



## wwPDB EM Validation Summary Report ⓘ

Sep 29, 2024 – 05:20 AM EDT

PDB ID : 7U9X  
EMDB ID : EMD-26409  
Title : Structure of PKA phosphorylated human RyR2-R2474S in the closed state  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2022-03-11  
Resolution : 2.58 Å(reported)  
Based on initial model : 7TZC

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

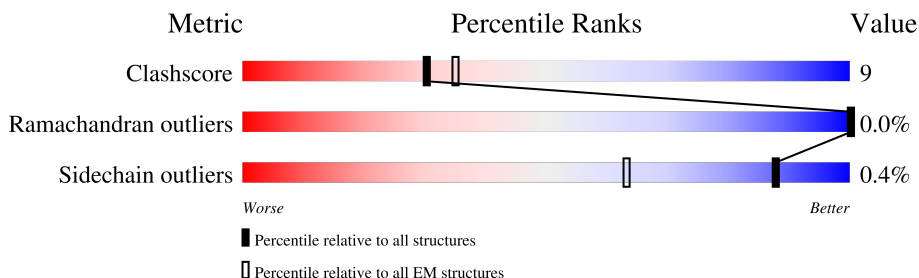
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.58 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  $\geq 3$ , 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>8%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	B	4967	<div> <div>8%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	C	4967	<div> <div>8%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	D	4967	<div> <div>8%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
2	E	108	<div> <div>76%</div> <div>23%</div> <div>.</div> </div>
2	F	108	<div> <div>76%</div> <div>23%</div> <div>.</div> </div>
2	G	108	<div> <div>76%</div> <div>23%</div> <div>.</div> </div>
2	H	108	<div> <div>75%</div> <div>24%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 138588 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
			33766	21513	5742	6281	230		
1	B	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	C	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	D	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2474	SER	ARG	variant	UNP Q92736
B	2474	SER	ARG	variant	UNP Q92736
C	2474	SER	ARG	variant	UNP Q92736
D	2474	SER	ARG	variant	UNP Q92736

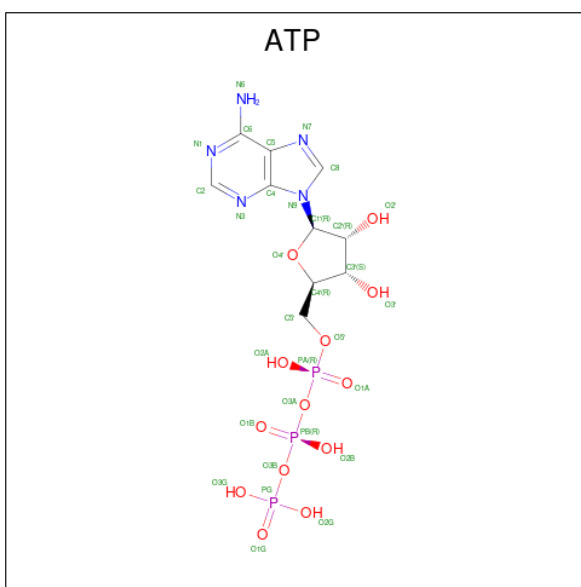
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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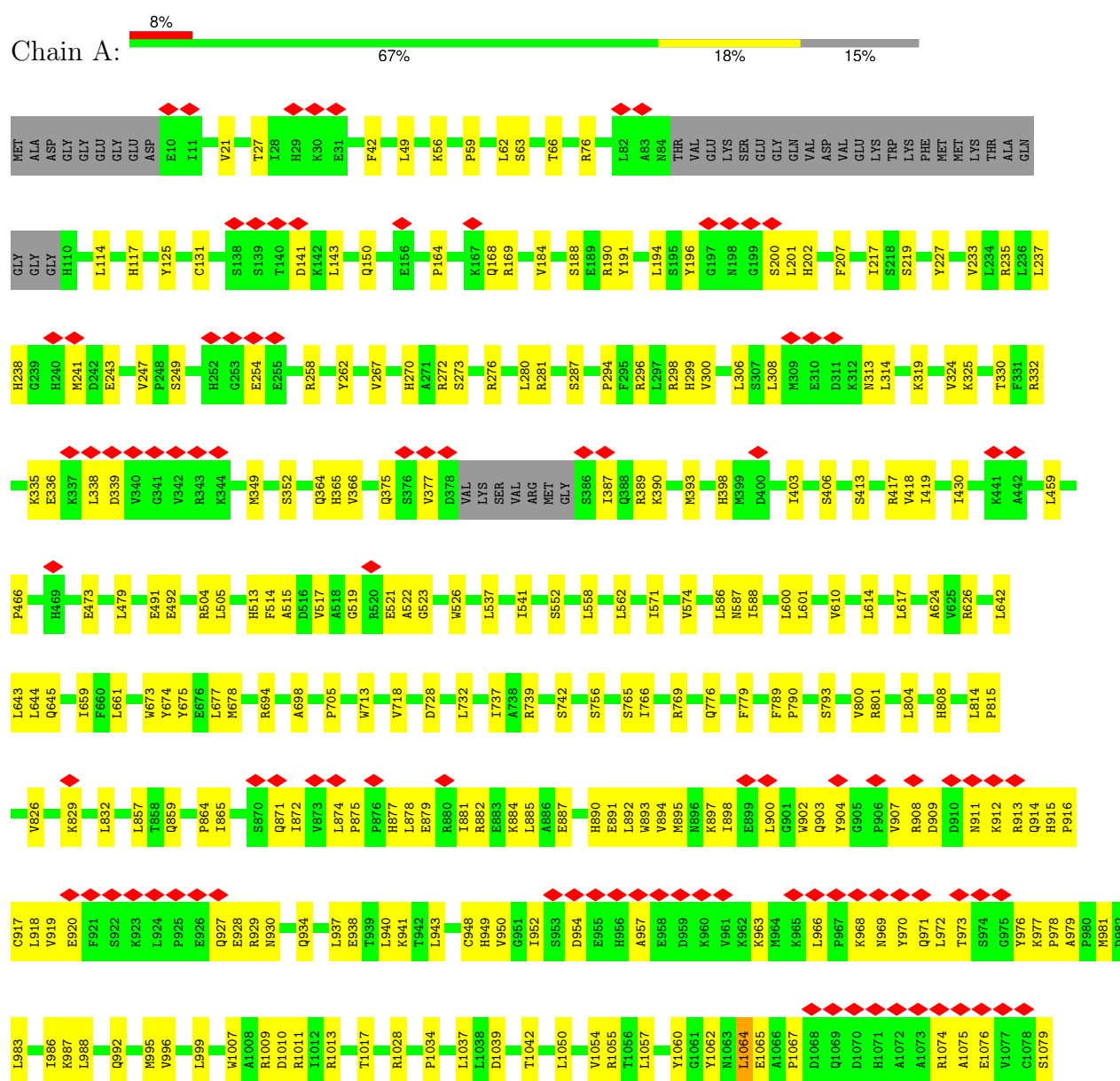
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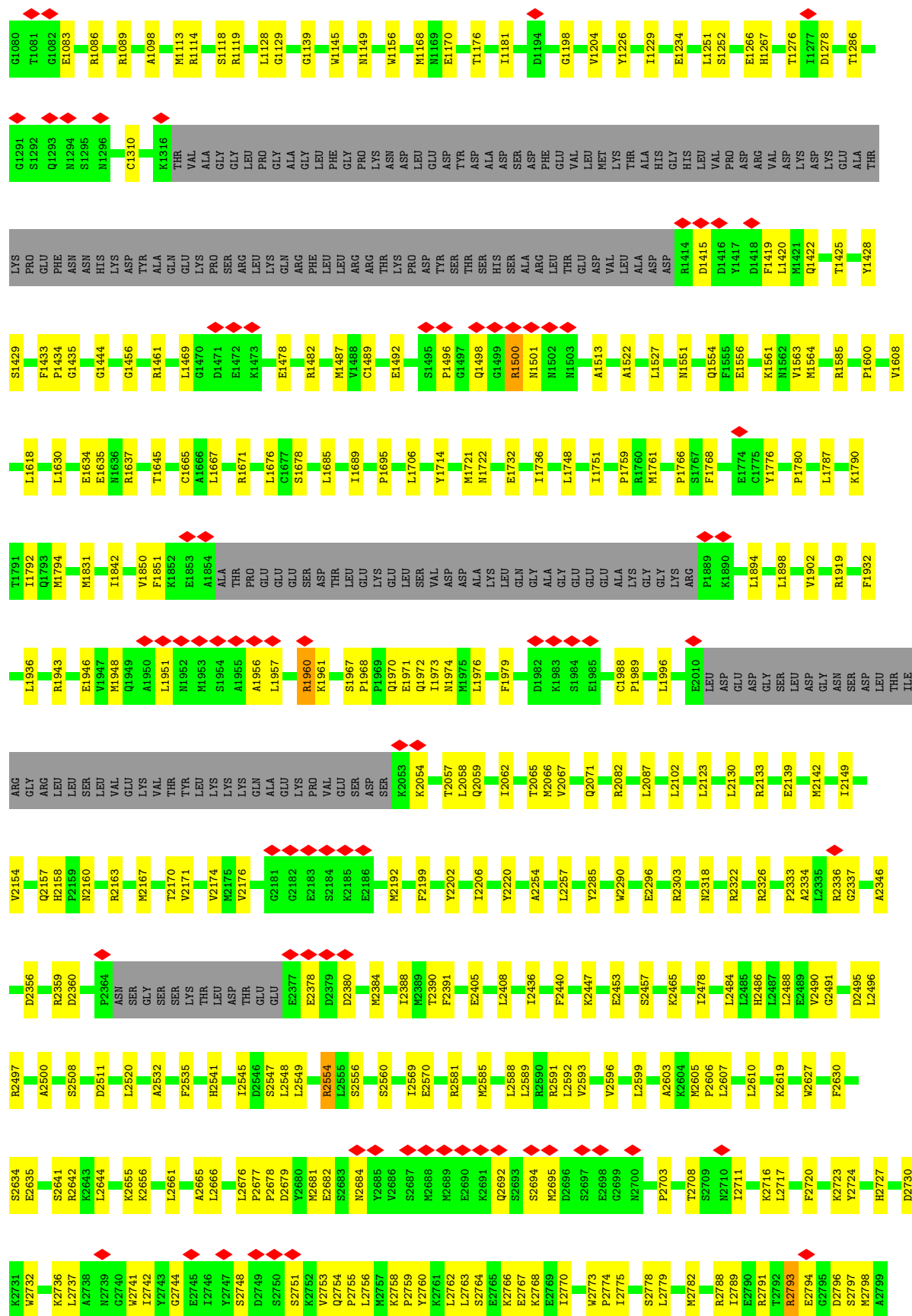
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	D	1	31	10	5	13	3	0

