



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 11:00 AM EDT

PDB ID : 5T9V
EMDB ID : EMD-8376
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

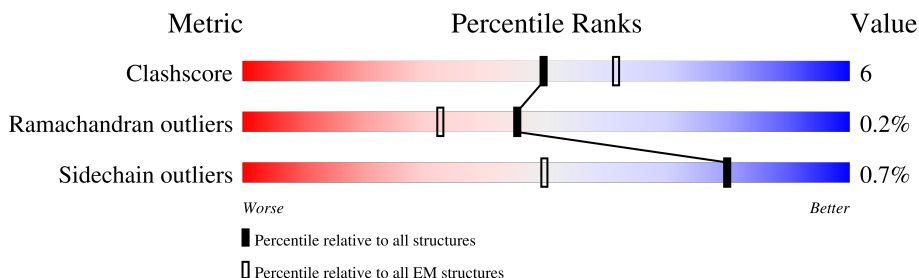
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>77%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	F	108	<div> <div>77%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	H	108	<div> <div>75%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	J	108	<div> <div>75%</div> <div> <div></div> <div>81%</div> <div>19%</div> <div>.</div> </div> </div>
2	B	4416	<div> <div>66%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
2	E	4416	<div> <div>66%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>
2	G	4416	<div> <div>65%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>
2	I	4416	<div> <div>65%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>

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.

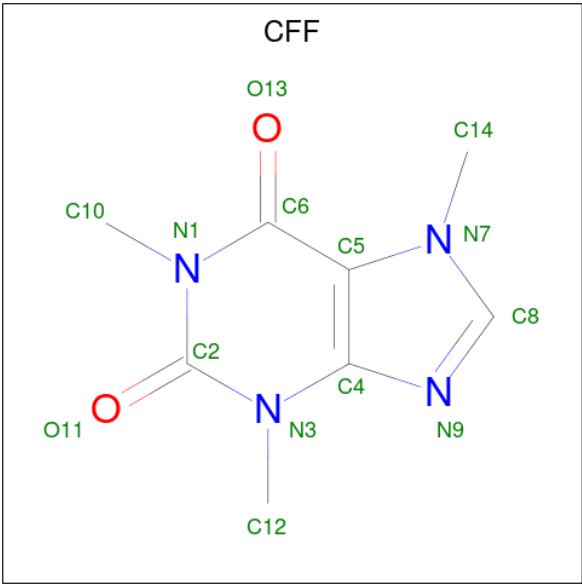
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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	G	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	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).



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

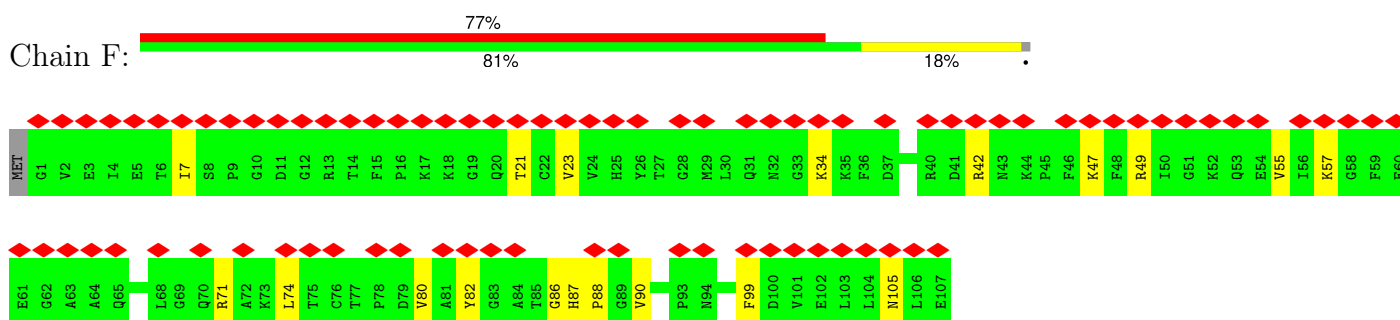
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

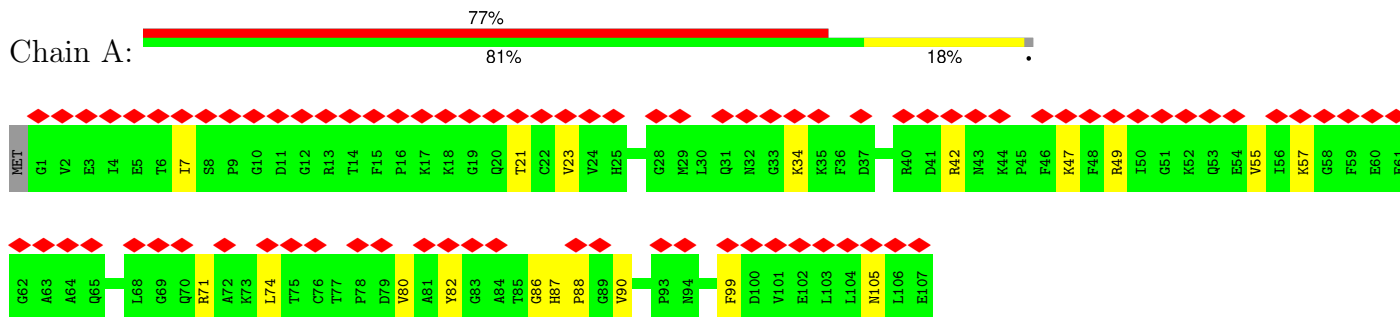
3 Residue-property plots [i](#)

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.

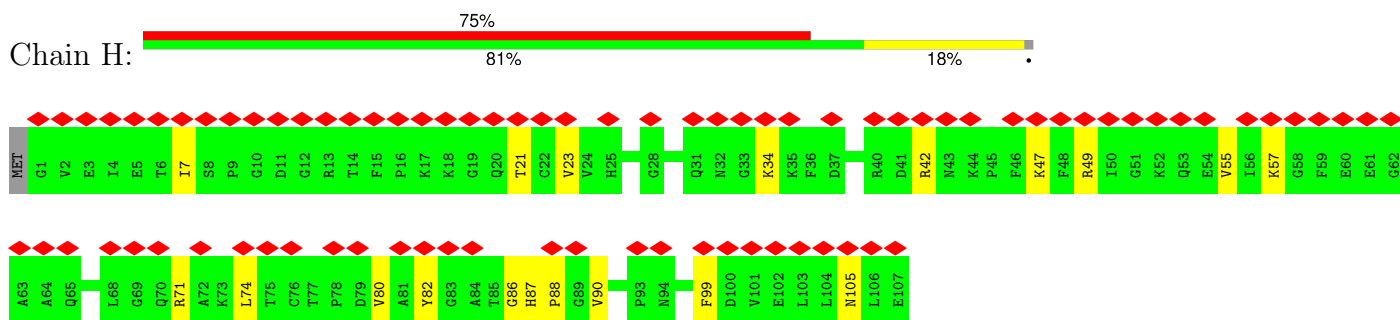
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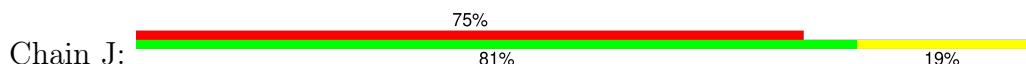
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

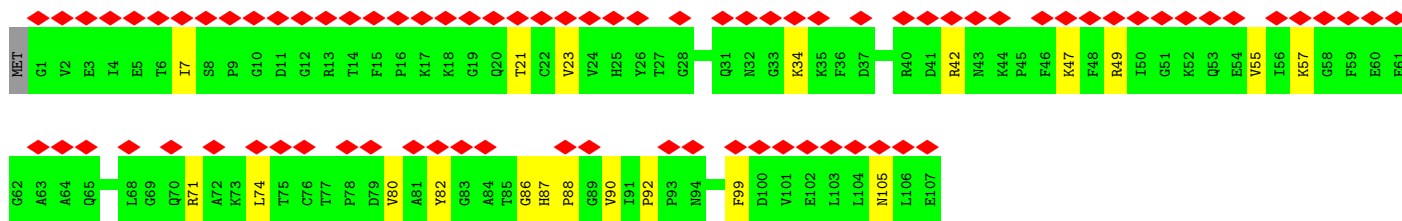


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

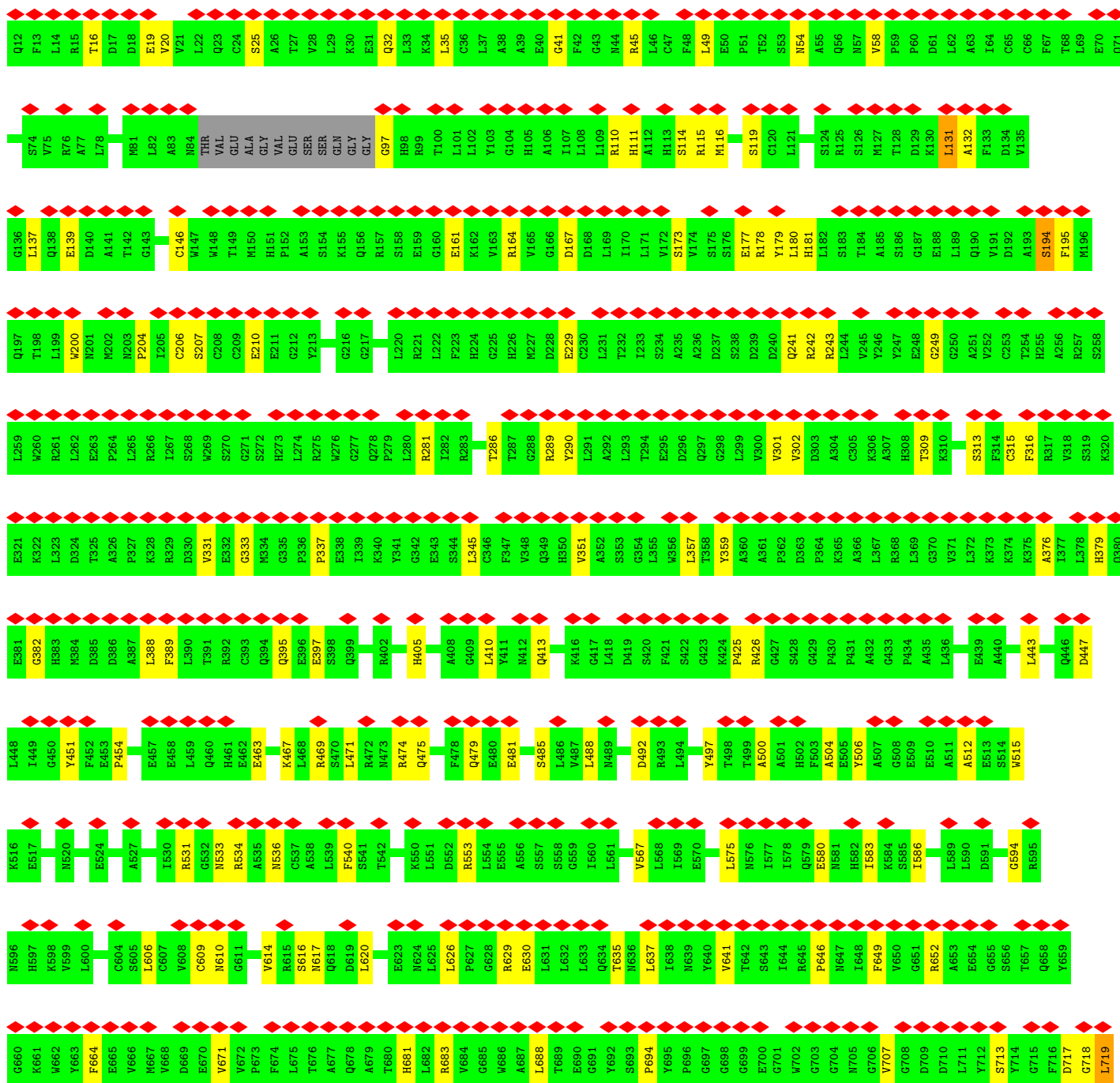
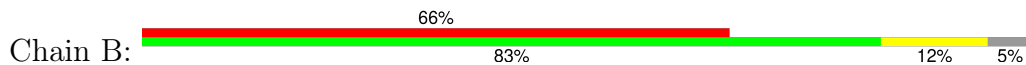


