



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 10:04 AM UTC

PDB ID : 8UXC / pdb_00008uxc
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

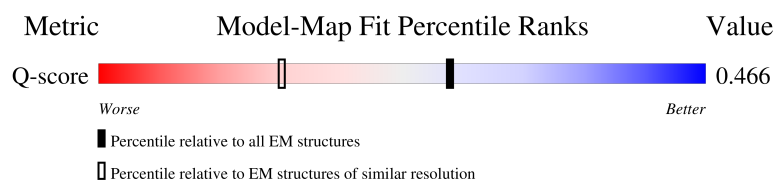
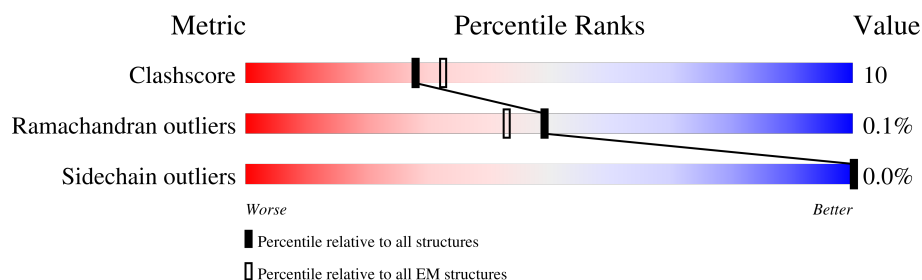
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



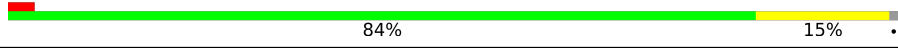
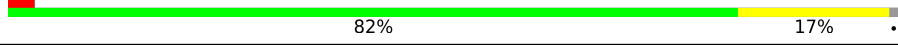
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12017 (2.36 - 3.36)

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	
1	B	4967	
1	C	4967	
1	D	4967	

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Mol	Chain	Length	Quality of chain
2	E	108	 82%17%
2	F	108	 83%16%
2	G	108	 84%15%
2	H	108	 82%17%

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

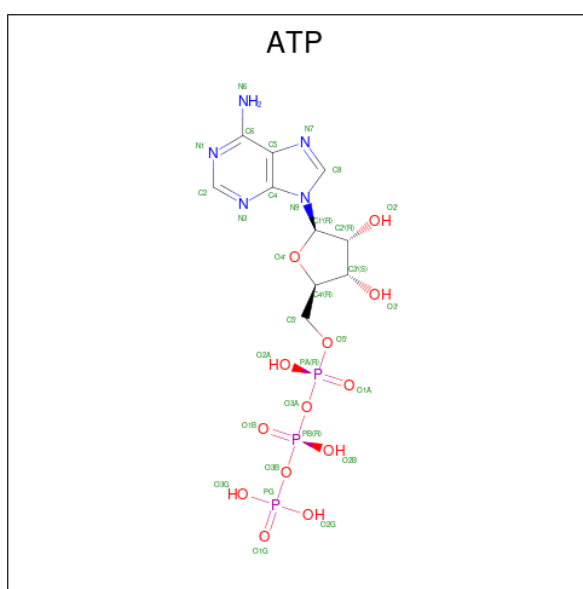
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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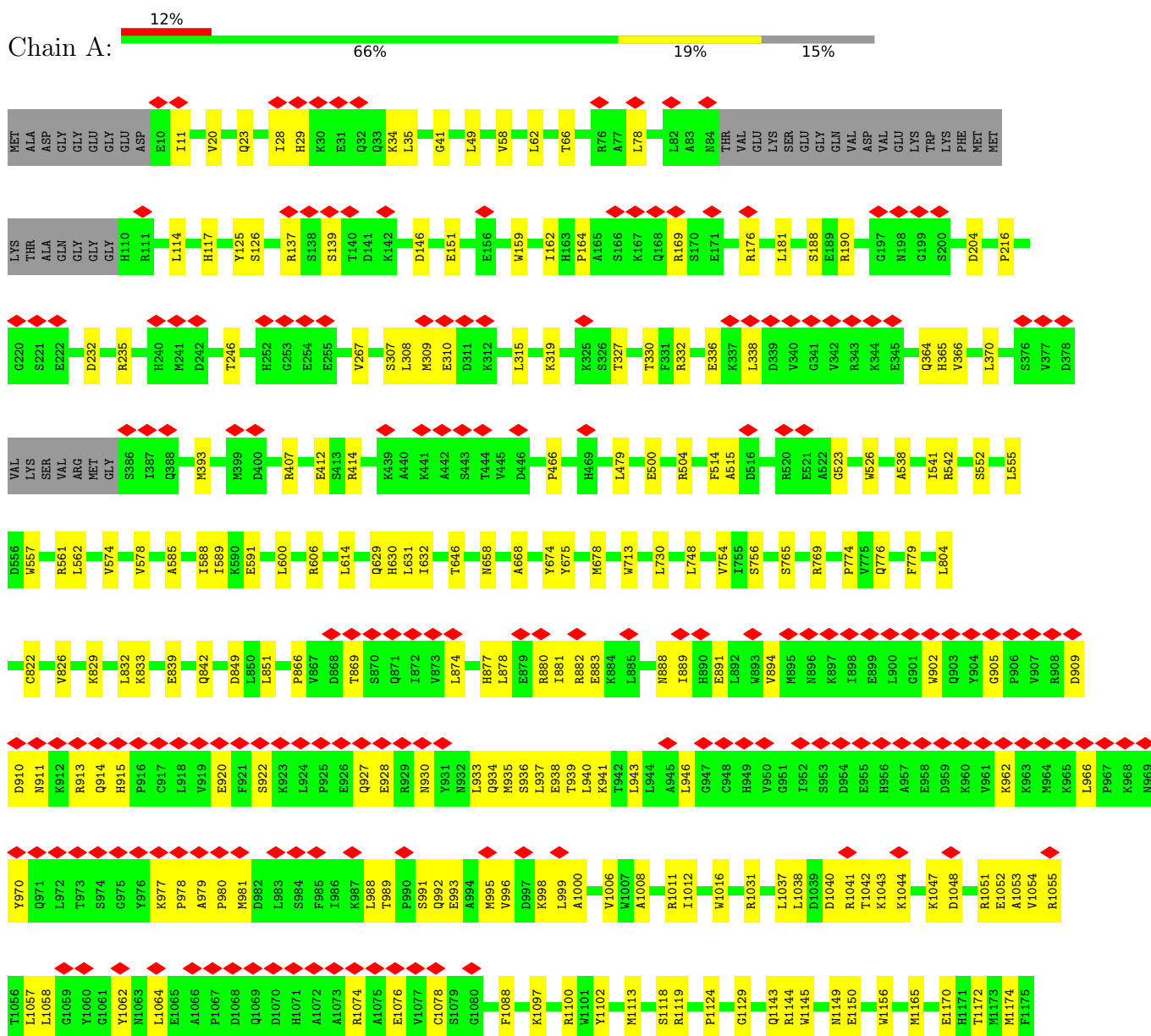
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	D	1	31	10	5	13	3	0

3 Residue-property plots [i](#)

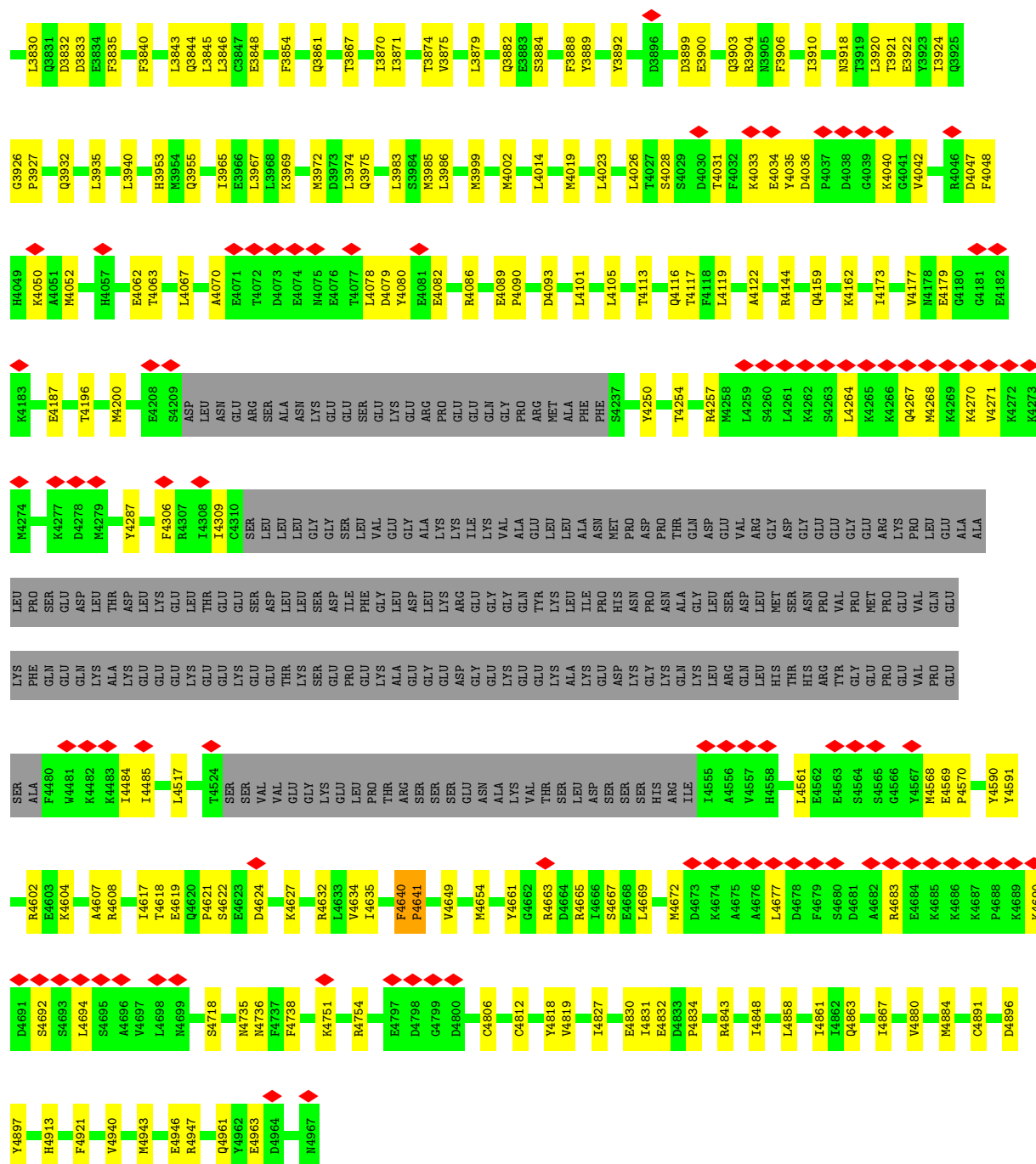
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