### 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.

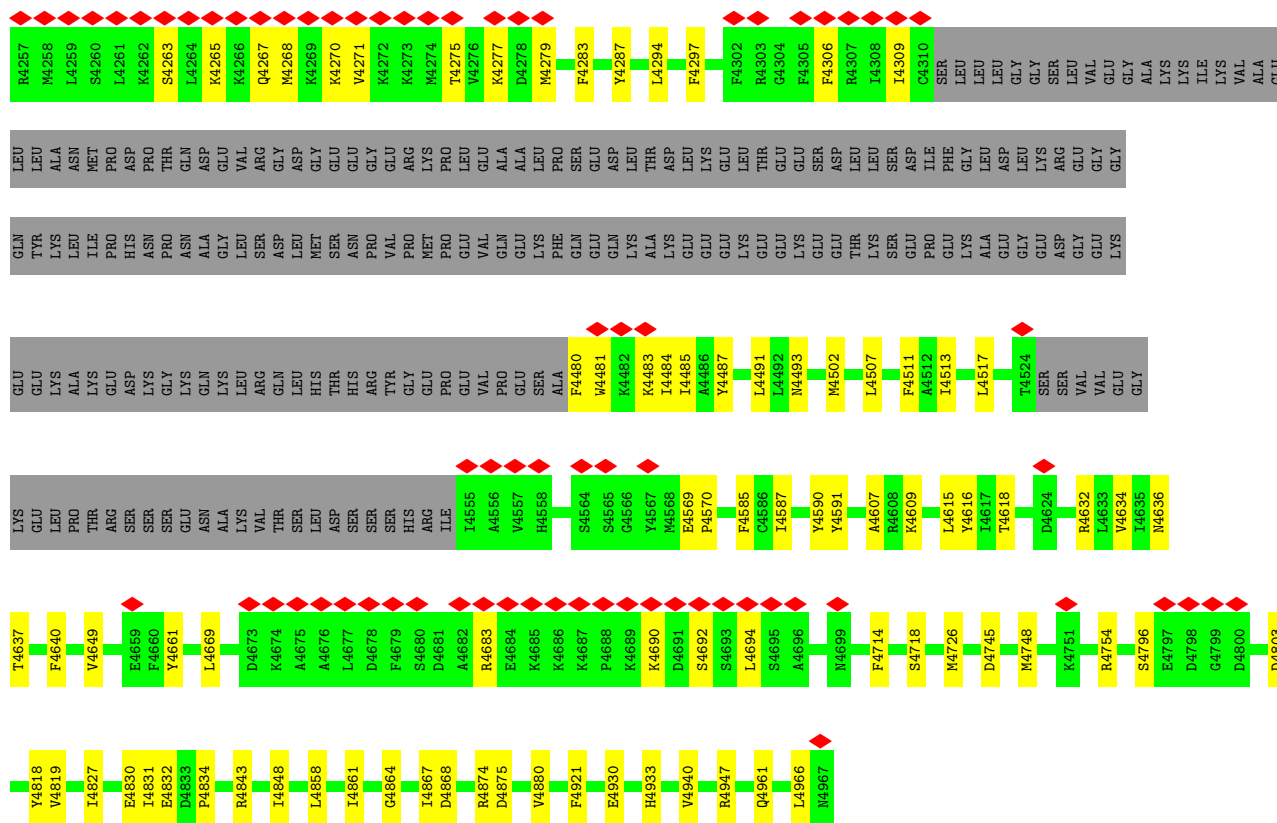
#### • Molecule 1: Ryanodine receptor 2



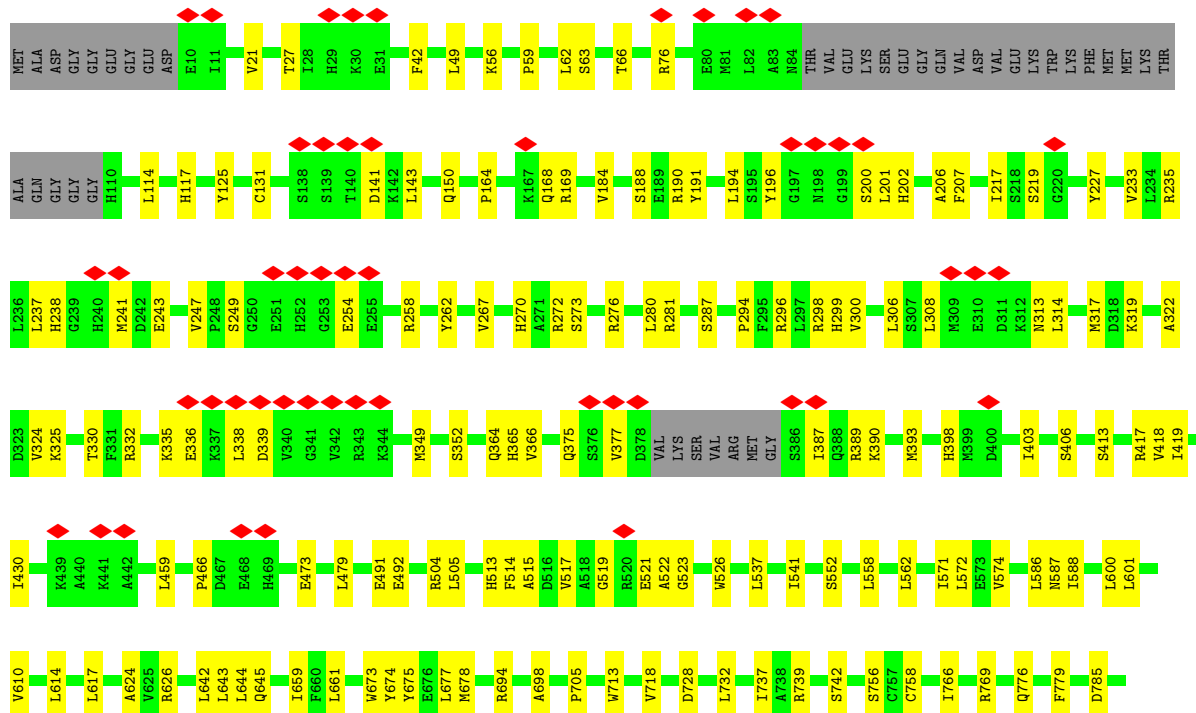






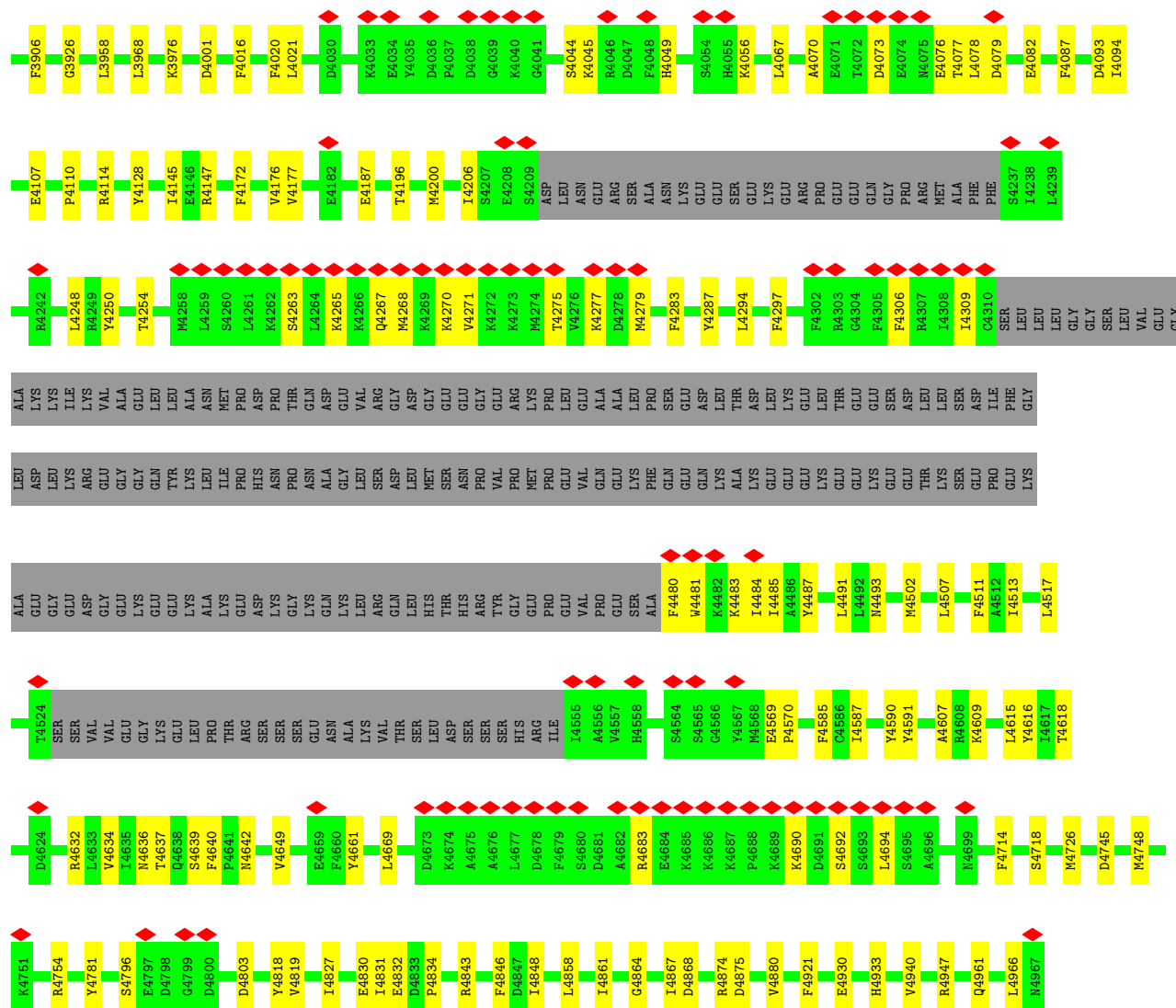


• Molecule 1: Ryanodine receptor 2

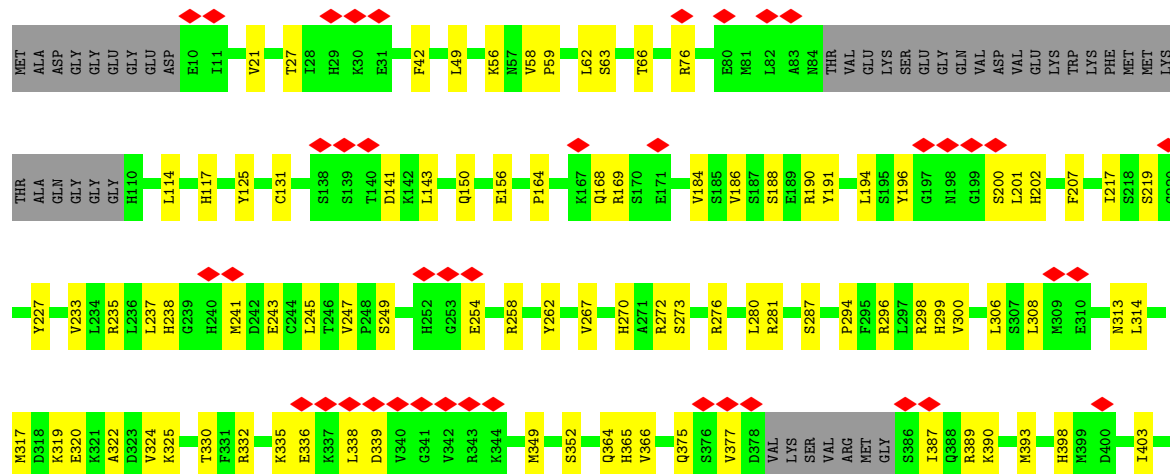


L2408	I2436	F2440	K2447	E2453	S2457	K2465	M2468	I2478	A2334	L2484	L2485	H2486	L2487	L2488	E2489	V2490	G2491	L2496	A2500	S2508	D2511	L2520	A2532	F2535	H2541	L2545	L2548	L2549	R2554	L2555	S2556	S2560	I2569	E2570	R2581	M2585																		
W2290	E2296	R2297	R2303	S2312	N2318	R2322	R2326	P2333	A2334	L2335	R2336	G2337	A2346	D2356	R2369	D2360	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLU	GLU	E2377	E2378	D2379	D2380	M2384	L2388	M2389	T2390	F2391	I2396	R2401	E2405													
R2082	L2087	L2102	L2123	L2130	R2133	E2139	M2142	I2149	V2154	Q2157	H2158	P2159	N2160	R2163	M2167	T2170	V2171	V2174	M2175	V2176	G2181	G2182	E2183	S2184	K2185	E2186	M2192	F2199	Y2202	I2206	Y2220	D2241	A2254	L2257	Y2285																			
L1996	E2010	LEU	ASP	GLU	GLY	ASP	SER	LEU	ASP	GLY	ASN	SER	ASP	LEU	THR	ILE	ARG	GLY	ARG	VAL	GLU	LYS	VAL	THR	LEU	LYS	GLN	ALA	GLU	LYS	GLU	VAL	SER	ASP	SER	T2057	L2058	Q2059	T2062	T2065	K2066	V2067	Q2071											
LYS	GLY	GLY	ARG	P1889	K1890	L1894	L1898	V1902	R1919	F1932	L1936	R1943	E1946	V1947	M1948	Q1949	A1950	L1951	M1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	K1961	S1967	P1968	P1969	Q1970	E1971	Q1972	I1973	N1974	M1975	L1976	F1979	D1982	K1983	S1984	E1985	C1988	P1989									
M1551	Q1554	F1555	E1556	K1561	M1562	V1563	M1564	R1585	P1600	V1608	L1618	L1630	E1634	E1635	N1636	R1637	T1645	C1665	A1666	L1667	R1671	L1676	C1677	S1678	L1685	I1689	P1695	L1706	Y1714	L1719	M1720	M1721	N1722	E1732	I1736	L1748	I1751																	
LEU	ALA	ASP	R1414	D1415	D1416	Y1417	D1418	F1419	L1420	M1421	Q1422	T1425	Y1428	S1429	F1433	P1434	G1444	G1456	R1461	L1469	G1470	D1471	E1472	K1473	E1478	R1482	M1487	V1488	C1489	E1492	S1495	P1496	G1497	Q1498	G1499	R1500	N1501	N1502	N1503	A1513	A1522	L1527												
ALA	HIS	HIS	LEU	VAL	PRO	ASP	ARG	VAL	ASP	LYS	ASP	THR	LYS	PRO	GLU	PHE	ASN	HIS	LYS	ASP	TTR	GLN	GLU	LYS	PRO	GLN	ARG	PHE	LEU	ARG	LYS	THR	PRO	ASP	TYR	SER	ALA	ARG	LEU	THR	GLU	ASP	VAL											
W902	Q903	Y904	G905	P906	V907	R908	D909	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Q934	L937	E938	T939	L940	K941	T942	L943	L944	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962	M964	K965	L966
F789	P790	S793	V800	R801	L804	H808	L814	P815	Y819	V826	K829	L832	S857	L858	Q859	I865	S870	Q871	I872	V873	L874	P875	P876	H877	L878	E879	R880	I881	R882	E883	K884	L885	A886	E887	H890	E891	L892	M893	V894	M895	N896	K897	I898	E899	L900	G901								

