



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 12:08 AM EST

PDB ID : 8UQ3
EMDB ID : EMD-42459
Title : Structure of human RyR2-S2808D in the closed state in the presence of ARM210
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-10-23
Resolution : 3.18 Å(reported)
Based on initial model : 7UA5

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

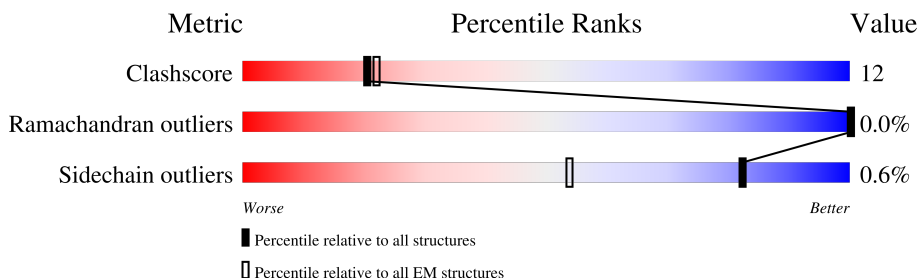
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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	4967	<div> <div>10%</div> <div>63%</div> <div>22%</div> <div>15%</div> </div>
1	B	4967	<div> <div>10%</div> <div>63%</div> <div>22%</div> <div>15%</div> </div>
1	C	4967	<div> <div>10%</div> <div>63%</div> <div>22%</div> <div>15%</div> </div>
1	D	4967	<div> <div>10%</div> <div>62%</div> <div>22%</div> <div>15%</div> </div>
2	E	108	<div> <div>67%</div> <div>31%</div> <div>..</div> </div>
2	F	108	<div> <div>68%</div> <div>31%</div> <div>..</div> </div>
2	G	108	<div> <div>65%</div> <div>33%</div> <div>..</div> </div>
2	H	108	<div> <div>67%</div> <div>31%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	A	5003	-	-	X	-
4	ATP	B	5003	-	-	X	-
4	ATP	C	5003	-	-	X	-
4	ATP	D	5003	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 138700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2808	ASP	SER	engineered mutation	UNP Q92736
B	2808	ASP	SER	engineered mutation	UNP Q92736
C	2808	ASP	SER	engineered mutation	UNP Q92736
D	2808	ASP	SER	engineered mutation	UNP Q92736

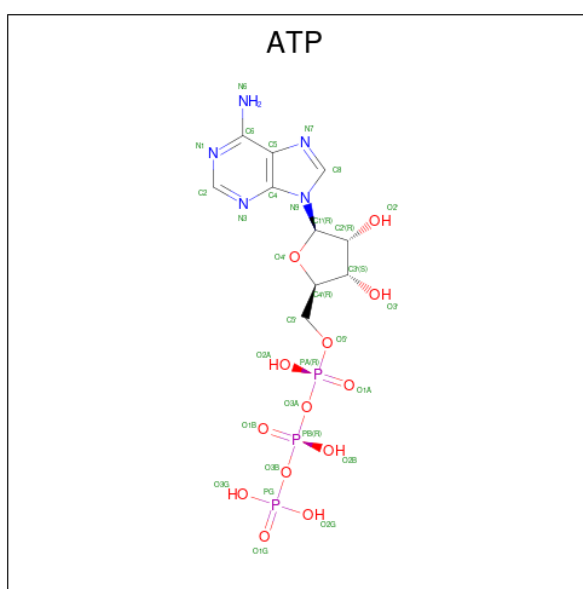
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



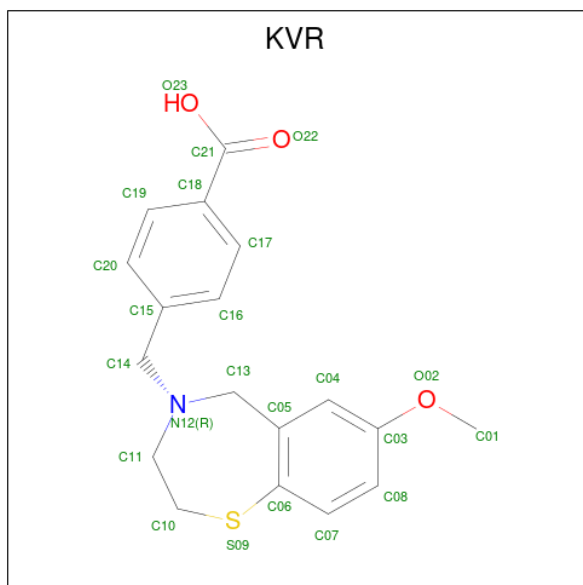
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: C₁₈H₁₉NO₃S).

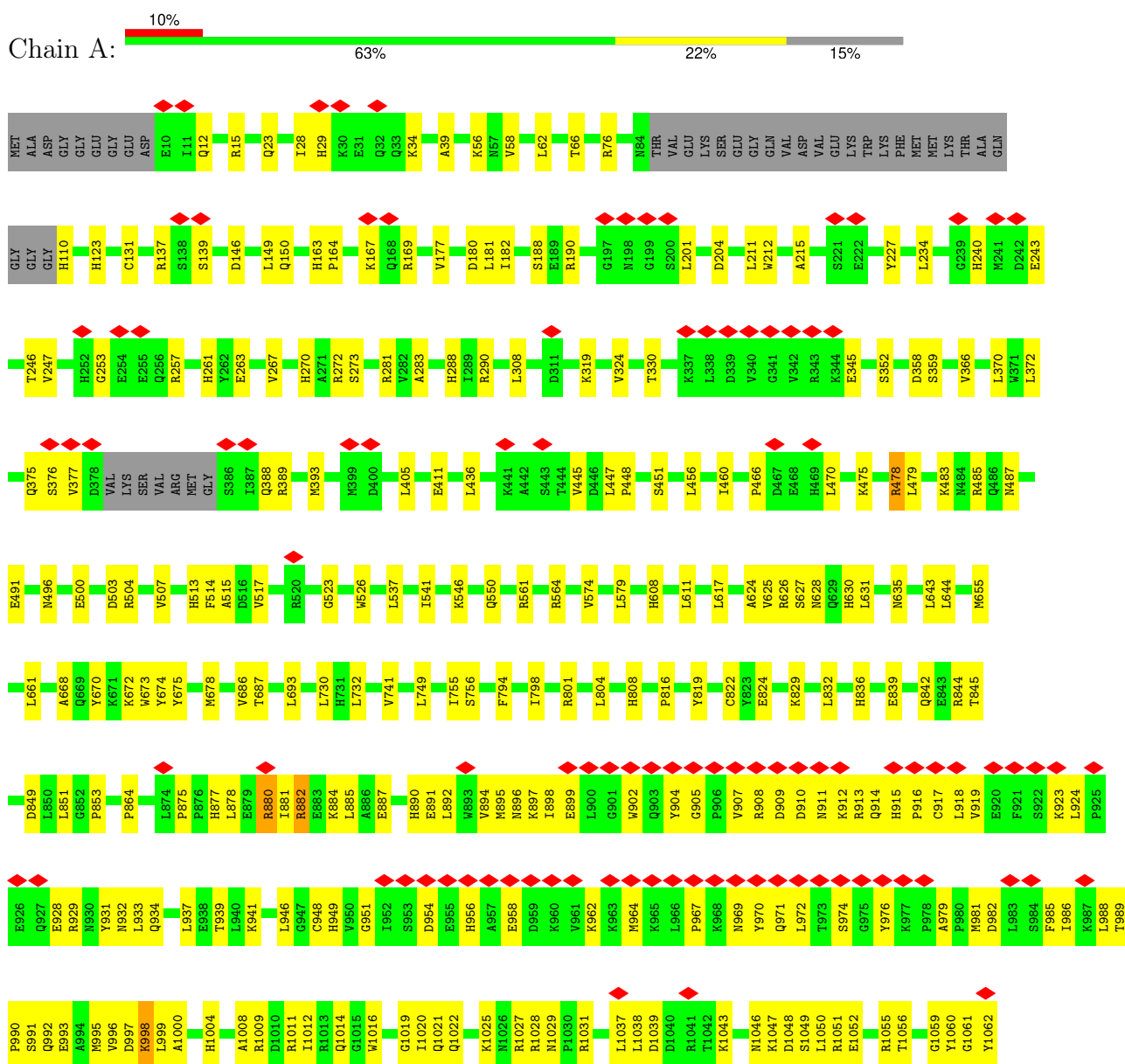


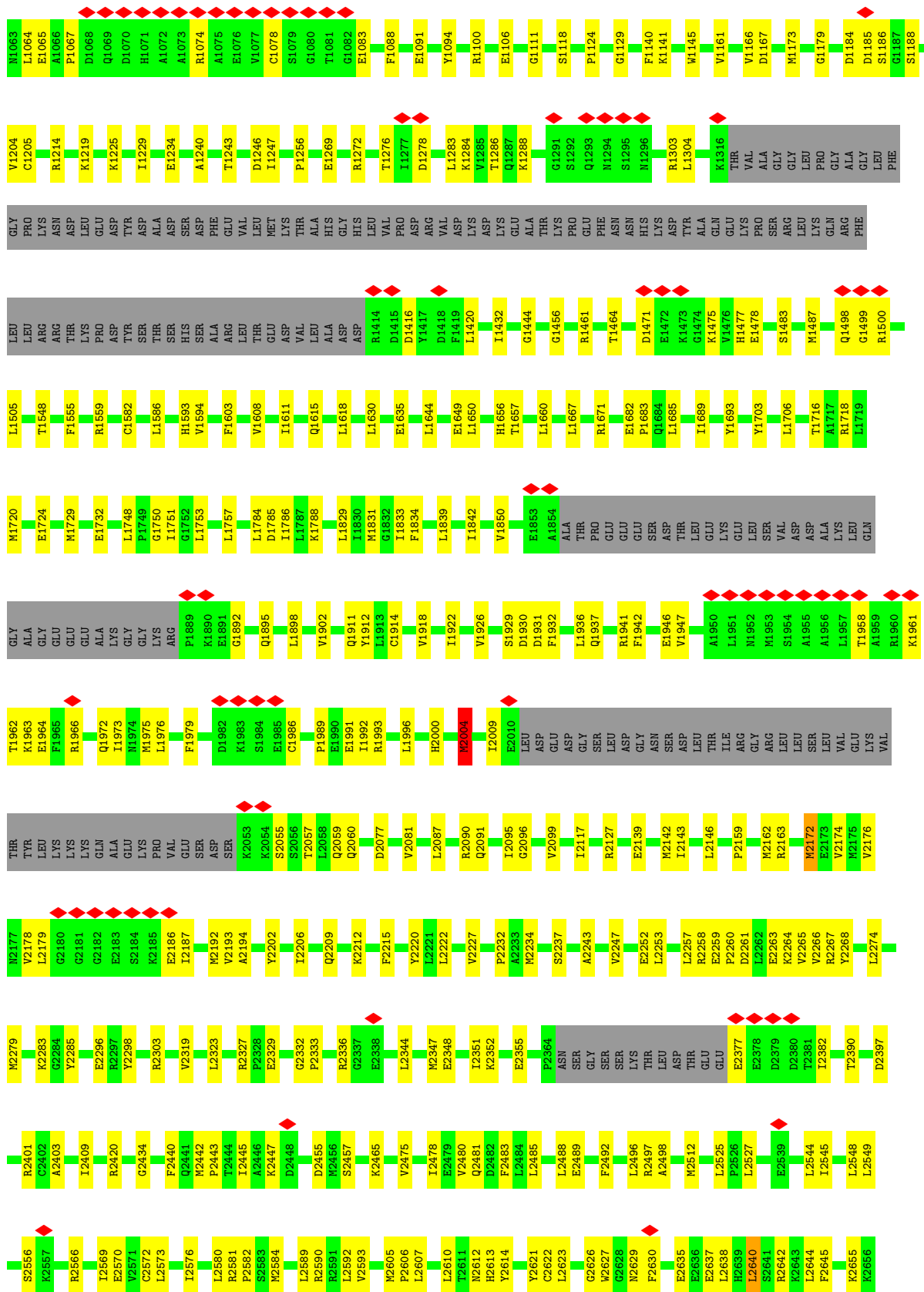
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	C	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	D	1	Total	C	N	O	S	0
			23	18	1	3	1	

3 Residue-property plots

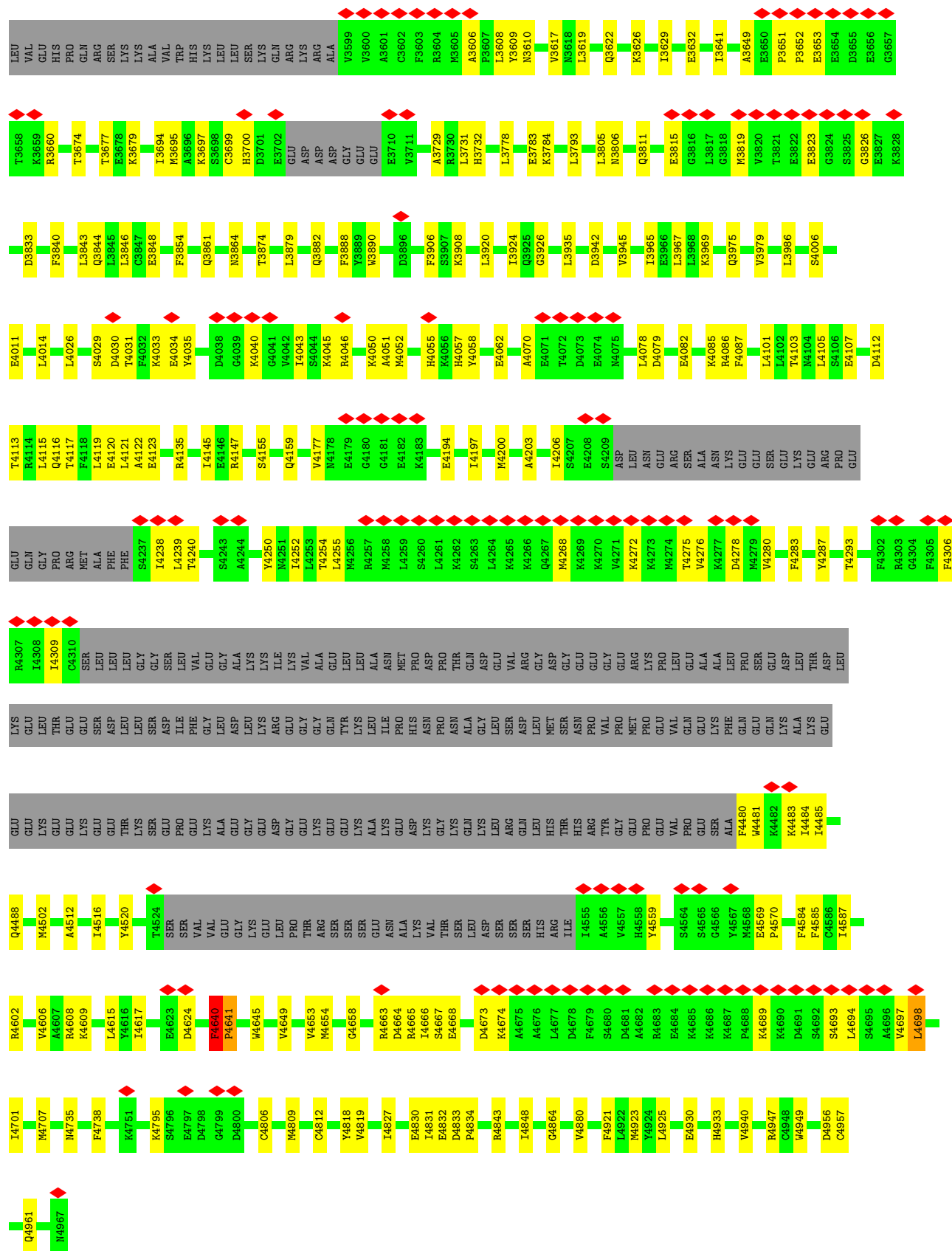
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

