



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 10:27 AM EDT

PDB ID : 8UXC
EMDB ID : EMD-42759
Title : Structure of PKA phosphorylated human RyR2-R420Q in the primed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 2.86 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

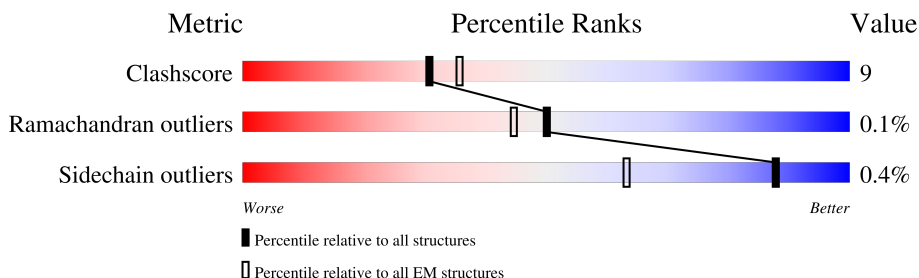
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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>12%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	B	4967	<div> <div>12%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	C	4967	<div> <div>12%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	D	4967	<div> <div>12%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
2	E	108	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	F	108	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	G	108	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	H	108	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 138600 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
			33769	21515	5743	6281	230		
1	B	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
1	C	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
1	D	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLN	ARG	engineered mutation	UNP Q92736
B	420	GLN	ARG	engineered mutation	UNP Q92736
C	420	GLN	ARG	engineered mutation	UNP Q92736
D	420	GLN	ARG	engineered mutation	UNP Q92736

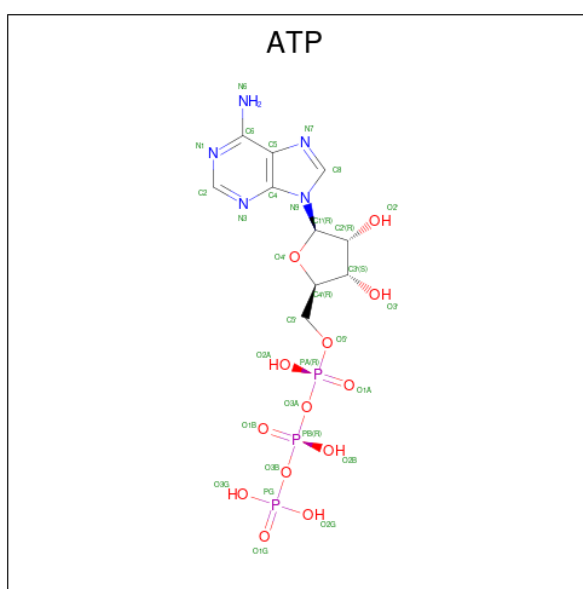
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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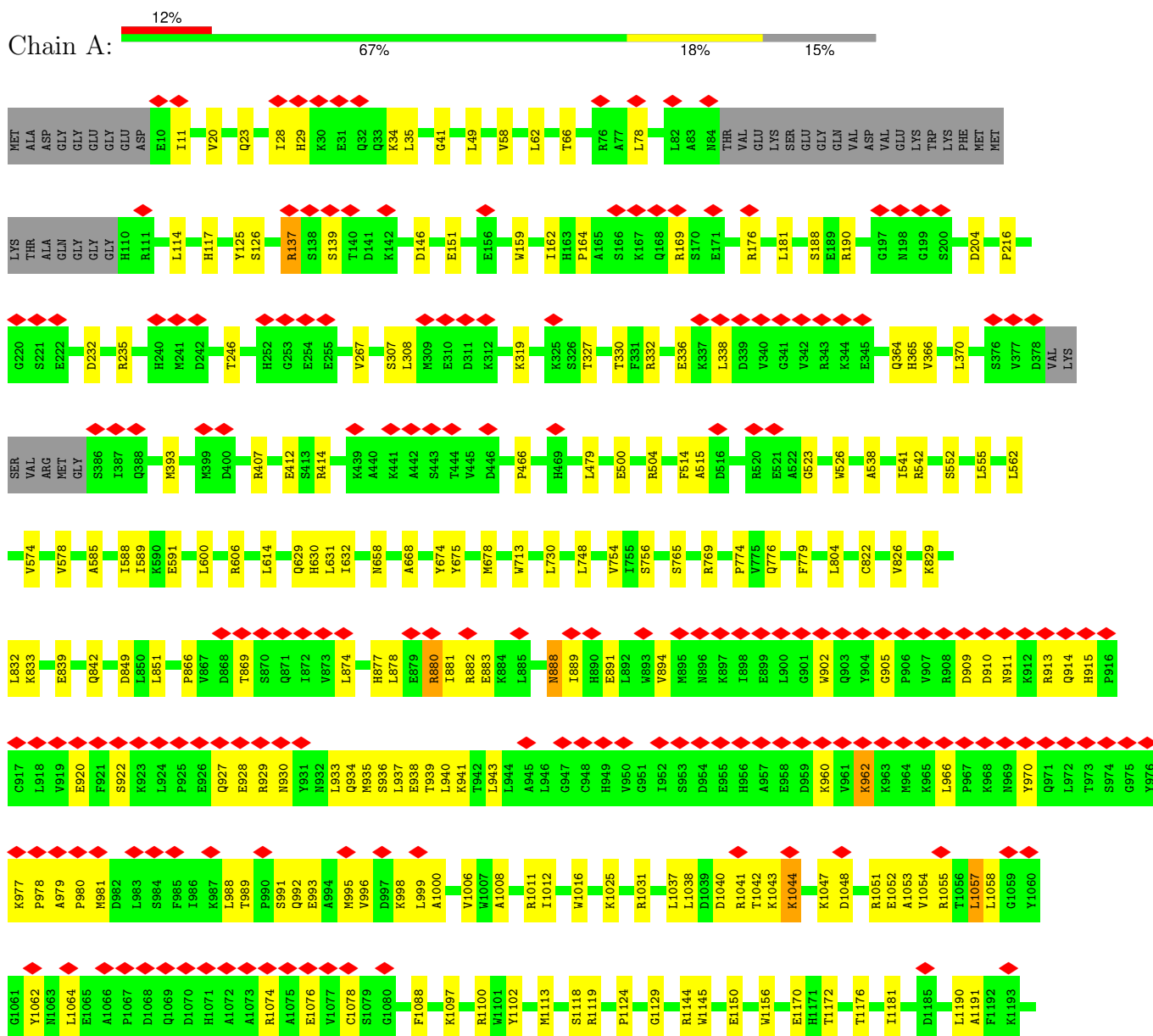
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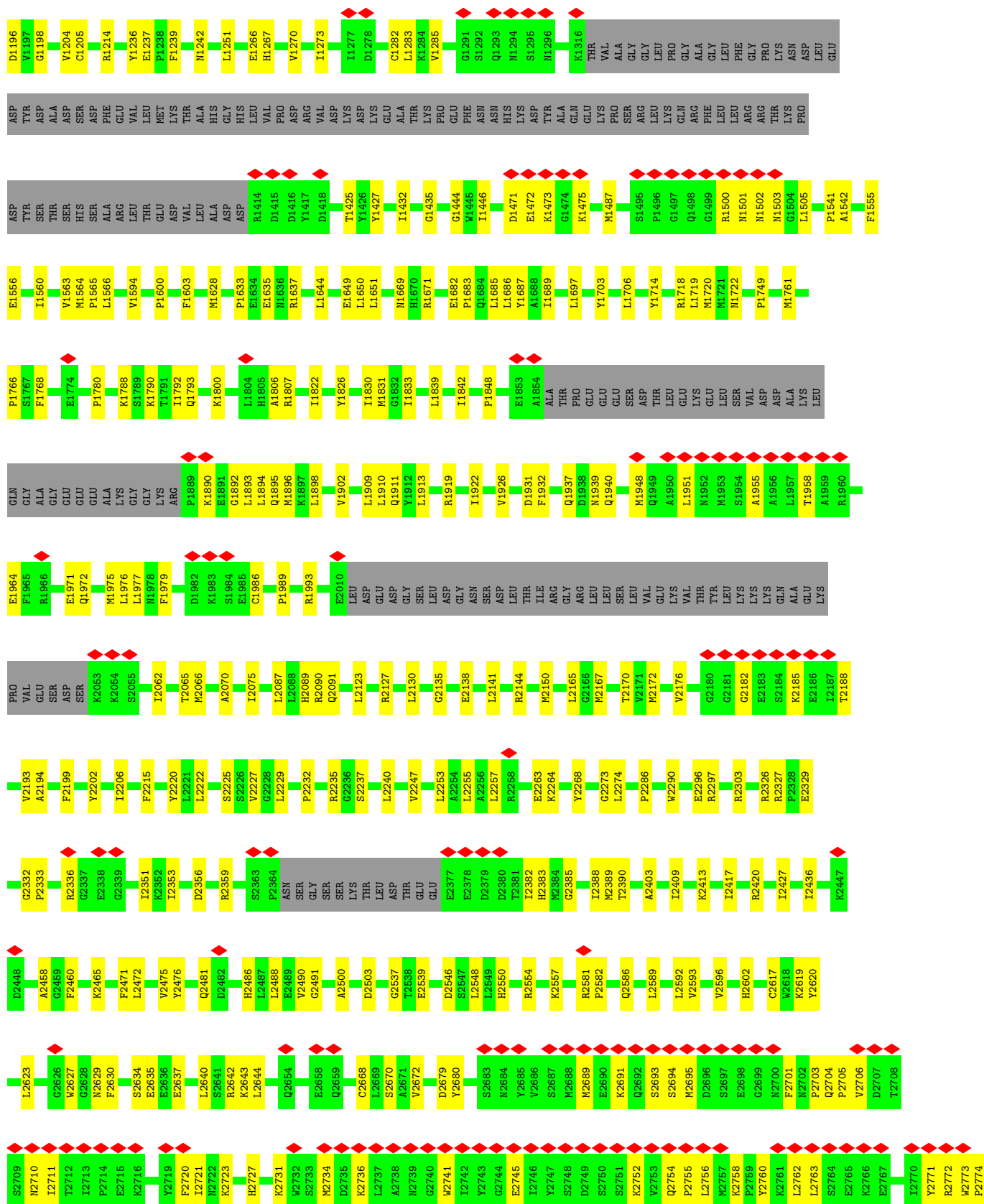
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	D	1	31	10	5	13	3	0

3 Residue-property plots [i](#)

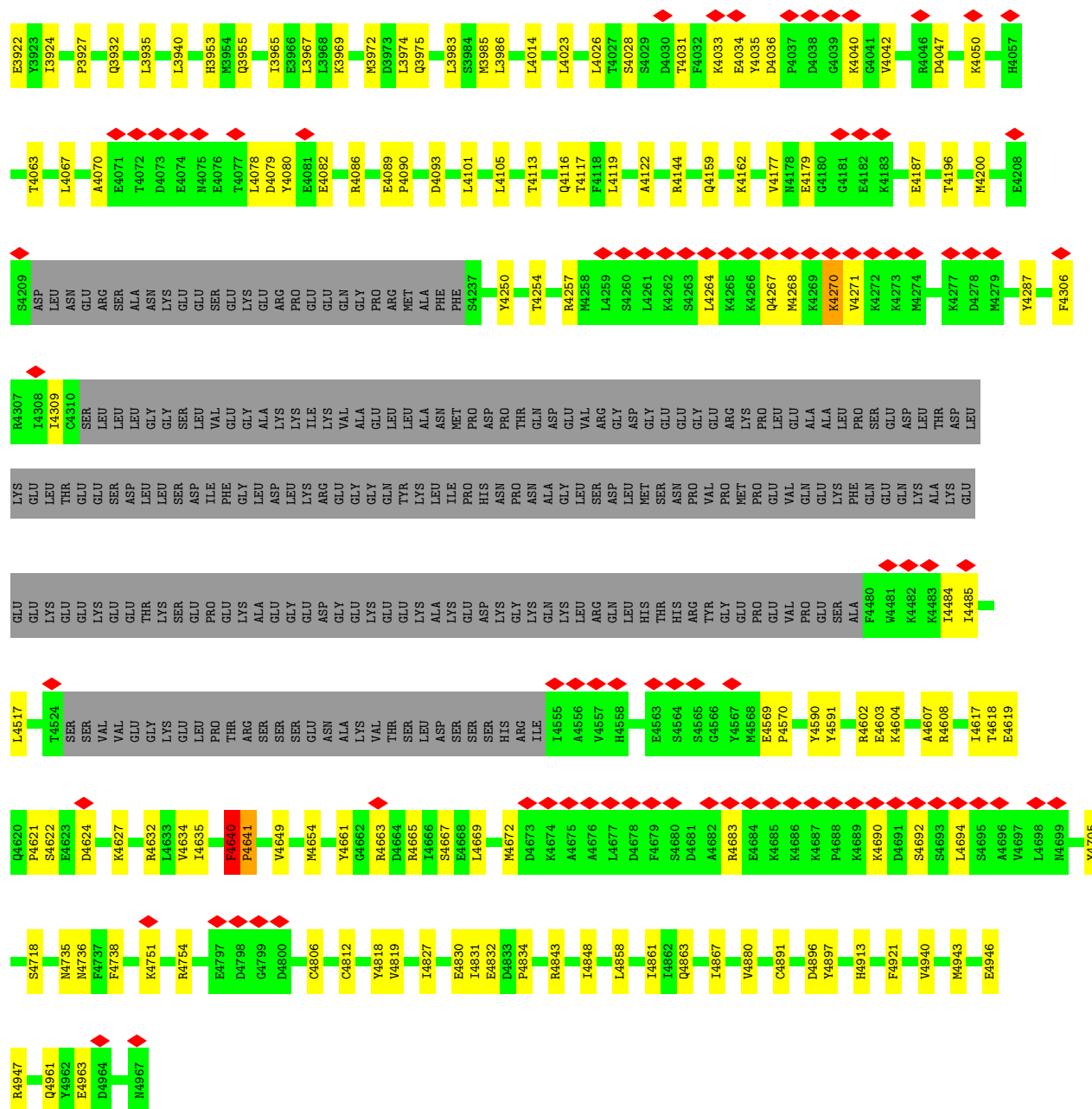
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 2