GLU	GLU	E3710	V3711	Q3727	Q3728	A3729	R3730	L3731	H3732	M3739	L3763	Y3780	K3784	L3803	E3815	G3816	G3817	G3818	M3819	V3820	T3821	E3822	E3823	G3824	G3825	E3827	G3828	D3832	F3835	D3838	L3839	F3840	K3851	S3852	D3853	F3854	Q3855	T3874	S3884	L3701	E3702	GLU	ASP	ASP	GLY						
LYS	ALA	VAL	TRP	HIS	LYS	LEU	LEU	LEU	ARG	LYS	ALA	V3599	V3600	A3601	C3602	F3603	R3604	M3605	A3606	H3614	R3615	E3625	K3639	E3642	A3649	E3650	P3651	P3652	E3653	E3654	D3655	E3656	G3657	T3658	K3659	R3660	L3676	L3687	K3697	H3700	D3701	E3702	GLU	ASP	ASP	GLY					
ILE	ARG	TRP	GLN	MET	LYS	LEU	TYR	ASP	PRO	ASN	ARG	THR	THR	ASP	THR	THR	ASP	PRO	GLY	GLU	VAL	VAL	GLU	VAL	ALA	VAL	GLN	HIS	GLN	GLY	ARG	ARG	TYR	CYS	VAL	GLU	GLY	ASP	ARG	HIS	PRO	GLN	ARG	PRO	LYS						
SER	LEU	ILE	VAL	VAL	ALA	ALA	LEU	LYS	ARG	PRO	ILE	GLY	GLN	LEU	ASN	ASN	ALA	PRO	GLY	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR						
ALA	ARG	GLY	ASP	MET	SER	GLU	ALA	GLU	LEU	LEU	ILE	LEU	LEU	ASP	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR						
E3271	H3272	M3273	N3274	L3277	G3278	N3279	L3280	L3283	L3284	L3288	D3291	E3292	G3293	L3299	F3302	S3303	T3306	T3307	K3311	P3312	Q3313	L3314	L3315	K3316	T3317	H3318	F3319	L3320	P3321	L3322	H3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	T3332	V3333	V3334	S3335	E3336	E3337	ASP	HIS	LEU	LYS	ALA	GLU
Y3184	N3185	T3186	K3187	R3190	E3191	A3193	A3194	L3195	S3196	L3197	P3198	E3202	D3203	V3204	C3205	I3208	L3214	M3215	E3216	E3217	I3218	V3219	E3220	L3221	A3222	E3223	I3226	R3227	Q3230	M3231	P3232	M3235	L3242	M3246	S3247	R3248	W3249	W3250	N3256	R3260	A3261	E3262	M3263	L3268	N3269	S3270					
Q3077	G3078	Q3079	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	G3089	V3090	T3091	I3094	T3098	M3104	I3112	F3117	G3118	E3119	D3120	D3125	V3126	Q3127	V3128	R3132	I3133	L3134	V3144	S3145	V3147	V3148	S3153	R3248	W3249	W3250	N3256	R3260	A3261	E3262	M3263	L3268	N3269	S3270						
E2952	H2953	F2954	P2955	Y2956	E2957	Q2958	E2959	L2960	V2966	V2967	L2968	P2969	L2970	L2971	D2972	K2976	R2979	A2986	R2987	P2988	P2989	L2990	C2991	L3011	V3015	R3018	I3019	S3020	L3021	F3022	G3023	N3024	D3025	I3029	L3033	H3034	I3035	L3036	G3037	Q3038	T3039	L3040	L3050	V3053	L3061	N3074					
G2864	G2865	G2866	N2867	H2868	E2869	L2870	L2871	Y2874	D2875	T2878	K2882	D2891	L2892	L2893	F2894	L2896	Q2897	L2898	Y2901	A2902	V2903	S2904	R2905	C2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	R2920	L2929	A2936	Y2939	I2940	F2943	D2944	G2945	G2946	S2947	R2948	G2949	G2951					
M2695	S2696	E2698	P2703	T2708	N2709	N2710	I2711	K2716	L2717	F2720	K2723	Y2724	H2727	M2730	K2731	W2732	K2736	L2737	A2738	N2739	W2741	L2742	Y2743	G2744	E2745	L2746	Y2747	D2748	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	I2826	D2827	R2835	D2836	L2837	M2840	A2841	K2854						
L2588	D2696	L2589	R2590	L2591	L2592	V2593	V2596	L2599	A2603	K2604	M2605	P2606	L2607	L2610	K2619	M2627	E2630	S2634	E2635	S2641	R2642	V2643	L2644	K2655	K2656	L2661	A2665	L2666	L2676	D2679	V2680	M2681	E2682	P2755	Q2756	L2757	M2757	K2758	P2759	Y2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	K2768	S2694		

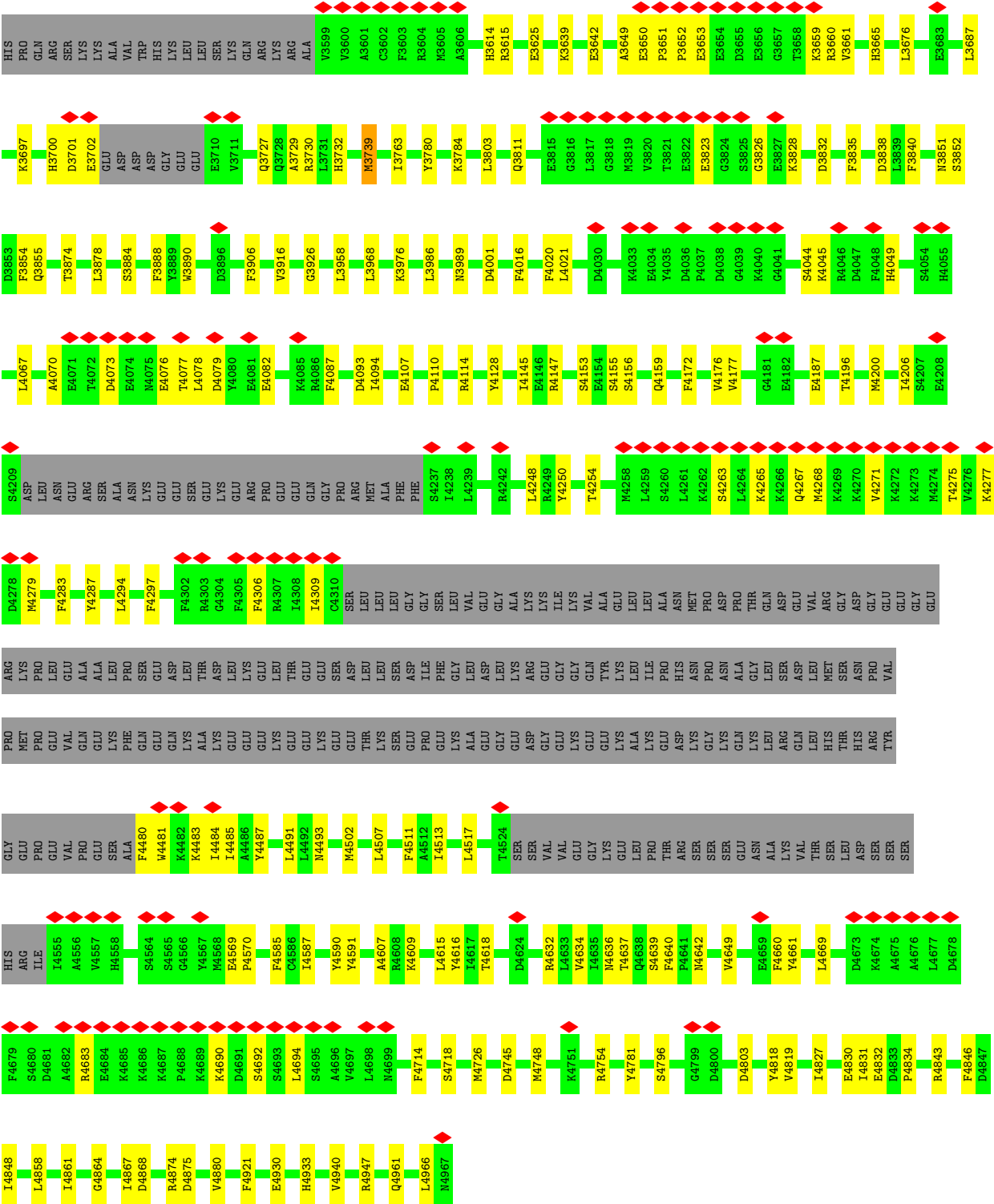


• Molecule 1: Ryanodine receptor 2

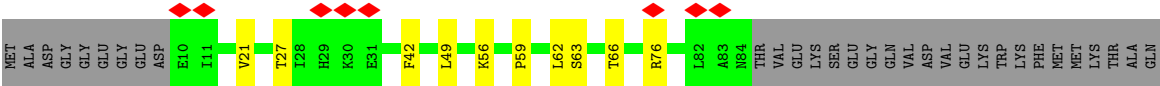








● Molecule 1: Ryanodine receptor 2

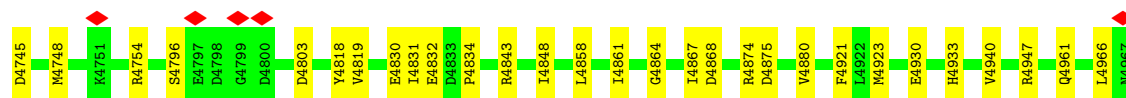






S3196	E3202	D3203	V3204	C3205	T3208	L3214	I3218	V3219	E3220	L3221	F3222	S3224	G3225	R3227	Q3230	K3231	P3232	K3235	L3239	L3242	K3246	R3247	W3249	N3256	R3260	A3261	E3262	L3268	N3269	S3270	E3271	H3272	N3273	N3274	L3277	G3278	N3279	I3280	I3283													
ASN	GLN	PRO	K3088	G3089	V3090	T3091	Q3092	I3093	I3094	T3098	M3104	I3112	F3117	G3118	E3119	D3125	V3126	Q3127	V3128	R3132	I3133	L3134	K3144	S3145	V3148	S3153	G3156	E3157	F3162	P3167	H3174	L3175	D3176	K3177	I3183	Y3184	N3185	T3186	K3187	R3190	R3279	F3080	T3081	HIS	THR	ARG						
E2957	Q2958	E2959	I2960	V2966	V2967	L2968	P2969	I2970	I2971	D2972	R2979	A2986	S2987	P2988	P2989	L2990	C2991	L3011	V3015	R3018	I3019	S3020	L3021	F3022	G3023	N3024	D3025	I3029	L3033	H3034	I3035	G3037	Q3038	T3039	L3040	L3050	V3053	N3074	Q3077	G3078	Q3079	F3080	T3081	HIS	THR	ARG						
P2869	L2870	L2871	Y2874	D2875	T2878	K2882	D2891	L2892	L2893	K2894	F2895	L2896	Q2897	L2898	Y2901	A2902	V2903	S2904	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	K2919	R2920	L2929	A2936	Y2939	I2940	F2943	D2944	G2945	G2946	S2947	R2948	G2949	K2950	G2951	E2952	H2953	F2954	Y2956				
W2782	R2788	I2789	E2790	R2791	T2792	R2793	E2794	G2795	D2796	S2797	W2798	A2799	L2800	Y2801	N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	I2826	D2827	N2830	R2835	D2836	L2837	M2840	A2841	K2854	G2864	G2865	G2866	N2867	H2868
T2708	S2709	N2710	I2711	K2716	L2717	F2720	Y2724	H2727	D2730	K2731	W2732	K2736	L2737	A2738	N2739	G2740	W2741	L2742	W2743	G2744	E2745	L2746	W2747	S2748	D2749	S2750	S2751	K2752	V2753	Q2754	P2755	K2758	P2759	Y2760	L2762	L2763	S2764	E2765	K2766	E2767	K2768	I2770	W2773	P2774	L2775	S2778	L2779					
V2596	L2599	K2603	K2604	M2605	P2606	L2607	L2610	K2619	W2627	F2630	S2634	E2635	S2641	K2642	K2643	L2644	K2655	K2656	L2661	A2665	L2666	L2676	D2679	Y2680	M2681	E2682	S2683	N2684	Y2685	V2686	S2687	M2688	E2689	K2691	Q2692	S2693	S2694	M2695	D2696	S2697	G2698	G2699	N2700	P2703								
R2303	N2318	R2322	R2326	P2333	L2334	L2335	R2336	G2337	A2346	D2356	R2359	D2360	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLU	E2377	E2378	D2379	D2380	M2384	I2388	M2389	T2390	F2391	I2396	E2405	L2408	I2436	F2440	K2447	E2453												
L2130	R2133	E2139	M2142	I2149	V2154	Q2157	H2158	P2159	N2160	R2163	M2167	T2170	V2171	V2174	M2175	V2176	G2181	G2182	E2183	S2184	K2185	E2186	M2192	F2199	Y2202	I2206	Y2220	A2254	L2257	V2285	Y2285	W2290	E2296	F2301	L2302																	
K1890	L1894	S1767	F1768	Y1776	P1780	K1790	T1792	H1793	M1794	M1831	I1842	V1850	F1851	K1852	E1853	A1854	ALA	THR	PRO	GLN	GLU	GLU	GLU	ASP	THR	LEU	GLU	LYS	LEU	VAL	ASP	Q1970	E1971	Q1972	I1973	N1974	M1975	L1976	F1979	D1982	K1983	S1984	E1985	L1996	E2010	LEU	ASP	GLU	ASP			





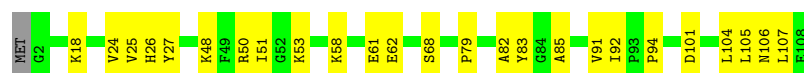
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 76% 23%



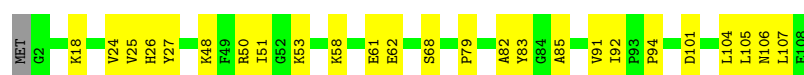
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 76% 23%



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

Chain G: 76% 23%



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

Chain H: 75% 24%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212141	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)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.859	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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, 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	0.26	0/34506	0.49	1/46608 (0.0%)
1	B	0.26	0/34506	0.49	1/46608 (0.0%)
1	C	0.26	0/34506	0.49	1/46608 (0.0%)
1	D	0.26	0/34506	0.49	1/46608 (0.0%)
2	E	0.37	0/834	0.57	0/1123
2	F	0.37	0/834	0.56	0/1123
2	G	0.37	0/834	0.57	0/1123
2	H	0.37	0/834	0.57	0/1123
All	All	0.26	0/141360	0.49	4/190924 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3202	GLU	CA-CB-CG	5.44	125.36	113.40
1	C	3202	GLU	CA-CB-CG	5.44	125.36	113.40
1	A	3202	GLU	CA-CB-CG	5.42	125.33	113.40
1	D	3202	GLU	CA-CB-CG	5.41	125.31	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3926	GLY	Peptide
1	B	3926	GLY	Peptide
1	C	3926	GLY	Peptide
1	D	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	33766	0	33447	613	0
1	B	33766	0	33447	611	0
1	C	33766	0	33447	619	0
1	D	33766	0	33447	609	0
2	E	818	0	821	15	0
2	F	818	0	821	14	0
2	G	818	0	821	15	0
2	H	818	0	821	15	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	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
All	All	138588	0	137168	2426	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 9.