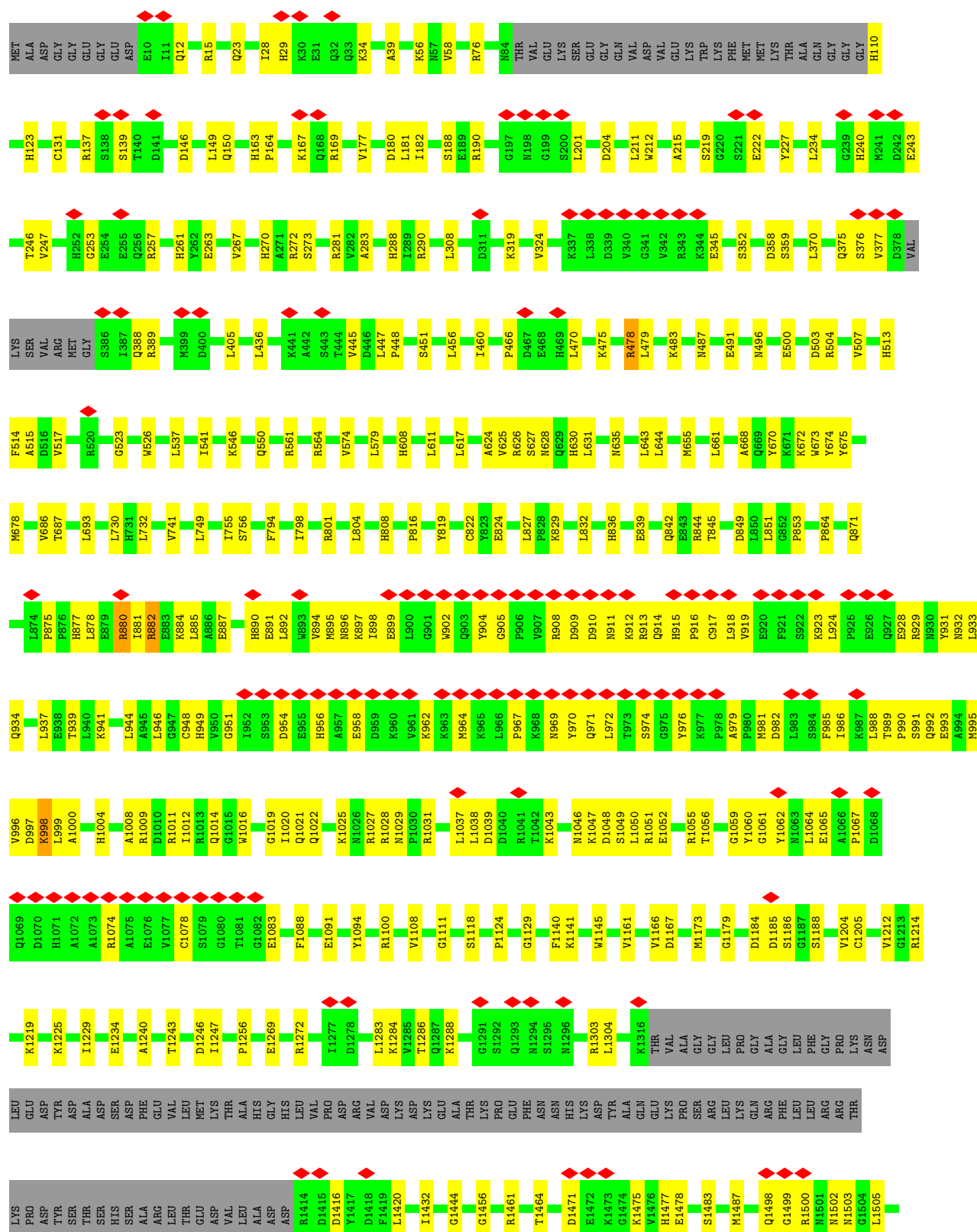
• Molecule 1: Ryanodine receptor 2











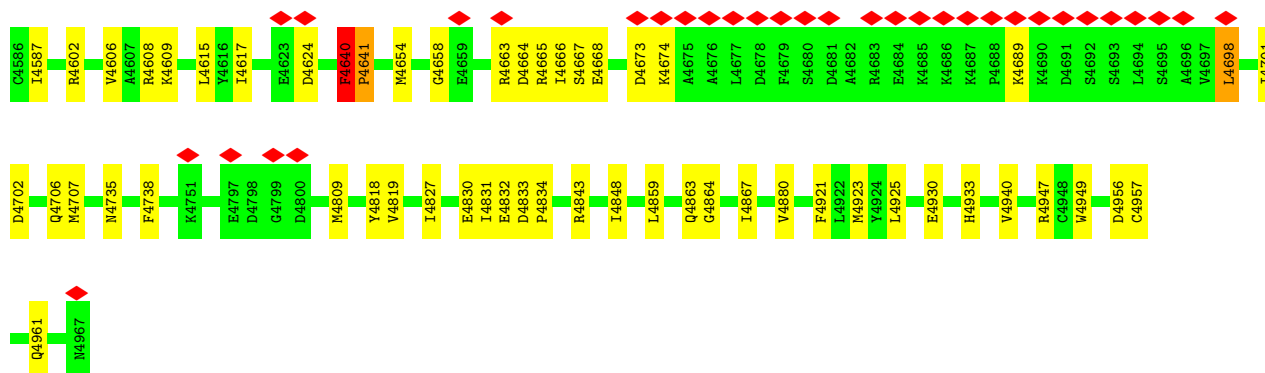


D4038	L3843	T3677	HIS	LEU	ARG	MET	ASP	T3275	P3209	S3145	Q3077	S3006	G2946
G4039	Q3844	E3678	PRO	GLU	TYR	VAL	HIS	L3276	S3210	I3146	G3078	L3007	S2947
K4040	L3845	K3679	GLN	ASP	SER	ALA	LEU	L3277	E3211	V3147	Q3079	K3010	R2948
G4041	L3846	L3846	SER	PRO	GLN	VAL	GLY	K3282	K3213	V3148	F3080	L3011	G2949
V4042	G3847	M3695	LYS	ALA	THR	PHE	ALA	L3283	L3214	R3150	HIS	L3014	K2950
L4043	E3848	A3696	ILE	ILE	SER	ILE	ALA	L3284	M3215	Q3151	THR	V3015	G2951
S4044	F3854	S3698	VAL	TRP	ILE	TRP	GLY	Y3285	E3216	R3152	ARG	R3016	E2952
K4045	S3699	S3699	GLN	GLN	VAL	TRP	ASP	N3286	I3218	S3153	ASN	H3017	H2953
R4046	T3874	H3700	HIS	MET	ALA	LYS	MET	K3287	L3221	A3154	GLN	R3018	F2954
K4050	L3879	D3701	LEU	LEU	ALA	LYS	SER	L3288	L3221	L3155	PRO	I3019	F2955
A4051	Q3882	E3702	LEU	TYR	LYS	ASN	ALA	G3289	S3224	G3156	K3088	S3020	V2956
N4052	F3888	GLU	SER	LYS	ARG	PHE	GLU	G3290	G3225	C3158	G3089	D3025	E2957
H4055	F3888	ASP	LYS	ASP	LEU	VAL	GLU	D3291	I3226	L3159	V3090	A3026	Q2958
Y4058	Y3889	ASP	ARG	PRO	LEU	GLU	ILE	G3292	R3227	A3160	T3091	I3029	I2960
E4062	K3890	GLY	LYS	ASN	ILE	GLU	LEU	A3294	T3228	F3162	Q3092	V3030	K2961
T4063	D3896	GLU	ARG	ARG	GLY	GLN	ASP	K3296	Q3230	A3163	I3093	I3094	F2962
L4067	E3710	E3710	ALA	THR	LEU	ASN	GLU	K3297	H3233	G3164	M3095	L3033	F2963
A4070	V3600	V3711	ASP	ASP	ASN	PHE	PHE	R3298	V3234	A3165	Y3096	H3034	K2964
E4071	A3601	Q3728	THR	THR	ILE	VAL	THR	A3300	K3235	F3166	T3097	L3036	K2965
T4072	C3602	R3729	ASP	SER	CYS	VAL	THR	V3301	E3236	P3167	L3101	L3037	V2966
D4073	F3603	R3730	PRO	ASP	ALA	GLN	LEU	F3302	V3237	V3168	L3102	Q3038	L2967
F4074	R3604	L3731	GLY	GLY	GLN	ASN	ASP	Q3303	I3238	A3169	P3103	T3039	L2968
N4075	M3605	H3732	THR	THR	GLU	ASN	LEU	Q3304	P3240	F3170	M3104	L3040	P2969
L4078	A3606	T3785	VAL	VAL	LEU	MET	ALA	F3305	M3241	E3172	L3108	D3041	I2970
D4079	P3607	L3778	GLU	GLU	ILE	SER	PHE	K3308	Y3245	T3173	F3109	A3042	I2971
E4082	L3608	K3784	ARG	ARG	ALA	PHE	TYR	K3309	M3246	H3174	E3110	R3043	Q2972
K4085	V3609	E3783	VAL	VAL	LEU	LEU	PRO	L3314	R3247	L3175	H3111	T3044	F2975
F4087	M3610	K3784	LEU	LEU	ALA	ILE	LEU	F3312	S3248	K3176	G3113	M3046	R2976
L4101	L3619	L3805	ASP	ASP	ASN	THR	ASP	Q3313	V3249	K3177	Q3114	K3047	H2978
T4102	Q3622	N3806	ALA	ALA	ARG	THR	THR	E3251	H3252	I3180	F3117	G3049	I2979
R4103	K3626	Q3811	VAL	VAL	PHE	LYS	PHE	E3252	H3252	T3183	G3118	L3050	L2980
L4105	I3629	E3815	LEU	LEU	LEU	LYS	ASP	E3255	E3255	Y3184	E3119	E3051	F2981
S4106	E3632	G3816	HIS	HIS	THR	ASP	ASN	N3256	N3257	N3185	D3120	V3052	L2982
E4107	I3641	L3817	GLU	GLU	THR	GLU	ARG	P3258	P3258	K3186	L3121	K3054	L2983
D4112	A3649	M3819	LEU	LEU	GLU	ALA	ALA	E3259	E3259	S3188	I3122	L3057	A2984
T4113	E3650	V3820	ARG	ARG	ASP	VAL	TRP	R3260	R3260	S3189	L3123	R3068	A2985
R4114	P3651	T3821	GLY	GLY	ILE	GLU	GLY	A3261	A3261	R3190	E3124	L3061	A2986
L4115	P3652	E3822	VAL	VAL	ASP	ASP	PRO	E3262	E3262	E3191	D3125	D3062	S2987
Q4116	E3653	E3823	ARG	ARG	ASP	GLN	ASN	K3263	C3264	R3192	V3126	N3063	R2988
T4117	E3654	G3824	ARG	ARG	SER	LYS	PRO	C3265	C3265	A3193	Q3127	L3066	L2990
F4118	S3825	S3826	THR	THR	ASN	LYS	GLU	T3266	T3266	A3194	Y3131	E3066	C2991
K4033	G3827	E3827	HIS	GLY	ILE	LYS	ALA	A3267	A3267	L3196	R3132	D3067	S2992
E4034	E3656	K3828	LEU	LEU	ARG	GLU	GLU	L3268	L3268	P3197	R3133	L3068	G2993
A4122	T3658	D3833	GLN	GLN	GLY	LEU	PHE	S3270	S3270	T3199	L3134	E3069	G2994
E4123	K3659	F3840	ASP	ASP	GLY	LEU	ARG	K3271	K3271	N3200	T3135	K3070	A2996
	R3660							H3272	H3272	V3201	L3137	T3071	S2997
	T3674							E3336	E3336	E3202	L3140	E3073	K2999
								E3337	E3337	D3203	G3141	N3074	E3000
										V3204	T3142	T3002	K3001
										T3208	S3143	Y3004	K3002
											K3144		T3005

