



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:54 PM UTC

PDB ID : 5TAS / pdb_00005tas
EMDB ID : EMD-8383
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 6.20 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

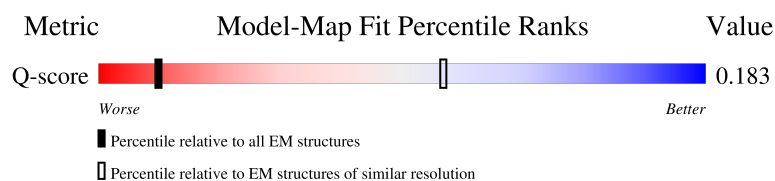
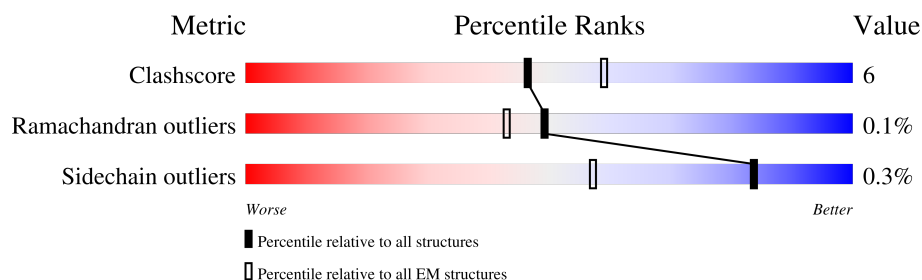
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 Å.

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



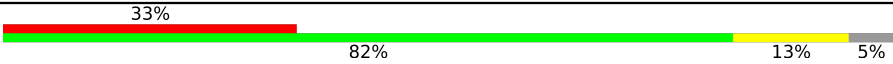
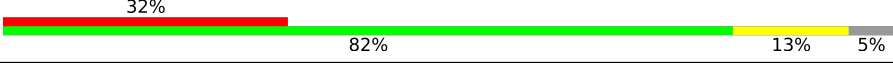
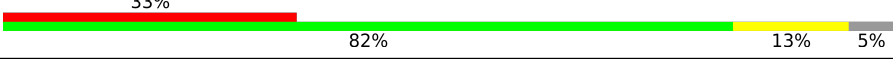
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	537 (5.70 - 6.70)

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	

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Mol	Chain	Length	Quality of chain
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

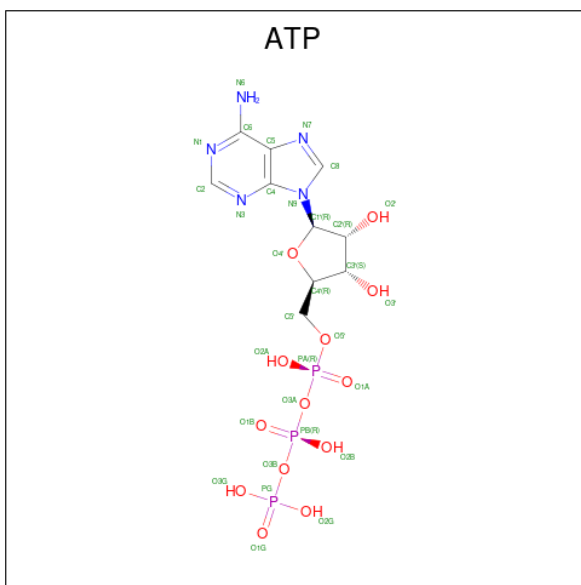
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

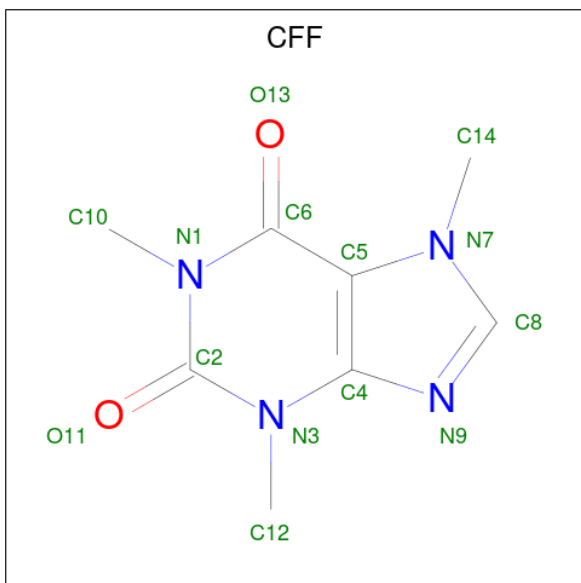
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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	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	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (CCD ID: 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	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

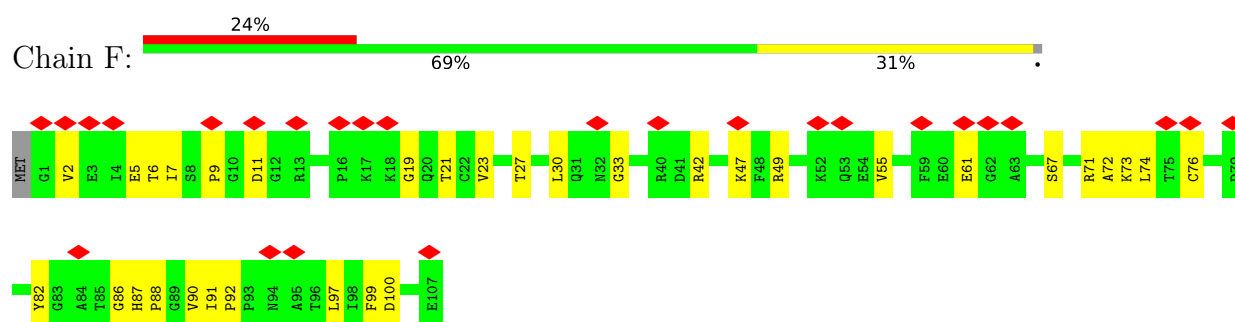
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

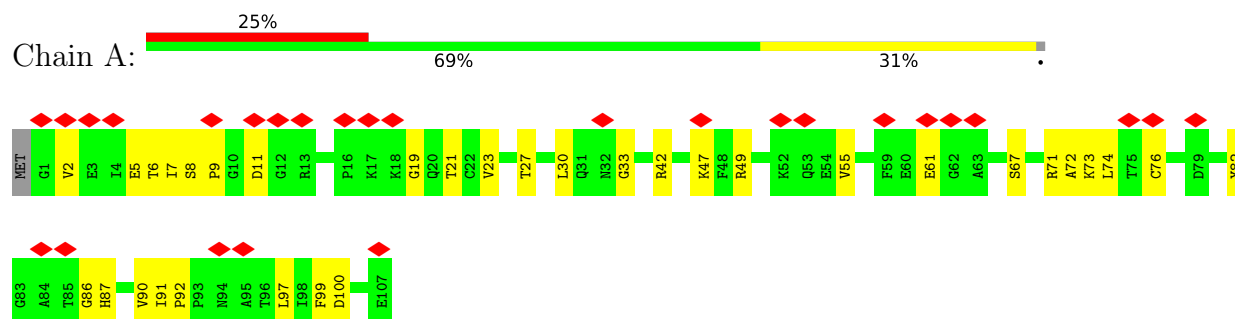
3 Residue-property plots [i](#)

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.

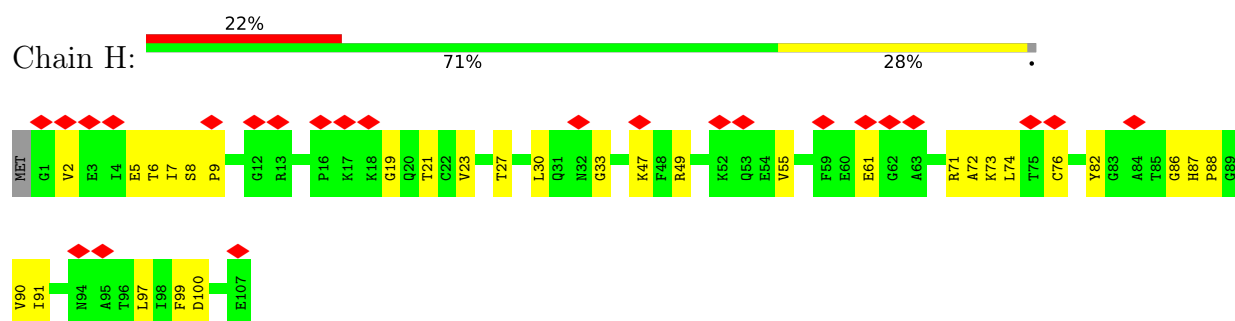
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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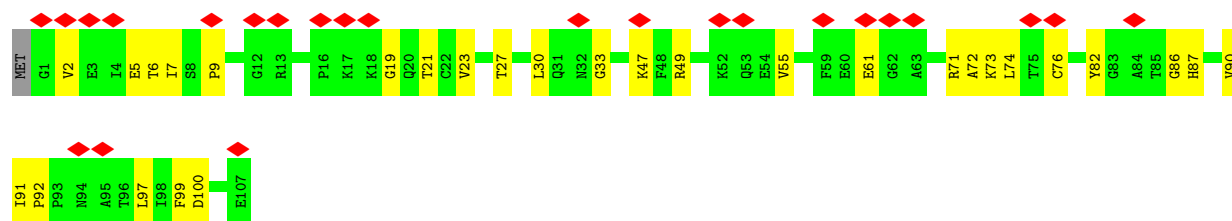


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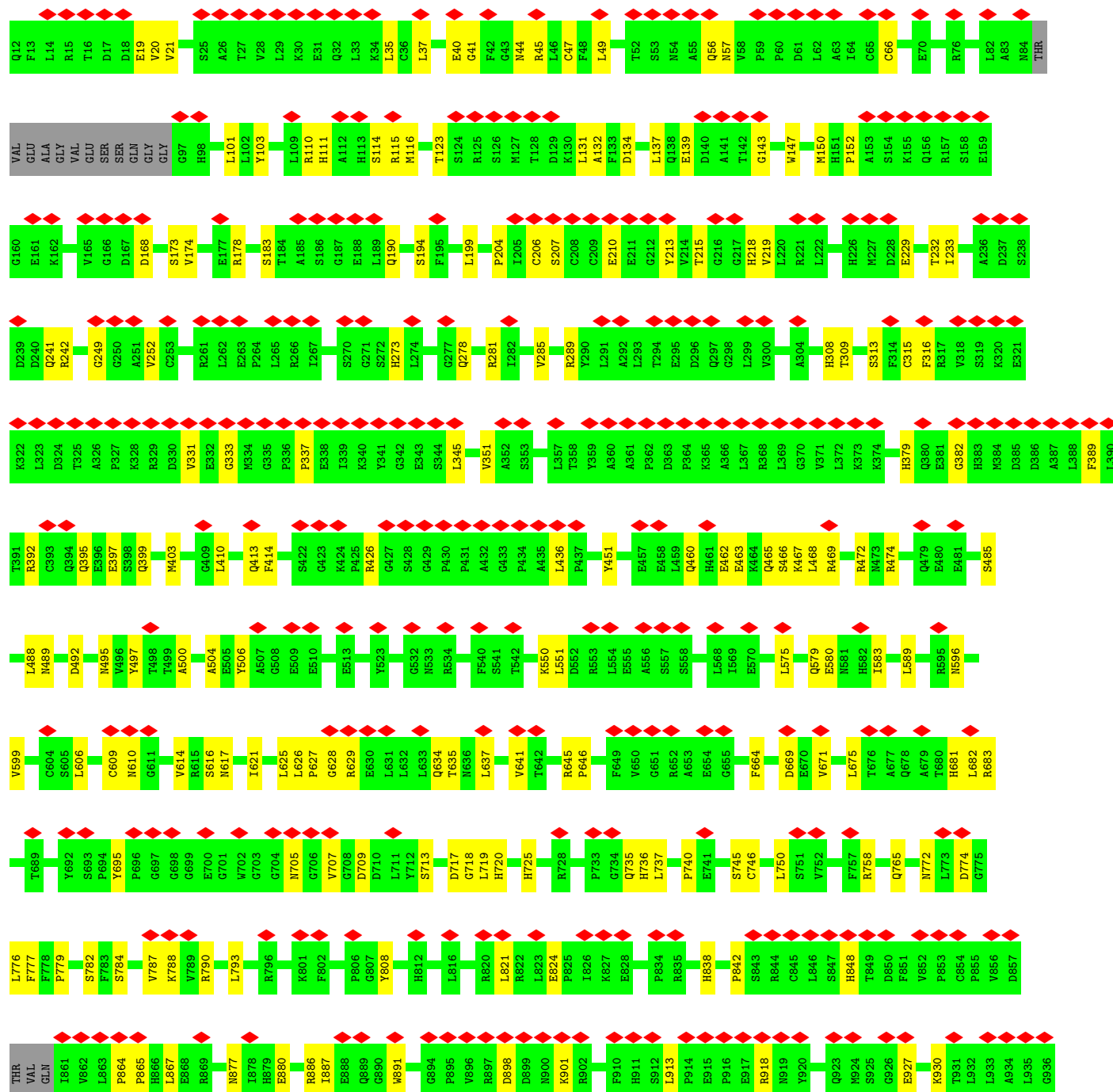
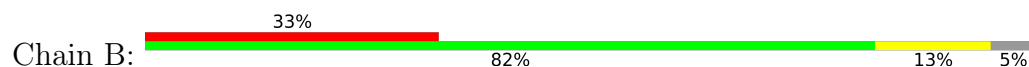