The worst 5 of 2426 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:4834:PRO:HB3	1:C:4843:ARG:HD3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4834:PRO:HB3	1:D:4843:ARG:HD3	1.60	0.83
1:A:4834:PRO:HB3	1:A:4843:ARG:HD3	1.60	0.83
1:B:4834:PRO:HB3	1:B:4843:ARG:HD3	1.60	0.82
1:A:2142:MET:HE3	1:A:2174:VAL:HG21	1.64	0.79

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	4102 (98%)	96 (2%)	0	100	100
1	B	4198/4967 (84%)	4102 (98%)	96 (2%)	0	100	100
1	C	4198/4967 (84%)	4101 (98%)	97 (2%)	0	100	100
1	D	4198/4967 (84%)	4103 (98%)	95 (2%)	0	100	100
2	E	105/108 (97%)	102 (97%)	2 (2%)	1 (1%)	13	27
2	F	105/108 (97%)	102 (97%)	2 (2%)	1 (1%)	13	27
2	G	105/108 (97%)	102 (97%)	2 (2%)	1 (1%)	13	27
2	H	105/108 (97%)	102 (97%)	2 (2%)	1 (1%)	13	27
All	All	17212/20300 (85%)	16816 (98%)	392 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	61	GLU
2	H	61	GLU
2	E	61	GLU
2	G	61	GLU

### 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%)	3693 (100%)	15 (0%)	89	96
1	B	3708/4358 (85%)	3693 (100%)	15 (0%)	89	96
1	C	3708/4358 (85%)	3693 (100%)	15 (0%)	89	96
1	D	3708/4358 (85%)	3693 (100%)	15 (0%)	89	96
2	E	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	G	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
All	All	15184/17788 (85%)	15124 (100%)	60 (0%)	88	96

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3202	GLU
1	D	2793	ARG
1	C	1960	ARG
1	D	2766	LYS
1	D	3739	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	934	GLN
1	D	3811	GLN
1	D	4636	ASN
1	D	3274	ASN
1	B	4636	ASN

### 5.3.3 RNA ⓘ

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
4	ATP	D	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	B	5002	-	28,33,33	0.61	0	34,52,52	0.60	1 (2%)
4	ATP	C	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	B	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	C	5002	-	28,33,33	0.61	0	34,52,52	0.60	1 (2%)
4	ATP	D	5002	-	28,33,33	0.61	0	34,52,52	0.60	1 (2%)
4	ATP	A	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	A	5002	-	28,33,33	0.61	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
4	ATP	D	5003	-	-	5/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	5/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	C	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	5/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	7/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5003	ATP	C5-C6-N6	2.36	123.90	120.31
4	B	5003	ATP	C5-C6-N6	2.36	123.90	120.31
4	D	5003	ATP	C5-C6-N6	2.36	123.90	120.31
4	A	5002	ATP	C5-C6-N6	2.34	123.87	120.31
4	D	5002	ATP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C3'-C4'-C5'-O5'
4	A	5003	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	C3'-C4'-C5'-O5'
4	B	5003	ATP	O4'-C4'-C5'-O5'
4	C	5002	ATP	C3'-C4'-C5'-O5'

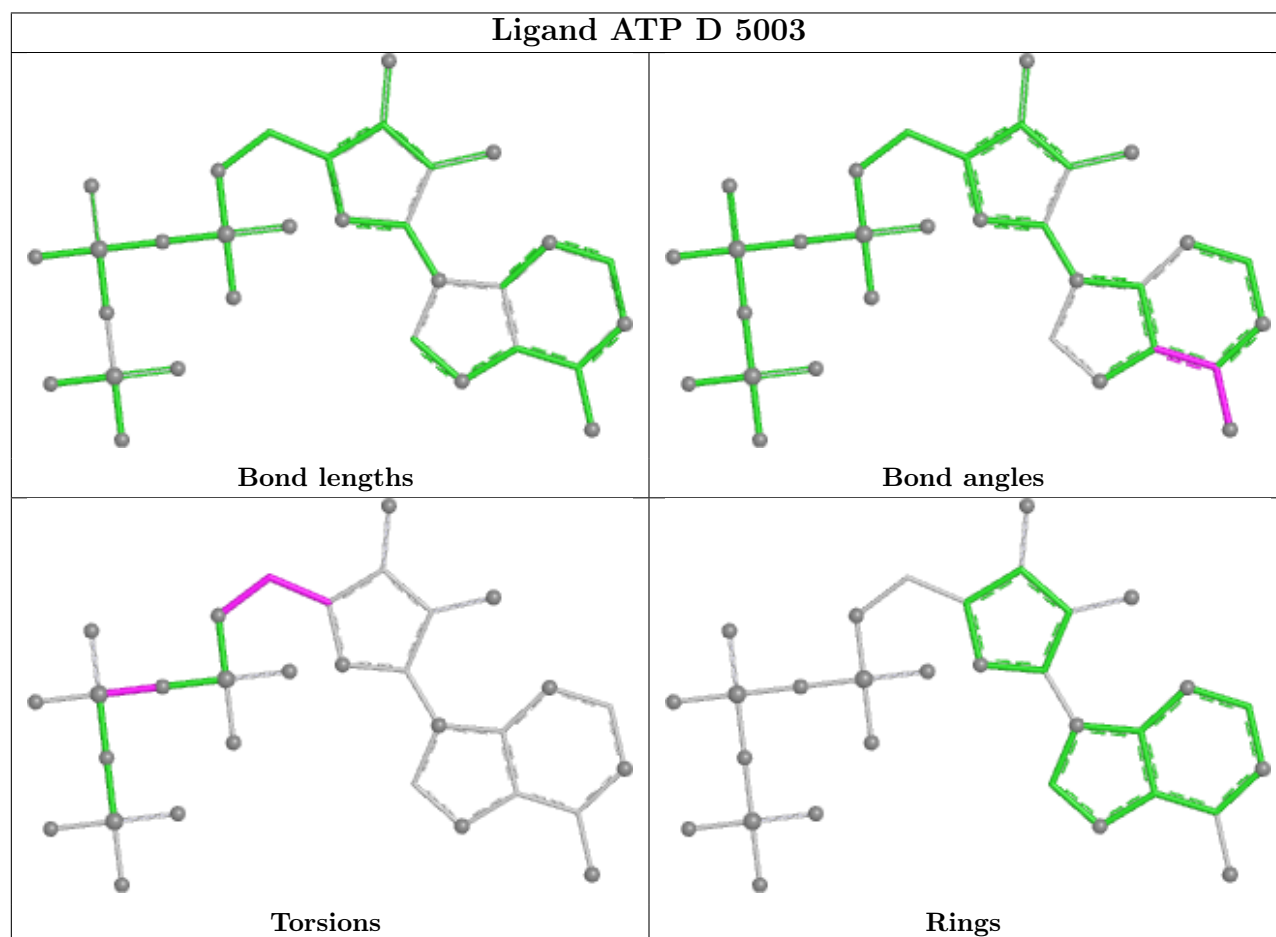
There are no ring outliers.

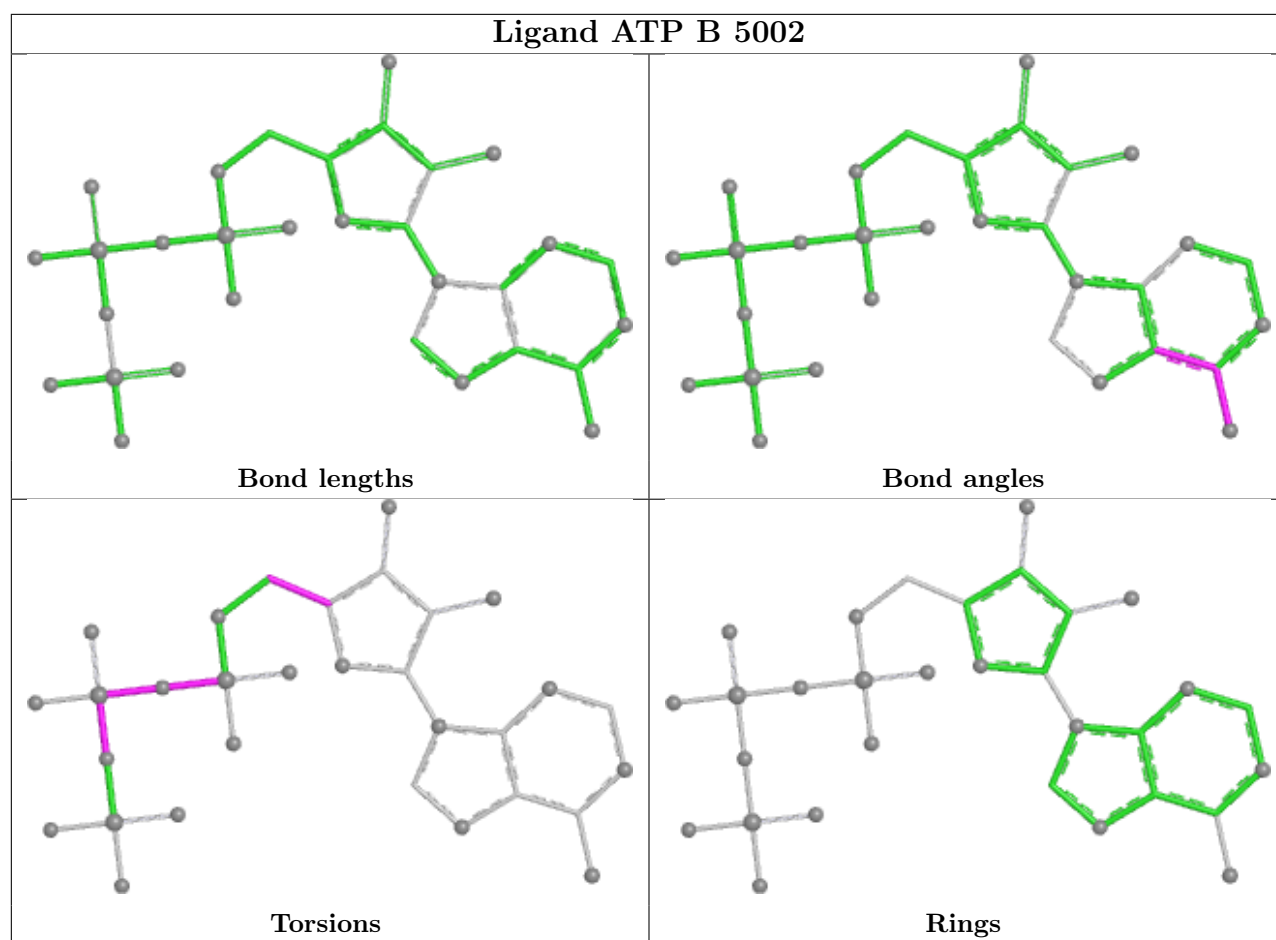
4 monomers are involved in 8 short contacts:

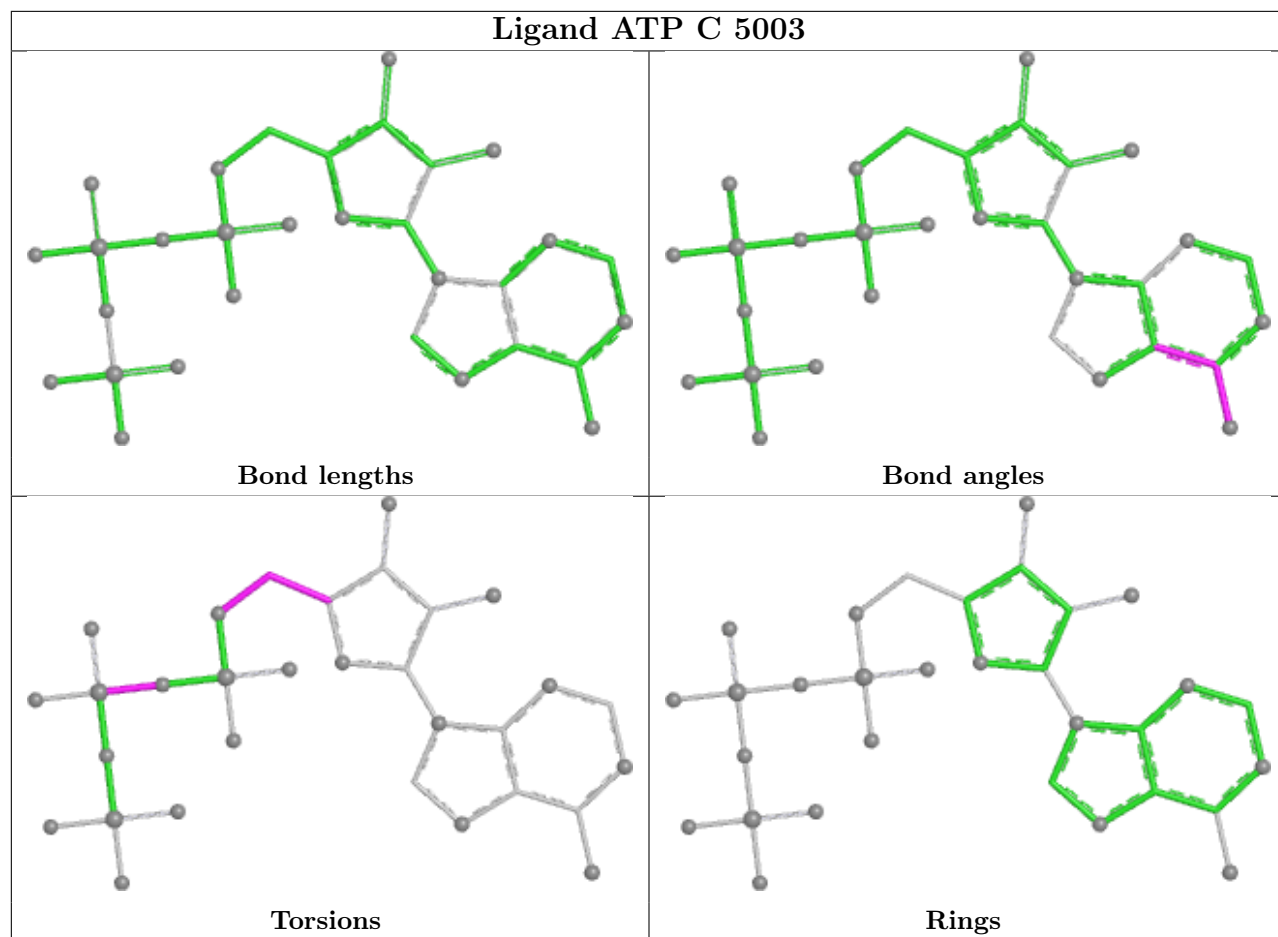
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5003	ATP	2	0
4	C	5003	ATP	2	0
4	B	5003	ATP	2	0
4	A	5003	ATP	2	0

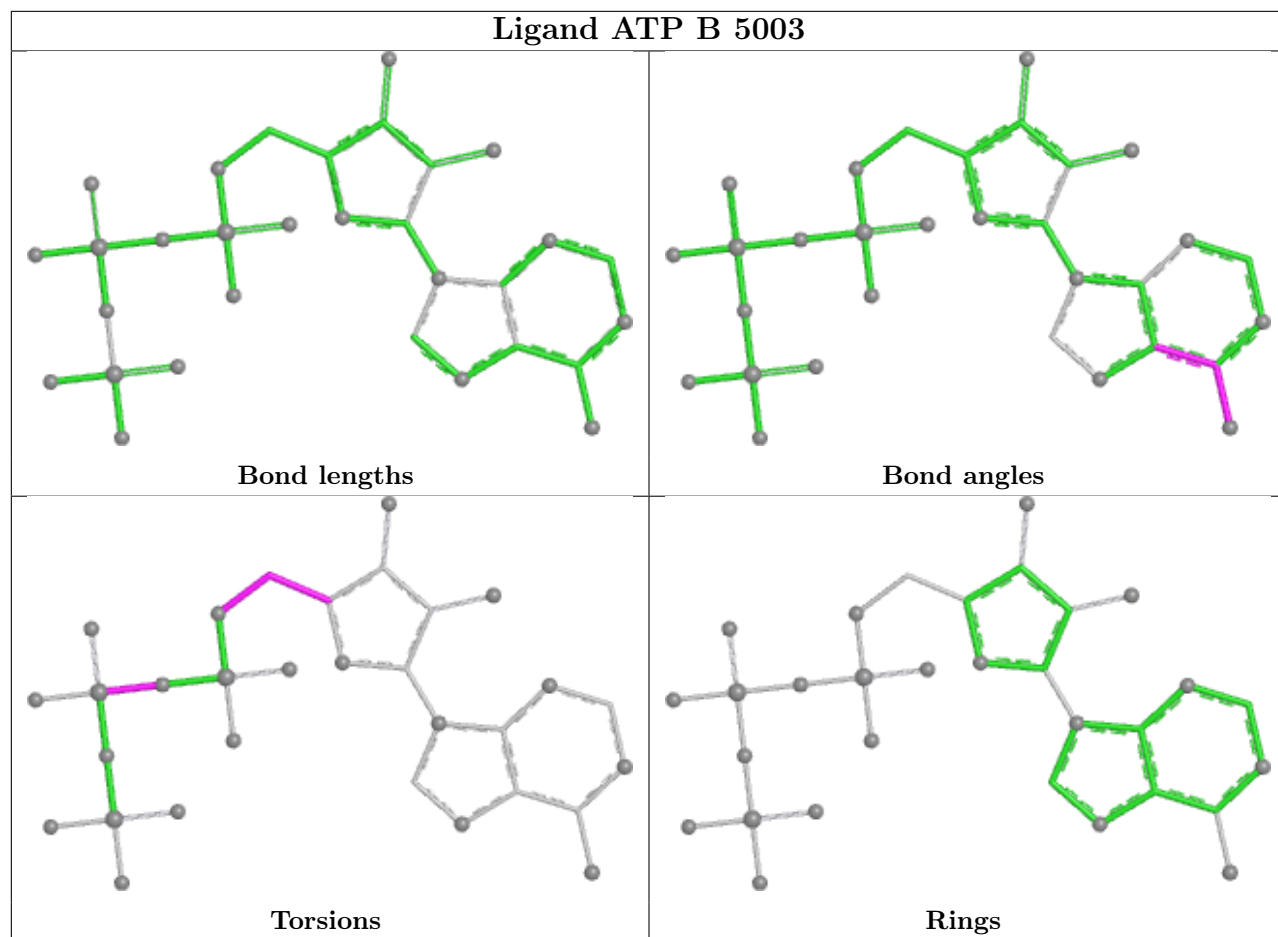
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

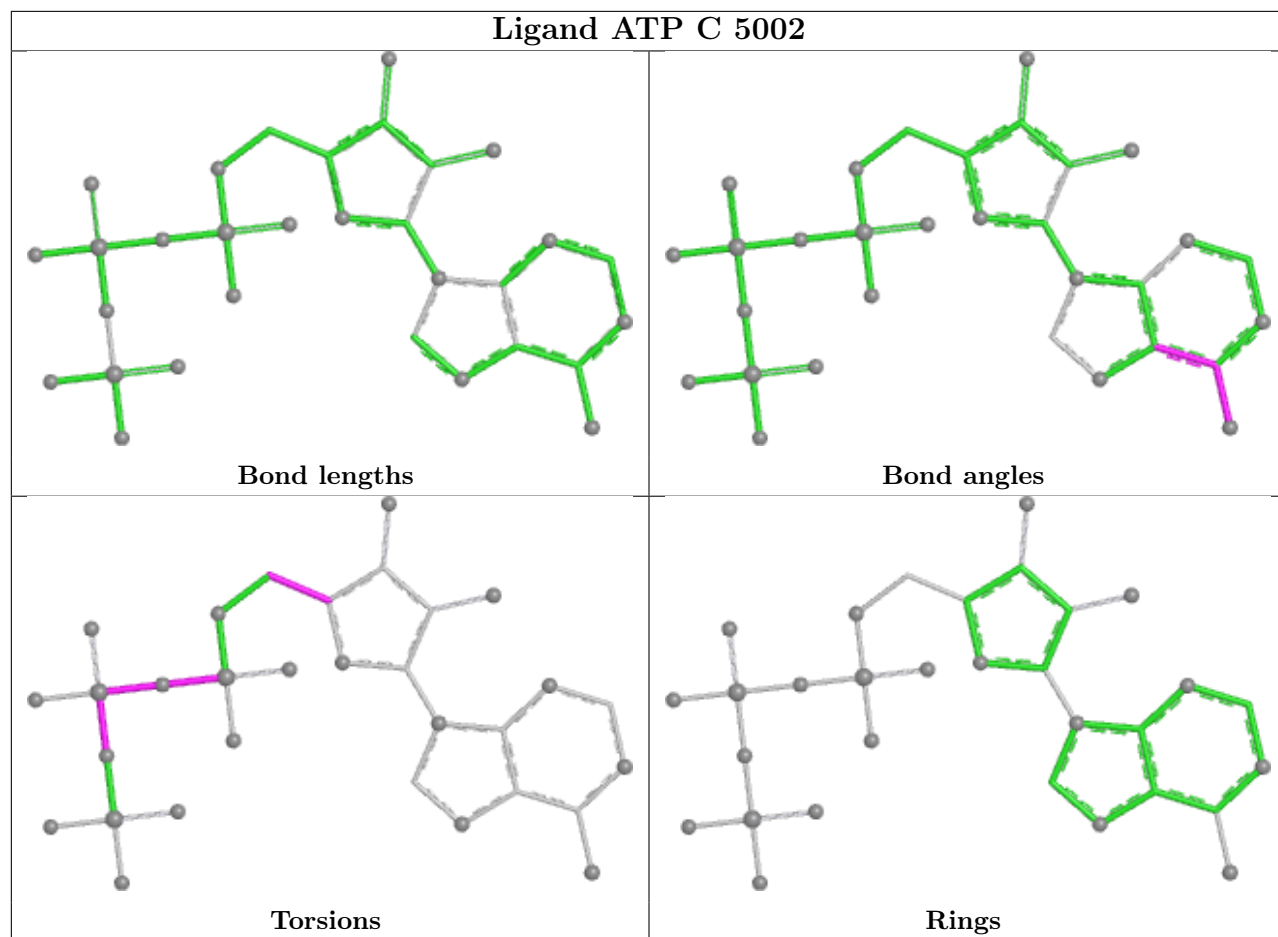
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