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: Ryanodine receptor 1

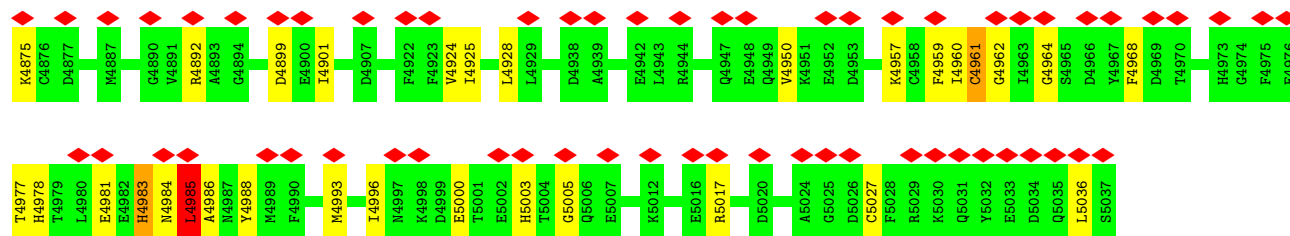


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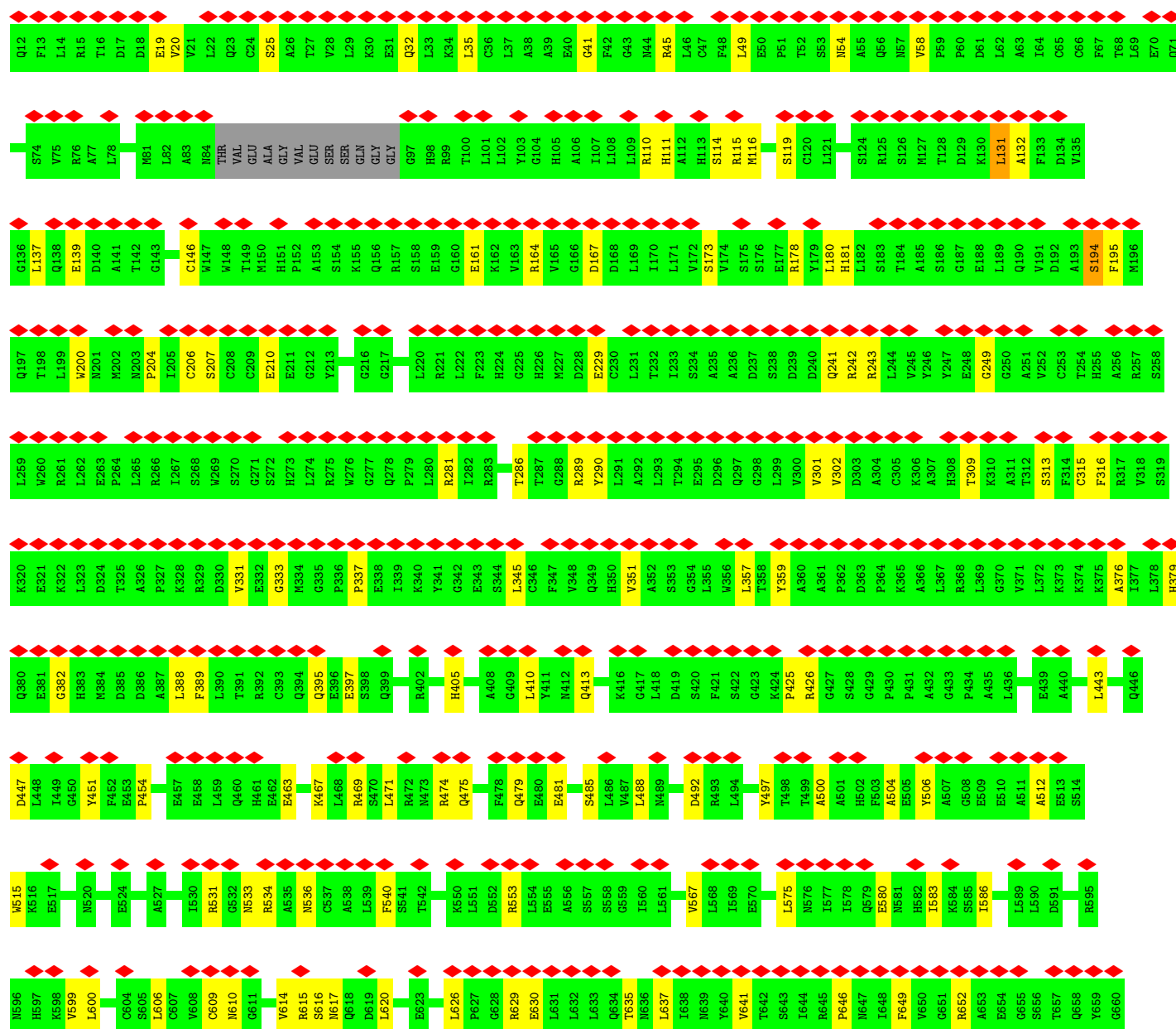
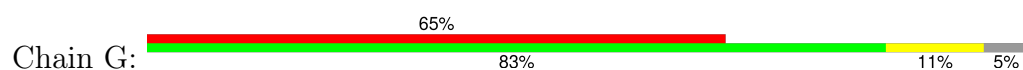


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X3577	X3517	X3415	X3355	X3295	X3225	X3159	X3029	X2951	K2889	G2829	D2769	X2679
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X3579	X3519	X3417	X3357	X3297	X3227	X3161	X3031	X2953	K2891	GLU	L2771	X2681
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X3581	X3521	X3419	X3359	X3299	X3229	X3163	X3033	X2955	E2893	THR	N2773	X2683
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• Molecule 2: Ryanodine receptor 1

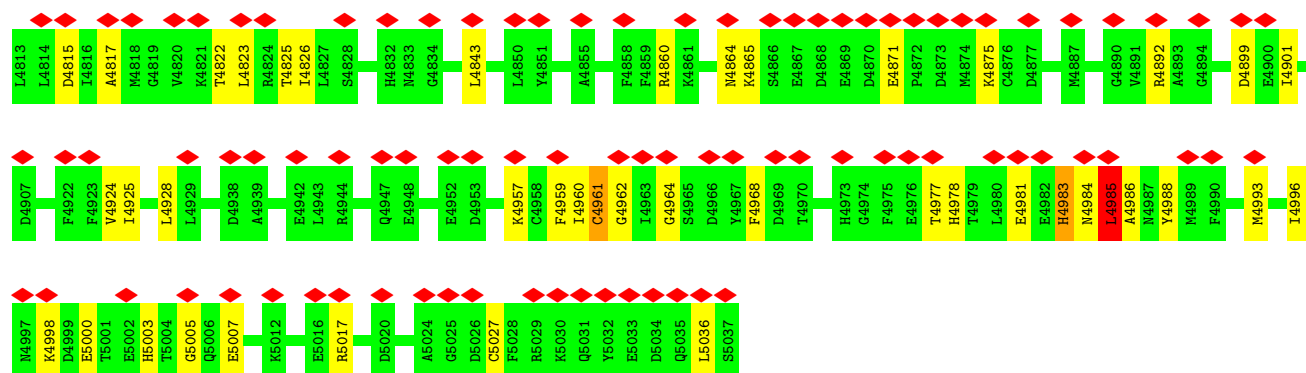


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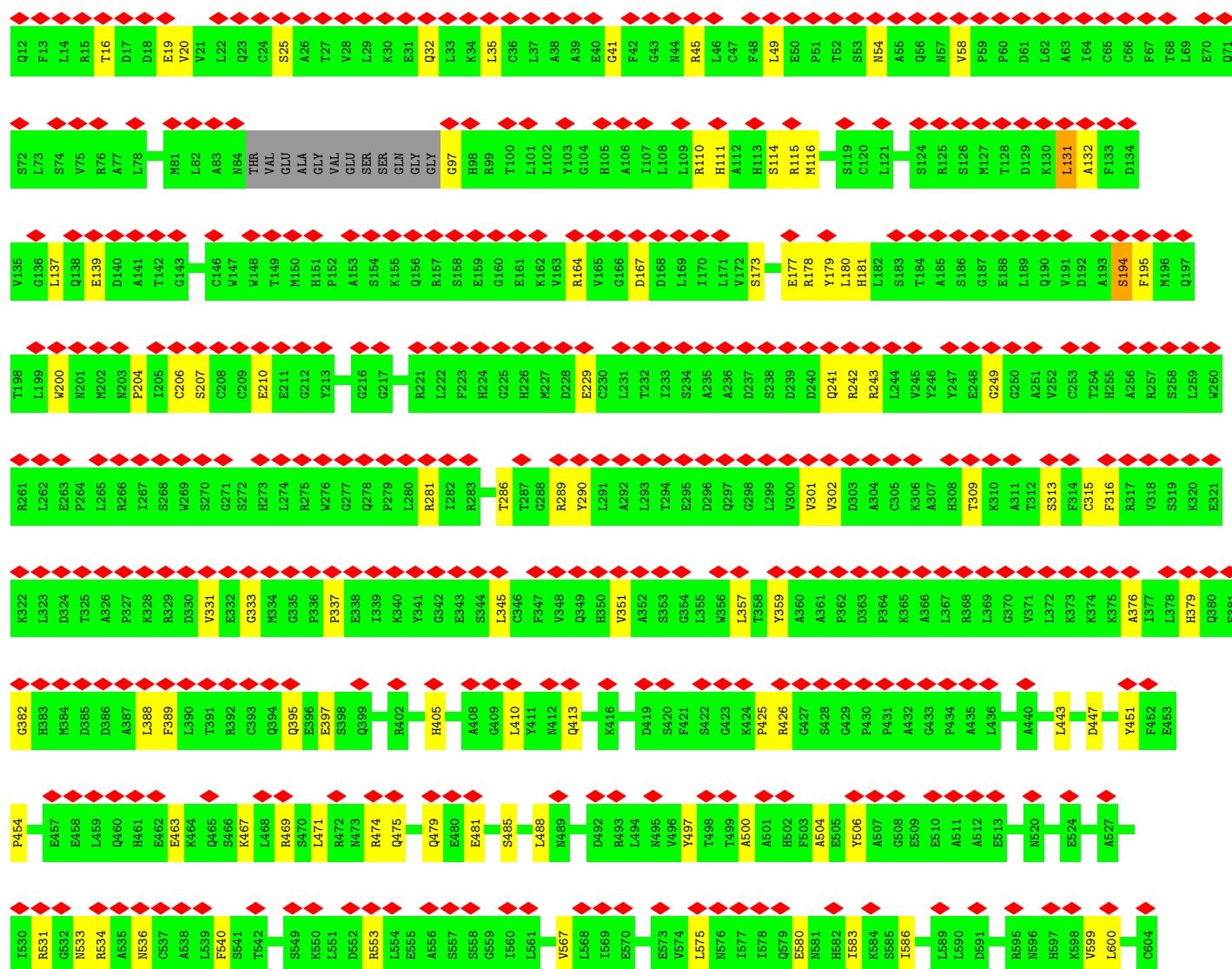
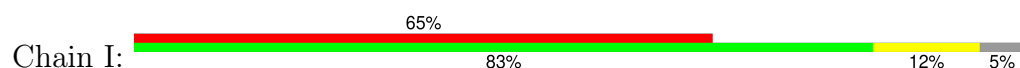


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• Molecule 2: Ryanodine receptor 1

