



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 02:38 AM UTC

PDB ID : 7UA5 / pdb_00007ua5
EMDB ID : EMD-26415
Title : Structure of dephosphorylated human RyR2 in the closed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 2.83 Å (reported)
Based on initial model : 7U9Q

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:

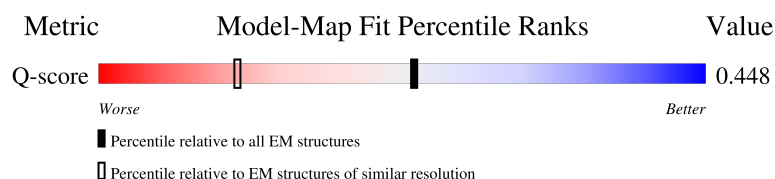
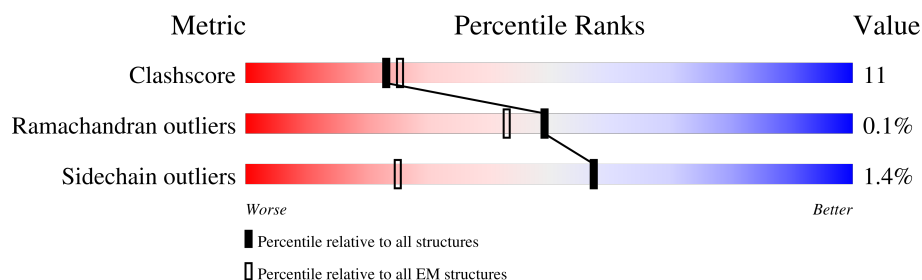
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 2.83 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	11847 (2.33 - 3.33)

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	 10% 63% 21% • 15%
1	B	4967	 10% 64% 21% • 15%
1	C	4967	 10% 64% 21% • 15%
1	D	4967	 10% 63% 21% • 15%

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Mol	Chain	Length	Quality of chain
2	E	108	 82%16%..
2	F	108	 82%16%..
2	G	108	 83%15%..
2	H	108	 81%17%..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 138608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

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

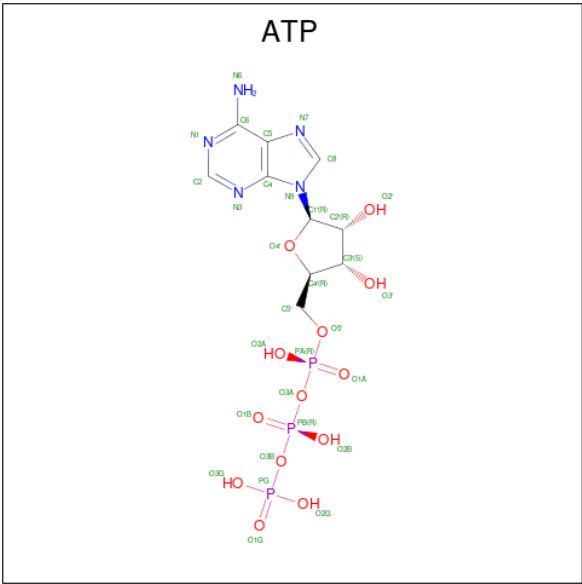
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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: C₁₀H₁₆N₅O₁₃P₃) (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	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots

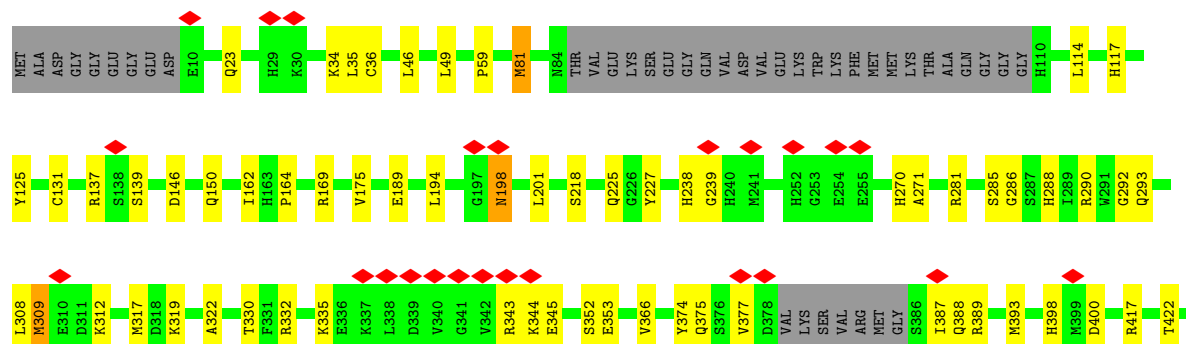
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



12711	E2636	L2520	D2380	E2952	M2142	LEU	P1938	F1851	S1713	T1548	TYR	A1191
T2712	E2637	L2527	T2381	L2253	R2143	LEU	M1939	K1852	Y1714	S1549	ASP	A1196
12713	H2638	L2527	I2382	L2255	R2144	LEU	V1947	E1853	L1719	P1550	ALA	D1196
P2714	S2641	L2548	G2385	K2264	Y2156	VAL	M1948	A1854	M1722	N1551	SER	V1197
E2715	R2642	L2549	N2386	V2266	L2165	GLU	Q1949	ALA	E1732	F1555	ASP	G1198
	K2643	Y2553	M2389	V2266	G2166	VAL	A1950	PRG	R1751	R1559	GLU	C1205
	L2644	Y2557	I2396	L2274	M2167	THR	L1951	GLU	G1752	K1560	VAL	V1209
Y2719	A2651	K2557	A2403	Q2275	H2168	TYR	M1952	GLU	L1753	N1562	LEU	A1210
F2720	L2652	L2561	Q2277	Q2276	V2171	LEU	A1955	SER	R1758	V1563	THR	K1225
N2721		Q2565	C2277	S2276	M2175	LYS	A1956	THR	P1759	M1564	ALA	T1228
K2723		Q2566	M2278	L2280	V2176	LYS	L1957	LEU	R1760	C1582	HIS	T1228
A2725		D2567	E2415	L2280	M2177	ALA	K1961	GLY	M1761	ASP	ASP	L1232
E2726					V2178	GLU	R1966	GLU	P1766	R1585	HIS	L1232
H2727					G2181	LYS	S1967	LEU	S1767	D1415	VAL	N1242
S2728					E2182	PRG	Q1972	SER	F1768	D1416	PRO	N1242
F2729					E2183	VAL	M1975	VAL	P1780	Y1417	ASP	R1245
D2730					S2184	GLU	N1978	ASP	D1785	D1418	ARG	R1245
K2731					K2053	ASP	F1979	ALA	I1786	F1433	VAL	L1251
V2732					S2054	SER	D1982	LYS	L1787	F1434	ASP	P1256
S2733					S2055	LEU	K1983	GLN	K1788	G1435	ASP	P1256
M2734					T2057	GLU	S1984	GLY	S1789	G1435	LYS	I1268
L2735					L2058	GLU	E1985	GLU	T1791	P1610	GLU	I1268
K2736					L2059	GLU	C1986	GLU	I1792	L1611	THR	R1272
L2737					Q2060	GLU	P1987	GLU	I1793	L1617	LYS	L1283
L2738					L2061	GLU	C1988	GLU	I1794	L1630	PRO	G1291
N2739					L2062	ALA	P1989	LYS	M1794	L1644	PHE	S1292
G2740					Q2071	LYS	E1990	GLY	E1797	E1649	ASN	Q1293
V2741					D2077	GLY	I1991	LYS	A1806	L1650	ASN	Q1293
L2742					M2214	LYS	I1992	LYS	R1807	L1651	LYS	M1294
Y2743					Y2220	GLU	R1993	ARG	D1808	L1667	ASP	M1300
E2745					L2222	GLU	D1994		V1819	H1670	TYR	K1316
L2746					L2222	GLU	Q1995		F1825	H1674	ALA	K1316
Y2747					S2225	LEU	E2010		V1826	H1674	GLN	VAL
S2748					S2226	ASP	LEU		T1827	E1682	LYS	ALA
D2749					V2227	GLU	ASP		I1830	E1682	PRO	GLY
S2750					G2228	GLU	GLU		M1831	P1683	ARG	GLY
S2751					L2229	GLY	ASP		L1910	Q1684	LYS	GLY
K2752					P2232	LYS	LEU		Q1911	L1685	GLN	ALA
V2753					A2233	THR	ASP		C1914	L1686	ARG	GLY
Q2754					R2234	LEU	GLY		R1919	Q1498	PHE	LEU
P2755					R2235	GLU	ASN		F1928	G1499	LEU	PHE
L2756					T2238	GLU	ASP		L1845	R1500	ARG	LYS
L2757					L2240	GLU	LEU		L1845	L1505	THR	LYS
P2758					N2250	GLU	THR		S1849	L1517	PRO	LYS
N2759					N2251	GLU	ILE		V1850	K1525	ASP	LEU
K2760							ARG			E1534	ASP	ASP
V2761							ARG					
L2762												
L2763												
S2764												
E2765												
K2766												
E2767												
K2768												
E2769												
12770												
Y2771												
R2772												