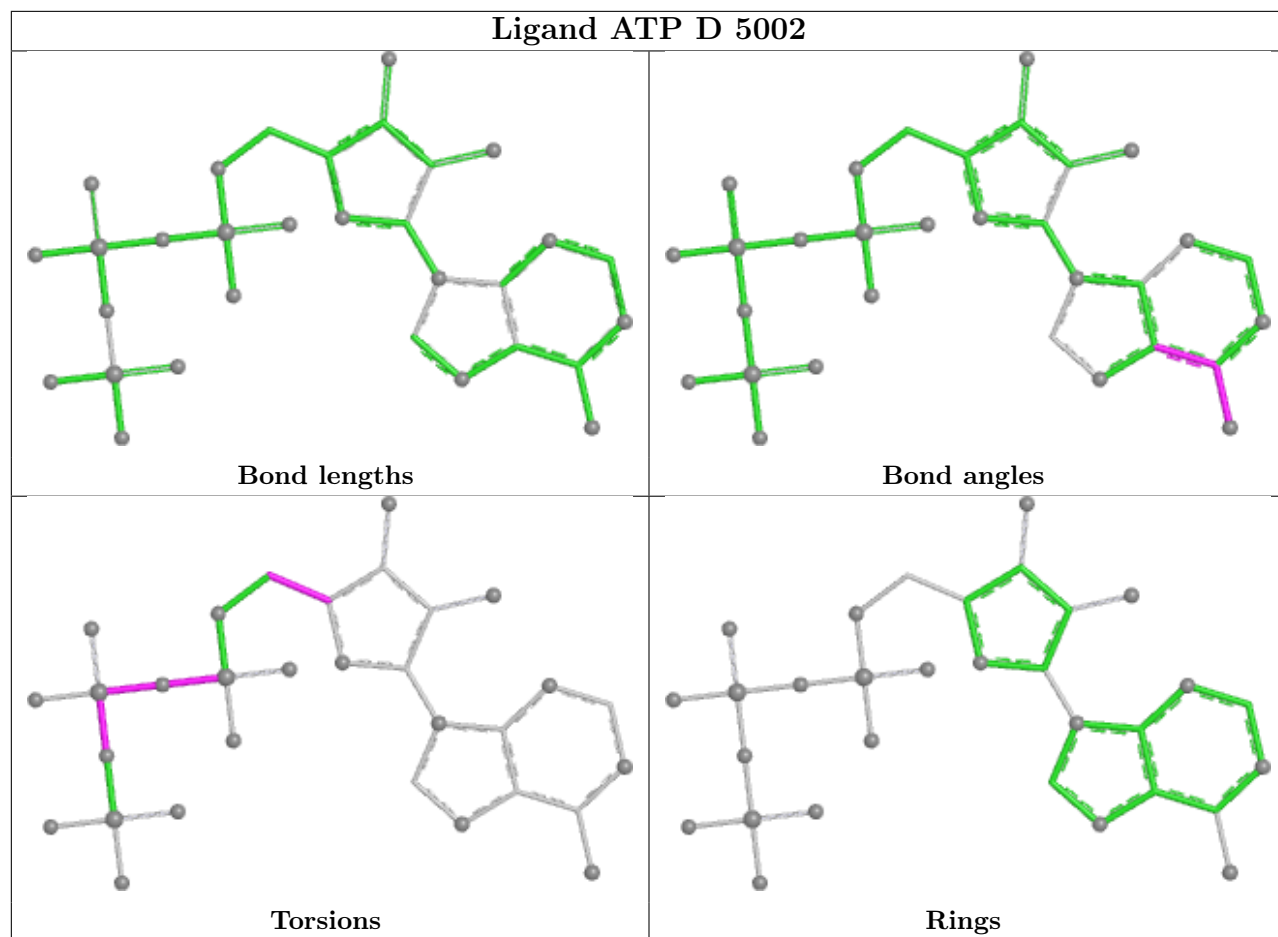




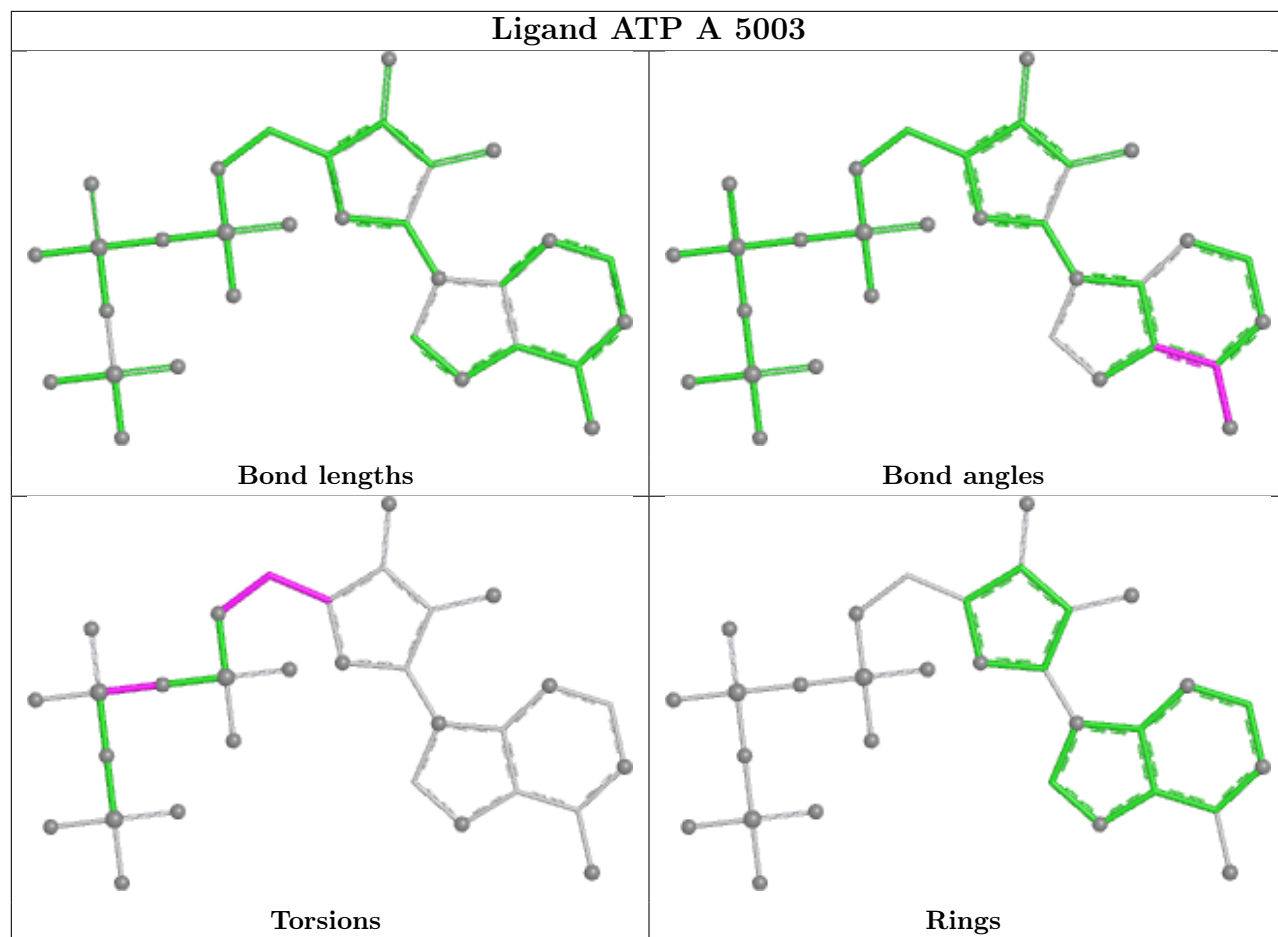


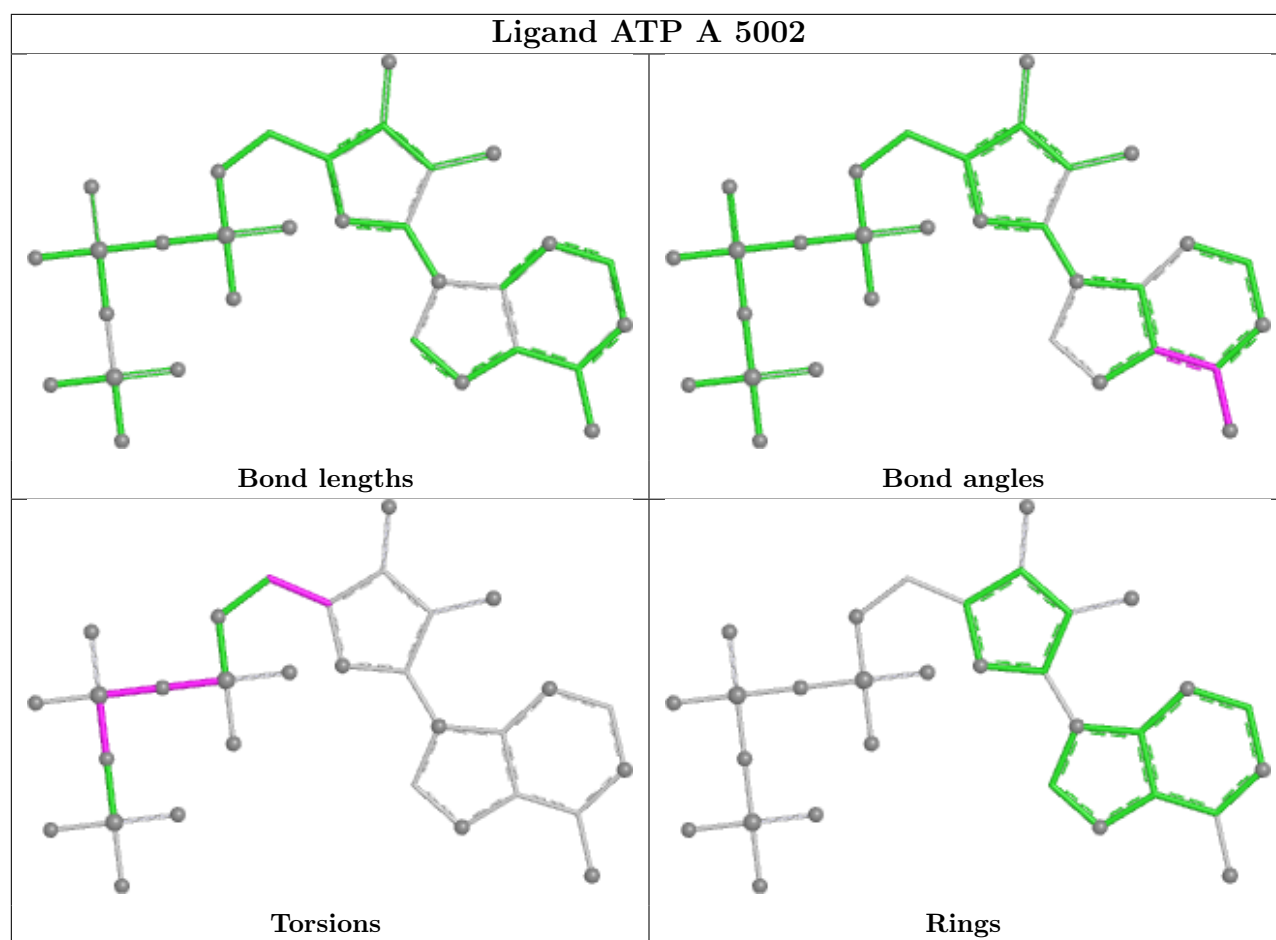












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

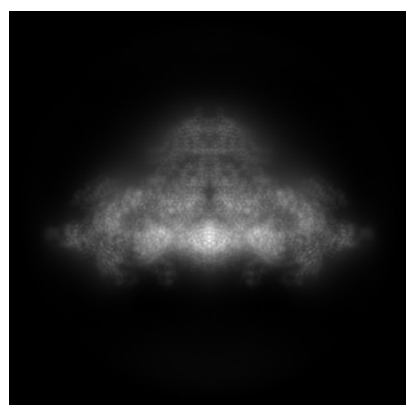
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26409. These allow visual inspection of the internal detail of the map and identification of artifacts.

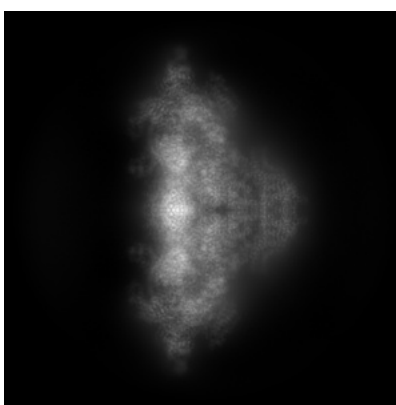
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

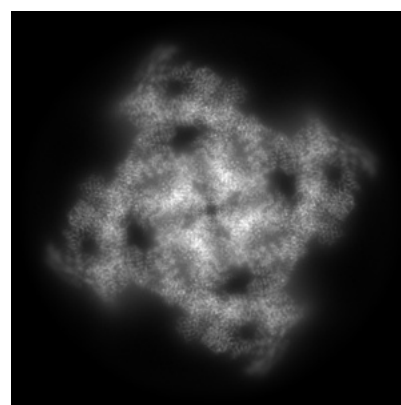
#### 6.1.1 Primary map



X



Y

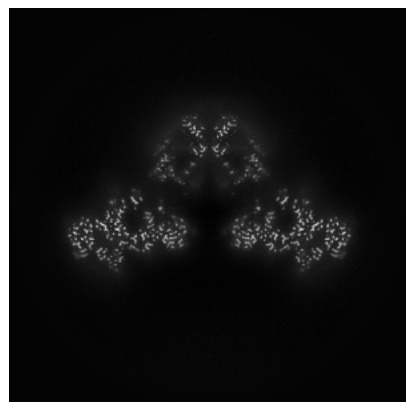


Z

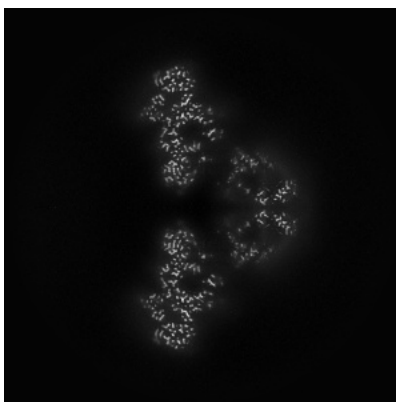
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

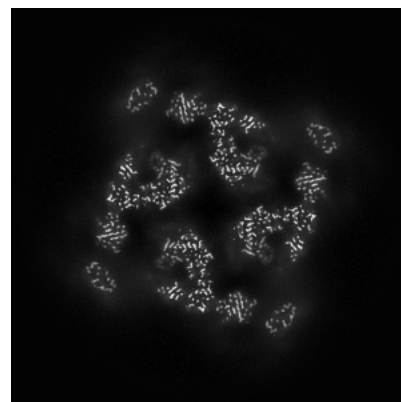
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