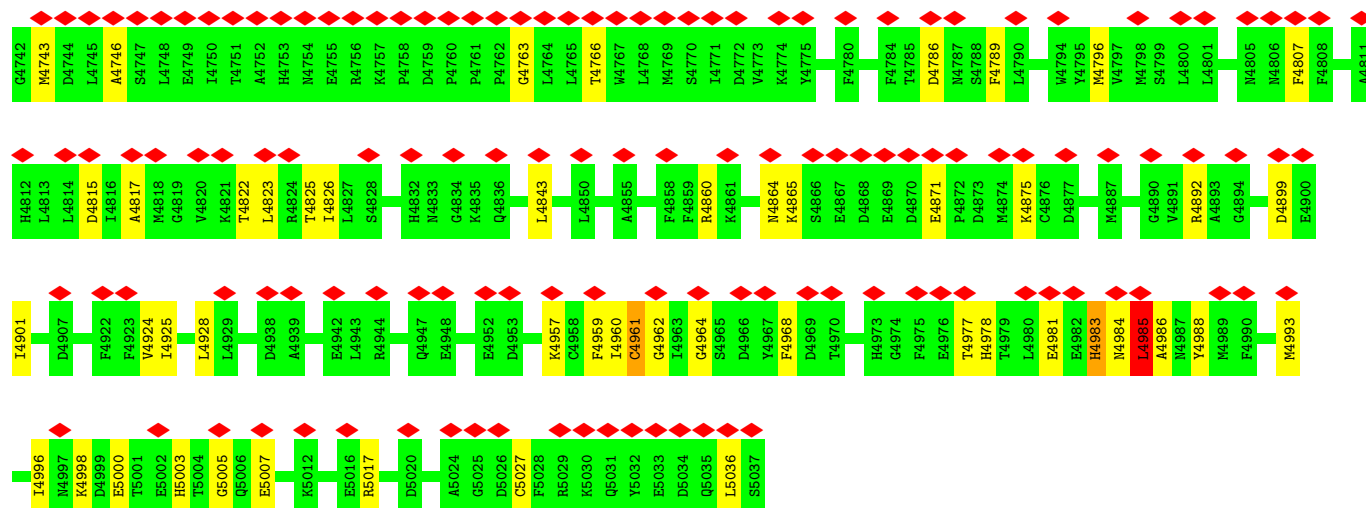


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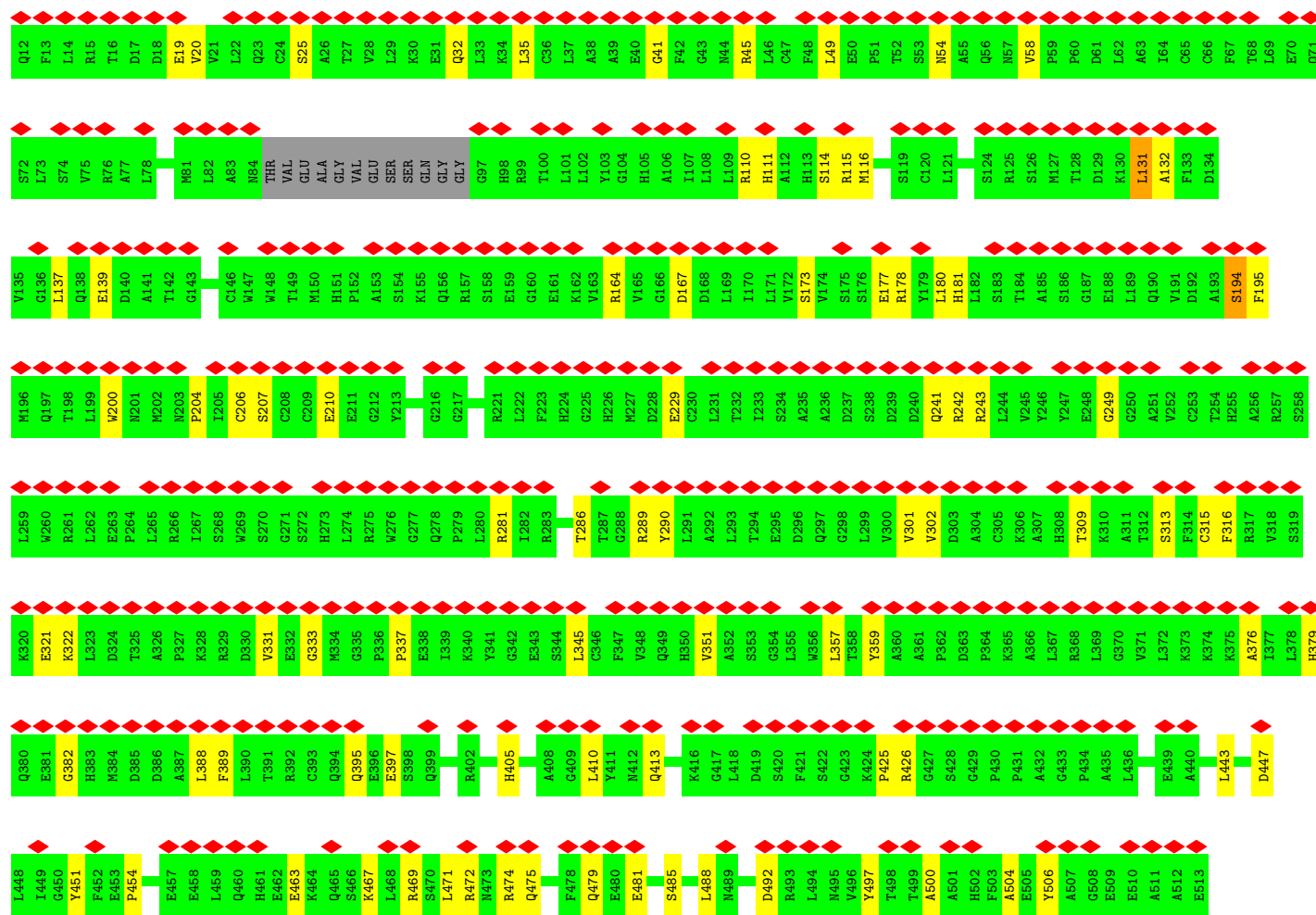
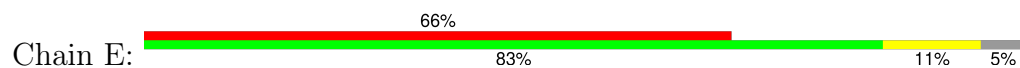


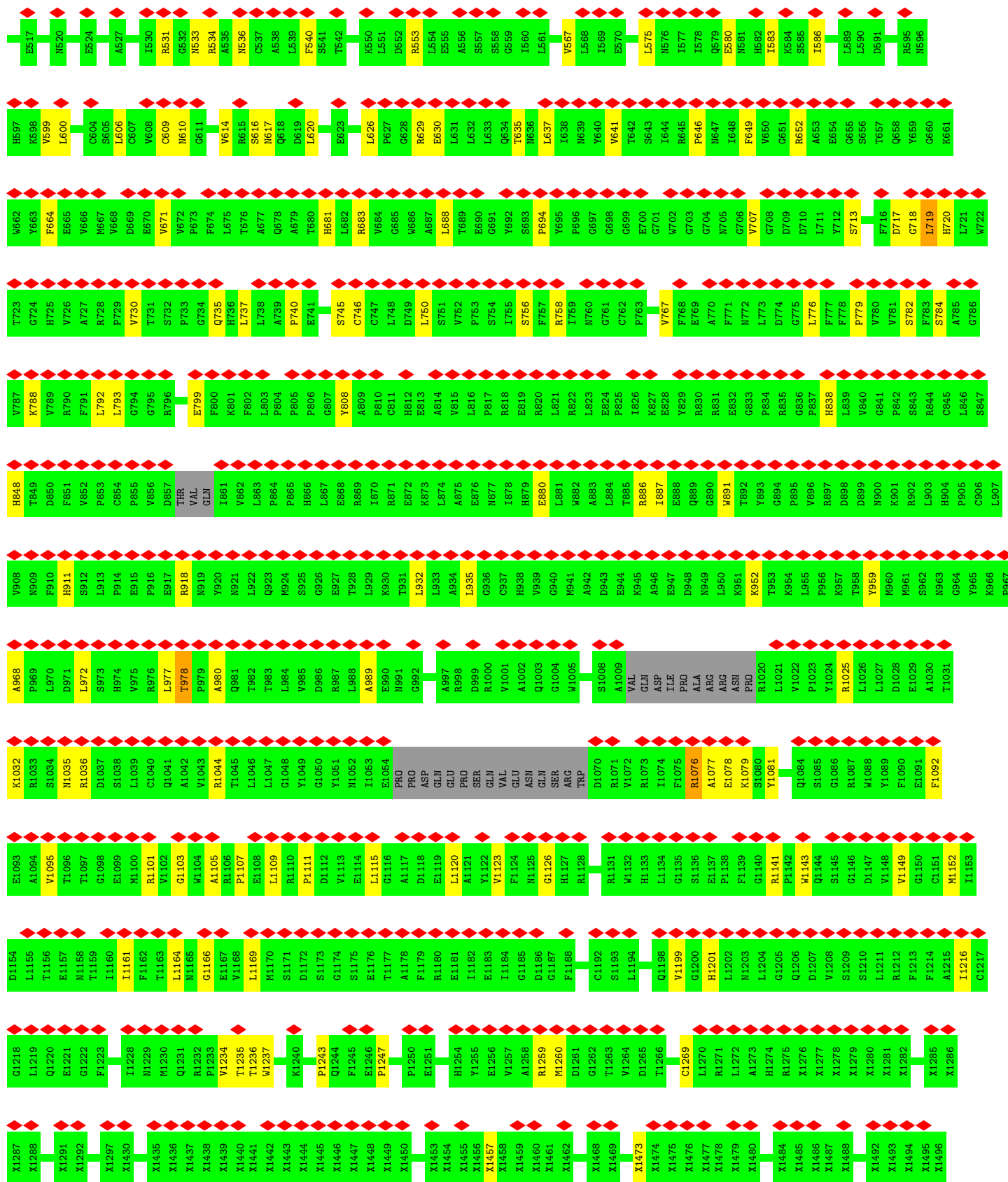
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• Molecule 2: Ryanodine receptor 1

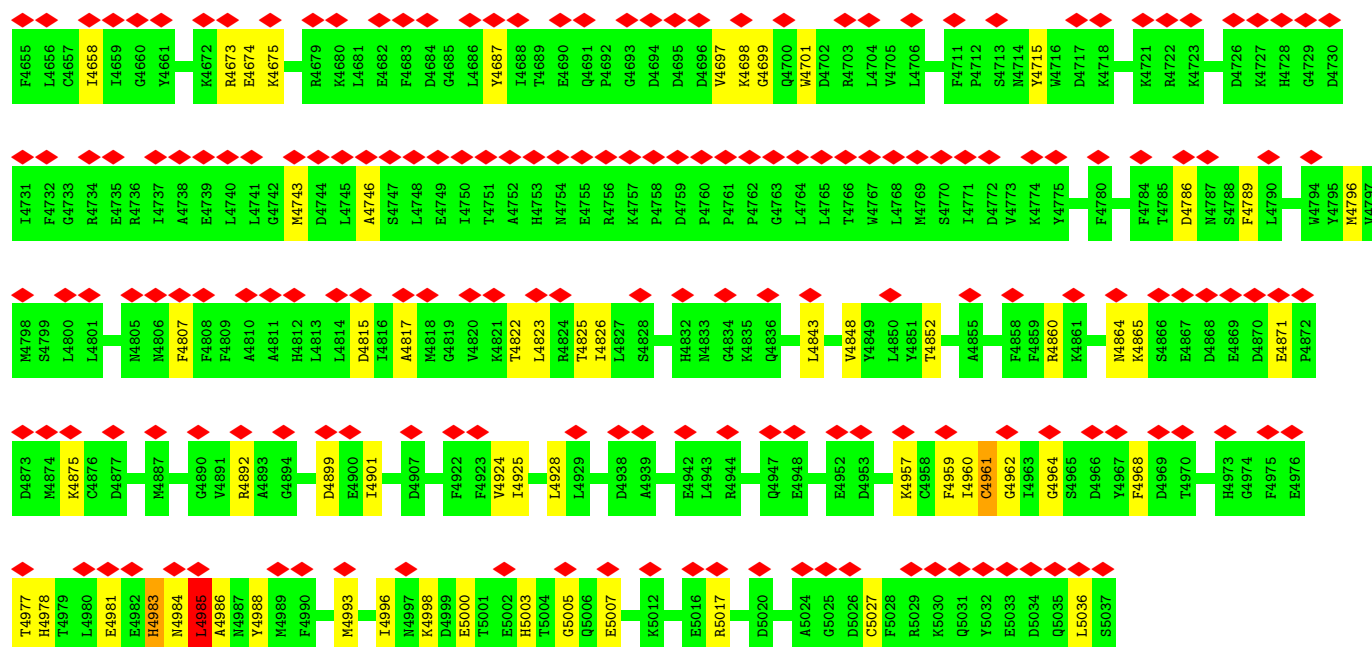






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X3357	X3297	X3227	X3161	X3031	X2953	K2891	GLU	L2771	X2681	X2620	L2469
X3358	X3298	X3228	X3162	X3032	X2954	Q2892	GLU	Q2772	X2682	X2621	L2470
X3359	X3299	X3229	X3163	X3033	X2955	E2893	ARG	N2773	X2683	X2622	S2471
X3360	X3300	X3230	X3170	X3034	X2956	L2894	GLU	N2774	X2684	X2623	L2472
X3361	X3301	X3231	X3171	X3035	X2957	E2895	LYS	W2775	X2685	X2624	P2473
X3362	X3302	X3232	X3172	X3036	X2958	A2896	LYS		X2686	X2625	L2474
X3363	X3303	X3233	X3173	X3037	X2959	K2897	THR	Y2777	X2687	X2626	Q2475
X3364	X3304	X3234	X3174	X3038	X2960	G2898	ARG	G2778	X2688	X2627	L2476
X3365	X3305	X3235	X3175	X3039	X2961	G2899	ILE	E2779	X2689	X2628	T2477
X3366	X3306	X3236	X3176	X3040	X2962	G2900	SER	N2780	X2690	X2629	L2478
X3367	X3307	X3237	X3177	X3041	X2963	T2901	GLN	V2781	X2691	X2630	K2487
X3368	X3308	X3242	X3178	X3042	X2964	H2902	THR	D2782	X2692	X2631	L2488
X3369	X3309	X3243	X3179	X3043	X2965	P2903	ALA	E2783	X2693	X2632	X2489
X3370	X3310	X3244	X3180	X3044	X2966	L2904	GLN	E2784	X2694	X2633	X2490
X3371	X3311	X3245	X3181	X3045	X2967	X2905	TVR	L2785	X2695	X2634	
X3372	X3312	X3246	X3182	X3046	X2968	V2906	ASP	L2786	X2696	X2635	X2493
X3373	X3313	X3247	X3183	X3047	X2969	P2907	PRO	T2787	X2697	X2636	X2494
X3374	X3314	X3248	X3184	X3048	X2970	V2908	GLU	H2788	X2698	X2637	X2495
X3375	X3315	X3249	X3185	X3049	X2971	D2909	GLY	P2789	X2699	X2638	X2496
X3376	X3316	X3250	X3186	X3050	X2972	T2910		M2790	X2700	X2639	X2497
X3377	X3317	X3251	X3187	X3051	X2973	L2911		L2791	X2701	X2640	X2498
X3378	X3318	X3252	X3188	X3052	X2974	T2912		R2792	X2702	X2641	X2499
X3379	X3319	X3253	X3189	X3053	X2975	A2913		P2793	X2703	X2642	X2500
X3380	X3320	X3254	X3190	X3054	X2976	K2914		T2794	X2704	X2643	L2501
X3381	X3321	X3261	X3191	X3055	X2977	E2915		K2795	X2705	X2644	X2502
X3382	X3322	X3262	X3192	X3056	X2978	K2916		T2796	X2706	X2645	
X3383	X3323	X3263	X3193	X3057	X2979	A2917		F2797	X2707	X2646	X2511
X3384	X3324	X3264	X3194	X3058	X2980	R2918		T2798	X2708	X2647	X2512
X3385	X3325	X3265	X3195	X3059	X2981	D2919		E2799	X2709	X2648	X2513
X3386	X3326	X3266	X3196	X3060	X2982	K2920		P2739	X2710	X2649	
X3387	X3327	X3267	X3197	X3061	X3001	E2921		V2740	X2711	X2650	