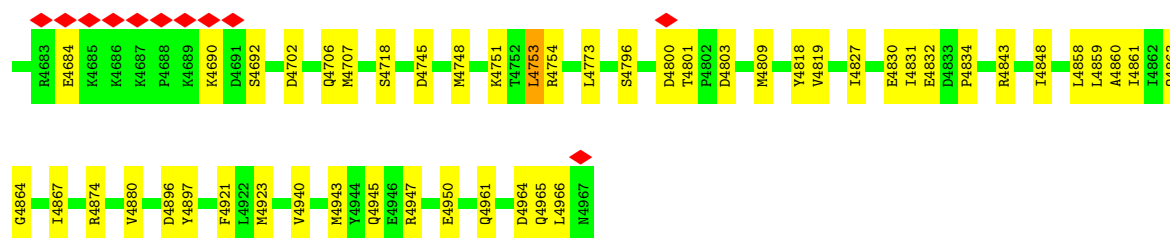




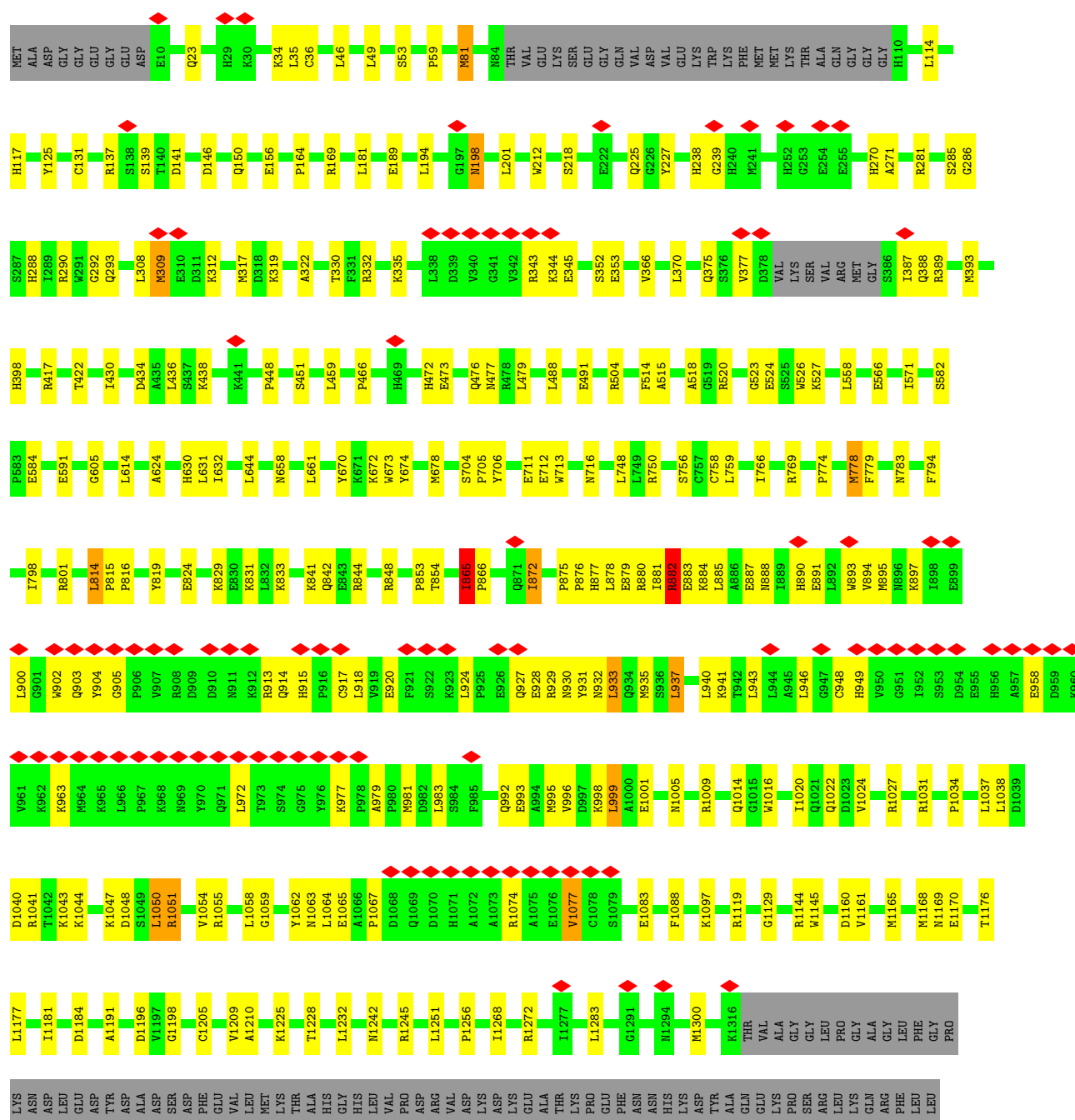




[illegible]



• Molecule 1: Ryanodine receptor 2





E3823	G3648	ILE	ASP	ILE	D2836	Y2901	V2966	R3043	E3119	N3185	Q3313	W3250	Q3250	Q3230	Q3231	Q3232	Q3233	Q3234	Q3235	Q3236	Q3237	Q3238	Q3239	Q3240	Q3241	Q3242	Q3243	Q3244	Q3245	Q3246	Q3247	Q3248	Q3249
G3824	A3649	ALA	THR	ALA	L2837	A2902	V2967	T3044	D3120	S3189	L3314	P3254	P3255	L3239	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258
S3825	E3650	ASN	LYS	VAL	H2838	A2903	L2968	M3045	I3121	R3190	L3315	E3256	E3257	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3830	P3651	LEU	MET	PHE	K2839	A2904	P2969	K3047	I3122	R3191	L3316	N3257	N3258	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
D3833	P3652	LEU	LYS	LEU	A2841	A2905	P2970	T3048	D3125	R3192	L3317	N3259	N3260	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
E3834	E3653	HIS	ASP	HIS	E2842	A2906	L2972	G3049	Q3127	N3261	L3318	E3261	E3262	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
F3835	D3654	LEU	LYS	GLU	E2843	A2907	L2973	L3050	Q3128	R3193	L3319	E3263	E3264	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
D3838	D3655	GLN	ALA	GLN	E2844	A2908	Q2973	K3054	S3129	R3194	L3320	E3265	E3266	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
Q3844	E3656	LYS	VAL	LYS	E2845	A2909	F2974	R3058	S3130	R3195	L3321	E3267	E3268	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3845	G3657	ARG	ASP	ARG	E2846	A2910	F2975	R3059	S3131	R3196	L3322	E3269	E3270	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3846	K3659	ARG	GLN	ARG	E2847	A2911	K2976	R3059	S3132	R3197	L3323	E3271	E3272	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
F3854	R3660	VAL	ILE	VAL	E2848	A2912	K2977	R3060	S3133	R3198	L3324	E3273	E3274	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
Q3861	L3687	ARG	GLY	ARG	E2849	A2913	F2978	R3061	S3134	R3199	L3325	E3275	E3276	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
T3862	L3687	GLY	GLY	GLY	E2850	A2914	F2979	R3062	S3135	R3200	L3326	E3277	E3278	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
T3867	L3687	GLY	GLY	GLY	E2851	A2915	F2980	R3063	S3136	R3201	L3327	E3279	E3280	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
I3870	L3687	GLY	GLY	GLY	E2852	A2916	F2981	R3064	S3137	R3202	L3328	E3281	E3282	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3879	L3687	GLY	GLY	GLY	E2853	A2917	F2982	R3065	S3138	R3203	L3329	E3283	E3284	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
Q3882	L3687	GLY	GLY	GLY	E2854	A2918	F2983	R3066	S3139	R3204	L3330	E3285	E3286	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
E3883	L3687	GLY	GLY	GLY	E2855	A2919	F2984	R3067	S3140	R3205	L3331	E3287	E3288	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
S3884	L3687	GLY	GLY	GLY	E2856	A2920	F2985	R3068	S3141	R3206	L3332	E3289	E3290	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
D3887	L3687	GLY	GLY	GLY	E2857	A2921	F2986	R3069	S3142	R3207	L3333	E3291	E3292	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
F3888	L3687	GLY	GLY	GLY	E2858	A2922	F2987	R3070	S3143	R3208	L3334	E3293	E3294	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
Y3891	L3687	GLY	GLY	GLY	E2859	A2923	F2988	R3071	S3144	R3209	L3335	E3295	E3296	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
Q3903	L3687	GLY	GLY	GLY	E2860	A2924	F2989	R3072	S3145	R3210	L3336	E3297	E3298	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
F3906	L3687	GLY	GLY	GLY	E2861	A2925	F2990	R3073	S3146	R3211	L3337	E3299	E3300	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
K3914	L3687	GLY	GLY	GLY	E2862	A2926	F2991	R3074	S3147	R3212	L3338	E3301	E3302	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
E3922	L3687	GLY	GLY	GLY	E2863	A2927	F2992	R3075	S3148	R3213	L3339	E3303	E3304	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
G3926	L3687	GLY	GLY	GLY	E2864	A2928	F2993	R3076	S3149	R3214	L3340	E3305	E3306	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
P3927	L3687	GLY	GLY	GLY	E2865	A2929	F2994	R3077	S3150	R3215	L3341	E3307	E3308	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
C3928	L3687	GLY	GLY	GLY	E2866	A2930	F2995	R3078	S3151	R3216	L3342	E3309	E3310	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3935	L3687	GLY	GLY	GLY	E2867	A2931	F2996	R3079	S3152	R3217	L3343	E3311	E3312	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3940	L3687	GLY	GLY	GLY	E2868	A2932	F2997	R3080	S3153	R3218	L3344	E3313	E3314	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
A3952	L3687	GLY	GLY	GLY	E2869	A2933	F2998	R3081	S3154	R3219	L3345	E3315	E3316	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
D3961	L3687	GLY	GLY	GLY	E2870	A2934	F2999	R3082	S3155	R3220	L3346	E3317	E3318	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3962	L3687	GLY	GLY	GLY	E2871	A2935	F3000	R3083	S3156	R3221	L3347	E3319	E3320	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
D3961	L3687	GLY	GLY	GLY	E2872	A2936	F3001	R3084	S3157	R3222	L3348	E3321	E3322	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3962	L3687	GLY	GLY	GLY	E2873	A2937	F3002	R3085	S3158	R3223	L3349	E3323	E3324	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
L3967	L3687	GLY	GLY	GLY	E2874	A2938	F3003	R3086	S3159	R3224	L3350	E3325	E3326	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
	L3967	GLY	GLY	GLY	E2875	A2939	F3004	R3087	S3160	R3225	L3351	E3327	E3328	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259
	L3967	GLY	GLY	GLY	E2876	A2940	F3005	R3088	S3161	R3226	L3352	E3329	E3330	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259

