



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 11:33 PM EDT

PDB ID : 7U9Z
EMDB ID : EMD-26410
Title : Structure of PKA phosphorylated human RyR2-R2474S in the open state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 3.29 Å(reported)
Based on initial model : 7U9X

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

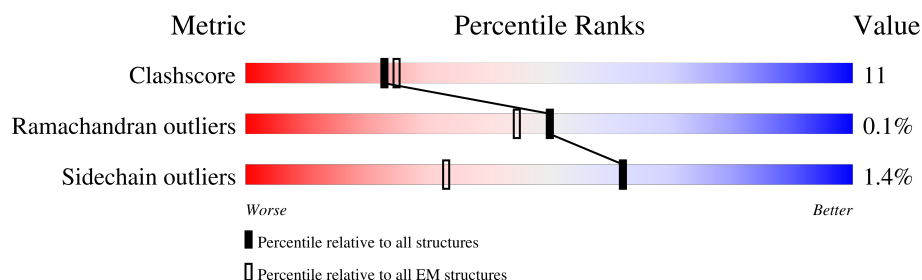
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 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>11%</div> <div>63%</div> <div>21%</div> <div>15%</div> </div>
1	B	4967	<div> <div>11%</div> <div>63%</div> <div>21%</div> <div>15%</div> </div>
1	C	4967	<div> <div>11%</div> <div>64%</div> <div>20%</div> <div>15%</div> </div>
1	D	4967	<div> <div>11%</div> <div>64%</div> <div>21%</div> <div>15%</div> </div>
2	E	108	<div> <div>77%</div> <div>20%</div> <div>..</div> </div>
2	F	108	<div> <div>77%</div> <div>20%</div> <div>..</div> </div>
2	G	108	<div> <div>77%</div> <div>20%</div> <div>..</div> </div>
2	H	108	<div> <div>77%</div> <div>20%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 138688 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	4226	Total	C	N	O	S	2	0
			33779	21520	5746	6283	230		
1	B	4226	Total	C	N	O	S	2	0
			33779	21520	5746	6283	230		
1	C	4226	Total	C	N	O	S	2	0
			33779	21520	5746	6283	230		
1	D	4226	Total	C	N	O	S	2	0
			33779	21520	5746	6283	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

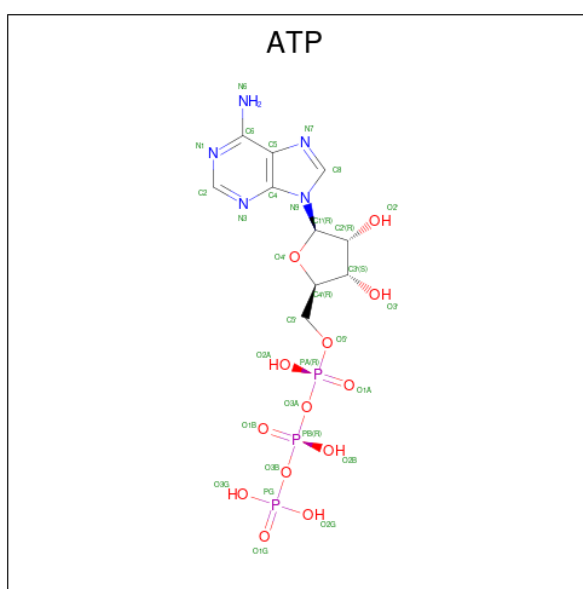
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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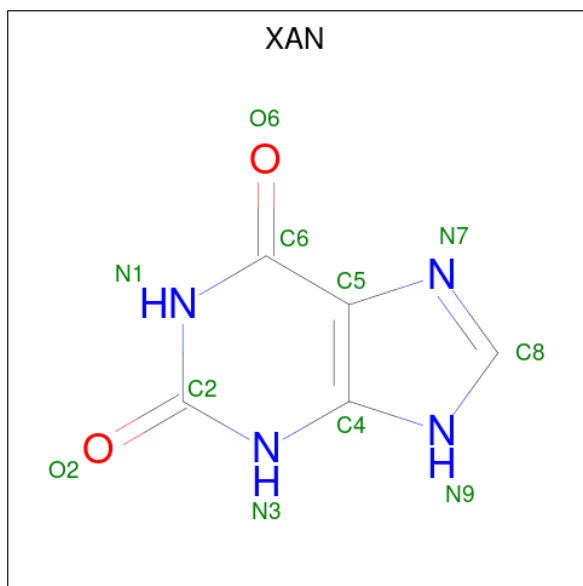
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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

- Molecule 6 is XANTHINE (three-letter code: XAN) (formula: C₅H₄N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			11	5	4	2	
6	B	1	Total	C	N	O	0
			11	5	4	2	
6	C	1	Total	C	N	O	0
			11	5	4	2	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	D	1	11	5	4	2	0

3 Residue-property plots

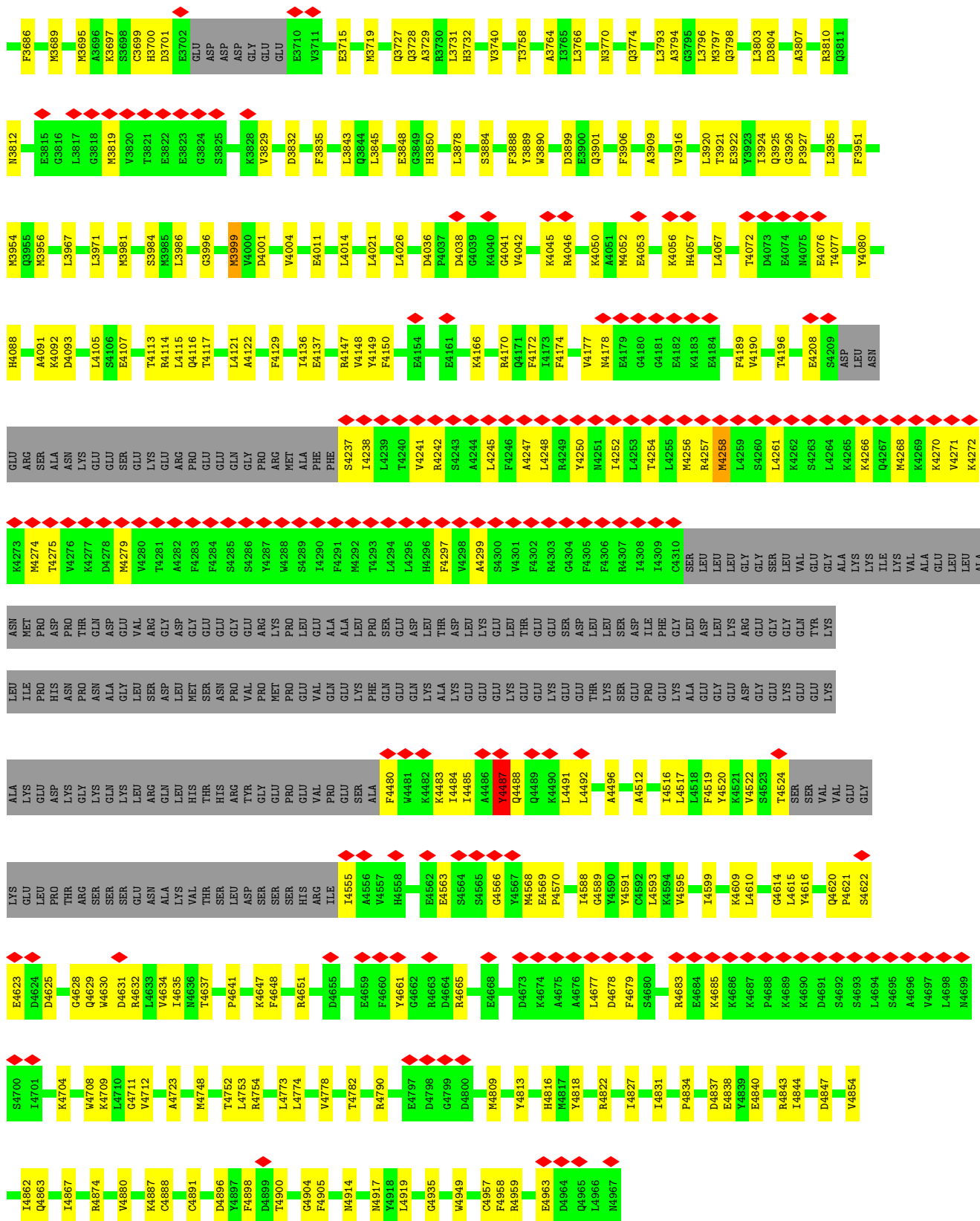
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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