GLY	X3388	X3612	X3937	L4017	H4156	S4236	H4156	E4196	M4626
GLU	X3389	X3613	S3938	D4018	D4157	E4239	D4157	E4199	M4627
ASP	X3390	T3639	Q3939	D4022	P4158	E4239	P4158	E4199	M4627
ASP	X3391	T3640	K3940	D4023	L4159	E4239	L4159	E4199	M4627
GLU	X3392	L3641	D3941	L4028	L4160	E4239	L4160	E4199	M4627
GLY	X3393	T3642	V3942	L4028	R4161	E4239	R4161	E4199	M4627
SER	X3394	N3643	T3943	S4029	F4162	E4239	F4162	E4199	M4627
ALA	X3395	L3644	E3944	L4030	F4163	E4239	F4163	E4199	M4627
ALA	X3396	T3645	E3945	L4030	L4164	E4239	L4164	E4199	M4627
GLY	X3397	T3646	Q3946	L4032	E4165	E4239	E4165	E4199	M4627
ASP	X3398	H3647	G3947	G4032	L4166	E4239	L4166	E4199	M4627
LEU	X3399	R3648	K3948	G4033	A4167	E4239	A4167	E4199	M4627
ALA	X3400	R3649	R3949	N4034	E4168	E4239	E4168	E4199	M4627
GLY	X3401	C3650	N3950	V4035	S4169	E4239	S4169	E4199	M4627
ALA	X3402	N3651	D3877	V4036	I4170	E4239	I4170	E4199	M4627
GLY	X3403	N3652	D3878	M4037	L4171	E4239	L4171	E4199	M4627
GLY	X3404	F3653	Q3882	M4037	E4172	E4239	E4172	E4199	M4627
GLY	X3405	F3653	D3883	G4038	Y4173	E4239	Y4173	E4199	M4627
GLY	X3406	X3656	L3884	M4039	E4174	E4239	E4174	E4199	M4627
GLY	X3407	X3657	F3885	I4040	P4106	E4239	P4106	E4199	M4627
TRP	X3408	X3658	R3886	A4041	E4109	E4239	E4109	E4199	M4627
SER	X3409	X3659	Q3889	R4042	F4110	E4239	F4110	E4199	M4627
GLY	X3410	A3660	L3890	D4046	L4111	E4239	L4111	E4199	M4627
GLY	X3411	X3661	M4047	M4047	L4112	E4239	L4112	E4199	M4627
GLY	X3412	L3663	L3891	L4048	S4113	E4239	S4113	E4199	M4627
GLU	X3413	T3664	C3892	V4049	E4116	E4239	E4116	E4199	M4627
ALA	X3414	E3665	E3893	E4050	A4117	E4239	A4117	E4199	M4627
ALA	X3415	E3666	N3896	M4054	E4118	E4239	E4118	E4199	M4627
GLY	X3416	H3667	N3897	V4055	D4119	E4239	D4119	E4199	M4627
ASP	X3417	S3668	D3898	E4056	E4120	E4239	E4120	E4199	M4627
ASP	X3418	F3669	F3899	E4056	E4121	E4239	E4121	E4199	M4627
GLU	X3419	X3672	N3901	L4059	T4200	E4239	T4200	E4199	M4627
GLY	X3420	GLY	Y3902	K4060	E4122	E4239	E4122	E4199	M4627
ALA	X3421	X3673	L3903	F4061	M4123	E4239	M4123	E4199	M4627
GLU	X3422	X3674	T3905	D4063	M4124	E4239	M4124	E4199	M4627
GLU	X3423	X3675	T3906	M4064	F4125	E4239	F4125	E4199	M4627
GLU	X3424	X3676	Q3906	F4065	E4126	E4239	E4126	E4199	M4627
GLU	X3425	X3677	T3907	L4066	E4127	E4239	E4127	E4199	M4627
GLU	X3426	X3678	G3908	K4067	F4128	E4239	F4128	E4199	M4627
GLU	X3427	X3679	N3909	L4068	A4129	E4239	A4129	E4199	M4627
GLU	X3428	X3680	T3910	K4069	M4130	E4239	M4130	E4199	M4627
GLU	X3429	X3681	T3911	D4070	R4131	E4239	R4131	E4199	M4627
GLU	X3430	X3682	T3912	I4071	F4132	E4239	F4132	E4199	M4627
GLU	X3431	Q3683	I3913	V4072	Q4133	E4239	Q4133	E4199	M4627
GLU	X3432	X3684	N3914	G4073	E4134	E4239	E4134	E4199	M4627
GLU	X3433	E3685	I3915	S4074	P4135	E4239	P4135	E4199	M4627
GLU	X3434	X3686	Q3916	E4075	A4136	E4239	A4136	E4199	M4627
GLU	X3435	X3687	D3921	A4076	R4137	E4239	R4137	E4199	M4627
GLU	X3436	X3688	R3925	F4077	D4138	E4239	D4138	E4199	M4627
GLU	X3437	X3689	S4007	F4078	I4139	E4239	I4139	E4199	M4627
GLU	X3438	V3690	S4007	Q4078	F4141	E4239	F4141	E4199	M4627
GLU	X3439	X3691	N3860	D4079	M4142	E4239	M4142	E4199	M4627
GLU	X3440	E3692	Q3929	Y4080	L4150	E4239	L4150	E4199	M4627
GLU	X3441	X3693	D3862	V4081	E4151	E4239	E4151	E4199	M4627
GLU	X3442	X3694	Q3863	T4082	E4152	E4239	E4152	E4199	M4627
GLU	X3443	X3695	T3864	D4083	H4153	E4239	H4153	E4199	M4627
GLU	X3444	X3696	Q3766	P4084	P4155	E4239	P4155	E4199	M4627
GLU	X3445	X3697	X3768	R4085	E4239	E4239	E4239	E4199	M4627
GLU	X3446	X3698	R3769	G4086	E4239	E4239	E4239	E4199	M4627
GLU	X3447	X3699							
GLU	X3448	X3700							
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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	0.060	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	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, ZN, ATP, CFF

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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	10/34534 (0.0%)
2	E	0.30	0/25428	0.54	10/34534 (0.0%)
2	G	0.30	0/25428	0.54	10/34534 (0.0%)
2	I	0.30	0/25428	0.54	10/34534 (0.0%)
All	All	0.30	0/105048	0.54	40/142628 (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
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	7.69	132.98	115.30
2	B	131	LEU	CA-CB-CG	7.67	132.95	115.30
2	E	131	LEU	CA-CB-CG	7.67	132.93	115.30
2	G	131	LEU	CA-CB-CG	7.65	132.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4985	LEU	CA-CB-CG	6.48	130.20	115.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	194	SER	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	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	818	0	824	13	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	15	0
2	B	29499	0	24748	311	0
2	E	29499	0	24748	298	0
2	G	29499	0	24748	300	0
2	I	29499	0	24748	305	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	102376	1234	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 1234 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:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.64	0.86
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.64	0.86
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.64	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.64	0.85
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.81	0.78

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%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	338 (10%)	7 (0%)	44	78
2	E	3235/4416 (73%)	2888 (89%)	340 (10%)	7 (0%)	44	78
2	G	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	44	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	44	78
All	All	13360/18096 (74%)	11932 (89%)	1400 (10%)	28 (0%)	45	78

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU

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%)	2474 (99%)	19 (1%)	79	85
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	79	85
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	79	85
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	79	85
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	80	87

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	131	LEU
2	E	4085	ARG
2	E	553	ARG
2	E	1964	ARG

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Mol	Chain	Res	Type
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	1775	HIS
2	E	3896	ASN
2	E	4983	HIS
2	G	838	HIS
2	G	725	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
4	CFF	G	5102	-	8,15,15	2.15	3 (37%)	8,23,23	1.31	1 (12%)
3	ATP	E	5101	-	28,33,33	0.85	0	34,52,52	1.27	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	E	5102	-	8,15,15	2.15	3 (37%)	8,23,23	1.31	1 (12%)
4	CFF	B	5102	-	8,15,15	2.15	3 (37%)	8,23,23	1.31	1 (12%)
3	ATP	B	5101	-	28,33,33	0.85	0	34,52,52	1.27	3 (8%)
3	ATP	I	5101	-	28,33,33	0.85	0	34,52,52	1.27	3 (8%)
4	CFF	I	5102	-	8,15,15	2.15	3 (37%)	8,23,23	1.31	1 (12%)
3	ATP	G	5101	-	28,33,33	0.86	0	34,52,52	1.26	3 (8%)

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
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	4/18/38/38	0/3/3/3
3	ATP	I	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	4/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C6-N1	-3.55	1.32	1.38
4	B	5102	CFF	C6-N1	-3.52	1.32	1.38
4	E	5102	CFF	C6-N1	-3.52	1.32	1.38
4	I	5102	CFF	C6-N1	-3.52	1.32	1.38
4	I	5102	CFF	C5-C4	-3.37	1.33	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-3.30	124.20	128.67
3	B	5101	ATP	N3-C2-N1	-3.27	124.23	128.67
3	G	5101	ATP	N3-C2-N1	-3.26	124.25	128.67
3	I	5101	ATP	N3-C2-N1	-3.25	124.26	128.67
3	E	5101	ATP	C4-C5-N7	-2.96	106.20	109.34

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

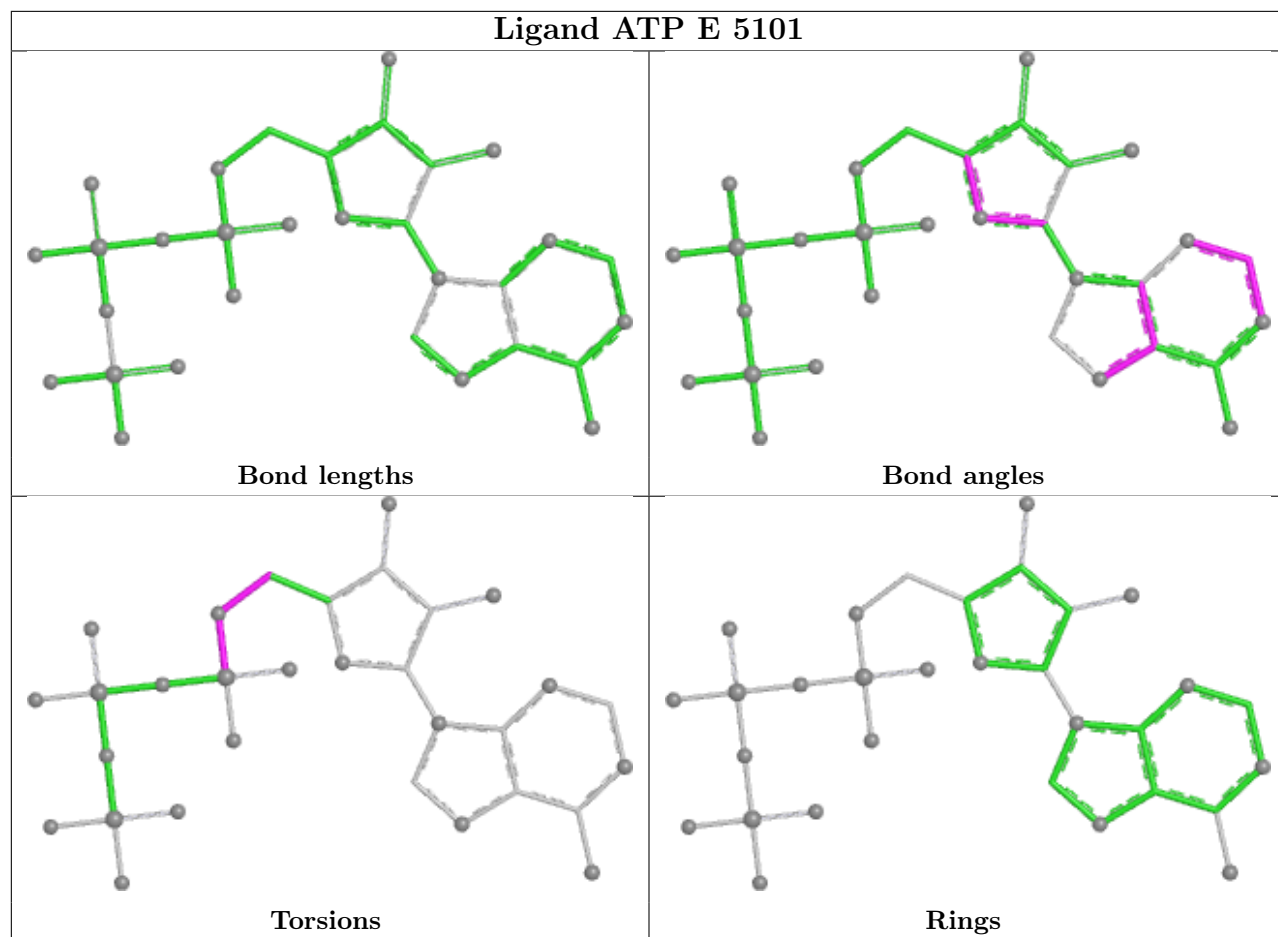
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C4'-C5'-O5'-PA