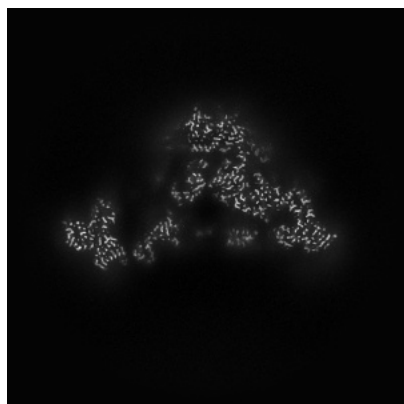


Z Index: 256

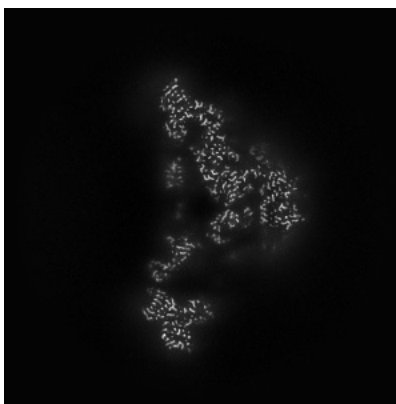
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

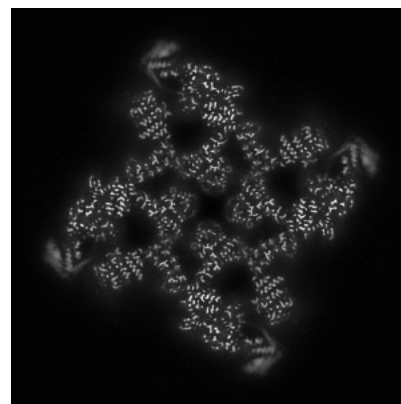
### 6.3.1 Primary map



X Index: 275



Y Index: 237

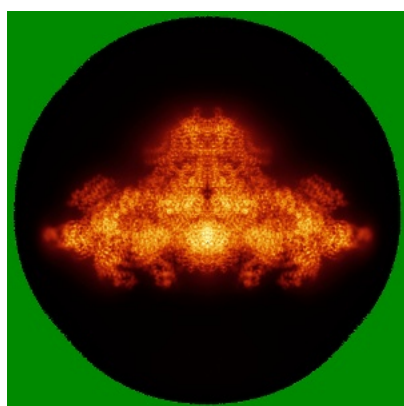


Z Index: 227

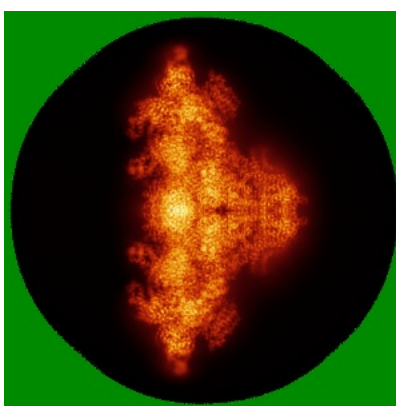
The images above show the largest variance slices of the map in three orthogonal directions.

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

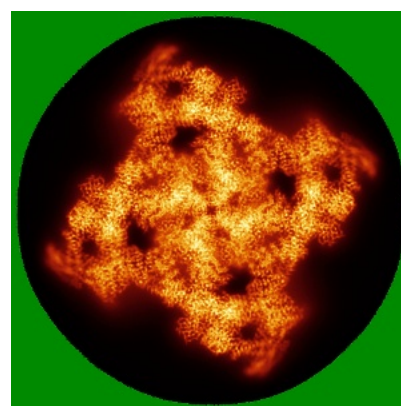
### 6.4.1 Primary map



X



Y

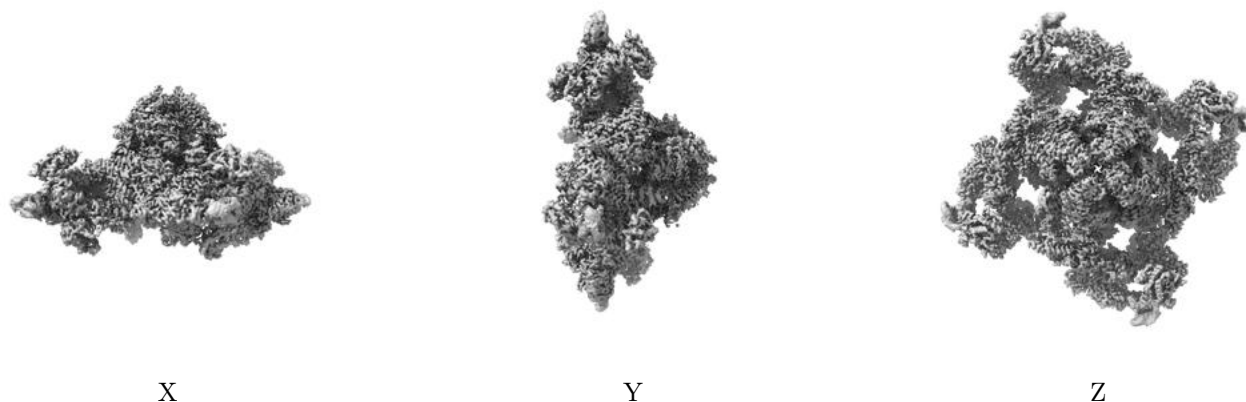


Z

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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

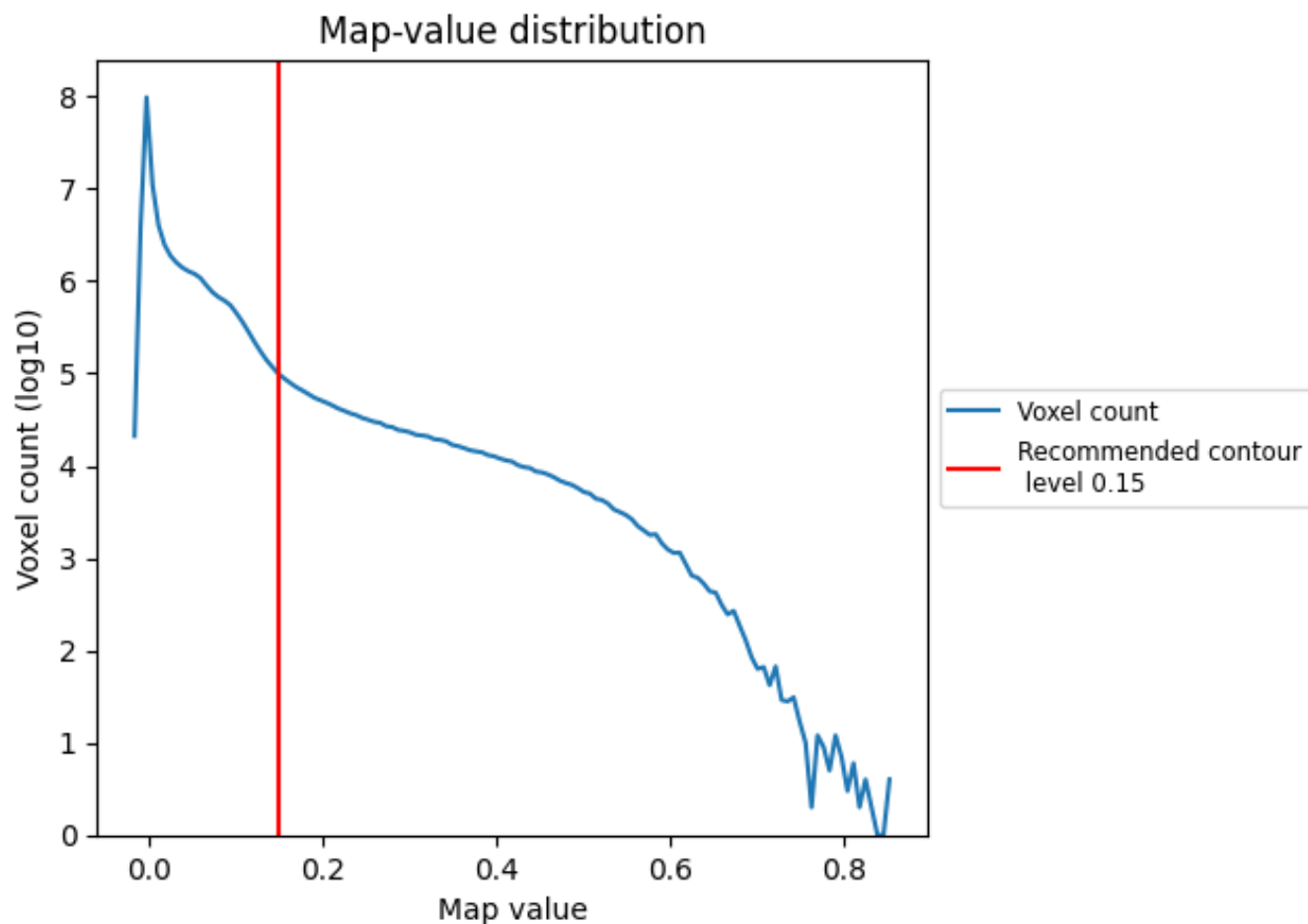
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

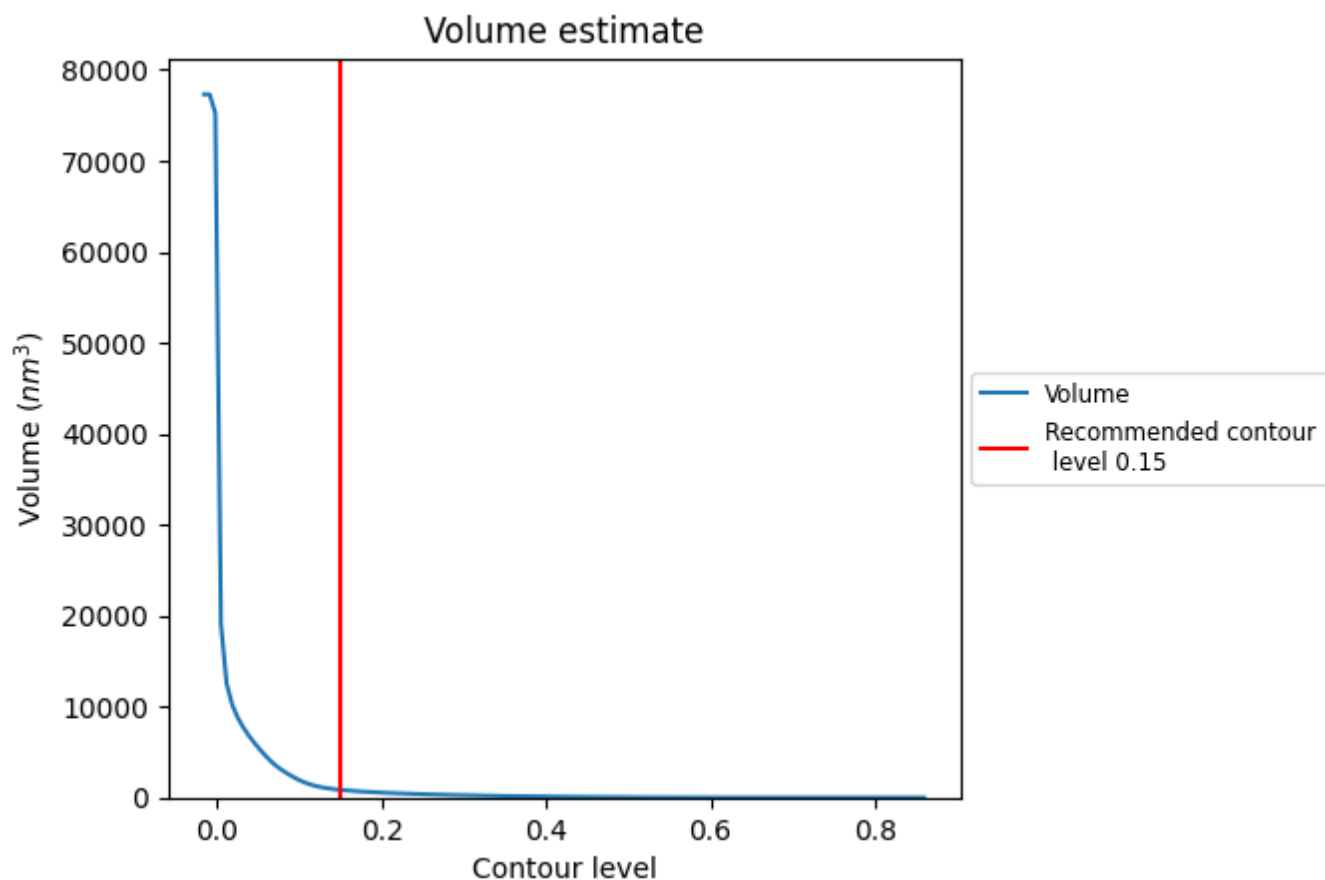
This section contains the results of statistical analysis of the map.