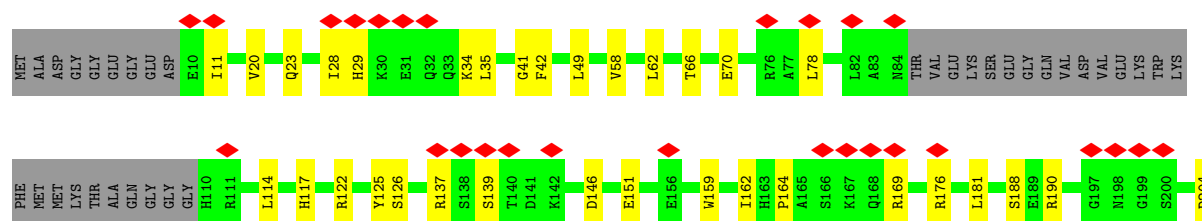








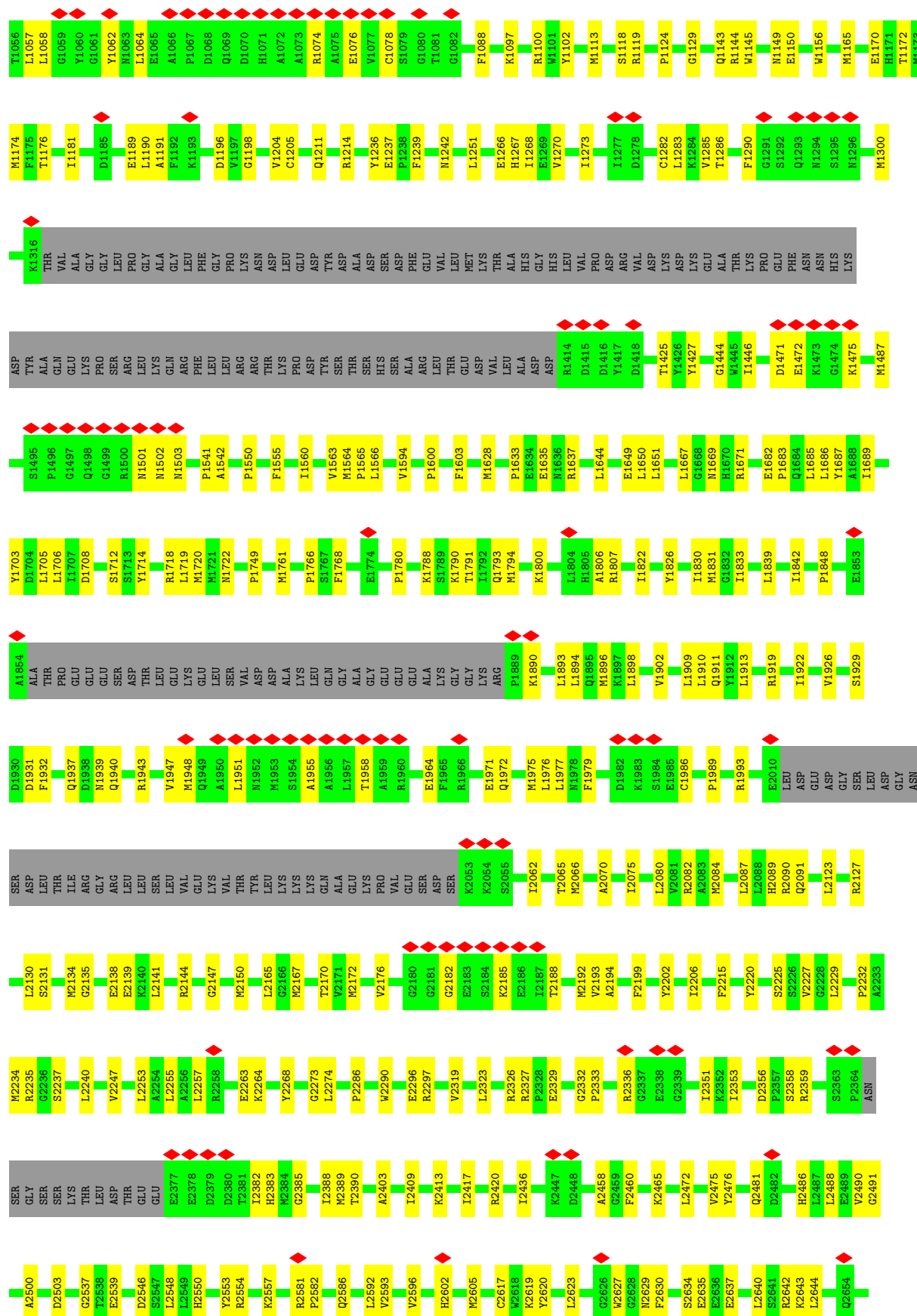
• Molecule 1: Ryanodine receptor 2





ARG	ASN	PRO	K3088	G3089	V3090	T3091	E3092	K3093	L3094	N3095	Y3096	T3097	T3098	Q3116	F3117	G3118	E3119	I3122	L3123	E3124	P3125	V3126	S3129	I3133	T3134	T3135	S3136	K3144	S3145	I3146	N3147	V3148	E3149	R3150	S3151	V3152	L3155	L3159	F3162	G3164	A3165	F3166	P3167	V3168	L3171	H3174	L3175	THR	T3071	M3072	E3073	N3074	L3075	K3076	Q3077	G3078	Q3079	F3080	T3081	THR	L2990	C2991	S2992	H2995	N2998	K2999	E3000	K3001	E3002	M3003	L3004	V3005	S3006	K3010	L3011	G3012	R3016	I3019	S3020	L3021	H3034	I3035	Q3038	T3039	L3040	D3041	A3042	P2955	T3044	V3045	E2957	Q2958	E2959	I2960	A2964	K2965	V2966	V2967	L2968	P2969	L2970	T2971	D2972	Q2973	R2979	L2980	Y2981	F2982	L2983	D2909	L2910	E2911	L2912	D2913	T2914	P2915	E2918	M2843	M2844	I2851	K2854	K2857	M2858	L2860	E2861	S2862	K2863	G2864	G2865	G2866	M2867	H2868	P2869	L2870	L2871	V2872	P2873	T2874	D2875	T2876	E2881	K2882	A2883	K2884	D2885	E2886	E2887	Q2890	D2891	I2892	L2893	K2894	F2895	L2896	M2899	R2905	G2906	F2907	T2908	T2909	L2910	E2911	L2912	D2913	T2914	P2915	E2918	M2782	W2785	G2786	W2787	R2788	E2789	R2791	T2792	E2793	G2794	G2795	D2796	S2797	M2798	A2799	L2800	Y2801	M2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	VAL	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	L2826	D2827	M2828	S2829	N2830	T2831	T2832	L2833	S2834	R2835	D2836	L2837	D2913	T2914	P2915	E2918	M2843	M2844	I2851	K2854	K2857	M2858	L2860	E2861	S2862	K2863	G2864	G2865	G2866	M2867	H2868	P2869	L2870	L2871	V2872	P2873	T2874	D2875	T2876	E2881	K2882	A2883	K2884	D2885	E2886	E2887	Q2890	D2891	I2892	L2893	K2894	F2895	L2896	M2899	R2905	G2906	F2907	T2908	T2909	L2910	E2911	L2912	D2913	T2914	P2915	E2918	M2714	E2715	K2716	Y2719	F2720	L2721	N2722	K2723	H2727	S2728	K2731	W2732	S2733	M2734	D2735	K2736	L2737	A2738	N2739	G2740	W2741	L2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	S2750	K2751	K2752	V2753	Q2754	P2755	L2756	M2757	K2758	P2759	Y2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	L2770	Y2771	R2772	W2773	P2774	K2775	L2776	L2779	W2627	G2628	N2629	F2630	S2634	E2635	E2636	E2637	L2640	S2641	R2642	K2643	L2644	Q2654	E2658	C2668	L2669	S2670	V2672	D2679	Y2680	S2683	N2684	V2685	V2686	S2687	M2688	M2689	E2690	K2691	Q2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	N2700	F2701	R2702	K2618	K2619	Y2620	L2623	D2707	T2708	N2710	I2711	T2712	I2713	G2626	H2486	L2487	L2488	E2489	Y2490	G2491	K2500	D2503	G2537	T2538	E2539	D2546	S2547	L2548	L2549	H2550	R2553	Y2554	K2557	R2581	P2582	Q2586	L2589	L2592	V2593	V2596	H2602	W2605	C2617	K2618	K2619	Y2620	L2623	D2707	T2708	N2710	I2711	T2712	I2713	G2626	K2352	I2353	D2356	R2359	S2363	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	LEU	ASP	THR	GLU	E2377	E2378	D2379	D2380	T2381	H2382	H2383	M2384	G2385	I2388	M2389	T2390	A2403	I2409	K2413	I2417	R2420	I2427	I2436	K2447	D2448	D2455	M2456	S2457	A2458	G2459	F2460	K2465	R2471	L2472	Y2475	Q2481	D2482	H2486	L2487	L2488	E2489	Y2490	G2491	K2500	D2503	G2537	T2538	E2539	D2546	S2547	L2548	L2549	H2550	R2553	Y2554	K2557	R2581	P2582	Q2586	L2589	L2592	V2593	V2596	H2602	W2605	C2617	K2618	K2619	Y2620	L2623	D2707	T2708	N2710	I2711	T2712	I2713	G2626	S2267	R2268	K2212	F2215	Y2220	S2225	S2226	V2227	G2228	L2229	P2232	A2233	M2234	R2235	G2236	S2237	L2240	Y2247	L2253	L2257	R2258	E2263	G2264	Y2268	G2273	L2274	P2286	W2290	E2296	R2297	R2326	R2327	F2328	E2329	G2332	P2333	R2336	G2337	E2338	G2339	I2351	V2081	R2082	M2083	L2087	L2088	H2089	R2090	Q2091	L2123	R2127	L2130	M2134	G2135	E2138	E2139	K2140	L2141	R2144	G2147	M2150	L2165	G2166	M2167	L2170	V2171	M2172	V2176	G2180	G2181	G2182	E2183	S2184	K2185	E2186	I2187	T2188	M2192	V2193	A2194	F2199	Y2202	I2206	D1982	K1983	S1984	E1985	C1986	P1989	R1993	E2010	LEU	ASP	GLU	GLY	SER	LEU	ASP	GLY	ASN	SER	ASP	LEU	THR	ILE	ARG	GLY	ARG	LEU	LEU	SER	LEU	VAL	GLU	LYS	VAL	THR	TYR	LEU	LYS	LYS	LYS	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911	V1912	L1913	R1919	I1922	V1926	S1929	D1930	I1931	F1932	Q1937	D1938	N1939	Q1940	R1943	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	E1964	F1965	R1966	E1971	Q1972	M1975	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	P1989	L1909	L1910	Q1911
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LYS	V3599	THR	PHE	L3276	L3197	Q3116	L3011	Y2939	M2867	L2800	K2736	E2658
LYS	V3600	SER	ILE	L3277	P3198	F3117	G3012	I2940	H2868	Y2801	L2737	C2668
VAL	V3601	TRP	TYR	L3281	T3199	G3117	R3016	L2941	P2869	M2802	A2738	L2669
TRP	V3602	VAL	ASP	K3282	N3200	E3119	R3016	E2942	S2870	ARG	N2739	S2670
HIS	V3603	MET	LYS	I3283	V3201	I3122	T3019	F2943	L2871	THR	G2740	A2671
LYS	V3604	SER	ALA	I3284	E3202	L3123	S3020	D2944	V2872	ARG	W2741	V2672
LEU	V3605	GLY	HIS	E3203	D3203	E3124	S3021	G2945	P2873	ARG		
LEU	V3606	LEU	ASP	N3285		D3125	L3021	G2946	Y2874	ILE	I2742	D2679
LEU	V3607	LEU	ASN	N3286	L3211	V3126	H3034	S2947	D2875	SER	Y2743	Y2680
LYS	V3608	LEU	GLY	N3287	E3212	V3126	I3035	R2948	T2876	GLN		
GLN	V3609	LEU	ARG	N3288	K3213	S3129	Q3038	G2949	L2877	THR	E2745	S2683
LEU	V3610	LEU	ILE	G3289	L3214		T3039	K2950	E2881	GLN	I2746	N2684
PRO	V3611	LEU	GLY	I3290	K3215	I3133	T3039	G2951	K2882	VAL	Y2747	Y2685
ASN	V3612	LEU	GLY	D3291	E3216	L3134	L3040	G2952	A2883	SER		Y2686
ARG	V3613	LEU	ASN	E3292	E3217	E3041	E3041	E2952	K2884	VAL	D2748	S2687
ALA	V3614	LEU	PHE	G3293	I3218	S3135	A3042	H2953	D2885	ASP	D2749	M2688
ASP	V3615	THR	THR	I3219	V3219	R3136	R3043	F2954	K2886	ALA	S2750	M2689
THR	V3616	LEU	VAL	E3220	E3220	K3144	T3044	P2955	E2887	ALA	S2751	M2690
GLN	V3617	LEU	GLN			S3145	V3045	Y2956		HIS	K2752	E2691
ALA	V3618	LEU	ASP	E3223		I3146	K3046	E2957	Q2890	G2820	V2753	K2691
PRO	V3619	ARG	ASP	I3226	R3227	V3147	X3047	E2958	D2891	Y2821	Q2754	Q2692
GLY	V3620	ARG	ILE	Y3228	Y3228	Y3148	L3050	E2959	I2892	S2822	P2755	S2693
LYS	V3621	TYR	ASN	T3229	E3149	E3149	S3051	I2960	L2893	P2823	L2756	S2694
THR	V3622	ALA	ALA	Q3304	R3305	R3150	V3053	A2964	K2894	R2824	L2756	M2695
VAL	V3623	GLY	PHE	I3306	I3306	Q3151	L3068	K2965	F2895	A2825	M2757	M2696
GLU	V3624	LEU	THR	I3307	I3307	Q3151	L3068	V2966	K2896	I2826	P2758	D2697
LEU	V3625	LEU	LEU	K3308	P3332	R3152	L3068	V2967	Q2897	D2827	K2759	E2698
LEU	V3626	LEU	LEU	H3333	H3333	R3152	L3068	L2968	I2898	M2828	Y2760	Q2699
ASP	V3627	LEU	THR	V3310	V3234	L3155	T3071	P2969	N2899	S2829	L2762	M2700
ILE	V3628	ILE	ARG	M3235	E3236	L3159	E3072	L2972	Q2906	V2831	L2763	F2701
ALA	V3629	ARG	LYS	E3237	V3237	F3162	X3074	L2973	K2907	T2832	S2764	N2702
ASN	V3630	VAL	VAL	I3238	I3238	A3163	L3075	D2909	F2907	T2833	K2765	P2703
VAL	V3631	LEU	ASP	L3239	L3239	G3164	L3076	L2980	K2908	L2833	K2766	Q2704
PHE	V3632	LEU	TYR	P3240	P3240	A3165	K3076	F2981	D2909	S2834	E2767	P2705
LEU	V3633	LEU	ASN	M3241	M3241	P3167	Q3077	L2982	L2910	P2836		V2706
ASN	V3634	ARG	ARG	H3318	H3318	P3167	Q3078	L2983	E2911	L2837	I2770	D2707
ALA	V3635	ALA	ALA	F3319	F3319	V3168	G3078	L2984	E2911	M2838	Y2771	T2708
GLY	V3636	GLY	VAL	K3246	K3246	V3168	F3080	S2984	D2913	A2839	S2772	S2709
LYS	V3637	LEU	LYS	S3247	S3247	L3171	T3081	A2985	D2913	M2840	W2773	N2710
ASP	V3638	LEU	LYS	R3248	R3248	H3174	THR	R2988	D2913	A2841	P2774	I2711
GLY	V3639	LEU	LYS	W3250	W3250	L3175	ARG	P2989	T2914	E2942	K2776	I2712
PRO	V3640	LEU	GLY	M3256	M3256	H3176	ASN	L2990	P2915	M2843		I2713
ALA	V3641	LEU	ALA	R3260	R3260	N3179	PRO	C2991	E2918	M2844	L2779	P2714
GLY	V3642	LEU	ALA	A3261	A3261	I3183	K3088	S2992	K2919	L2851		E2715
ASP	V3643	LEU	GLY	E3262	E3262	Y3184	G3089	S2992	R2920	K2854	M2782	K2716
ARG	V3644	LEU	PHE	C3264	C3264	K3187	T3091	H2995	F2921			Y2719
GLY	V3645	LEU	GLY	C3265	C3265	S3188	Q3092	K2999	Y2923	K2857	W2785	F2720
ASP	V3646	LEU	ARG	L3268	L3268	R3190	T3093	E3000	L2926	M2858	G2786	G2720
ARG	V3647	LEU	VAL	M3269	M3269	E3191	N3094	K3001	Q2927	P2859	W2787	I2721
GLY	V3648	LEU	ALA	S3270	S3270	A3192	N3095	E3002	Q2928	L2860	R2788	K2722
MET	V3649	LEU	GLY	N3273	N3273	A3193	Y3096	M3003	L2929	F2861	I2789	K2723
VAL	V3650	VAL	GLY			A3194	T3097	V3004	I2930	E2790	E2790	
ASP	V3651	ASP	ASP				T3098	T3005	E2935	R2791	R2791	H2727
HIS	V3652	HIS	HIS				S3107	S3006	K2936	R2792	R2792	S2728
LEU	V3653	LEU	LEU						H2937	R2793	R2793	K2731
LYS	V3654	LYS	LYS						Q2938	E2794	E2794	W2732
PRO	V3655	PRO	GLN							G2795	G2795	S2733
GLN	V3656	GLN	ARG							D2796	D2796	S2734
ASP	V3657	ASP	SER							S2797	S2797	M2734
THR	V3658	THR	PRO							M2798	M2798	M2735
LYS	V3659	LYS	LYS									
GLY	V3660	GLY	GLY									
VAL	V3661	VAL	VAL									
ASP	V3662	ASP	ASP									
THR	V3663	THR	THR									
LEU	V3664	LEU	LEU									
GLY	V3665	GLY	GLY									
ASP	V3666	ASP	ASP									
THR	V3667	THR	THR									
LYS	V3668	LYS	LYS									
GLY	V3669	GLY	GLY									
VAL	V3670	VAL	VAL									
ASP	V3671	ASP	ASP									
THR	V3672	THR	THR									
LEU	V3673	LEU	LEU									
GLY	V3674	GLY	GLY									
ASP	V3675	ASP	ASP									
THR	V3676	THR	THR									
LYS	V3677	LYS	LYS									
GLY	V3678	GLY	GLY									
VAL	V3679	VAL	VAL									
ASP	V3680	ASP	ASP									
THR	V3681	THR	THR									
LYS	V3682	LYS	LYS									
GLY	V3683	GLY	GLY									
VAL	V3684	VAL	VAL									
ASP	V3685	ASP	ASP									
THR	V3686	THR	THR									
LYS	V3687	LYS	LYS									
GLY	V3688	GLY	GLY									
VAL	V3689	VAL	VAL									
ASP	V3690	ASP	ASP									
THR	V3691	THR	THR									
LYS	V3692	LYS	LYS									
GLY	V3693	GLY	GLY									
VAL	V3694	VAL	VAL									
ASP	V3695	ASP	ASP									
THR	V3696	THR	THR									
LYS	V3697	LYS	LYS									
GLY	V3698	GLY	GLY									
VAL	V3699	VAL	VAL									