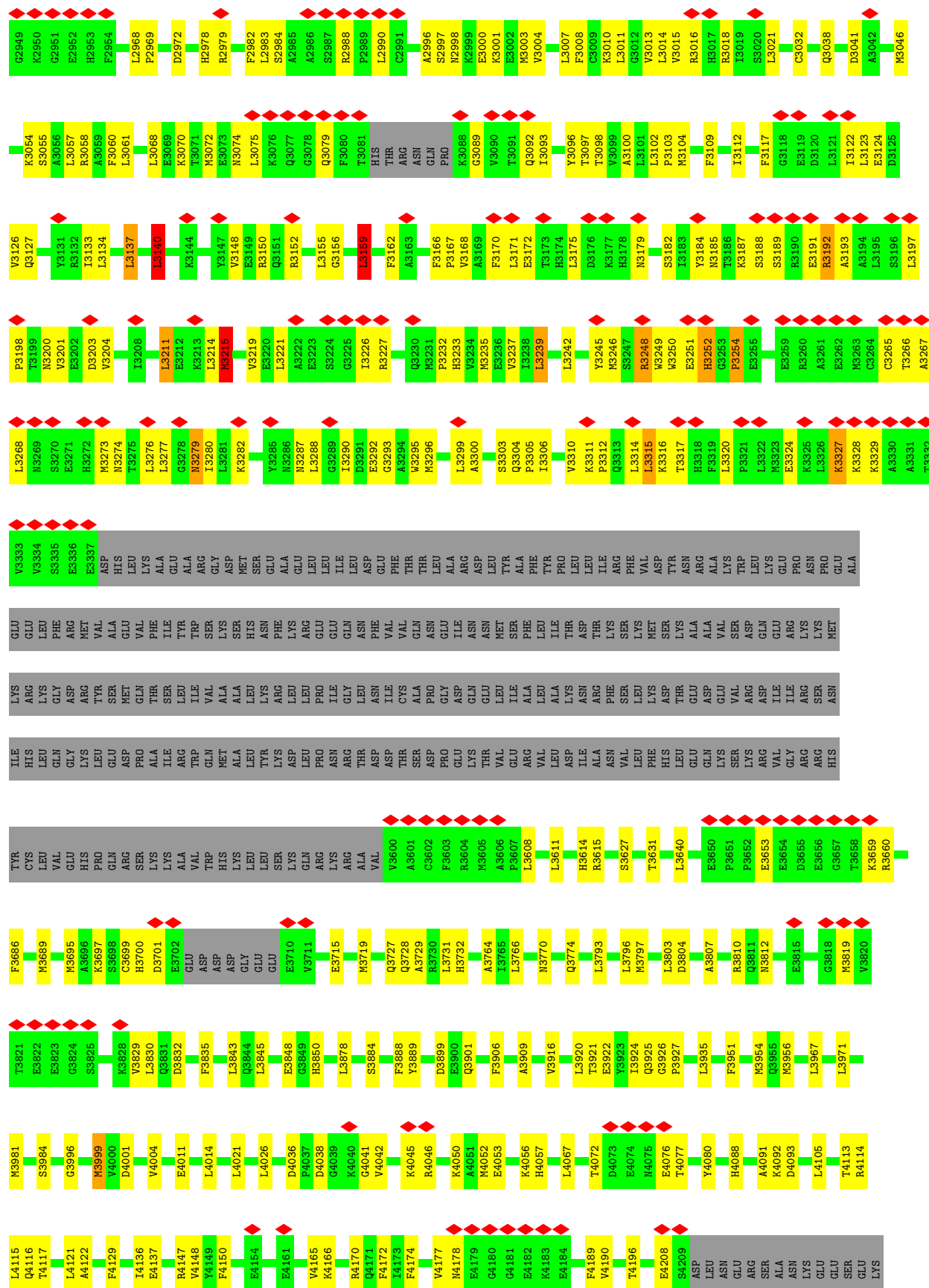


- Molecule 1: Ryanodine receptor 2

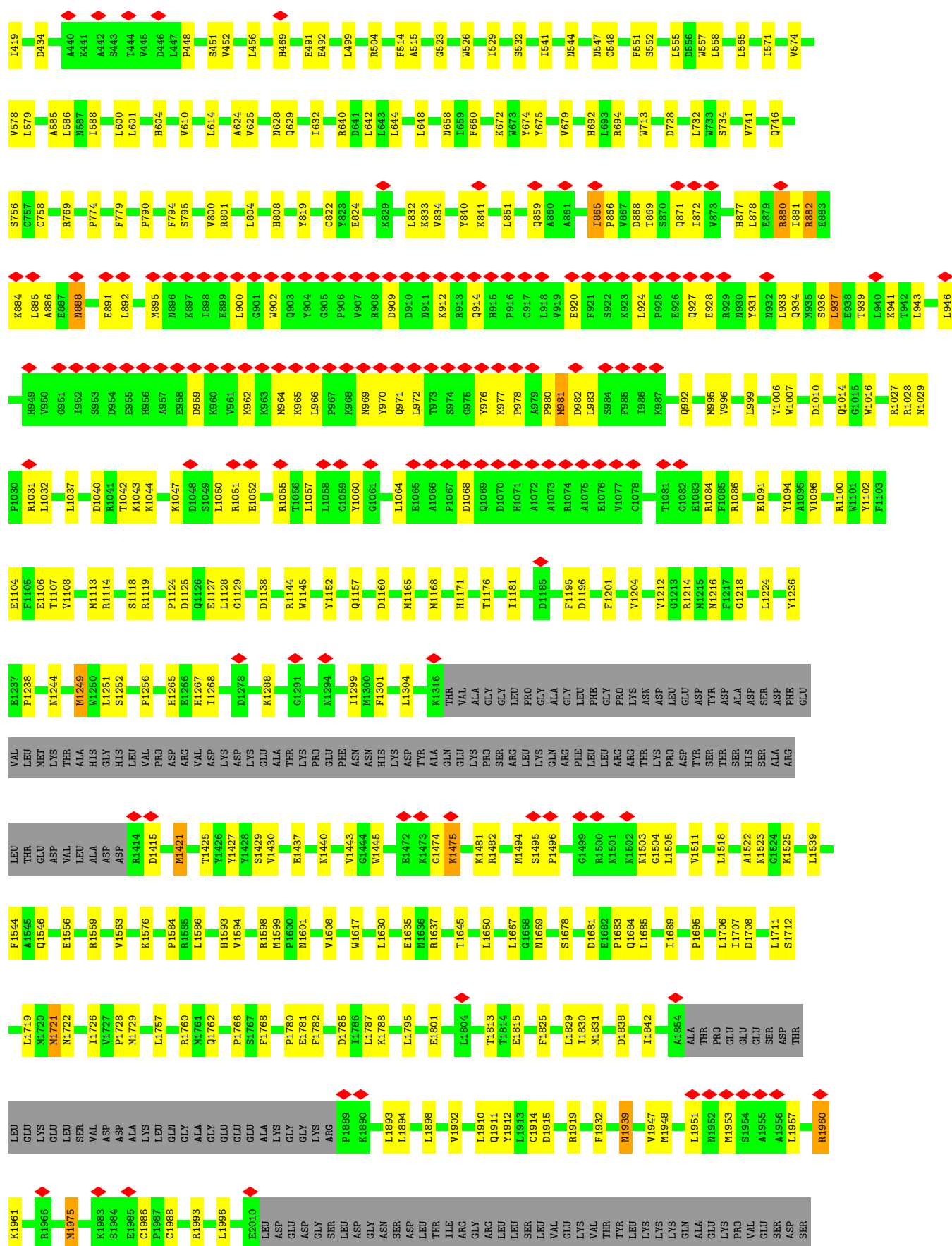


MET	D311	G397	D556	R694	V867	R929	V996	T1081	V1204
ALA	K312	H398	W557	W713	D868	N930	L999	G1082	V1212
ASP	N813	M399	L558	D728	S870	Y931	V1006	R1083	G1213
GLY	L314	L405	L565	L732	Q871	N932	D1010	F1084	R1214
PHE	L315	R417	I571	L732	I872	L933	Q1014	F1085	M1215
MET	L316	I419	V574	W734	V873	Q934	Q1015	R1086	N1216
GLY	M317	I419	V574	S734	L874	M935	Q1016	F1217	A1217
GLY	D323	D434	V578	V741	H877	S936	W1015	E1091	K1219
ASP	V324	D434	L579	Q746	L878	L937	W1016	Y1094	K1220
THR	K325	A440	A585	Q746	E879	T939	W1017	A1095	D1220
ALA	L234	K441	L586	V754	R880	K941	R1027	Y1096	T1223
GLY	L234	A442	N587	I755	R882	T942	R1028	Y1236	Y1236
GLY	L234	T444	I588	S756	R883	L943	M1029	E1237	P1238
THR	L237	V445	L600	C757	K884	L946	P1030	E1104	L1244
VAL	L237	D446	L601	C758	L885	L946	L1031	F1105	M1244
LYS	L237	L447	H604	R769	A886	L946	L1032	E1106	M1249
GLN	L237	P448	V610	P774	E887	L946	Y1035	T1107	W1250
GLY	L237	S451	L614	F779	N888	L946	L1037	V1108	L1251
GLY	L237	V452	A624	F794	E891	L946	L1037	M1113	S1252
GLY	L237	L456	V625	S795	L892	L946	D1040	R1114	P1256
GLY	L237	H469	N628	S795	W893	L946	E1041	S1118	P1256
GLY	L237	E491	Q629	V800	L893	L946	T1042	R1119	H1265
GLY	L237	E492	I632	R801	Y893	L946	K1043	P1124	H1265
GLY	L237	L499	R640	L804	E899	L946	K1044	E1127	H1267
GLY	L237	A271	L641	H808	L900	L946	E1052	L1128	I1268
GLY	L237	R272	L642	Y819	G901	L946	R1055	G1129	K1288
GLY	L237	W275	L644	C822	W902	L946	T1056	Y1152	N1294
GLY	L237	R276	L644	E824	Q903	L946	L1057	Q1157	S1295
GLY	L237	L280	L648	E824	G905	L946	L1058	D1160	N1296
GLY	L237	W291	N658	K829	P906	L946	G1059	M1165	I1299
GLY	L237	P294	I659	L832	V907	L946	Y1060	M1168	M1300
GLY	L237	F295	L661	K833	R908	L946	G1061	H1171	F1301
GLY	L237	R296	A668	Y840	D909	L946	L1064	T1176	L1304
GLY	L237	L297	K672	K841	D910	L946	E1065	Y1181	K1316
GLY	L237	R298	W673	L851	N911	L946	A1066	F1195	THR
GLY	L237	V300	Y674	L851	R912	L946	P1067	D1196	THR
GLY	L237	T302	Y675	Q859	R913	L946	D1068	PHE	THR
GLY	L237	G303	M678	A860	Q914	L946	Q1069	LEU	THR
GLY	L237	MET	V679	A861	H915	L946	D1070	GLY	THR
GLY	L237	K304	H692	I865	P916	L946	H1071	GLY	THR
GLY	L237	Y365	L693	P866	C917	L946	A1072	GLY	THR
GLY	L237	L306	L693	P866	L918	L946	A1073	GLY	THR
GLY	L237	S307	L693	P866	L919	L946	R1074	GLY	THR
GLY	L237	L308	L693	P866	E920	L946	A1075	GLY	THR
GLY	L237	M309	L693	P866	F921	L946	E1076	GLY	THR
GLY	L237	ASP	L693	P866	S922	L946	V1077	GLY	THR
GLY	L237	VAL	L693	P866	K923	L946	C1078	GLY	THR
GLY	L237	ASP	L693	P866	L924	L946	L988	GLY	THR
GLY	L237	VAL	L693	P866	P925	L946	L988	GLY	THR
GLY	L237	VAL	L693	P866	E926	L946	L988	GLY	THR
GLY	L237	VAL	L693	P866	Q927	L946	L988	GLY	THR
GLY	L237	VAL	L693	P866	E928	L946	L988	GLY	THR
GLY	L237	VAL	L693	P866	E928	L946	L988	GLY	THR

S2862	K2863	G2864	G2865	G2866	N2867	H2868	H2869	L2870	L2877	E2881	K2884	E2887	L2893	K2894	F2895	L2896	Y2901	A2902	V2903	S2904	R2905	G2906	F2907	L2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	S2916	I2917	E2918	K2919	R2920	S2924	Q2927	Q2928	L2929	I2930	V2933	Y2939	I2940	F2943	S2947	R2948						
K2780	N2781	M2782	L2783	A2784	V2785	R2788	L2789	E2790	R2791	E2792	R2793	E2794	G2795	M2798	N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	VAL	ASP	A2817	A2818	H2819	G2820	P2823	S2824	S2829	N2830	R2835	A2841	E2842	M2843	H2849	K2854	K2857	N2858	E2859	L2860	E2861						
P2703	V2706	D2707	T2708	S2709	N2710	E2715	K2716	L2717	E2718	Y2719	F2720	L2721	N2722	K2723	Y2724	A2725	E2726	K2731	D2735	K2736	L2737	A2738	N2739	G2740	N2741	L2742	Y2743	G2744	E2745	I2746	Y2747	S2748	D2749	S2750	S2751	K2752	V2753	Q2754	P2755	L2756	N2757	K2758	P2759	Y2760	K2761	L2762	L2763	E2769	I2770	Y2771	R2772	Q2773	I2775
E2615	R2616	Y2621	C2622	L2623	P2624	G2625	E2635	E2636	E2637	L2638	H2639	L2640	R2642	K2643	L2644	F2645	W2646	D2650	Q2654	L2664	A2665	G2666	P2667	C2668	L2669	V2672	V2676	L2677	P2678	D2679	Y2680	M2681	Q2682	S2683	N2684	Y2685	V2686	N2687	M2688	E2689	R2690	L2691	V2692	F2693	L2694	L2695	H2696	L2697	H2613	Y2614			
G2491	P2494	A2499	T2504	L2507	S2508	R2530	H2541	L2544	I2545	D2546	S2547	L2548	L2549	R2554	L2555	S2556	L2561	R2566	I2569	C2572	I2576	L2580	M2584	Q2585	H2587	L2588	L2589	R2590	L2591	V2593	F2594	L2599	H2602	P2606	L2607	H2613	Y2614																
A2354	P2357	S2358	P2364	ASN	GLY	SER	SER	THR	LEU	ASP	E2377	E2378	D2379	T2381	I2382	K2383	M2384	G2385	N2386	A2387	L2388	K2389	L2390	F2391	I2396	M2406	H2410	K2413	T2417	G2434	K2447	A2458	M2468	D2473	T2478	L2484	L2485	L2488															
L2146	I2149	M2150	Q2157	L2165	G2166	M2167	V2176	L2179	G2180	Q2181	G2182	E2183	S2184	K2185	E2186	I2187	F2199	L2200	M2214	Y2220	L2229	R2235	A2245	S2246	V2247	M2248	L2257	R2258	E2259	P2260	M2279	Y2285	I2288	G2289	W2290	R2297	R2322	R2326	L2344														
ARG	LEU	SER	LEU	VAL	GLU	LYS	VAL	THR	LEU	LYS	LYS	LYS	GLN	ALA	GLU	LYS	PRO	VAL	GLU	SER	ASP	K2053	K2054	Q2059	T2065	M2066	V2067	Q2071	L2087	Q2090	Q2091	V2092	R2100	I2117	L2120	I2126	R2127	L2130	R2133	L2141	M2142	L2143	R2144	G2145									
L1913	C1914	D1915	R1919	F1932	M1939	V1947	M1948	L1951	H1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	K1961	R1965	M1975	D1981	D1982	K1983	S1984	C1985	F1987	C1988	R1993	L1996	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	ASN	SER	ASP	LEU	THR	ILE	ARG	GLY							
E1815	F1825	I1829	L1829	M1831	D1838	I1842	A1854	ALA	THR	PRO	GLU	GLU	SER	THR	LEU	GLU	LYS	GLU	SER	VAL	ASP	ASP	ALA	LYS	GLY	GLY	GLU	GLU	ALA	LYS	GLY	LYS	ARG	P1889	K1890	L1893	L1894	L1898	V1902	L1910	Q1911	Y1912											
L1667	G1668	M1669	L1676	G1677	S1678	D1681	E1682	P1683	Q1684	L1685	I1689	P1695	L1706	I1707	D1708	L1711	S1712	L1719	M1720	N1721	N1722	I1726	V1727	P1728	M1729	L1767	R1760	M1761	Q1762	P1766	S1767	F1768	P1780	E1781	F1782	D1785	I1786	L1787	K1788	L1795	E1801	T1813	T1814										
G1499	R1500	N1501	N1503	G1504	L1505	V1511	L1518	A1522	N1523	G1524	K1525	L1539	F1544	A1545	Q1546	E1556	R1559	V1563	K1576	P1584	R1585	L1586	L1591	S1592	H1593	V1594	M1599	V1608	W1617	L1618	V1619	L1630	E1635	G1674	R1637	T1645	L1660	V1664															
ARG	THR	LYS	PRO	ASP	TVR	SER	THR	SER	HIS	SER	ALA	ARG	LEU	THR	GLU	ASP	VAL	LEU	ALA	ASP	R1414	D1415	D1416	Y1417	H1421	T1425	V1426	Y1427	V1428	S1429	V1430	G1435	Q1436	E1437	N1440	V1443	G1444	V1445	Y1453	E1472	K1473	G1474	K1475	R1482	M1494	S1495	P1496	G1497	Q1498				