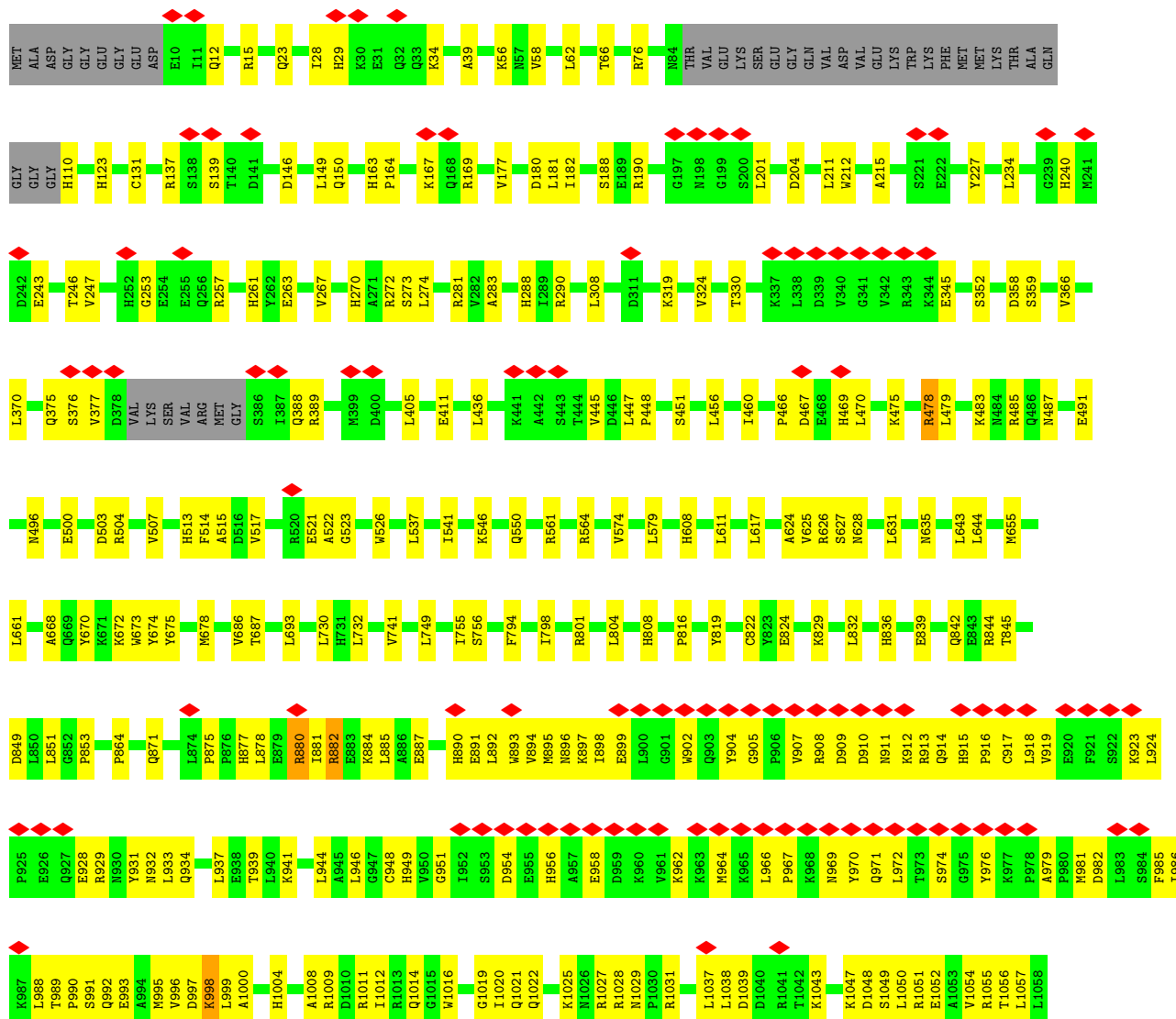


T3266	L3134	E3066	A2996	V2933	E2861	R2791	K2723	L2644	D3397	K2283
A3267	T3135	D3067	S2997	V2937	S2862	T2792	A2724	F2645	R2401	G2284
L3268	L3136	E3068	N2998	H2937	K2863	T2793	E2726	K2655	C2402	Y2285
N3269	N3200	K3070	E3000	Y2938	C2864	E2794	S2727	K2656	A2403	E2296
E3270	E3201	K3071	E3002	Y2939	G2865	D2795	H2728	Y2657	E2297	Y2298
E3271	E3202	M3072	E3003	F2943	G2866	D2796	D2729	E2658	I2409	
H3272	D3203	E3073	M3004	D2944	N2867	S2797	D2730	K2557	R2420	R2303
H3273	V3204	M3074	S3005	G2945	H2868	W2798	K2731	R2557	R2421	
S3274	S3143	E3075	L3007	G2946	P2869	A2799		R2566	D2431	V2319
S3275	S3144	Q3077	K3010	S2947	L2870	N2802	W2732	I2569	G2434	L2323
L3276	S3145	G3078	L3011	R2948	L2871	ARG	K2663	E2570	V2435	
L3277	V3147	Q3079	L3012	G2949	P2872	THR	L2664	I2571	F2440	R2327
L3281	V3148	F3080	L3013	G2949	P2873	ARG	K2665	E2572	M2442	P2328
K3282	E3149	T3081	L3014	G2949	P2874	ARG	L2666	E2573	P2443	E2329
L3283	R3150	HIS	L3015	K2950	D2875	ILE	L2667	I2576	F2444	G2332
L3284	Q3151	THR	L3016	G2951	D2876	ASP	S2670	L2580	M2445	P2333
Y3285	R3152	ARG	R3017	E2952	T2876	GLN	P2677	R2581	I2446	G2337
K3286	S3153	ASN	H3018	H2953	L2877	THR	Y2680	P2582	K2447	G2336
K3287	L3154	GLN	R3019	F2954	E2881	SER	Y2681	S2583	D2448	G2337
L3288	L3155	PRO	S3020	F2955	K2884	VAL	G2744	M2584		G2338
G3289	G3156	K3088	D3025	Y2956	D2885	SER	E2745	L2589	D2455	L2344
I3290	E3157	G3089	A3026	E2957	E2886	VAL	I2746	R2590	M2456	
G3295	G3158	V3090	A3026	Q2958	E2887	ASP	Y2747	R2591	S2457	M2347
I3296	L3159	T3091	A3026	E2959	E2887	ALA	S2748	L2592	K2485	E2348
E3297	A3160	Q3092	I3029	I2960	E2887	ALA	D2749	V2593		
E3298	F3162	I3093	V3030	K2961	E2887	HIS	S2750	M2605		
E3299	A3163	I3094	L3033	F2962	Q2890	Q2820	K2691	P2606		
E3300	G3164	I3095	H3034	F2963	D2891	Y2821	Q2692	M2607		
E3301	A3165	Y3096	H3034	A2964	L2892	S2822	K2692	L2610		
E3302	F3166	T3097	L3035	K2965	L2893	S2823	S2693	N2612		
E3303	P3167	L3101	L3036	Y2966	K2894	E2824	S2694	H2613		
E3304	V3168	Q3038	Q3037	L2967	L2896	R2824	M2695	Y2614		
E3305	A3169	T3039	Q3038	L2968	Q2897	A2825	D2696	Y2621		
E3306	F3170	M3104	L3040	P2969	L2898	R2826	C2622	C2626		
E3307	L3171	L3108	D3041	L2971	N2899	D2827	W2701	W2627		
E3308	E3172	F3109	A3042	D2972	A2902	M2828	Q2704	G2628		
E3309	T3173	G3110	R3043	Y2974	C2906	S2697	L2496	N2629		
E3310	H3111	E3110	T3044	F2975	F2907	E2698	R2497	P2630		
E3311	I3112	H3111	V3045	K2976	K2908	E2699	A2498	E2635		
E3312	G3113	I3112	M3046	N2977	D2909	G2699	M2512	E2636		
E3313	Q3114	Q3114	K3047	H2978	D2909	T2700	L2526	E2637		
E3314	G3115	G3115	T3048	L2980	L2910	N2701	L2638	L2639		
E3315	I3180	F3117	G3049	Y2981	E2911	F2701	H2640	S2641		
E3316	I3183	G3118	L3050	F2982	E2912	Q2704	L2642	Q2643		
E3317	Y3184	E3119	E3051	L2983	D2913	D2707	E2635			
E3318	N3185	S3052	V3053	S2984	T2914	T2708	E2636			
E3319	T3186	L3120	K3054	A2985	P2915	S2709	E2637			
E3320	K3187	L3121	A2986	A2986	P2916	W2772	L2638			
E3321	S3188	I3122	L3057	S2987	I2917	W2773	H2639			
E3322	S3189	L3123	R3058	S2987	E2918	L2711	L2640			
E3323	R3190	E3124	L3061	R2988	K2919	L2712	S2641			
E3324	K3191	D3125	D3062	P2989	R2920	L2713	E2642			
E3325	R3192	V3126	N3063	L2990	P2921	E2714	R2643			
E3326	A3193	Q3127		C2991	Y2923	K2715				
E3327	A3194	Y3131		G2993	L2929	E2716				
E3328	L3195	I3133		G2994	I2930	L2717				
E3329	S3196			H2995		E2718				
						Y2719				
						F2720				



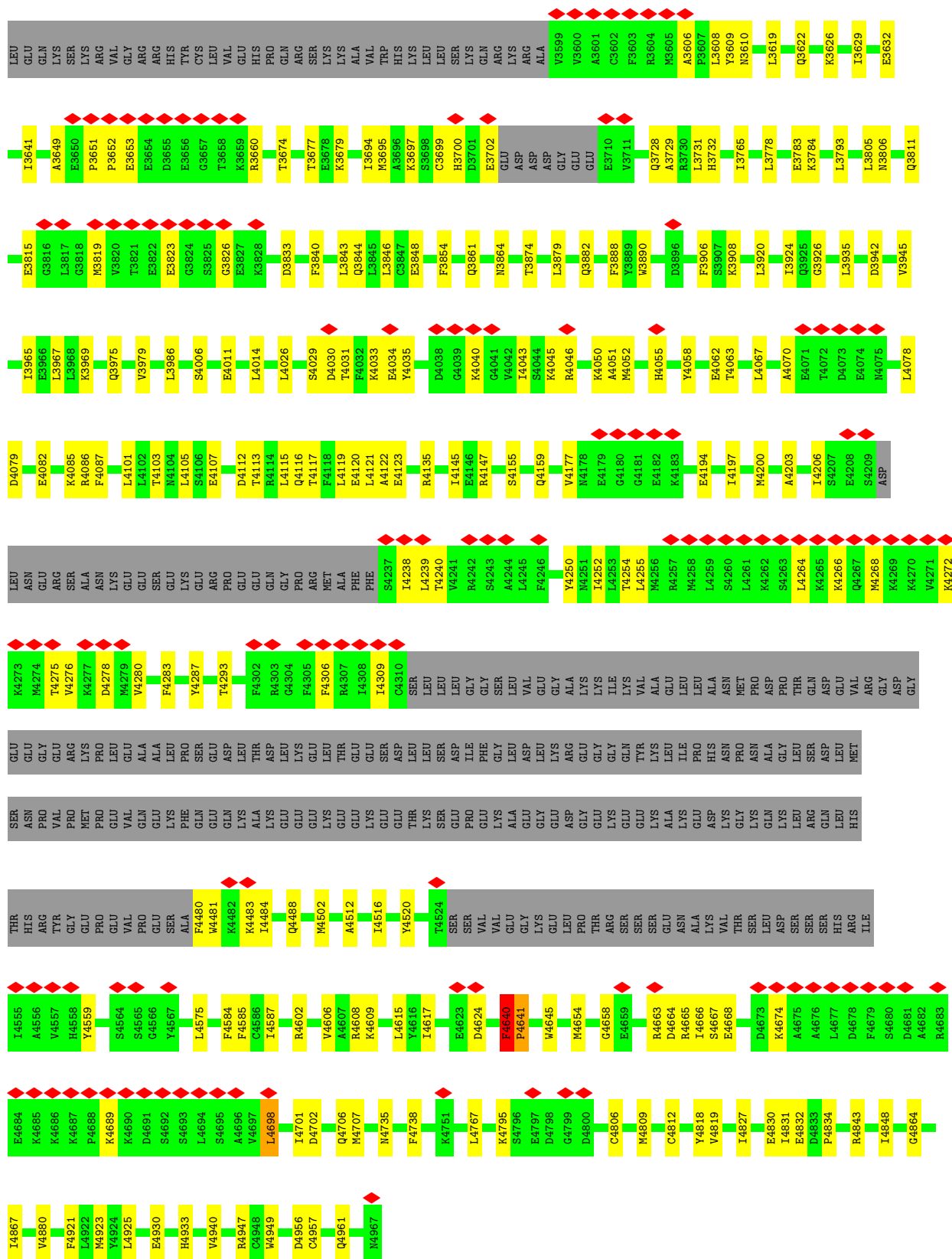


• Molecule 1: Ryanodine receptor 2

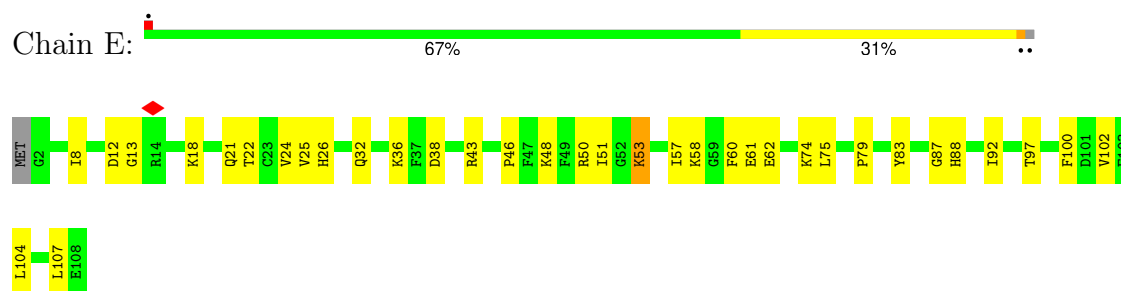




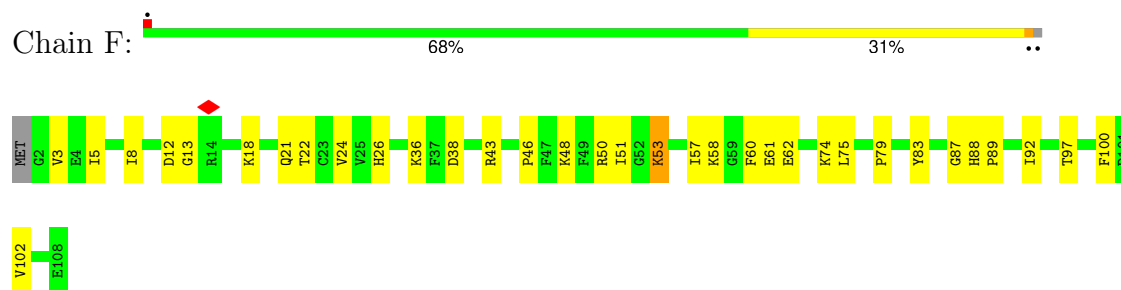




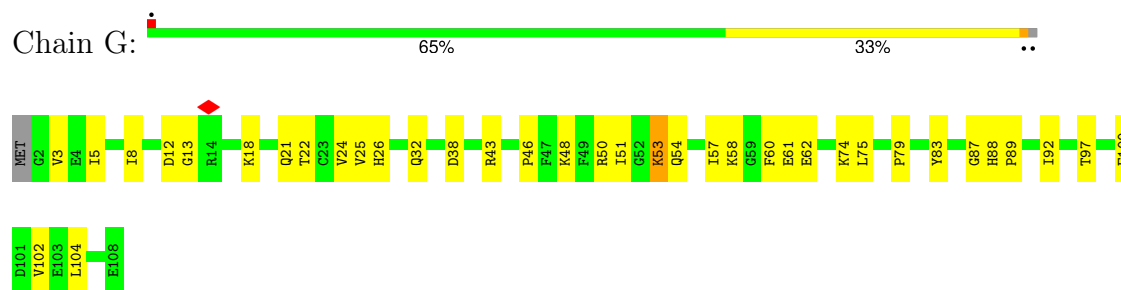
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