EL649	LI650	LI651	LI667	LI668	LI669	LI670	LI671	LI682	LI683	LI684	LI685	LI686	LI687	LI688	LI689	LI703	LI706	LI707	LI708	SI712	SI713	SI714	LI718	LI719	LI720	LI721	LI722	PI749	MI761	PI766	SI767	FI768	SI774	PI780	LI788	SI789	LI790	LI791	LI792	QI793	MI794	KI800	LI804	HI805	AI806														
Y1427	TI1432	G1435	G1444	PI445	HI446	D1471	E1472	K1473	G1474	K1475	MI487	S1495	PI496	G1497	Q1498	G1499	R1500	Y1501	NI502	NI503	G1504	LI505	PI541	PI542	PI550	FI555	LI560	VI563	MI564	PI565	LI566	VI594	PI600	FI603	MI628	PI633	FI634	LI635	NI636	PI637	LI644																		
GLU	ALA	THR	LYS	PRO	GLU	PHE	ASN	HIS	LYS	ASP	TYR	ALA	GLU	LYS	PRO	SER	ARG	LEU	LYS	ASN	ASP	LEU	GLU	TYR	THR	SER	HIS	SER	ALA	ARG	LEU	THR	GLU	ASP	VAL	LEU	ALA	ASP	R1414	D1415	D1416	Y1417	D1418	F1419	LI420	TI425	Y1426												
NI1149	EI1150	WI1156	MI1165	EI1170	HI1171	MI1172	MI1173	MI1174	MI1175	TI1176	II1181	D11185	EI1189	LI1190	AI1191	FI1192	KI1193	D11196	VI1197	G11198	LI1204	C1205	Q1211	R1214	Y1236	E1237	PI238	FI239	NI242	LI251	E1266	HI267	I1268	V1269	V1270	LI273	LI277	D1278	C1282	LI283	K1284	V1285																	
TI1286	FI1290	SI1292	NI1294	SI1295	NI1296	MI300	K1316	THR	VAL	ALA	GLY	GLY	LEU	PRO	GLY	ALA	GLY	LEU	PHE	GLY	PRO	LYS	ASN	ASP	LEU	GLU	TYR	ASP	ALA	SER	ASP	PHE	GLU	VAL	LEU	HIS	HIS	LEU	VAL	PRO	ASP	ARG	VAL	ASP	LYS	ASP	LYS												
DI048	RI051	EI052	AI053	VI054	RI055	TI056	LI057	LI058	GI059	YI060	GI061	YI062	NI063	LI064	EI065	AI066	PI067	DI068	QI069	DI070	HI071	AI072	AI073	RI074	AI075	EI076	YI077	C1078	SI079	GI080	TI081	GI082	FI088	KI097	RI100	WI101	YI102	MI113	SI118	RI119	PI120	GI121	PI124	GI129	RI133	Q1143	RI144	WI145											
K963	M964	K965	L966	P967	K968	K969	Y970	Q971	L972	T973	S974	G975	Y976	K977	P978	A979	P980	M981	D982	L983	S984	P985	I986	K987	L988	T989	P990	S991	Q992	E993	A994	M995	V996	D997	K998	L999	AI000	VI006	WI007	AI008	RI011	II012	WI016	RI031	LI037	LI038	DI039	DI040	RI041	T1042	K1043	K1044	K1047						
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
K963	M964	K965	L966	P967	K968	K969	Y970	Q971	L972	T973	S974	G975	Y976	K977	P978	A979	P980	M981	D982	L983	S984	P985	I986	K987	L988	T989	P990	S991	Q992	E993	A994	M995	V996	D997	K998	L999	AI000	VI006	WI007	AI008	RI011	II012	WI016	RI031	LI037	LI038	DI039	DI040	RI041	T1042	K1043	K1044	K1047						
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P																																														





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	0.14	0/34509	0.41	2/46612 (0.0%)
1	B	0.14	0/34509	0.41	2/46612 (0.0%)
1	C	0.14	0/34509	0.41	2/46612 (0.0%)
1	D	0.14	0/34509	0.41	2/46612 (0.0%)
2	E	0.13	0/834	0.35	0/1123
2	F	0.14	0/834	0.35	0/1123
2	G	0.14	0/834	0.35	0/1123
2	H	0.13	0/834	0.35	0/1123
All	All	0.14	0/141372	0.41	8/190940 (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 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3072	MET	CB-CG-SD	-6.03	94.61	112.70
1	B	3072	MET	CB-CG-SD	-6.03	94.62	112.70
1	C	3072	MET	CB-CG-SD	-6.03	94.62	112.70
1	D	3072	MET	CB-CG-SD	-6.03	94.62	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3235	MET	CB-CG-SD	-5.20	97.09	112.70

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	655	0
1	B	33769	0	33450	659	0
1	C	33769	0	33450	659	0
1	D	33769	0	33450	650	0
2	E	818	0	821	13	0
2	F	818	0	821	12	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	2640	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 10.