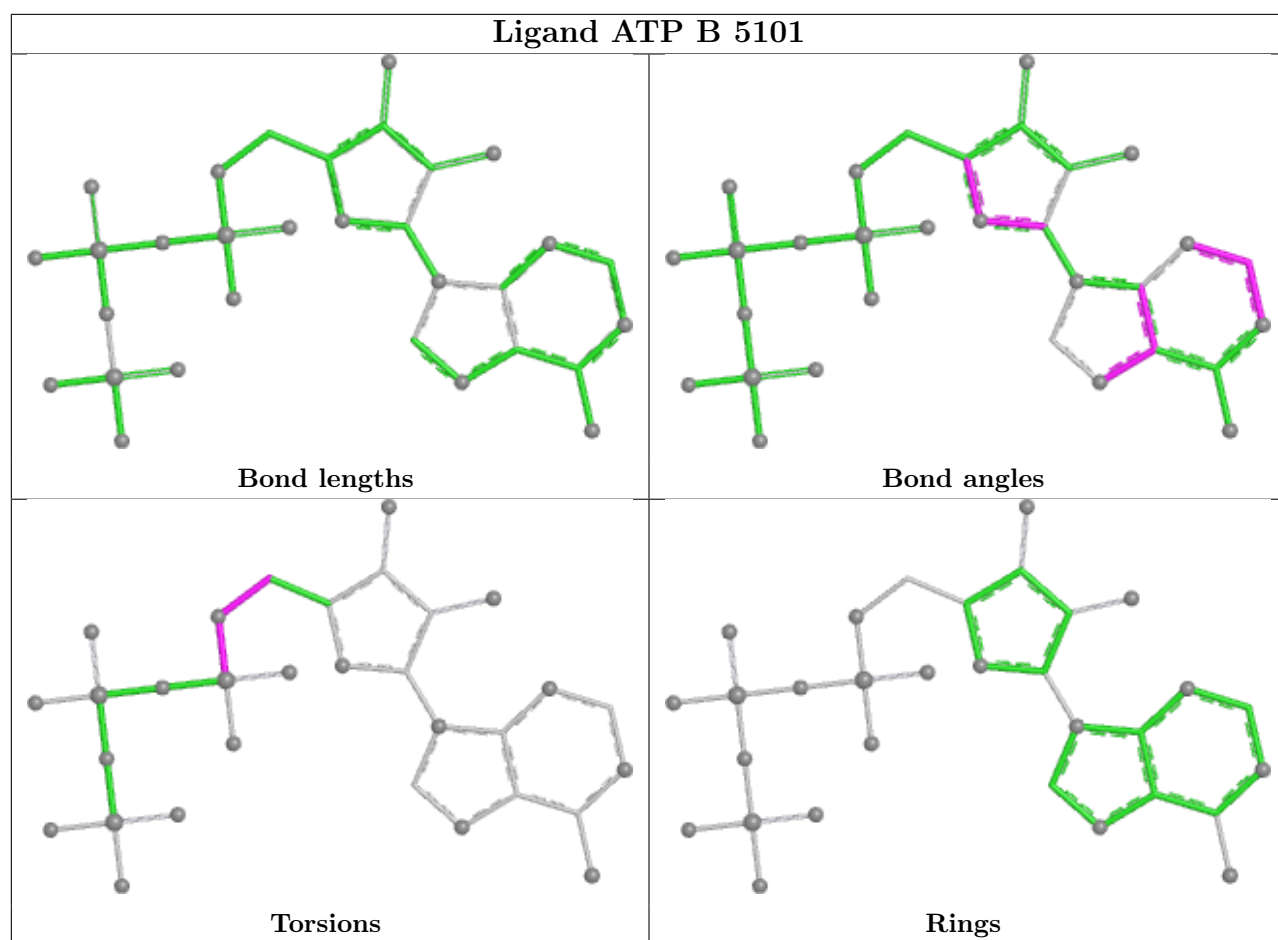
There are no ring outliers.

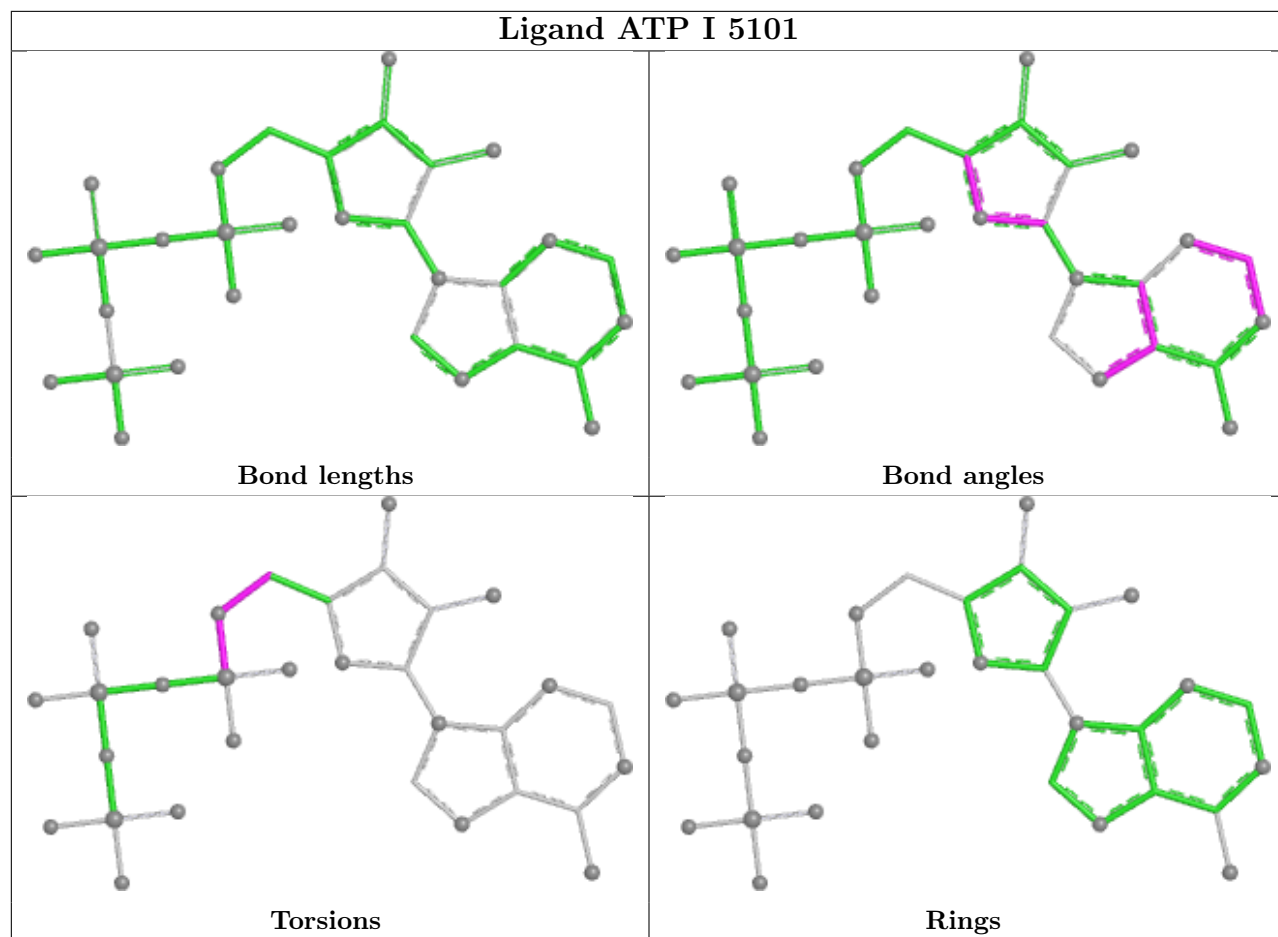
4 monomers are involved in 4 short contacts:

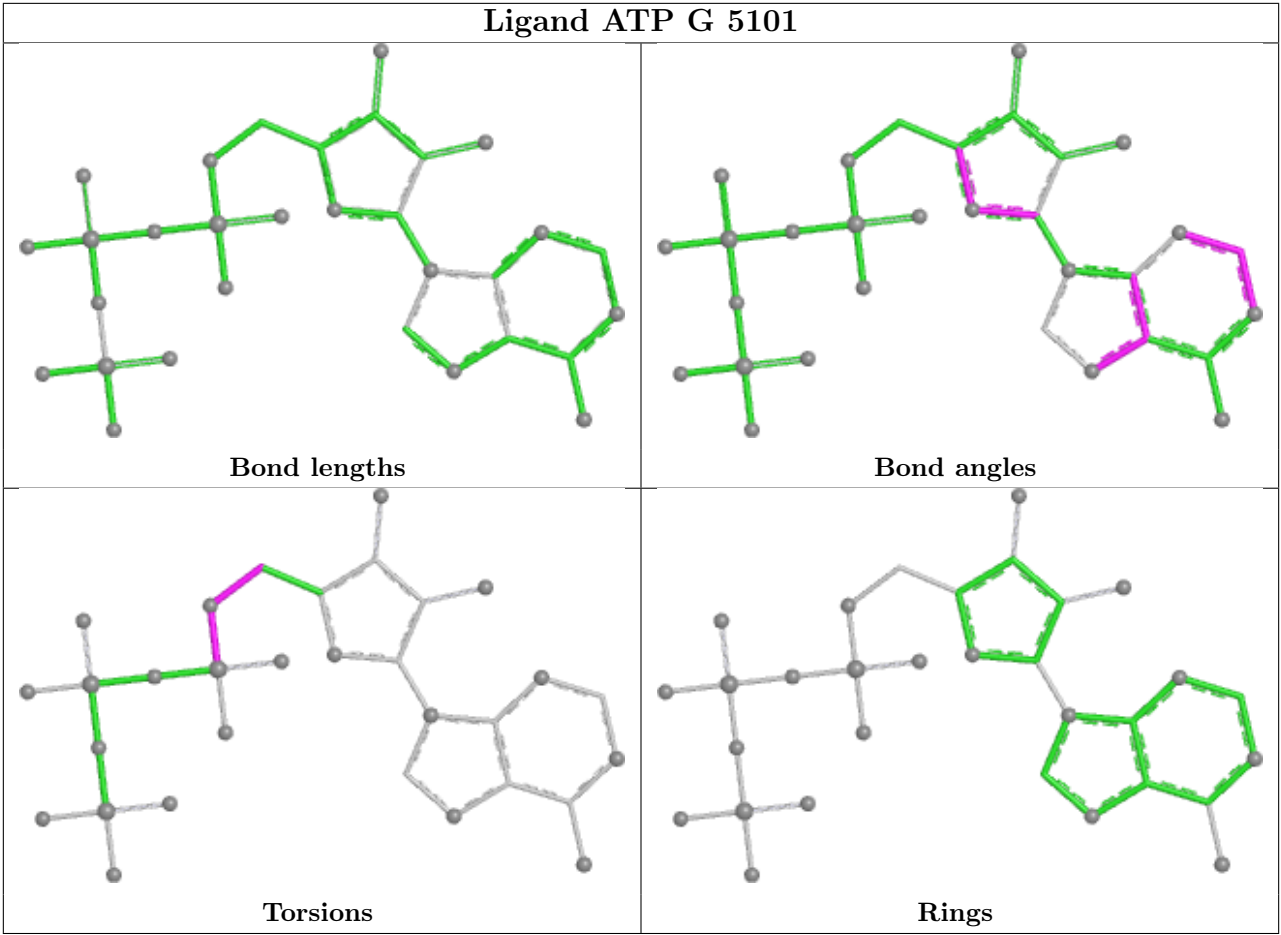
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	1	0
3	B	5101	ATP	1	0
3	I	5101	ATP	1	0
3	G	5101	ATP	1	0

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	B	14
2	G	14
2	I	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.47
1	G	4345:UNK	C	4540:PHE	N	73.47

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Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.47
1	E	4345:UNK	C	4540:PHE	N	73.47
1	B	3613:UNK	C	3639:THR	N	45.62

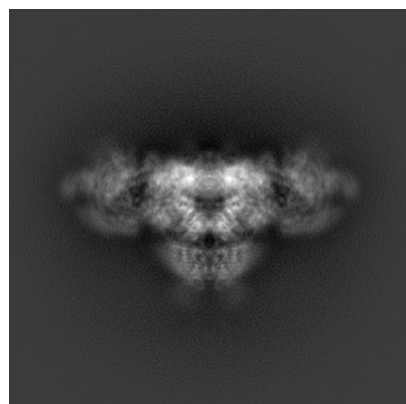
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8376. These allow visual inspection of the internal detail of the map and identification of artifacts.