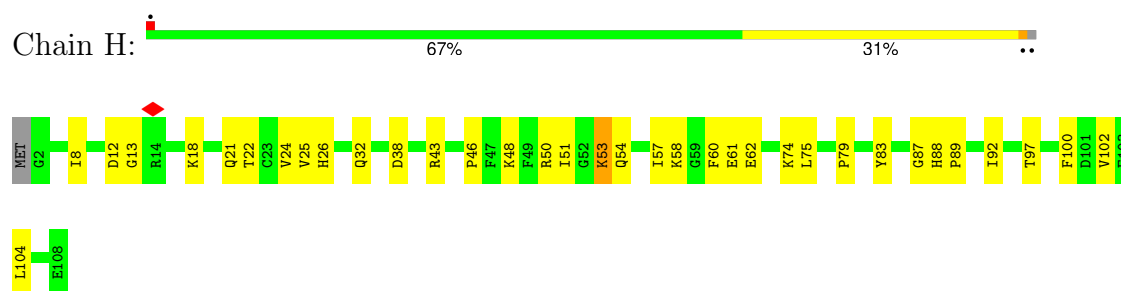
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	83460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.550	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, KVR, 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	0.27	0/34511	0.51	9/46614 (0.0%)
1	B	0.27	0/34511	0.51	9/46614 (0.0%)
1	C	0.27	0/34511	0.51	9/46614 (0.0%)
1	D	0.27	0/34511	0.51	9/46614 (0.0%)
2	E	0.29	0/834	0.53	0/1123
2	F	0.29	0/834	0.53	0/1123
2	G	0.29	0/834	0.53	0/1123
2	H	0.29	0/834	0.53	0/1123
All	All	0.27	0/141380	0.51	36/190948 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3277	LEU	CA-CB-CG	8.45	134.73	115.30
1	A	3277	LEU	CA-CB-CG	8.43	134.69	115.30
1	C	3277	LEU	CA-CB-CG	8.42	134.67	115.30
1	B	3277	LEU	CA-CB-CG	8.42	134.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2640	LEU	CB-CG-CD2	-7.00	99.11	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3192	ARG	Sidechain
1	A	3926	GLY	Peptide
1	A	4640	PHE	Peptide
1	B	3192	ARG	Sidechain
1	B	3926	GLY	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	33771	0	33455	796	0
1	B	33771	0	33455	790	0
1	C	33771	0	33455	799	0
1	D	33771	0	33455	809	0
2	E	818	0	821	24	0
2	F	818	0	821	23	0
2	G	818	0	821	25	0
2	H	818	0	821	26	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	9	0
4	B	62	0	24	9	0
4	C	62	0	24	9	0
4	D	62	0	24	10	0
5	A	23	0	0	7	0
5	B	23	0	0	7	0
5	C	23	0	0	7	0
5	D	23	0	0	7	0
All	All	138700	0	137200	3276	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 12.

The worst 5 of 3276 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3227:ARG:HE	1:C:3228:TYR:H	1.13	0.92
1:B:4834:PRO:HB3	1:B:4843:ARG:HD3	1.51	0.92
1:D:4834:PRO:HB3	1:D:4843:ARG:HD3	1.51	0.92
1:A:3227:ARG:HE	1:A:3228:TYR:H	1.13	0.91
1:A:4834:PRO:HB3	1:A:4843:ARG:HD3	1.51	0.91

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	4198/4967 (84%)	4073 (97%)	123 (3%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4075 (97%)	121 (3%)	2 (0%)	100	100
1	C	4198/4967 (84%)	4073 (97%)	123 (3%)	2 (0%)	100	100
1	D	4198/4967 (84%)	4075 (97%)	121 (3%)	2 (0%)	100	100
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17212/20300 (85%)	16700 (97%)	504 (3%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4641	PRO

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Mol	Chain	Res	Type
1	B	4641	PRO
1	C	4641	PRO
1	D	4641	PRO
1	A	2770	ILE

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	3708/4358 (85%)	3687 (99%)	21 (1%)	84	92
1	B	3708/4358 (85%)	3687 (99%)	21 (1%)	84	92
1	C	3708/4358 (85%)	3687 (99%)	21 (1%)	84	92
1	D	3708/4358 (85%)	3687 (99%)	21 (1%)	84	92
2	E	88/89 (99%)	87 (99%)	1 (1%)	70	84
2	F	88/89 (99%)	87 (99%)	1 (1%)	70	84
2	G	88/89 (99%)	87 (99%)	1 (1%)	70	84
2	H	88/89 (99%)	87 (99%)	1 (1%)	70	84
All	All	15184/17788 (85%)	15096 (99%)	88 (1%)	82	92

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2950	LYS
1	D	998	LYS
1	C	3140	LEU
1	C	4698	LEU
1	D	2303	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	650	ASN

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Mol	Chain	Res	Type
1	D	4933	HIS
1	D	1593	HIS
1	D	3111	HIS
1	B	2802	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
5	KVR	B	5004	-	24,25,25	1.43	3 (12%)	31,34,34	1.71	4 (12%)
4	ATP	D	5003	-	28,33,33	0.63	0	34,52,52	0.62	1 (2%)
4	ATP	B	5002	-	28,33,33	0.65	0	34,52,52	0.61	1 (2%)
5	KVR	A	5004	-	24,25,25	1.44	3 (12%)	31,34,34	1.71	4 (12%)
5	KVR	C	5004	-	24,25,25	1.44	3 (12%)	31,34,34	1.71	4 (12%)
4	ATP	C	5002	-	28,33,33	0.65	0	34,52,52	0.61	1 (2%)
4	ATP	A	5003	-	28,33,33	0.63	0	34,52,52	0.62	1 (2%)
4	ATP	D	5002	-	28,33,33	0.64	0	34,52,52	0.62	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	KVR	D	5004	-	24,25,25	1.44	3 (12%)	31,34,34	1.71	3 (9%)
4	ATP	C	5003	-	28,33,33	0.63	0	34,52,52	0.62	1 (2%)
4	ATP	B	5003	-	28,33,33	0.62	0	34,52,52	0.62	1 (2%)
4	ATP	A	5002	-	28,33,33	0.65	0	34,52,52	0.61	1 (2%)

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
5	KVR	B	5004	-	-	8/10/20/20	0/2/3/3
4	ATP	D	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	3/18/38/38	0/3/3/3
5	KVR	A	5004	-	-	8/10/20/20	0/2/3/3
5	KVR	C	5004	-	-	8/10/20/20	0/2/3/3
4	ATP	C	5002	-	-	3/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	3/18/38/38	0/3/3/3
5	KVR	D	5004	-	-	8/10/20/20	0/2/3/3
4	ATP	C	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	3/18/38/38	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)
5	C	5004	KVR	C06-S09	4.90	1.82	1.77
5	D	5004	KVR	C06-S09	4.90	1.82	1.77
5	A	5004	KVR	C06-S09	4.88	1.82	1.77
5	B	5004	KVR	C06-S09	4.86	1.82	1.77
5	A	5004	KVR	C13-C05	2.61	1.55	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5004	KVR	C10-S09-C06	7.29	113.03	102.71
5	A	5004	KVR	C10-S09-C06	7.27	113.02	102.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5004	KVR	C10-S09-C06	7.27	113.00	102.71
5	B	5004	KVR	C10-S09-C06	7.25	112.99	102.71
5	C	5004	KVR	C15-C14-N12	-2.91	107.20	113.15

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

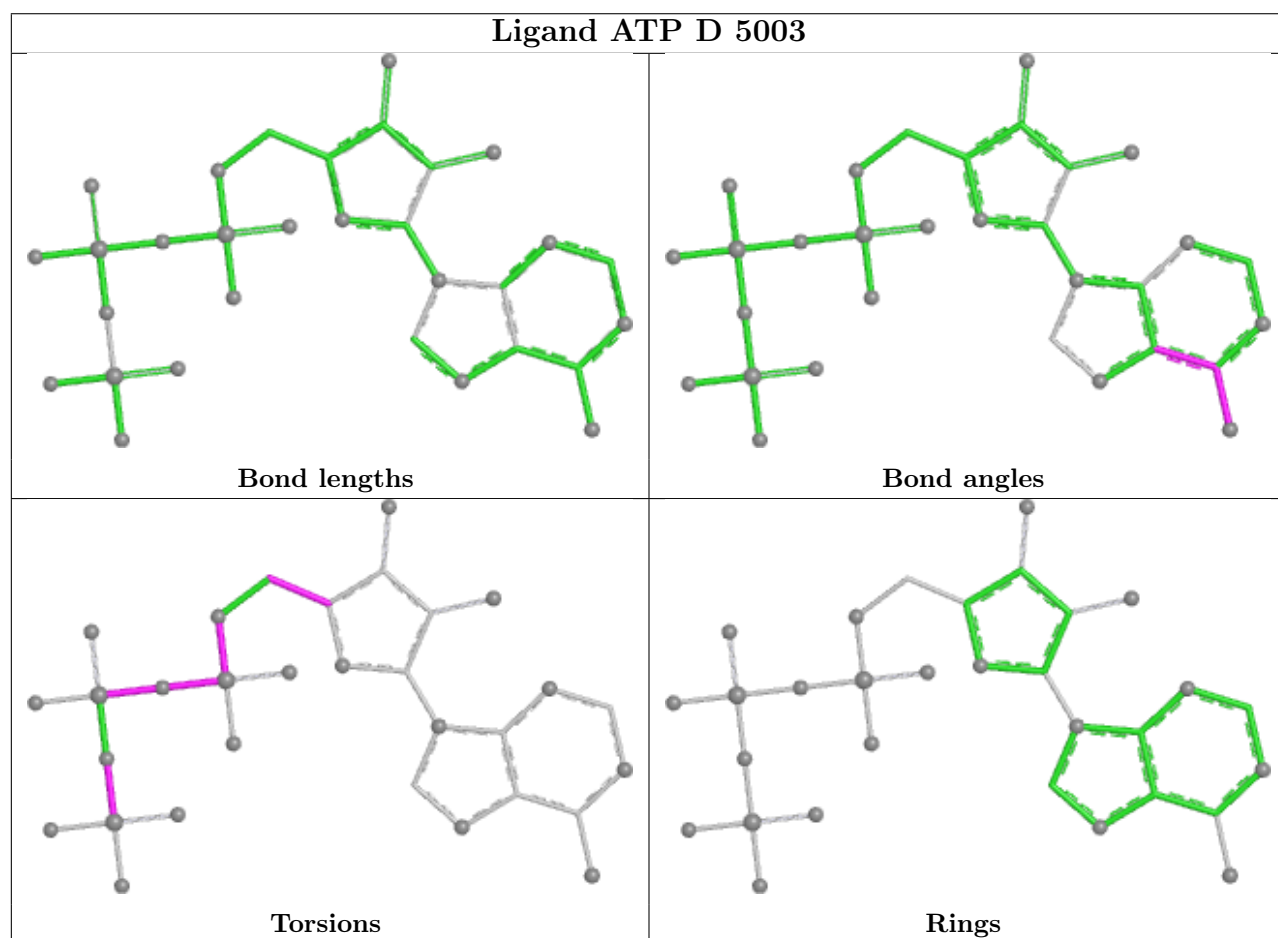
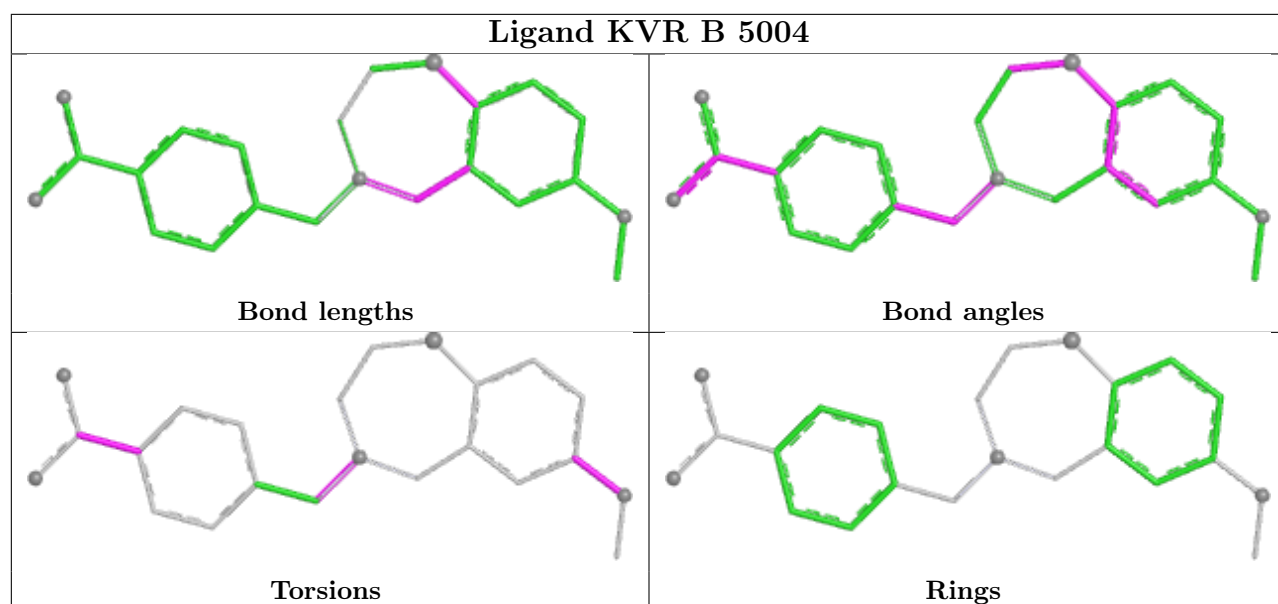
Mol	Chain	Res	Type	Atoms
4	A	5003	ATP	PB-O3B-PG-O2G
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	B	5003	ATP	PB-O3B-PG-O2G