The worst 5 of 2640 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:1940:GLN:HE22	1:C:1972:GLN:HE21	1.16	0.90
1:D:1940:GLN:HE22	1:D:1972:GLN:HE21	1.16	0.90
1:A:3293:GLY:H	1:A:3296:MET:HE1	1.37	0.89
1:A:1940:GLN:HE22	1:A:1972:GLN:HE21	1.16	0.89
1:B:1940:GLN:HE22	1:B:1972:GLN:HE21	1.16	0.89

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	4092/4967 (82%)	3982 (97%)	108 (3%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4087 (97%)	108 (3%)	3 (0%)	48	68
1	C	2662/4967 (54%)	2597 (98%)	62 (2%)	3 (0%)	48	68
1	D	4198/4967 (84%)	4087 (97%)	108 (3%)	3 (0%)	48	68
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	15570/20300 (77%)	15169 (97%)	390 (2%)	11 (0%)	49	68

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4641	PRO
1	B	3927	PRO
1	B	4641	PRO
1	C	3927	PRO
1	C	4641	PRO

5.3.2 Protein sidechains [i](#)

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%)	3707 (100%)	1 (0%)	100	100
1	B	3708/4358 (85%)	3707 (100%)	1 (0%)	100	100
1	C	3708/4358 (85%)	3707 (100%)	1 (0%)	100	100
1	D	1044/4358 (24%)	1044 (100%)	0	100	100
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	12520/17788 (70%)	12517 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3719	MET
1	B	3719	MET
1	C	3719	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2722	ASN
1	D	731	HIS
1	C	3287	ASN
1	C	4055	HIS
1	B	544	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 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	5002	-	32,33,33	0.27	0	48,52,52	0.30	0
4	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	C	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	B	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	D	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	A	5002	-	32,33,33	0.27	0	48,52,52	0.30	0
4	ATP	A	5003	-	32,33,33	0.25	0	48,52,52	0.27	0

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	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	C	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

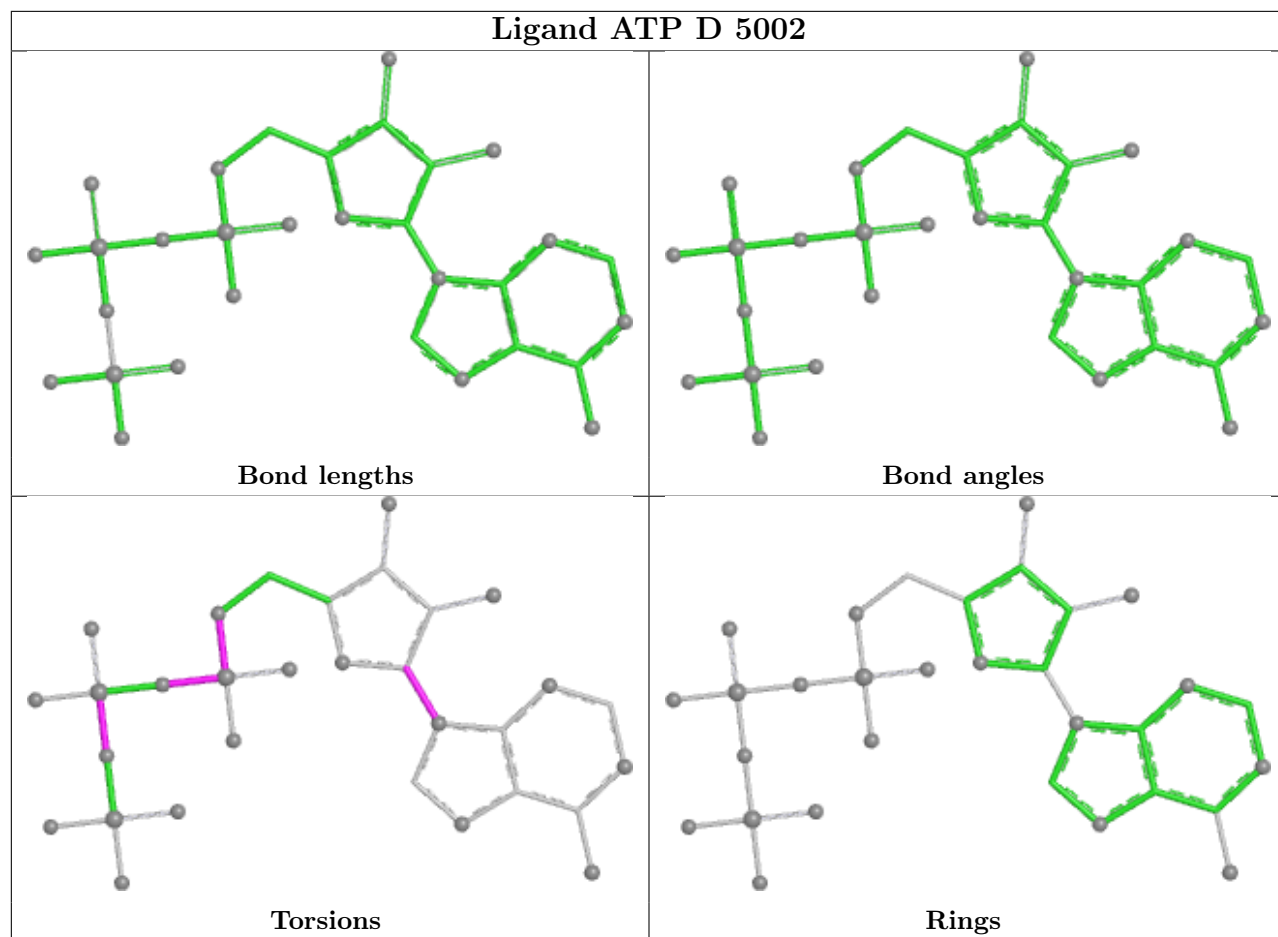
Mol	Chain	Res	Type	Atoms
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	B	5003	ATP	C5'-O5'-PA-O1A
4	B	5003	ATP	C5'-O5'-PA-O2A

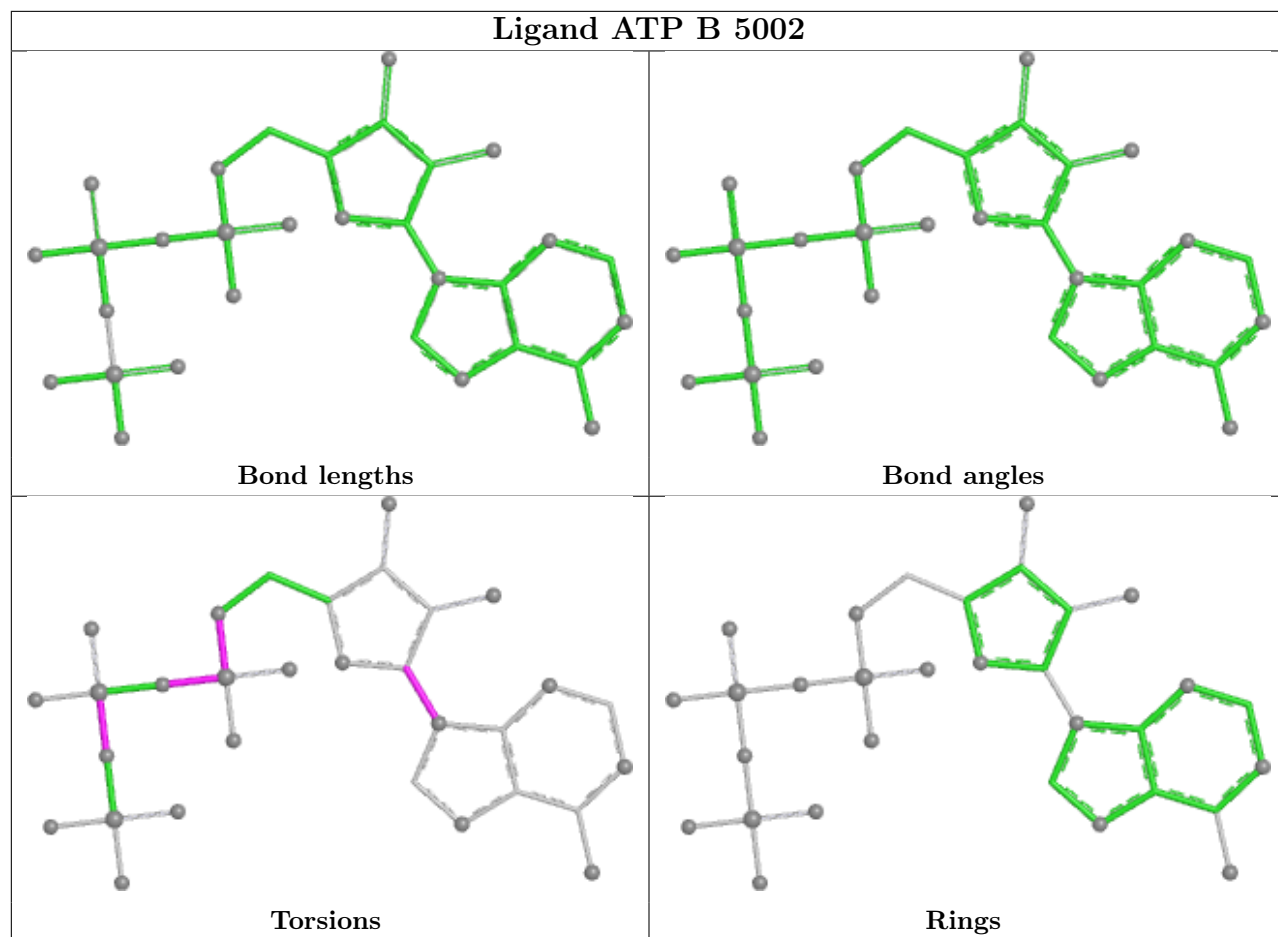
There are no ring outliers.

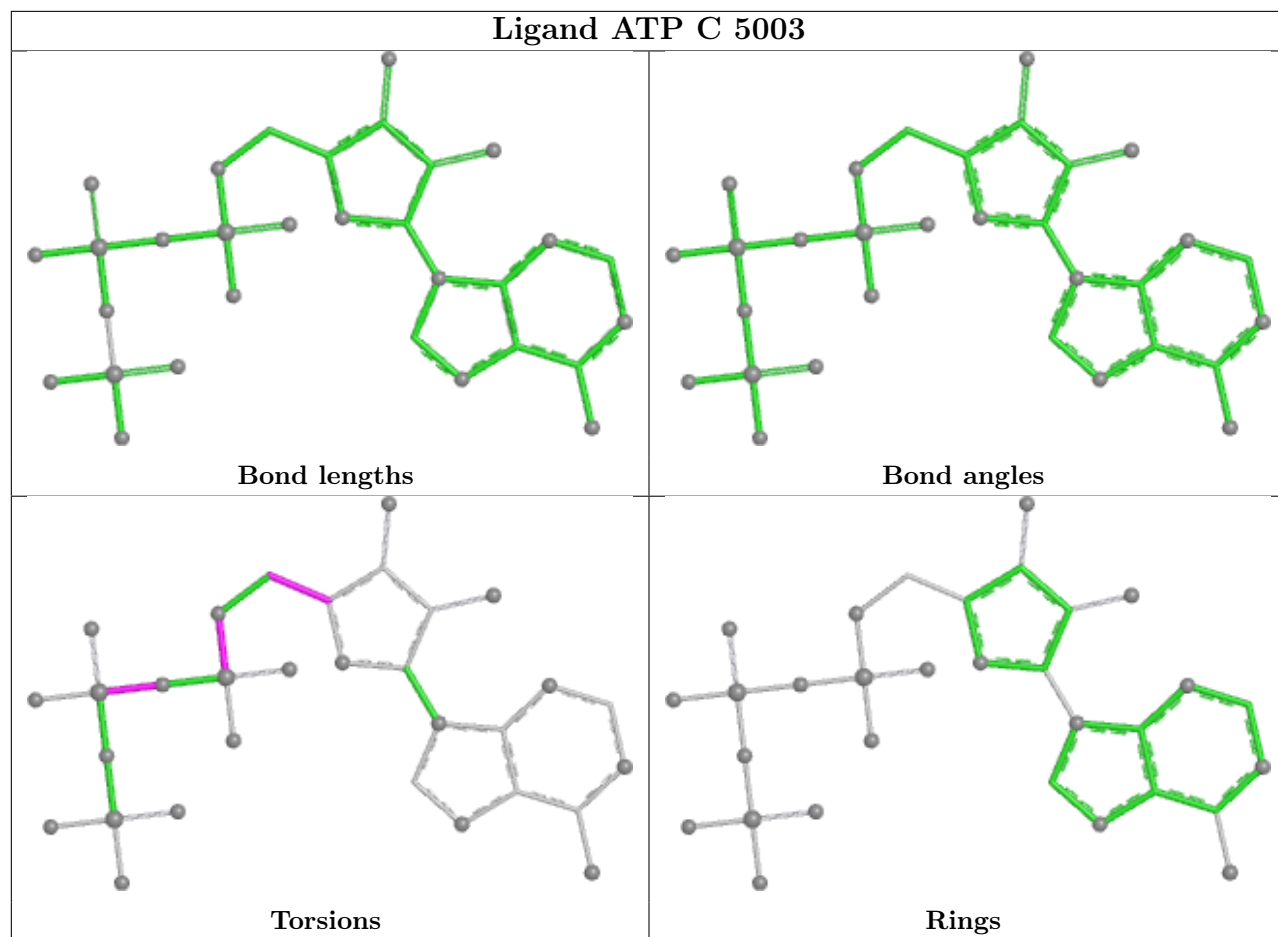
4 monomers are involved in 4 short contacts:

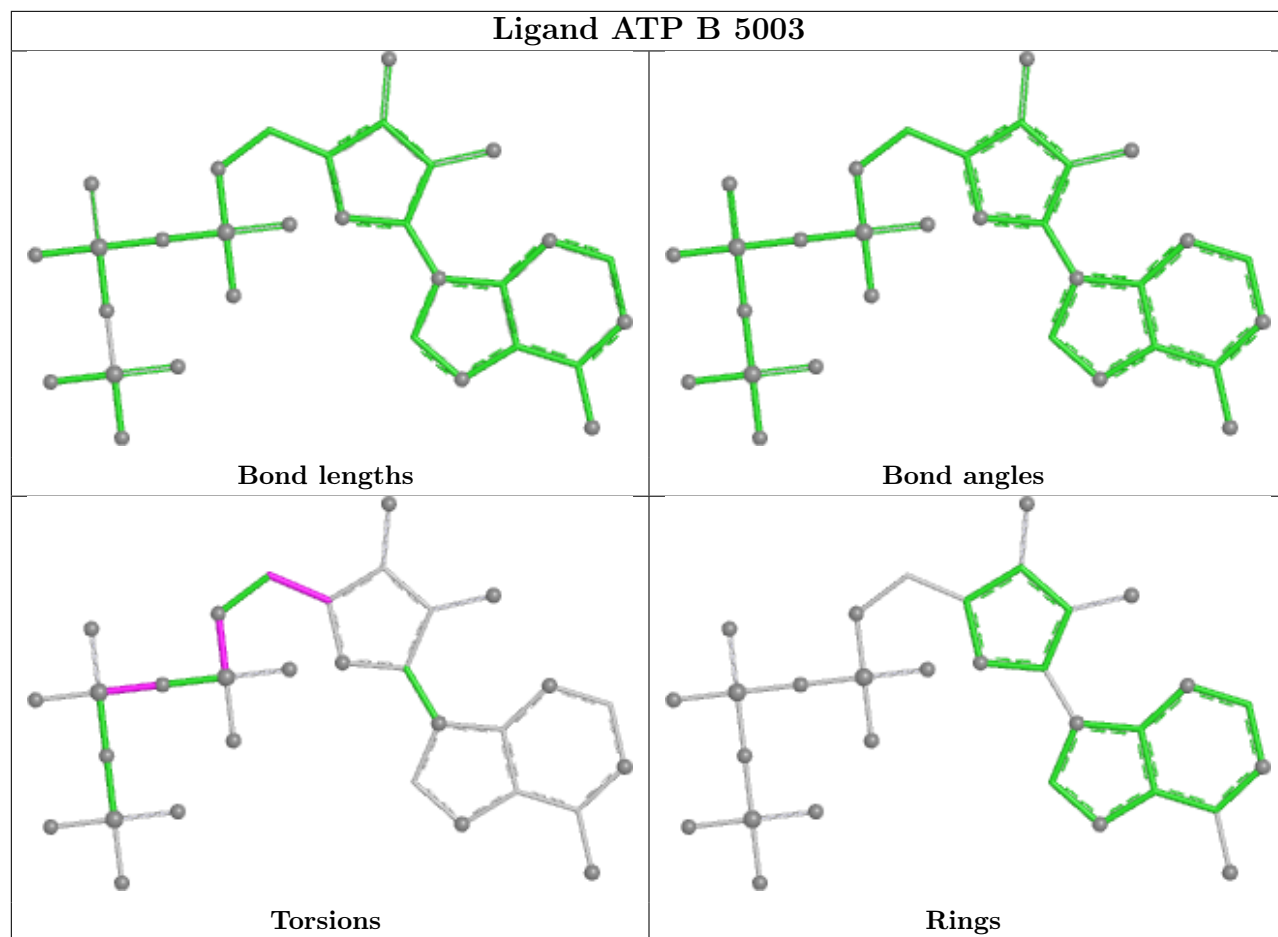
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5003	ATP	1	0
4	B	5003	ATP	1	0
4	D	5003	ATP	1	0
4	A	5003	ATP	1	0

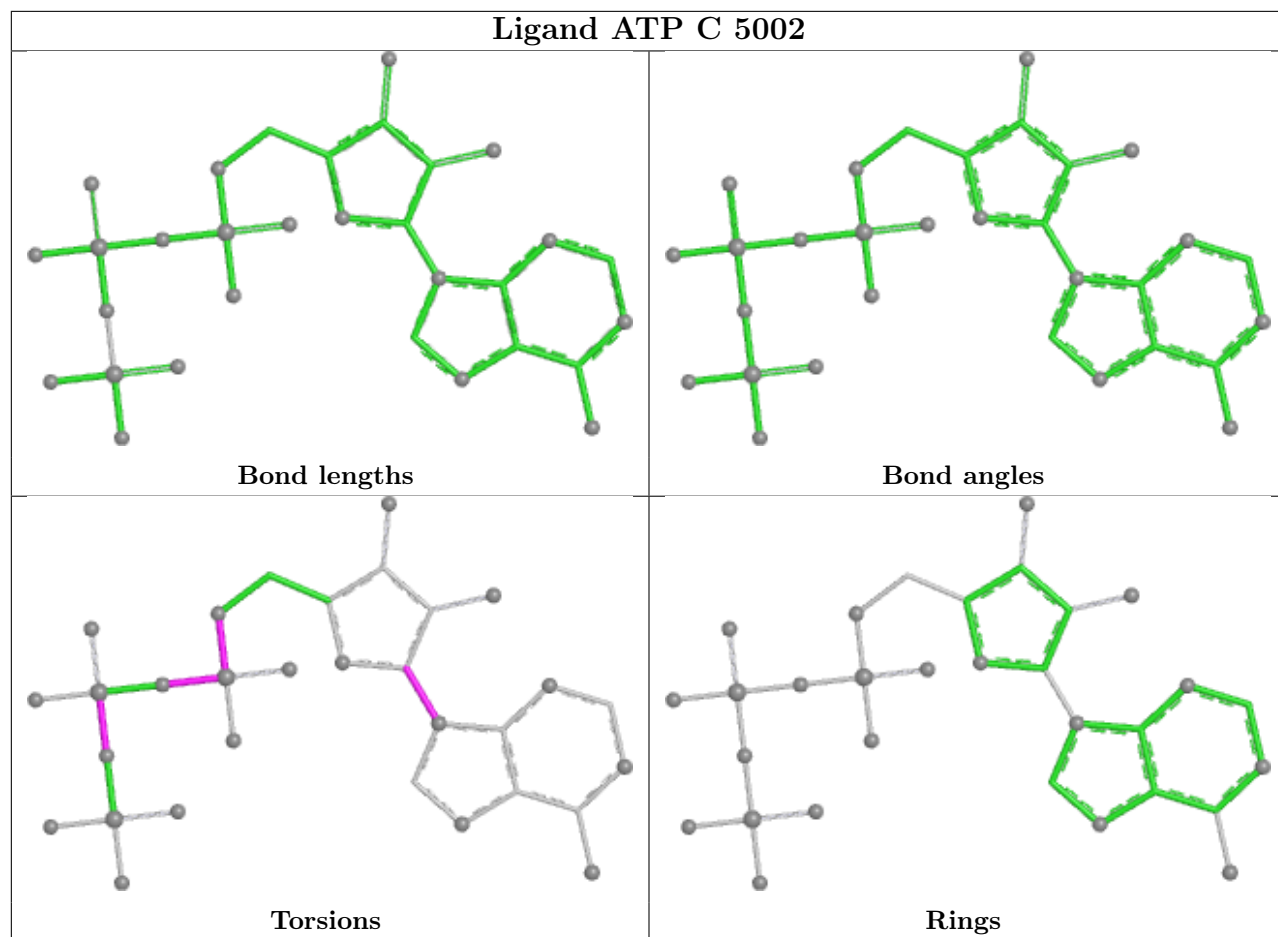
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