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



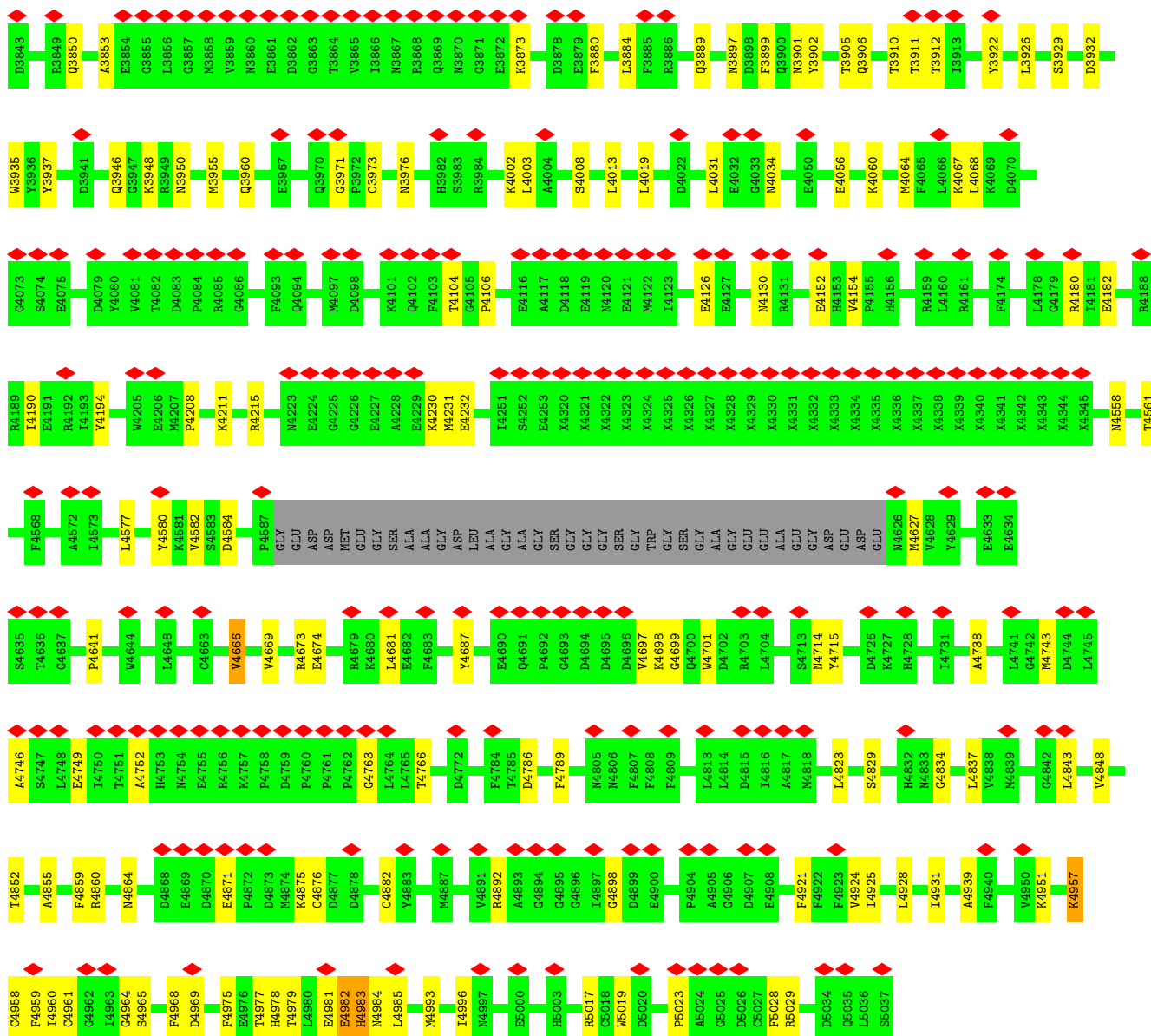


• Molecule 2: Ryanodine receptor 1

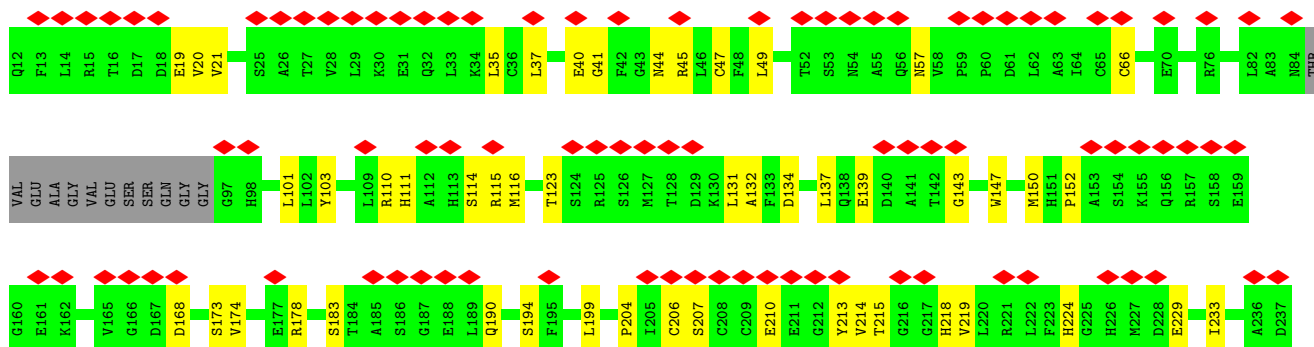
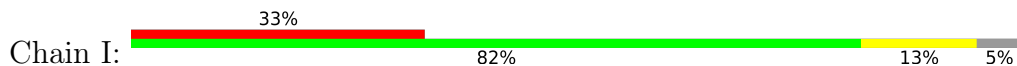




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L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	L2752	S2753	P2754	L2755	L2756	K2757	P2758	A2759	E2760	Y2761	T2762	E2763	E2764	K2765	W2766	A2767	P2768	D2769	K2770	L2771	Q2772	N2773	N2774	S2775	P2776	Y2777	Q2778	E2779	N2780	L2781	D2782	E2783	E2784	L2785	K2786	L2787	H2788	P2789	M2790	L2791	L2792	P2793	Y2794	K2795	L2796	P2797	S2798	E2799	D2800	K2802																																																																																																																																																																																																																																																																																																																																																																																																																						
E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	Y2821	W2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LVS	LVS	ARG	LVS	ILE	THR	GLN	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862																																																																																																																																																																																																																																																																																																																																																																																																																								
S2863	Q2864	V2865	L2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	E2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	L2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922																																																																																																																																																																																																																																																																																																																																																																																																																					
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X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3469	X3470	X3471	X3472	X3473	X3474	X3475	X3476	X3477	X3478	X3479	X3480	X3481	X3482	X3483	X3484	X3485	X3486	X3487	X3488	X3489	X3490	X3491	X3492	X3493	X3494	X3495	X3496	X3497	X3498	X3499	X3500	X3501	X3502	X3503	X3504	X3505	X3506	X3507	X3508	X3509	X3510	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588																																																																																																																									
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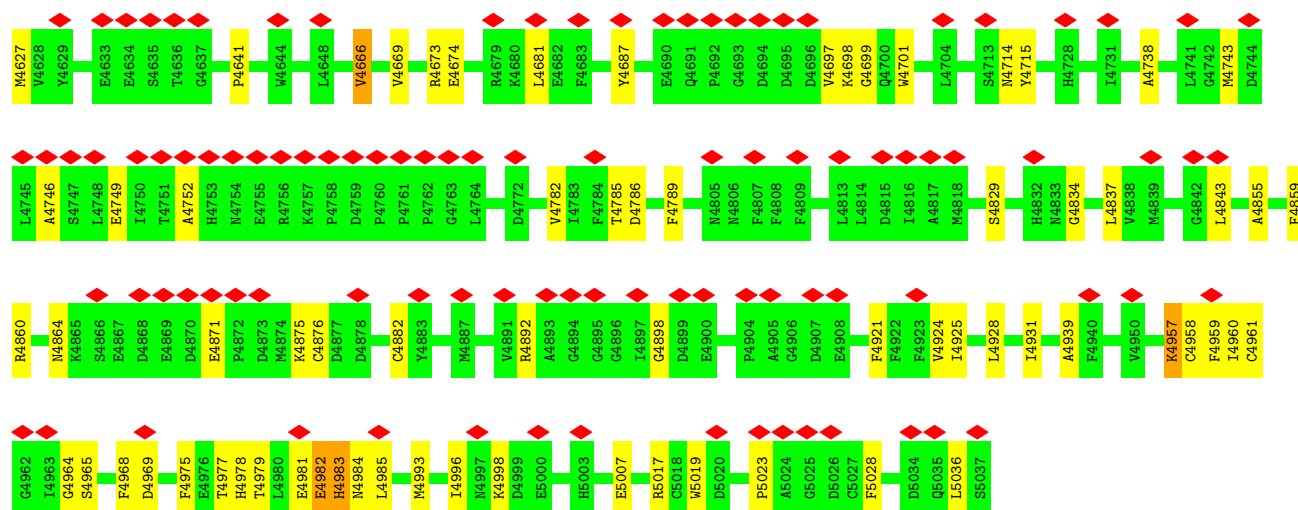
● Molecule 2: Ryanodine receptor 1



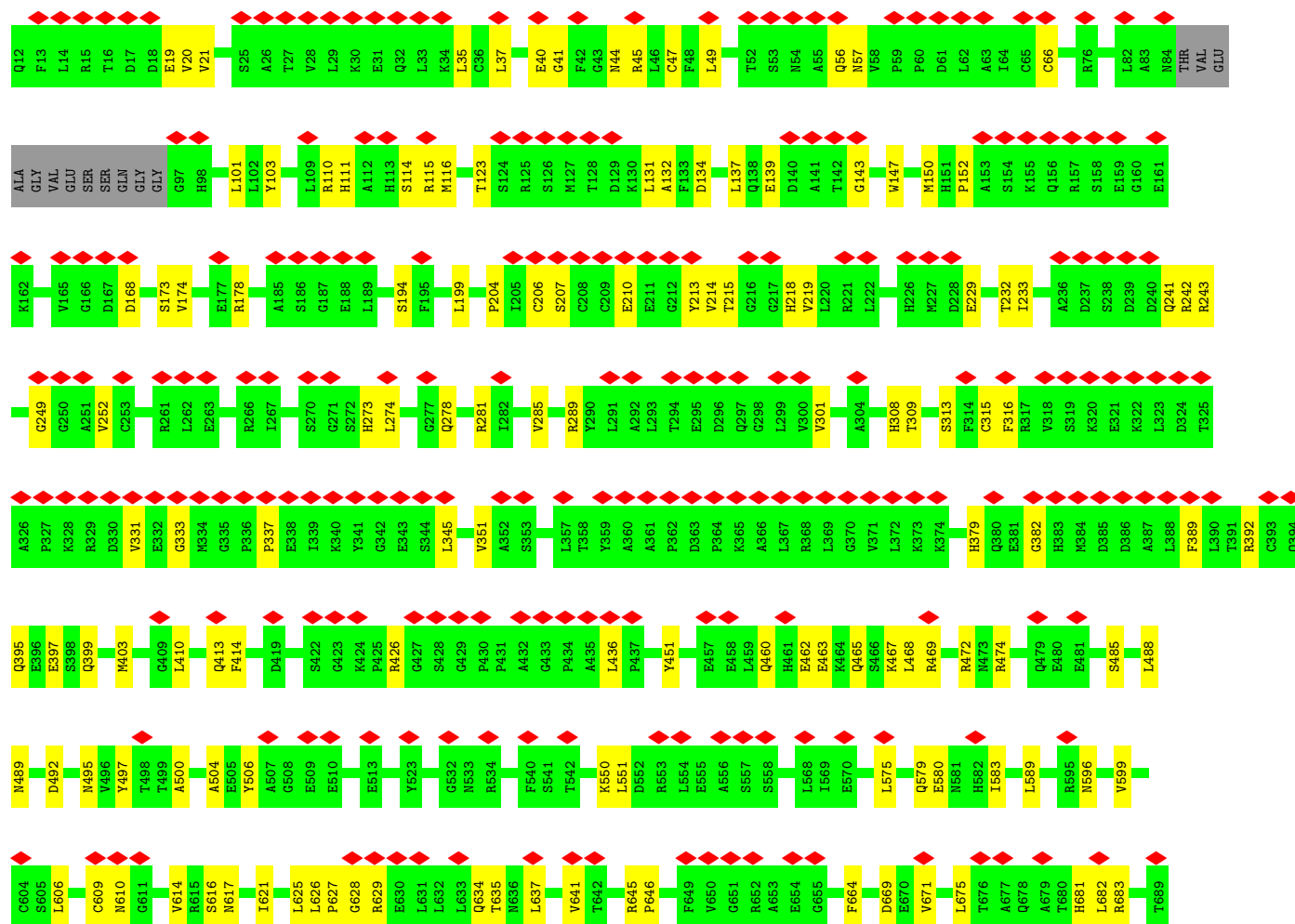
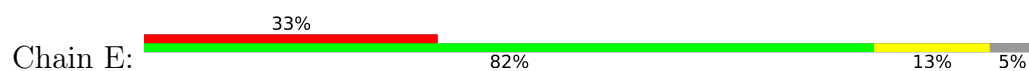
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ARG	ARG	ASN	PRO	R1020	A1030	T1031	M1035	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	M1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	SER	ARG	TRP	D1070	R1071	V1072	R1073	E1074	F1075	R1076	A1077	E1078	L1079	S1080	Y1081	F1090	E1091	F1092	E1093	A1094	V1095		
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P855	V856	D857	THR	GLN	I861	V862	L863	P864	P865	H866	L867	E868	R869	N877	I878	H879	E880	R886	T887	E888	Q889	G890	N891	G894	P895	V896	R897	D898	D899	N900	K901	R902	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	V920	Q923	H924	S925	G926	E927	K930	T931	L932	L933			
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K322	L323	D324	T325	A326	P327	K328	R329	D330	V331	E332	G333	M334	G335	P336	P337	E338	I339	K340	Y341	G342	E343	S344	L345	V351	A352	S353	L357	T358	Y359	A360	A361	P362	D363	P364	K365	A366	L367	R368	L369	V371	L372	K373	K374	H379	Q380	E381	G382	H383	M384	D385	D386	A387	L388	F389	L390



