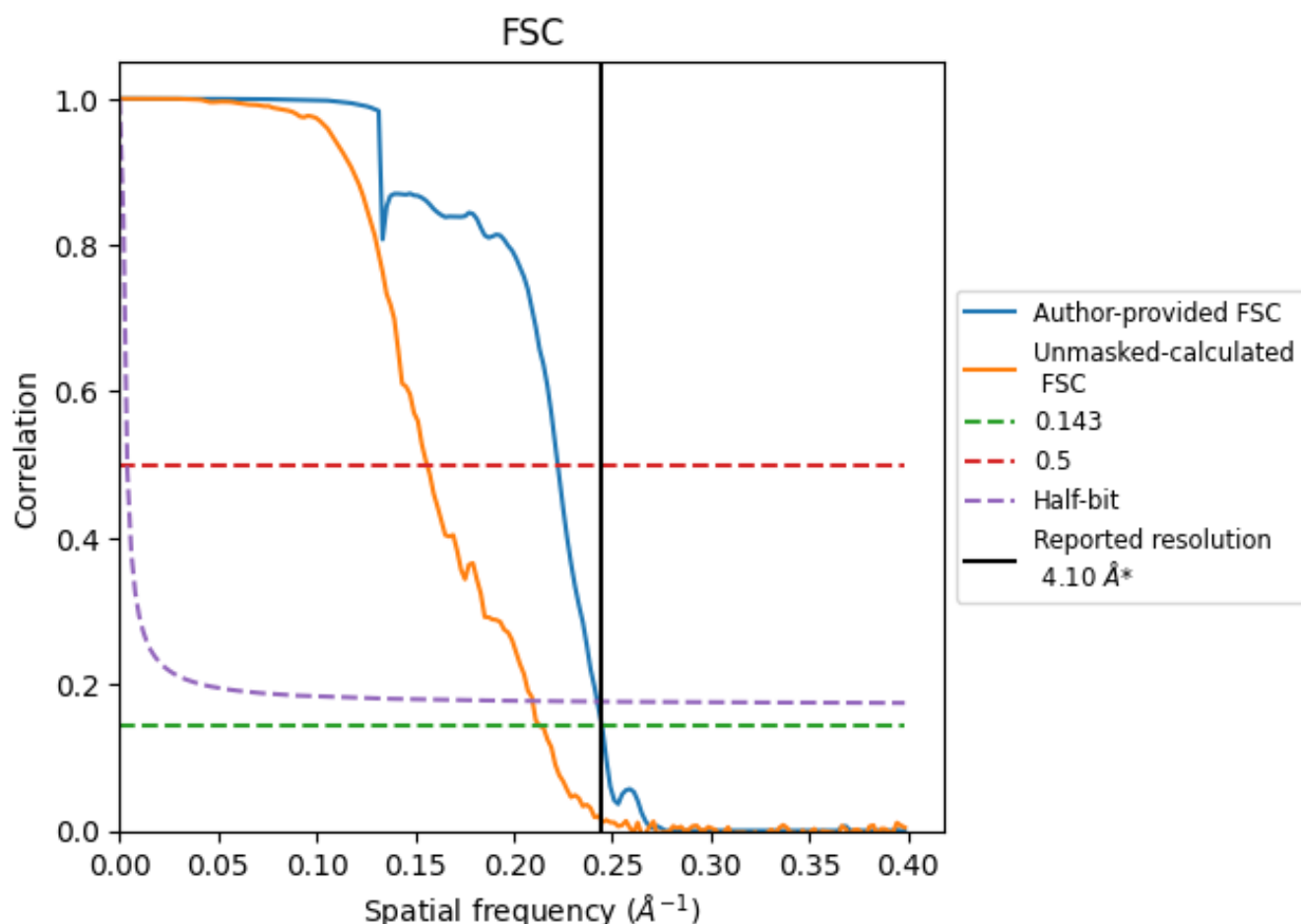


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

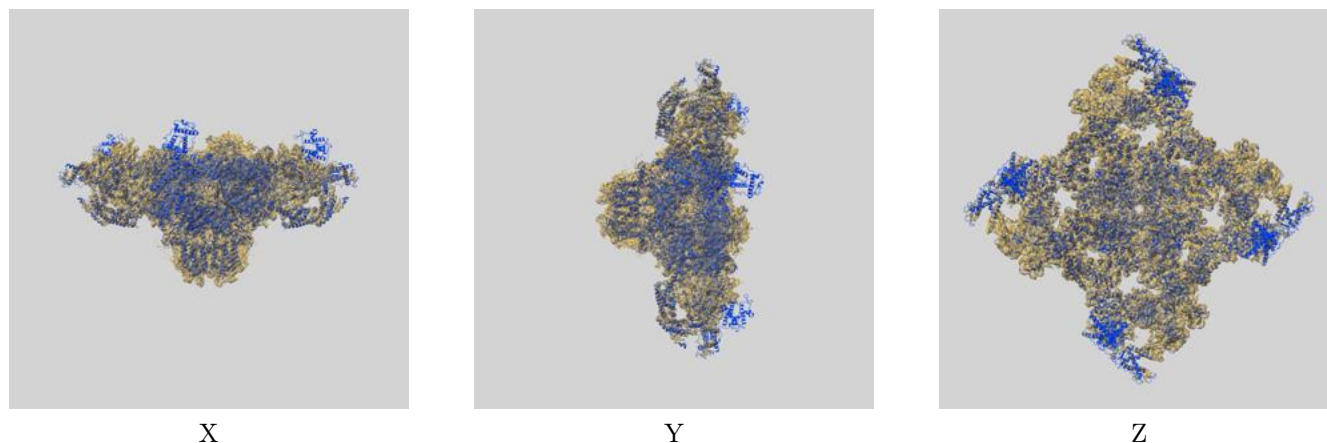
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	4.50	4.13
Unmasked-calculated*	4.69	6.41	4.77

*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 4.69 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