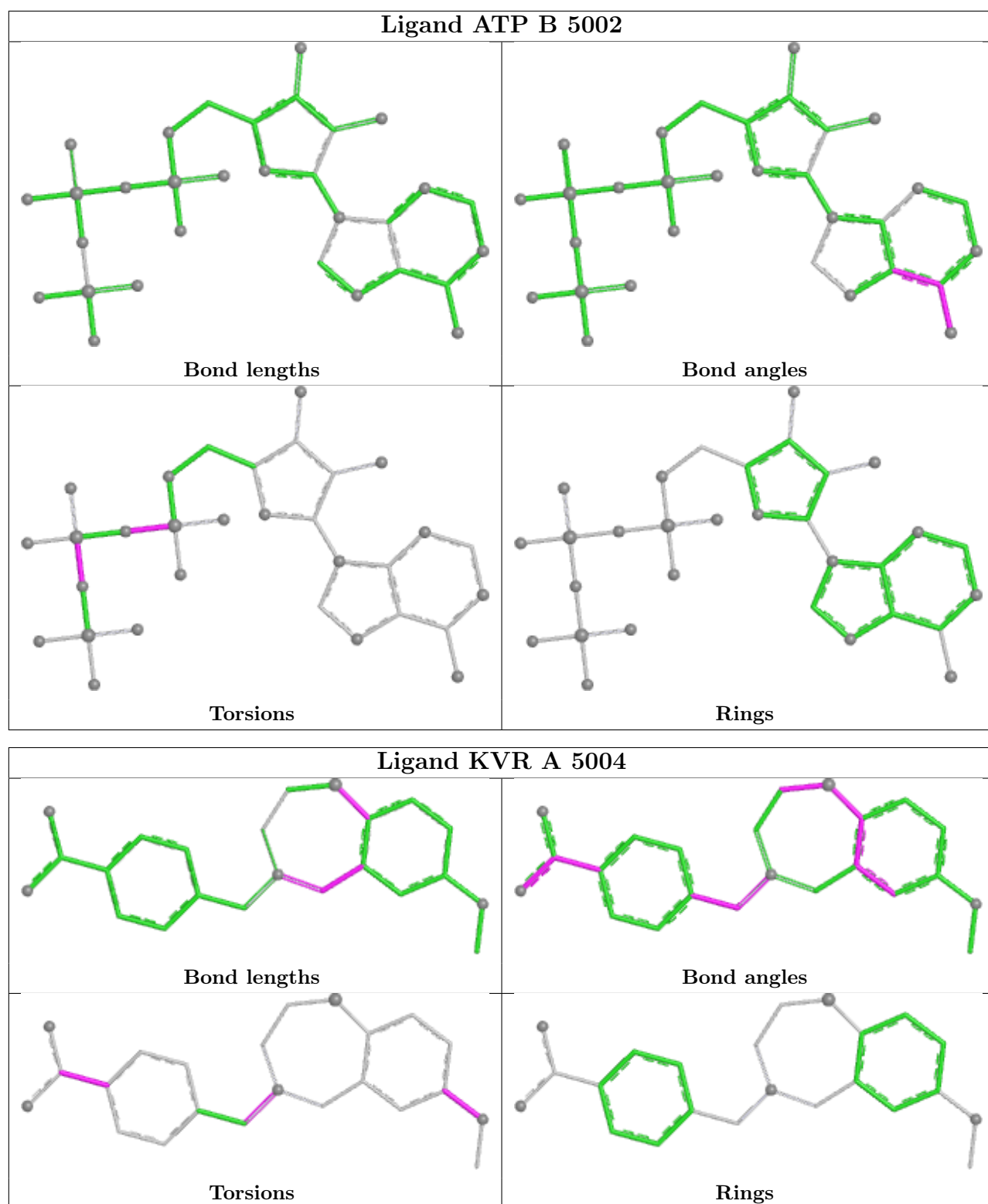
There are no ring outliers.

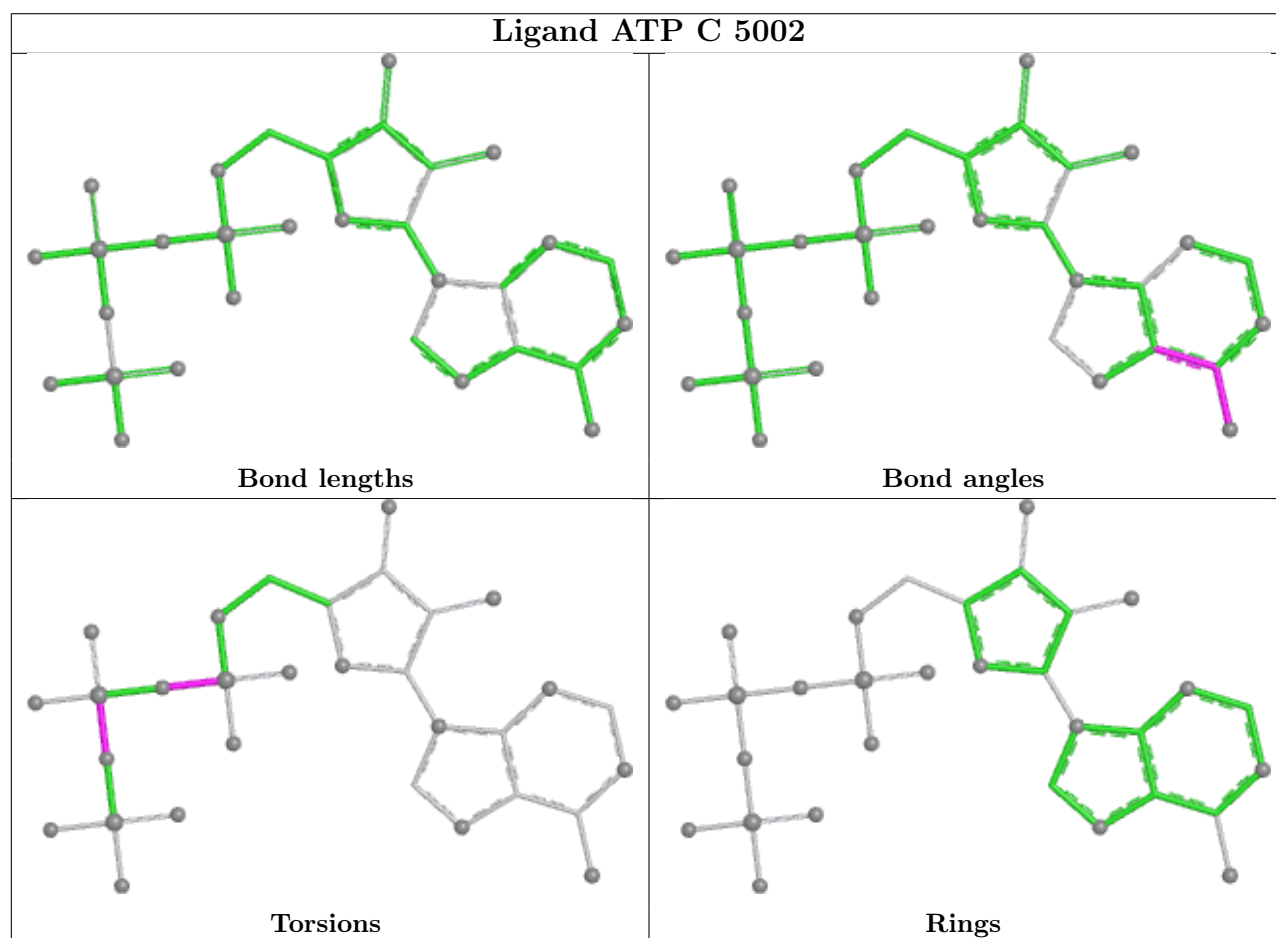
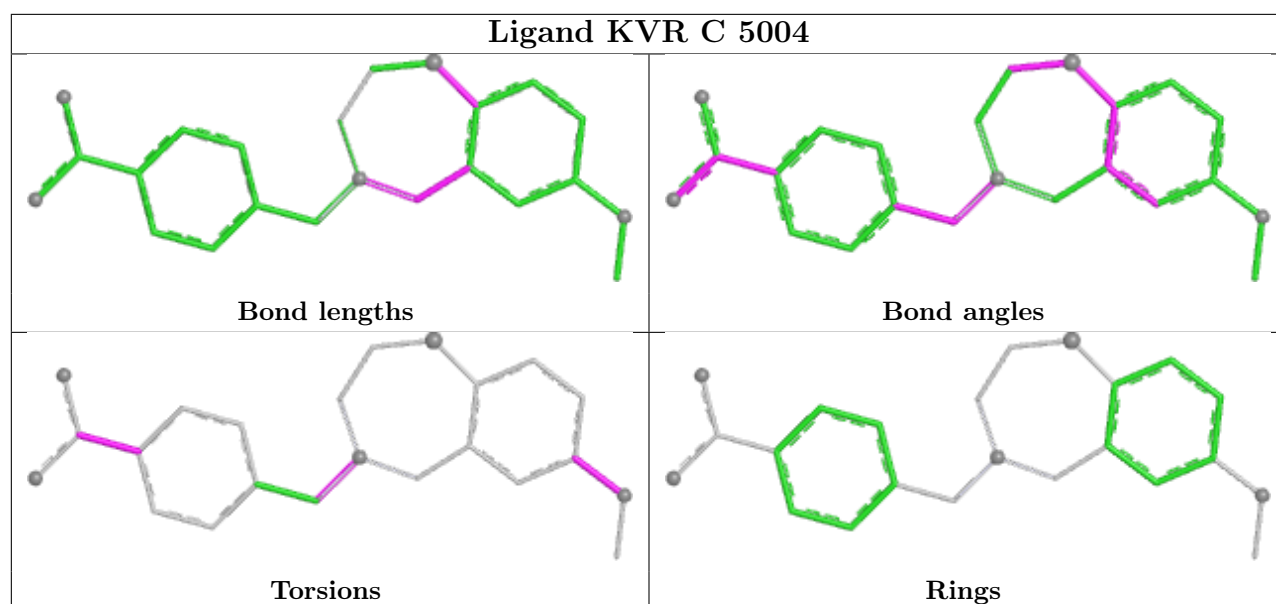
8 monomers are involved in 41 short contacts:

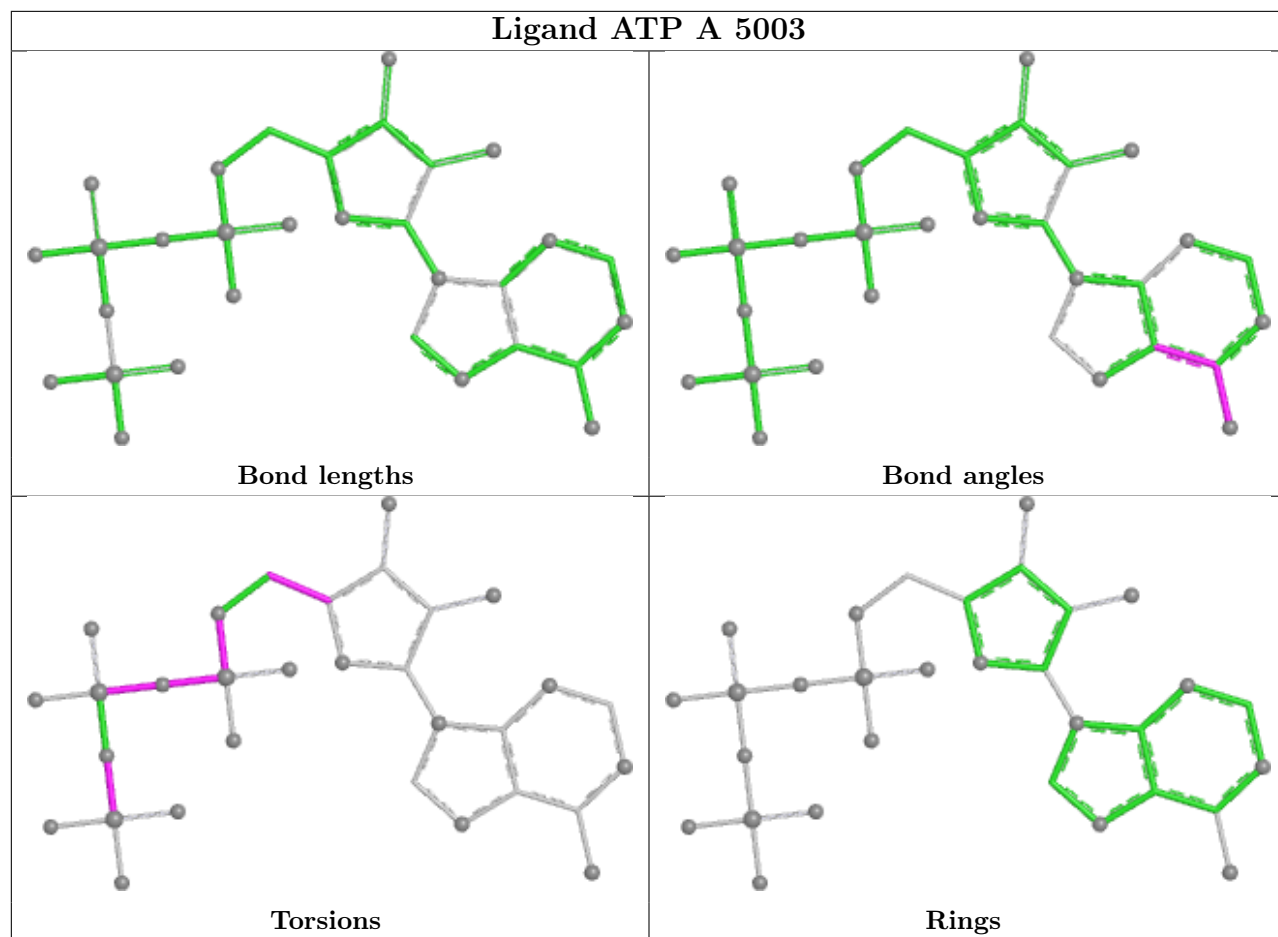
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5004	KVR	7	0
4	D	5003	ATP	10	0
5	A	5004	KVR	7	0
5	C	5004	KVR	7	0
4	A	5003	ATP	9	0
5	D	5004	KVR	7	0
4	C	5003	ATP	9	0
4	B	5003	ATP	9	0