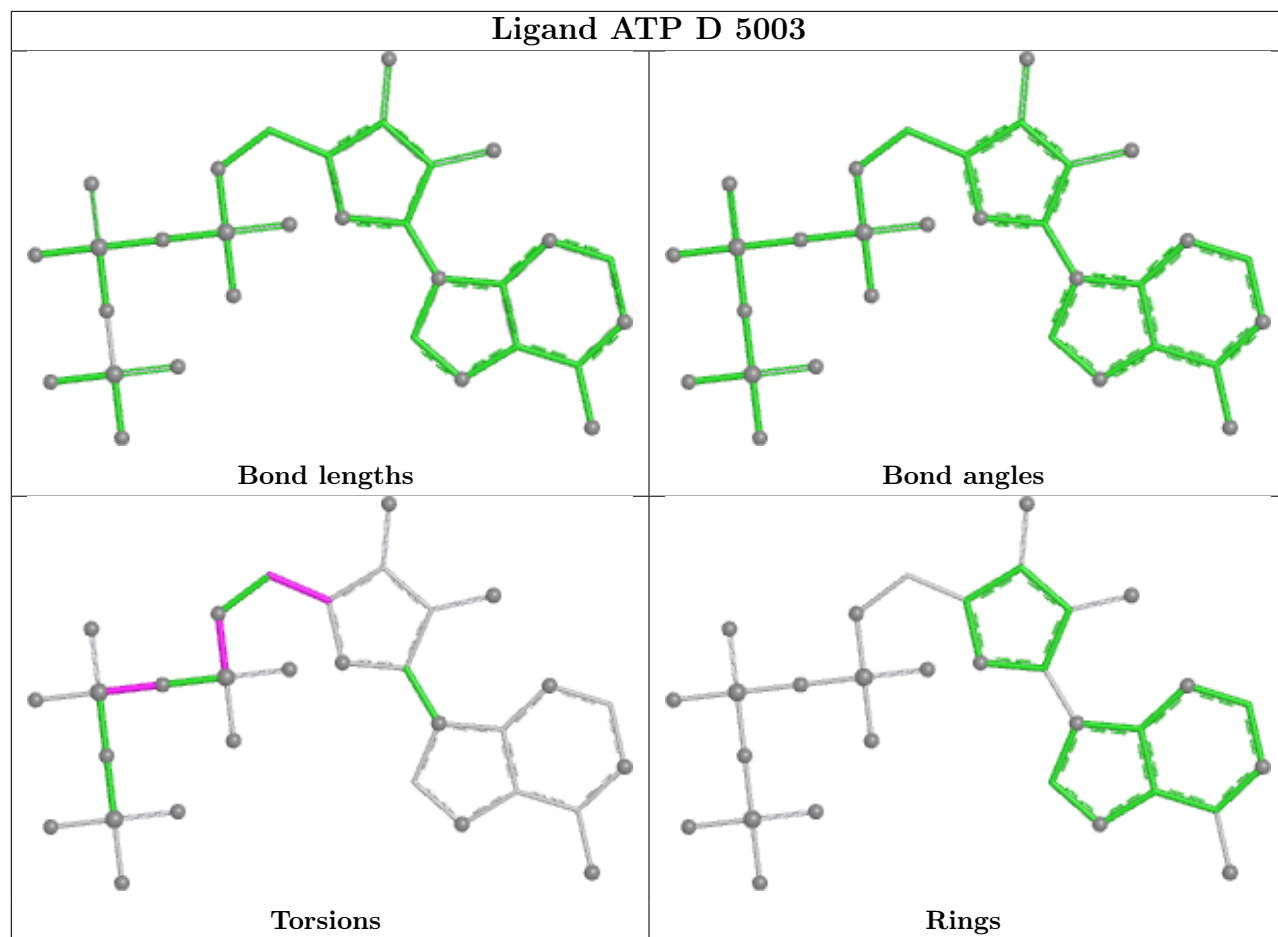


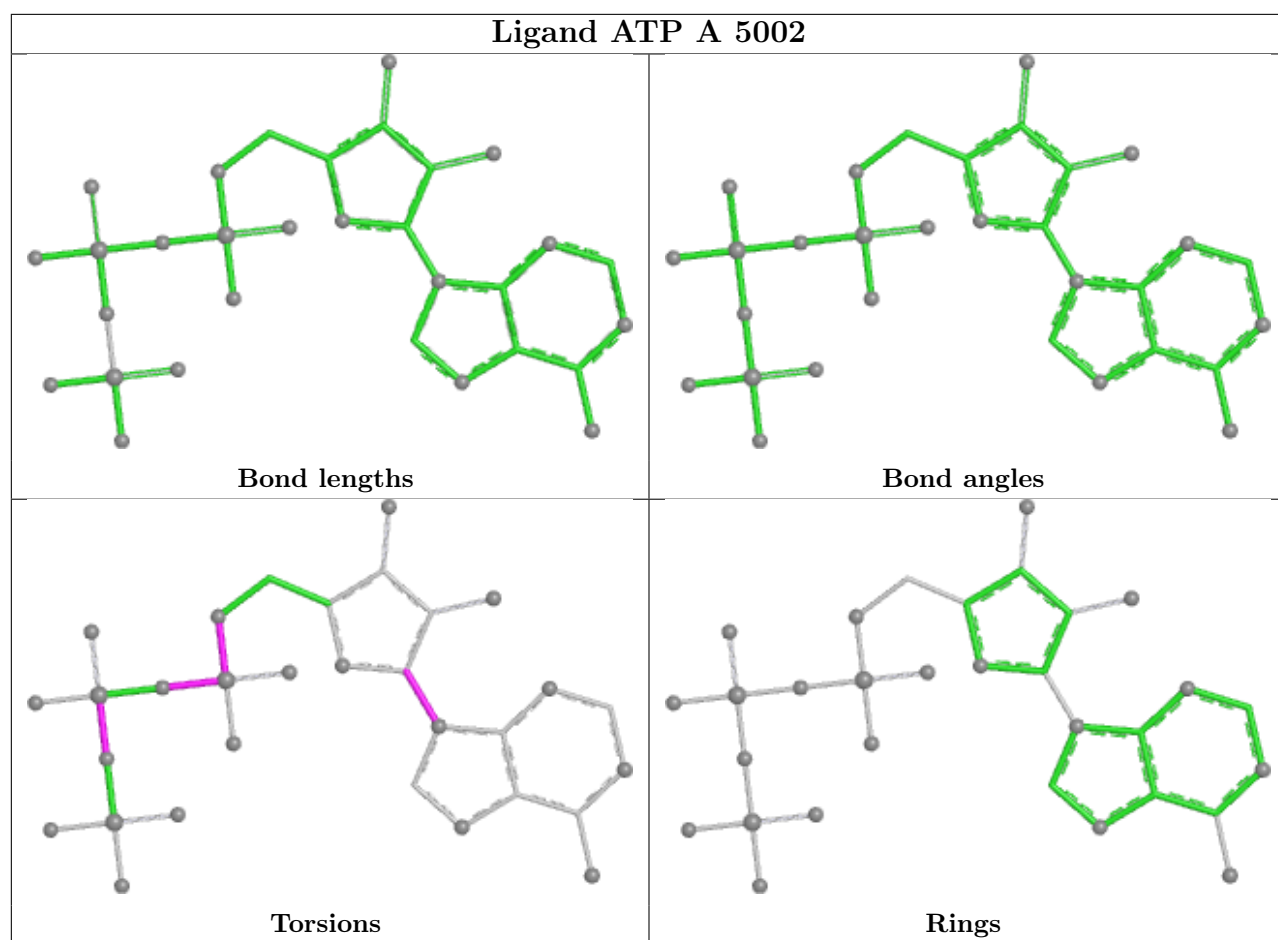


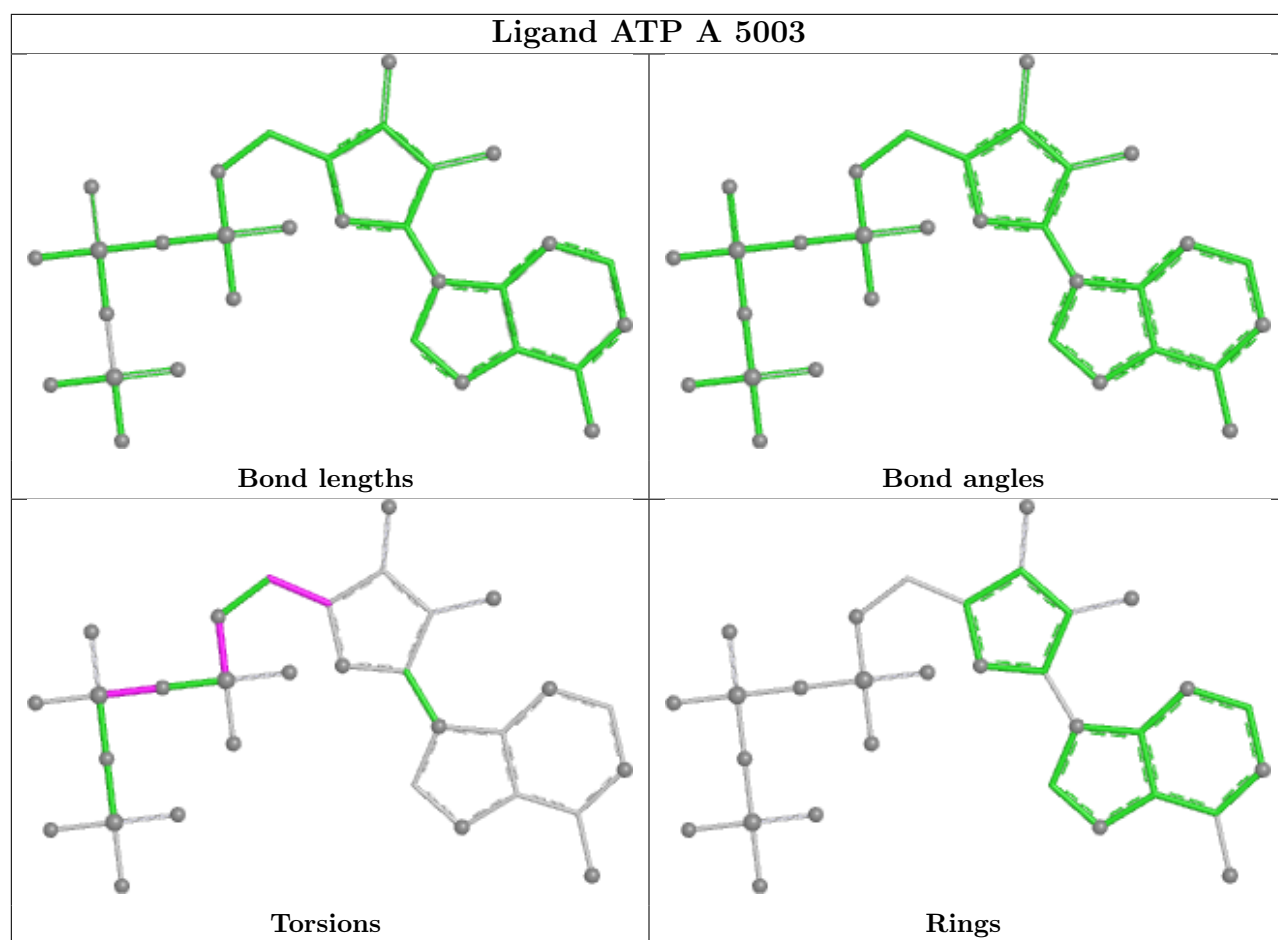












5.7 Other polymers [i](#)

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.

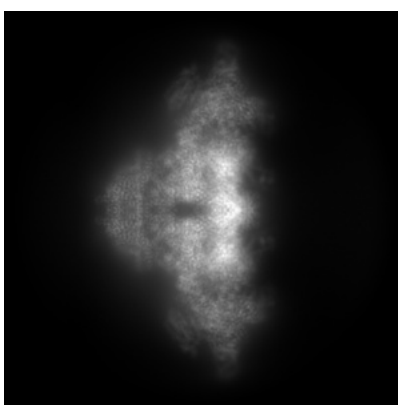
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

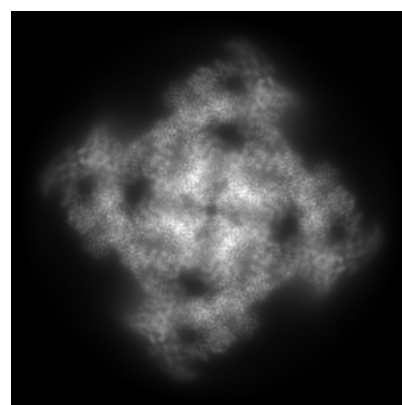
6.1.1 Primary map



X



Y



Z

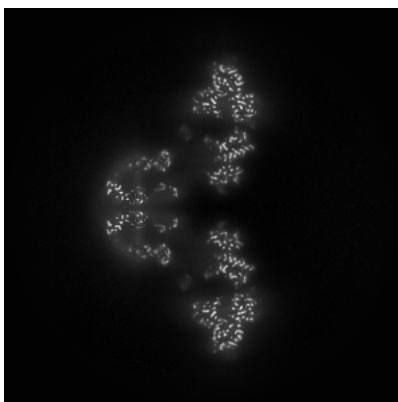
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

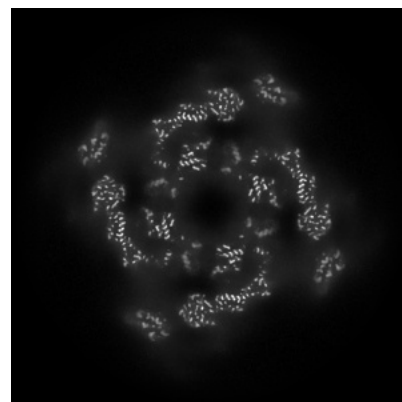
6.2.1 Primary map



X Index: 256



Y Index: 256

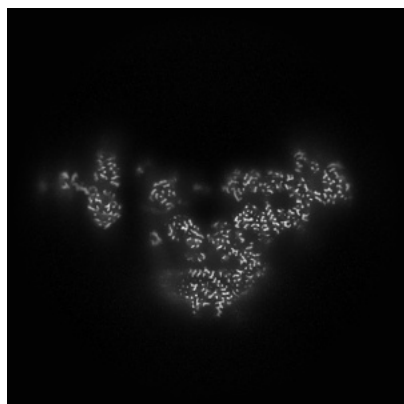


Z Index: 256

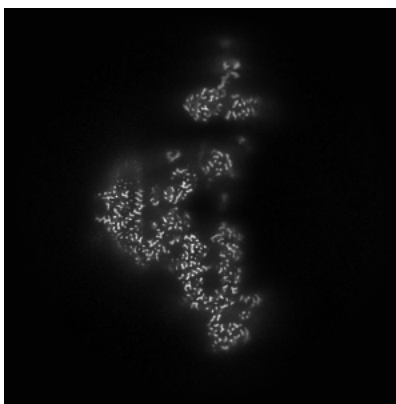
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

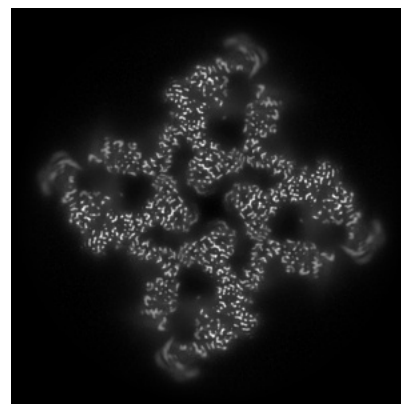
6.3.1 Primary map



X Index: 238



Y Index: 238

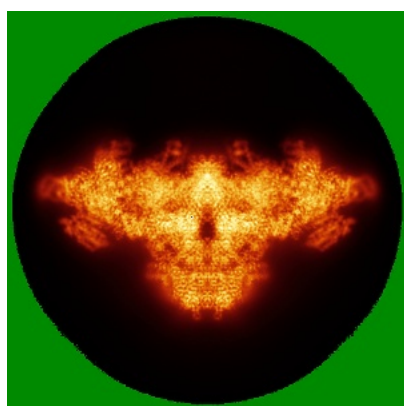


Z Index: 282

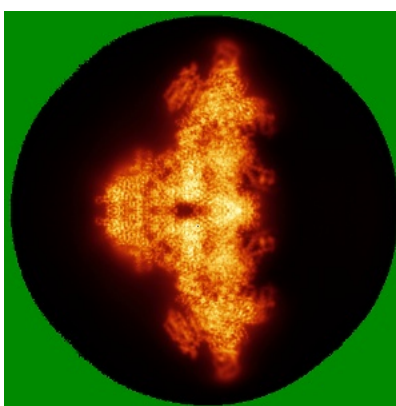
The images above show the largest variance slices of the map in three orthogonal directions.