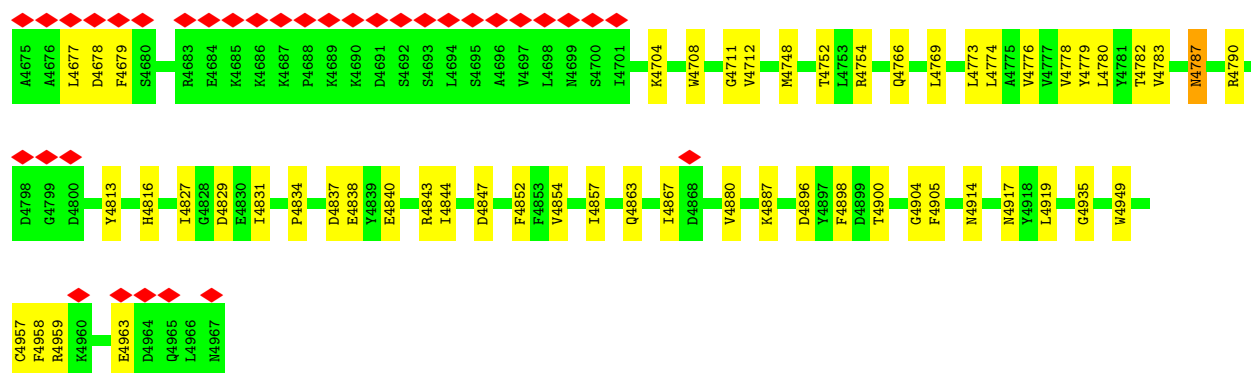




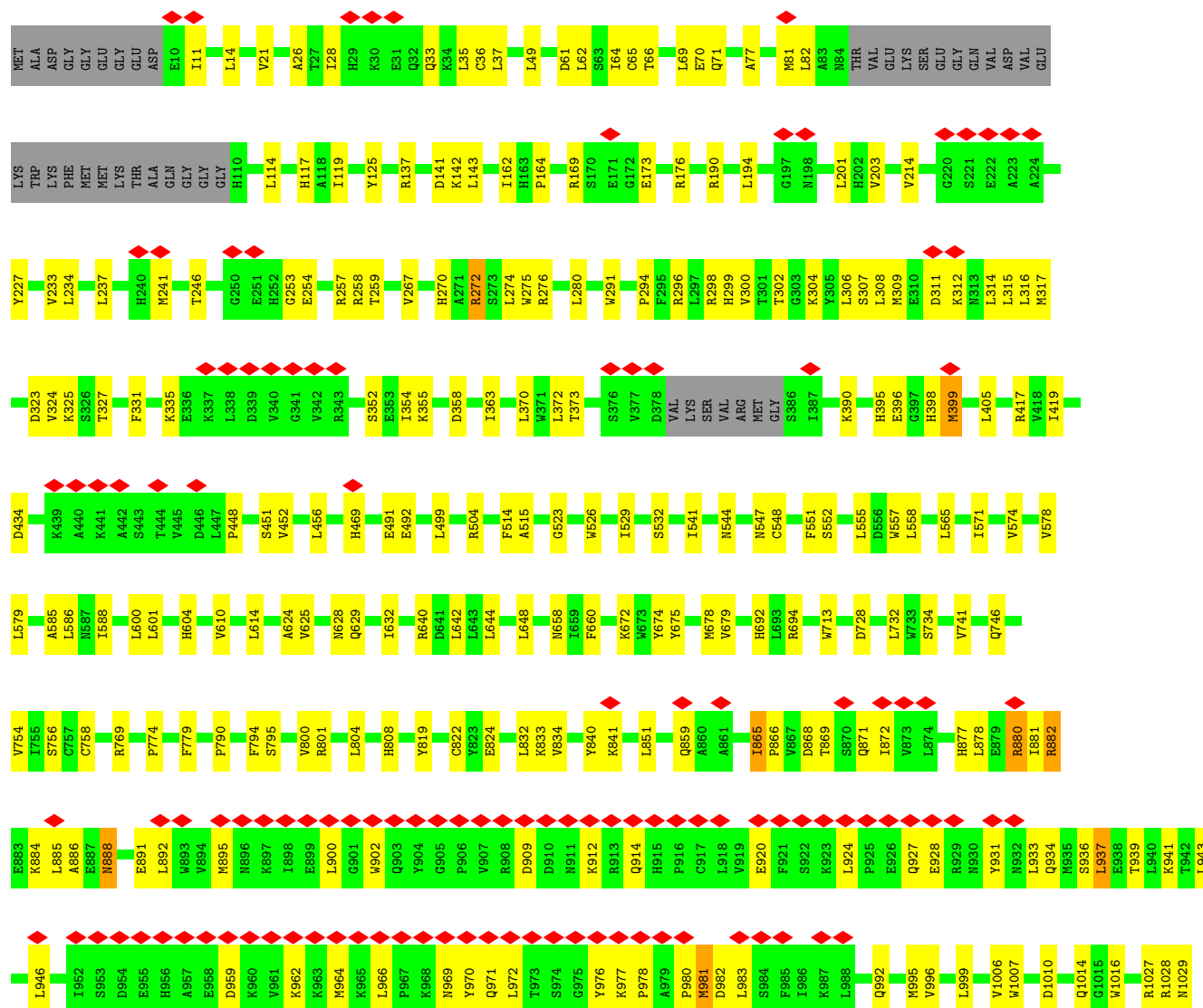


L3288	G3289	L3290	D3291	E3292	G3293	A3294	N3295	M3296	L3299	A3300	S3303	Q3304	P3305	I3306	V3310	K3311	P3312	Q3313	L3314	L3315	M3316	K3317	H3318	F3319	L3320	P3321	L3322	K3323	E3324	K3325	L3326	E3327	E3328	R3329	A3330	A3331	T3332	V3333	V3334	S3335	E3336	E3337	ASP	HIS	LEU	LYS	ALA	GLU	ALA	ARG	GLY	ASP	MET	SER	GLU	ALA
Q3151	R3152	L3155	G3156	L3159	A3160	A3161	F3162	A3163	F3166	P3167	V3168	A3169	F3170	L3171	E3172	T3173	H3174	L3175	D3176	K3177	H3178	N3179	S3182	I3183	Y3184	N3185	T3186	K3187	S3188	R3189	R3190	E3191	R3192	A3193	A3194	L3195	S3196	L3197	P3198	T3199	N3200	V3201	E3202	D3203	V3204	I3208	L3211	E3212	K3213	L3214	N3215	V3219				
E3220	L3221	A3222	E3223	S3224	G3225	L3226	R3227	Q3230	M3231	P3232	H3233	V3234	M3235	E3236	V3237	L3238	L3239	L3242	Y3245	M3246	S3247	R3248	V3249	V3250	E3251	H3252	G3253	P3254	E3255	E3259	R3260	A3261	E3262	M3263	C3264	C3265	T3266	A3267	L3268	M3269	S3270	E3271	H3272	M3273	N3274	T3275	L3276	L3277	K3278	M3279	I3280	Y3285	N3286	N3287		
Q3077	G3078	Q3079	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	V3089	T3091	Q3092	L3093	T3094	K3095	Y3096	T3097	T3098	V3099	A3100	L3101	L3102	P3103	M3104	F3109	E3110	H3111	I3112	F3117	G3118	E3119	D3120	L3121	I3122	L3123	E3124	D3125	V3126	Q3127	R3132	I3133	L3134	L3137	L3140	F3144	Y3147	E3148	E3149	R3150					
S2987	R2988	P2989	L2990	C2991	A2996	S2997	N2998	K2999	K3000	K3001	M3002	V3003	V3004	L3007	F3008	C3009	K3010	L3011	G3012	V3013	L3014	V3015	R3016	H3017	R3018	L3019	S3020	L3021	C3032	Q3038	T3039	L3040	D3041	A3042	M3046	K3054	S3055	A3056	K3058	L3057	R3059	F3060	L3061	L3068	P3070	K3071	M3072	E3073	N3074	L3075	K3076					
N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	VAL	ASP	A2817	A2818	H2819	R2824	M2828	S2829	R2835	A2841	F2842	M2843	H2849	K2854	K2857	M2858	E2859	L2860	E2861	S2862	K2863	G2864	G2865	G2866	N2867	H2868	P2869	L2870	L2877	E2881	K2884	E2887	L2893	K2894											
K2736	L2737	A2738	N2739	G2740	V2741	L2742	Y2743	G2744	E2745	I2746	Y2747	S2748	D2749	S2750	S2751	K2752	V2753	P2754	P2755	L2756	M2757	K2758	P2759	Y2760	K2761	L2762	L2763	K2766	E2769	I2770	Y2771	R2772	V2773	P2774	L2775	K2776	T2777	S2778	L2779	K2780	M2781	N2782	L2783	A2784	V2785	R2788	I2789	E2790	R2791	T2792	R2793	G2795	M2798	A2799		
E2665	L2666	C2667	L2668	L2669	V2672	L2676	P2677	D2679	M2680	M2681	E2682	S2683	H2684	V2685	V2687	L2688	M2689	E2690	K2691	Q2692	M2695	D2696	S2697	E2698	G2699	N2700	F2701	N2702	P2703	V2706	D2707	T2708	S2709	N2710	I2711	E2715	K2716	L2717	E2718	V2719	F2720	I2721	N2722	K2723	Y2724	A2725	E2726	K2731	W2732	D2735						
L2555	S2556	L2561	R2566	I2569	C2572	L2576	L2580	M2584	Q2585	H2587	L2588	S2589	R2590	L2592	V2593	F2594	L2599	H2602	P2606	L2607	Y2614	E2615	R2616	L2623	P2624	G2625	E2635	E2636	E2637	L2638	H2639	S2640	K2641	R2642	L2644	F2645	W2646	D2650	Q2654	L2664																
M2214	Y2220	L2229	R2235	A2245	S2246	V2247	M2248	L2257	R2258	E2259	P2260	M2279	Y2285	W2290	R2297	R2322	R2326	E2338	L2344	A2354	P2357	S2358	P2364	ASN	SER	GLY	SER	SER	SER	LYS	THR	LEU	ASP	THR	GLU	GLU	E2377	E2378	E2379	D2379	D2380	T2381	I2382	H2383												
K2053	K2054	Q2059	T2065	M2066	V2067	Q2071	L2087	R2090	Q2091	Y2092	R2100	I2117	L2120	I2126	R2127	L2130	R2133	L2141	M2142	L2143	R2144	G2145	L2146	Q2157	L2165	G2166	M2167	V2176	L2179	G2180	G2181	G2182	E2183	S2184	K2185	E2186	I2187	F2199	L2200																	



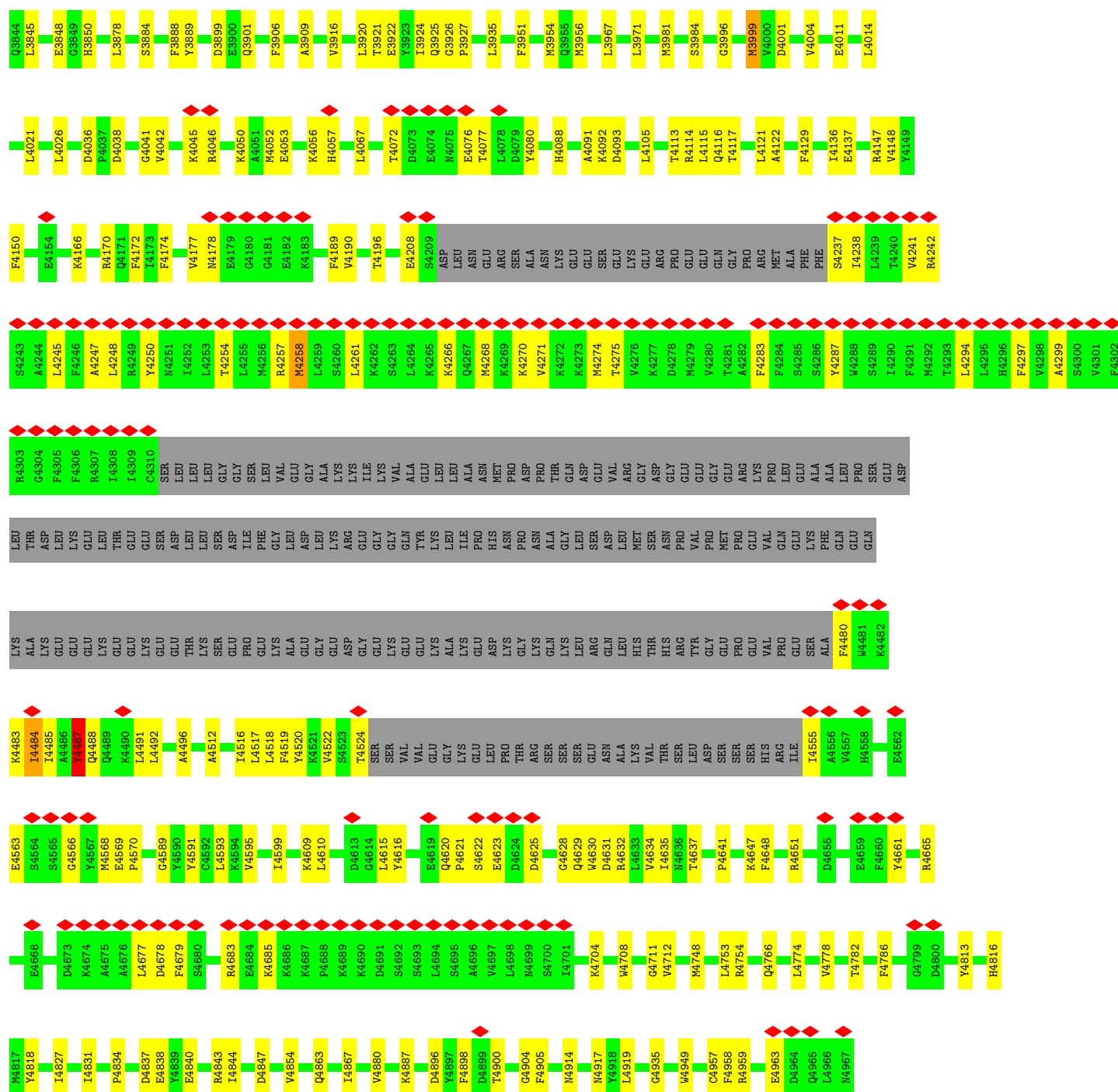


• Molecule 1: Ryanodine receptor 2



L2644	L2645	W2646	D2650	Q2654	L2661	R2666	L2667	C2668	L2669	V2672	L2676	P2677	P2678	Z2679	Y2680	W2681	H2682	S2683	H2684	R2685	V2686	S2687	W2688	L2689	F2690	D2691	Q2692	M2695	D2696	S2697	E2698	N2701	N2702	P2703	V2706	Z2707	E2715	K2716	L2717	E2718	T2719	F2720	L2721	N2722	S2641	R2642	K2643	K2725	E2726	K2731						
L2548	L2549	L2555	S2556	L2561	R2566	L2569	C2572	L2576	C2577	L2580	L2584	Q2585	Q2586	H2587	L2588	L2589	R2590	Z2591	L2592	V2593	F2594	L2599	H2602	P2606	L2607	K2608	L2609	H2613	Y2614	E2615	R2616	Y2621	C2622	L2623	P2624	L2625	E2635	L2636	E2637	L2638	F2639	L2640	S2641	K2642	K2643											
F2199	L2200	M2214	Y2220	L2229	R2235	A2245	S2246	V2247	M2248	L2257	R2258	Y2259	P2260	M2279	Y2285	W2290	R2297	R2322	R2326	L2344	A2354	P2357	S2358	S2363	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLU	G2180	G2181	G2182	E2183	S2184	D2379	D2380	T2381	L2382											
H2383	H2384	G2385	G2386	A2387	L2388	L2389	F2391	L2396	W2406	H2410	K2413	L2417	G2434	K2447	A2458	H2464	M2468	D2473	T2478	L2484	L2485	L2488	G2491	P2494	A2499	L2502	D2503	T2504	L2507	S2508	R2530	H2541	L2544	L2545	D2546	S2547																				
L2548	L2649	L2655	S2656	L2661	R2666	L2667	C2668	L2669	V2672	L2676	P2677	P2678	Z2679	Y2680	W2681	H2682	S2683	H2684	R2685	V2686	S2687	W2688	L2689	F2690	D2691	Q2692	M2695	D2696	S2697	E2698	N2701	N2702	P2703	V2706	Z2707	E2715	K2716	L2717	E2718	T2719	F2720	L2721	N2722	S2641	R2642	K2643	K2725	E2726	K2731							
ASP	SER	K2053	K2054	Q2059	T2065	W2066	V2067	Q2071	L2087	R2090	Q2091	Y2092	R2100	T2117	L2120	T2126	R2127	L2130	L2141	M2142	R2144	G2145	L2146	L2149	M2150	Q2157	L2165	G2166	M2167	V2174	V2176	L2179	G2180	G2181	G2182	E2183	S2184	D2379	D2380	T2381	L2382															
K1961	R1966	M1975	D1981	D1982	K1983	L1984	E1985	C1986	C1987	R1993	L1996	E2010	LEU	ASP	GLU	GLY	SER	LEU	ASP	GLY	LEU	ASN	SER	ASP	LEU	SER	LEU	VAL	GLU	LYS	THR	TYR	LEU	LYS	LYS	GLN	ALA	GLU	LYS	PRO	GLU	GLU	GLU	GLU	ASP	THR										
L1711	S1712	L1719	M1720	M1721	M1722	I1726	P1727	P1728	M1729	L1757	R1760	M1761	Q1762	P1766	S1767	F1768	P1780	E1781	F1782	D1785	I1786	L1787	K1788	L1795	E1801	T1813	T1814	E1815	F1825	L1829	I1830	M1831	D1838	I1842	A1854	ALA	THR	PRO	GLU	GLU	GLU	GLU	SER	ASP	THR											
E1556	R1559	V1563	K1576	P1584	L1586	H1593	V1594	R1598	M1599	P1600	N1601	V1608	W1617	L1618	V1619	L1630	E1635	N1636	L1637	T1645	L1650	V1664	L1667	G1668	N1669	L1676	G1677	S1678	D1681	E1682	P1683	Q1684	L1685	I1689	P1695	L1706	I1707	D1708																		
R1414	D1415	D1416	M1421	T1425	Y1426	Y1427	Y1428	S1429	V1430	E1437	P1438	N1439	N1440	V1443	G1444	W1445	Y1453	E1472	K1473	G1474	K1475	R1482	A1490	M1494	S1495	P1496	G1499	R1500	N1501	N1502	N1503	G1504	L1505	V1511	L1518	A1522	N1523	G1524	K1525	L1539	F1544	Q1546														
LEU	VAL	PRO	ARG	VAL	ASP	LYS	GLU	ALA	THR	LYS	PRO	PHE	ASN	ASN	HIS	LYS	ASP	TYR	ALA	GLN	GLU	LYS	PRO	GLY	SER	ARG	LEU	LYS	ASN	THR	LYS	PRO	ASP	GLU	GLU	TYR	THR	SER	HIS	ALA	ARG	LEU	VAL	THR	GLU	ASP	VAL	MET	LYS	THR	ALA	HIS	GLY	HIS		
P1030	R1031	L1032	L1037	D1040	R1041	T1042	K1043	K1044	K1047	L1050	R1051	E1052	R1055	T1056	L1057	L1058	G1059	Y1060	L1064	E1065	A1066	P1067	D1068	D1070	H1071	A1072	R1073	R1074	A1075	E1076	V1077	C1078	T1081	G1082	E1083	R1084	F1085	R1086	E1091	Y1094	A1095	V1096	R1100	E1104	F1105	E1106	T1107									
V1108	M1113	R1114	S1118	R1119	P1124	E1127	L1128	G1129	D1138	W1144	Y1145	Y1152	Q1157	D1160	M1165	M1168	H1171	T1176	I1181	F1195	D1196	F1201	V1204	V1212	G1213	R1214	M1215	N1216	F1217	G1218	K1219	D1220	T1223	Y1236	F1237	P1238	N1244																			
H1249	W1250	L1251	S1252	P1256	H1265	E1266	L1267	I1268	K1268	N1294	I1299	H1300	F1301	L1304	K1316	THR	VAL	ALA	GLY	PRO	GLY	SER	PRO	GLY	LEU	ALA	GLY	LEU	PHE	LEU	GLY	LYS	ASN	ASP	LEU	GLU	TYR	ASP	THR	SER	ASP	PHE	GLU	VAL	LEU	THR	GLU	ASP	VAL	MET	LYS	THR	ALA	HIS	GLY	HIS
LEU	VAL	PRO	ARG	VAL	ASP	LYS	GLU	ALA	THR	LYS	PRO	PHE	ASN	ASN	HIS	LYS	ASP	TYR	ALA	GLN	GLU	LYS	PRO	GLY	SER	ARG	LEU	LYS	ASN	THR	LYS	PRO	ASP	GLU	GLU	TYR	THR	SER	HIS	ALA	ARG	LEU	VAL	THR	GLU	ASP	VAL	MET	LYS	THR	ALA	HIS	GLY	HIS		






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

Chain E:




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

Chain F:  77% 20% ..




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

Chain G:  77% 20% ..



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

Chain H:  77% 20% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41126	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	0.643	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.13	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: ZN, ATP, XAN, CA

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	1/34520 (0.0%)	0.53	21/46627 (0.0%)
1	B	0.26	1/34520 (0.0%)	0.53	20/46627 (0.0%)
1	C	0.26	1/34520 (0.0%)	0.53	20/46627 (0.0%)
1	D	0.26	1/34520 (0.0%)	0.53	21/46627 (0.0%)
2	E	0.32	0/834	0.62	0/1123
2	F	0.32	0/834	0.62	0/1123
2	G	0.32	0/834	0.62	0/1123
2	H	0.32	0/834	0.62	0/1123
All	All	0.26	4/141416 (0.0%)	0.53	82/191000 (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	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3254	PRO	CG-CD	-6.09	1.30	1.50
1	B	3254	PRO	CG-CD	-6.09	1.30	1.50
1	D	3254	PRO	CG-CD	-6.08	1.30	1.50
1	A	3254	PRO	CG-CD	-6.08	1.30	1.50

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3159	LEU	CA-CB-CG	8.40	134.62	115.30
1	C	3159	LEU	CA-CB-CG	8.37	134.56	115.30
1	A	3159	LEU	CA-CB-CG	8.36	134.53	115.30
1	D	3159	LEU	CA-CB-CG	8.35	134.51	115.30
1	A	3254	PRO	N-CD-CG	-7.48	91.98	103.20

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2793	ARG	Sidechain
1	A	2835	ARG	Sidechain
1	A	2905	ARG	Sidechain
1	A	3248	ARG	Sidechain
1	A	3252	HIS	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	33779	0	33454	770	0
1	B	33779	0	33454	768	0
1	C	33779	0	33454	746	0
1	D	33779	0	33454	747	0
2	E	818	0	821	21	0
2	F	818	0	821	20	0
2	G	818	0	821	18	0
2	H	818	0	821	20	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	3	0
4	D	62	0	24	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	11	0	4	0	0
6	B	11	0	4	0	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
All	All	138688	0	137212	3039	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 11.