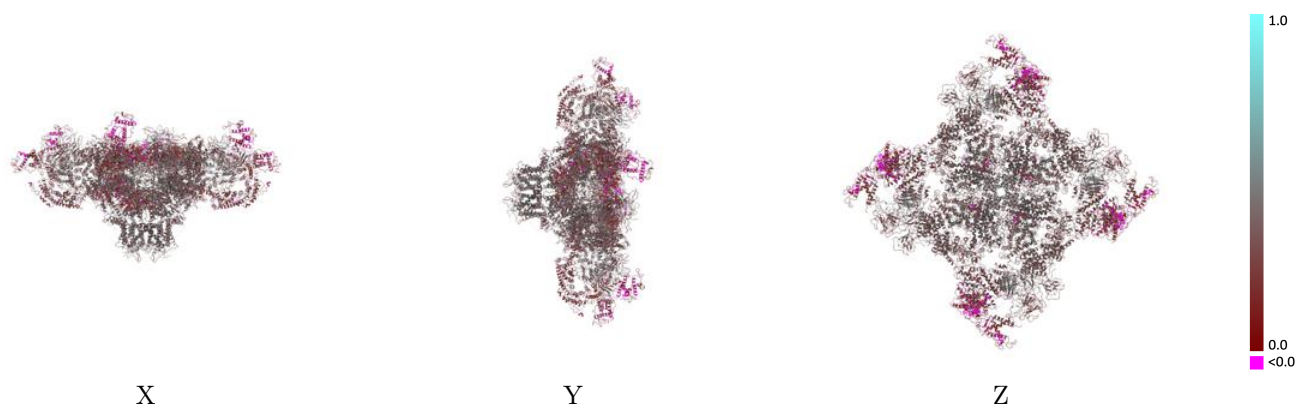
This section contains information regarding the fit between EMDB map EMD-8382 and PDB model 5TAQ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



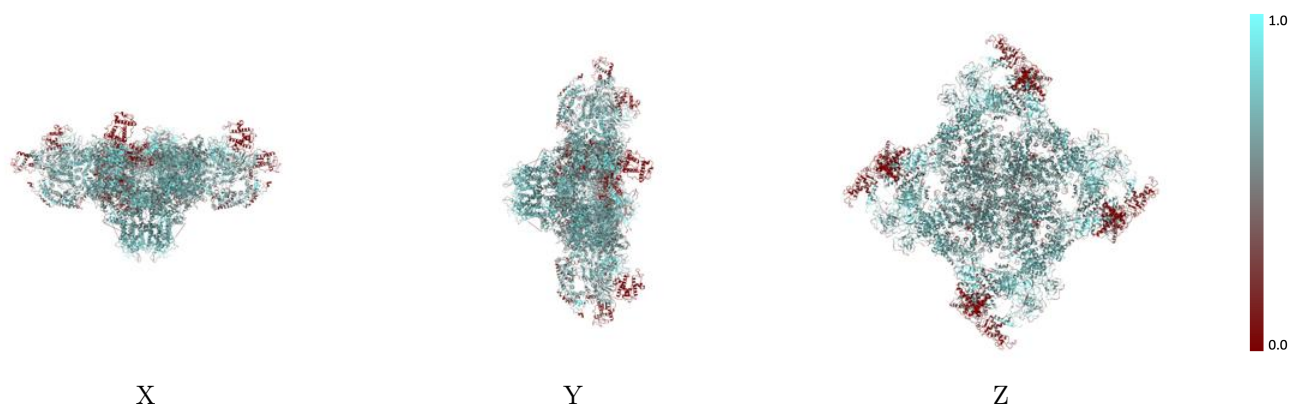
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