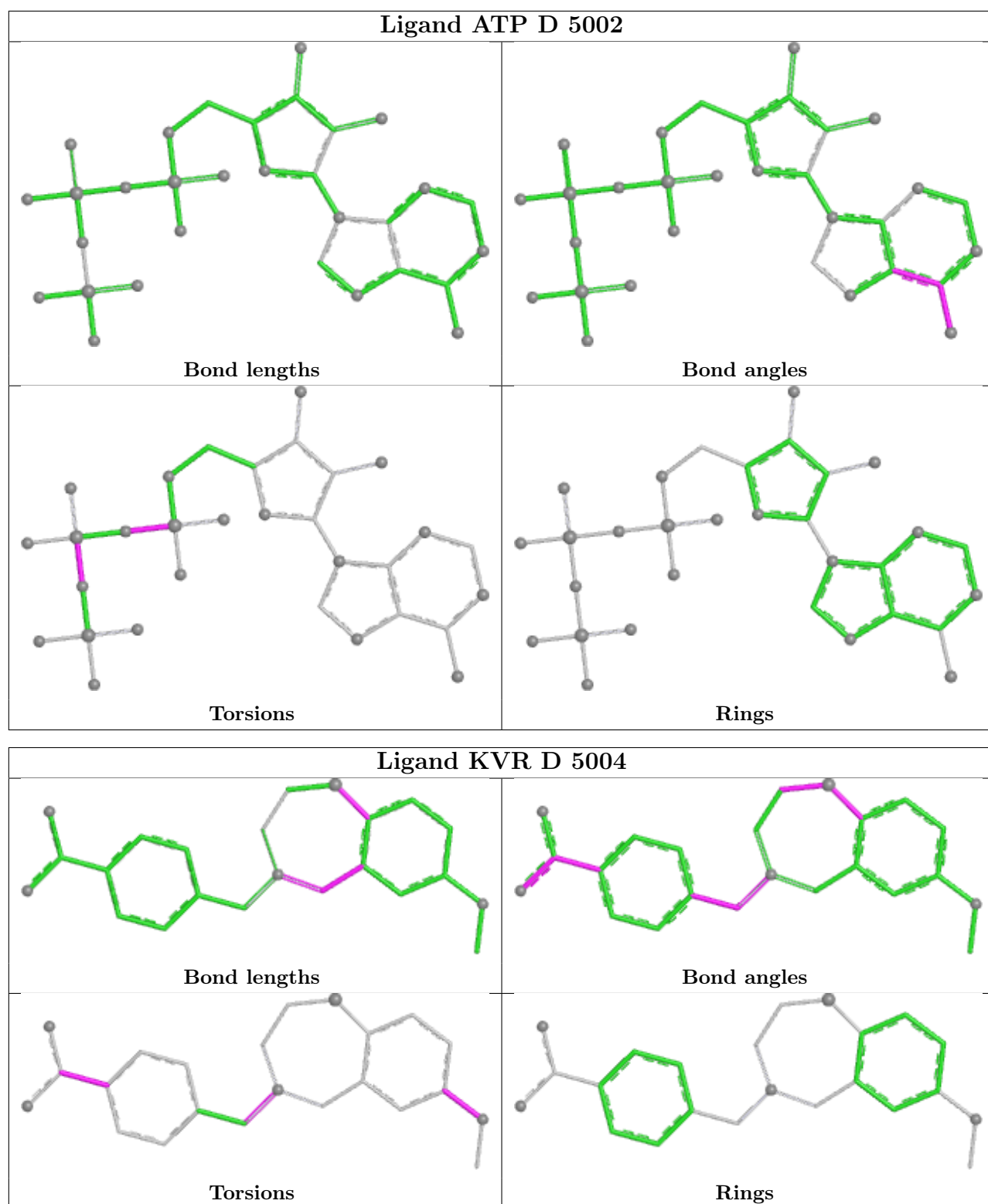
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

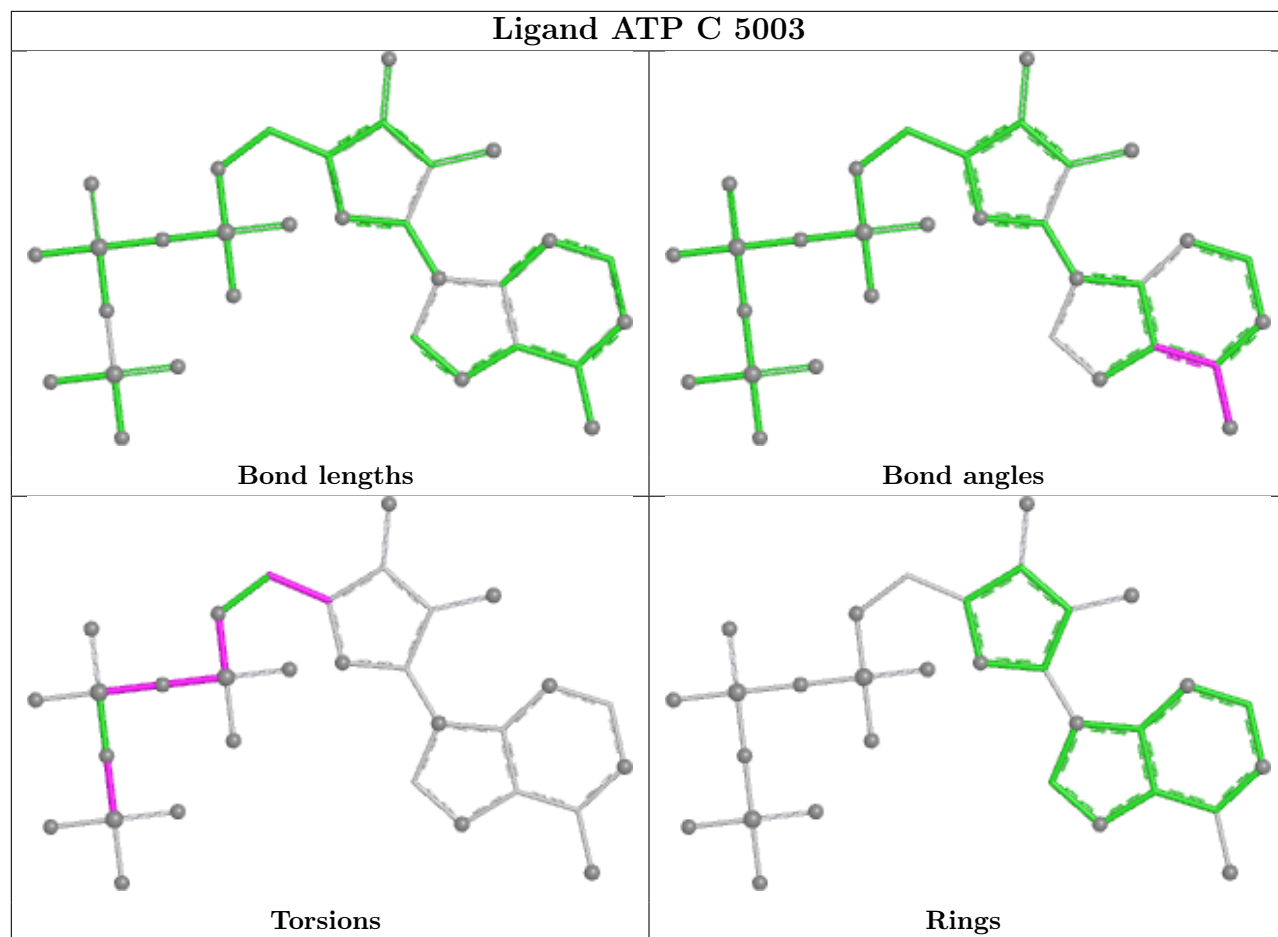


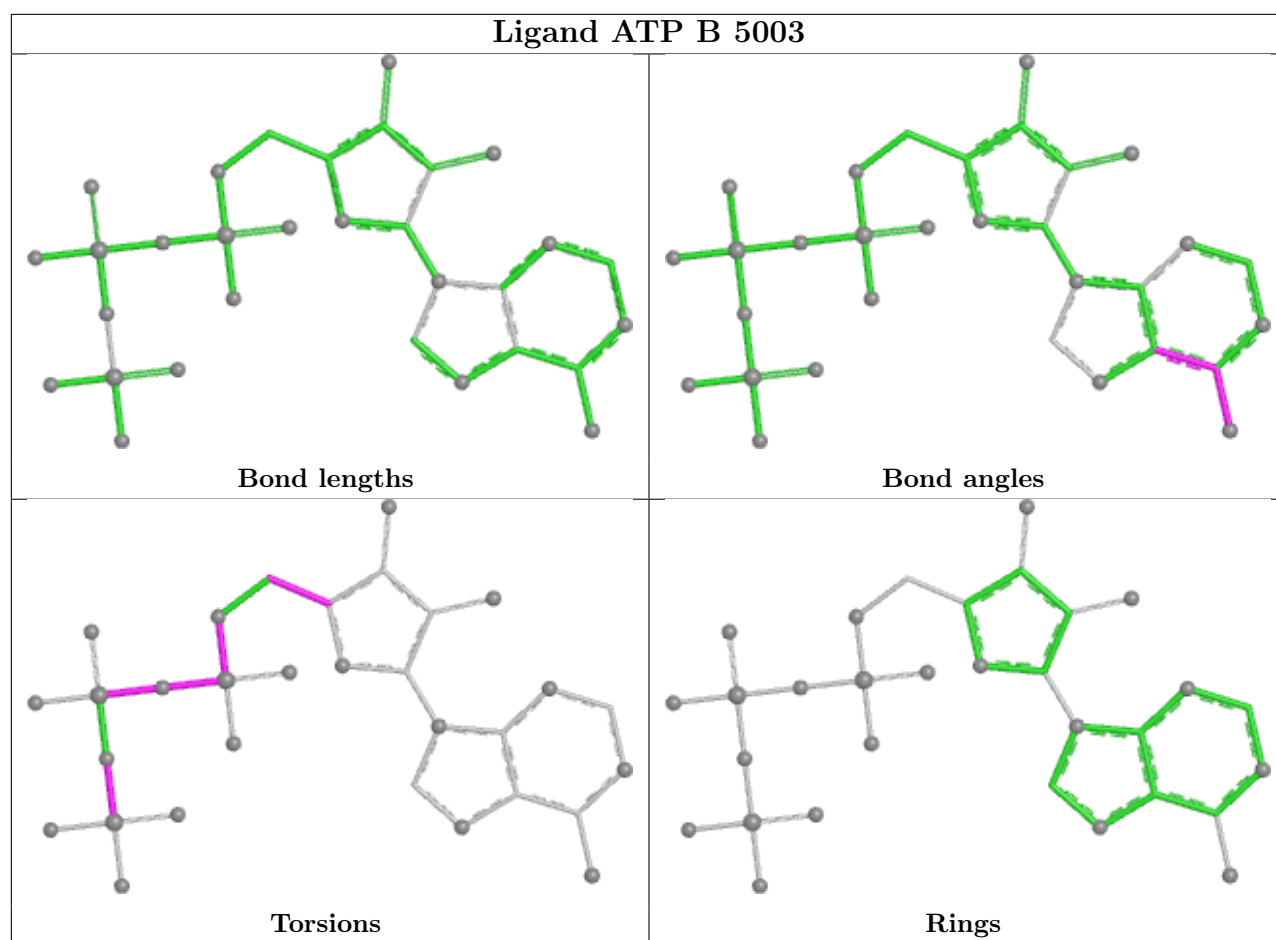


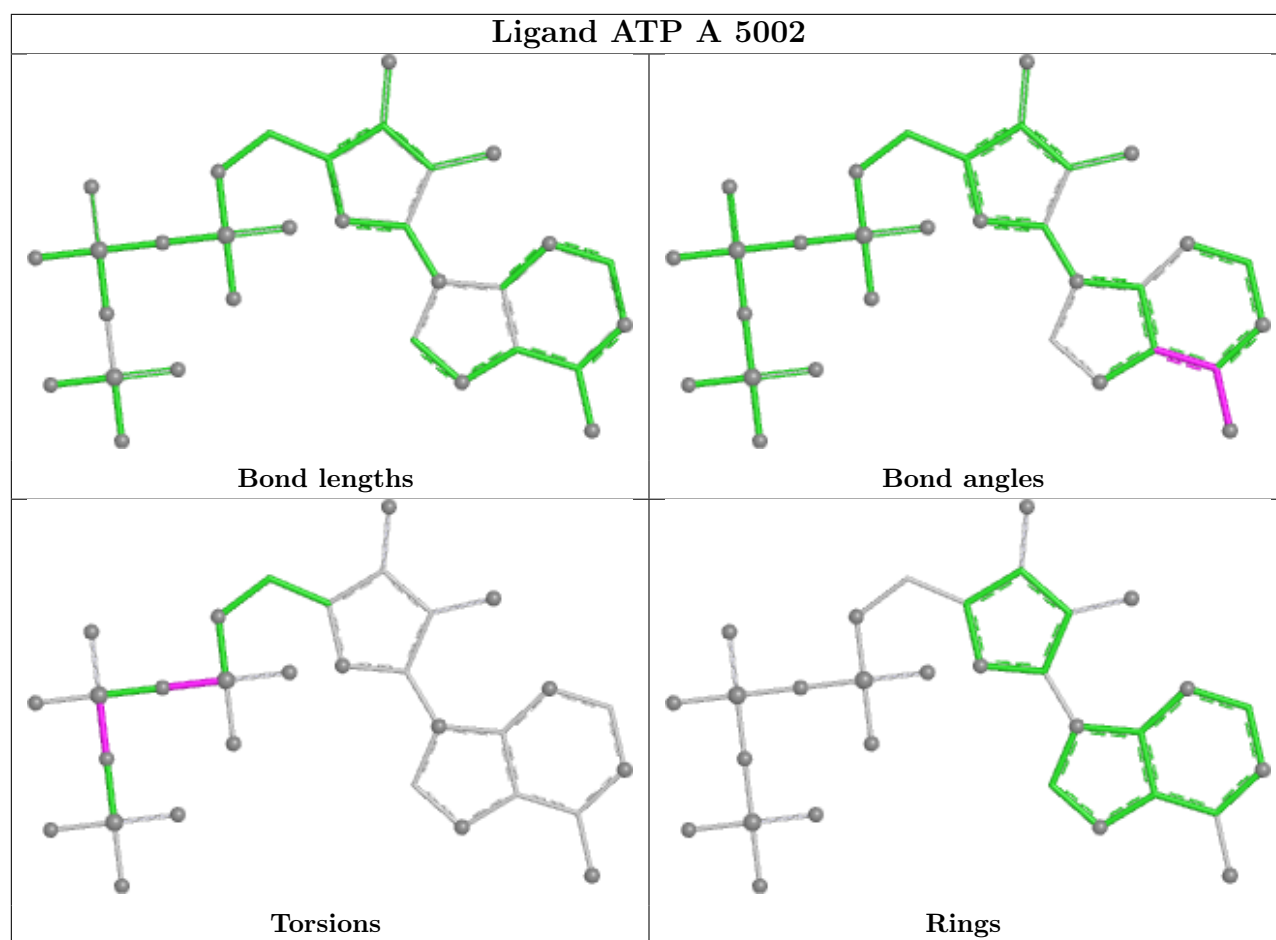












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

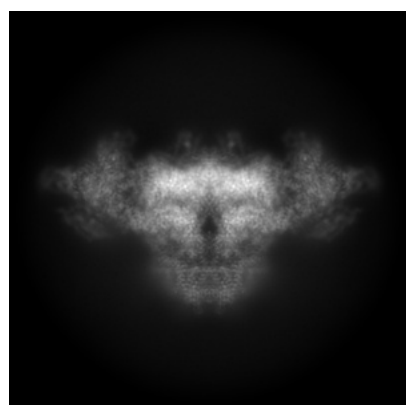
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42459. These allow visual inspection of the internal detail of the map and identification of artifacts.