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E4206	I4193	D4080	E3854	GLY	X3595	X3531	X3397	X3333	X3248	X3061	Y2927
M4207	Y4194	Y4081	G3855	GLU	X3596	X3532	X3398	X3334	X3249	X3062	R2928
P4208	T4082	V4081	L3856	ALA	X3597	X3533	X3399	X3335	X3250	X3063	F2929
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A4228	D4098	D4098	T3864	V3751	X3612	X3541	X3409	X3345	X3258	X3158	X3158
GLY	P4106	P4106	V3865	F3752	X3613	X3542	X3410	X3346	X3259	X3159	T2938
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ALA	Q4102	Q4102	T3664	Q3767	T3663	X3544	X3412	X3348	X3261	X3161	X2942
ALA	F4103	F4103	S3768	S3768	S3663	X3545	X3413	X3349	X3262	X3162	X2943
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ASP	G4105	G4105	L3770	R3771	E3665	X3547	X3431	X3351	X3264	X3170	X2945
ASP	P4106	P4106	H3771	T3772	X3548	X3550	X3432	X3352	X3265	X3171	X2946
LEU	A4004	A4004	T3773	G3774	X3549	X3551	X3433	X3353	X3266	X3172	X2947
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GLY	A4117	A4117	L3780	L3780	X3553	X3553	X3435	X3355	X3268	X3176	X2949
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GLY	M4120	M4120	S3784	S3784	X3555	X3555	X3439	X3357	X3270	X3191	X2952
GLY	E4121	E4121	F3885	F3885	X3556	X3556	X3440	X3358	X3271	X3192	X2973
GLY	X4322	X4322	R3886	R3886	X3557	X3557	X3441	X3359	X3272	X3193	X2974
GLY	X4323	X4323	Q3889	Q3889	X3558	X3558	X3442	X3360	X3273	X3194	X2975
GLY	X4324	X4324	F3889	F3889	X3559	X3559	X3443	X3361	X3274	X3195	X2976
TRP	X4325	X4325	L3805	L3805	X3560	X3560	X3443	X3362	X3281	X3196	X2995
GLY	X4326	X4326	E3684	E3684	X3561	X3561	X3453	X3363	X3282	X3197	X2995
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• Molecule 2: Ryanodine receptor 1

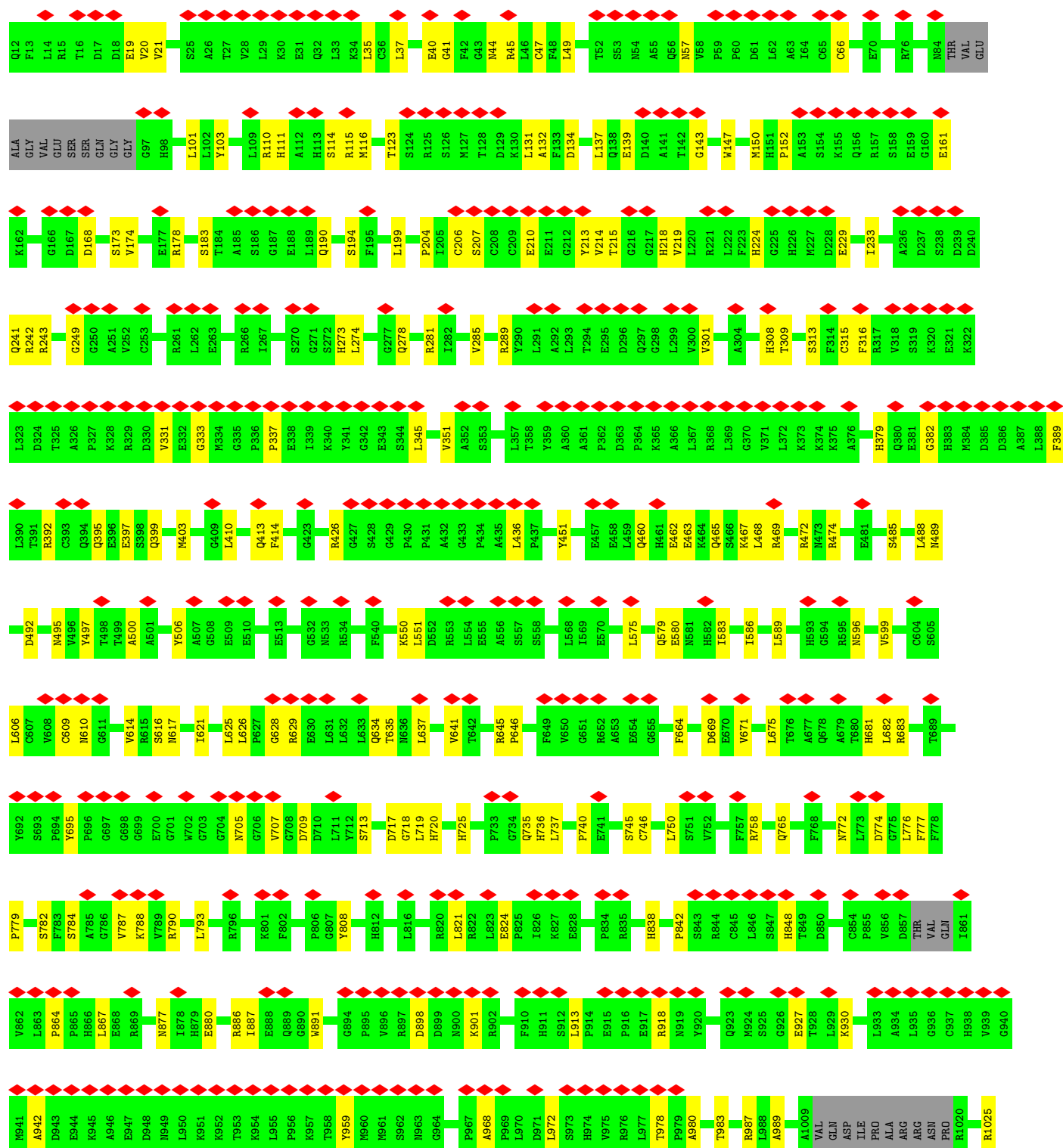
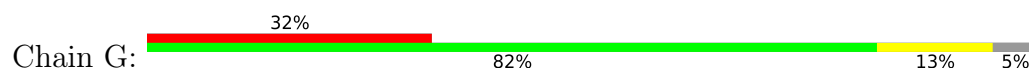