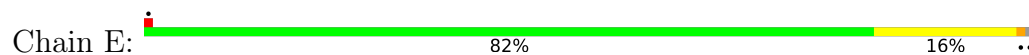




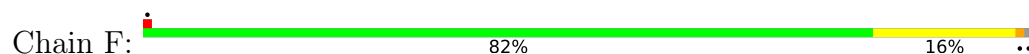




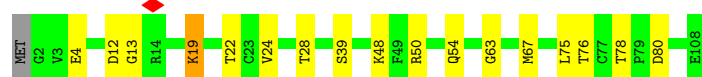
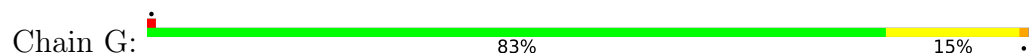
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



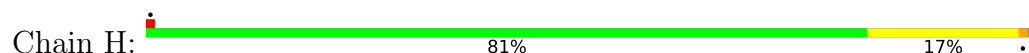
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90375	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	0.667	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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	0.16	0/34511	0.45	11/46614 (0.0%)
1	B	0.16	0/34511	0.45	11/46614 (0.0%)
1	C	0.16	0/34511	0.45	10/46614 (0.0%)
1	D	0.16	0/34511	0.45	11/46614 (0.0%)
2	E	0.17	0/834	0.41	0/1123
2	F	0.17	0/834	0.41	0/1123
2	G	0.17	0/834	0.41	0/1123
2	H	0.17	0/834	0.41	0/1123
All	All	0.16	0/141380	0.45	43/190948 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3315	LEU	CA-CB-CG	7.52	142.62	116.30
1	B	3315	LEU	CA-CB-CG	7.52	142.61	116.30
1	A	3315	LEU	CA-CB-CG	7.51	142.60	116.30
1	D	3315	LEU	CA-CB-CG	7.51	142.59	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2840	MET	CB-CG-SD	6.67	132.72	112.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1051	ARG	Sidechain
1	A	4640	PHE	Peptide
1	A	882	ARG	Sidechain
1	B	1051	ARG	Sidechain
1	B	882	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33771	0	33455	784	0
1	B	33771	0	33455	772	0
1	C	33771	0	33455	771	0
1	D	33771	0	33455	784	0
2	E	818	0	821	11	0
2	F	818	0	821	11	0
2	G	818	0	821	10	0
2	H	818	0	821	12	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	138608	0	137200	3061	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 3061 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:A:1498:GLN:NE2	1:D:2899:ASN:O	1.91	1.04
1:A:4060:GLN:HE21	1:A:4060:GLN:HA	1.21	1.04
1:A:882:ARG:NH2	1:A:933:LEU:O	1.92	1.03
1:B:4060:GLN:HA	1:B:4060:GLN:HE21	1.21	1.02
1:C:4060:GLN:HA	1:C:4060:GLN:HE21	1.21	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4198/4967 (84%)	4067 (97%)	127 (3%)	4 (0%)	48	69
1	B	4198/4967 (84%)	4065 (97%)	129 (3%)	4 (0%)	48	69
1	C	4198/4967 (84%)	4064 (97%)	130 (3%)	4 (0%)	48	69
1	D	4198/4967 (84%)	4063 (97%)	131 (3%)	4 (0%)	48	69
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17212/20300 (85%)	16667 (97%)	529 (3%)	16 (0%)	49	69

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2988	ARG
1	A	3927	PRO
1	A	4641	PRO
1	B	2988	ARG

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Mol	Chain	Res	Type
1	B	3927	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3708/4358 (85%)	3656 (99%)	52 (1%)	59	78
1	B	3708/4358 (85%)	3656 (99%)	52 (1%)	59	78
1	C	3708/4358 (85%)	3656 (99%)	52 (1%)	59	78
1	D	3708/4358 (85%)	3654 (98%)	54 (2%)	57	77
2	E	88/89 (99%)	87 (99%)	1 (1%)	65	81
2	F	88/89 (99%)	87 (99%)	1 (1%)	65	81
2	G	88/89 (99%)	87 (99%)	1 (1%)	65	81
2	H	88/89 (99%)	87 (99%)	1 (1%)	65	81
All	All	15184/17788 (85%)	14970 (99%)	214 (1%)	57	78

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	865	ILE
1	C	3050	LEU
1	D	3116	GLN
1	C	940	LEU
1	C	2592	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4879	GLN
1	D	3614	HIS
1	D	270	HIS
1	D	1972	GLN

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Mol	Chain	Res	Type
1	D	3933	GLN

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	0.31	0
4	ATP	C	5002	-	32,33,33	0.27	0	48,52,52	0.31	0
4	ATP	B	5002	-	32,33,33	0.27	0	48,52,52	0.31	0
4	ATP	D	5003	-	32,33,33	0.26	0	48,52,52	0.28	0
4	ATP	A	5003	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	C	5003	-	32,33,33	0.26	0	48,52,52	0.28	0
4	ATP	B	5003	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.31	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	-	-	4/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	4/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	4/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	13/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	13/22/38/38	0/3/3/3
4	ATP	C	5003	-	-	13/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	13/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3A-PA-O5'
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	PB-O3A-PA-O5'

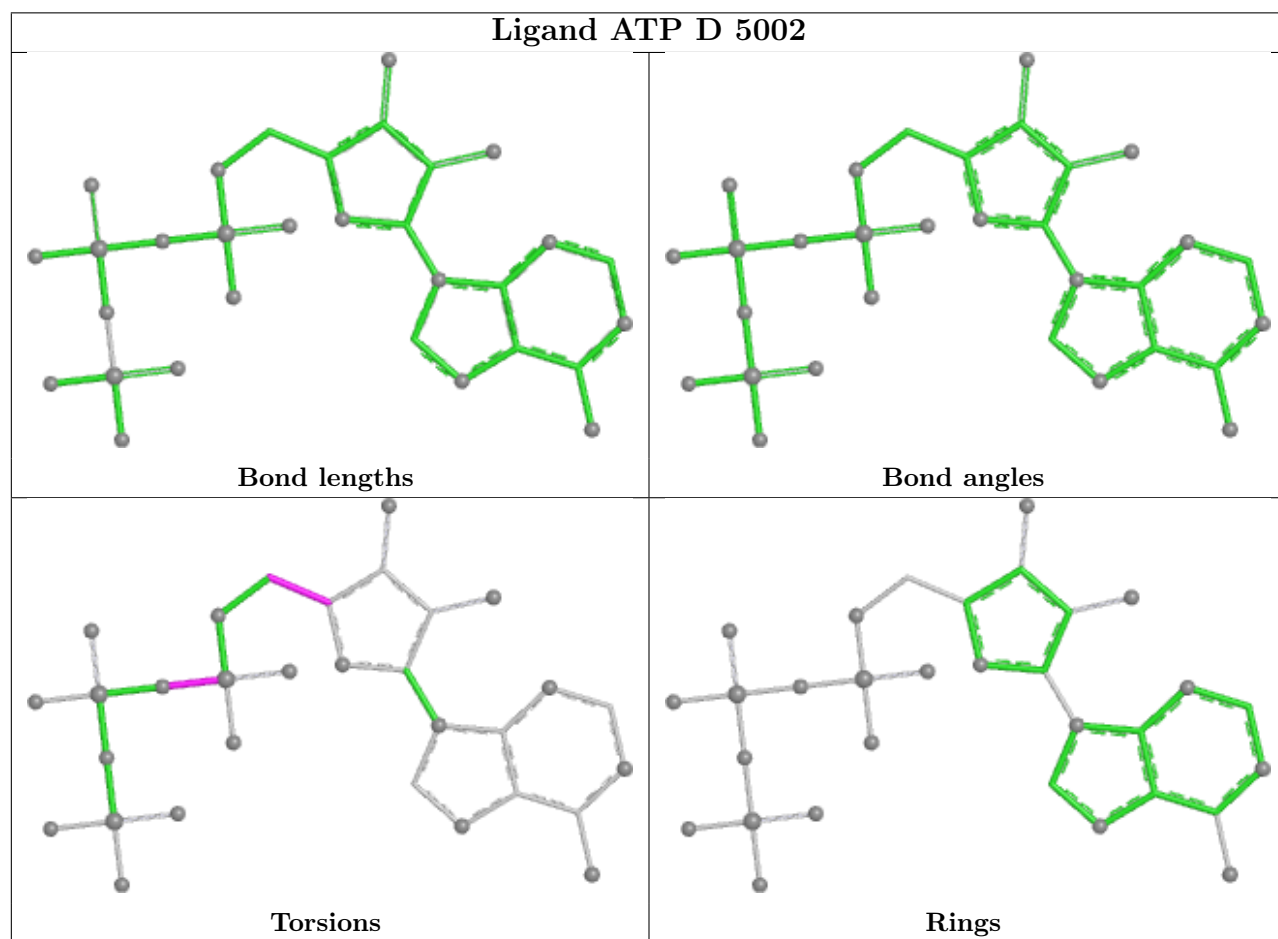
There are no ring outliers.