The worst 5 of 3039 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:B:3166:PHE:O	1:B:3248:ARG:NH1	1.94	1.00
1:D:3166:PHE:O	1:D:3248:ARG:NH1	1.94	1.00
1:A:3166:PHE:O	1:A:3248:ARG:NH1	1.94	1.00
1:C:3166:PHE:O	1:C:3248:ARG:NH1	1.94	1.00
1:A:2741:TRP:HB3	1:A:2754:GLN:HB2	1.50	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4200/4967 (85%)	4001 (95%)	193 (5%)	6 (0%)	48	76
1	B	4200/4967 (85%)	4000 (95%)	194 (5%)	6 (0%)	48	76
1	C	4200/4967 (85%)	4000 (95%)	194 (5%)	6 (0%)	48	76
1	D	4200/4967 (85%)	4000 (95%)	194 (5%)	6 (0%)	48	76
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17220/20300 (85%)	16405 (95%)	791 (5%)	24 (0%)	50	76

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2681	MET
1	A	2686	VAL
1	A	2915	PRO
1	B	2681	MET
1	B	2686	VAL

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%)	3660 (99%)	48 (1%)	65	79
1	B	3708/4358 (85%)	3660 (99%)	48 (1%)	65	79
1	C	3708/4358 (85%)	3659 (99%)	49 (1%)	65	79
1	D	3708/4358 (85%)	3660 (99%)	48 (1%)	65	79
2	E	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	F	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	G	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	H	88/89 (99%)	85 (97%)	3 (3%)	32	59
All	All	15184/17788 (85%)	14979 (99%)	205 (1%)	62	78

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	882	ARG

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Mol	Chain	Res	Type
1	C	3192	ARG
1	D	3819	MET
1	C	1165	MET
1	C	2584	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2849	HIS
1	D	1014	GLN
1	C	3949	HIS
1	D	2830	ASN
2	F	26	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	D	5005	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)
6	XAN	C	5004	-	7,12,12	1.18	1 (14%)	6,17,17	2.78	2 (33%)
4	ATP	B	5002	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	A	5005	-	28,33,33	0.65	0	34,52,52	0.58	1 (2%)
6	XAN	B	5004	-	7,12,12	1.18	1 (14%)	6,17,17	2.79	2 (33%)
4	ATP	D	5002	-	28,33,33	0.63	0	34,52,52	0.60	1 (2%)
4	ATP	C	5002	-	28,33,33	0.62	0	34,52,52	0.60	1 (2%)
6	XAN	D	5004	-	7,12,12	1.18	1 (14%)	6,17,17	2.79	2 (33%)
4	ATP	B	5005	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
6	XAN	A	5004	-	7,12,12	1.18	1 (14%)	6,17,17	2.80	2 (33%)
4	ATP	C	5005	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
4	ATP	A	5002	-	28,33,33	0.63	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	D	5005	-	-	7/18/38/38	0/3/3/3
6	XAN	C	5004	-	-	-	0/2/2/2
4	ATP	B	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5005	-	-	7/18/38/38	0/3/3/3
6	XAN	B	5004	-	-	-	0/2/2/2
4	ATP	D	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	7/18/38/38	0/3/3/3
6	XAN	D	5004	-	-	-	0/2/2/2
4	ATP	B	5005	-	-	7/18/38/38	0/3/3/3
6	XAN	A	5004	-	-	-	0/2/2/2
4	ATP	C	5005	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	7/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5004	XAN	O6-C6	-2.36	1.18	1.24
6	D	5004	XAN	O6-C6	-2.36	1.18	1.24
6	B	5004	XAN	O6-C6	-2.35	1.19	1.24

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5004	XAN	O6-C6	-2.34	1.19	1.24

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5004	XAN	C2-N1-C6	5.85	120.03	115.09
6	D	5004	XAN	C2-N1-C6	5.84	120.03	115.09
6	B	5004	XAN	C2-N1-C6	5.84	120.02	115.09
6	C	5004	XAN	C2-N1-C6	5.81	120.00	115.09
6	A	5004	XAN	C5-C6-N1	-2.58	119.97	123.42

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5005	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O3A

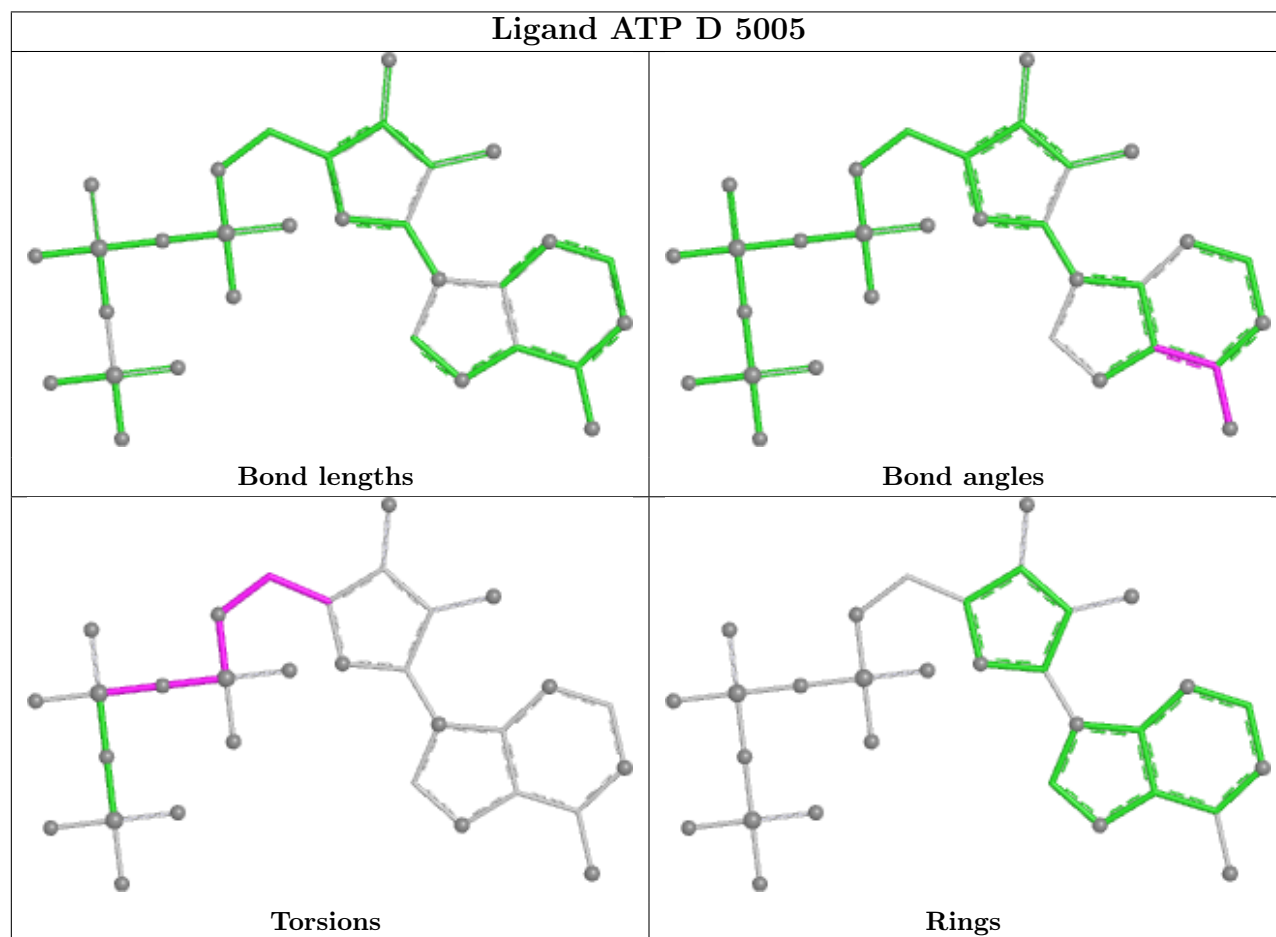
There are no ring outliers.

8 monomers are involved in 10 short contacts:

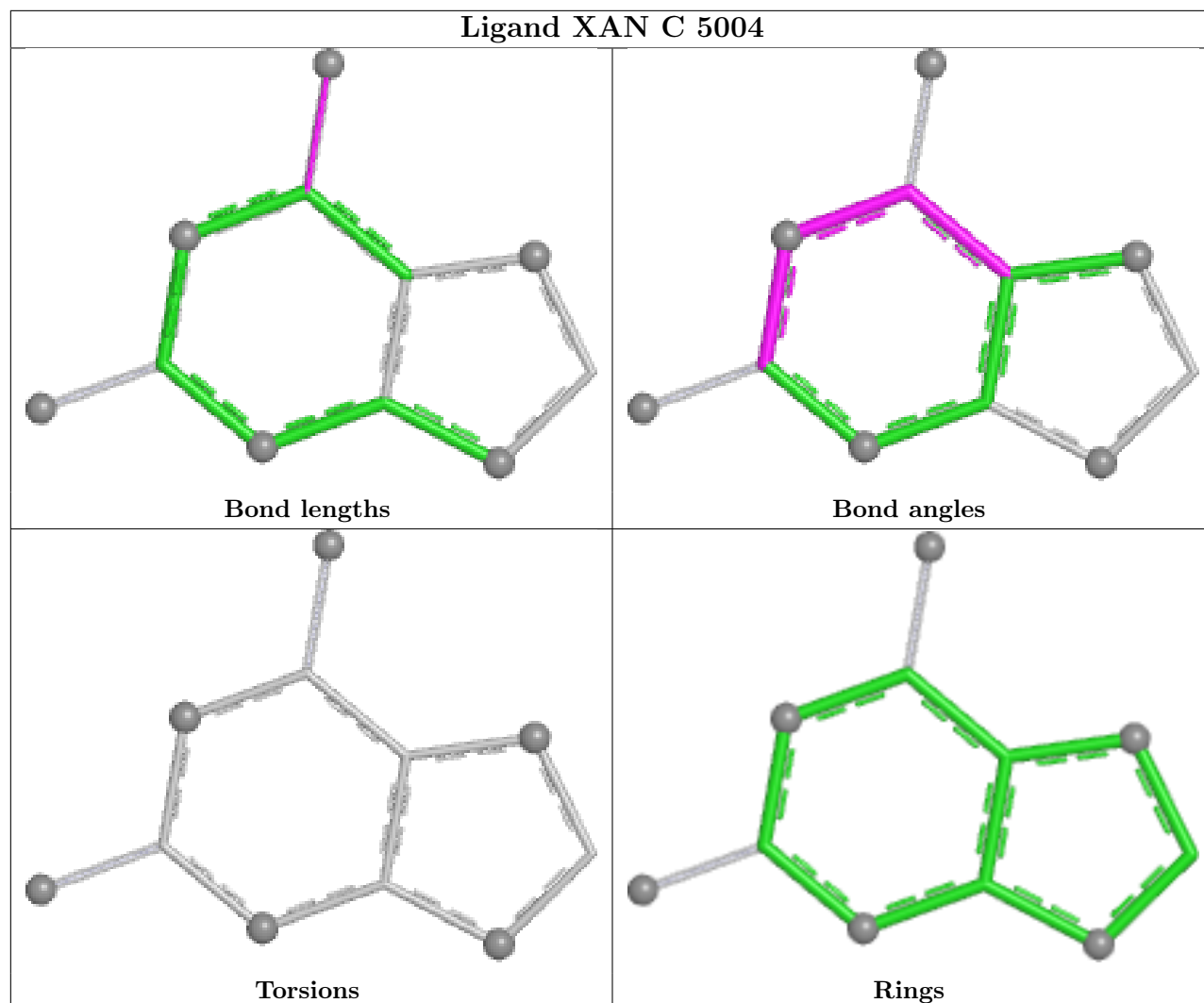
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5005	ATP	2	0
4	B	5002	ATP	1	0
4	A	5005	ATP	1	0
4	D	5002	ATP	1	0
4	C	5002	ATP	1	0
4	B	5005	ATP	1	0
4	C	5005	ATP	2	0
4	A	5002	ATP	1	0

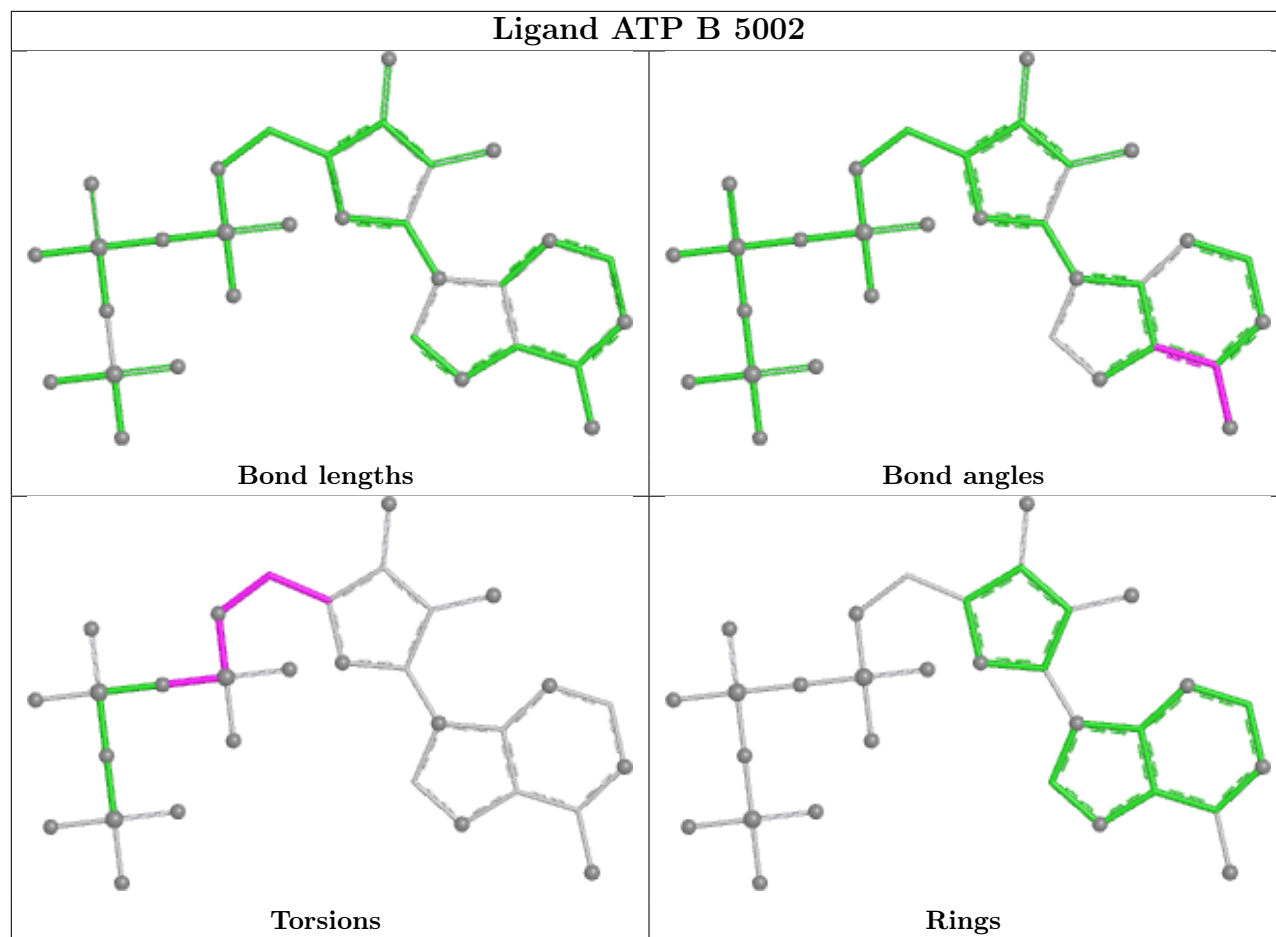
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