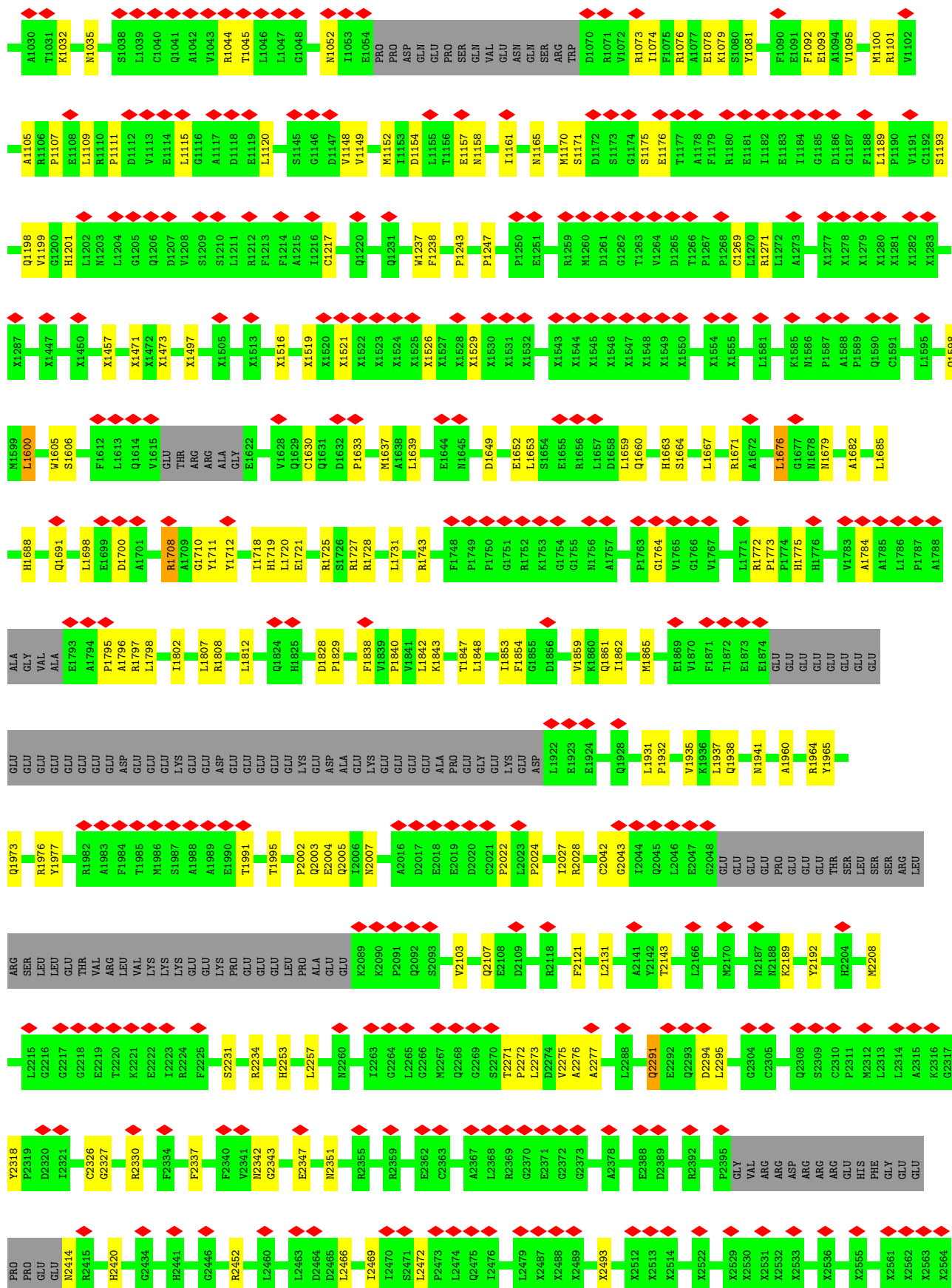


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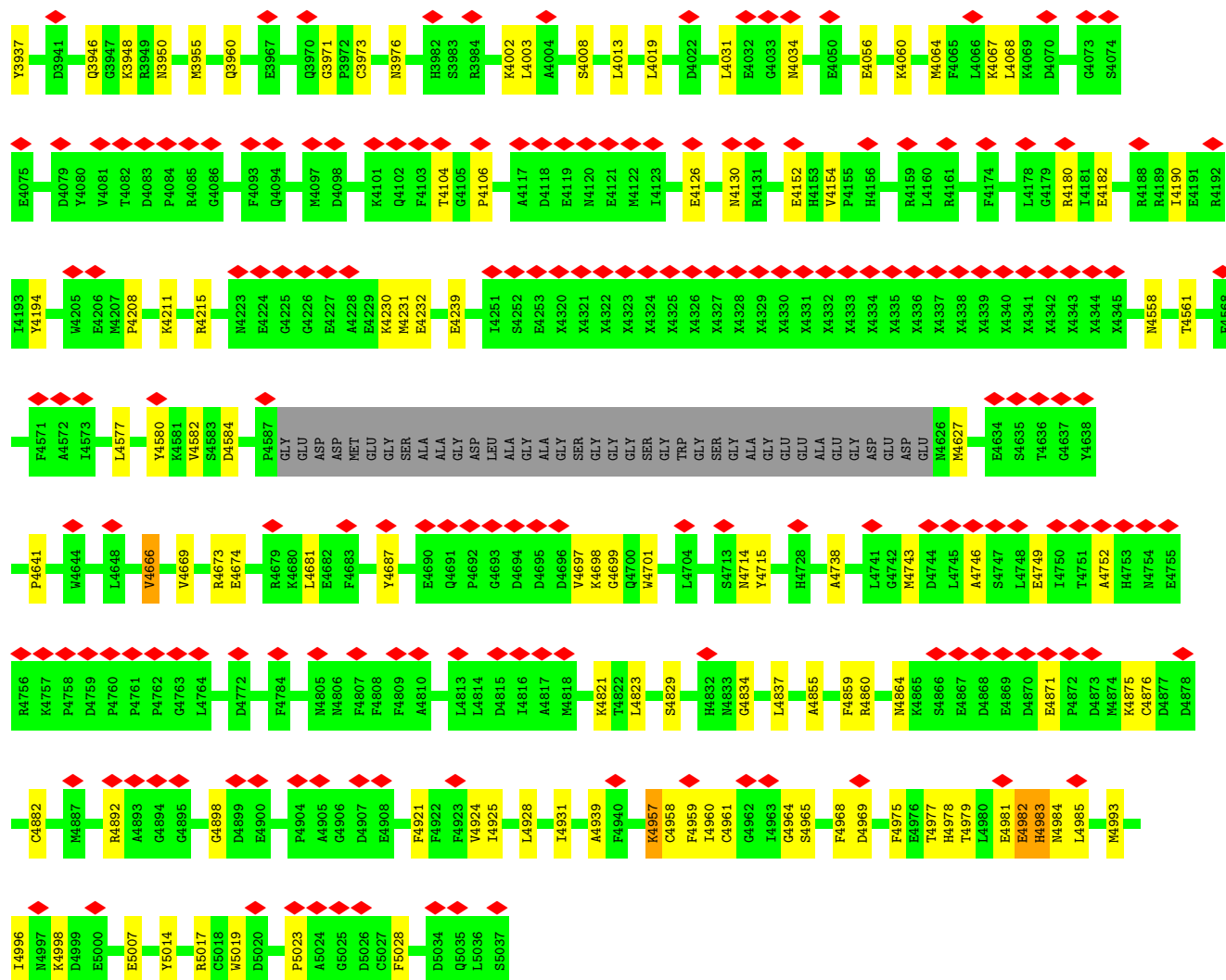
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E5000	E5000	D4694	D4694	D4694	GLY	X4320	N4120	L4019	L3884	X3554	X3666	X3554
H5003	H5003	D4695	D4695	D4695	GLY	X4321	E4121	D4022	L3884	X3555	X3667	X3555
E5007	E5007	V4696	V4696	V4696	GLY	X4322	M4122	G4033	F3885	X3556	X3668	X3556
Y5014	Y5014	K4697	K4697	K4697	GLY	X4323	E4123	N4034	F3886	X3557	X3669	X3557
R5017	R5017	Q4700	Q4700	Q4700	TRP	X4324	E4126	E4050	Q3889	X3558	X3670	X3558
C5018	C5018	G4699	G4699	G4699	GLY	X4325	E4127	E4050	D3897	X3559	X3671	X3559
D5020	D5020	V4701	V4701	V4701	GLY	X4326	E4127	E4050	F3889	X3560	X3681	X3560
P5023	P5023	L4704	L4704	L4704	ALA	X4327	M4130	E4050	L3805	X3561	X3682	X3561
A5024	A5024	S4713	S4713	S4713	GLY	X4328	R4131	E4050	K3787	X3562	X3683	X3562
G5025	G5025	M4714	M4714	M4714	GLY	X4329	E4152	E4050	Q3788	X3563	X3684	X3563
D5026	D5026	Y4715	Y4715	Y4715	GLY	X4330	R4153	E4050	E3789	X3564	X3685	X3564
C5027	C5027	D4726	D4726	D4726	ASP	X4331	V4154	E4050	T3790	X3565	X3686	X3565
R5028	R5028	H4727	H4727	H4727	GLY	X4332	H4155	E4050	N3806	X3566	X3687	X3566
R5029	R5029	H4728	H4728	H4728	GLY	X4333	H4156	E4050	N3809	X3567	X3688	X3567
D5034	D5034	A4738	A4738	A4738	ASP	X4334	R4159	E4050	K3815	X3568	X3689	X3568
Q5035	Q5035	L4742	L4742	L4742	GLY	X4335	L4160	E4050	M3816	X3572	V3690	X3572
L5036	L5036	M4743	M4743	M4743	GLY	X4336	R4161	E4050	L3817	X3573	E3692	X3573
						X4337	L4166	E4050	D3922	X3574	R3707	X3574
						X4338	L4166	E4050	T3911	X3575	L3710	X3575
						X4339	L4166	E4050	T3912	X3576	E3712	X3576
						X4340	L4166	E4050	T3913	X3577	L3711	X3577
						X4341	L4166	E4050	Y3922	X3578	E3712	X3578
						X4342	L4166	E4050	L3926	X3579	K3713	X3579
							F4174	E4050		X3580	S3714	X3580
										X3581	L3715	X3581
										X3582	L3716	X3582
										X3583	D3717	X3583
										X3584		X3584
										X3585		X3585

• Molecule 2: Ryanodine receptor 1









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	0.077	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.028	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: CFF, ATP, 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	0.19	0/834	0.48	0/1123
1	F	0.19	0/834	0.48	0/1123
1	H	0.19	0/834	0.48	0/1123
1	J	0.19	0/834	0.48	0/1123
2	B	0.19	0/25428	0.51	4/34534 (0.0%)
2	E	0.19	0/25428	0.51	4/34534 (0.0%)
2	G	0.19	0/25428	0.51	4/34534 (0.0%)
2	I	0.19	0/25428	0.51	4/34534 (0.0%)
All	All	0.19	0/105048	0.51	16/142628 (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	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

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(°)
2	G	4984	ASN	N-CA-C	-6.66	103.75	112.41
2	B	4984	ASN	N-CA-C	-6.65	103.76	112.41
2	I	4984	ASN	N-CA-C	-6.62	103.81	112.41
2	E	4984	ASN	N-CA-C	-6.59	103.84	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1829	PRO	N-CA-C	5.41	119.71	111.11

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	808	TYR	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	21	0
1	F	818	0	824	21	0
1	H	818	0	824	18	0
1	J	818	0	824	18	0
2	B	29499	0	24746	329	0
2	E	29499	0	24746	336	0
2	G	29499	0	24746	330	0
2	I	29499	0	24746	328	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	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
All	All	121452	0	102368	1374	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 1374 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:4230:LYS:HD2	2:G:4959:PHE:CE2	1.25	1.69
2:E:4230:LYS:HD2	2:E:4959:PHE:CE2	1.25	1.64
2:I:4230:LYS:HD2	2:I:4959:PHE:CE2	1.25	1.60
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.25	1.58
2:B:4230:LYS:HD2	2:B:4959:PHE:CZ	1.55	1.42

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%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	302 (9%)	4 (0%)	48	83
2	E	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	48	83
2	G	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	48	83
2	I	3235/4416 (73%)	2928 (90%)	303 (9%)	4 (0%)	48	83
All	All	13360/18096 (74%)	12101 (91%)	1243 (9%)	16 (0%)	49	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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Mol	Chain	Res	Type
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1840	PRO

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%)	2484 (100%)	9 (0%)	84	84
2	E	2493/3022 (82%)	2484 (100%)	9 (0%)	84	84
2	G	2493/3022 (82%)	2484 (100%)	9 (0%)	84	84
2	I	2493/3022 (82%)	2484 (100%)	9 (0%)	84	84
All	All	10324/12444 (83%)	10288 (100%)	36 (0%)	84	85

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1600	LEU
2	G	4983	HIS
2	G	1676	LEU
2	G	4154	VAL
2	I	3663	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 237 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	4034	ASN

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Mol	Chain	Res	Type
2	G	3896	ASN
2	E	1679	ASN
2	G	3830	GLN
2	G	5003	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 12 ligands modelled in this entry, 4 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	-	32,33,33	1.38	5 (15%)	48,52,52	1.72	9 (18%)
3	ATP	I	5101	-	32,33,33	1.39	5 (15%)	48,52,52	1.73	9 (18%)
4	CFF	E	5102	-	15,15,15	1.76	5 (33%)	23,23,23	2.80	10 (43%)
4	CFF	I	5102	-	15,15,15	1.76	5 (33%)	23,23,23	2.80	10 (43%)
3	ATP	G	5101	-	32,33,33	1.40	5 (15%)	48,52,52	1.73	9 (18%)
3	ATP	B	5101	-	32,33,33	1.39	5 (15%)	48,52,52	1.73	9 (18%)
4	CFF	B	5102	-	15,15,15	1.76	5 (33%)	23,23,23	2.80	10 (43%)
4	CFF	G	5102	-	15,15,15	1.76	5 (33%)	23,23,23	2.79	10 (43%)

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	-	-	6/22/38/38	0/3/3/3
3	ATP	I	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	5101	ATP	C5-C4	4.63	1.47	1.39
3	I	5101	ATP	C5-C4	4.61	1.47	1.39
3	E	5101	ATP	C5-C4	4.61	1.47	1.39
3	B	5101	ATP	C5-C4	4.61	1.47	1.39
4	B	5102	CFF	C6-N1	-3.74	1.32	1.40

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	C14-N7-C8	-7.71	111.86	126.28
4	G	5102	CFF	C14-N7-C8	-7.70	111.87	126.28
4	I	5102	CFF	C14-N7-C8	-7.70	111.87	126.28
4	E	5102	CFF	C14-N7-C8	-7.69	111.89	126.28
3	G	5101	ATP	C5-C4-N3	-5.60	119.01	126.72

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

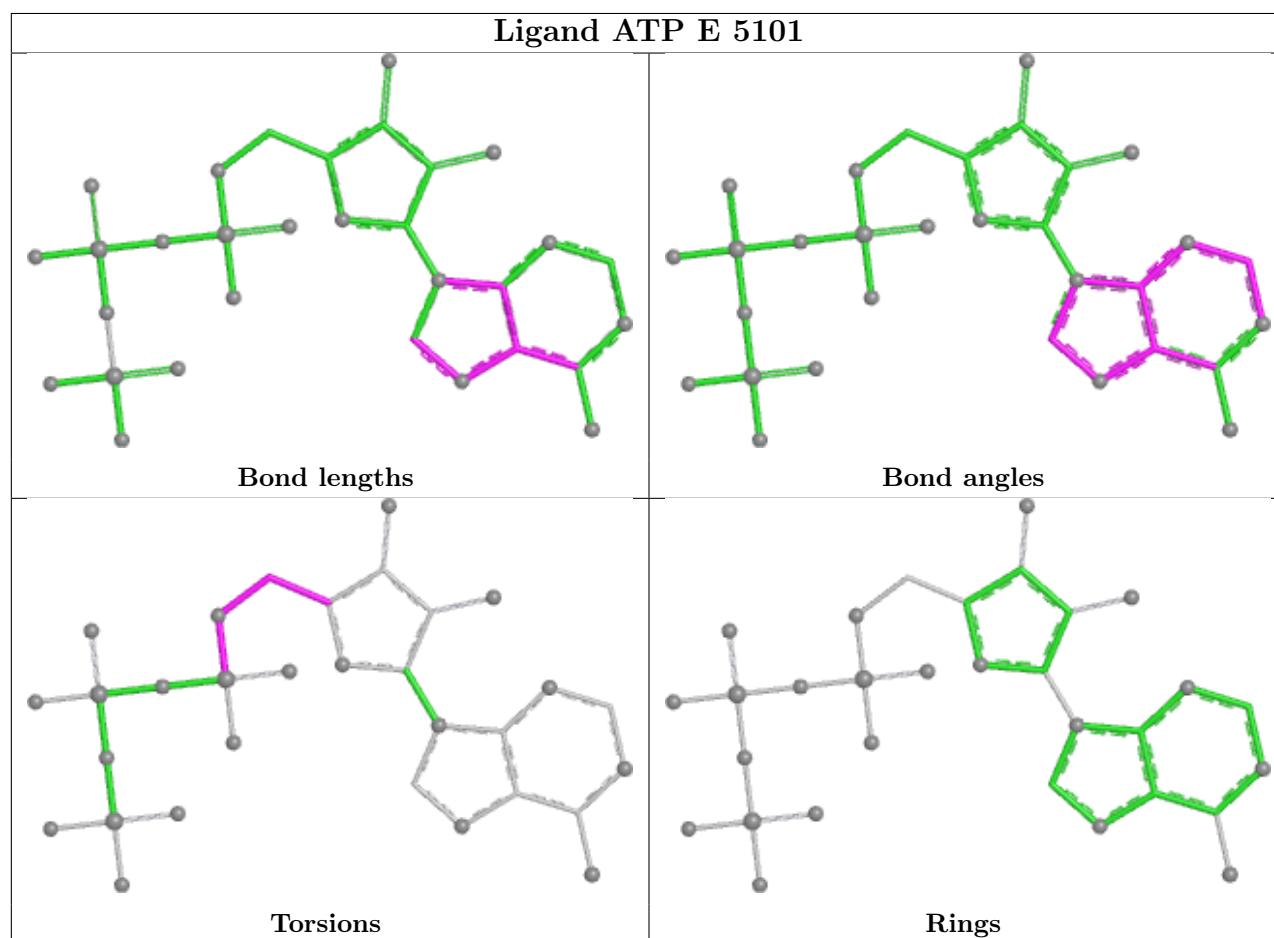
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A