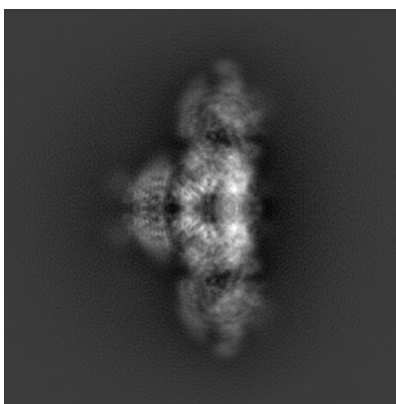
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

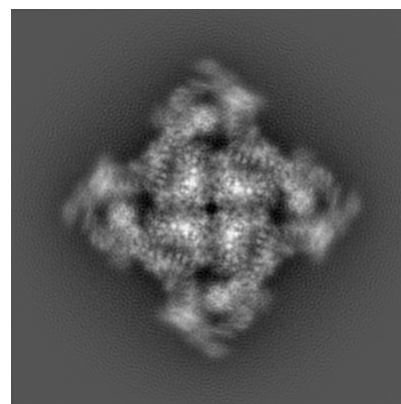
6.1.1 Primary map



X

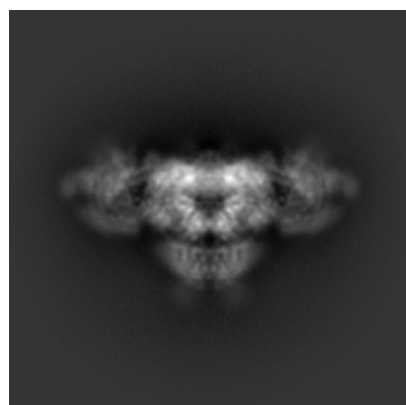


Y

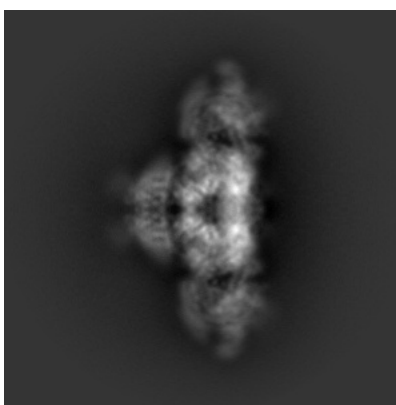


Z

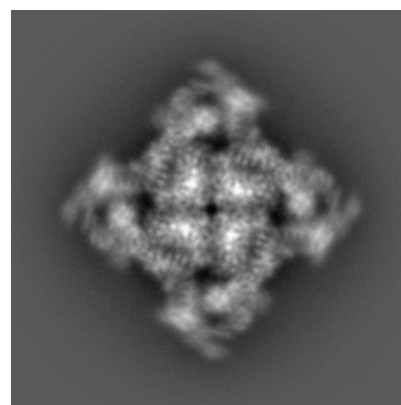
6.1.2 Raw map



X



Y

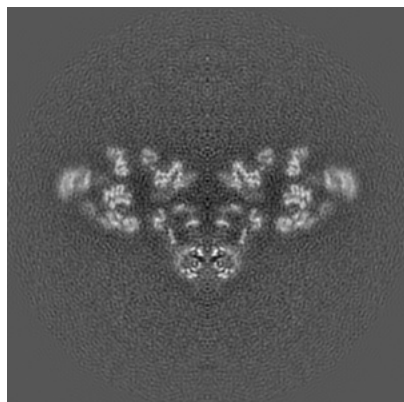


Z

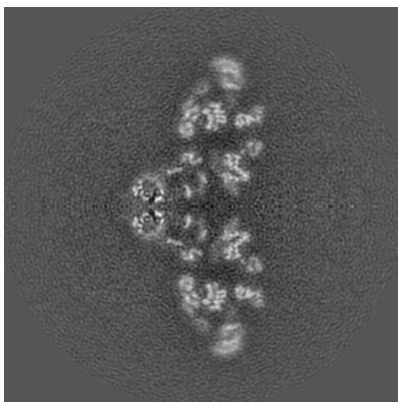
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

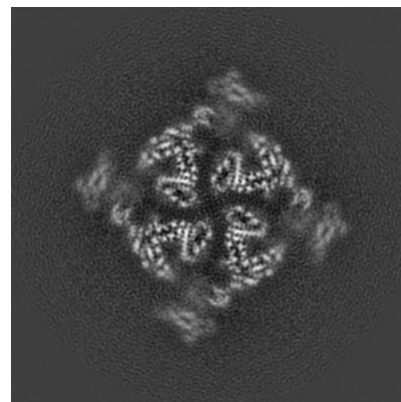
6.2.1 Primary map



X Index: 200

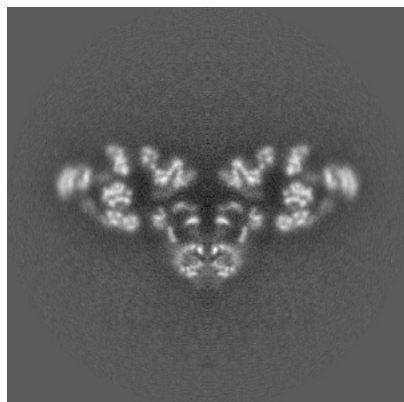


Y Index: 200

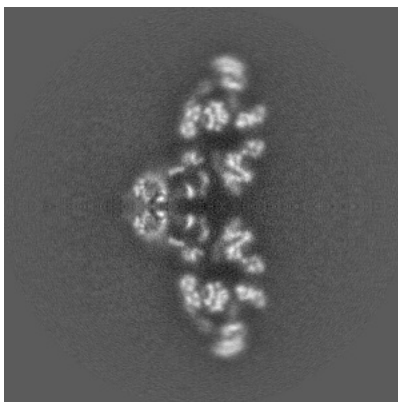


Z Index: 200

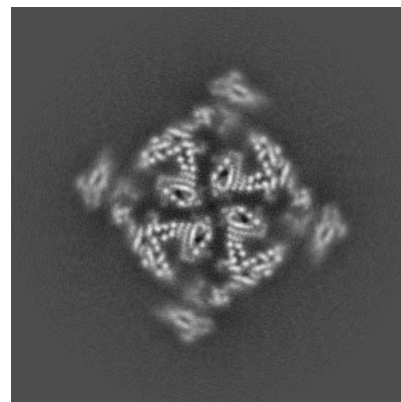
6.2.2 Raw map



X Index: 200



Y Index: 200

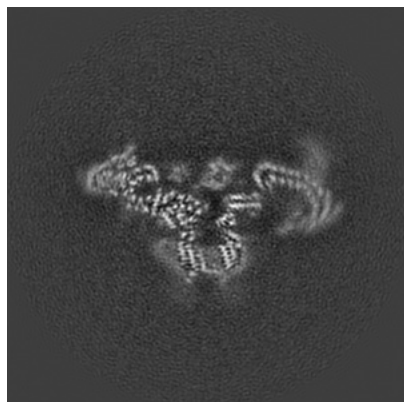


Z Index: 200

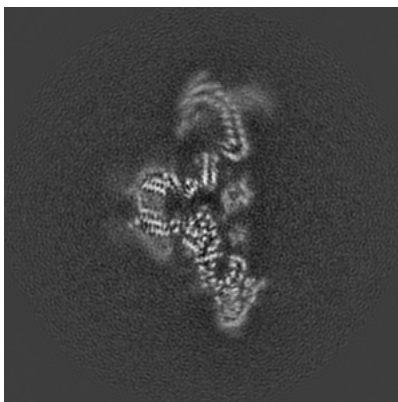
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

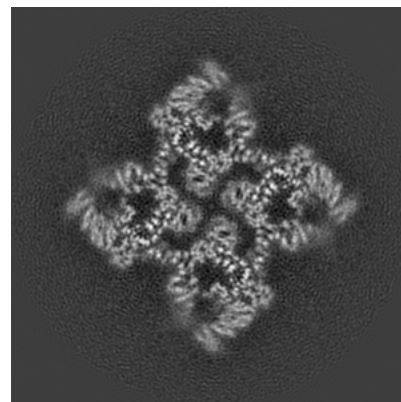
6.3.1 Primary map



X Index: 225

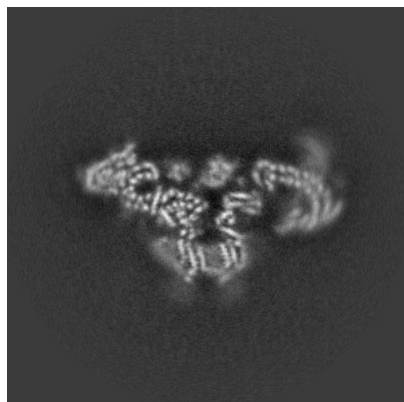


Y Index: 175

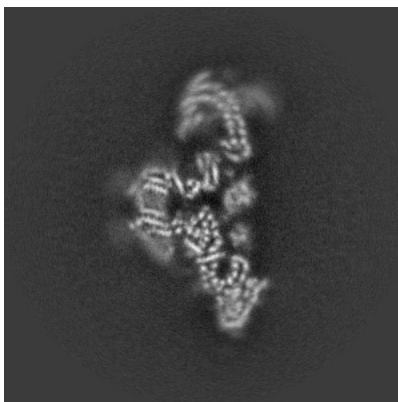


Z Index: 232

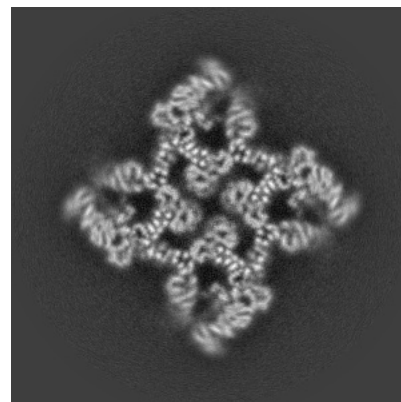
6.3.2 Raw map



X Index: 224



Y Index: 176



Z Index: 232

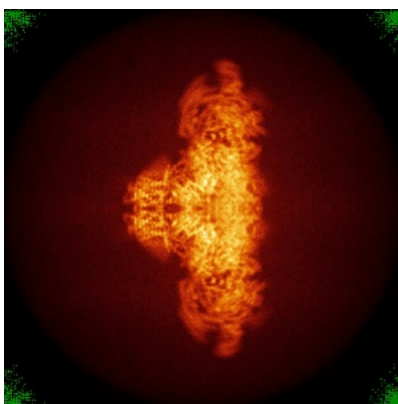
The images above show the largest variance slices of the map in three orthogonal directions.

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

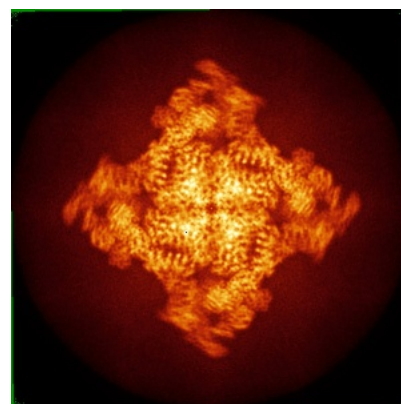
6.4.1 Primary map



X

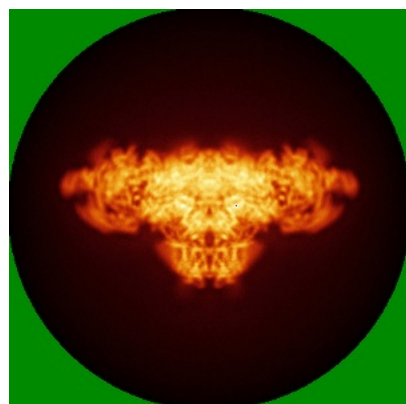


Y

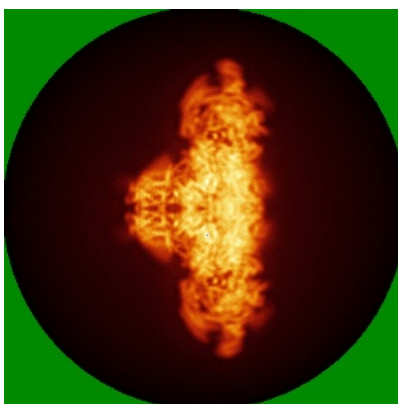


Z

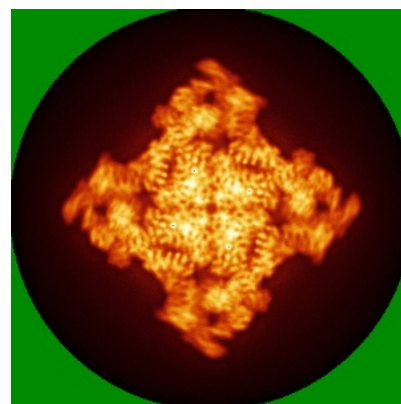
6.4.2 Raw map



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 0.025. 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.