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

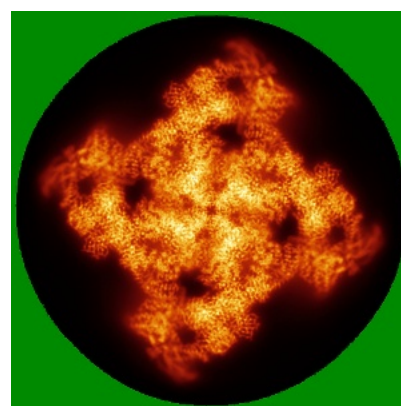
6.4.1 Primary map



X



Y

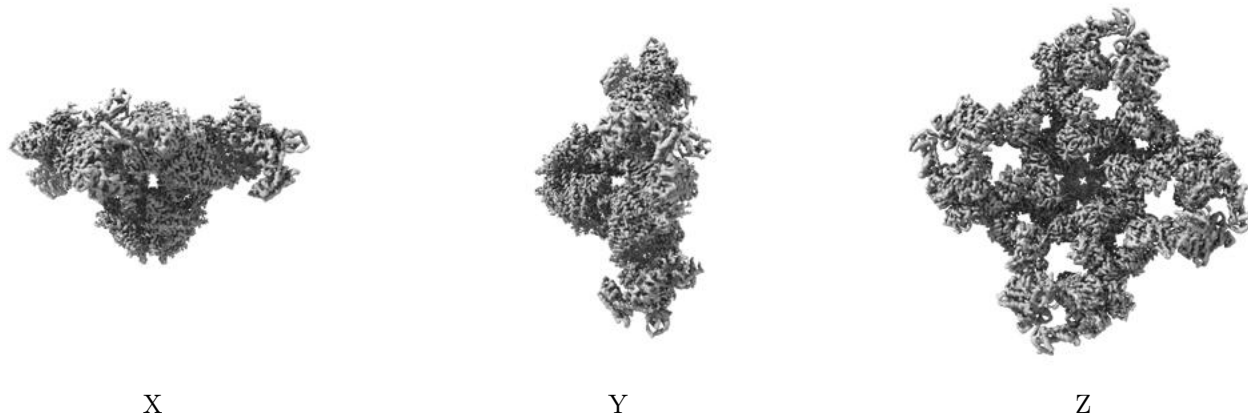


Z

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.

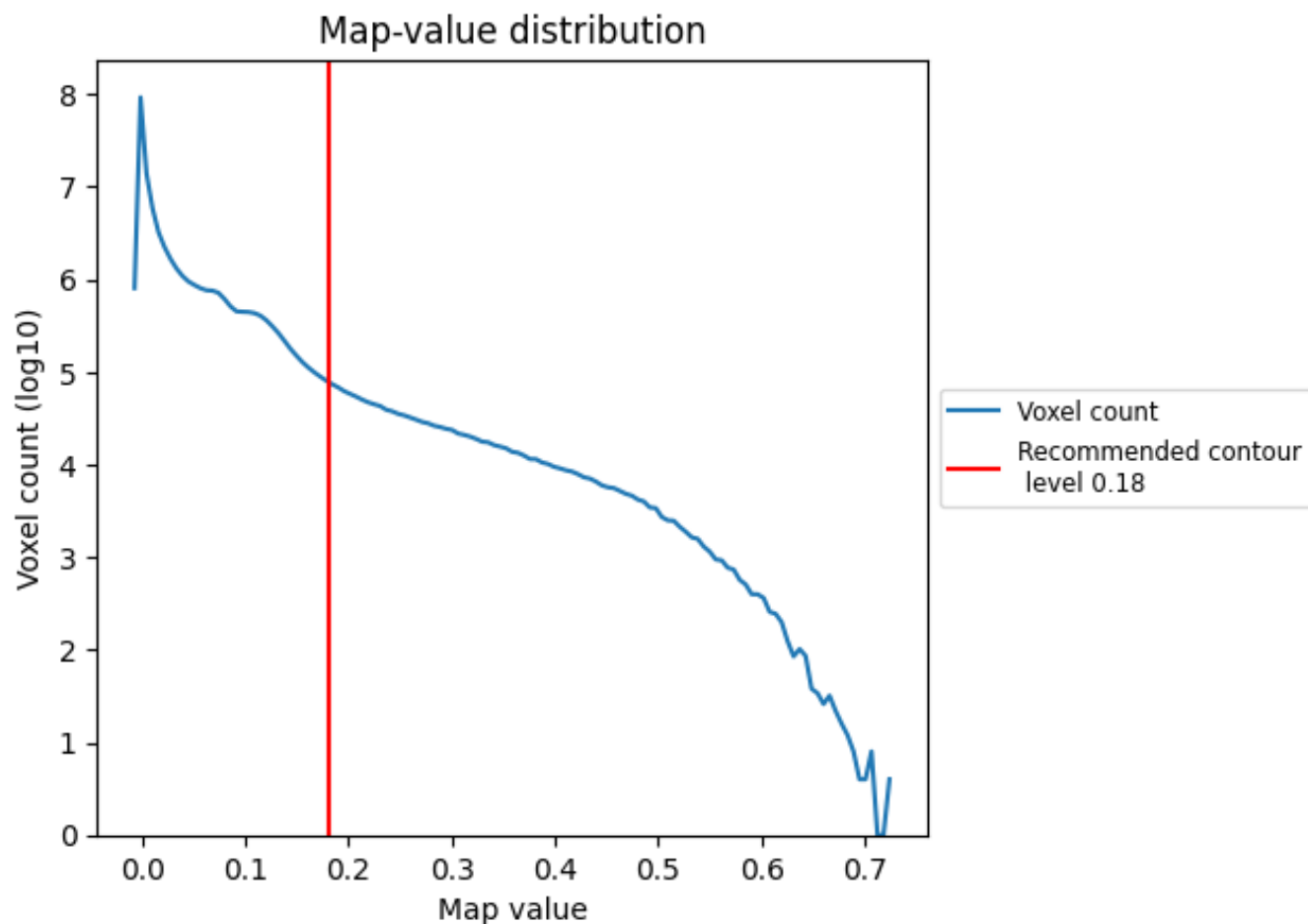
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

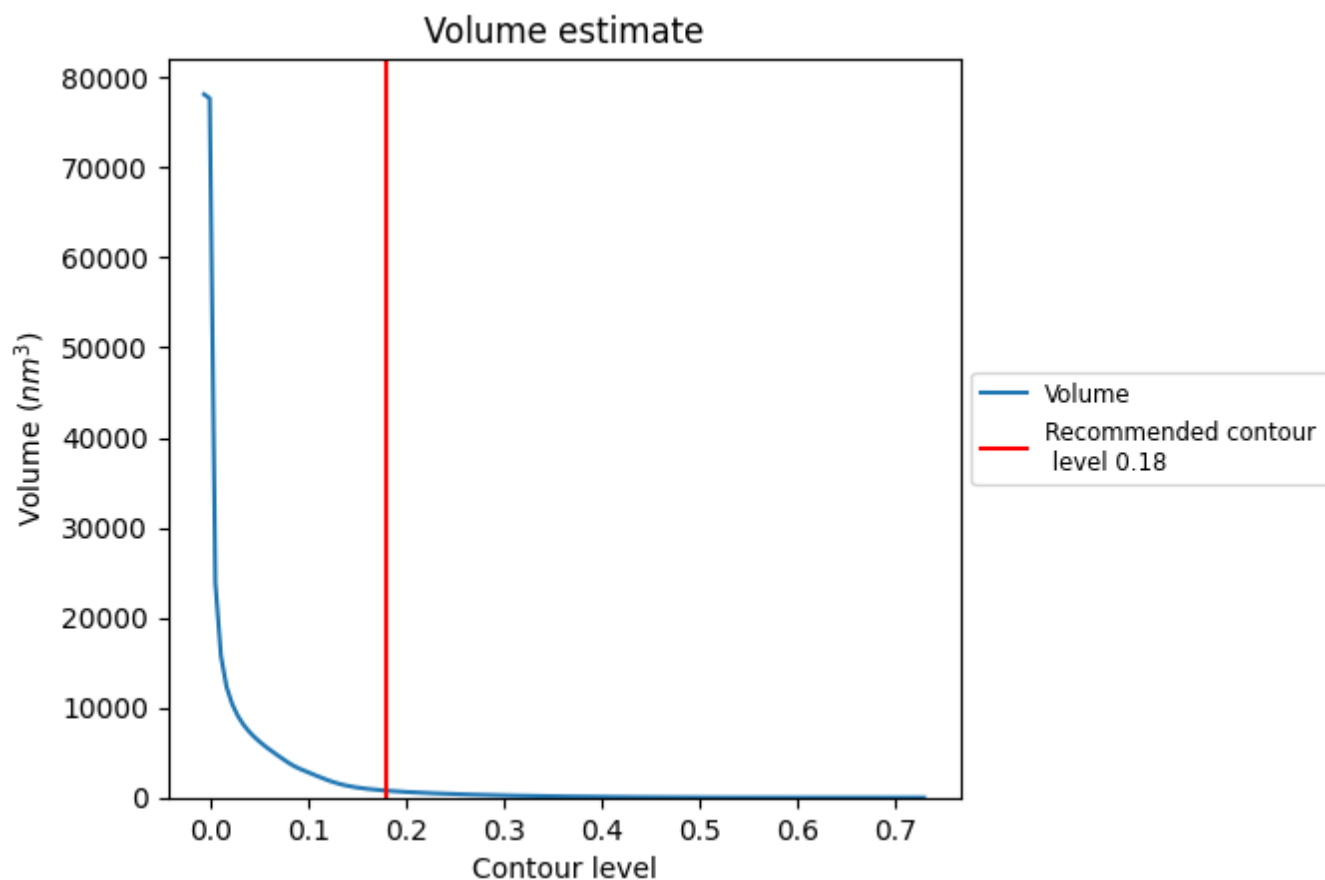
This section contains the results of statistical analysis of the map.

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.