### 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.

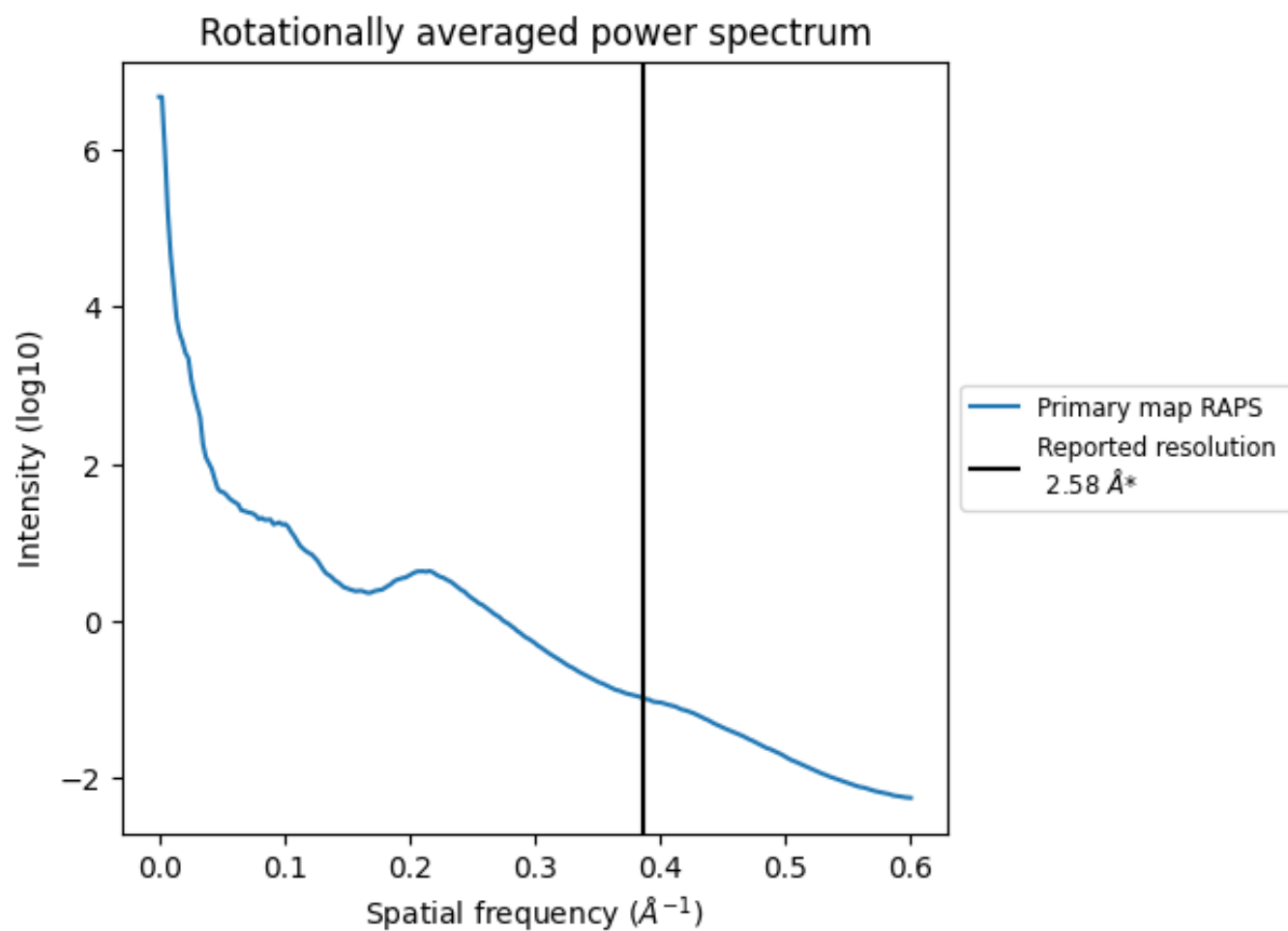
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 847 nm<sup>3</sup>; this corresponds to an approximate mass of 765 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 0.388 Å<sup>-1</sup>



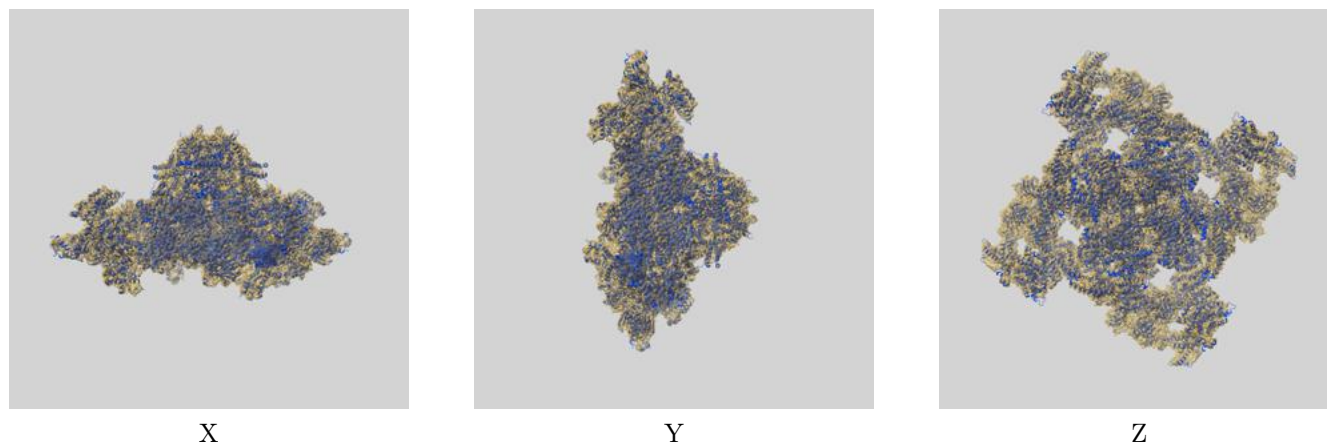
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

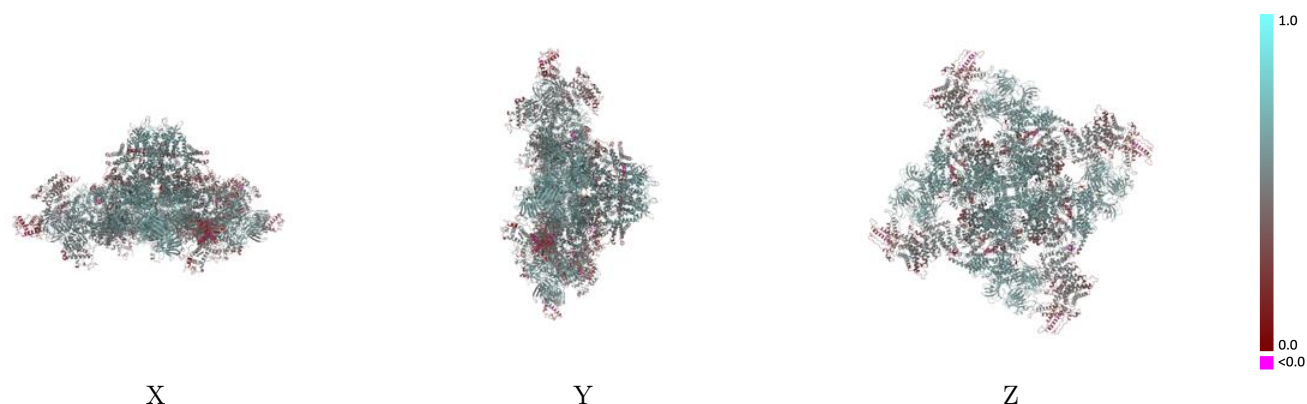
This section contains information regarding the fit between EMDB map EMD-26409 and PDB model 7U9X. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

### 9.1 Map-model overlay [i](#)



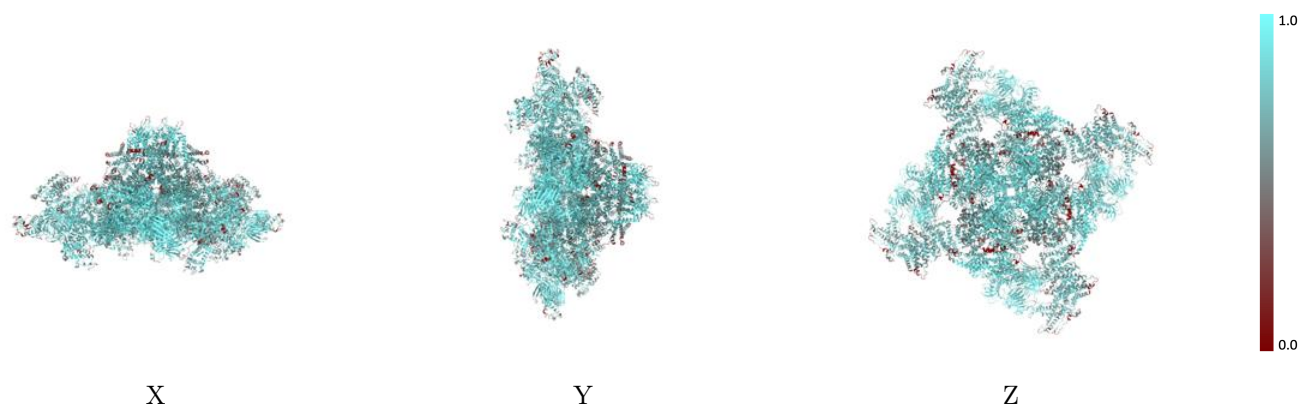
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



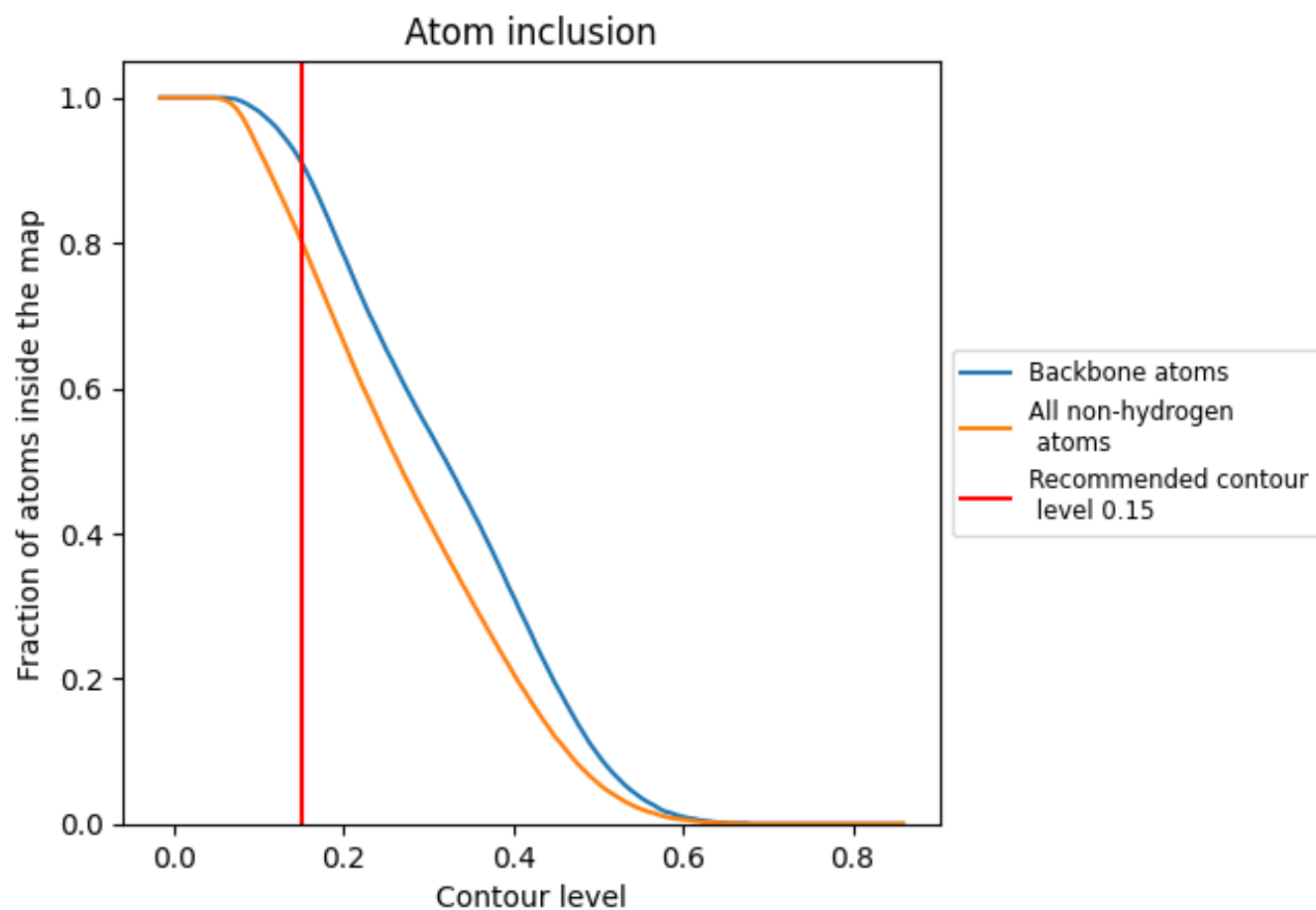
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8030	<div><div></div></div> 0.5150
A	<div><div></div></div> 0.8010	<div><div></div></div> 0.5150
B	<div><div></div></div> 0.8000	<div><div></div></div> 0.5100
C	<div><div></div></div> 0.8000	<div><div></div></div> 0.5100
D	<div><div></div></div> 0.8020	<div><div></div></div> 0.5170
E	<div><div></div></div> 0.9070	<div><div></div></div> 0.5880
F	<div><div></div></div> 0.8930	<div><div></div></div> 0.5750
G	<div><div></div></div> 0.9060	<div><div></div></div> 0.5720
H	<div><div></div></div> 0.9160	<div><div></div></div> 0.5910

1.0

0.0

<0.0