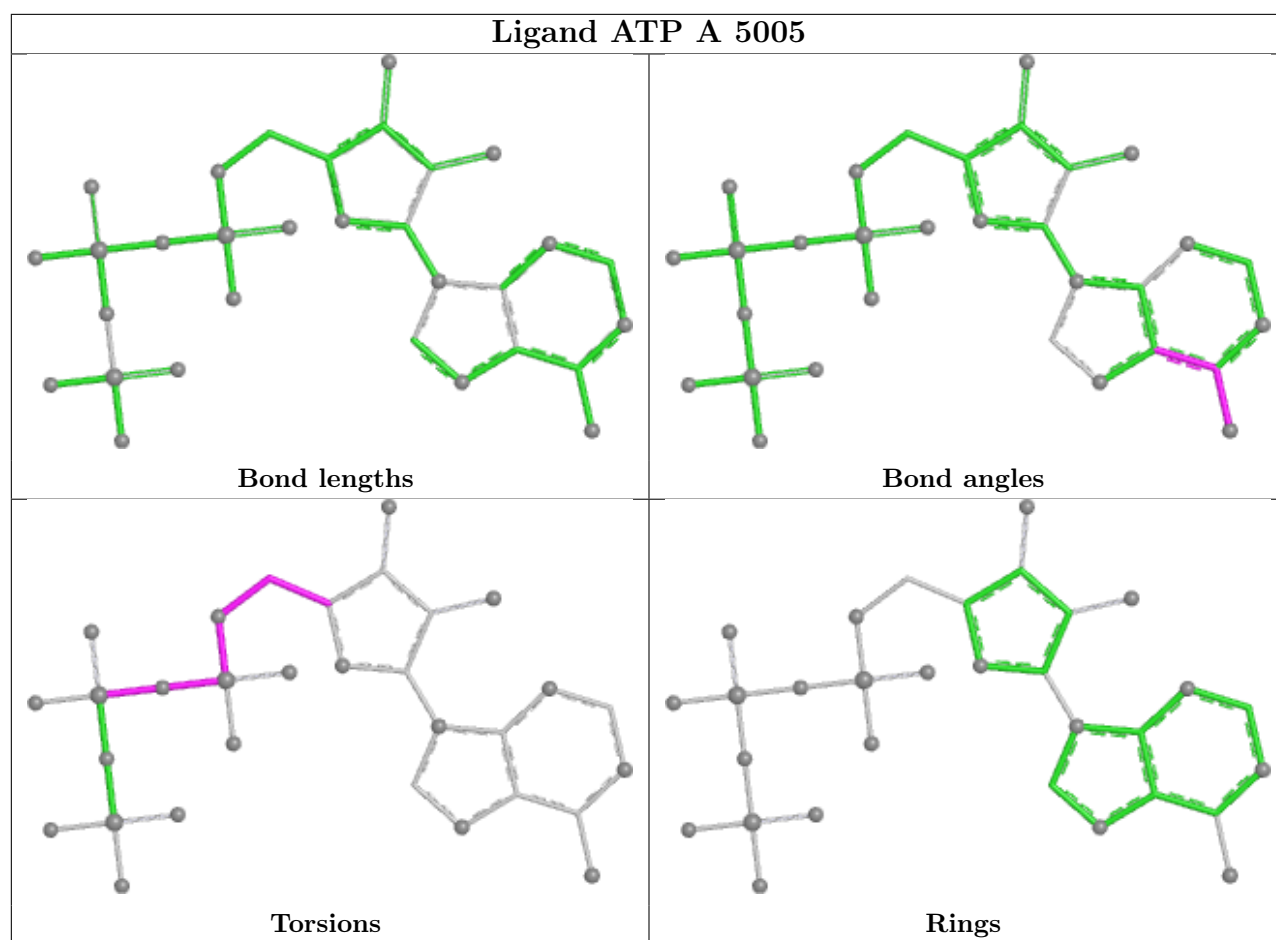
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