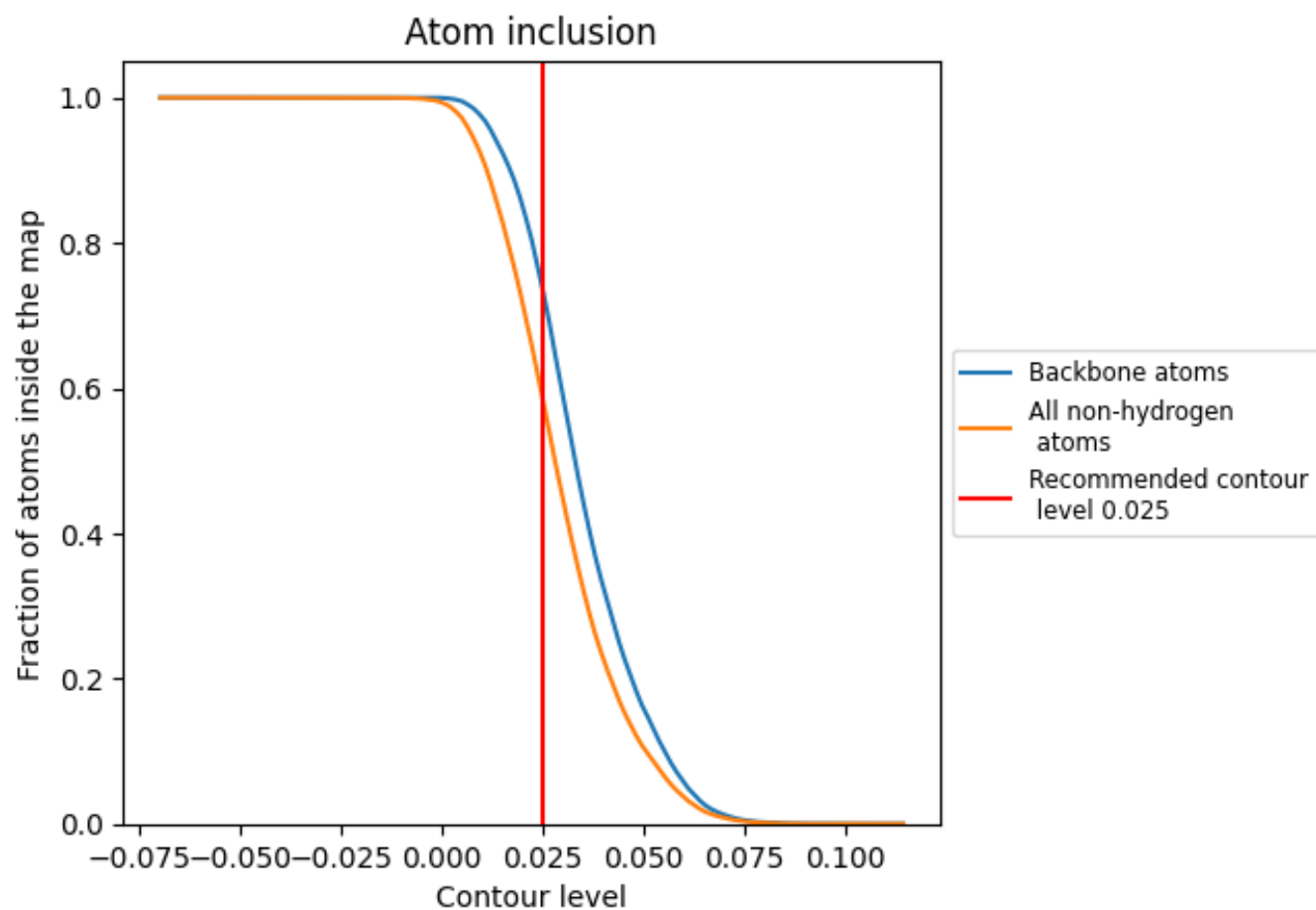
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 58% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5829	<div></div> 0.3350
A	<div></div> 0.5571	<div></div> 0.3500
B	<div></div> 0.5830	<div></div> 0.3340
E	<div></div> 0.5836	<div></div> 0.3340
F	<div></div> 0.5596	<div></div> 0.3560
G	<div></div> 0.5841	<div></div> 0.3350
H	<div></div> 0.5558	<div></div> 0.3530
I	<div></div> 0.5838	<div></div> 0.3350
J	<div></div> 0.5620	<div></div> 0.3490