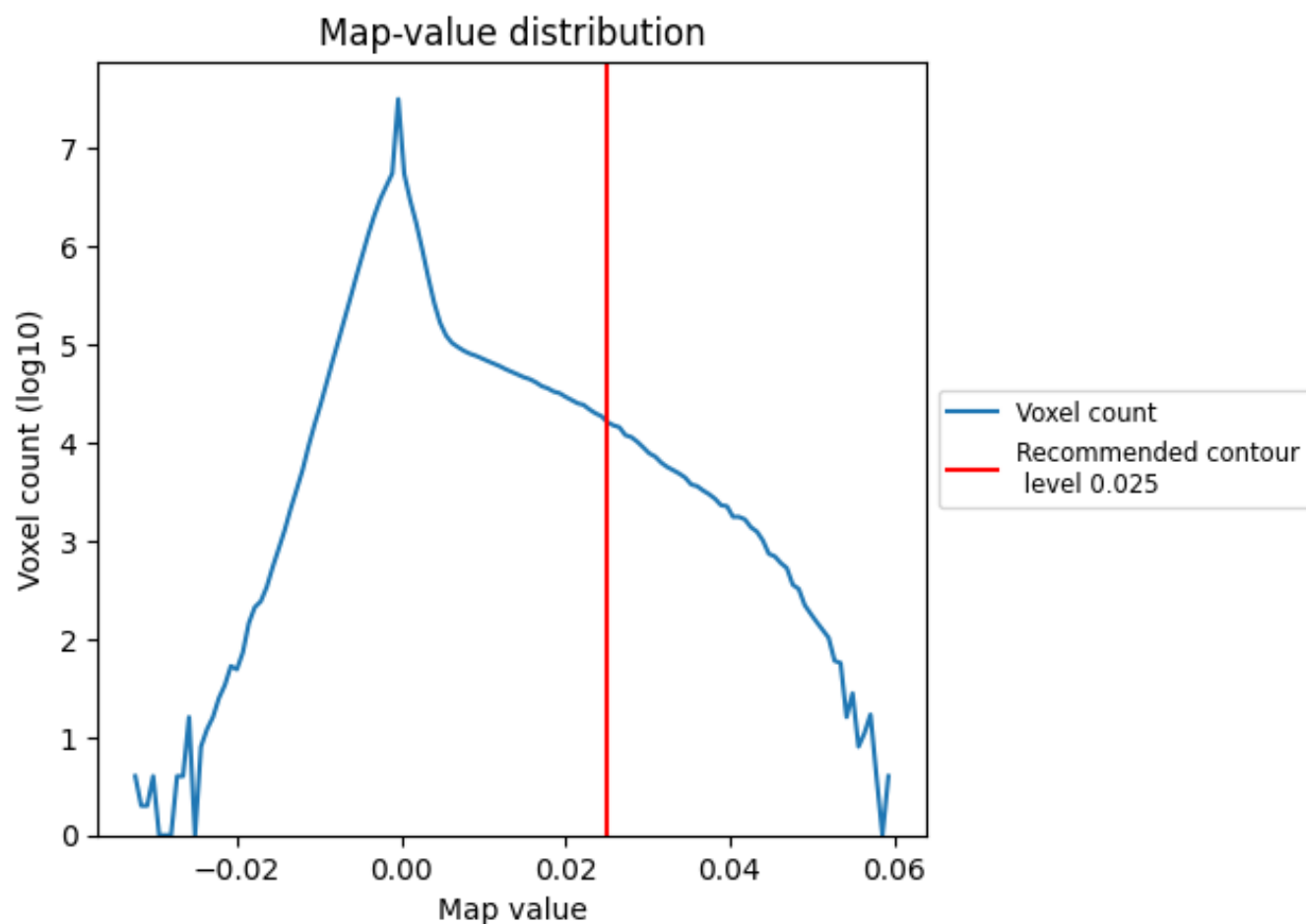
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

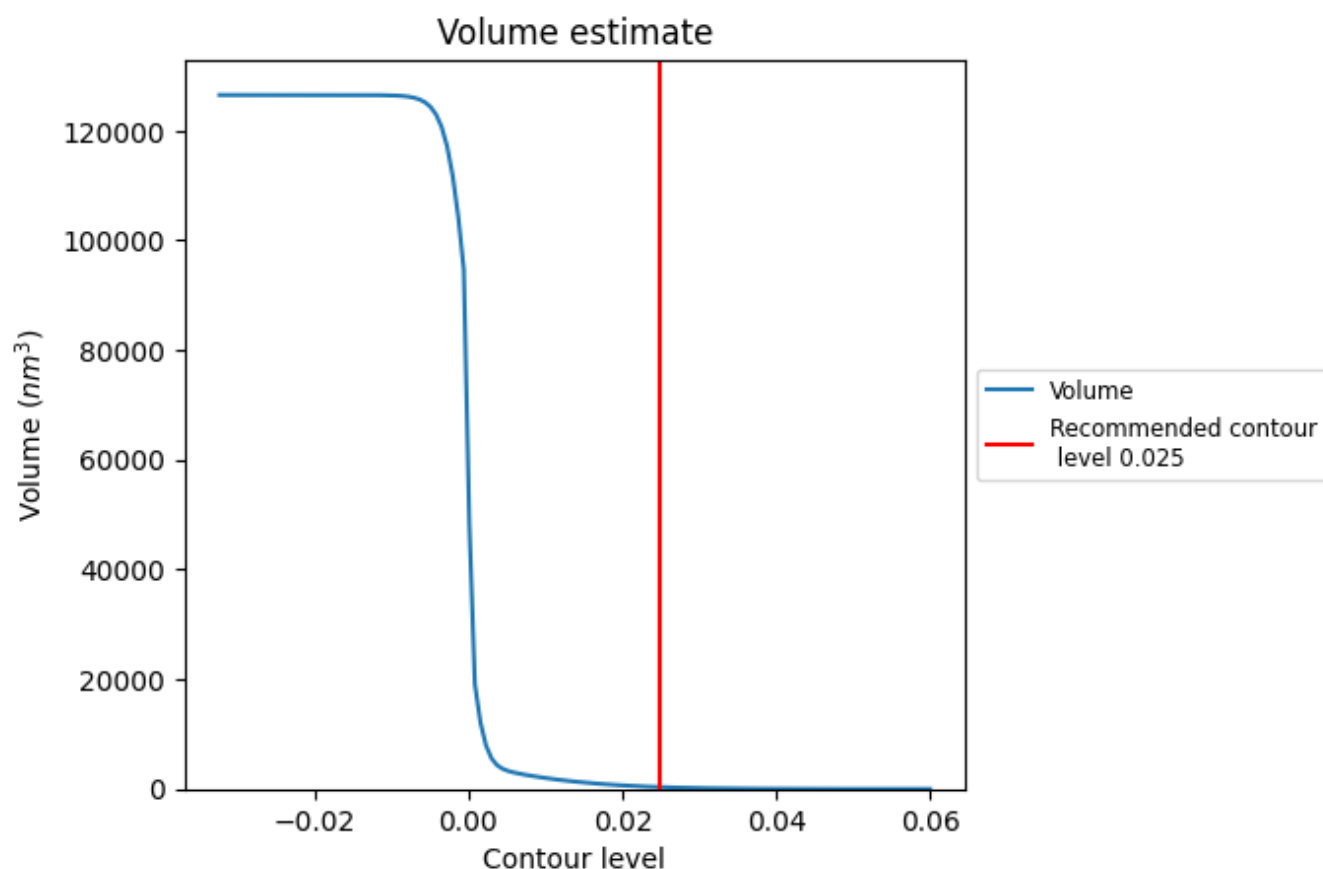
This section contains the results of statistical analysis of the map.

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.

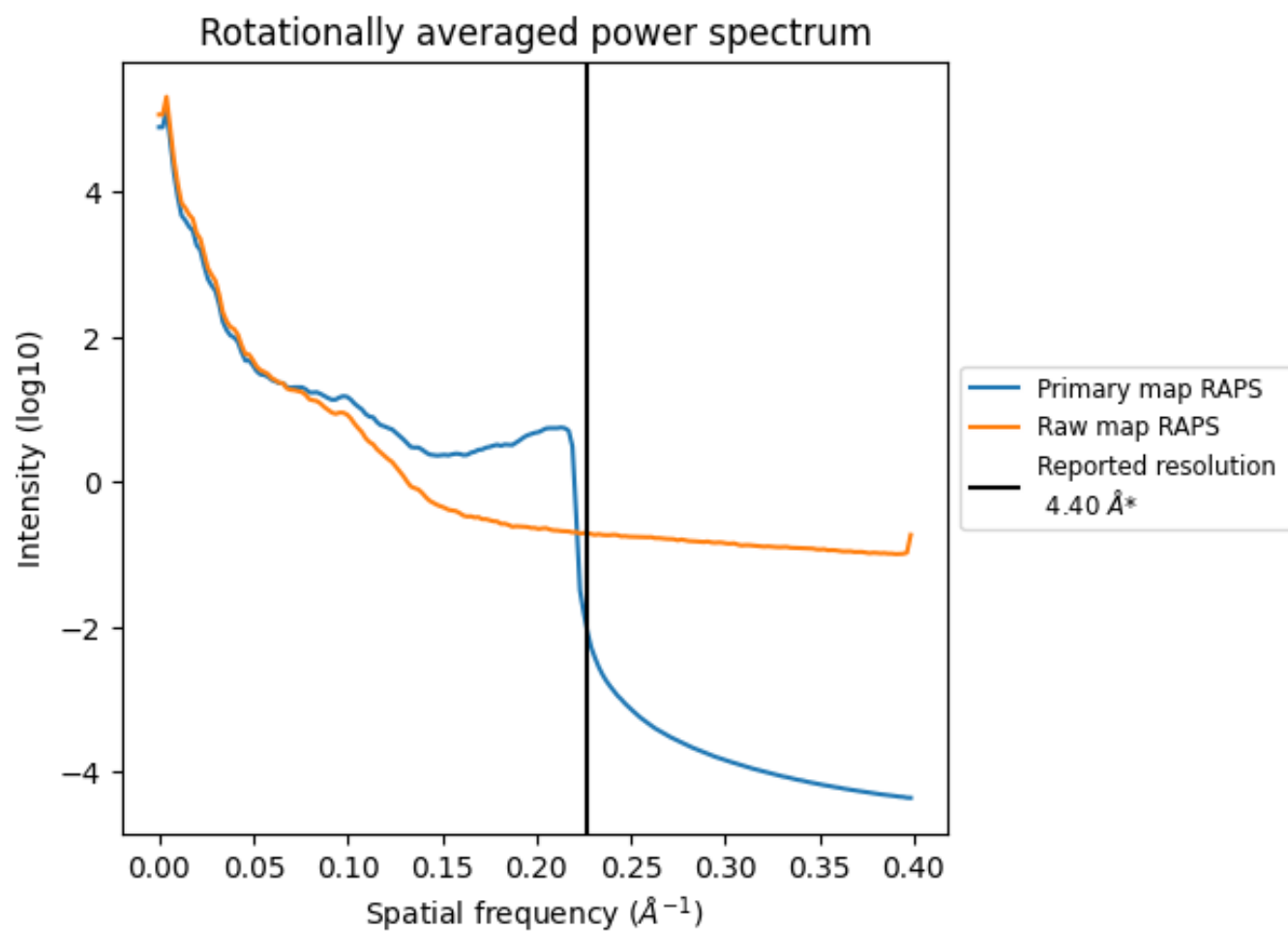
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm^3 ; this corresponds to an approximate mass of 299 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 ⓘ