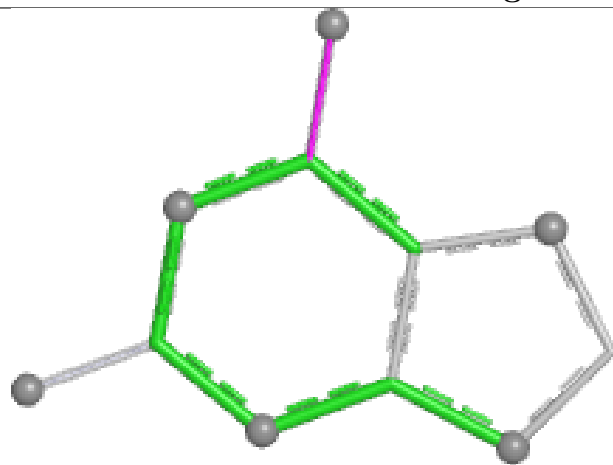
Ligand XAN C 5004



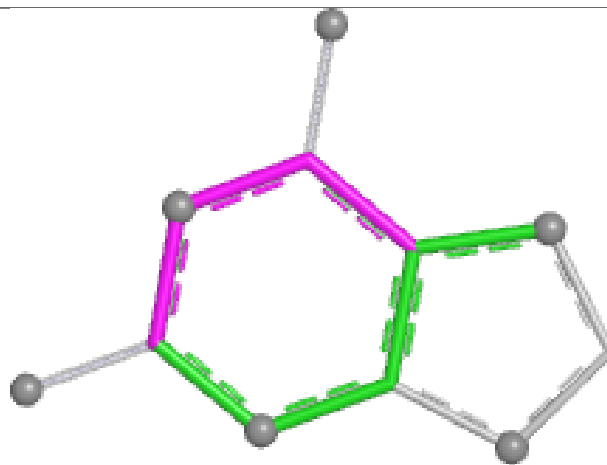




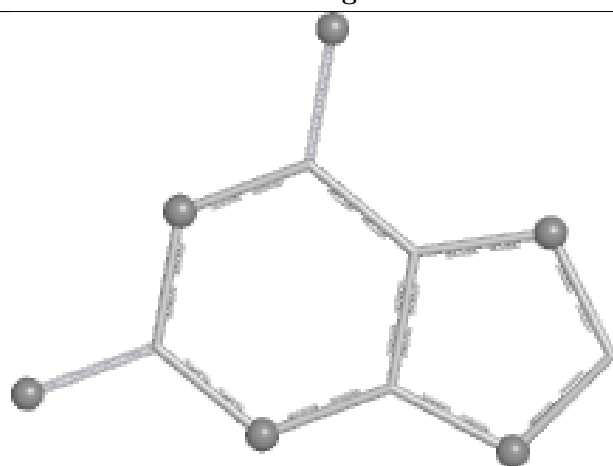
Ligand XAN B 5004



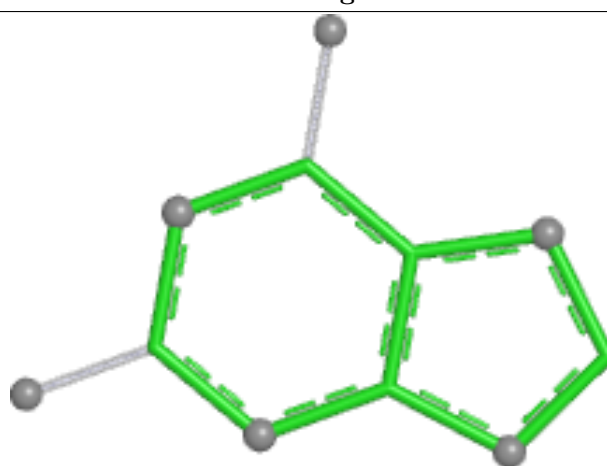
Bond lengths



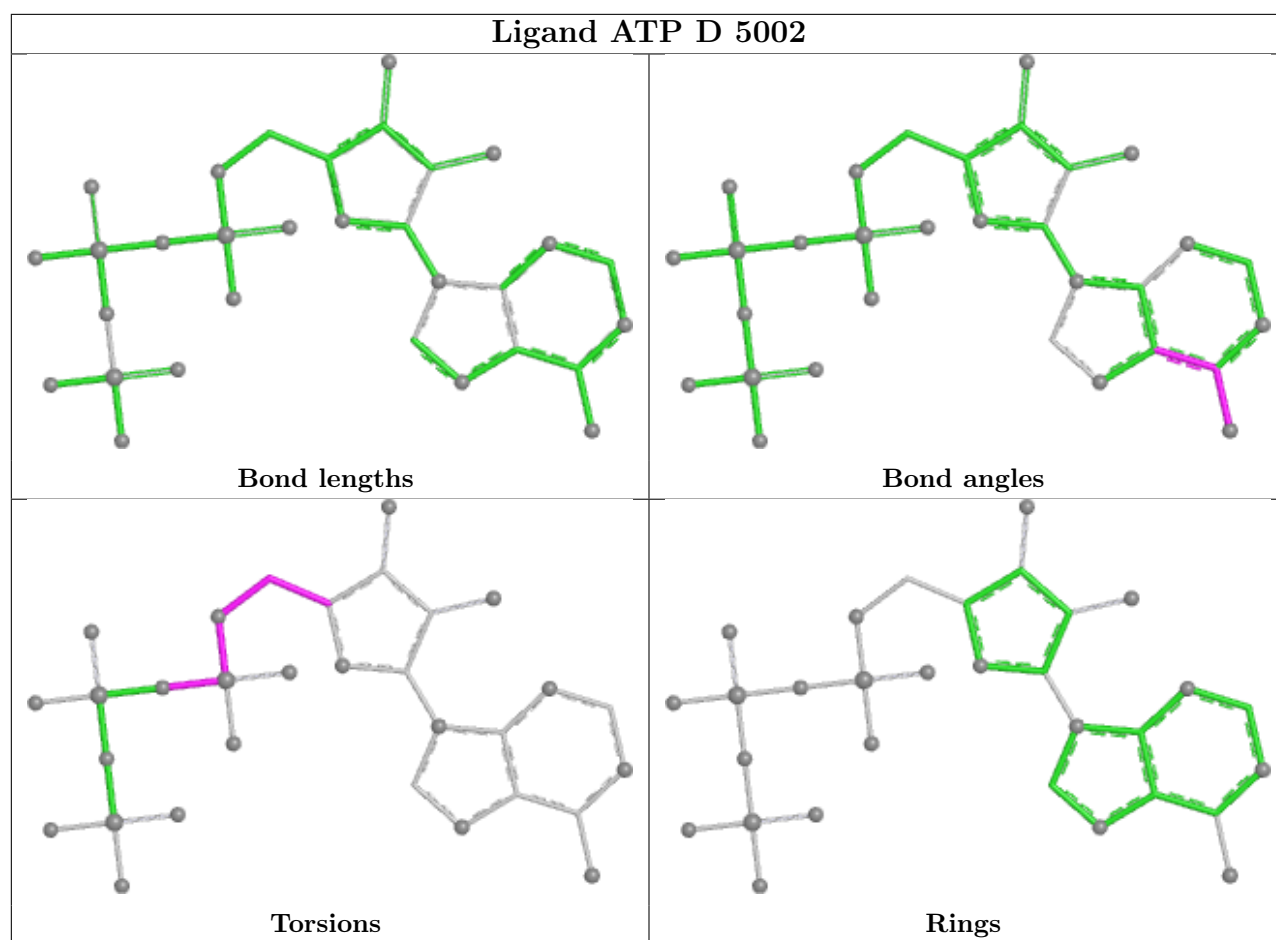
Bond angles

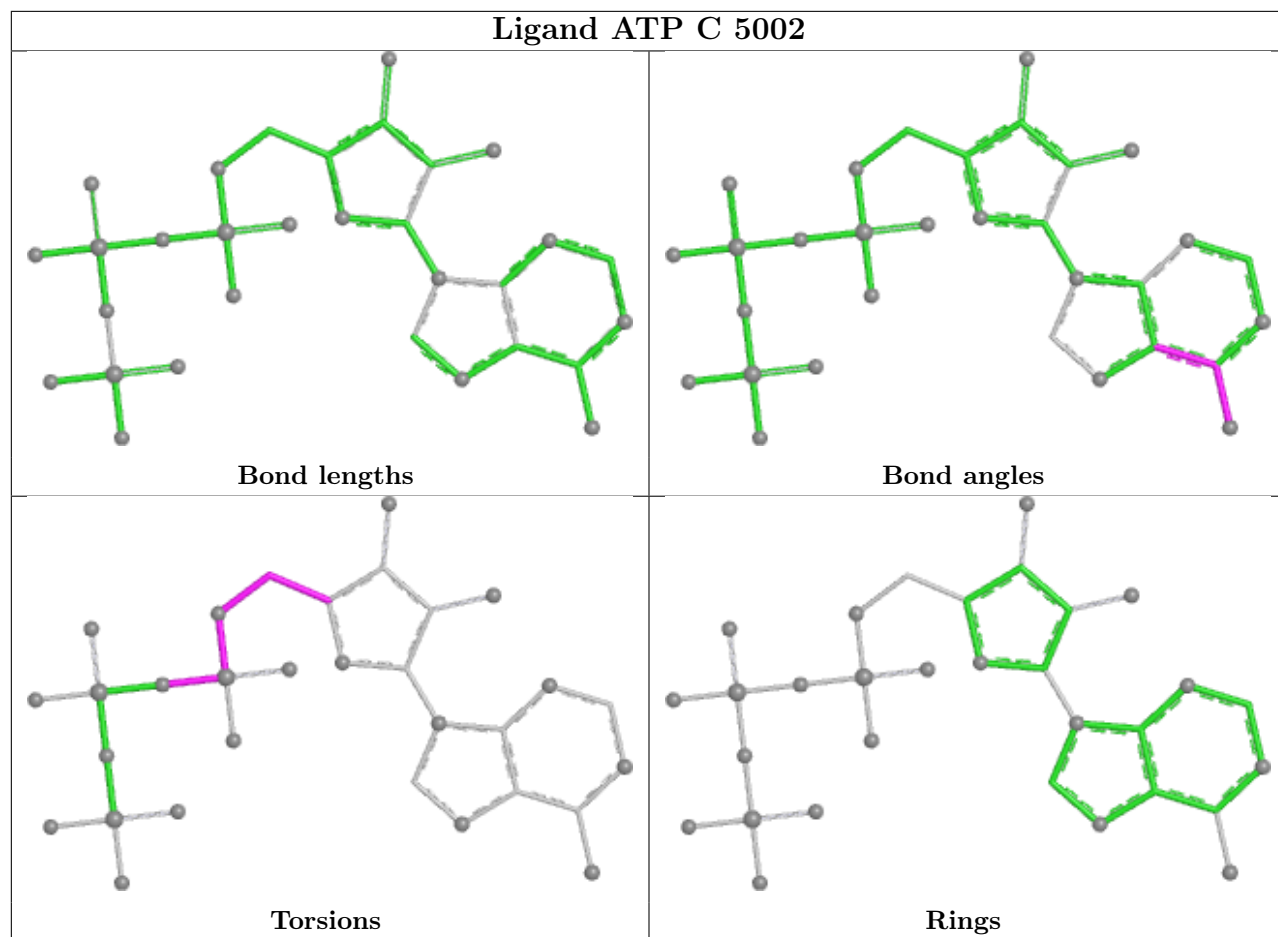


Torsions

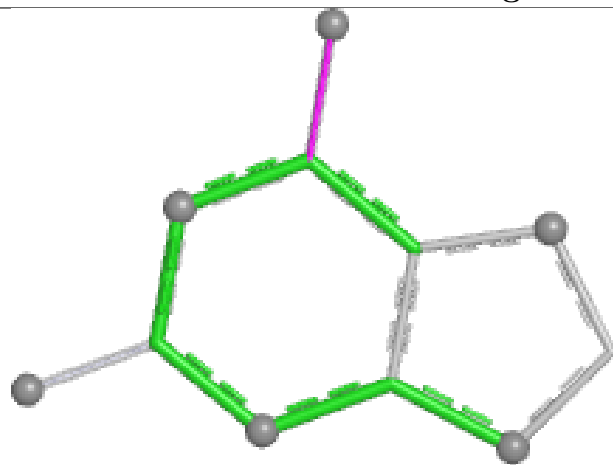


Rings

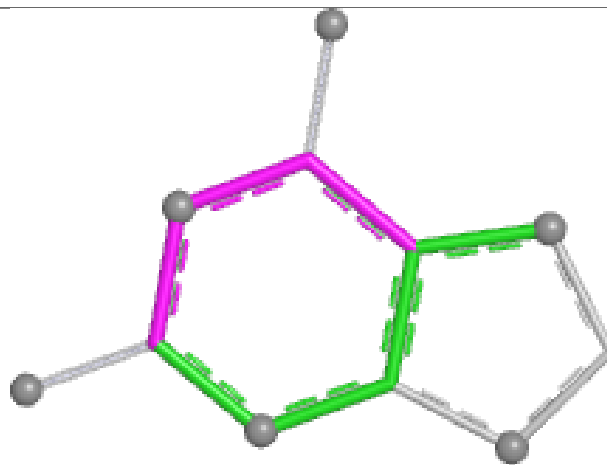




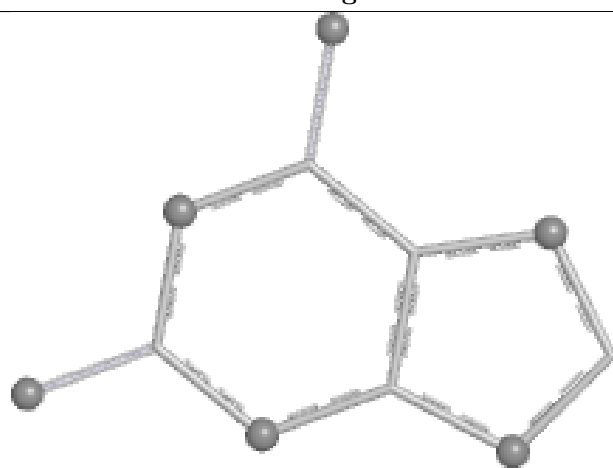
Ligand XAN D 5004



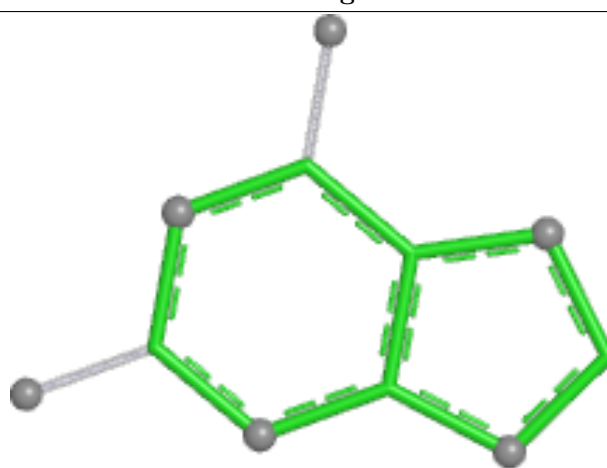
Bond lengths



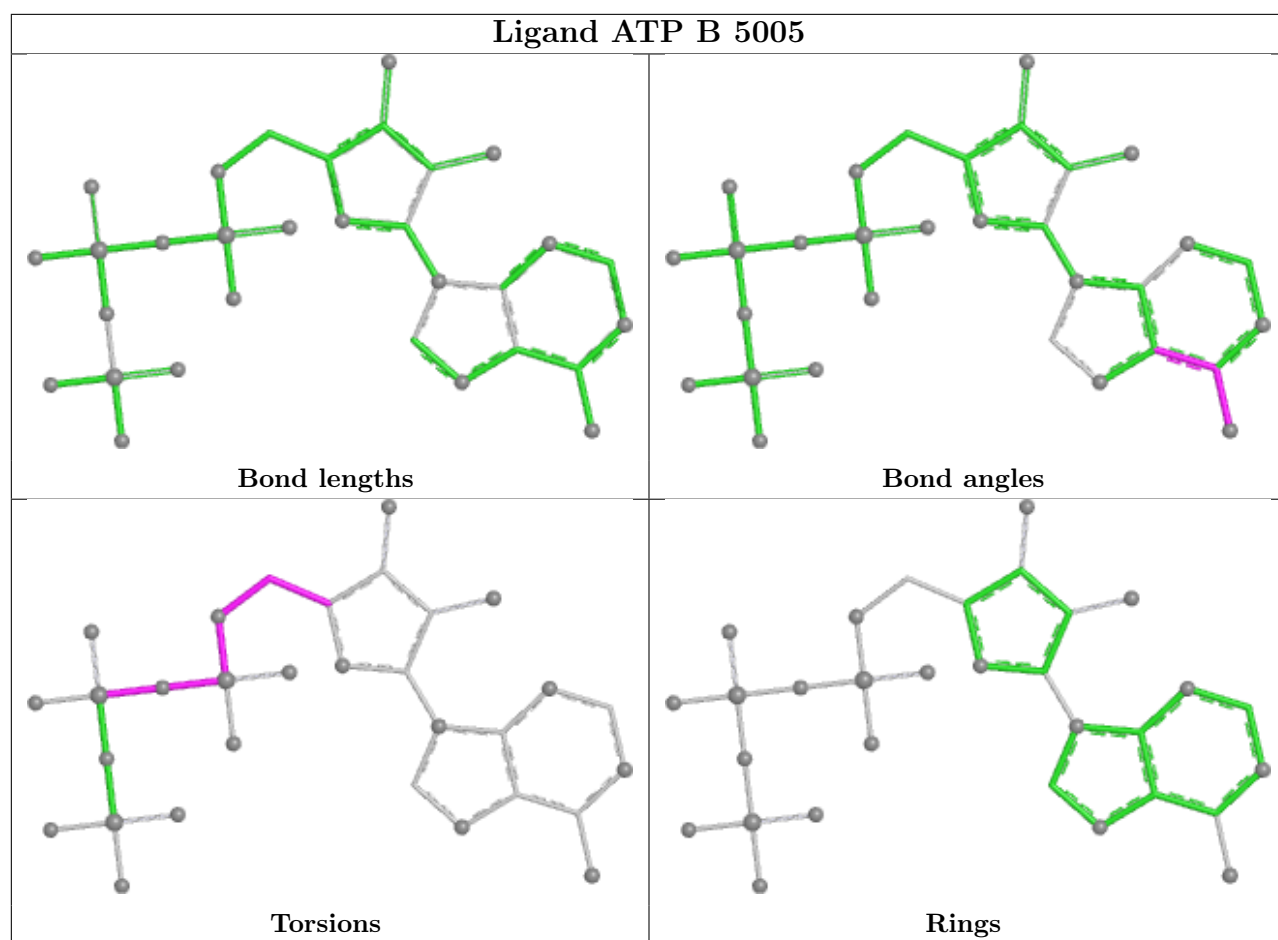
Bond angles



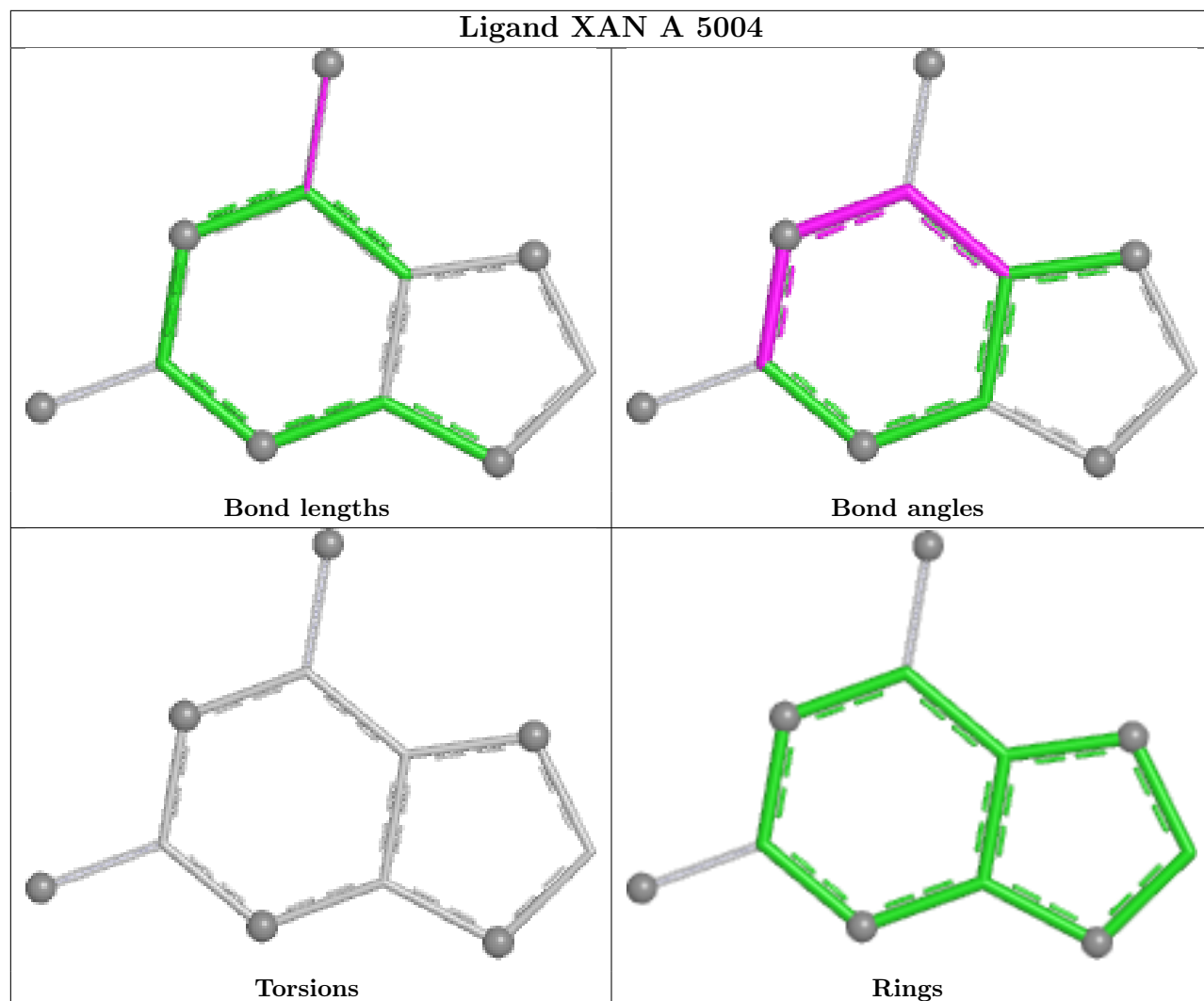
Torsions

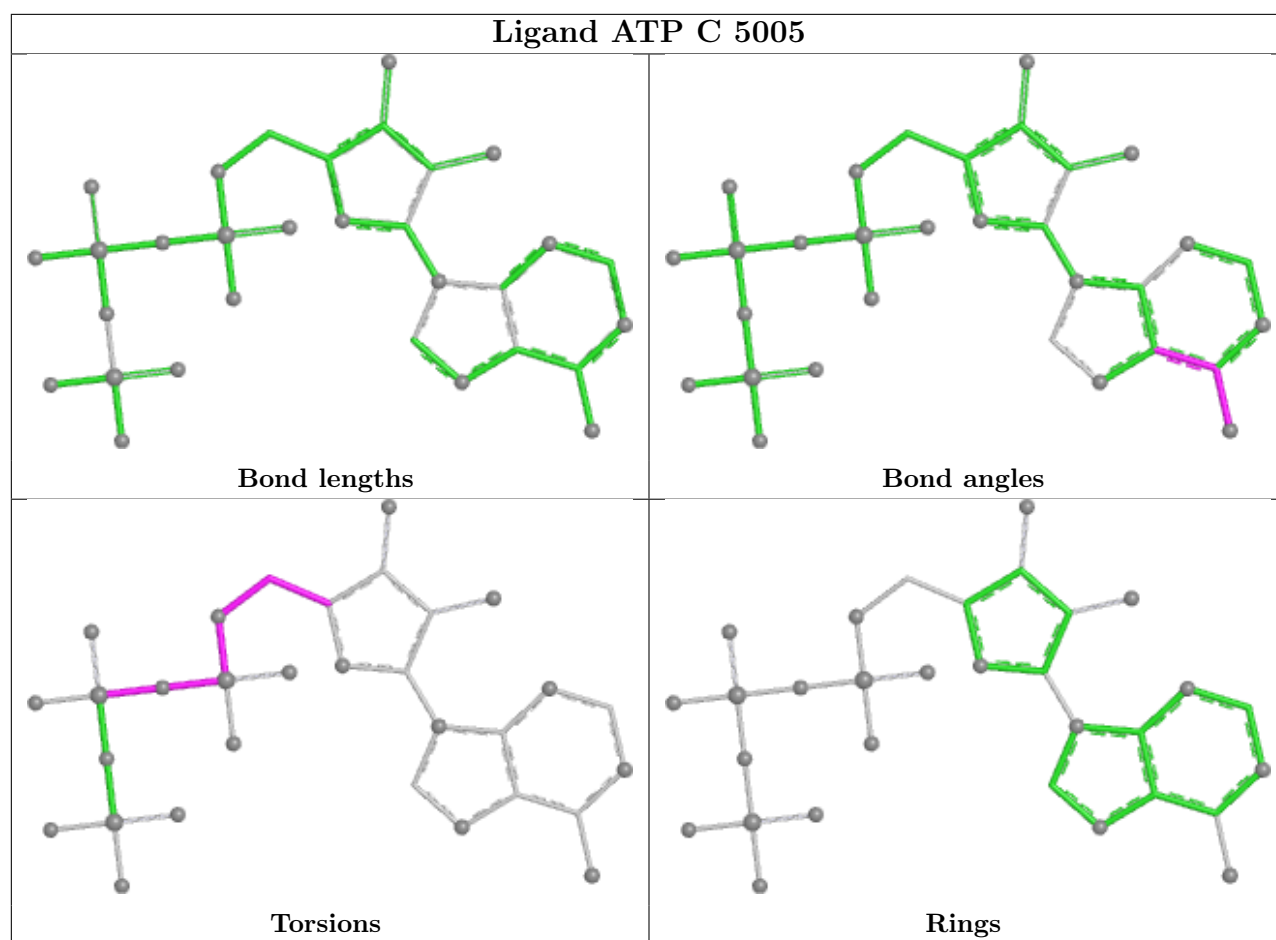


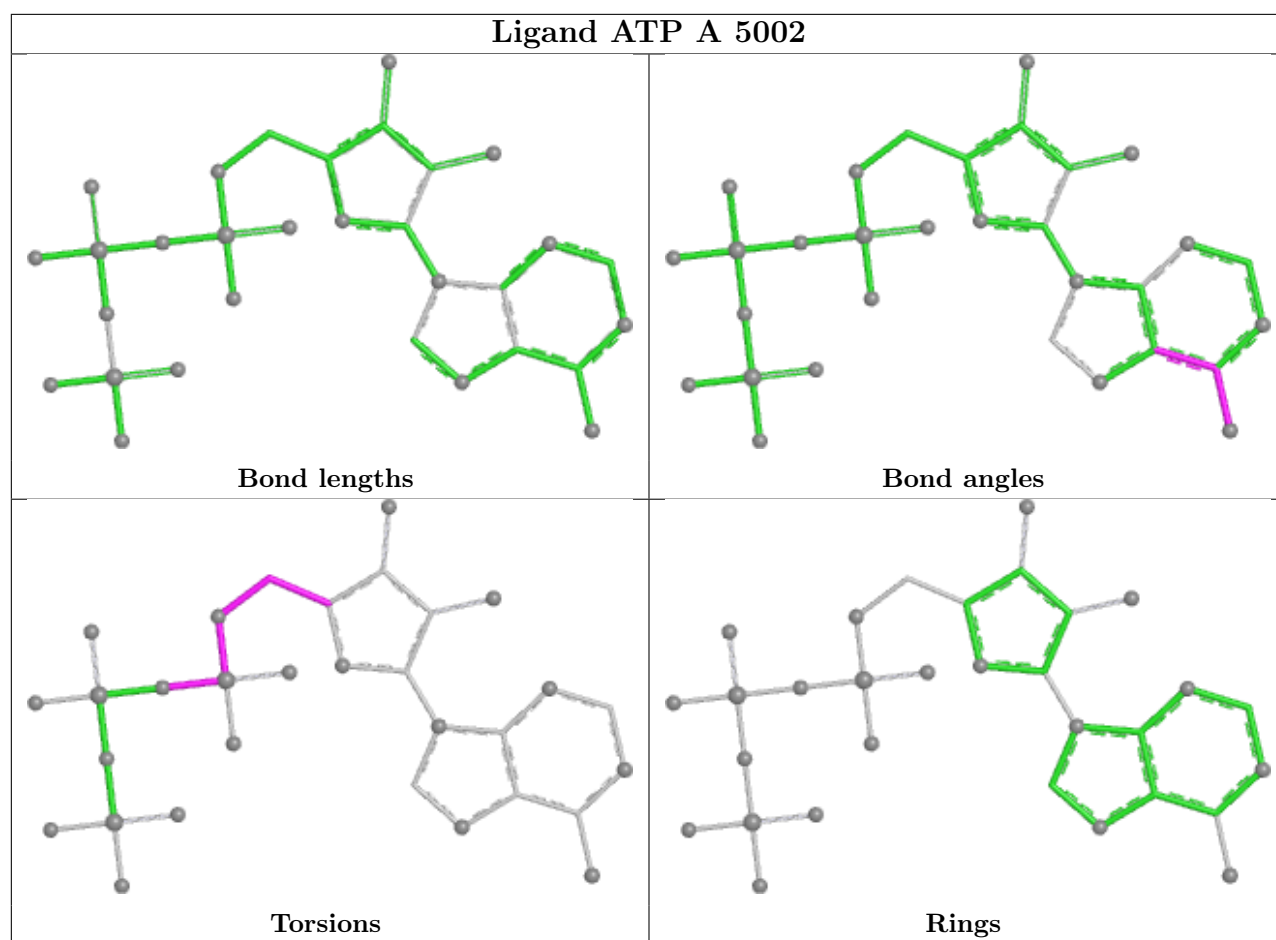
Rings



Ligand XAN A 5004







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.