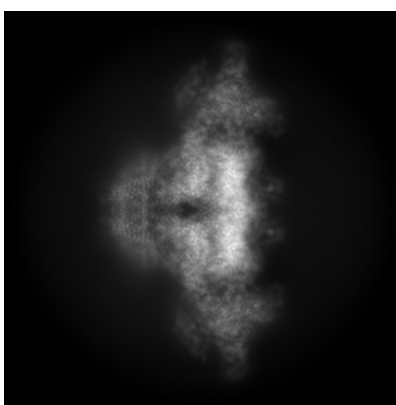
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

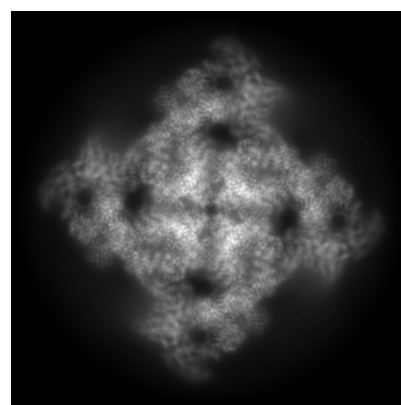
6.1.1 Primary map



X



Y

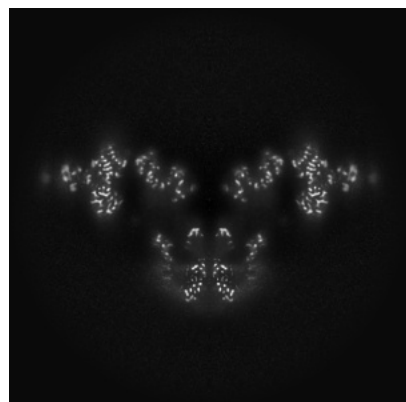


Z

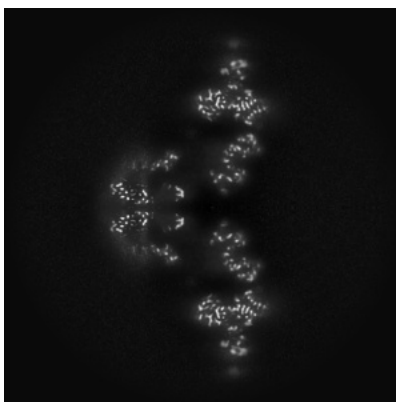
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

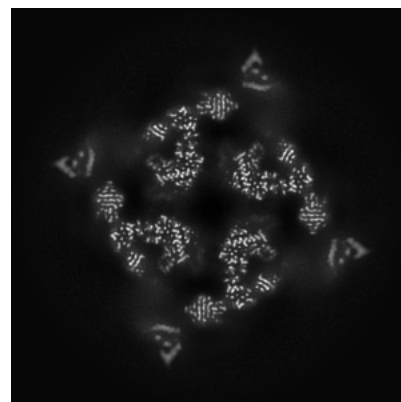
6.2.1 Primary map



X Index: 256



Y Index: 256

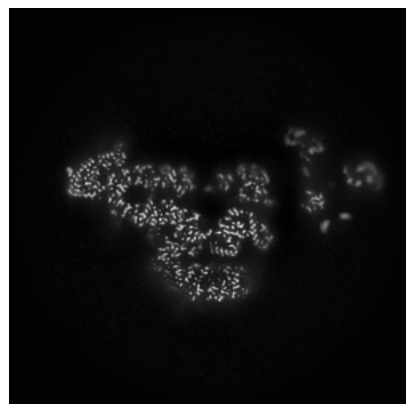


Z Index: 256

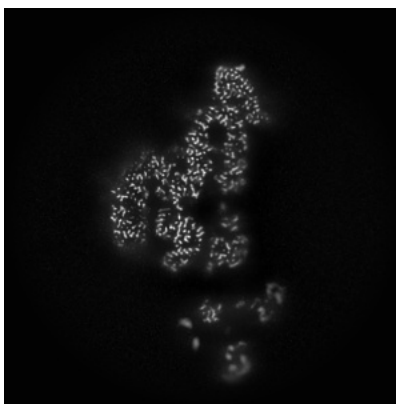
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

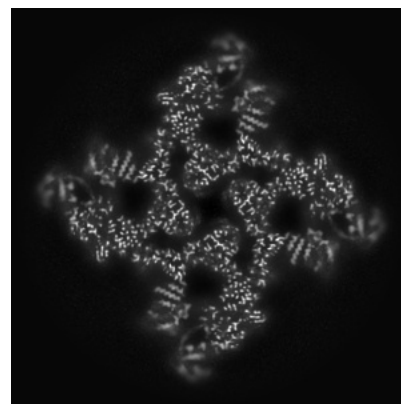
6.3.1 Primary map



X Index: 279



Y Index: 279

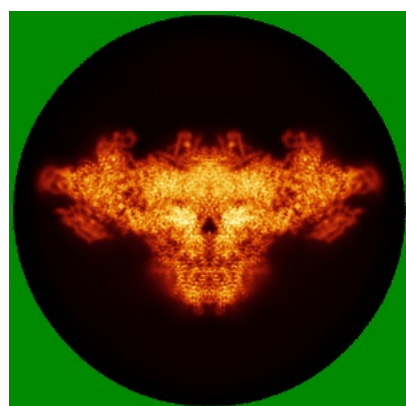


Z Index: 287

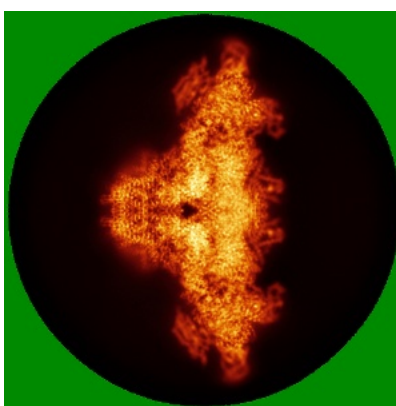
The images above show the largest variance slices of the map in three orthogonal directions.

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

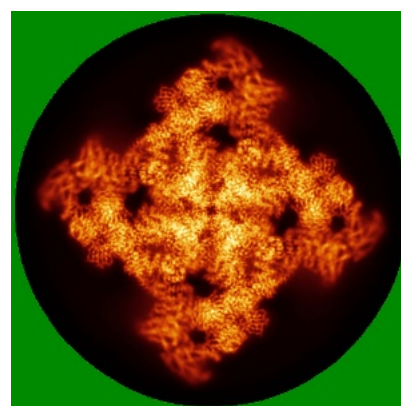
6.4.1 Primary map



X



Y

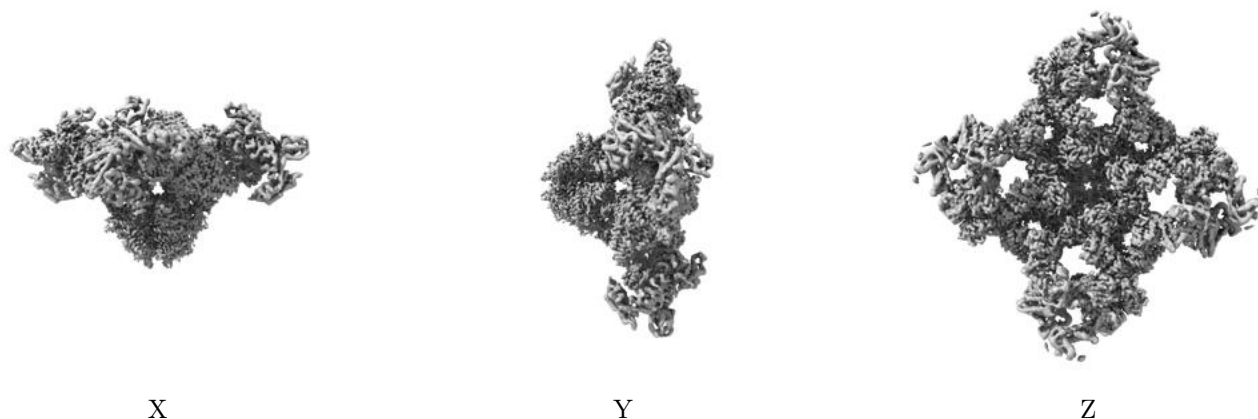


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

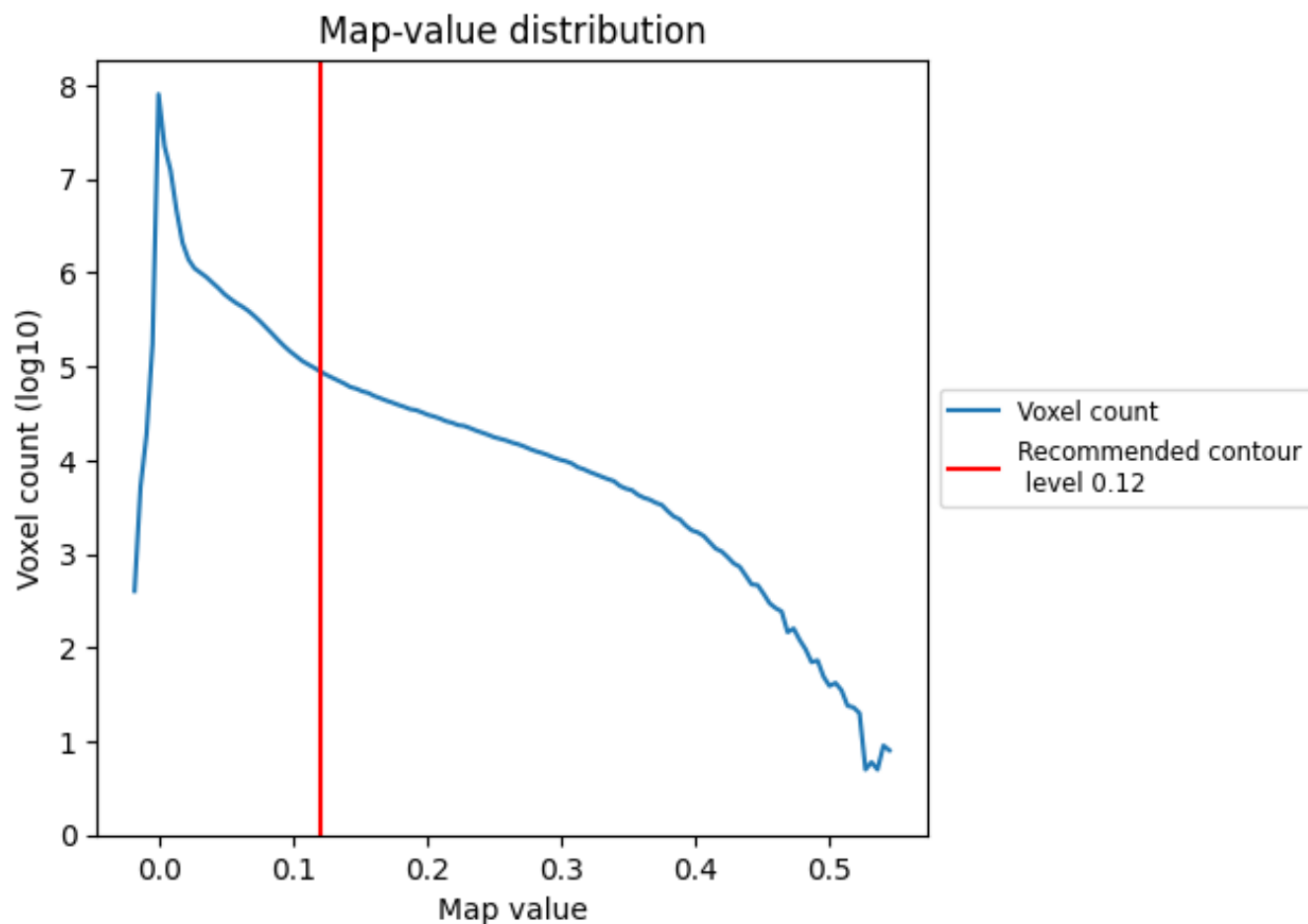
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

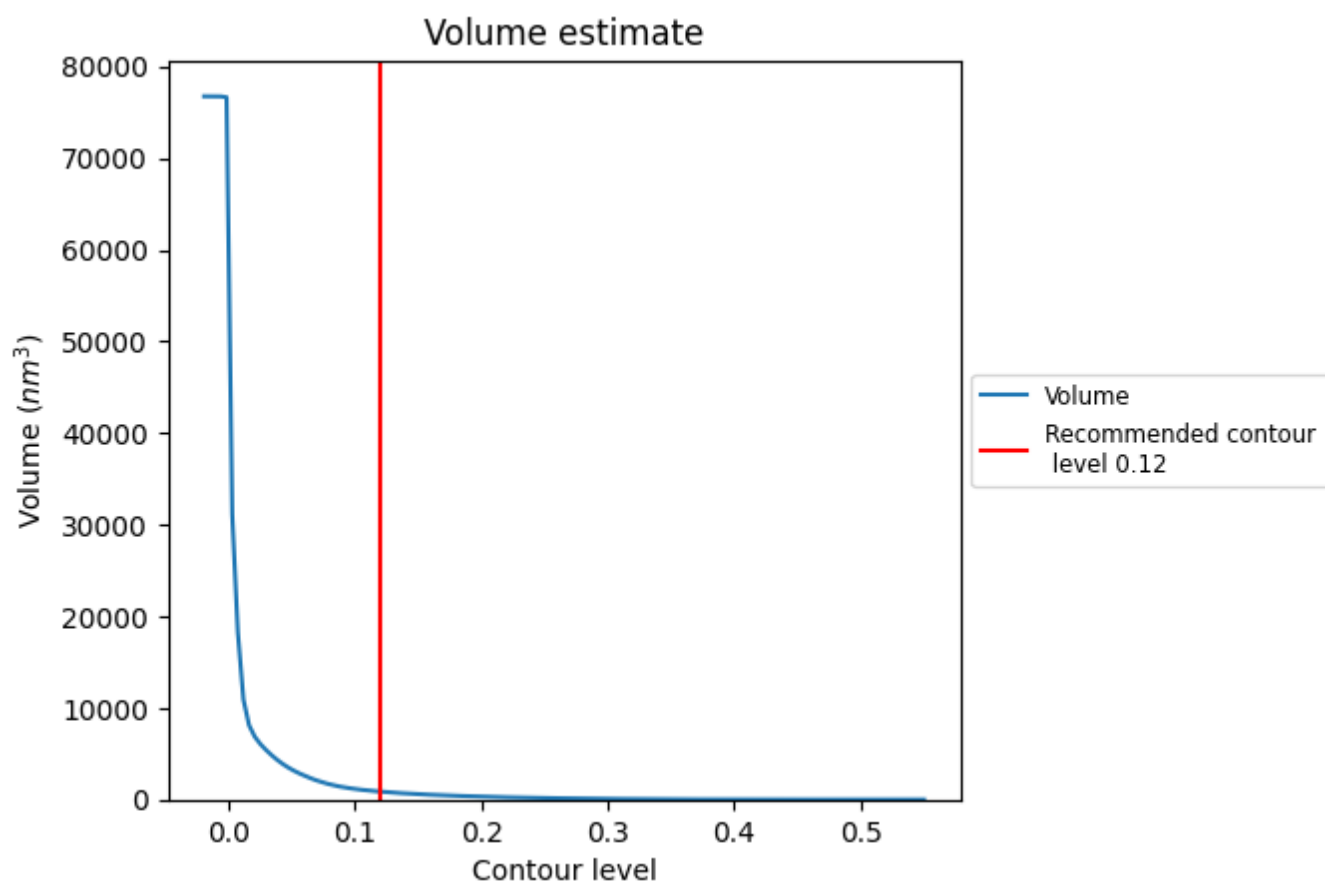
This section contains the results of statistical analysis of the map.