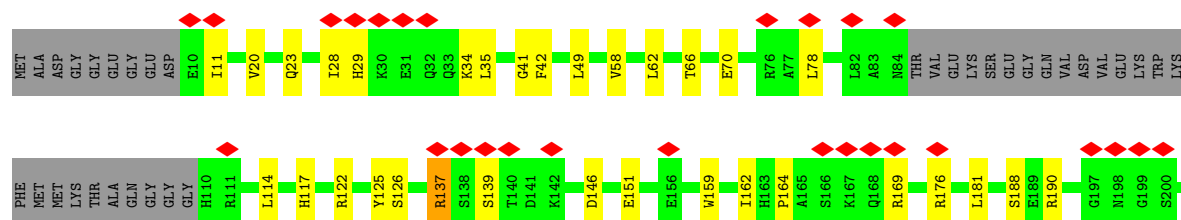








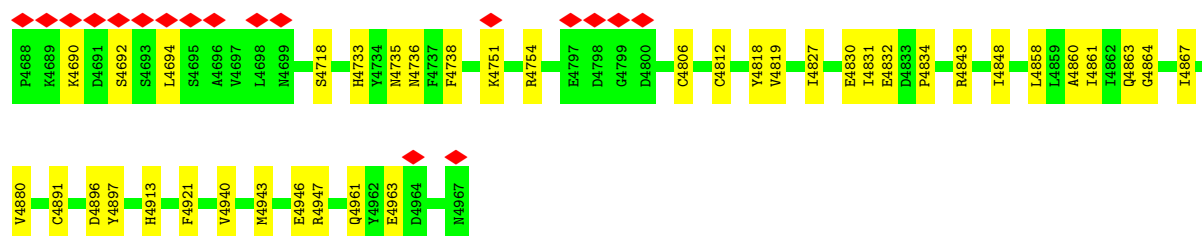
• Molecule 1: Ryanodine receptor 2



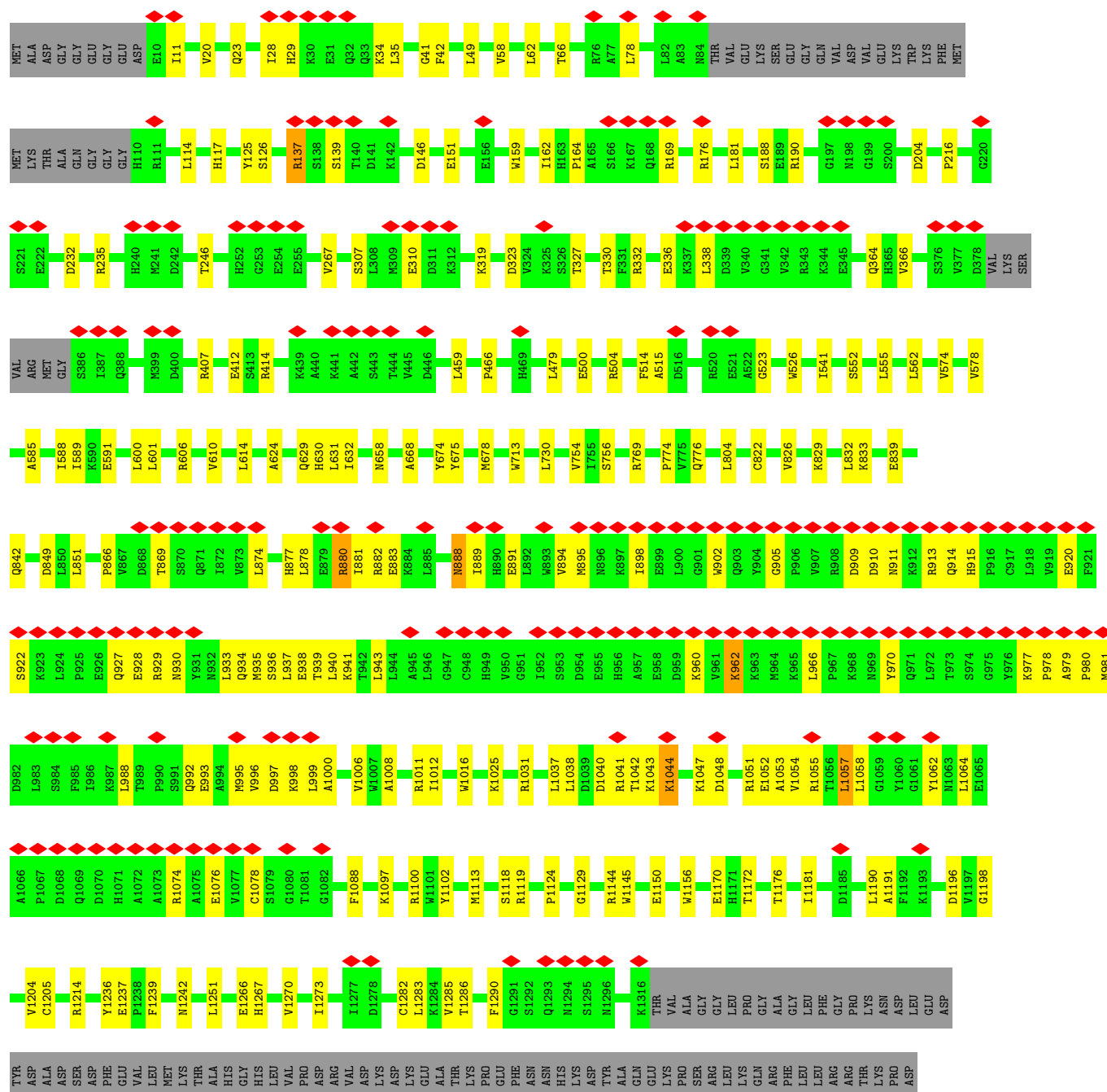


L3238	A3163	L3068	L2970	R2905	N2830	L2762	S2697	L2689	T2409	P2286	N2167	LEU
L3239	G3164	T3071	I2971	R2906	T2831	L2763	E2698	V2689	K2413	W2290	T2170	SER
F3240	F3166	M3072	D2972	C2906	T2832	S2764	G2699	V2693	L2417	R2297	V2171	LEU
M3246	F3167	E3073	Q2973	F2907	S2834	E2765	N2700	V2696	R2420	R2303	M2172	VAL
S3247	V3168	N3074	R2979	R2908	R2835	K2766	D2702	H2602	R2427	R2303	V2176	GLU
R3248	L3171	L3075	L2980	D2909	R2836	E2767	P2703	H2602	L2436	R2326	G2180	LYS
M3249	L3175	K3076	Y2981	L2910	D2836	I2770	Q2704	C2617	I2436	R2326	G2181	THR
N3250	H3178	Q3077	L2982	E2911	A2841	R2771	P2705	W2618	R2327	R2326	G2181	LYS
N3256	N3179	Q3079	L2984	D2912	E2842	R2772	V2706	K2619	E2328	E2329	E2183	LYS
R3260	H3178	F3080	A2985	L2913	M2843	R2773	T2708	Y2620	K2447	E2329	E2183	GLN
A3261	I3183	T3081	R2988	D2914	M2844	P2774	T2708	L2623	D2448	G2332	S2184	ALA
F3262	HIS	P2989	P2989	T2914	Y2848	K2776	S2709	L2623	A2458	P2333	K2185	GLU
K3263	THR	L2990	L2990	P2915	Y2848	K2776	N2710	G2626	G2459	R2336	E2186	LYS
C3264	ARG	C2991	C2991	E2918	I2851	W2785	I2711	W2627	G2459	R2336	E2186	PRO
C3265	ASN	S2992	S2992	R2920	I2851	G2786	T2712	W2627	F2460	G2337	I2187	VAL
L3268	GLN	H2995	H2995	F2921	K2854	W2787	L2713	N2629	K2465	E2338	T2188	GLU
S3270	PRO	N2995	N2995	Y2923	K2854	I2789	P2714	F2630	F2471	E2339	V2193	SER
M3273	K3088	N2998	N2998	L2926	K2857	E2790	E2715	S2634	L2472	I2351	A2194	ASP
L3276	G3089	K2999	K2999	Q2927	M2858	R2791	K2716	E2635	L2472	I2351	F2189	K2063
L3277	V3090	E3000	E3000	Q2928	E2859	T2792	N2719	E2635	D2482	K2352	Y2202	K2064
L3281	T3091	K3001	K3001	L2930	L2860	E2793	F2720	E2637	Y2476	I2353	Y2202	M2066
L3282	Q3092	E3002	E3002	L2930	E2861	E2794	L2721	L2640	Q2481	D2356	L2206	T2065
M3283	L3093	M3004	M3004	R2931	S2862	E2795	N2722	S2641	D2482	R2359	F2215	M2066
L3284	T3094	T3005	T3005	R2931	K2863	E2796	K2723	L2644	H2486	D2356	Y2220	A2070
Y3285	Y3095	S3006	S3006	E2935	E2864	D2796	H2727	E2659	L2487	S2363	L2206	T2065
L3288	K3010	K3010	K3010	A2996	G2866	S2797	K2731	Q2654	L2488	P2364	Y2220	A2070
G3289	L3011	L3011	L3011	H2997	G2866	M2798	E2732	E2659	E2489	ASN	S2226	L2087
L3290	C3012	C3012	C3012	Y2939	E2866	A2799	N2733	E2659	E2489	SER	S2226	L2087
D3291	R3016	R3016	R3016	L2941	N2867	L2800	S2733	E2659	G2491	GLY	V2227	H2089
E3292	I3019	I3019	I3019	E2942	E2868	Y2801	S2733	E2659	A2500	SER	G2228	R2090
G3293	S3020	S3020	S3020	F2943	L2870	N2802	N2734	E2659	D2503	THR	L2229	Q2091
A3294	H3034	H3034	H3034	D2944	L2871	ARG	D2735	E2659	D2503	THR	L2229	L2087
M3295	I3035	I3035	I3035	G2945	V2872	THR	K2736	E2659	D2503	THR	L2229	L2087
N3296	Q3038	Q3038	Q3038	G2946	Y2874	ARG	L2737	E2659	D2503	THR	L2229	L2087
K3297	L3040	L3040	L3040	S2947	D2875	ARG	A2738	E2659	D2503	THR	L2229	L2087
R3298	L3040	L3040	L3040	R2948	T2876	ILE	N2739	E2659	D2503	THR	L2229	L2087
L3299	L3040	L3040	L3040	R2948	L2877	SER	G2740	E2659	D2503	THR	L2229	L2087
Q3304	L3040	L3040	L3040	Q2949	L2877	THR	N2741	E2659	D2503	THR	L2229	L2087
F3305	L3040	L3040	L3040	K2950	E2881	SER	L2742	E2659	D2503	THR	L2229	L2087
L3306	L3040	L3040	L3040	G2951	K2882	GLN	Y2743	E2659	D2503	THR	L2229	L2087
R3307	L3040	L3040	L3040	E2952	A2883	VAL	N2684	E2659	D2503	THR	L2229	L2087
M3308	L3040	L3040	L3040	H2953	K2884	SER	Y2686	E2659	D2503	THR	L2229	L2087
N3309	L3040	L3040	L3040	F2954	D2886	VAL	E2745	E2659	D2503	THR	L2229	L2087
V3310	L3040	L3040	L3040	P2955	R2887	ASP	L2746	E2659	D2503	THR	L2229	L2087
Q3313	L3040	L3040	L3040	Y2956	E2887	ALA	Y2747	E2659	D2503	THR	L2229	L2087
L3314	L3040	L3040	L3040	E2957	Q2890	HIS	S2748	E2659	D2503	THR	L2229	L2087
K3315	L3040	L3040	L3040	Q2958	D2891	THR	D2749	E2659	D2503	THR	L2229	L2087
T3317	L3040	L3040	L3040	E2959	L2892	SER	S2750	E2659	D2503	THR	L2229	L2087
L3316	L3040	L3040	L3040	I2960	L2893	VAL	S2751	E2659	D2503	THR	L2229	L2087
L3317	L3040	L3040	L3040	L2966	K2894	VAL	V2753	E2659	D2503	THR	L2229	L2087
L3318	L3040	L3040	L3040	V2967	F2895	ASP	Q2754	E2659	D2503	THR	L2229	L2087
L3319	L3040	L3040	L3040	L2968	L2896	ALA	P2755	E2659	D2503	THR	L2229	L2087
L3320	L3040	L3040	L3040	P2969	L2899	ALA	L2756	E2659	D2503	THR	L2229	L2087
L3321	L3040	L3040	L3040	N2899	N2899	HIS	N2757	E2659	D2503	THR	L2229	L2087
L3322	L3040	L3040	L3040	N2899	N2899	HIS	K2758	E2659	D2503	THR	L2229	L2087
L3323	L3040	L3040	L3040	N2899	N2899	HIS	Y2760	E2659	D2503	THR	L2229	L2087
L3324	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3325	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3326	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3327	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3328	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3329	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3330	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3331	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3332	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3333	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3334	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3335	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3336	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087
L3337	L3040	L3040	L3040	N2899	N2899	HIS	K2761	E2659	D2503	THR	L2229	L2087