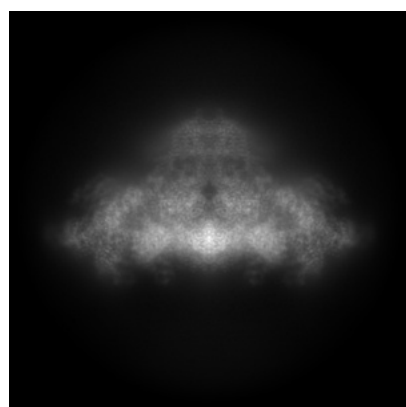
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26410. These allow visual inspection of the internal detail of the map and identification of artifacts.

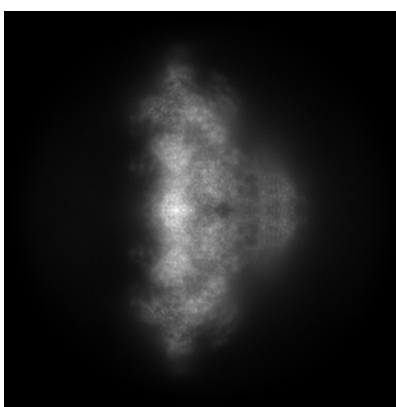
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

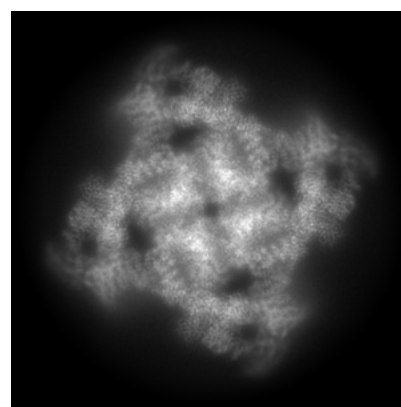
6.1.1 Primary map



X



Y

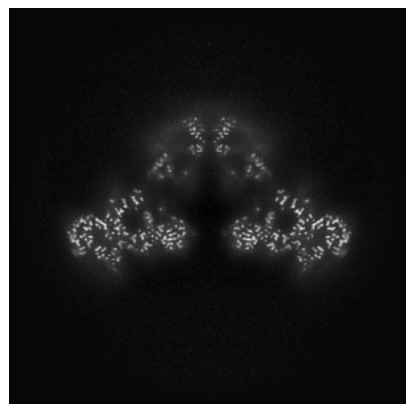


Z

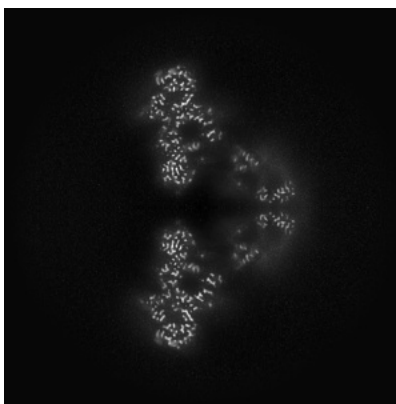
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

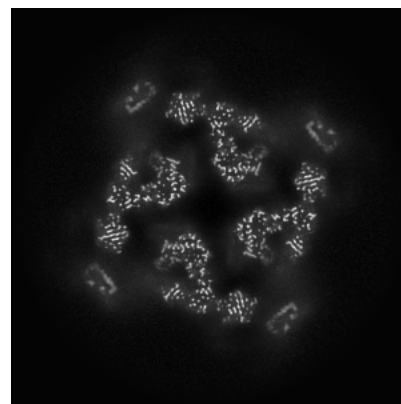
6.2.1 Primary map



X Index: 256



Y Index: 256

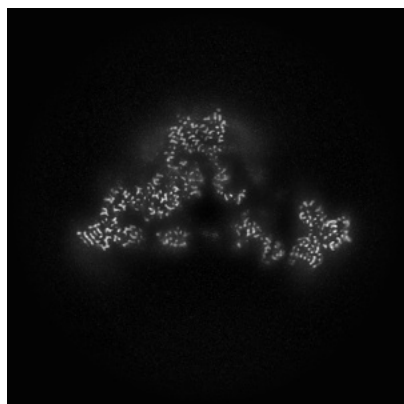


Z Index: 256

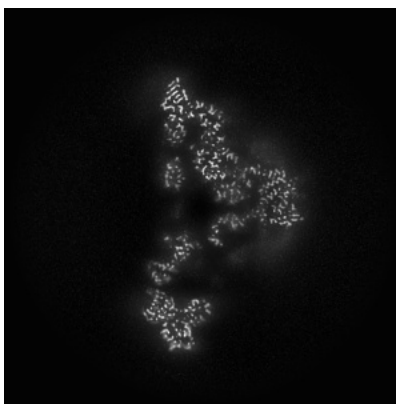
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

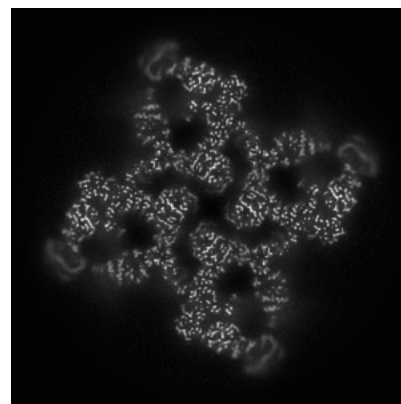
6.3.1 Primary map



X Index: 238



Y Index: 238

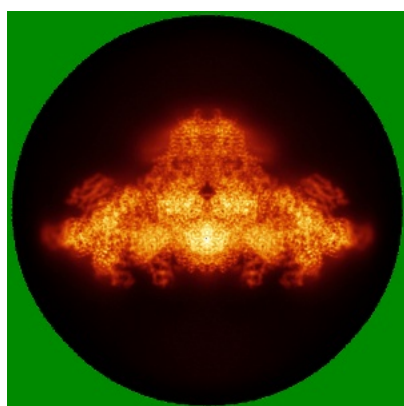


Z Index: 220

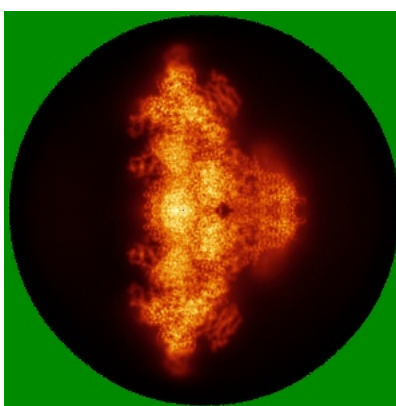
The images above show the largest variance slices of the map in three orthogonal directions.

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

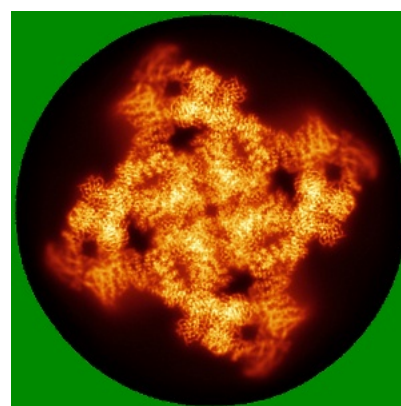
6.4.1 Primary map



X



Y

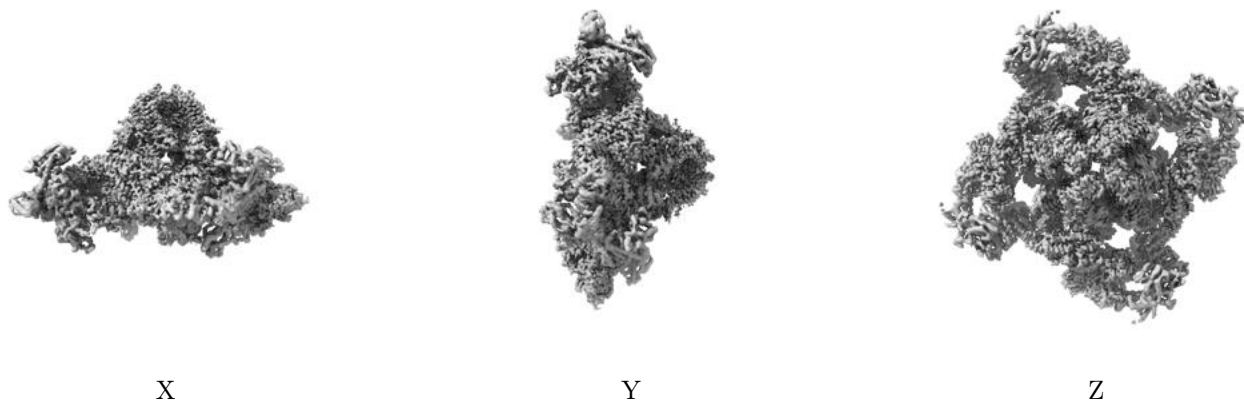


Z

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

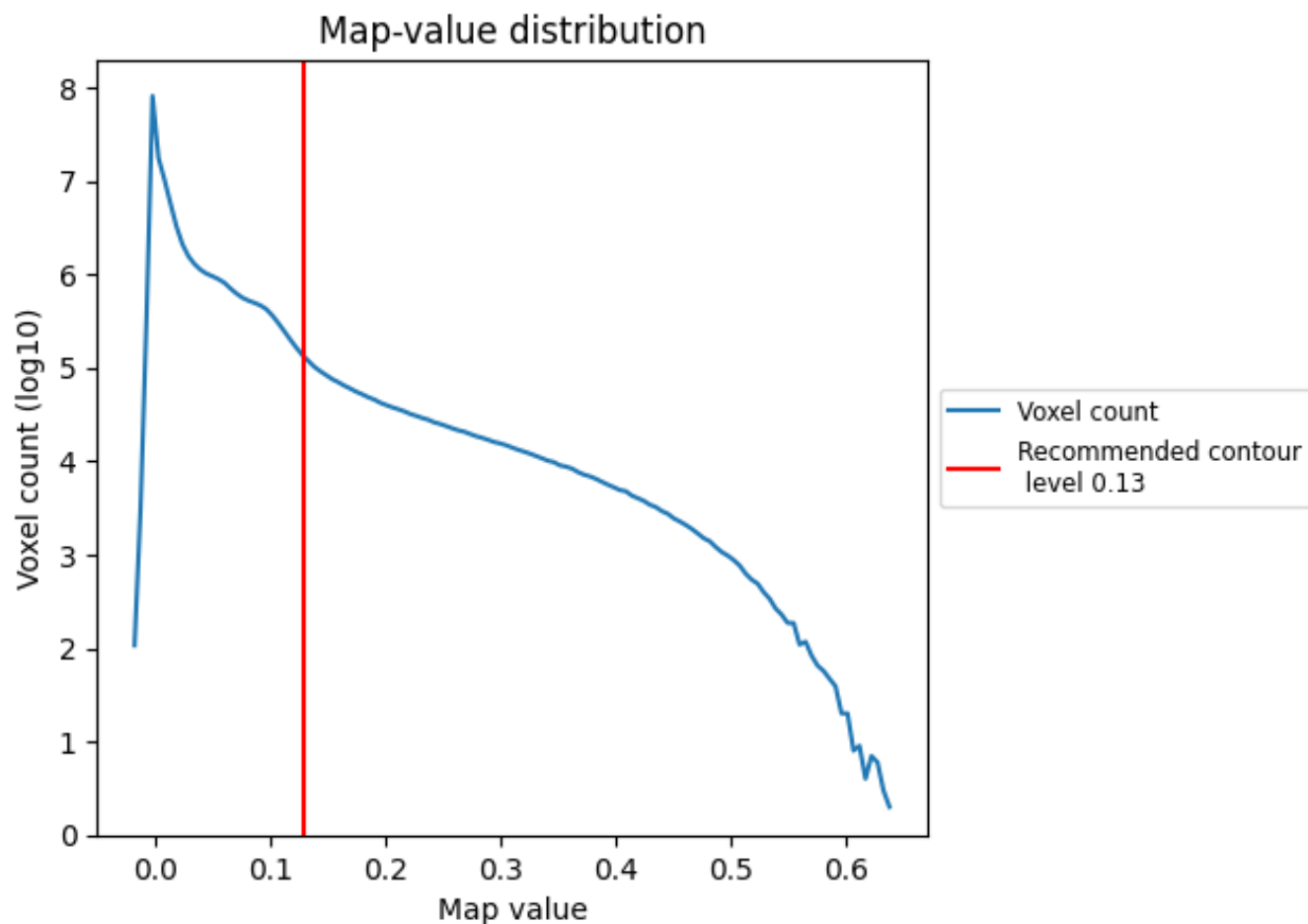
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