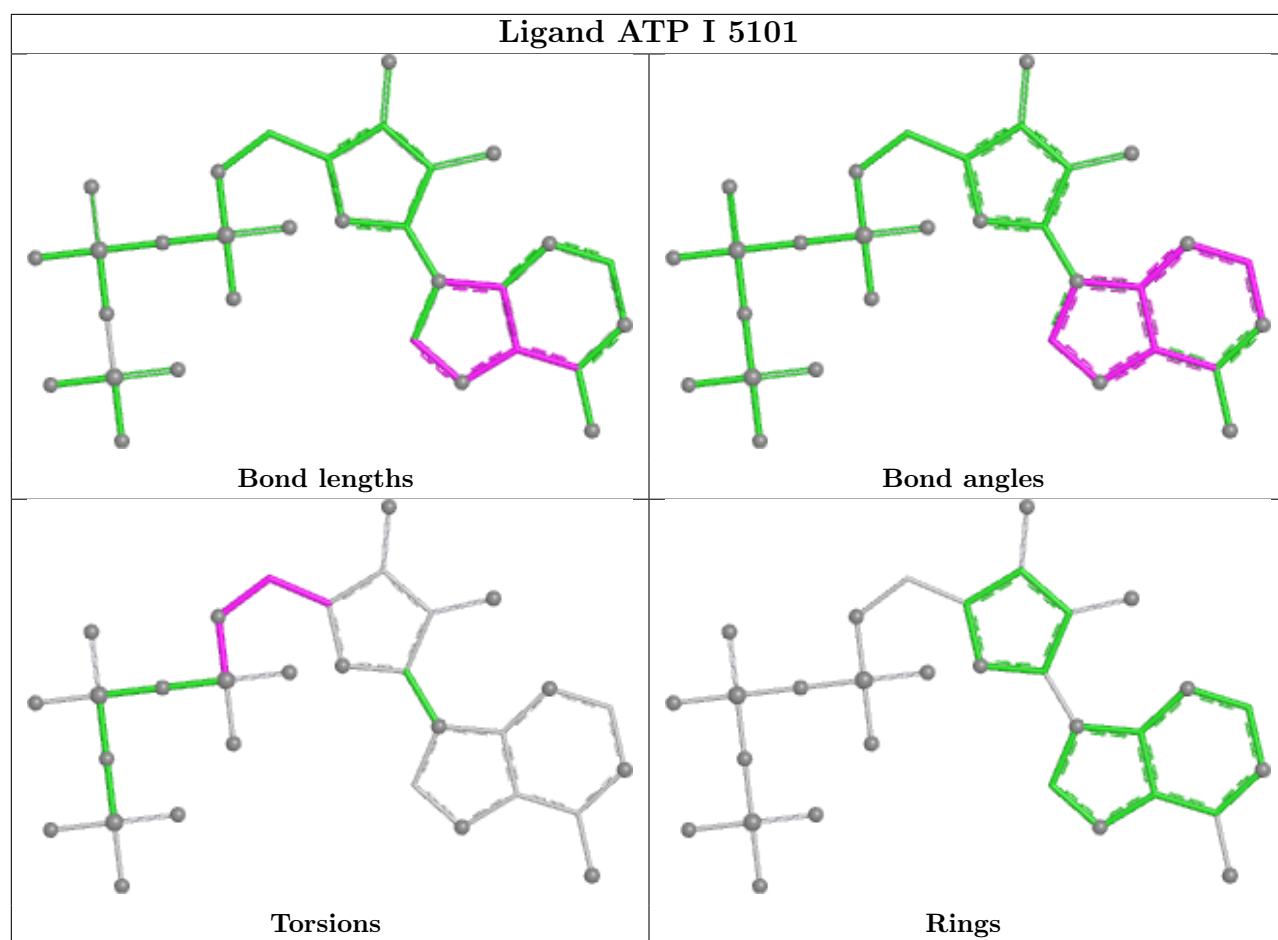
There are no ring outliers.

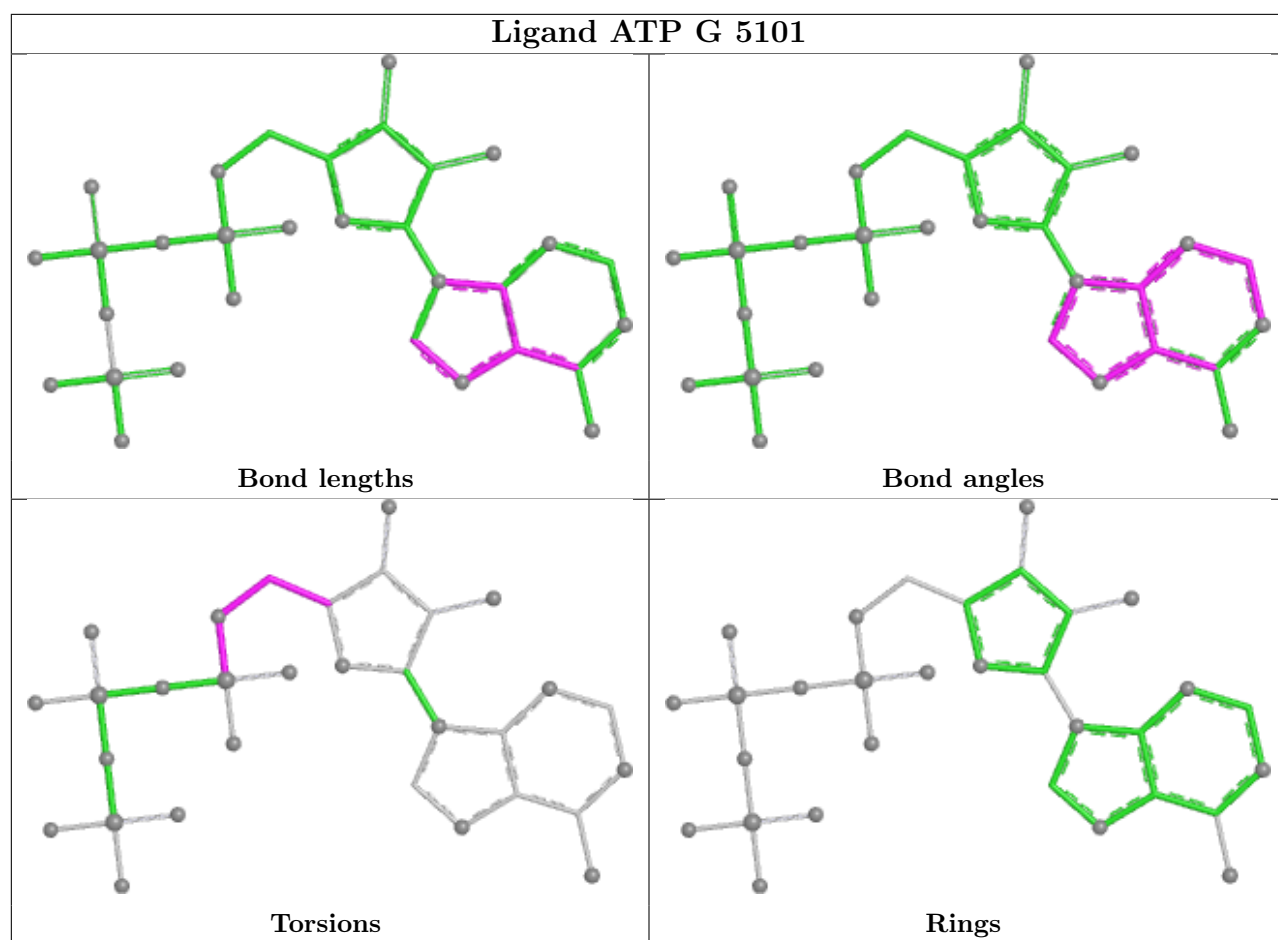
4 monomers are involved in 8 short contacts:

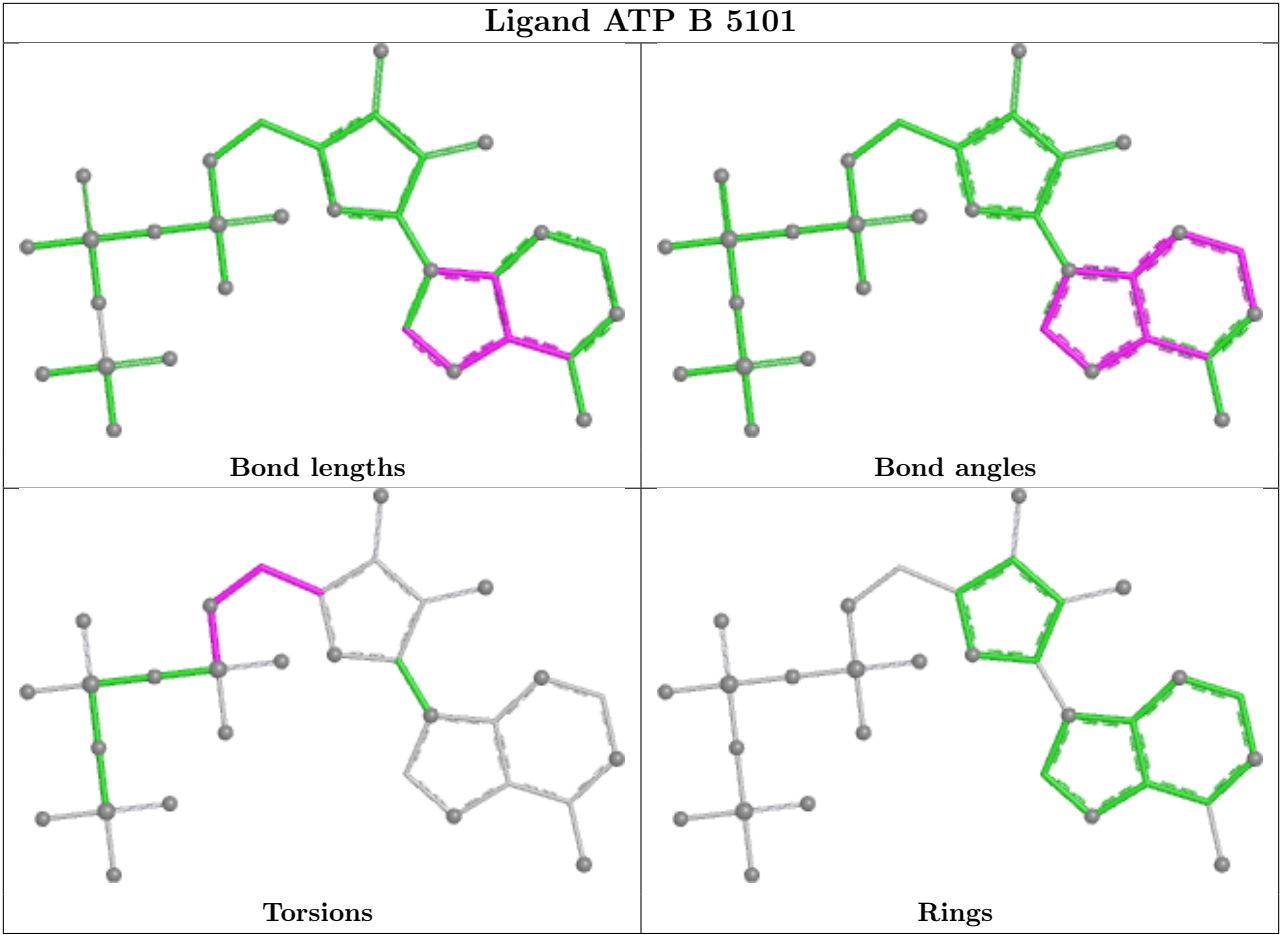
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	2	0
3	I	5101	ATP	2	0
3	G	5101	ATP	2	0
3	B	5101	ATP	2	0

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	I	14
2	E	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	B	4345:UNK	C	4540:PHE	N	73.19
1	I	4345:UNK	C	4540:PHE	N	73.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	73.19
1	G	4345:UNK	C	4540:PHE	N	73.19
1	B	3613:UNK	C	3639:THR	N	44.63

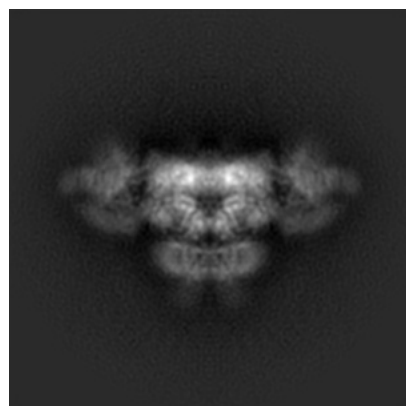
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8383. These allow visual inspection of the internal detail of the map and identification of artifacts.