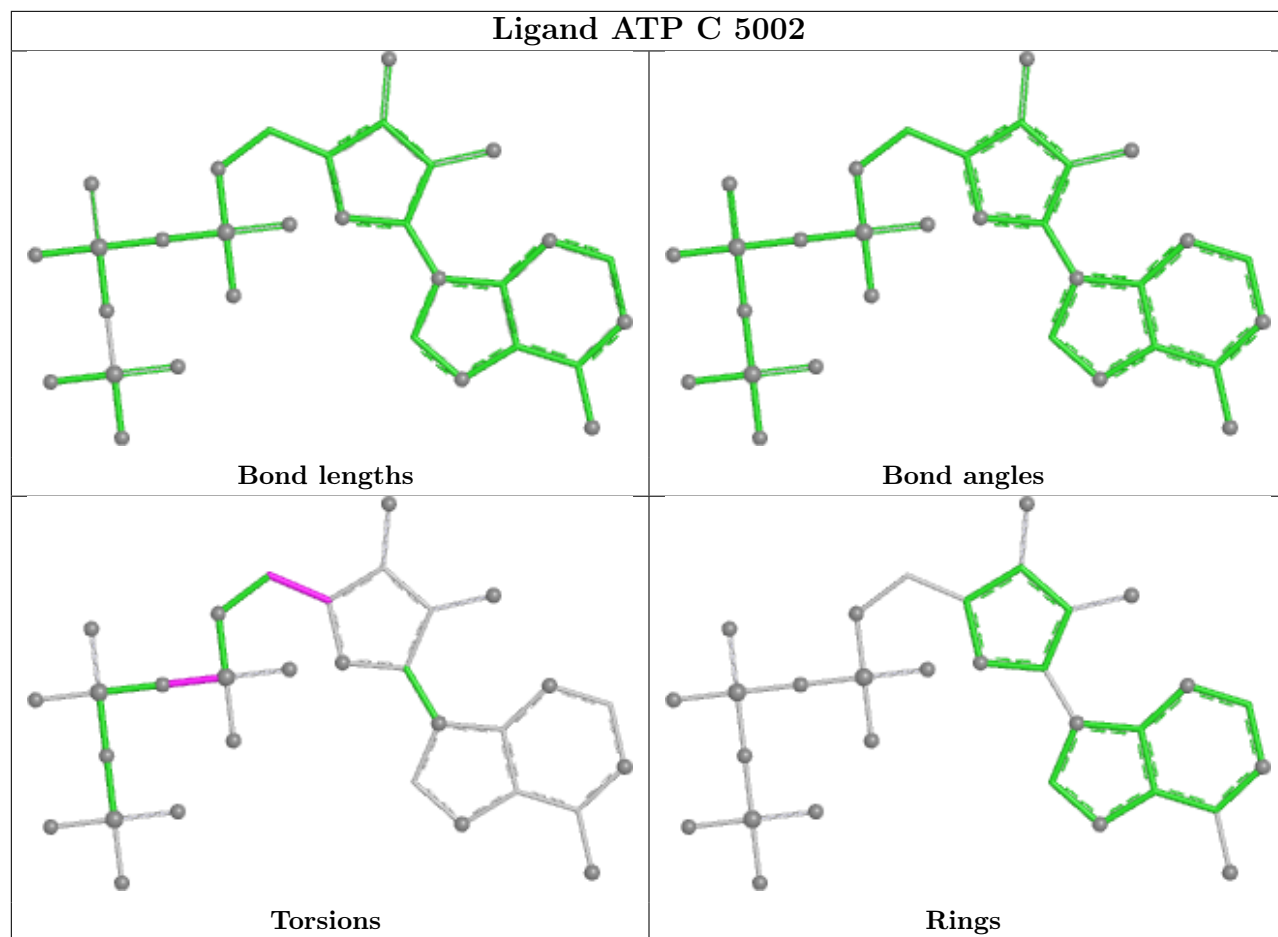
4 monomers are involved in 4 short contacts:

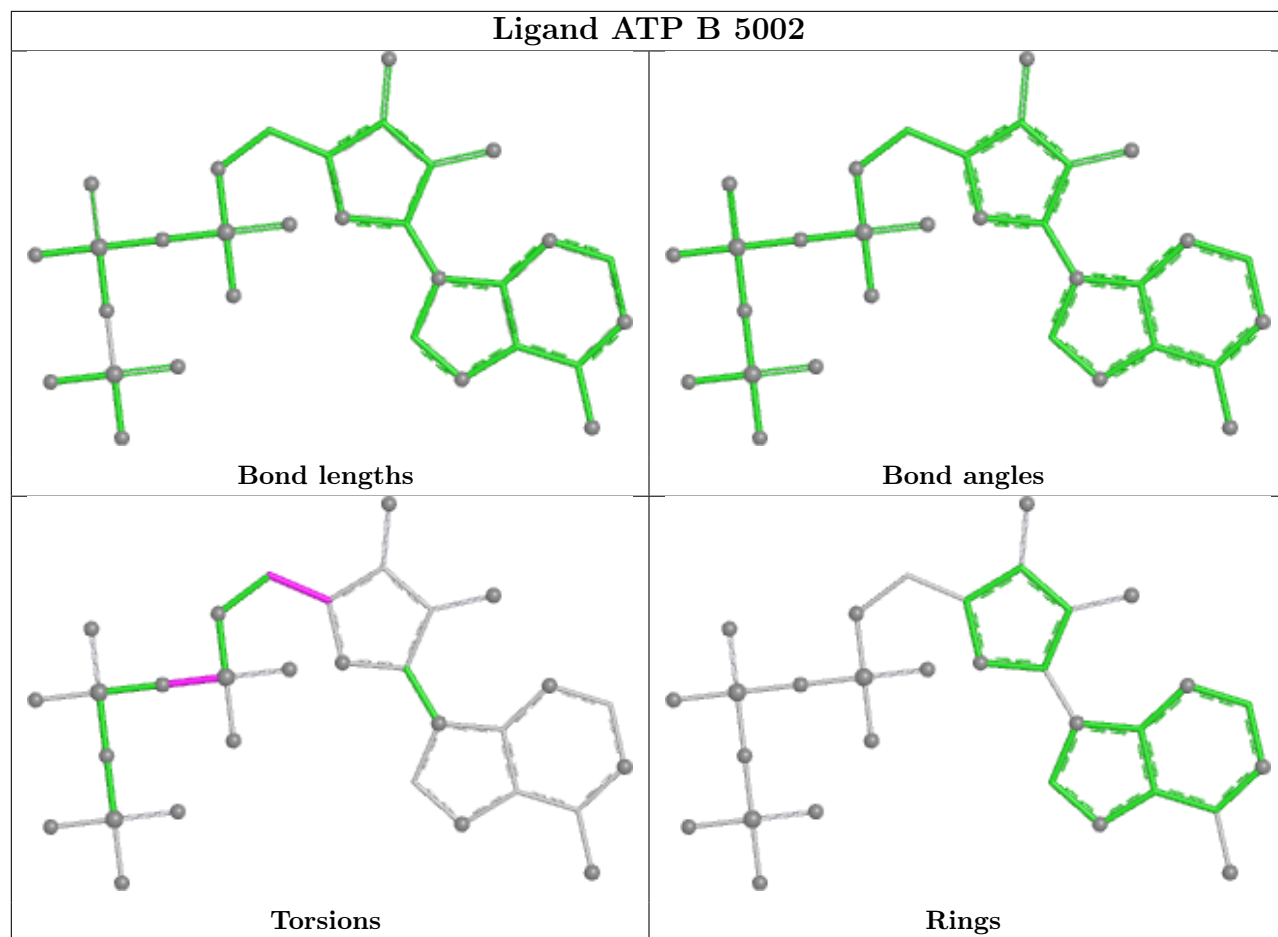
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5002	ATP	1	0
4	C	5002	ATP	1	0
4	B	5002	ATP	1	0
4	A	5002	ATP	1	0

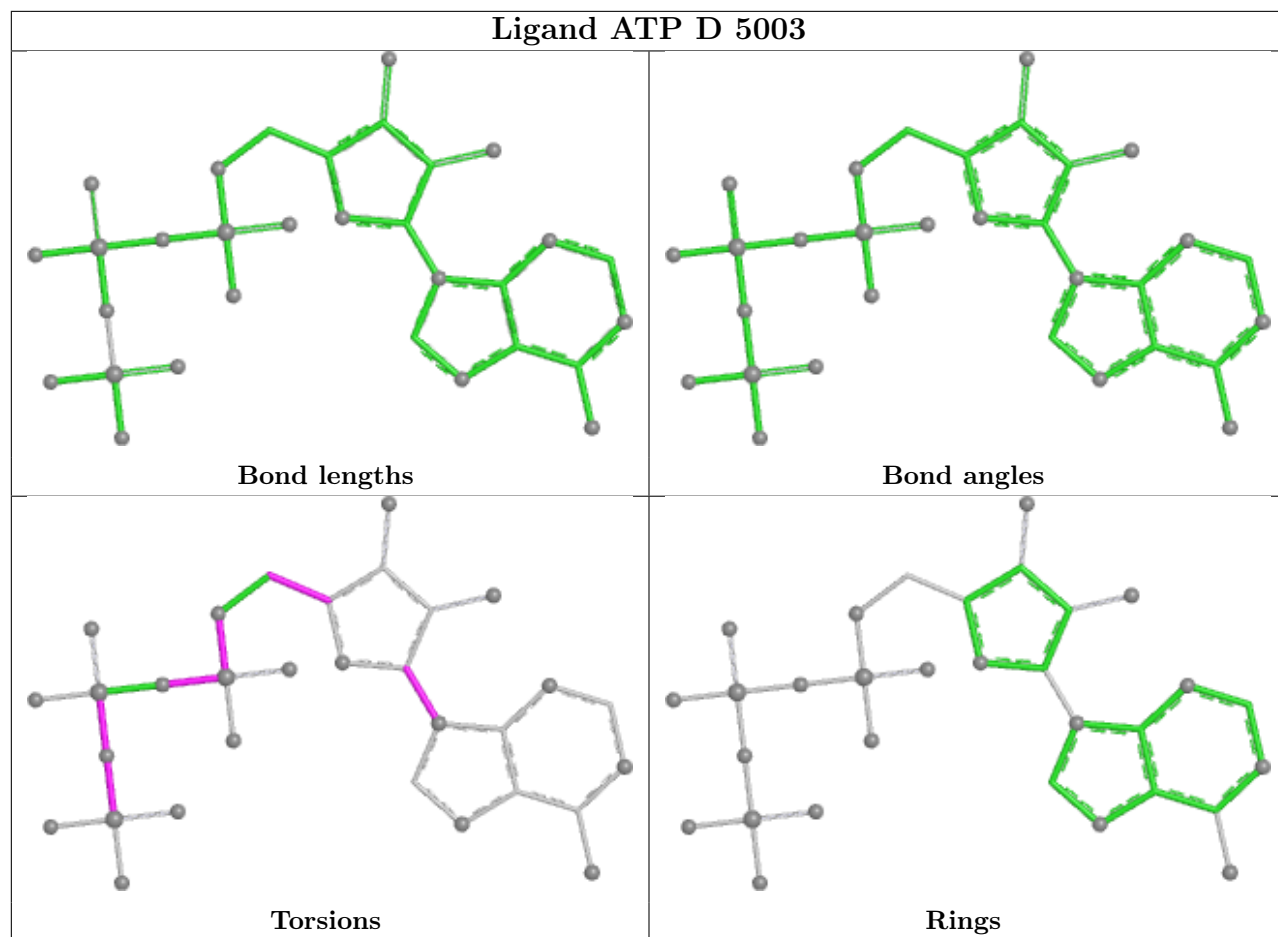
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