• Molecule 1: Ryanodine receptor 2



E2842	M2843	M2844	Y2848	L2851	K2854	K2857	M2858	E2859	L2860	E2861	S2862	K2863	G2864	G2865	G2866	M2867	H2868	F2869	L2870	L2871	V2872	Y2873	Y2874	D2875	L2876	L2877	E2881	K2882	K2883	K2884	L2885	R2886	E2887	Q2890	D2891	L2892	L2893	K2894	F2895	L2896	Q2897	L2898	M2899	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913																																		
S2709	N2710	I2711	T2712	P2713	P2714	E2715	K2716	Y2719	F2720	L2721	K2723	H2727	K2731	S2732	S2733	M2734	D2735	K2736	L2737	A2738	N2739	G2740	G2741	L2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	S2750	S2751	K2752	K2753	Q2754	P2755	L2756	M2757	K2758	P2759	Y2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	L2770	Y2771	R2772	W2773	P2774																																
I2775	K2776	W2785	G2786	M2787	R2788	L2789	E2790	R2791	T2792	R2793	E2794	G2795	D2796	S2797	M2798	A2799	L2800	Y2801	M2802	ARG	THR	ARG	ILE	SER	GLN	THR	GLN	VAL	SER	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	L2826	D2827	M2828	S2829	M2830	V2831	L2832	L2833	S2834	D2835	L2837	H2838	M2840	A2841																																
E2842	H2843	M2844	Y2848	L2851	K2854	K2857	M2858	E2859	L2860	E2861	S2862	K2863	G2864	G2865	G2866	M2867	H2868	F2869	L2870	L2871	V2872	Y2873	Y2874	D2875	L2876	L2877	E2881	K2882	K2883	K2884	L2885	R2886	E2887	Q2890	D2891	L2892	L2893	K2894	F2895	L2896	Q2897	L2898	M2899	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913																																		
P1565	L1566	V1594	P1600	F1603	M1628	P1633	E1634	E1635	M1636	R1637	L1644	E1649	L1650	L1651	L1667	G1668	M1669	H1670	R1671	E1682	M1683	Q1684	L1685	L1686	Y1687	A1688	I1689	Y1703	D1704	L1705	L1706	I1707	D1708	S1712	S1713	Y1714	R1718	L1719	M1720	M1721	N1722	P1749	M1761	P1766																																										
S1767	F1768	E1774	P1780	K1788	S1789	K1790	Q1793	M1794	K1800	L1804	H1805	A1806	R1807	I1822	Y1826	I1830	M1831	G1832	I1833	L1839	I1842	P1848	S1849	K1852	E1853	A1854	ALA	THR	PRO	GLU	GLU	GLU	SER	ASP	THR	LEU	GLU	LYS	LYS	LEU	SER	VAL	ASP	ASP	LYS	LYS	LYS	ALA																																						
LEU	GLN	GLY	ALA	GLY	GLU	GLU	ALA	LYS	GLY	LYS	LYS	ARG	P1889	K1890	L1893	L1894	Q1895	M1896	K1897	L1898	V1902	L1909	L1910	Q1911	Y1912	L1913	R1919	I1922	Y1926	S1929	D1930	L1931	F1932	Q1937	D1938	N1939	Q1940	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	L1956	L1957	T1958	A1959																																					
R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	M1978	F1979	D1982	K1983	S1984	C1986	P1989	R1993	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	SER	ASP	LEU	THR	ILE	ARG	GLY	ARG	LEU	LEU	SER	VAL	GLU	LYS	VAL	THR	TYR	LEU	LYS	LYS	GLN	ALA																																					
E2186	I2187	T2188	V2193	A2194	F2199	Y2202	I2206	F2215	Y2220	S2225	S2226	V2227	G2228	L2229	P2232	R2235	G2236	S2237	L2240	V2247	L2253	A2254	L2255	A2256	L2257	R2258	E2263	K2264	Y2268	G2273	L2274	P2286	W2290	E2296	R2297	R2303	V2319	L2323	R2326	R2327	E2329	G2332	P2333	R2336	G2337	E2338	G2339	I2351	K2352	L2353	D2356	F2357	S2358	R2359	S2363	P2364	ASN	SER	GLY	SER	LYS	THR	LEU	ASP	THR	GLU	E2377	E2378	D2379	T2381	L2382	H2383	R2384	G2385	L2388	M2389	T2390	A2403	L2409	K2413	L2417	R2420				
I2436	K2447	D2448	A2458	G2459	F2460	K2465	L2472	V2475	Y2476	Q2481	D2482	H2486	L2487	L2488	E2489	V2490	G2491	A2500	D2503	G2537	T2538	E2539	D2546	S2547	L2548	H2550	R2554	K2557	R2581	P2582	Q2586	L2592	V2593	Y2596	H2602	C2617	W2618	K2619	R2626	G2627	G2628	F2630	S2634	E2635	E2636	E2637	L2640	S2641	R2642	K2643	L2644	Q2654	E2658	C2668	L2669	S2670	A2671	V2672	D2679	Y2680	S2683	N2684	Y2685	V2686	S2687	M2688	E2689	E2690	K2691	Q2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	H2700	F2701	M2702	P2703	Q2704	P2705	V2706	D2707	T2708
Y2620	L2623	G2626	W2627	G2628	N2629	F2630	S2634	E2635	E2636	E2637	L2640	S2641	R2642	K2643	L2644	Q2654	E2658	C2668	L2669	S2670	A2671	V2672	D2679	Y2680	S2683	N2684	Y2685	V2686	S2687	M2688	E2689	E2690	K2691	Q2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	H2700	F2701	M2702	P2703	Q2704	P2705	V2706	D2707	T2708																																				
S2709	N2710	I2711	T2712	P2713	P2714	E2715	K2716	Y2719	F2720	L2721	K2723	H2727	K2731	S2732	S2733	M2734	D2735	K2736	L2737	A2738	N2739	G2740	G2741	L2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	S2750	S2751	K2752	K2753	Q2754	P2755	L2756	M2757	K2758	P2759	Y2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	L2770	Y2771	R2772	W2773	P2774																																
I2775	K2776	W2785	G2786	M2787	R2788	L2789	E2790	R2791	T2792	R2793	E2794	G2795	D2796	S2797	M2798	A2799	L2800	Y2801	M2802	ARG	THR	ARG	ILE	SER	GLN	THR	GLN	VAL	SER	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	L2826	D2827	M2828	S2829	M2830	V2831	L2832	L2833	S2834	D2835	L2837	H2838	M2840	A2841																																
E2842	H2843	M2844	Y2848	L2851	K2854	K2857	M2858	E2859	L2860	E2861	S2862	K2863	G2864	G2865	G2866	M2867	H2868	F2869	L2870	L2871	V2872	Y2873	Y2874	D2875	L2876	L2877	E2881	K2882	K2883	K2884	L2885	R2886	E2887	Q2890	D2891	L2892	L2893	K2894	F2895	L2896	Q2897	L2898	M2899	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913																																		



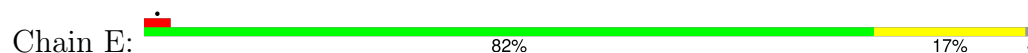




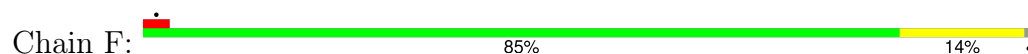
WORLDWIDE
PDB
PROTEIN DATA BANK



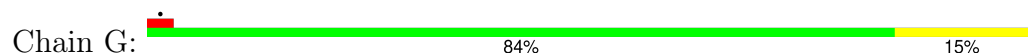
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



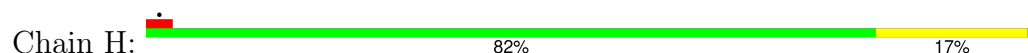
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- 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, Not provided	
Number of particles used	143933	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	0.730	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/34509	0.48	6/46612 (0.0%)
1	B	0.25	0/34509	0.48	6/46612 (0.0%)
1	C	0.25	0/34509	0.48	6/46612 (0.0%)
1	D	0.25	0/34509	0.48	6/46612 (0.0%)
2	E	0.26	0/834	0.48	0/1123
2	F	0.27	0/834	0.48	0/1123
2	G	0.27	0/834	0.48	0/1123
2	H	0.27	0/834	0.48	0/1123
All	All	0.25	0/141372	0.48	24/190940 (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.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4640	PHE	C-N-CD	-6.73	105.79	120.60
1	C	4640	PHE	C-N-CD	-6.71	105.83	120.60
1	A	4640	PHE	C-N-CD	-6.71	105.84	120.60
1	D	4640	PHE	C-N-CD	-6.70	105.86	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2990	LEU	CA-CB-CG	6.38	129.96	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4640	PHE	Peptide
1	B	4640	PHE	Peptide
1	C	4640	PHE	Peptide
1	D	4640	PHE	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	33769	0	33450	598	0
1	B	33769	0	33450	602	0
1	C	33769	0	33450	599	0
1	D	33769	0	33450	592	0
2	E	818	0	821	13	0
2	F	818	0	821	11	0
2	G	818	0	821	11	0
2	H	818	0	821	11	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	1	0
4	B	62	0	24	1	0
4	C	62	0	24	1	0
4	D	62	0	24	1	0
All	All	138600	0	137180	2407	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 2407 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:D:3293:GLY:H	1:D:3296:MET:HE1	1.32	0.94
1:C:3293:GLY:H	1:C:3296:MET:HE1	1.33	0.94
1:A:3293:GLY:H	1:A:3296:MET:HE1	1.33	0.93
1:B:3293:GLY:H	1:B:3296:MET:HE1	1.32	0.91
1:C:1940:GLN:HE22	1:C:1972:GLN:HE21	1.16	0.90