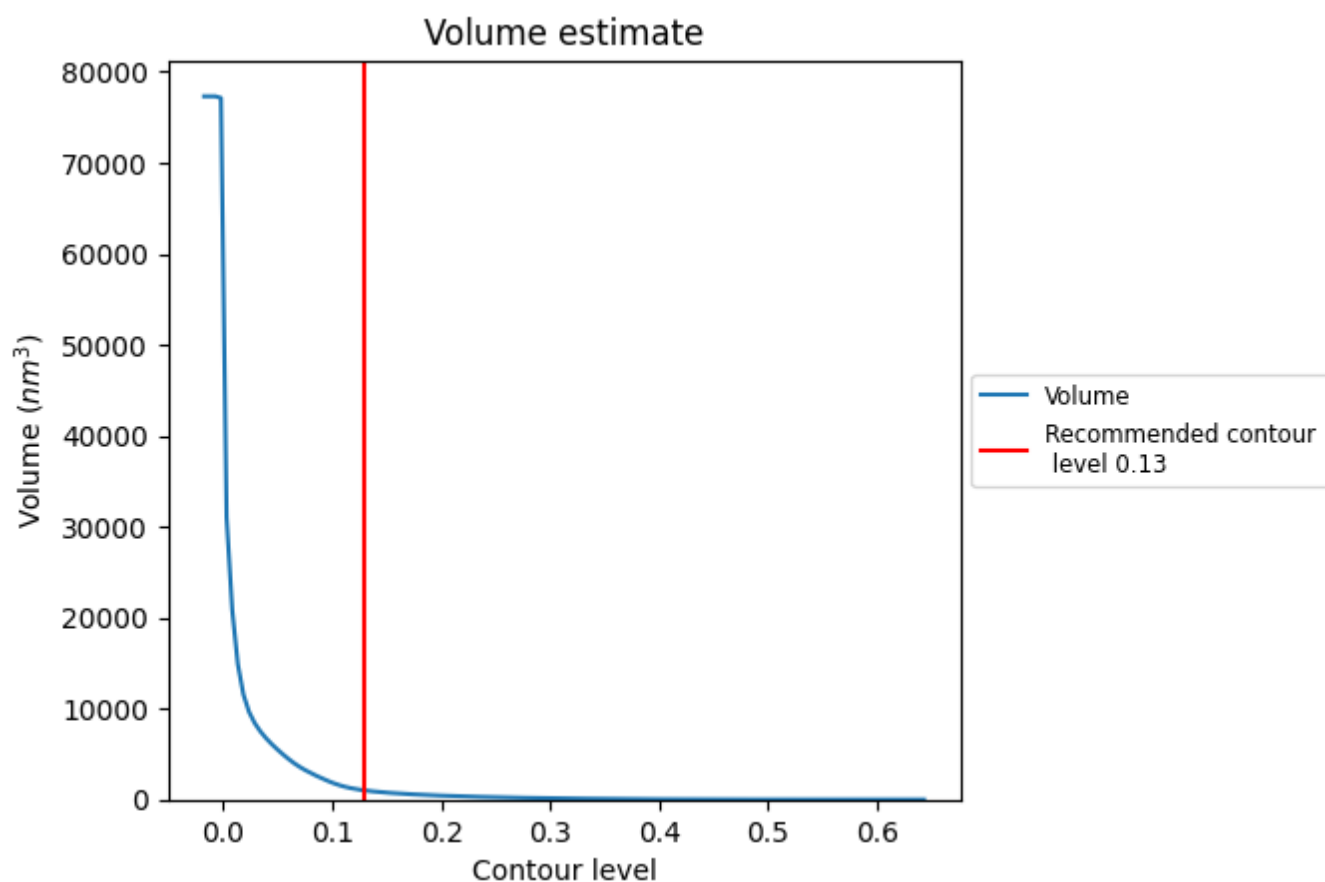
This section contains the results of statistical analysis of the map.

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.

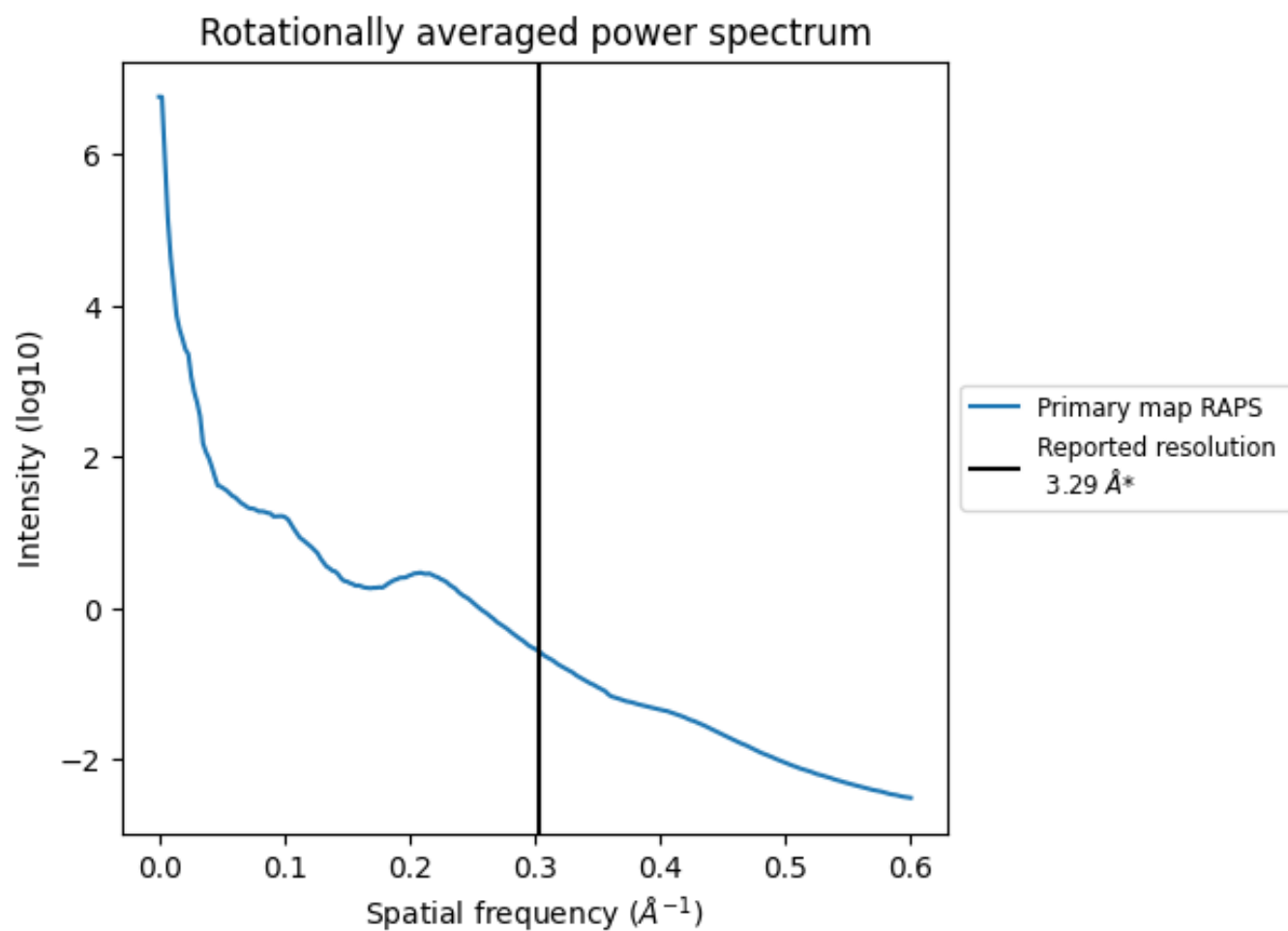
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1001 nm³; this corresponds to an approximate mass of 904 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 0.304 Å⁻¹

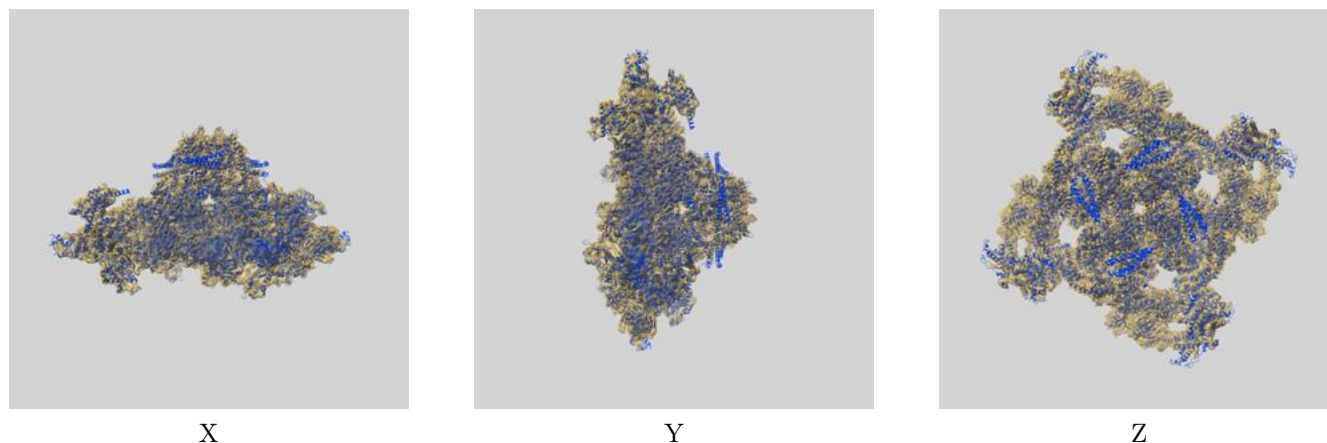
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

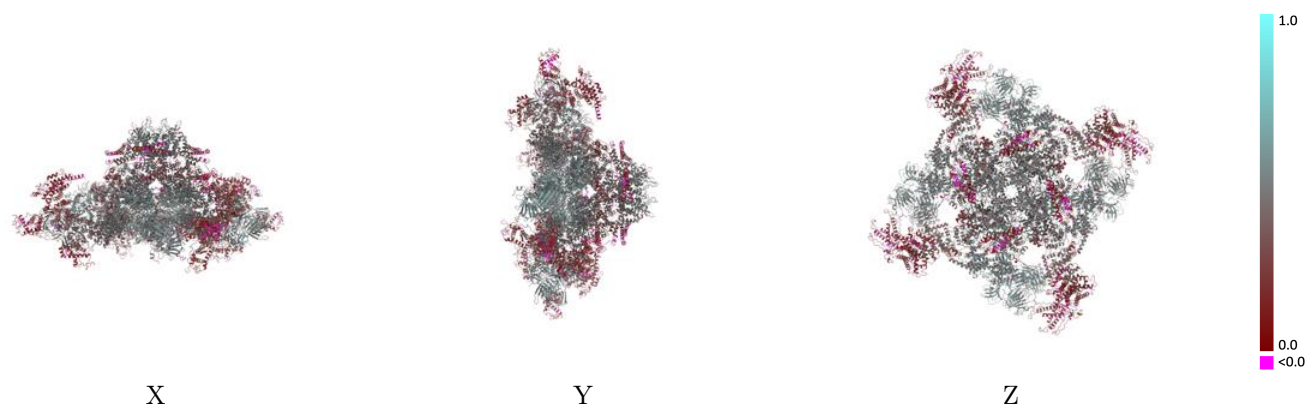
This section contains information regarding the fit between EMDB map EMD-26410 and PDB model 7U9Z. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



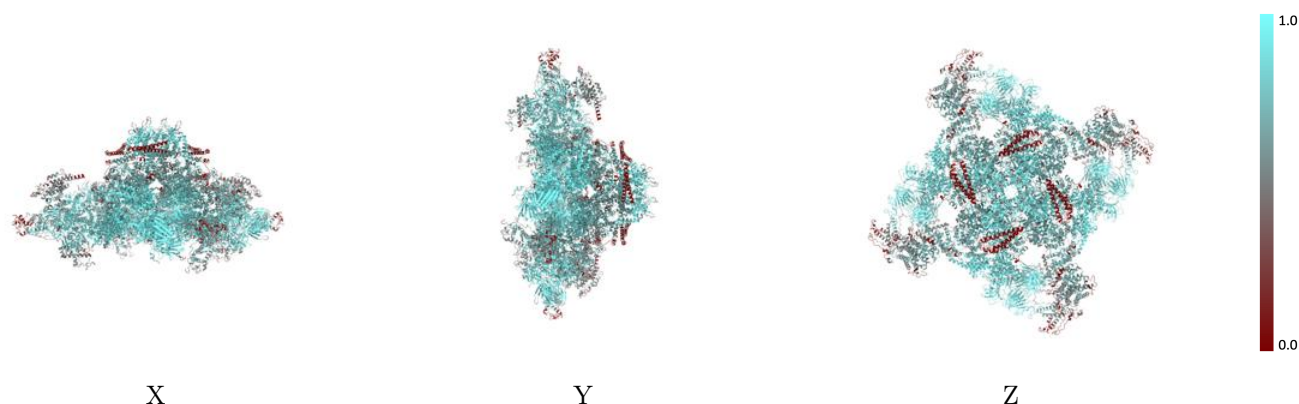
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



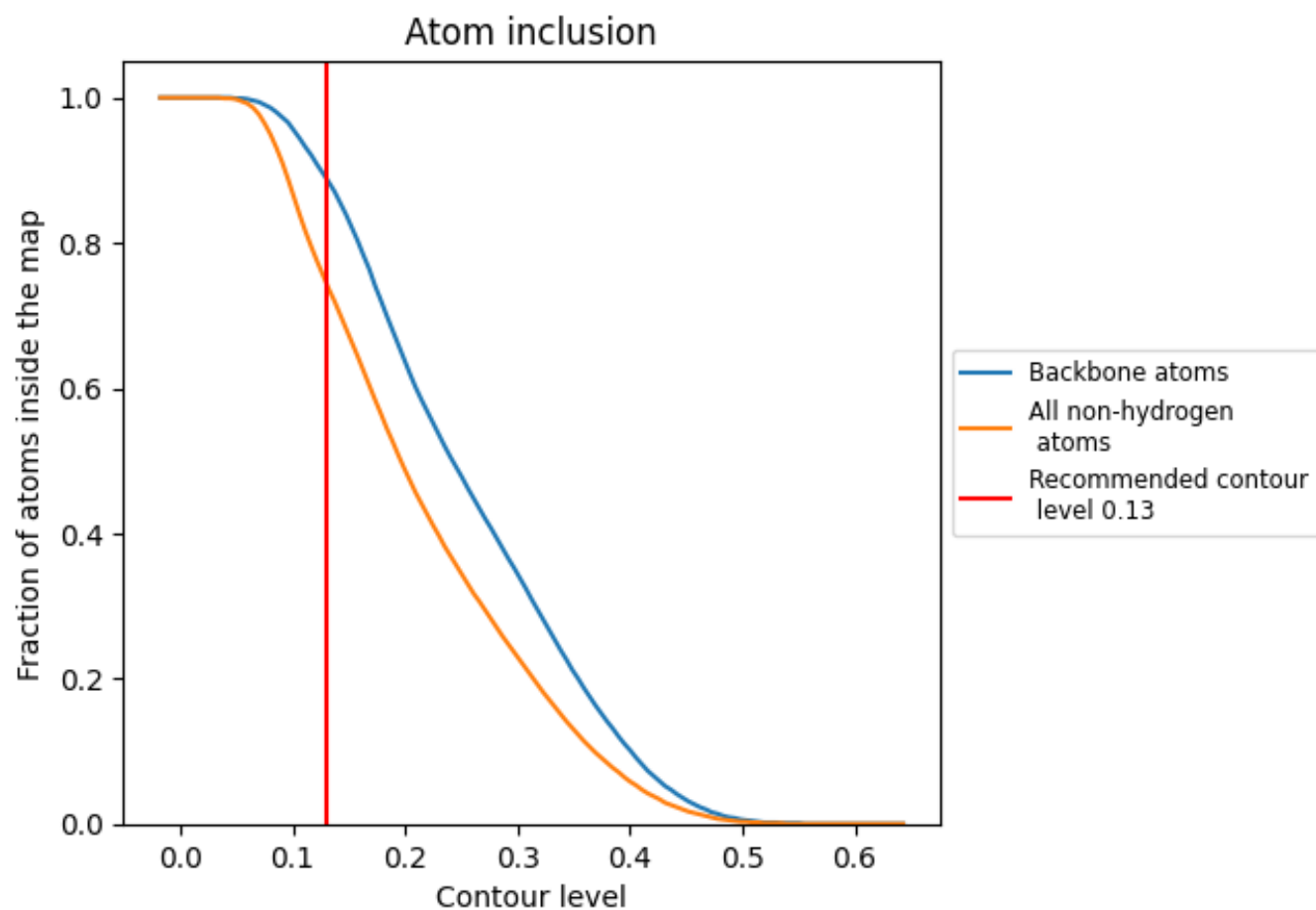
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 74% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7440	<div></div> 0.3940
A	<div></div> 0.7370	<div></div> 0.3860
B	<div></div> 0.7430	<div></div> 0.3980
C	<div></div> 0.7380	<div></div> 0.3850
D	<div></div> 0.7420	<div></div> 0.3940
E	<div></div> 0.9180	<div></div> 0.5420
F	<div></div> 0.9130	<div></div> 0.5260
G	<div></div> 0.9160	<div></div> 0.5250
H	<div></div> 0.9210	<div></div> 0.5450

1.0

0.0

<0.0