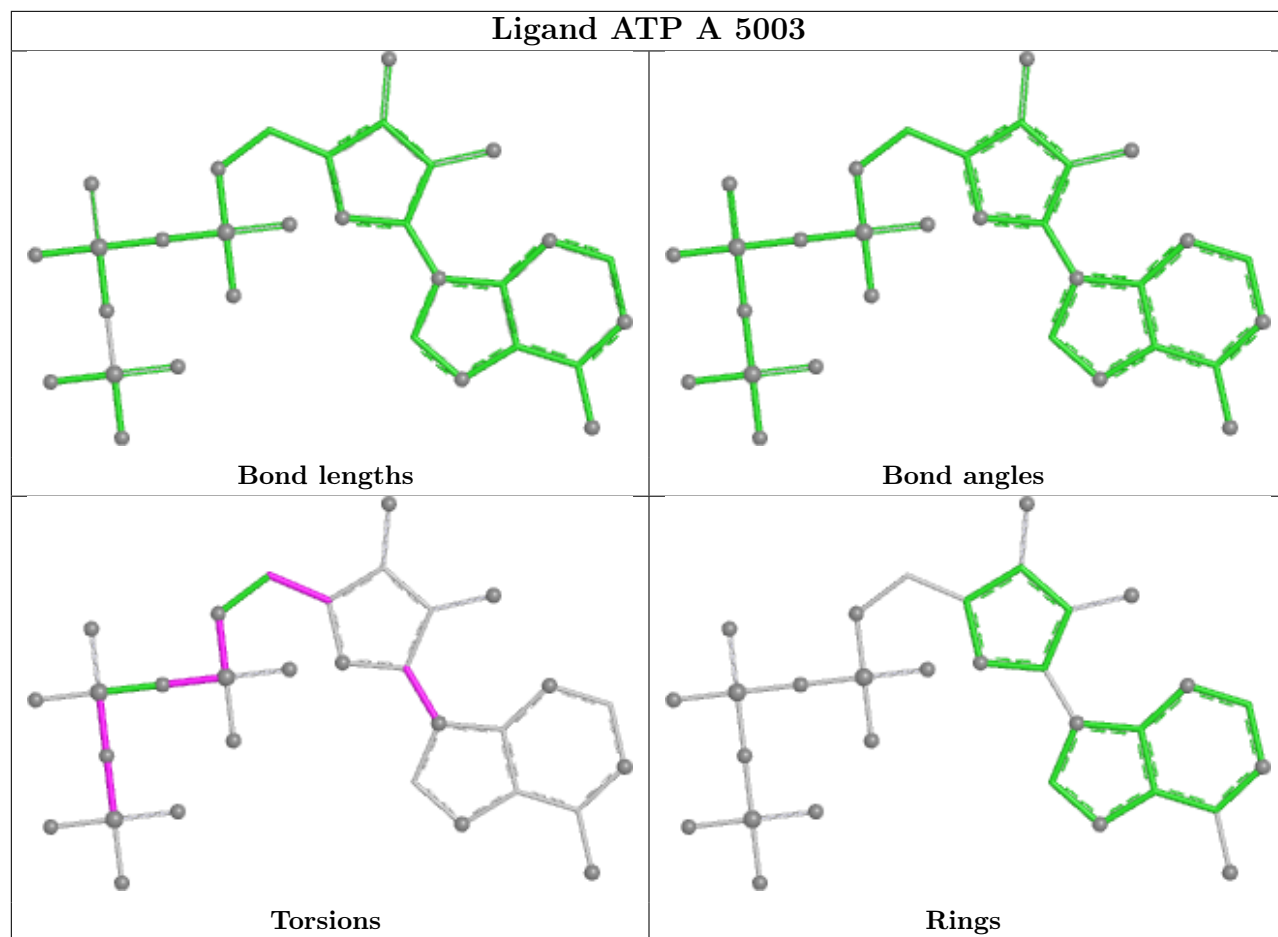
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