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%)	4086 (97%)	109 (3%)	3 (0%)	48	69
1	B	4198/4967 (84%)	4087 (97%)	108 (3%)	3 (0%)	48	69
1	C	4198/4967 (84%)	4086 (97%)	109 (3%)	3 (0%)	48	69
1	D	4198/4967 (84%)	4087 (97%)	108 (3%)	3 (0%)	48	69
2	E	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
2	F	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
2	G	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
2	H	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
All	All	17212/20300 (85%)	16762 (97%)	438 (2%)	12 (0%)	50	69

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3927	PRO
1	A	4641	PRO
1	B	3927	PRO
1	B	4641	PRO
1	C	3927	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	3708/4358 (85%)	3691 (100%)	17 (0%)	86	94
1	B	3708/4358 (85%)	3691 (100%)	17 (0%)	86	94
1	C	3708/4358 (85%)	3691 (100%)	17 (0%)	86	94
1	D	3708/4358 (85%)	3691 (100%)	17 (0%)	86	94
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%)	15116 (100%)	68 (0%)	88	95

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

Mol	Chain	Res	Type
1	D	1025	LYS
1	D	1473	LYS
1	D	3227	ARG
1	B	1044	LYS
1	B	1025	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	934	GLN
1	C	3955	GLN
1	C	1267	HIS
1	C	2704	GLN
1	D	658	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	A	5002	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)
4	ATP	B	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	B	5002	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
4	ATP	A	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	D	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	C	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	C	5002	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
4	ATP	D	5002	-	28,33,33	0.65	0	34,52,52	0.59	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	A	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	D	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	D	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	5002	ATP	C5-C6-N6	2.35	123.89	120.31
4	B	5003	ATP	C5-C6-N6	2.35	123.89	120.31
4	D	5003	ATP	C5-C6-N6	2.34	123.87	120.31
4	A	5003	ATP	C5-C6-N6	2.33	123.86	120.31
4	C	5002	ATP	C5-C6-N6	2.31	123.84	120.31

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C5'-O5'-PA-O1A
4	B	5003	ATP	C5'-O5'-PA-O2A

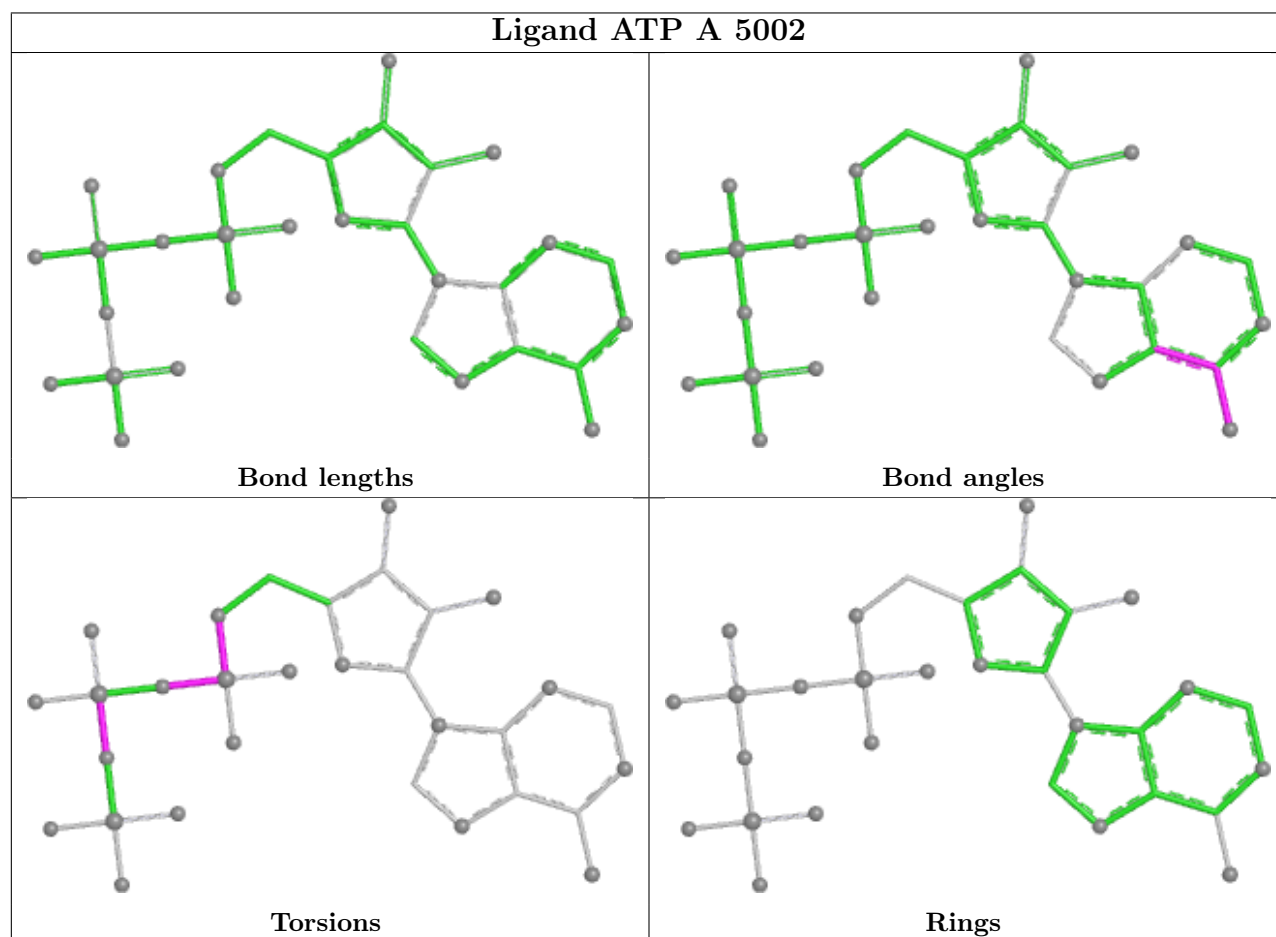
There are no ring outliers.

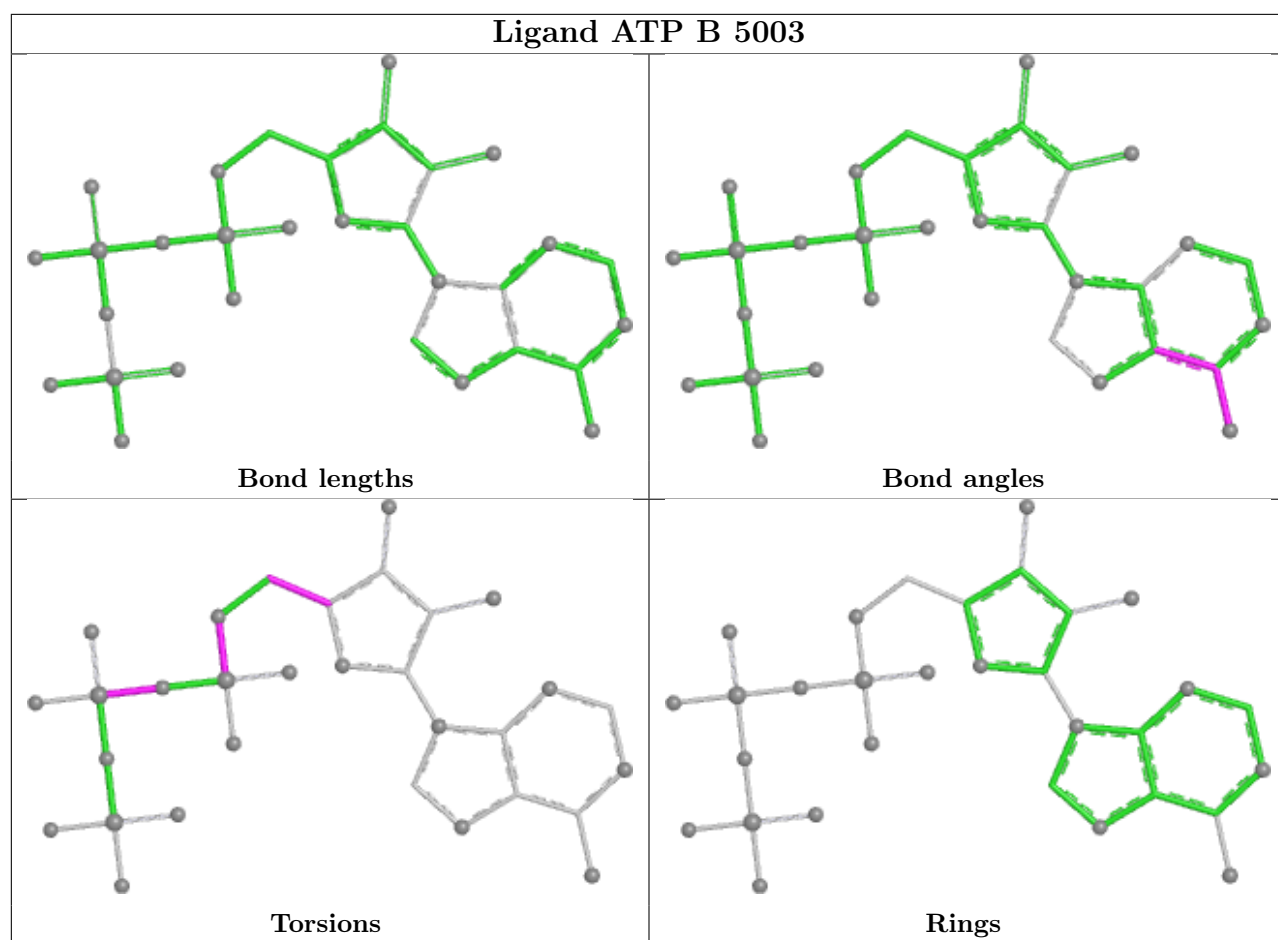
4 monomers are involved in 4 short contacts:

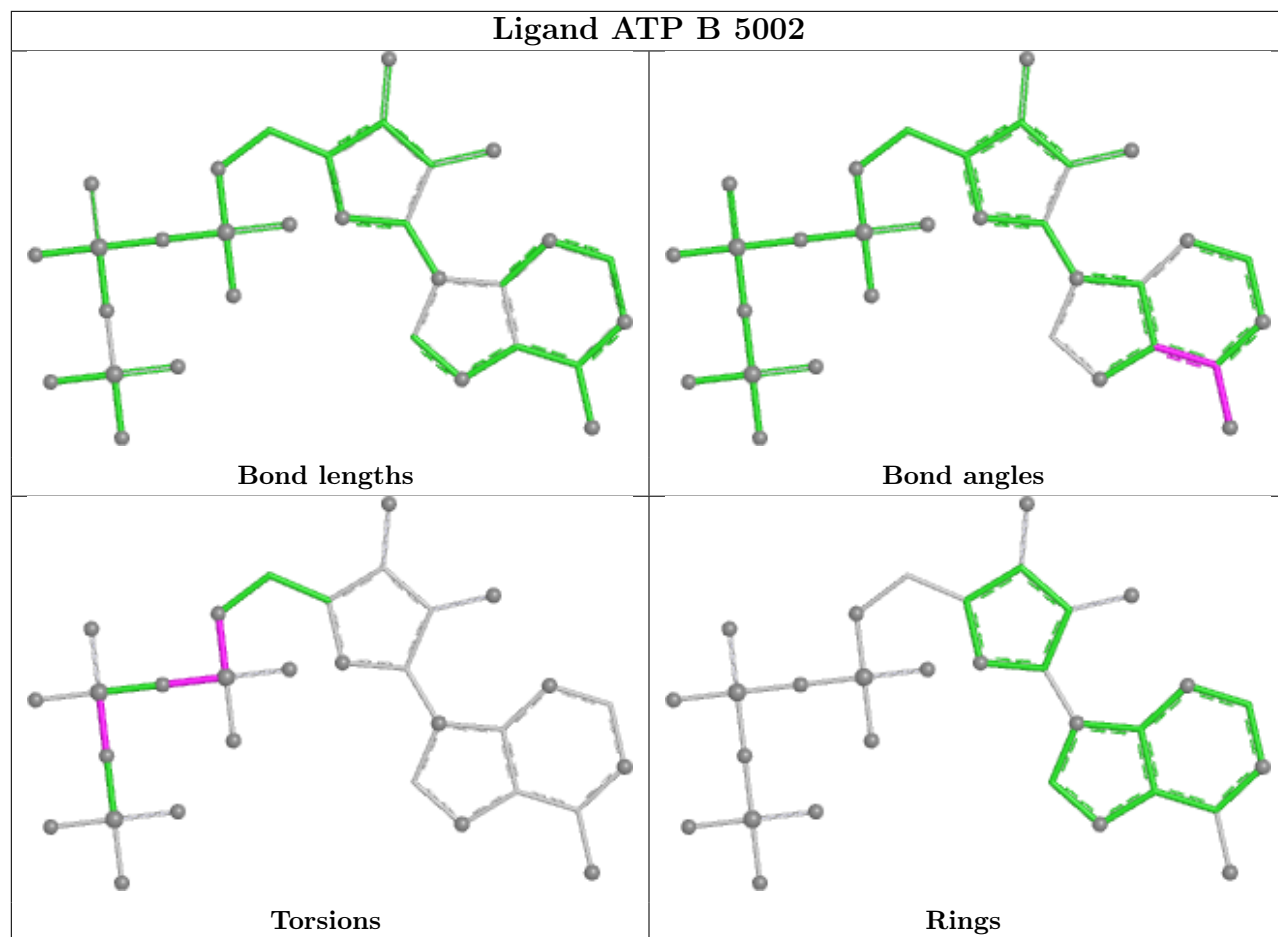
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5003	ATP	1	0
4	A	5003	ATP	1	0
4	D	5003	ATP	1	0
4	C	5003	ATP	1	0