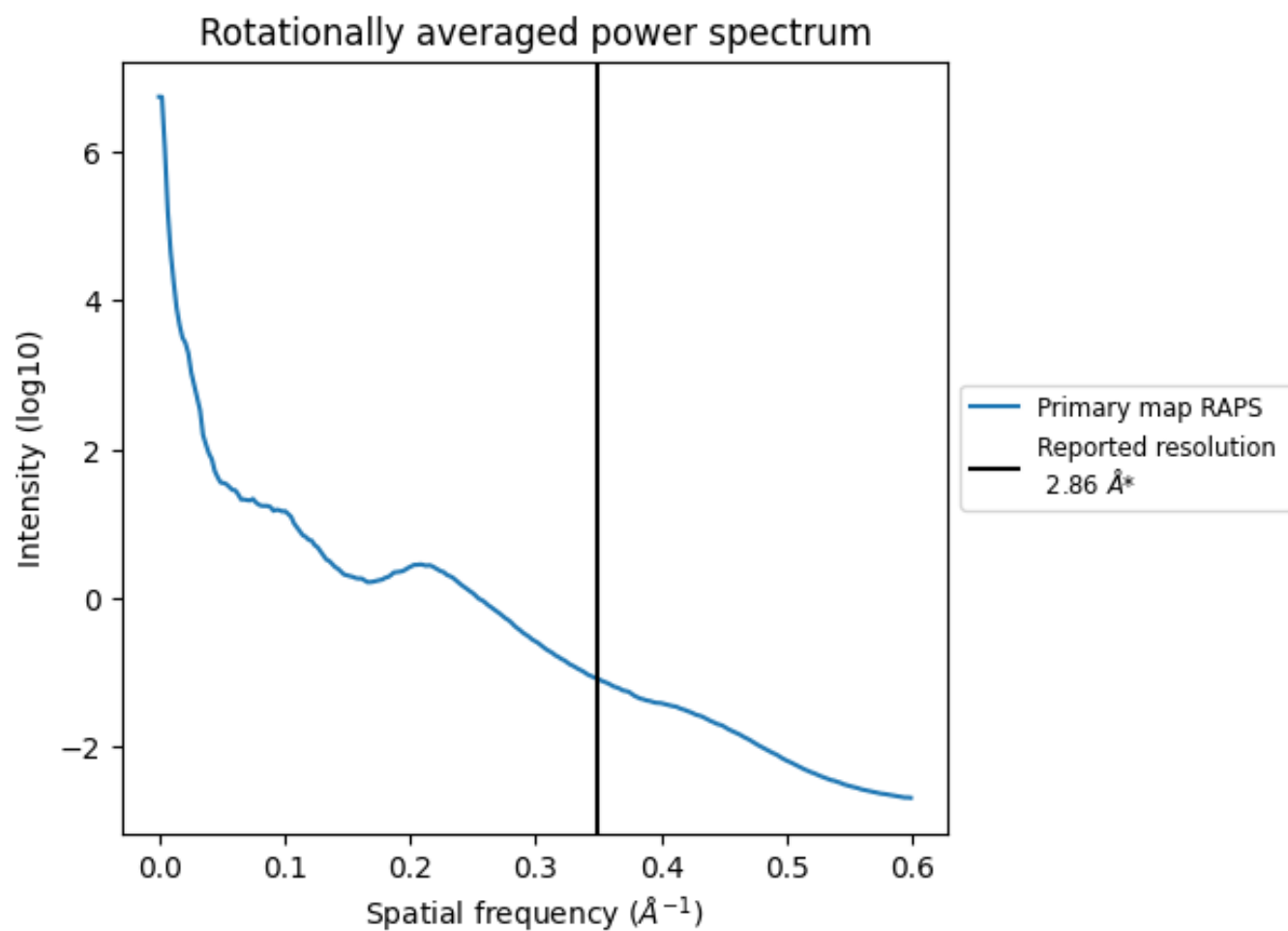
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 763 nm³; 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

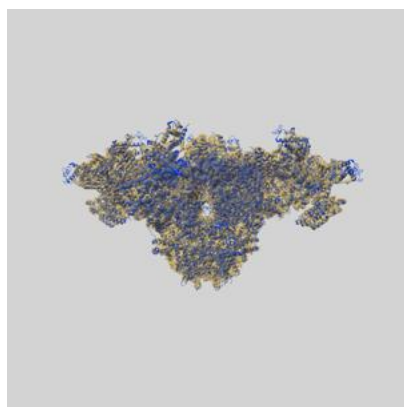
8 Fourier-Shell correlation

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

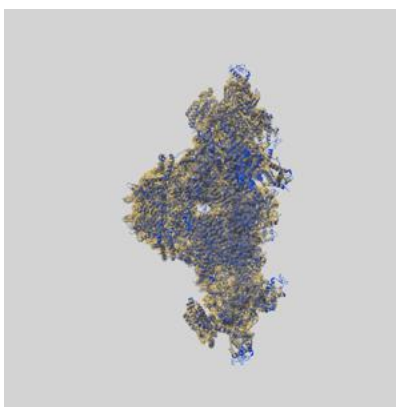
9 Map-model fit [i](#)

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 [7](#).

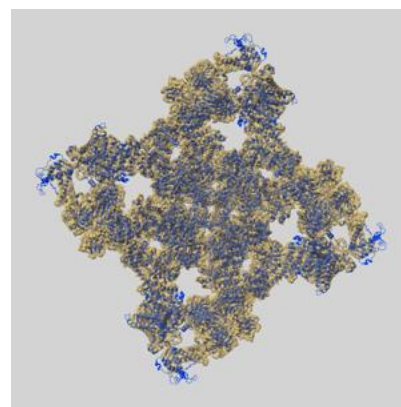
9.1 Map-model overlay [i](#)



X



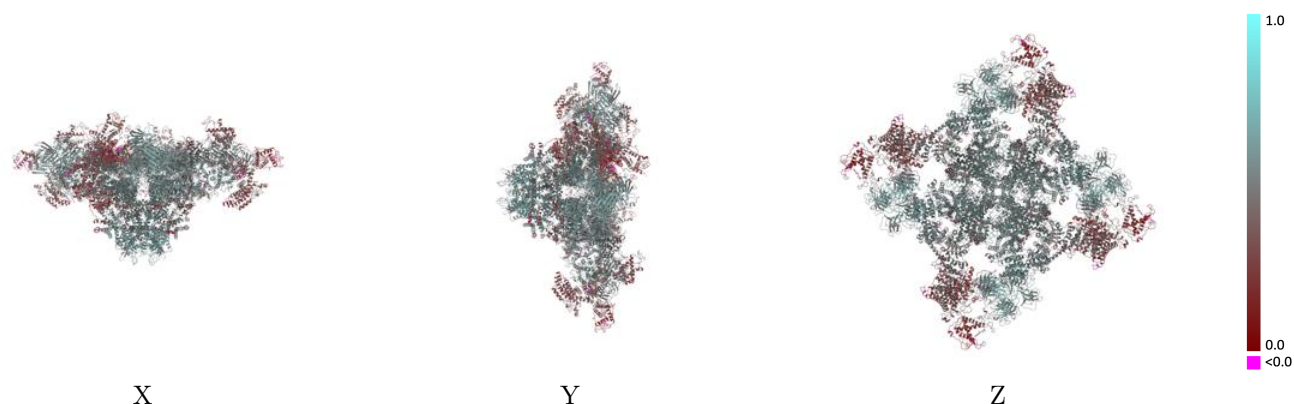
Y



Z

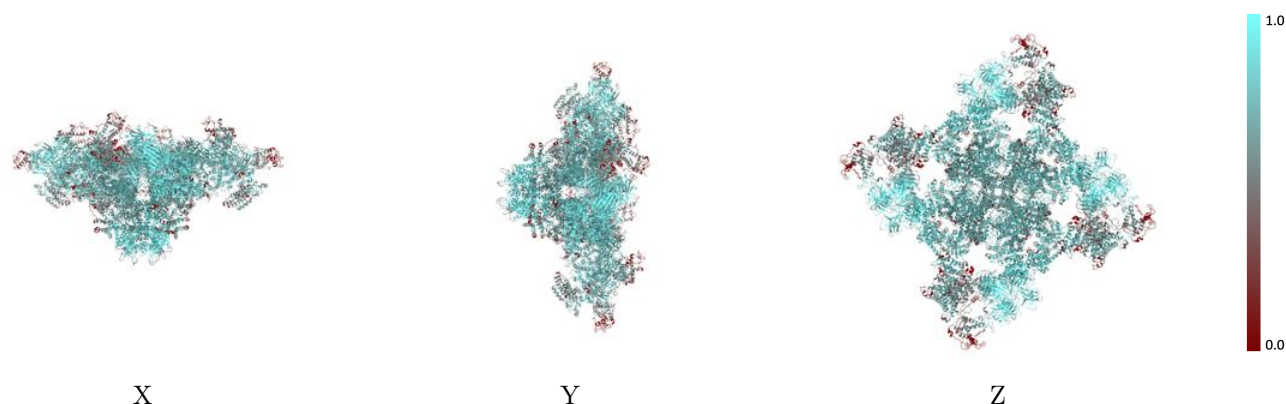
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



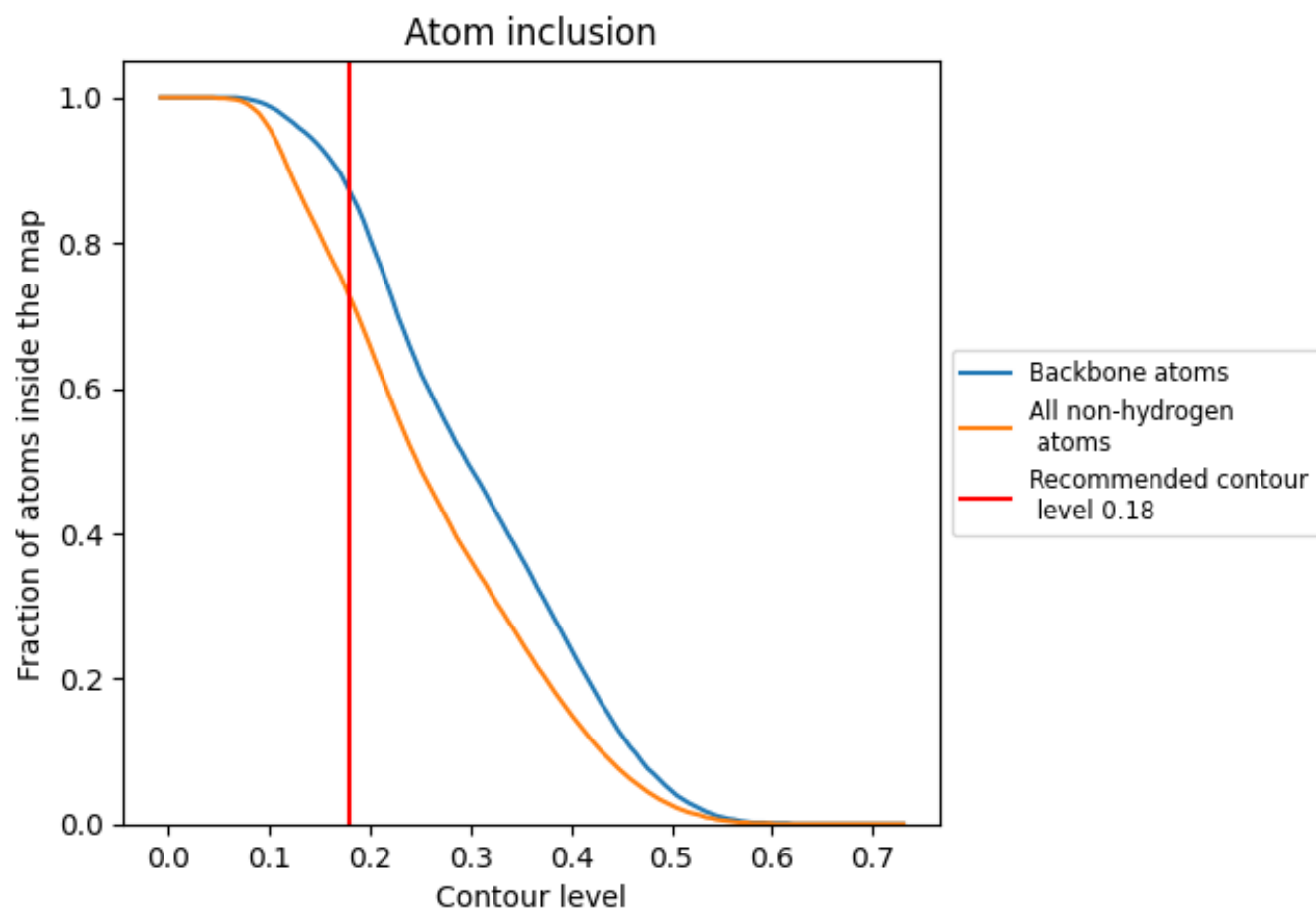
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	0.7270	0.4660
A	0.7240	0.4640
B	0.7240	0.4640
C	0.7240	0.4640
D	0.7240	0.4640
E	0.8490	0.5520
F	0.8440	0.5520
G	0.8500	0.5520
H	0.8500	0.5510

1.0

0.0

<0.0