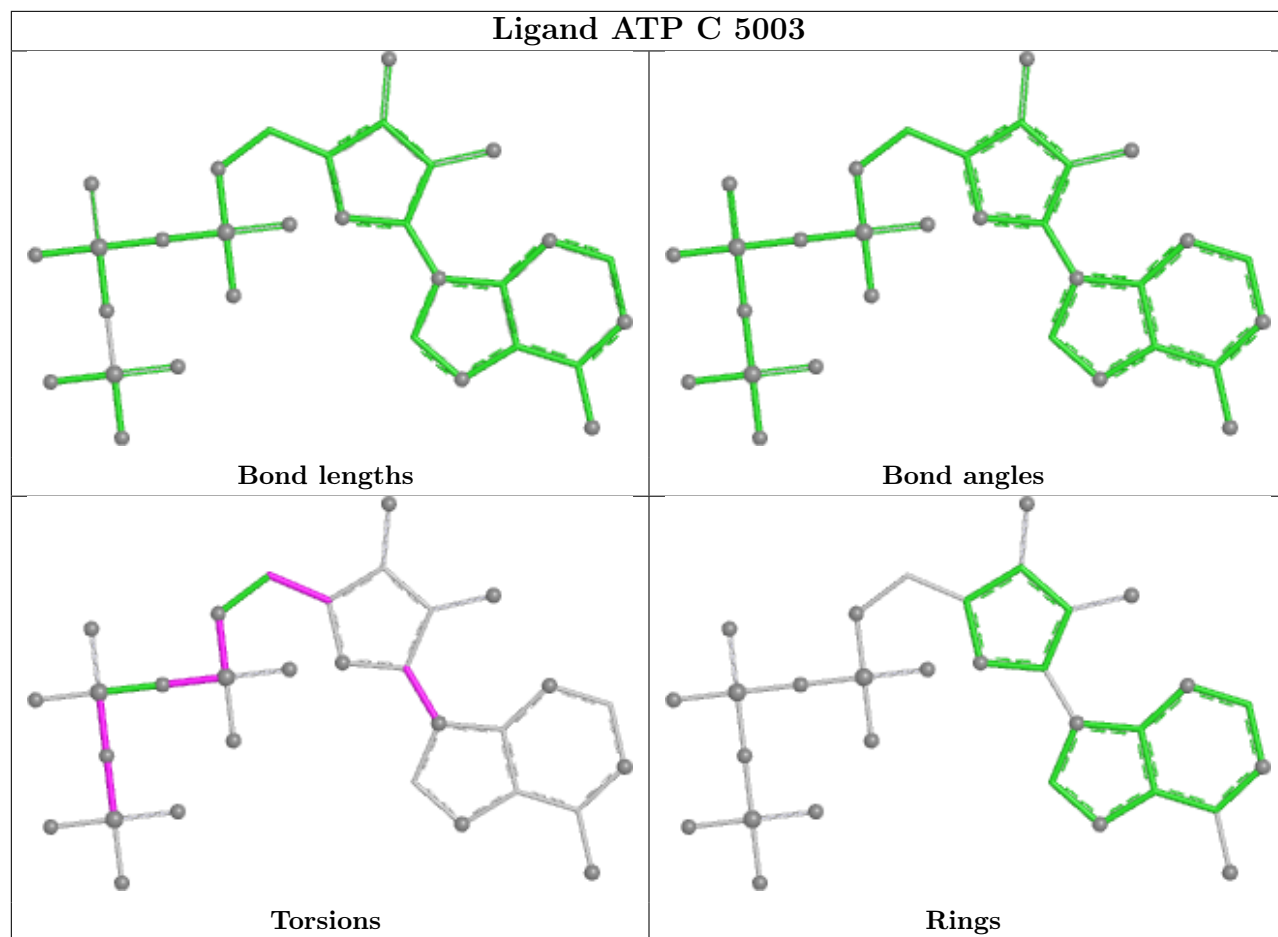


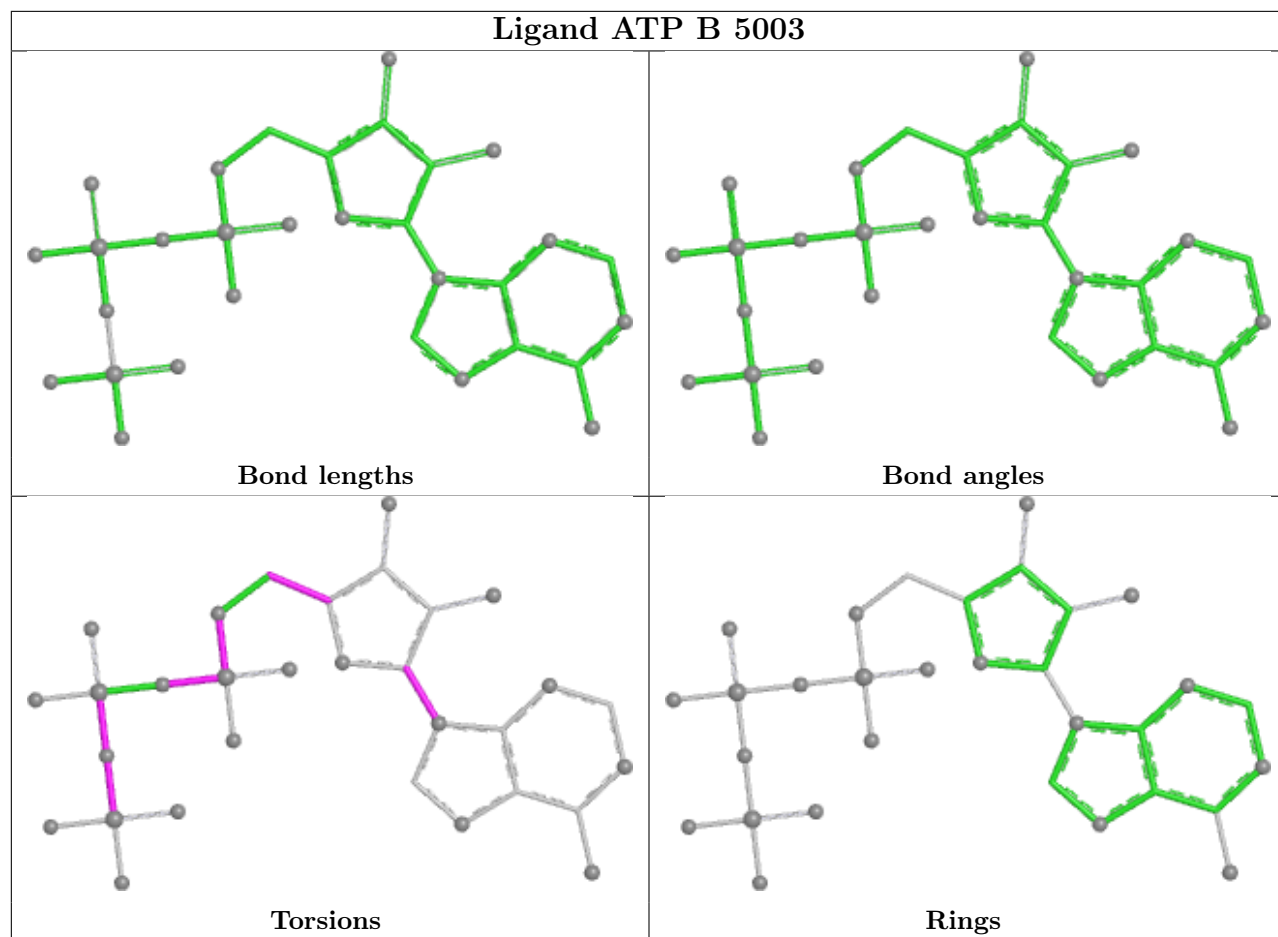


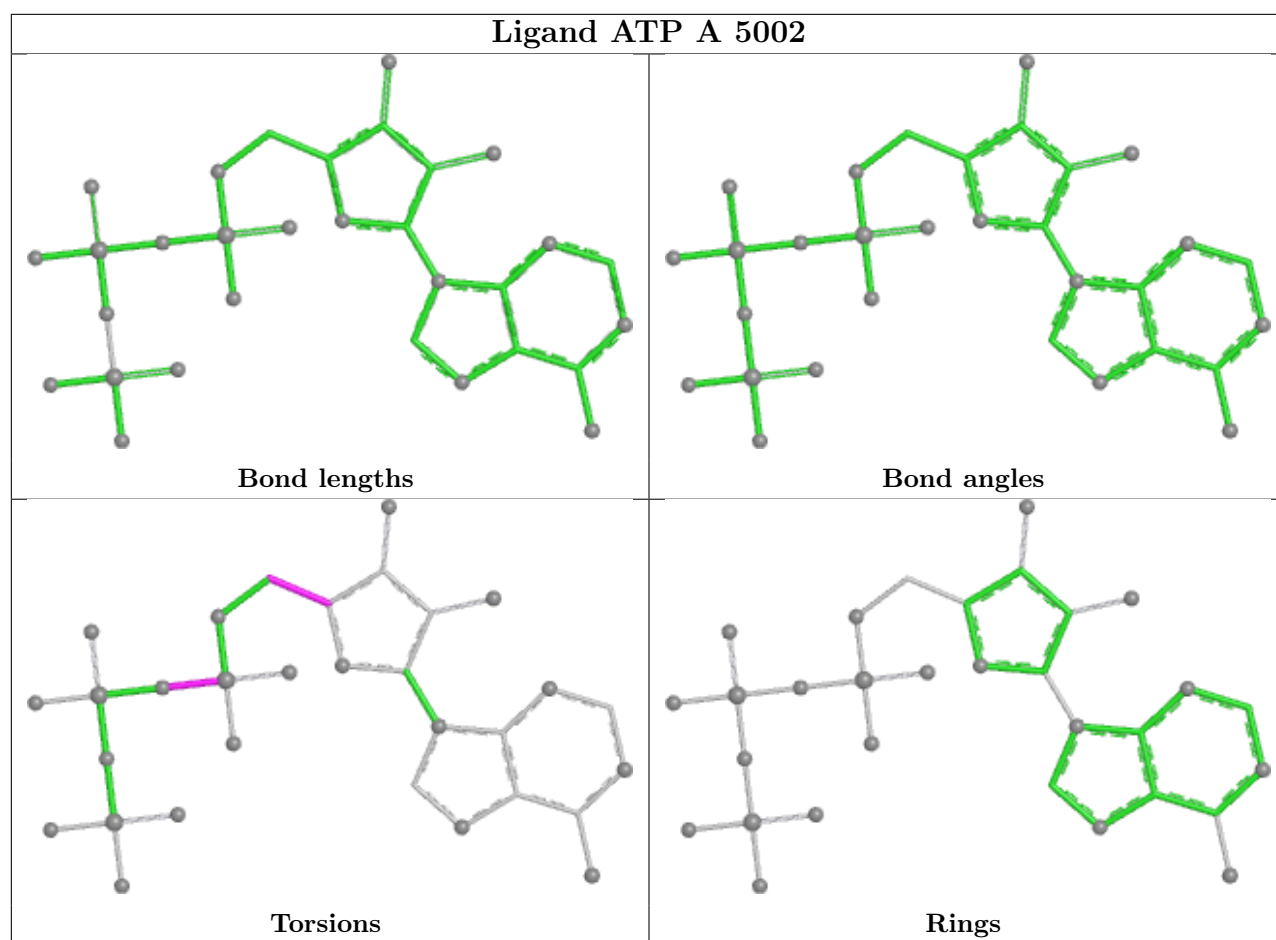












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

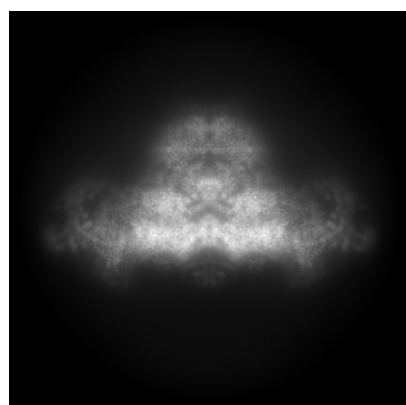
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26415. These allow visual inspection of the internal detail of the map and identification of artifacts.

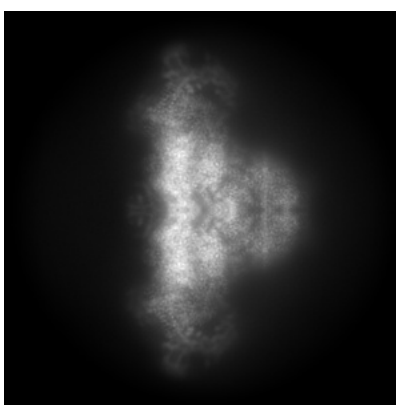
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

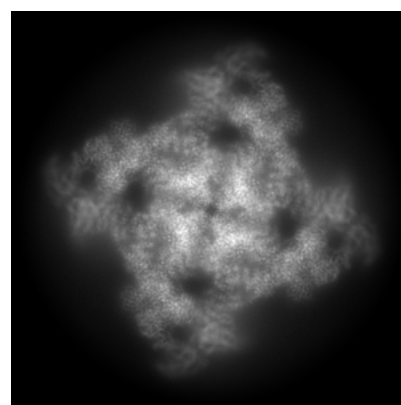
6.1.1 Primary map



X



Y

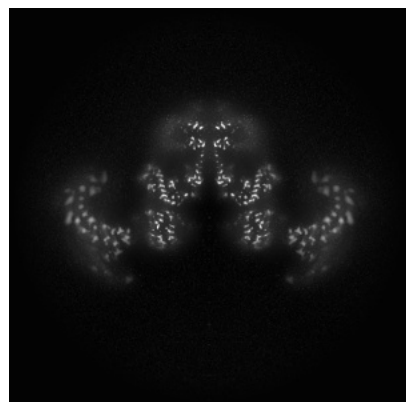


Z

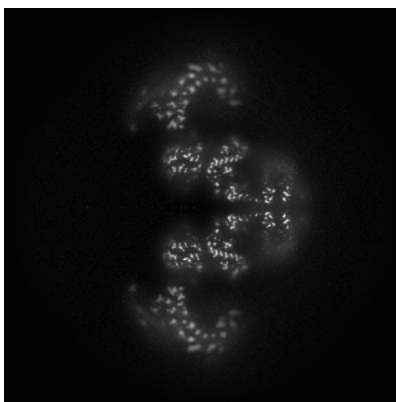
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

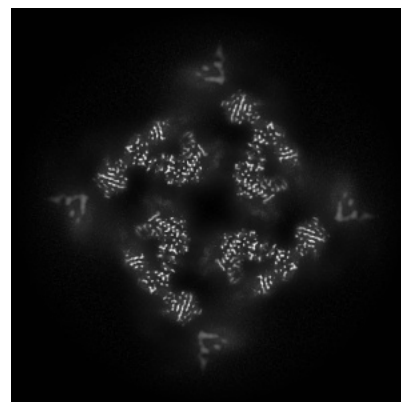
6.2.1 Primary map



X Index: 256



Y Index: 256

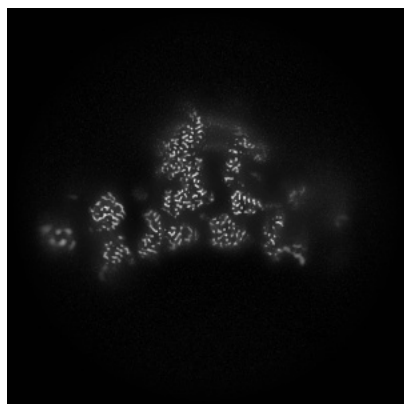


Z Index: 256

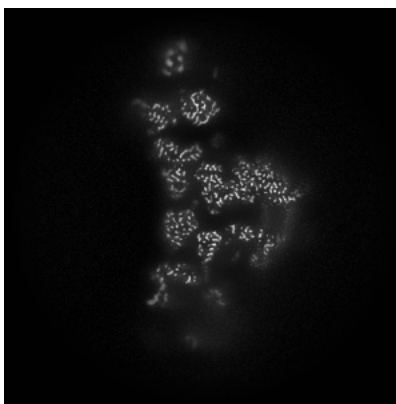
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