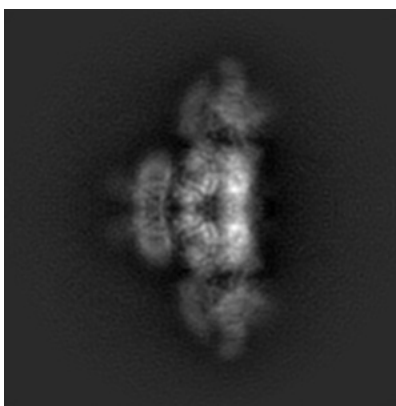
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

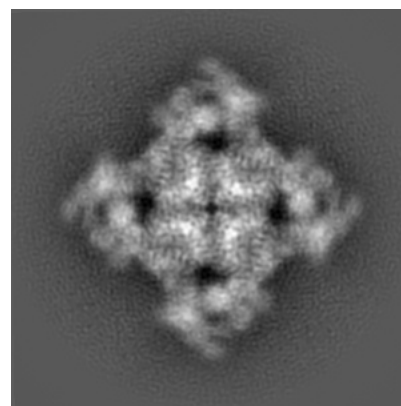
6.1.1 Primary map



X

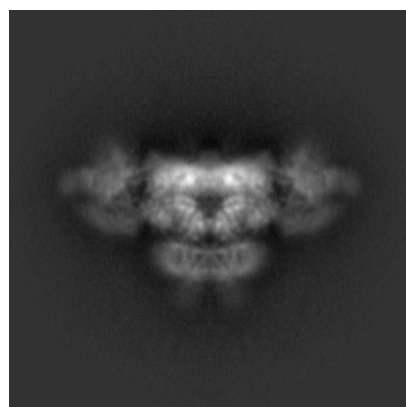


Y

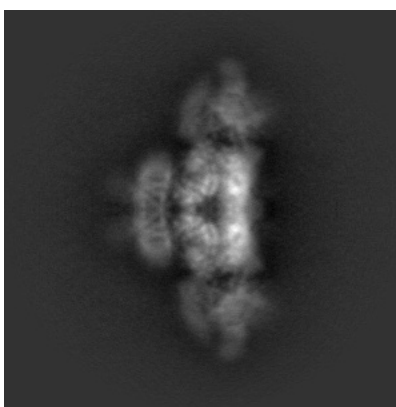


Z

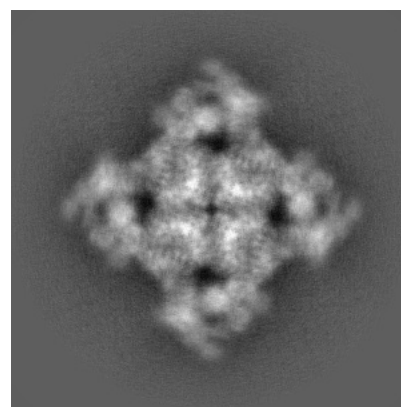
6.1.2 Raw map



X



Y

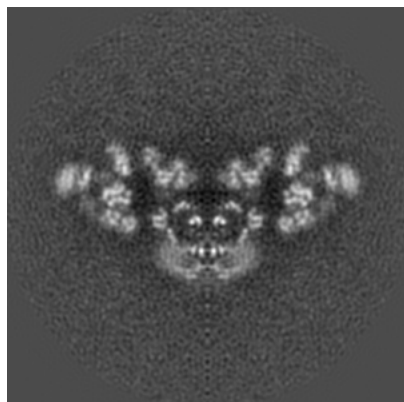


Z

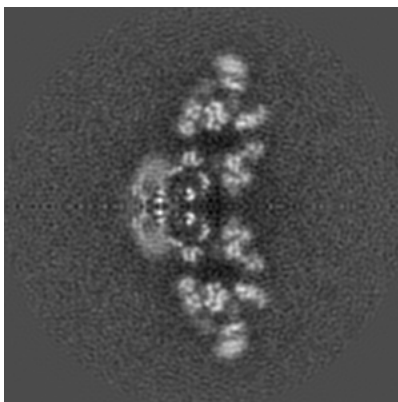
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

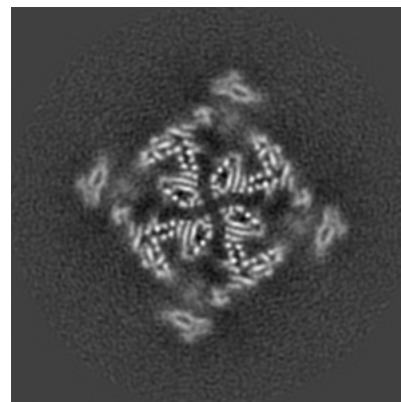
6.2.1 Primary map



X Index: 200

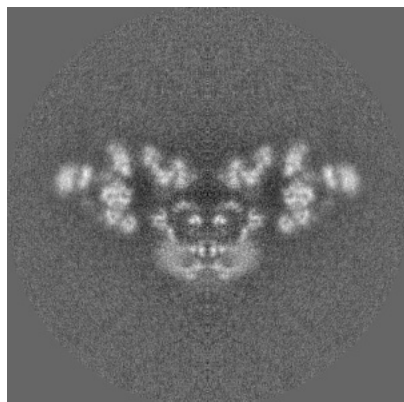


Y Index: 200

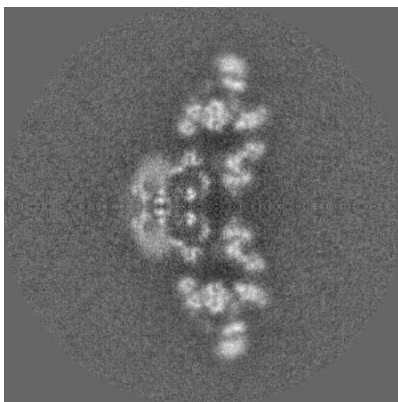


Z Index: 200

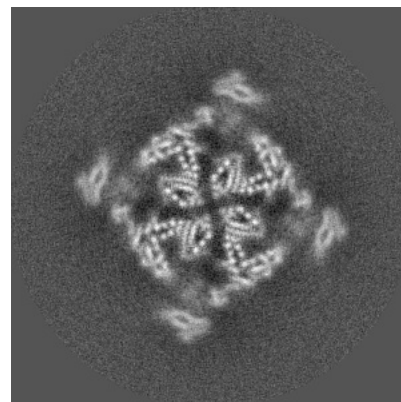
6.2.2 Raw map



X Index: 200



Y Index: 200

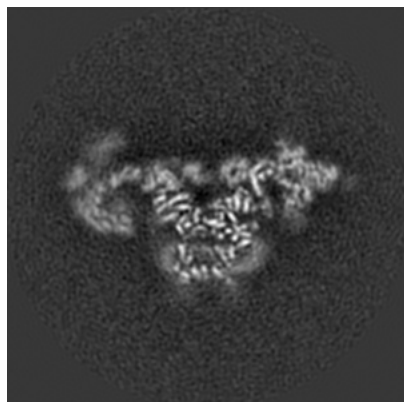


Z Index: 200

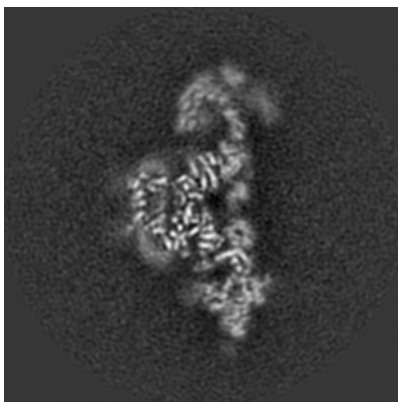
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

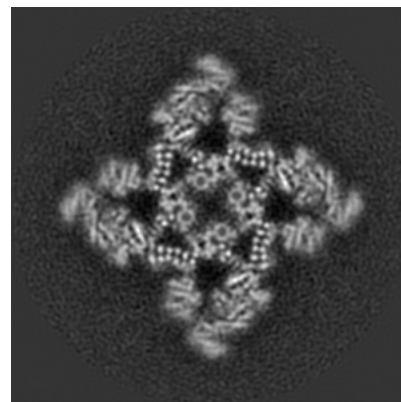
6.3.1 Primary map



X Index: 183

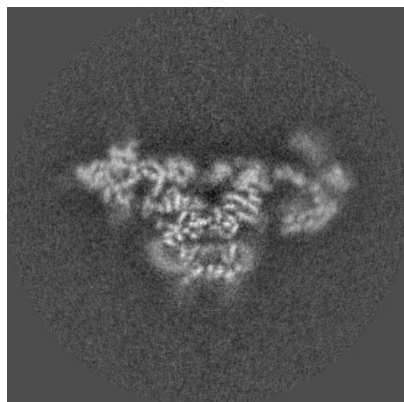


Y Index: 183

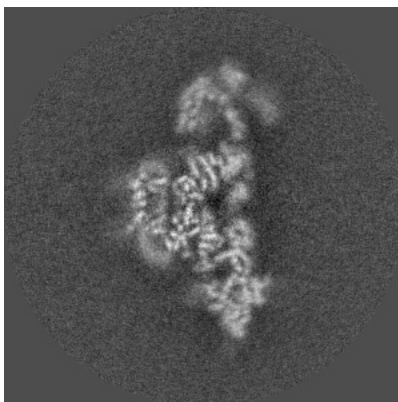


Z Index: 226

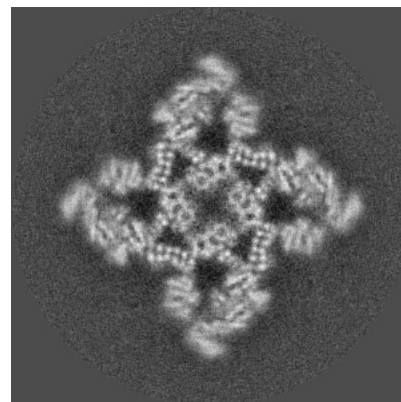
6.3.2 Raw map



X Index: 217



Y Index: 183

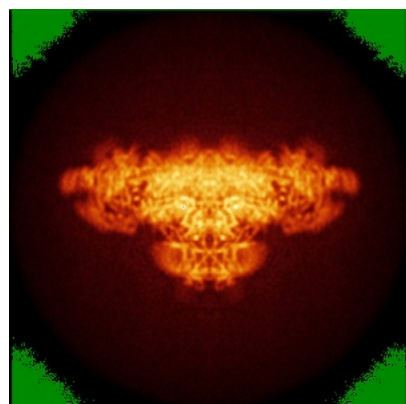


Z Index: 227

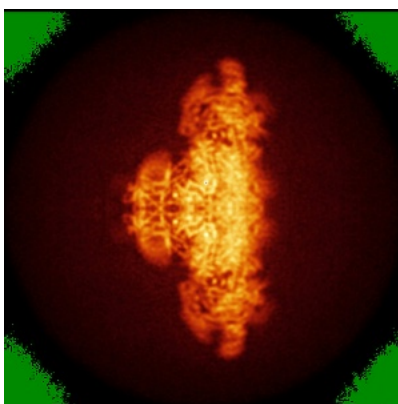
The images above show the largest variance slices of the map in three orthogonal directions.

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

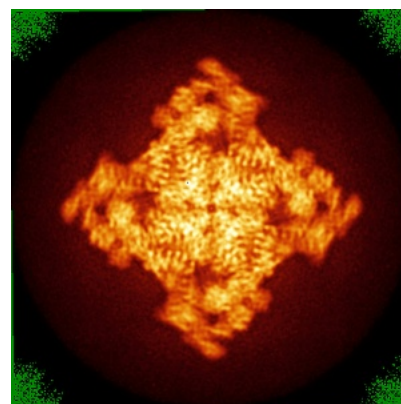
6.4.1 Primary map



X

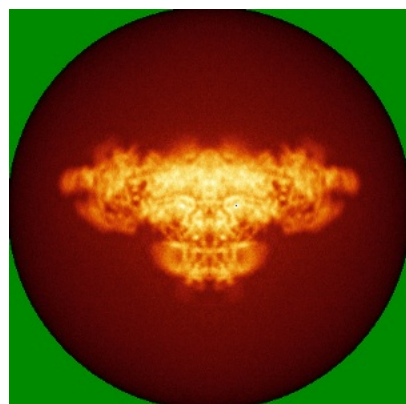


Y

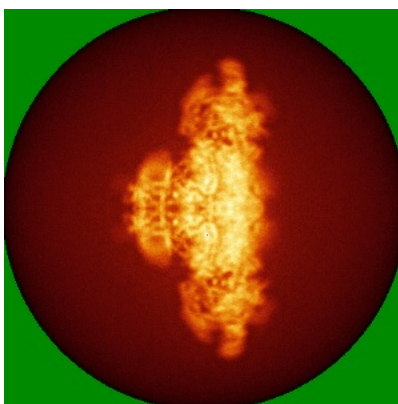


Z

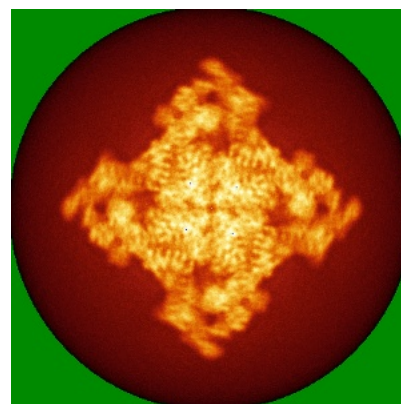
6.4.2 Raw map



X



Y

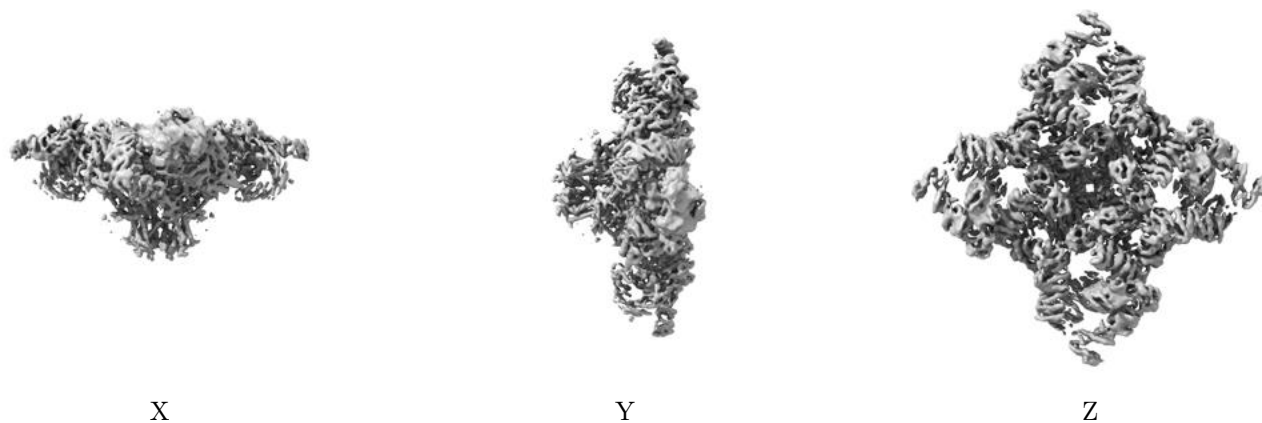


Z

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.