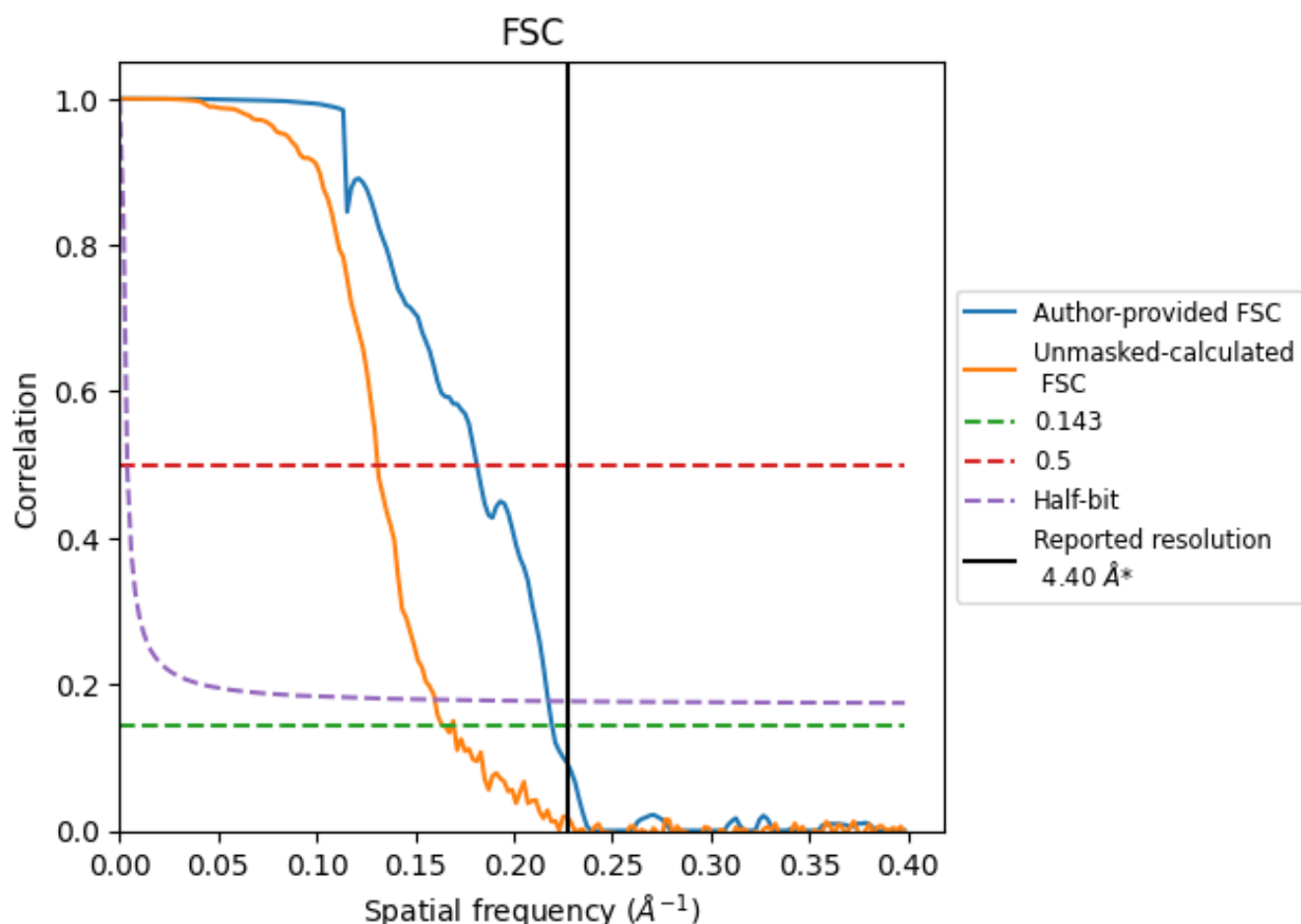


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

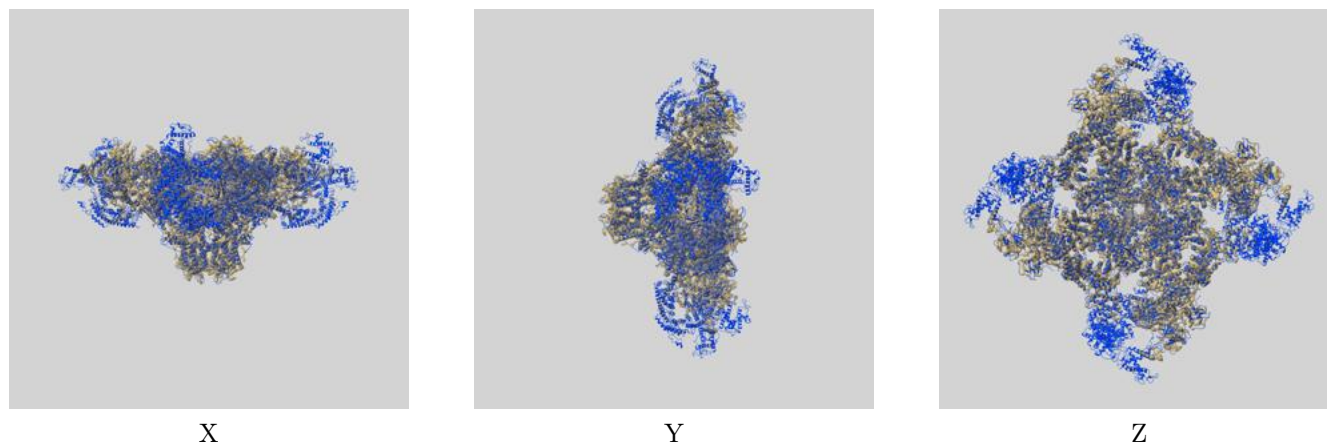
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.56	5.52	4.60
Unmasked-calculated*	6.06	7.64	6.25

*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 6.06 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

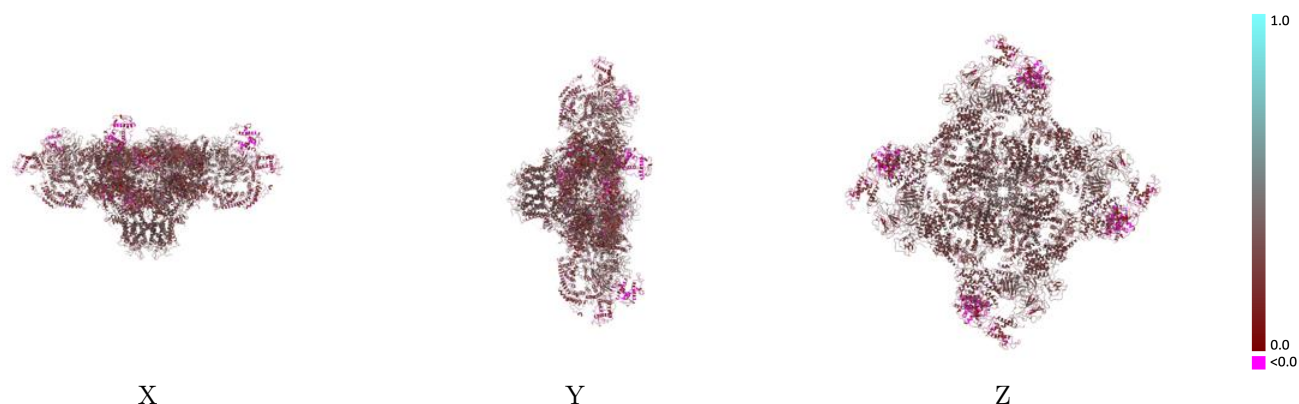
This section contains information regarding the fit between EMDB map EMD-8376 and PDB model 5T9V. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



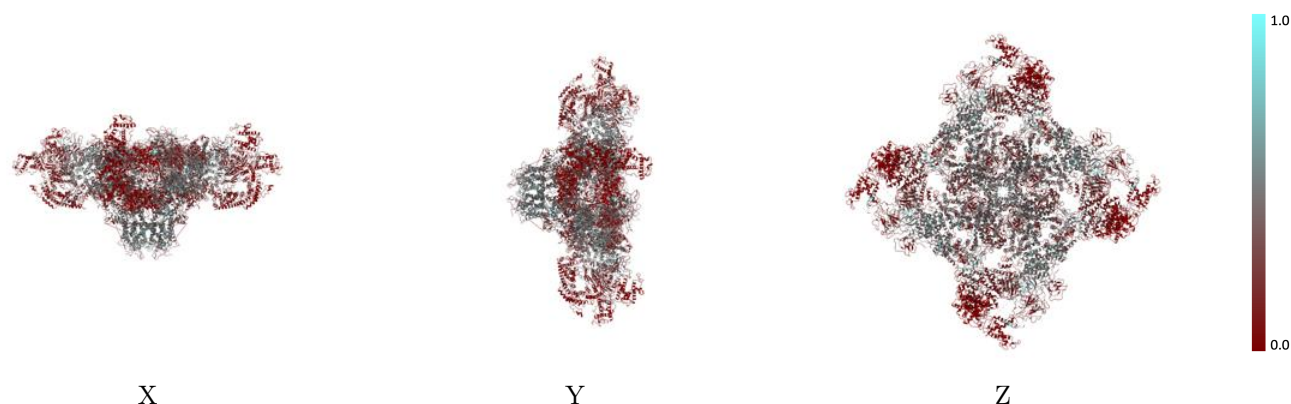
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



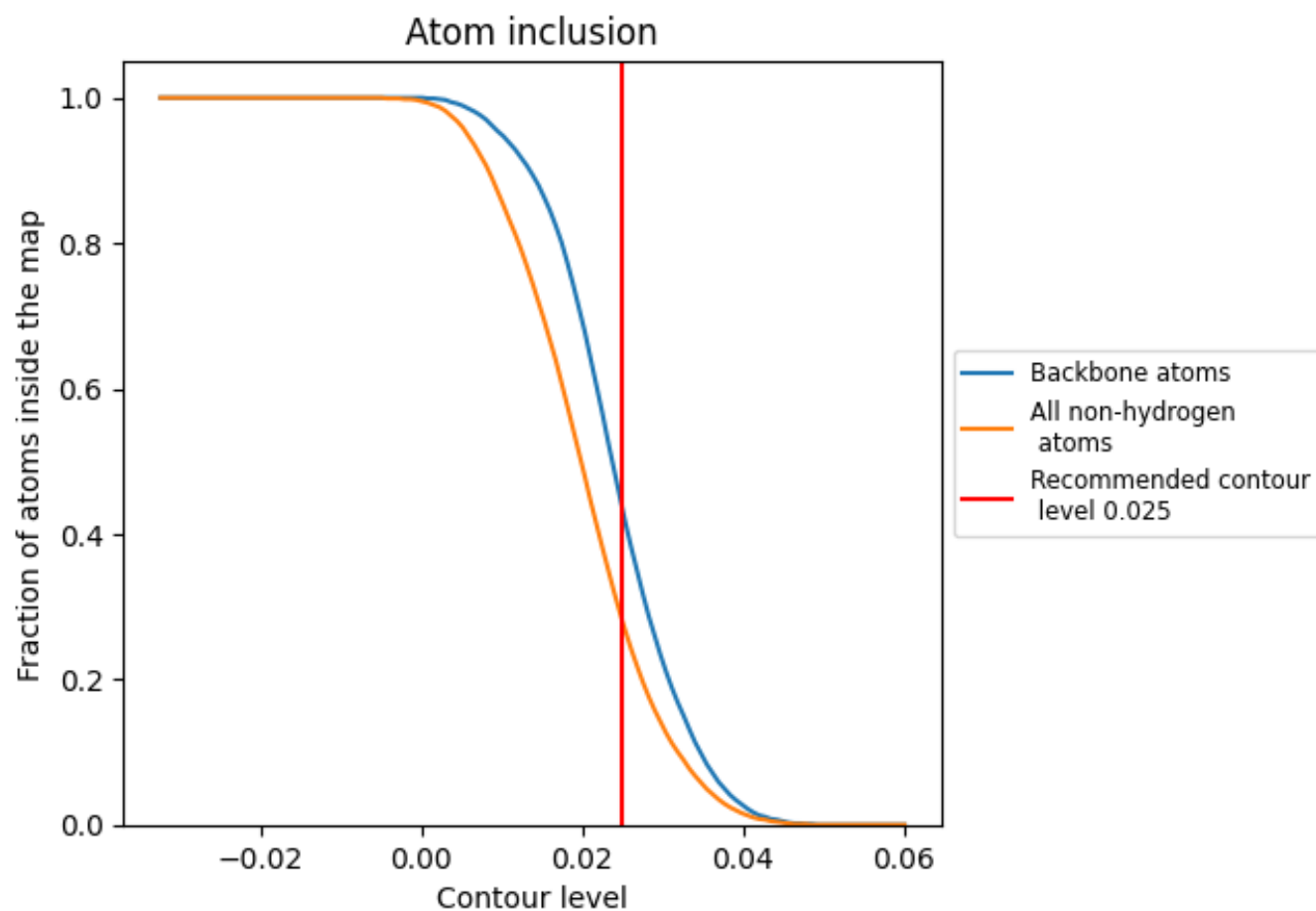
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 44% of all backbone atoms, 28% 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></div></div> 0.2800	<div><div></div></div> 0.2680
A	<div><div></div></div> 0.2690	<div><div></div></div> 0.3040
B	<div><div></div></div> 0.2810	<div><div></div></div> 0.2690
E	<div><div></div></div> 0.2800	<div><div></div></div> 0.2650
F	<div><div></div></div> 0.2680	<div><div></div></div> 0.3070
G	<div><div></div></div> 0.2800	<div><div></div></div> 0.2680
H	<div><div></div></div> 0.2710	<div><div></div></div> 0.3040
I	<div><div></div></div> 0.2800	<div><div></div></div> 0.2660
J	<div><div></div></div> 0.2720	<div><div></div></div> 0.3050

1.0

0.0

<0.0