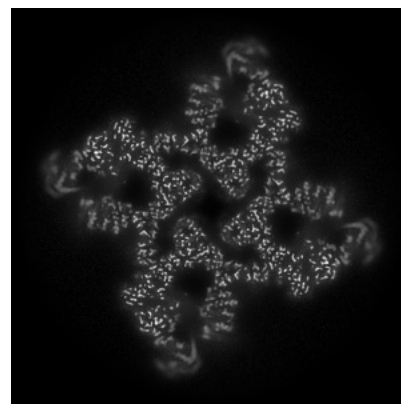
6.3.1 Primary map



X Index: 219



Y Index: 219

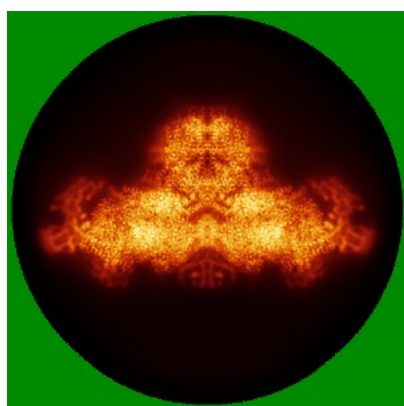


Z Index: 223

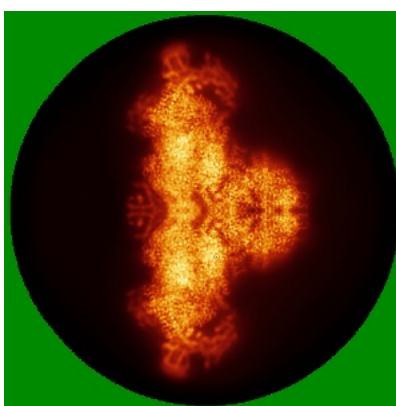
The images above show the largest variance slices of the map in three orthogonal directions.

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

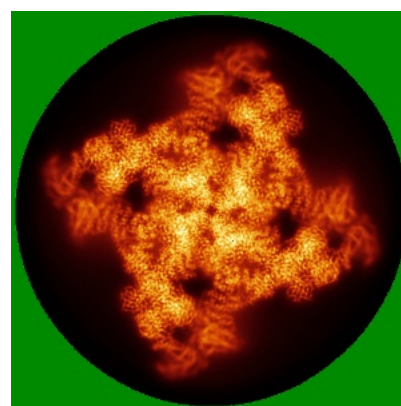
6.4.1 Primary map



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.

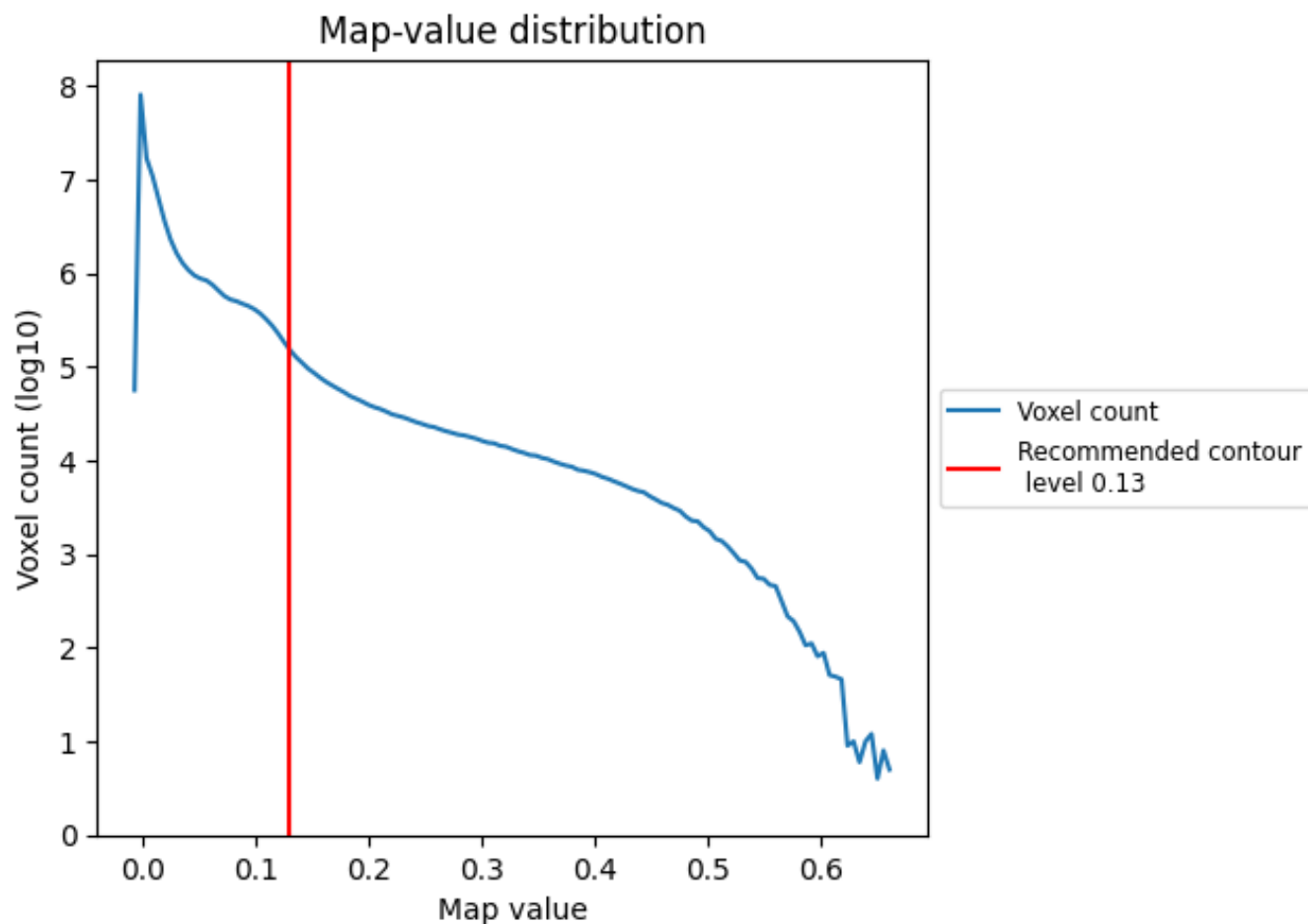
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

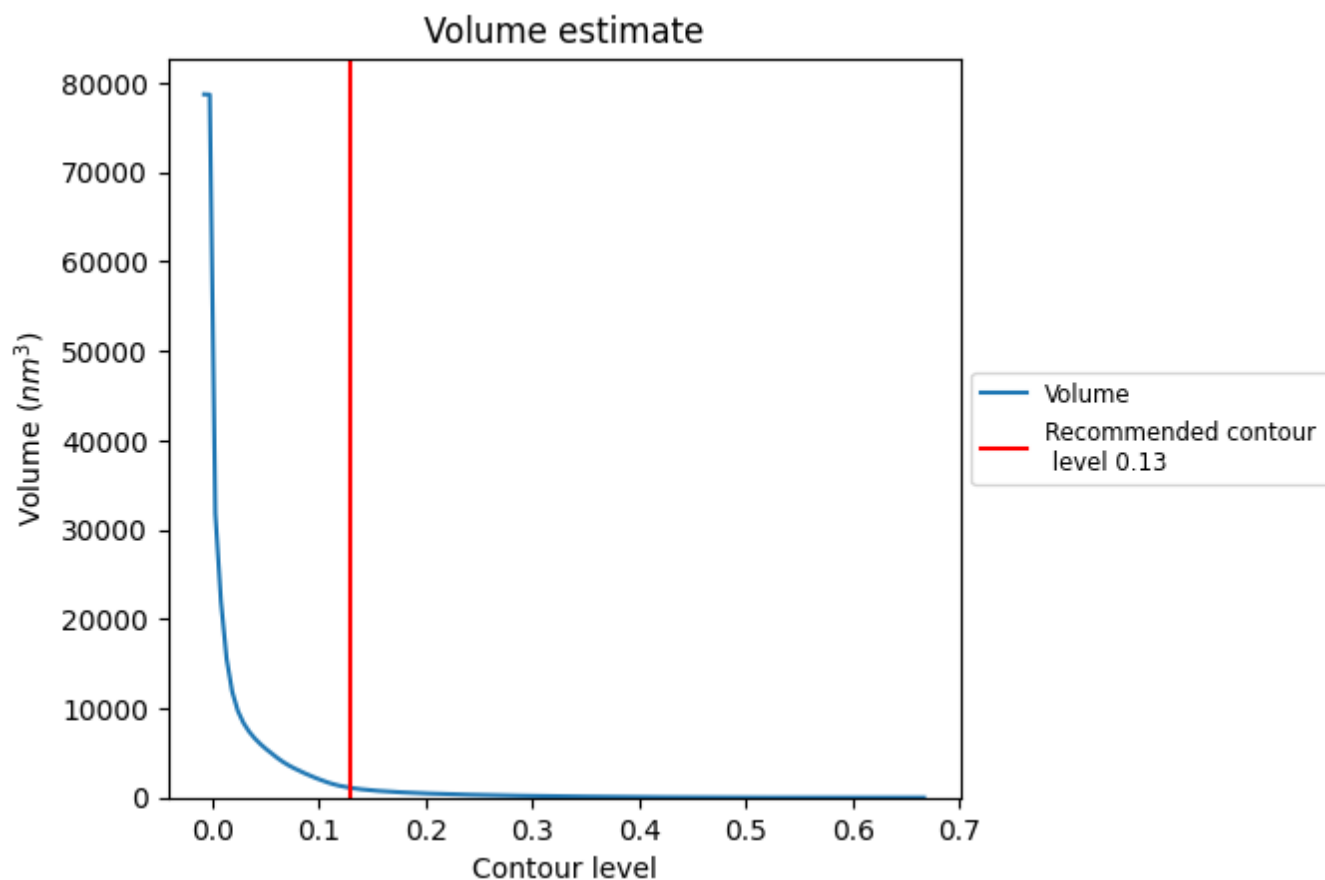
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