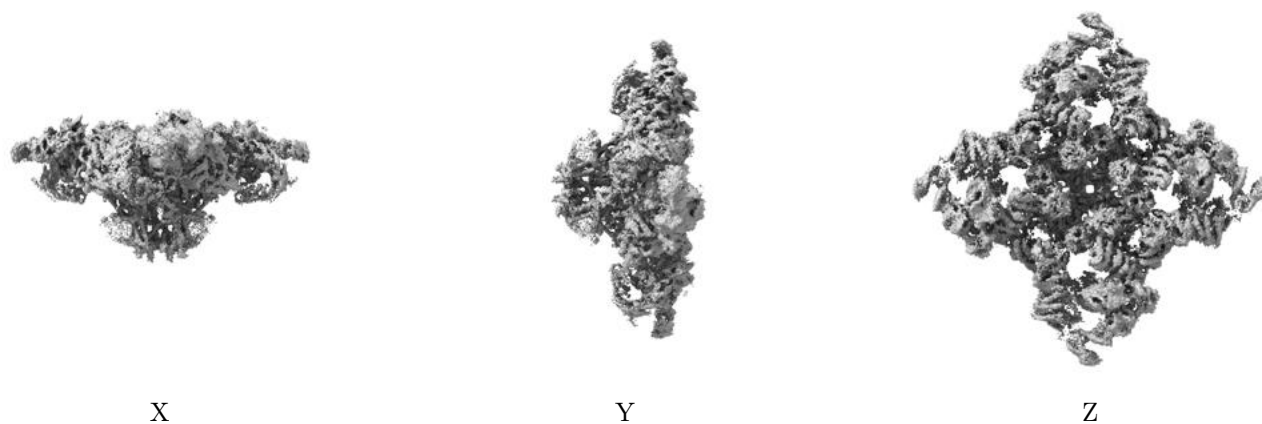
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. 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.

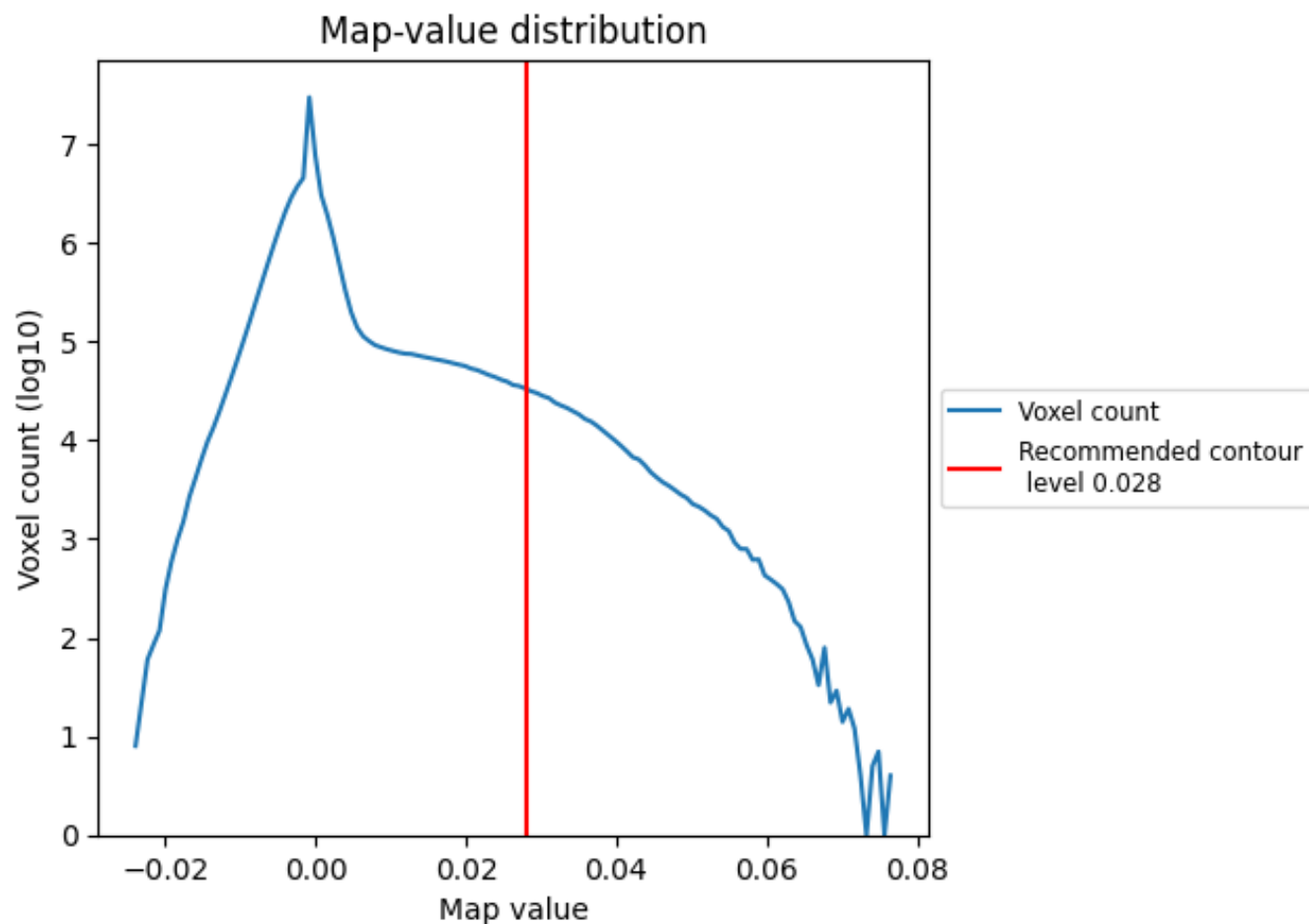
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

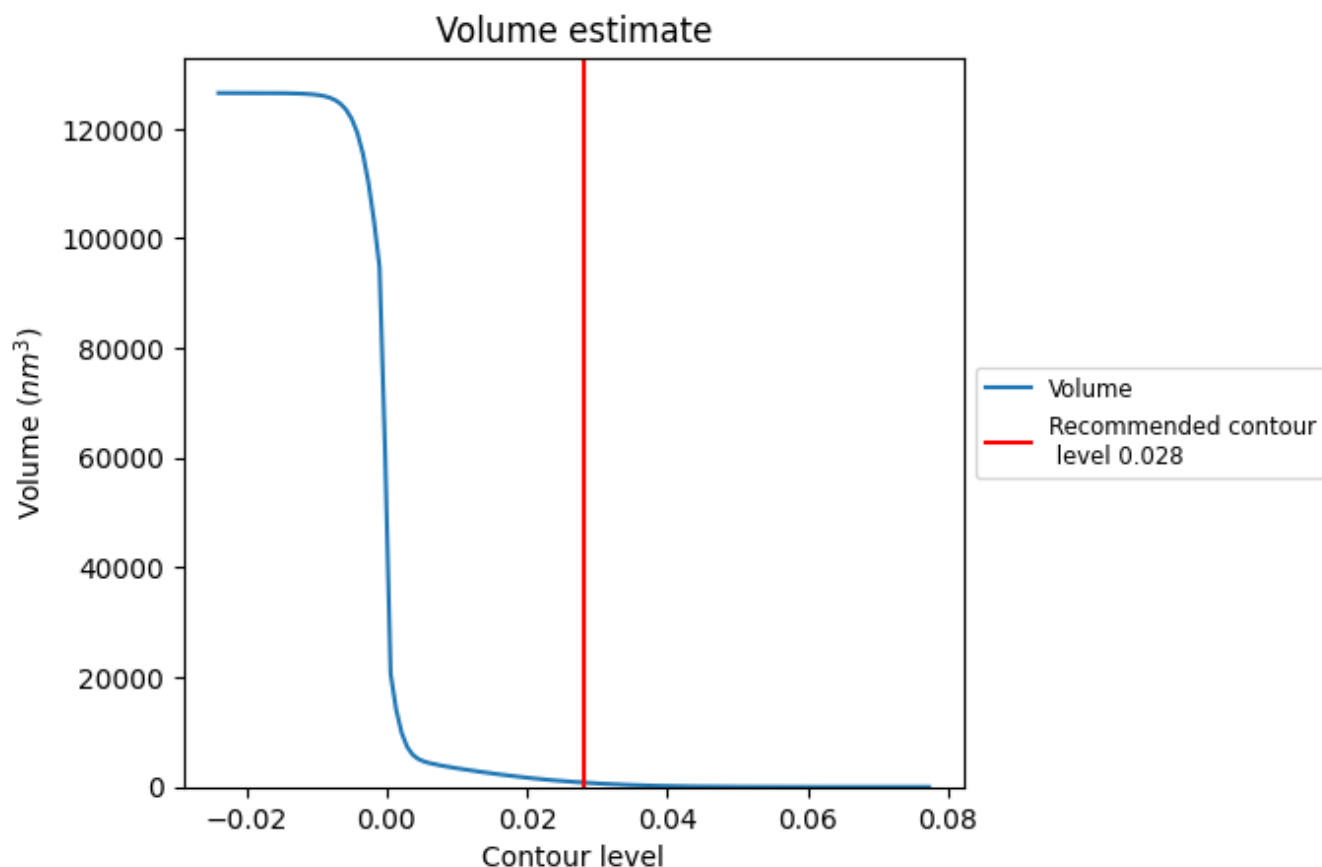
This section contains the results of statistical analysis of the map.

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.

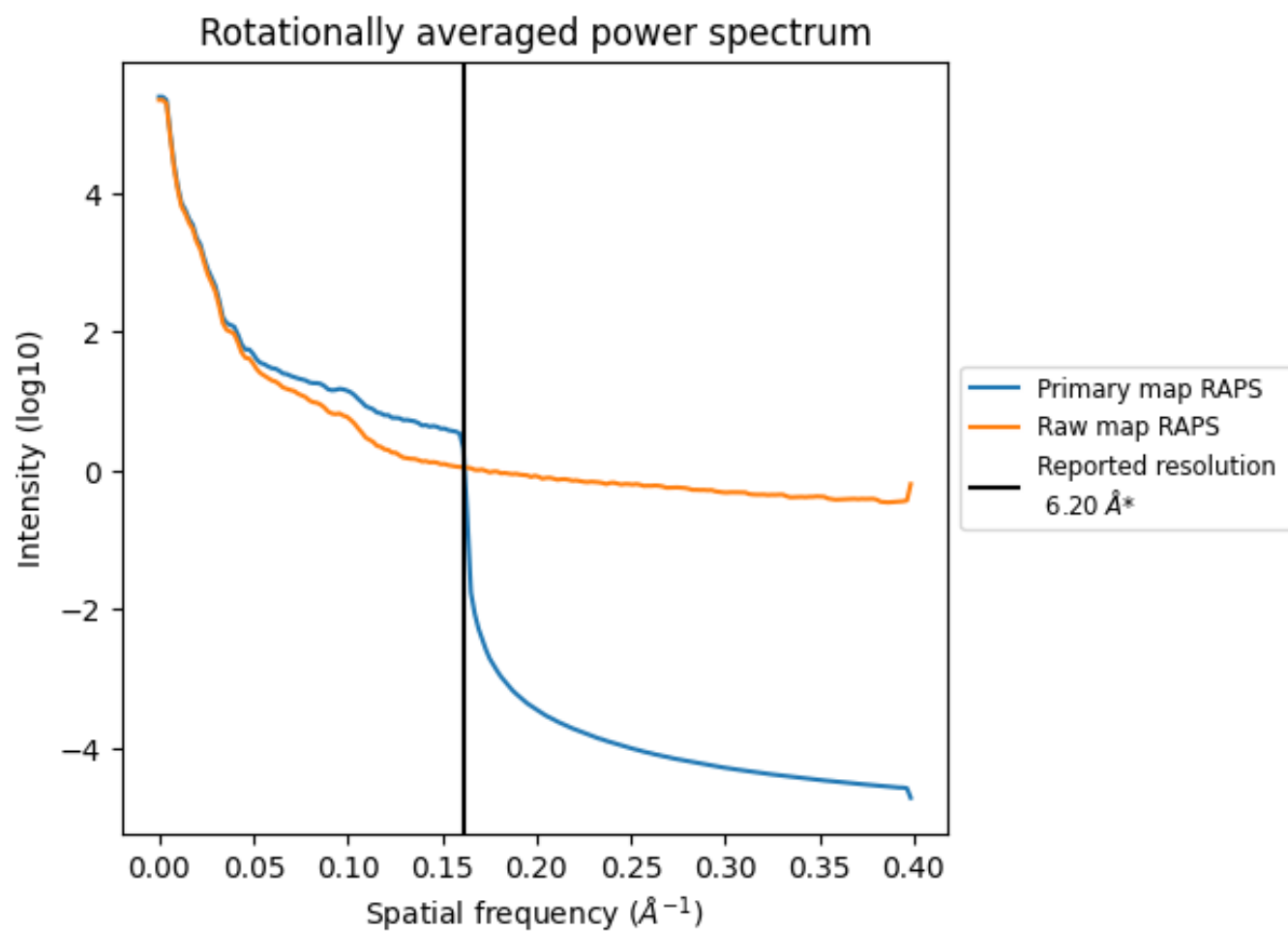
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 804 nm^3 ; this corresponds to an approximate mass of 726 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 ⓘ