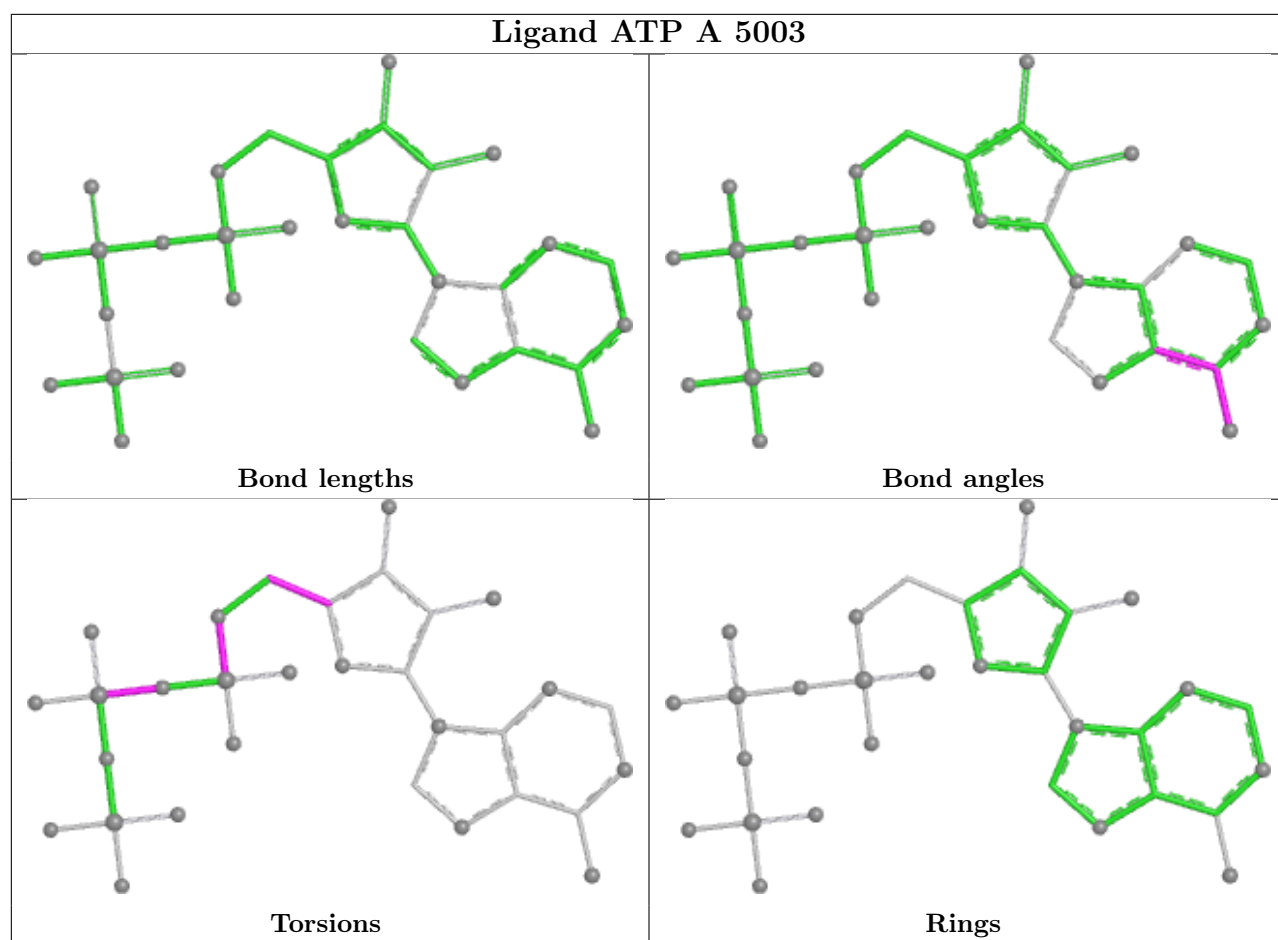
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

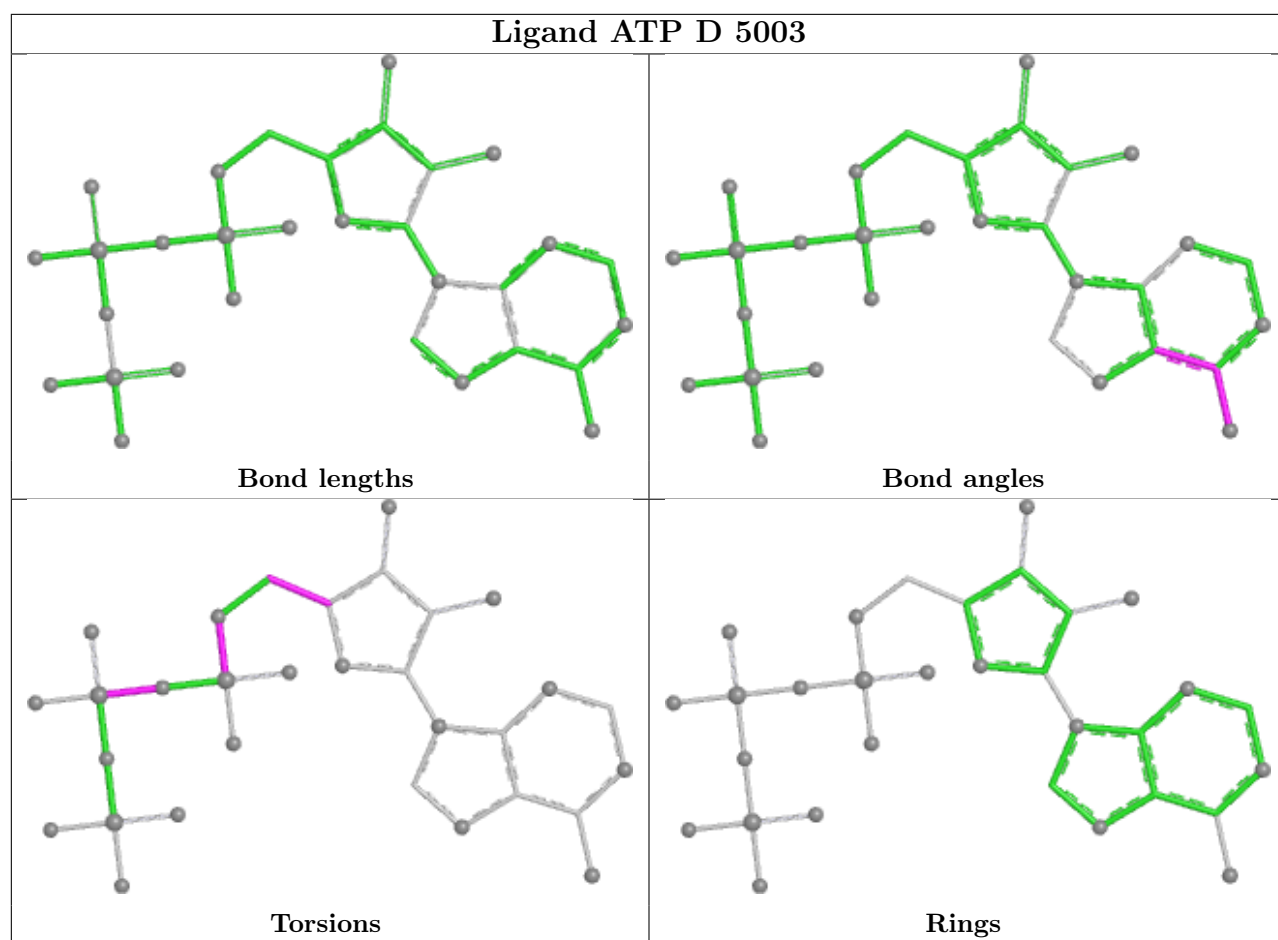
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