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.

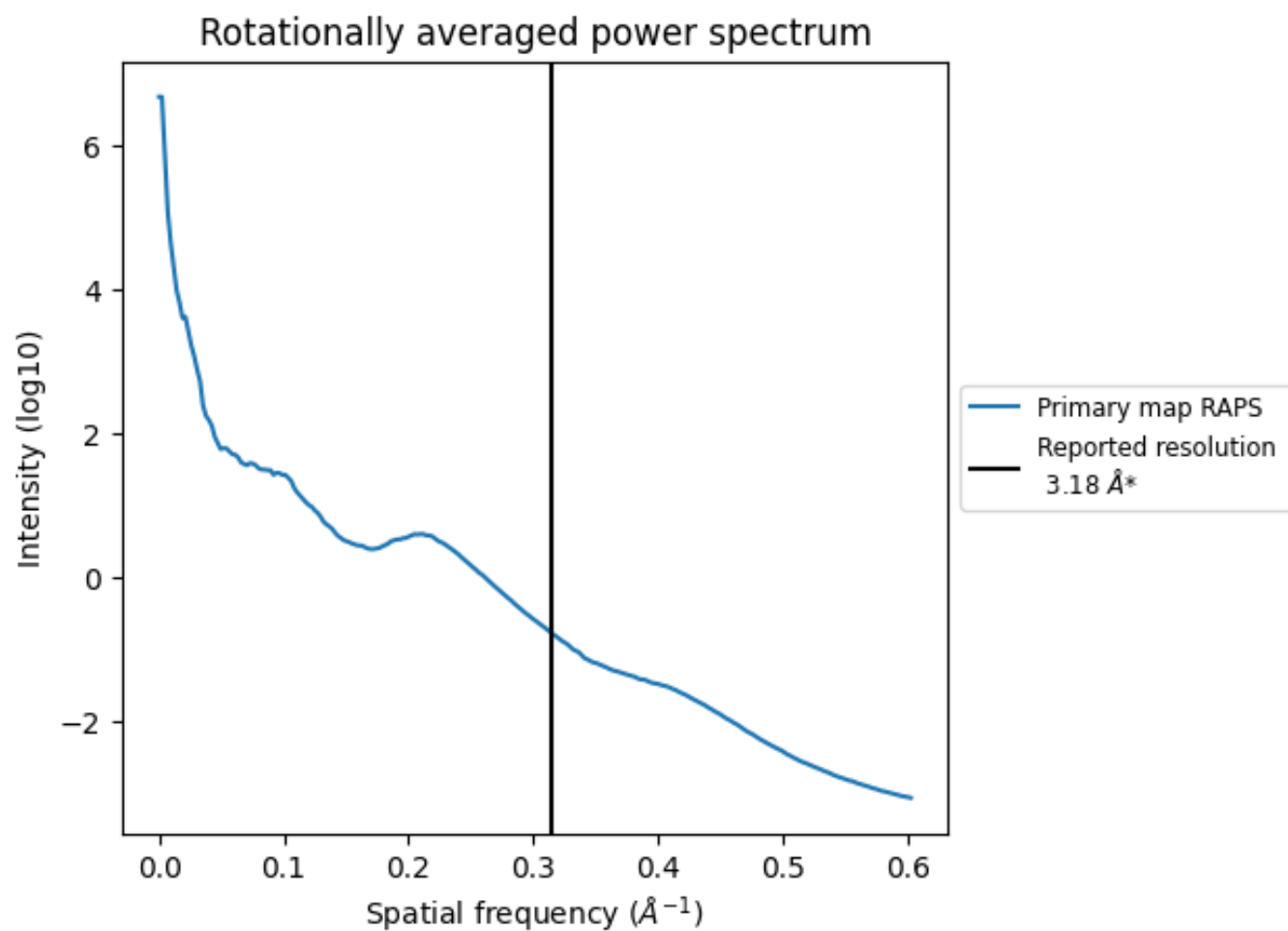
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 868 nm³; this corresponds to an approximate mass of 784 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 0.314 \AA^{-1}

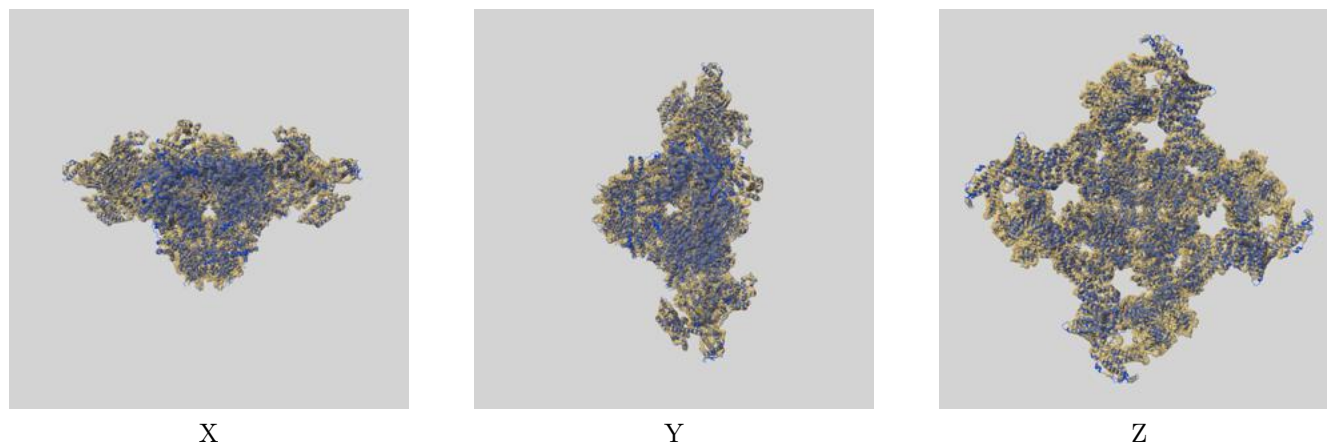
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

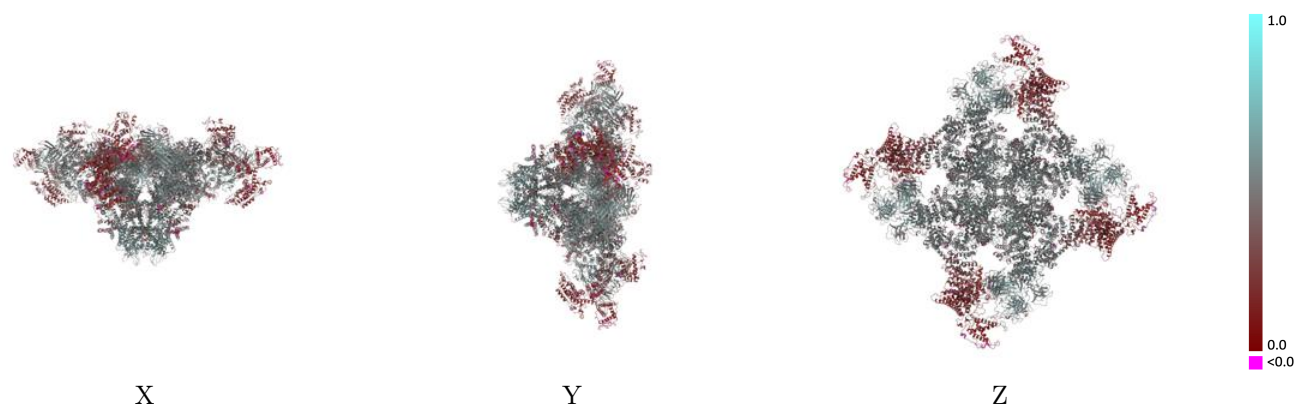
This section contains information regarding the fit between EMDB map EMD-42459 and PDB model 8UQ3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



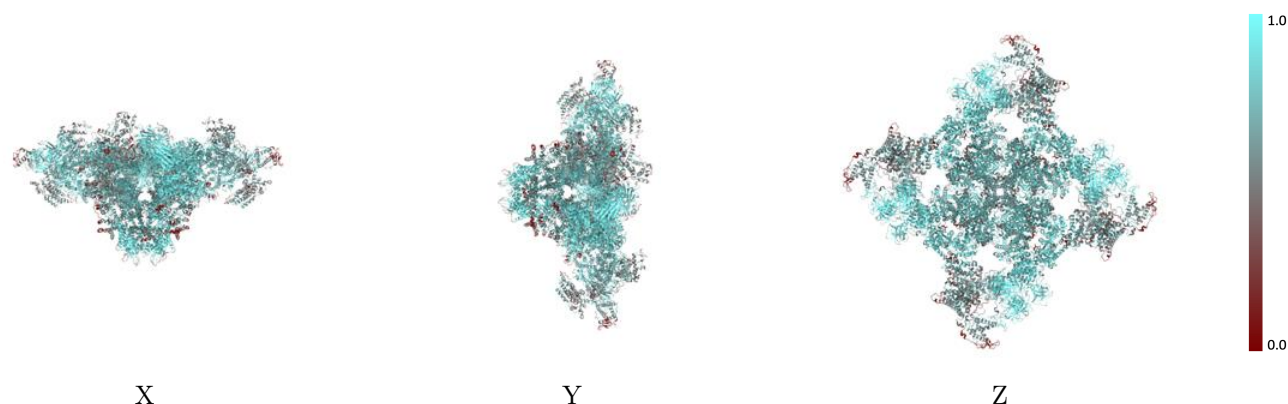
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



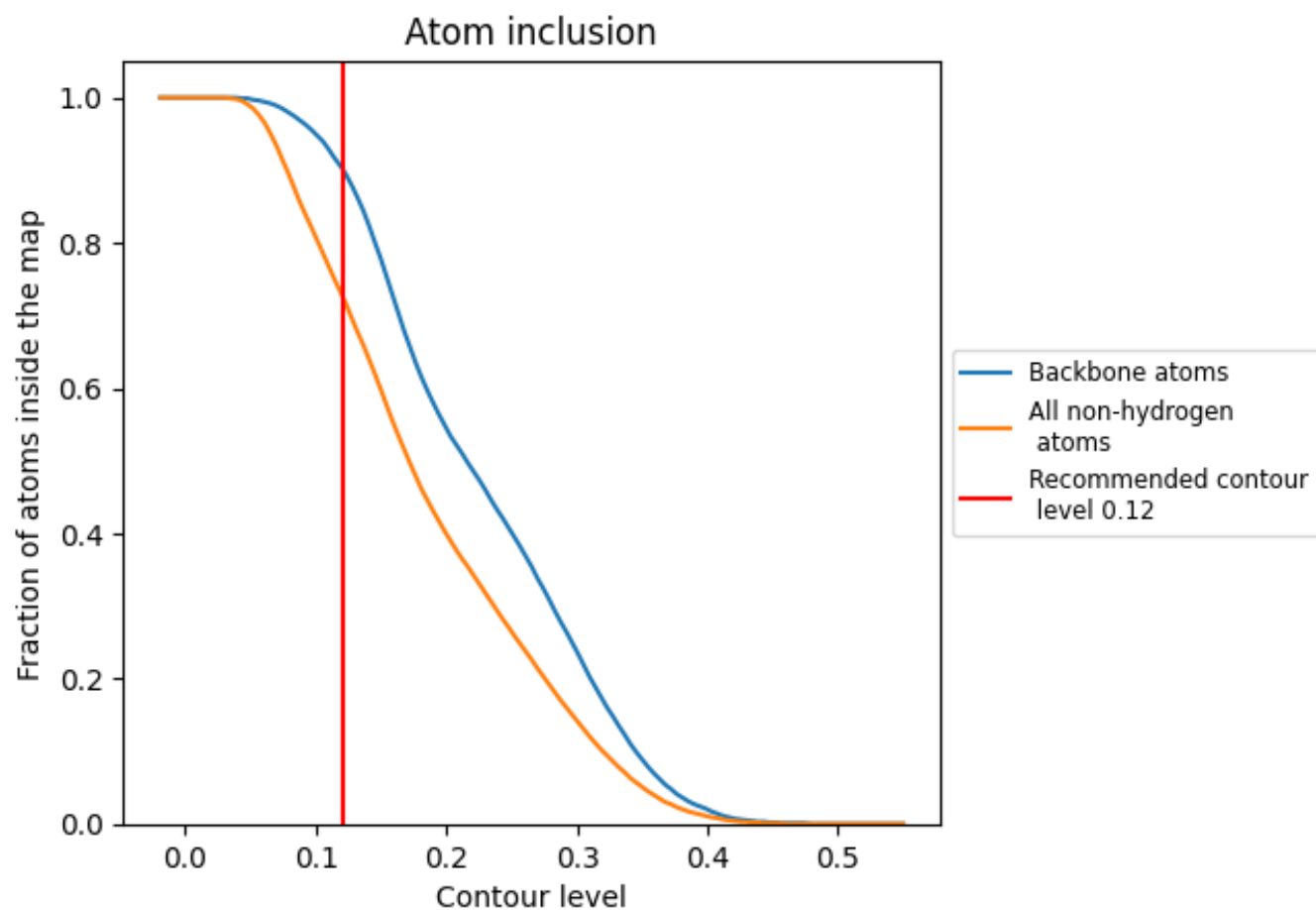
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7280	<div><div></div></div> 0.4180
A	<div><div></div></div> 0.7260	<div><div></div></div> 0.4160
B	<div><div></div></div> 0.7260	<div><div></div></div> 0.4160
C	<div><div></div></div> 0.7250	<div><div></div></div> 0.4150
D	<div><div></div></div> 0.7250	<div><div></div></div> 0.4160
E	<div><div></div></div> 0.8490	<div><div></div></div> 0.5070
F	<div><div></div></div> 0.8500	<div><div></div></div> 0.5100
G	<div><div></div></div> 0.8540	<div><div></div></div> 0.5100
H	<div><div></div></div> 0.8490	<div><div></div></div> 0.5110

1.0

0.0

<0.0