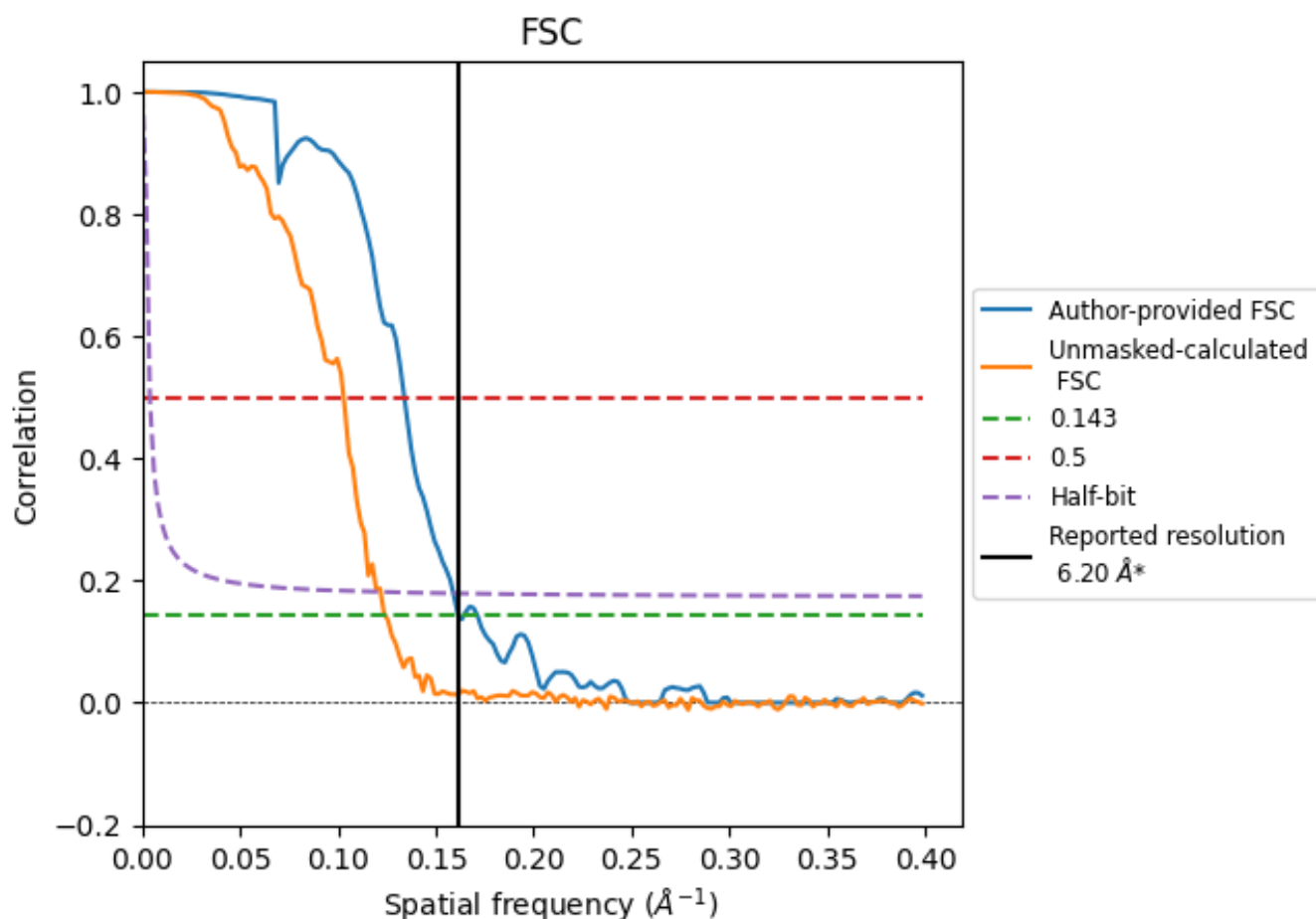


*Reported resolution corresponds to spatial frequency of 0.161 $\text{\AA}^{-1}$

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 0.161 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

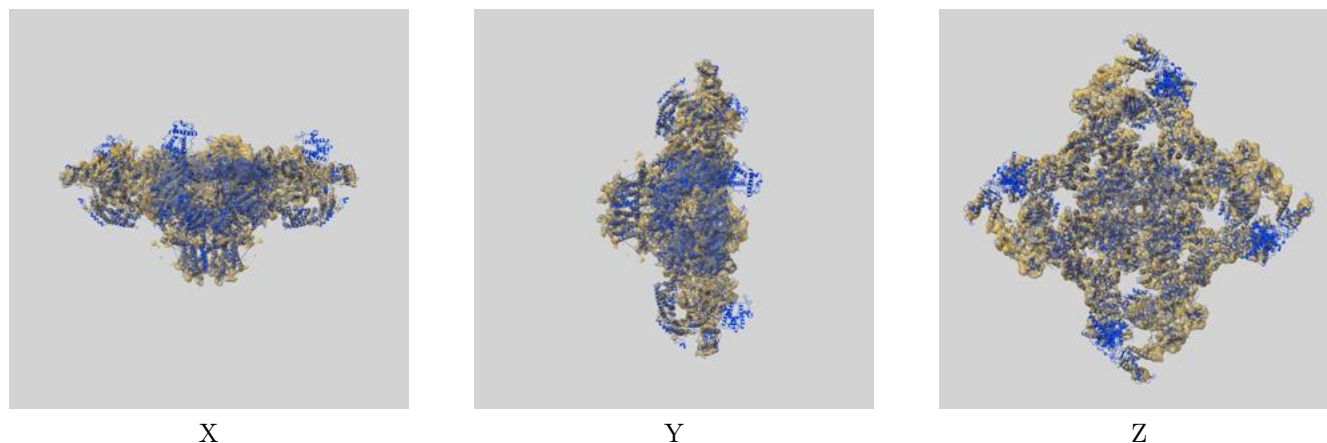
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.19	7.47	6.29
Unmasked-calculated*	8.06	9.72	8.21

*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 8.06 differs from the reported value 6.2 by more than 10 %

9 Map-model fit [i](#)

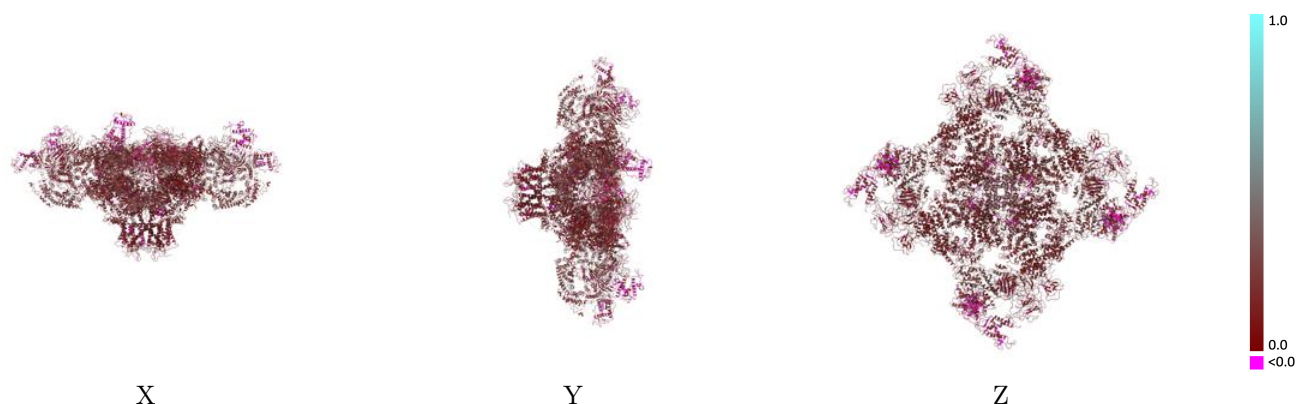
This section contains information regarding the fit between EMDB map EMD-8383 and PDB model 5TAS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

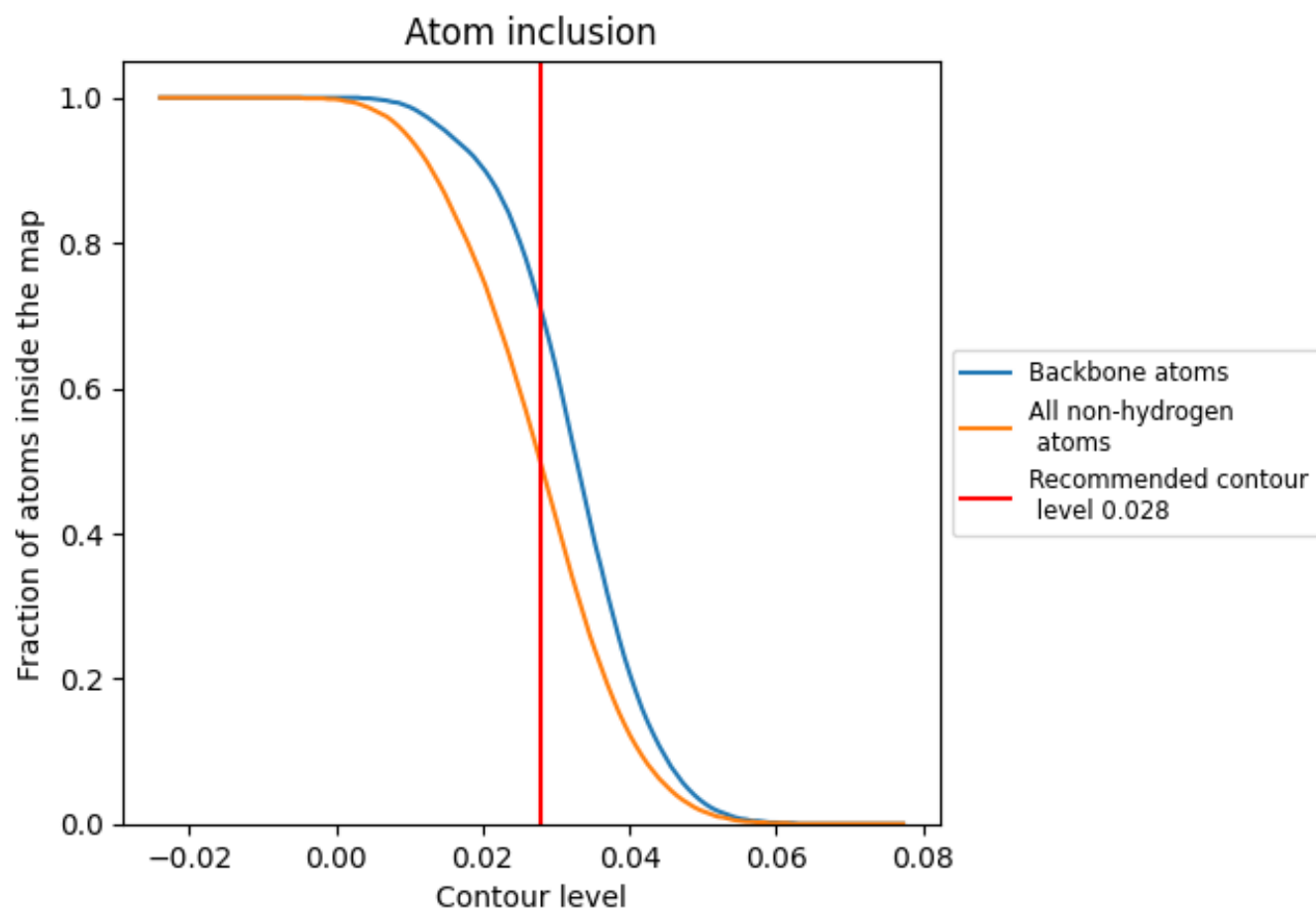


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 49% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4930	0.1830
A	0.5400	0.1700
B	0.4910	0.1840
E	0.4910	0.1830
F	0.5470	0.1750
G	0.4930	0.1840
H	0.5450	0.1730
I	0.4920	0.1830
J	0.5450	0.1720

1.0

0.0

<0.0