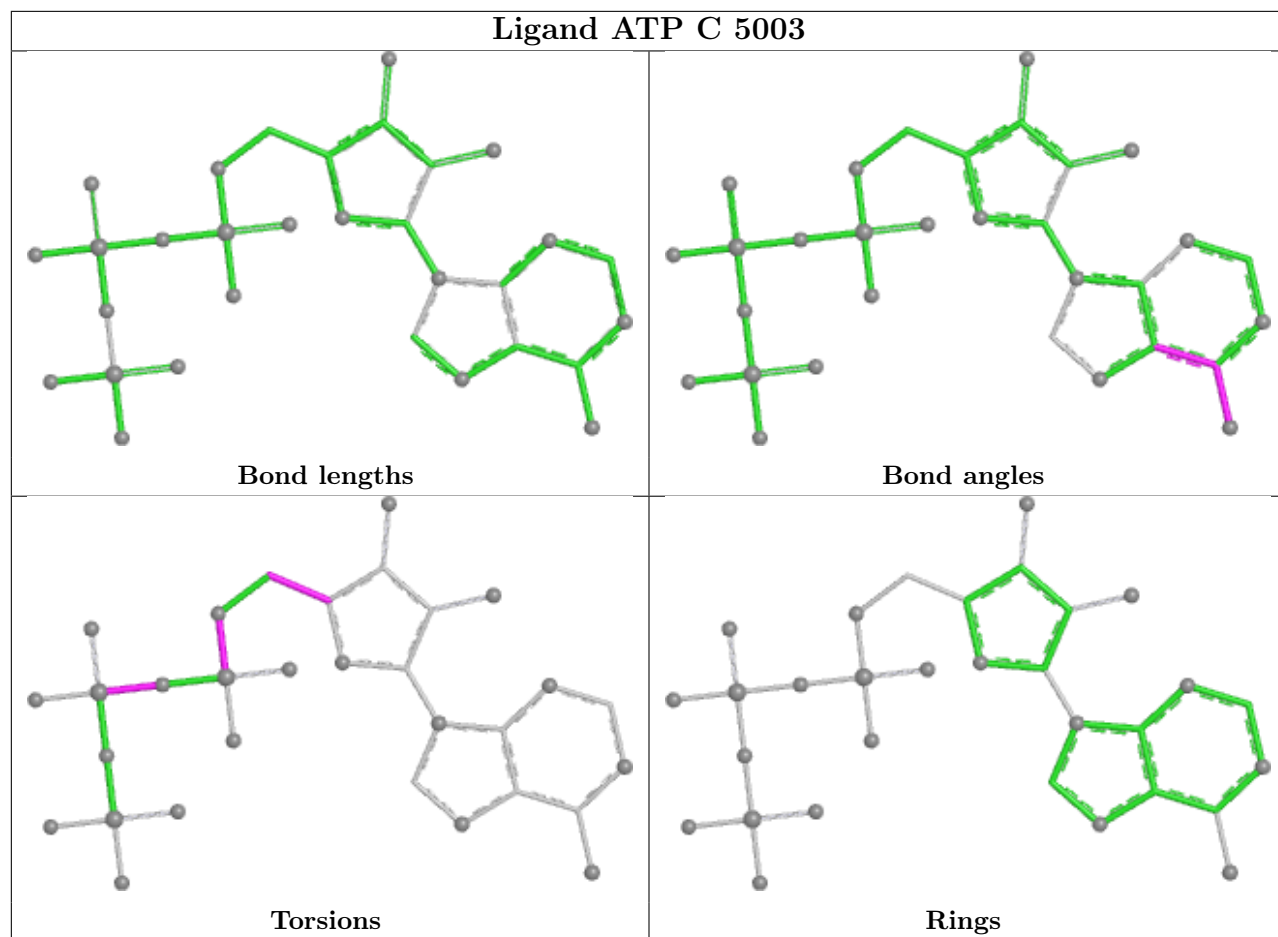


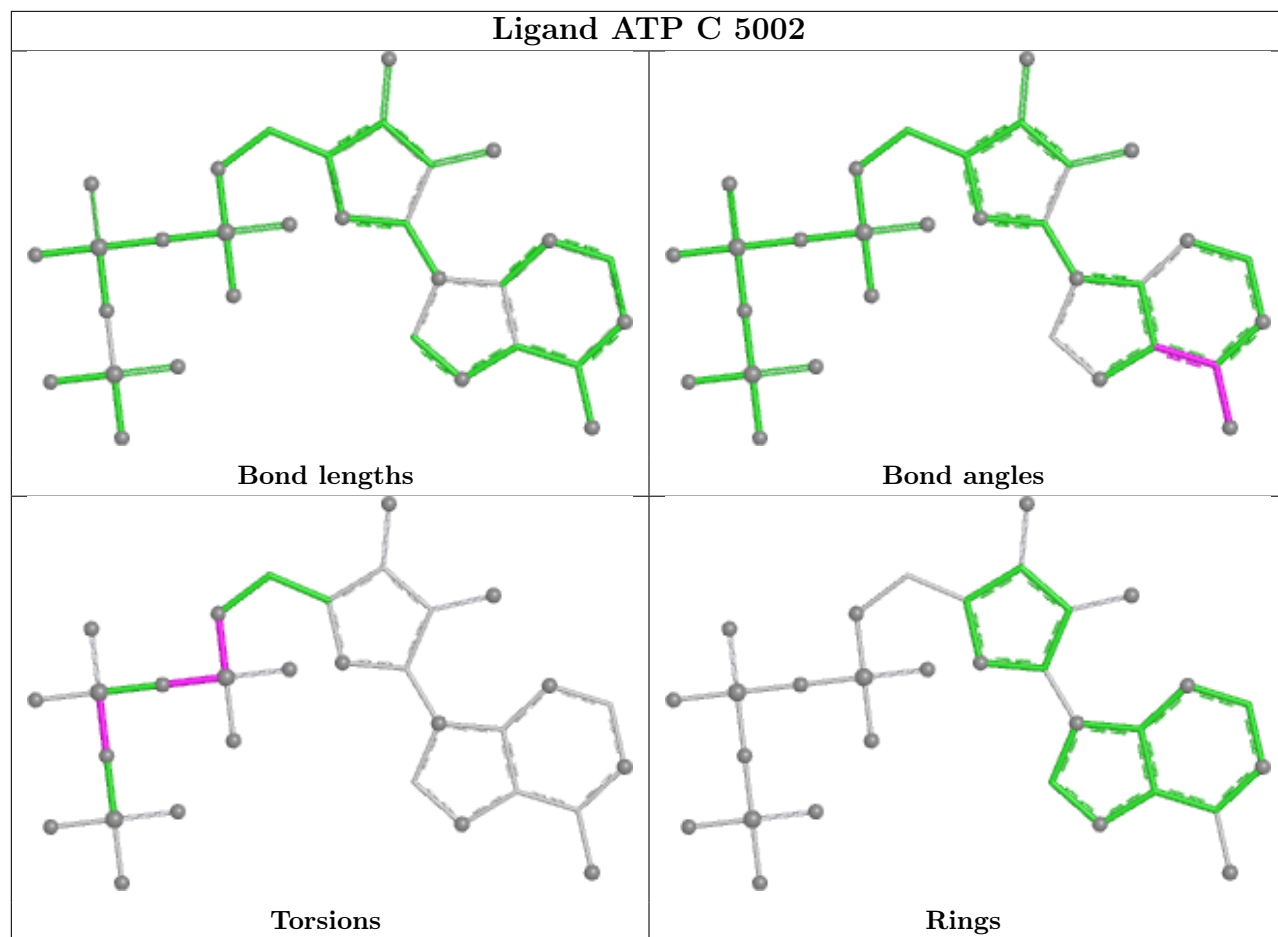


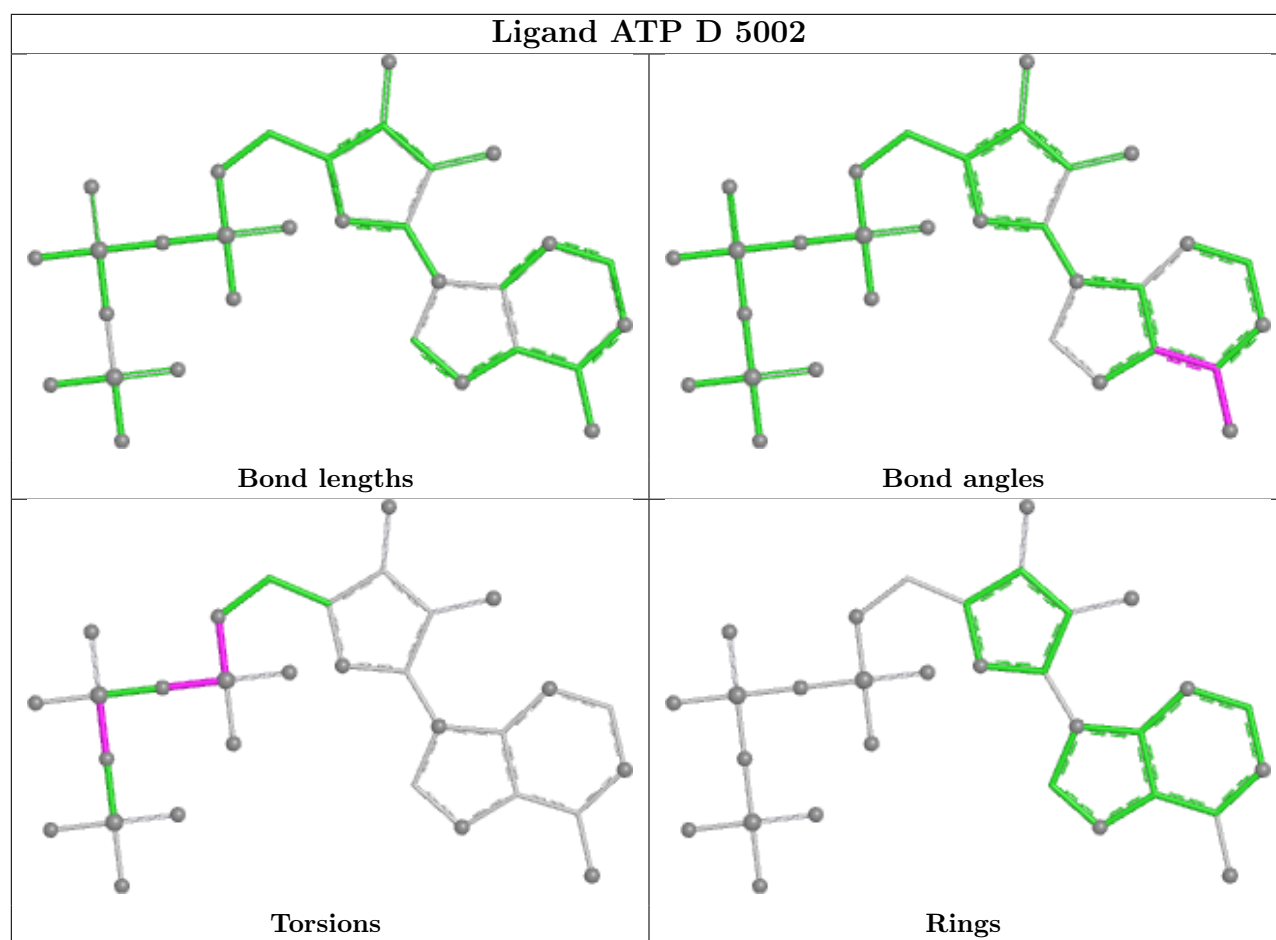












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42759. These allow visual inspection of the internal detail of the map and identification of artifacts.

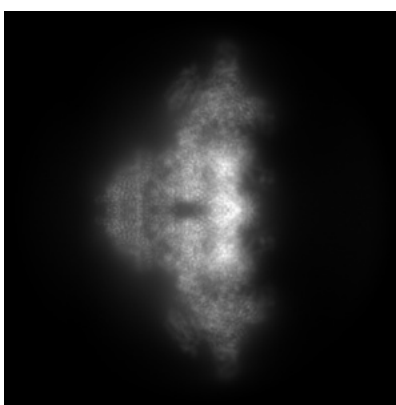
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

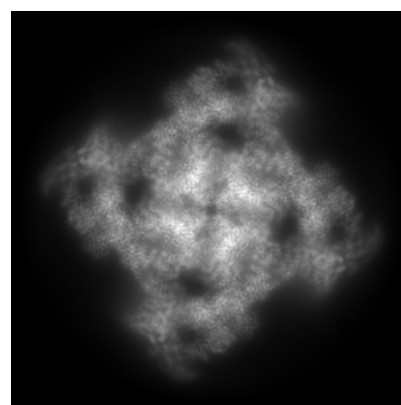
6.1.1 Primary map



X



Y

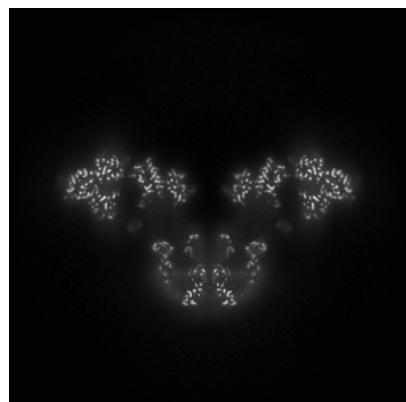


Z

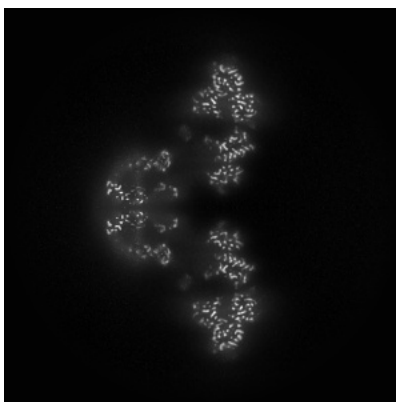
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

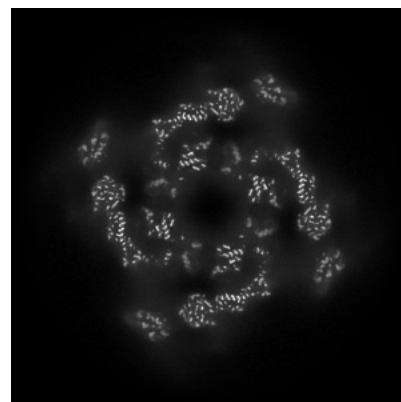
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

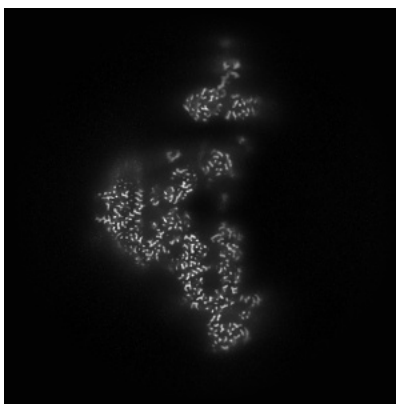
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

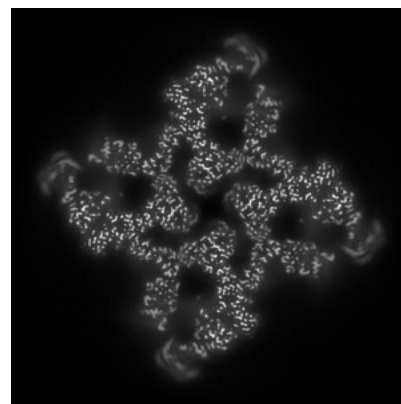
6.3.1 Primary map



X Index: 238



Y Index: 238

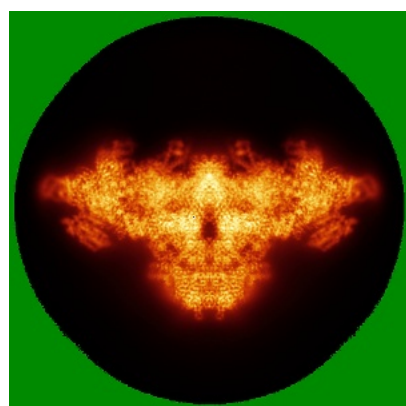


Z Index: 282

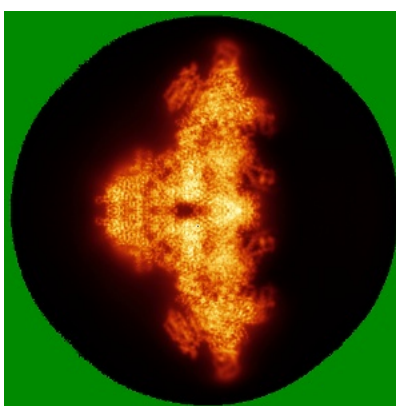
The images above show the largest variance slices of the map in three orthogonal directions.

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

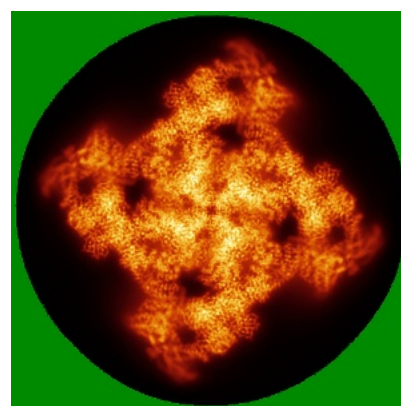
6.4.1 Primary map



X



Y

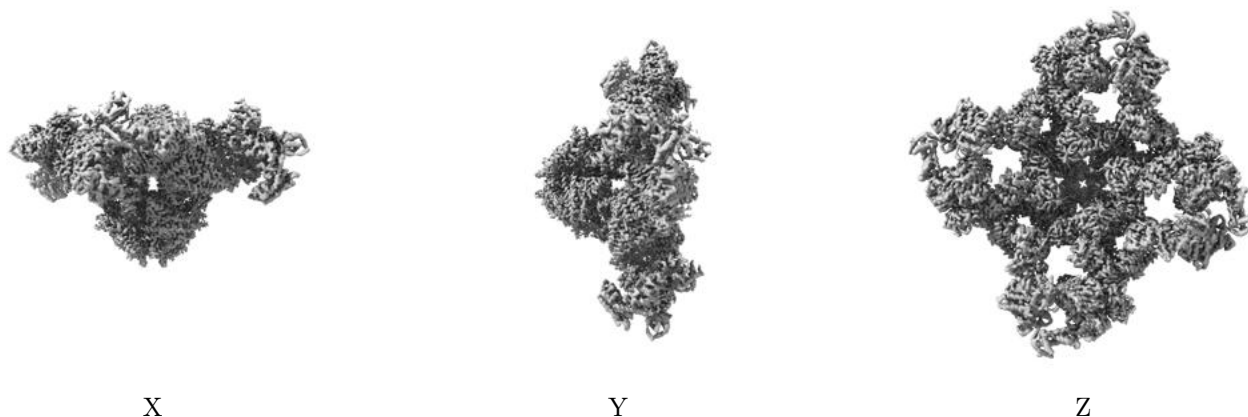


Z

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

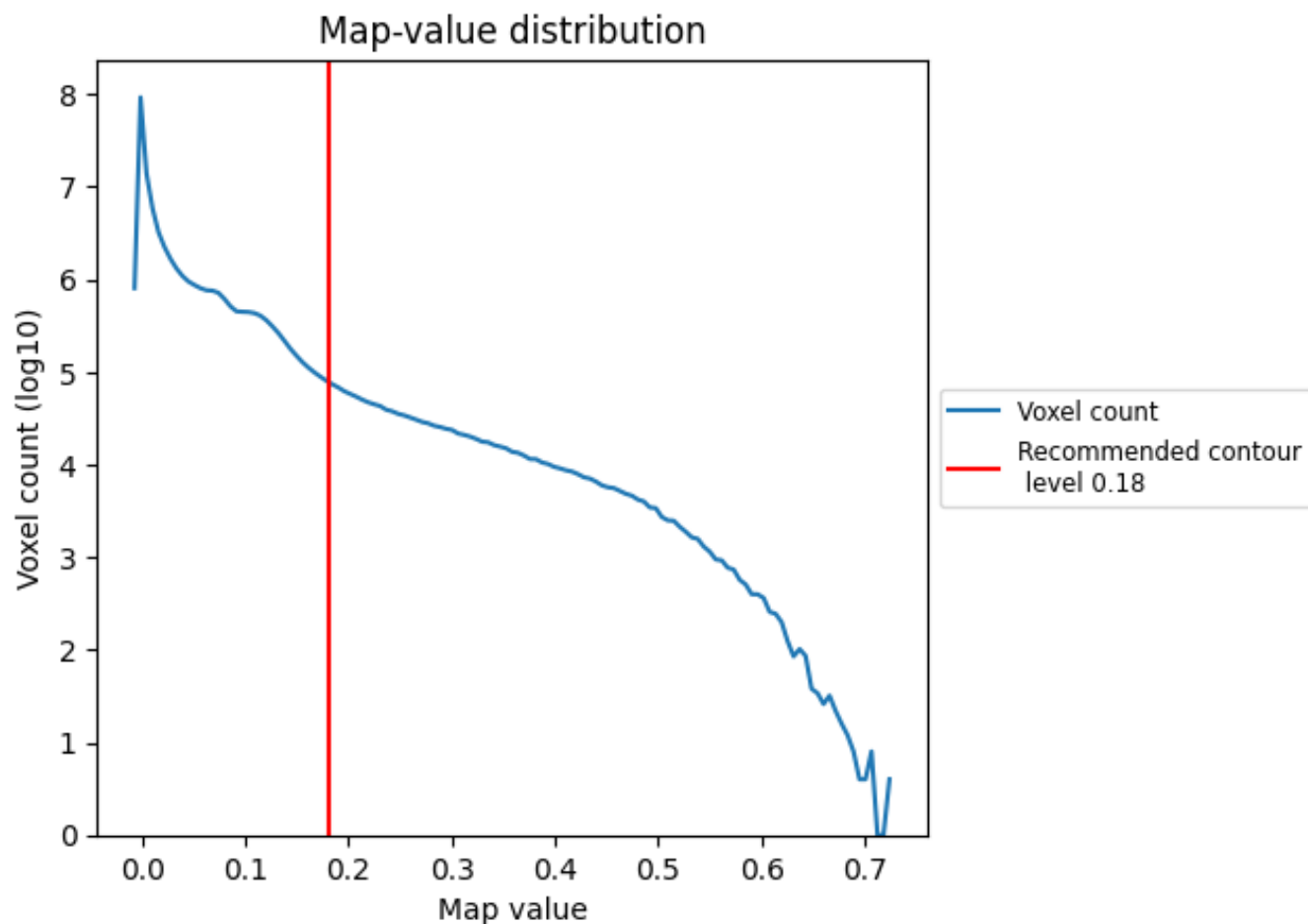
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

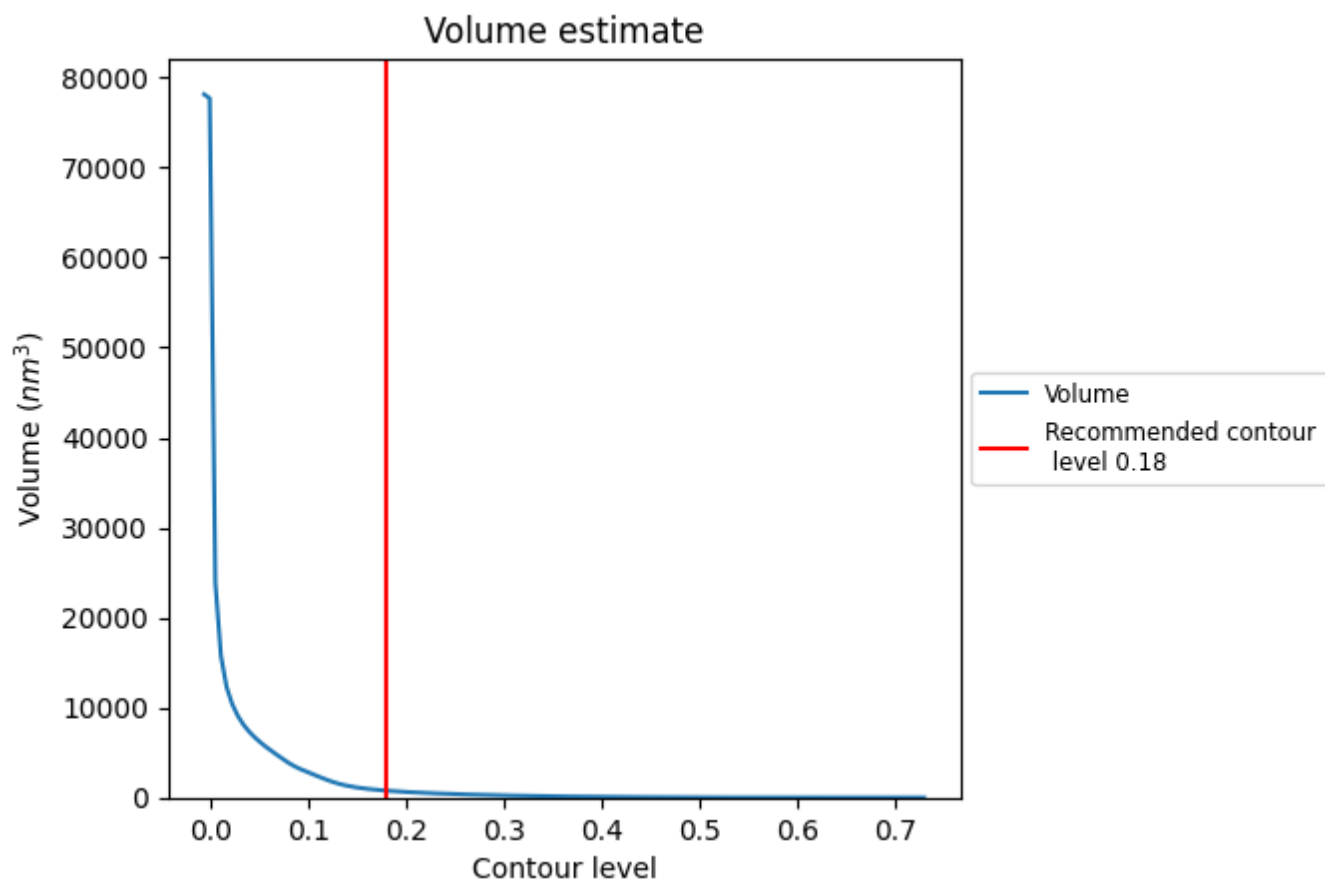
This section contains the results of statistical analysis of the map.

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.

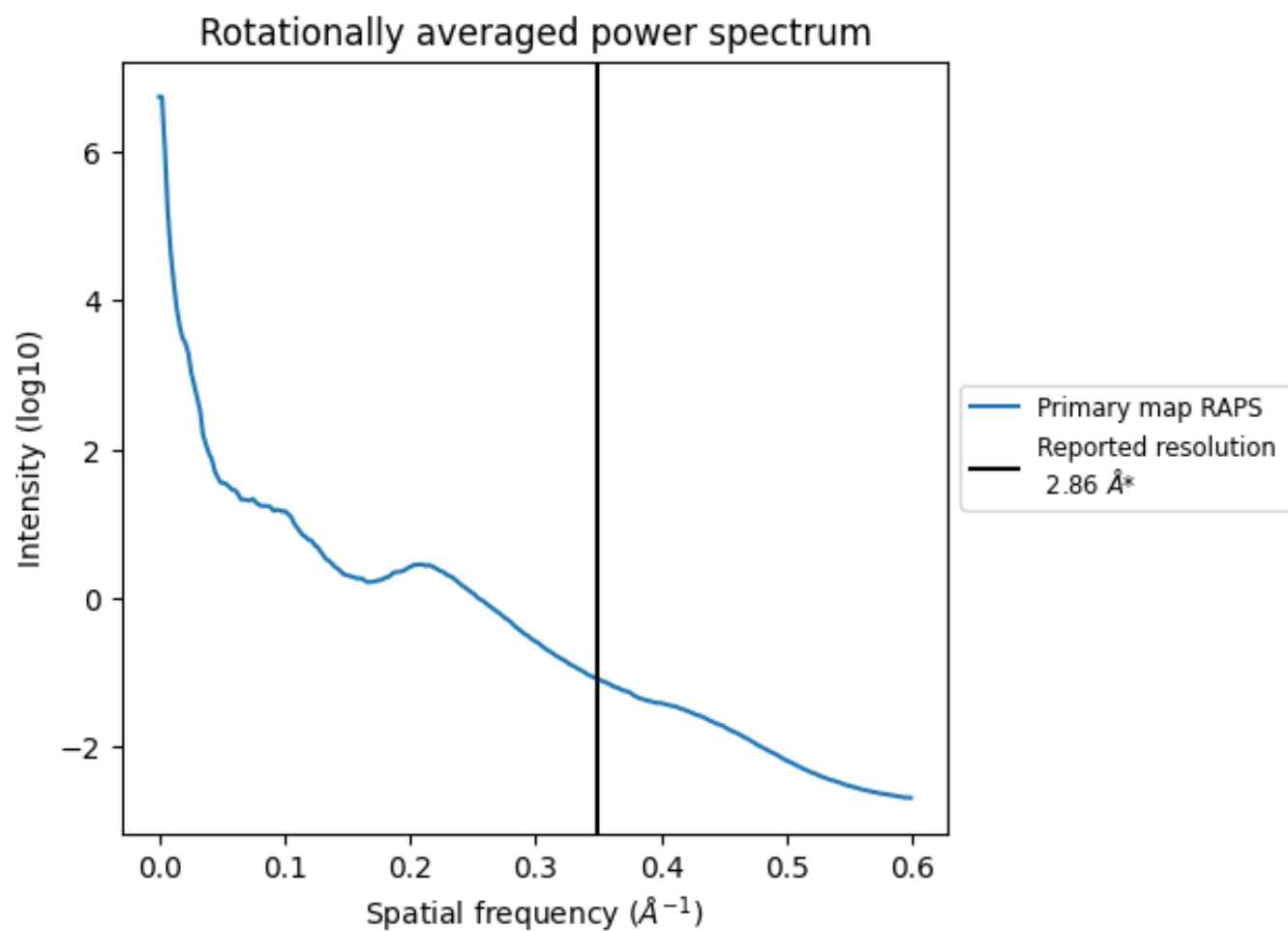
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 763 nm^3 ; this corresponds to an approximate mass of 689 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 0.350 Å⁻¹

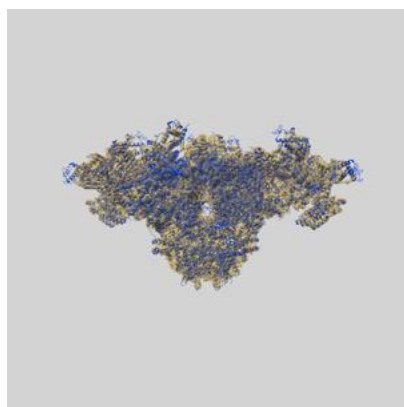
8 Fourier-Shell correlation

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

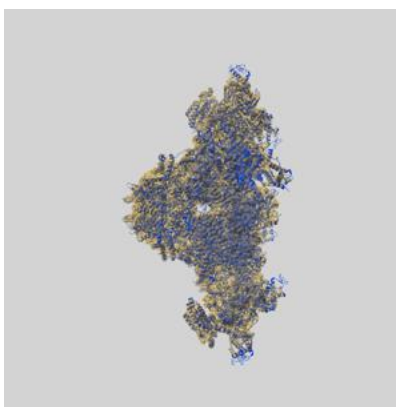
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42759 and PDB model 8UXC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

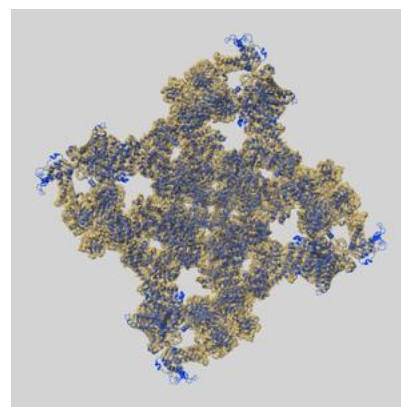
9.1 Map-model overlay [i](#)



X



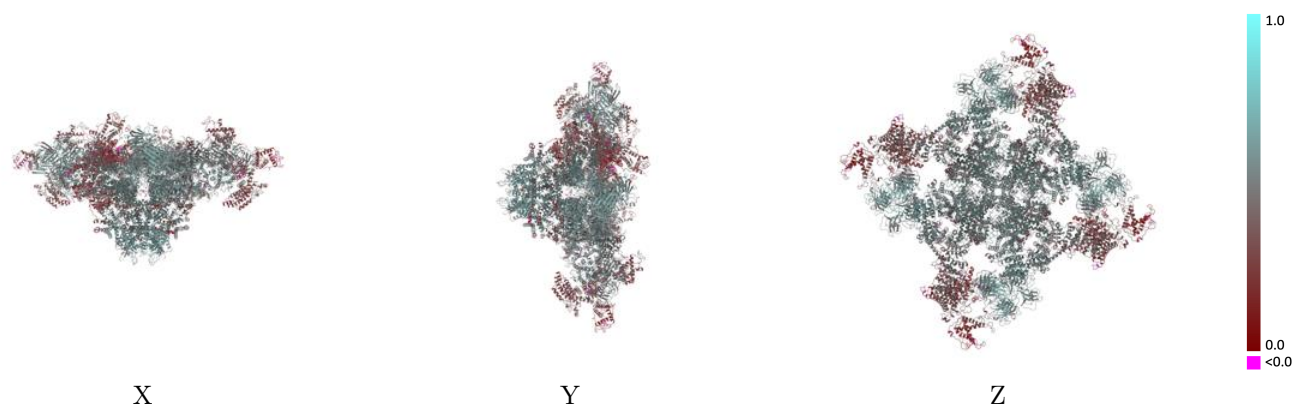
Y



Z

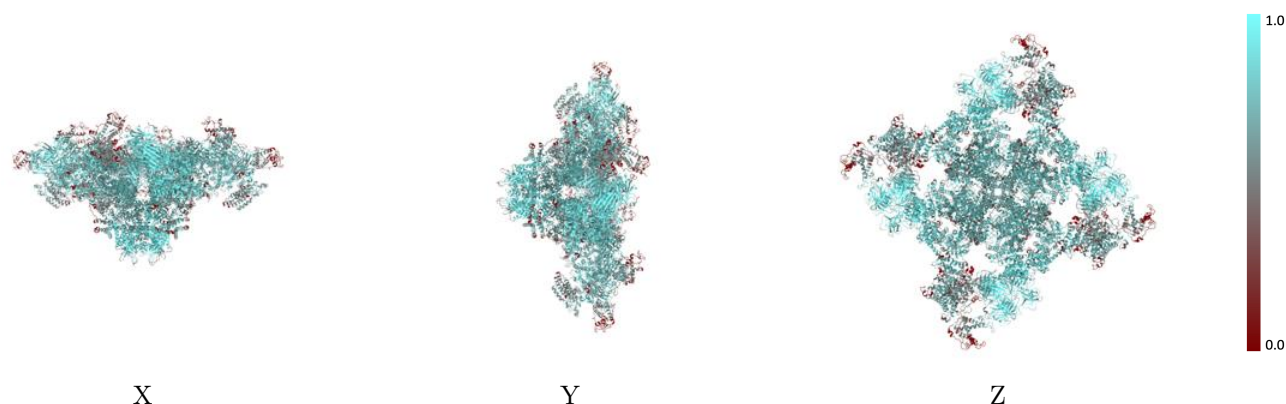
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



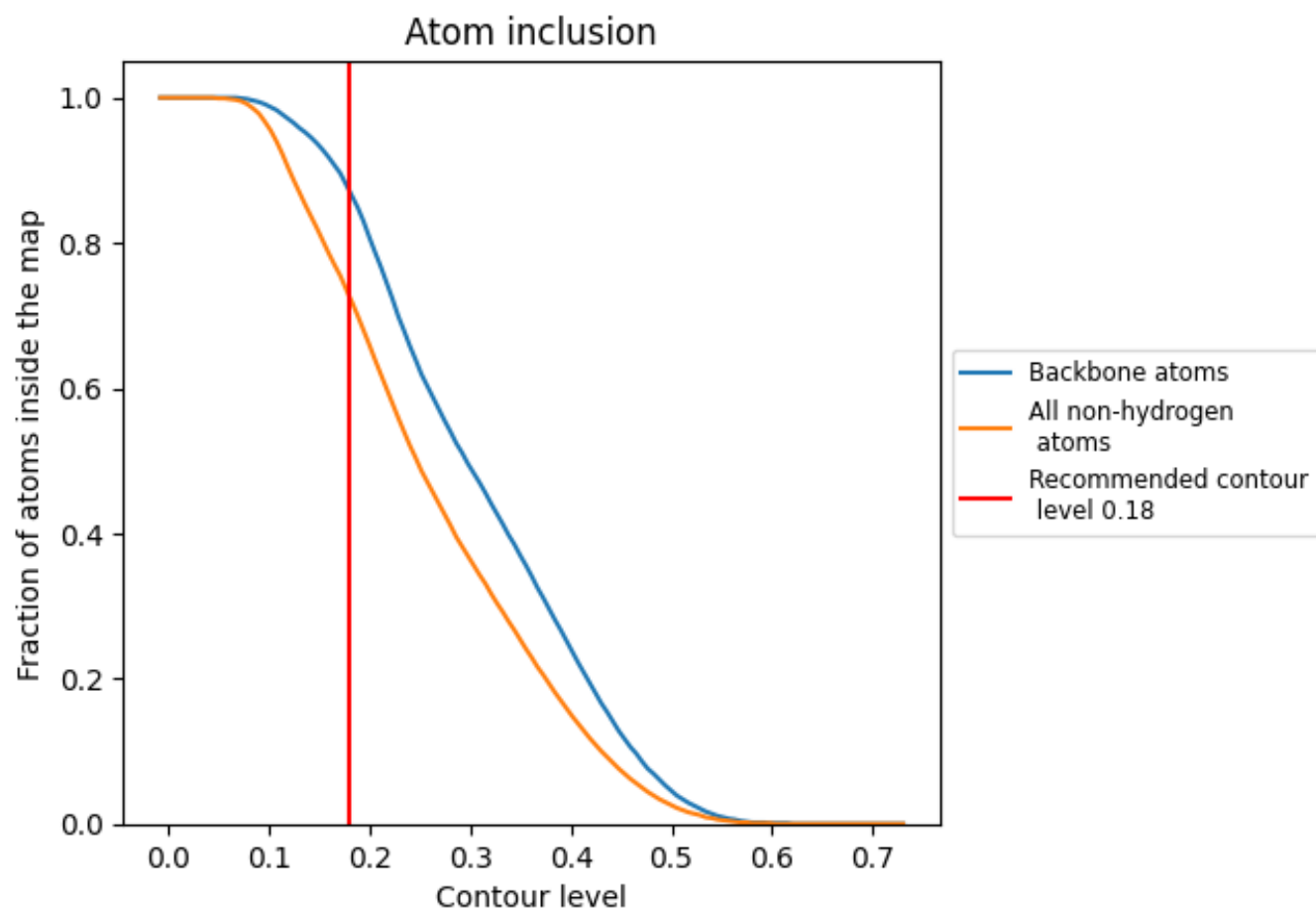
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7270	<div><div></div></div> 0.4660
A	<div><div></div></div> 0.7240	<div><div></div></div> 0.4640
B	<div><div></div></div> 0.7240	<div><div></div></div> 0.4640
C	<div><div></div></div> 0.7240	<div><div></div></div> 0.4640
D	<div><div></div></div> 0.7240	<div><div></div></div> 0.4640
E	<div><div></div></div> 0.8490	<div><div></div></div> 0.5520
F	<div><div></div></div> 0.8440	<div><div></div></div> 0.5520
G	<div><div></div></div> 0.8500	<div><div></div></div> 0.5520
H	<div><div></div></div> 0.8500	<div><div></div></div> 0.5510

1.0

0.0

<0.0