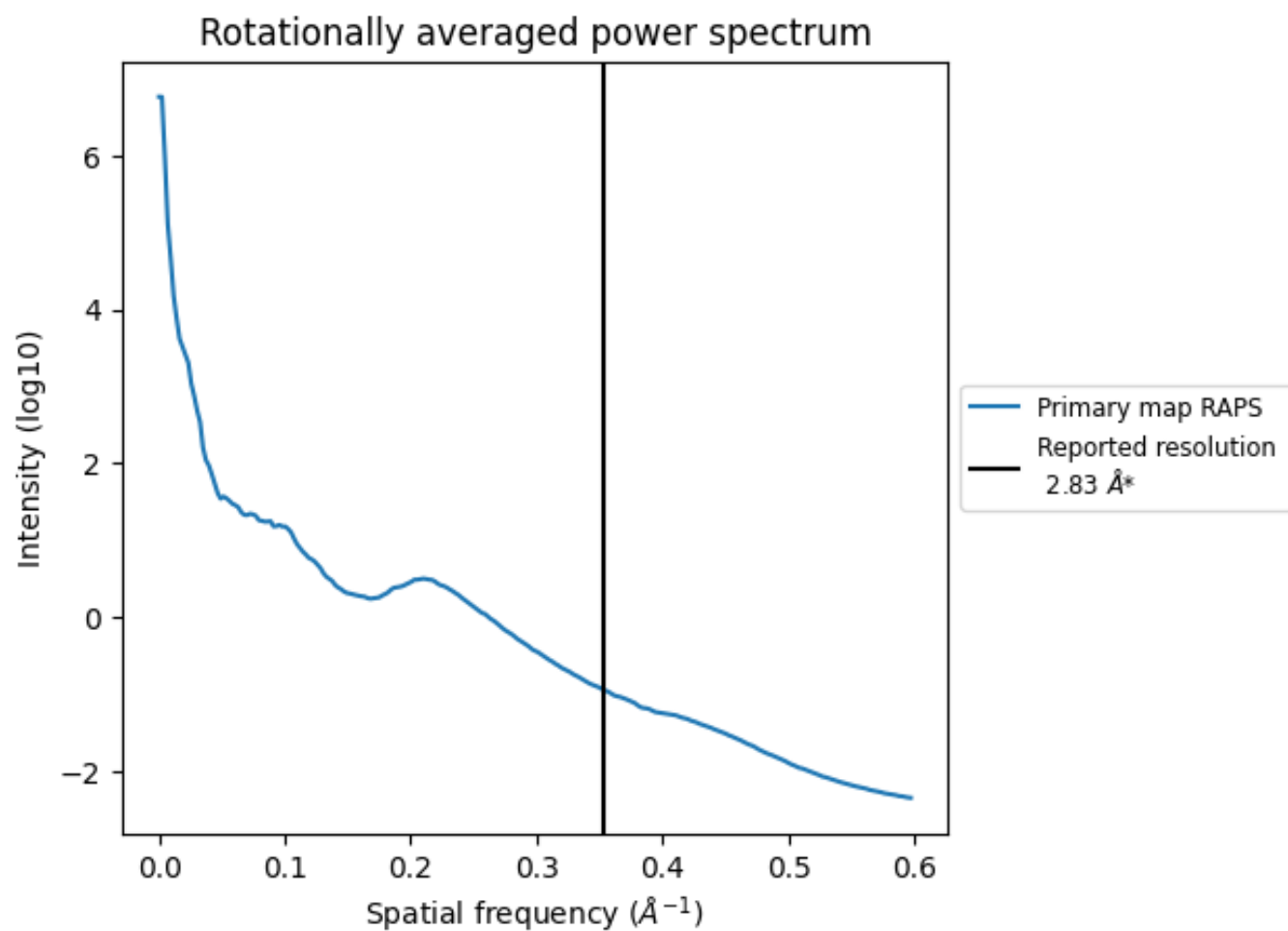
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1083 nm³; this corresponds to an approximate mass of 978 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 0.353 Å⁻¹

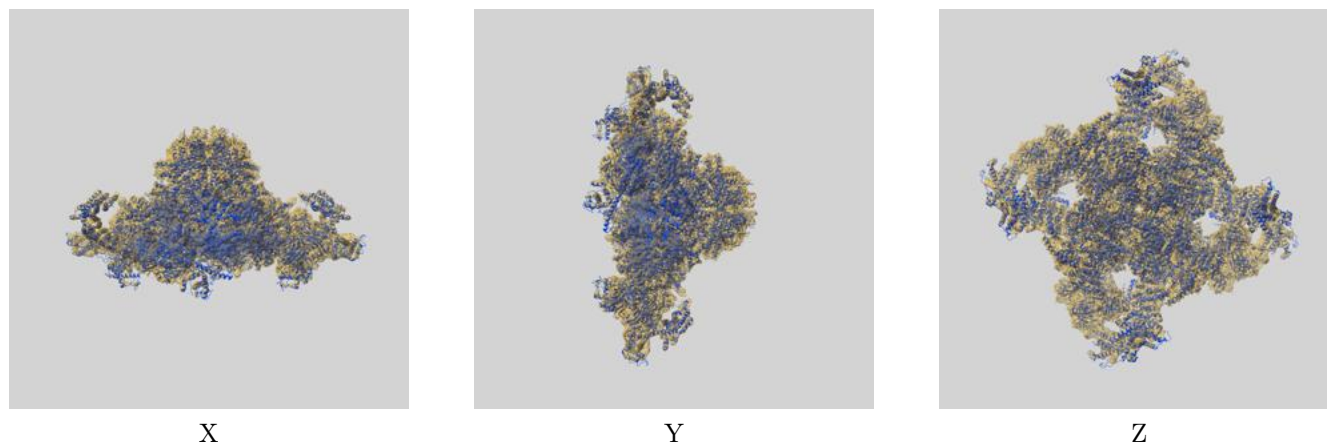
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

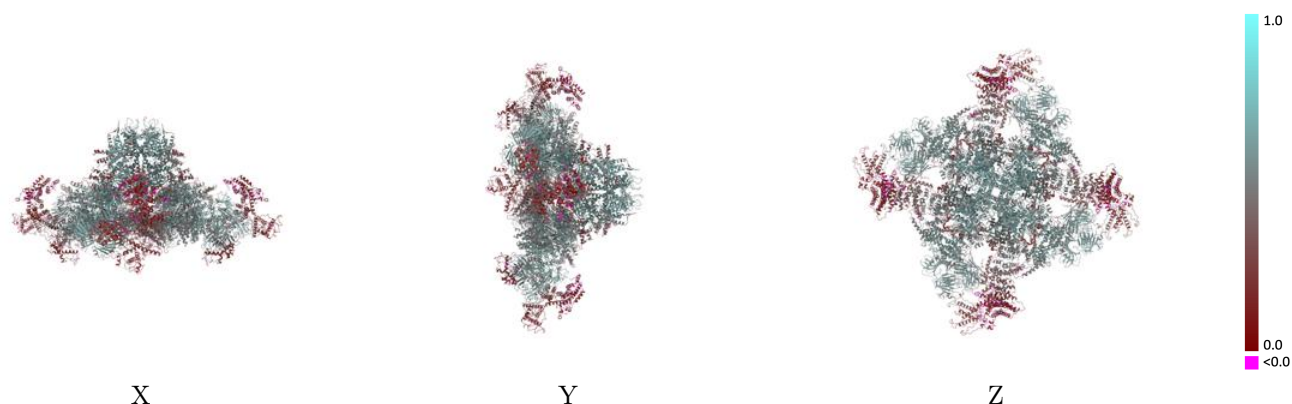
This section contains information regarding the fit between EMDB map EMD-26415 and PDB model 7UA5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



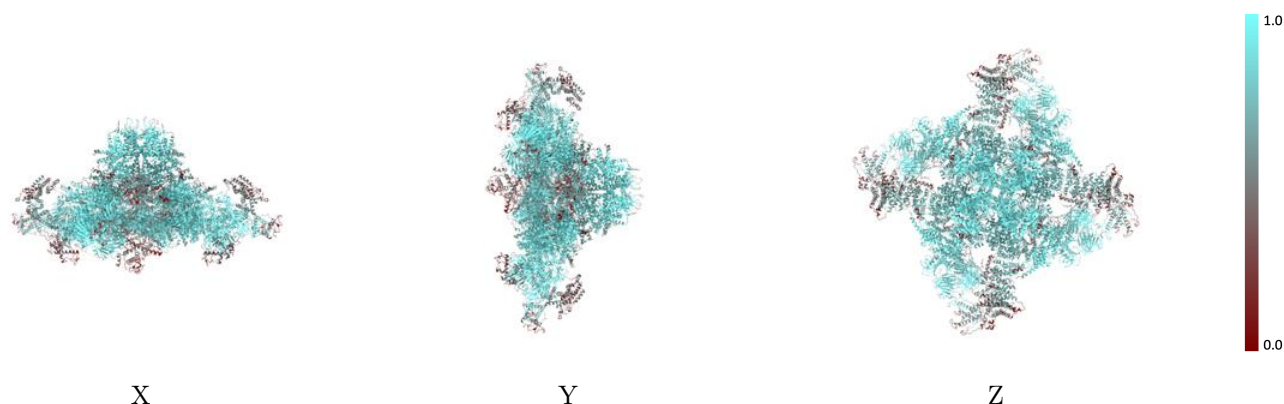
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



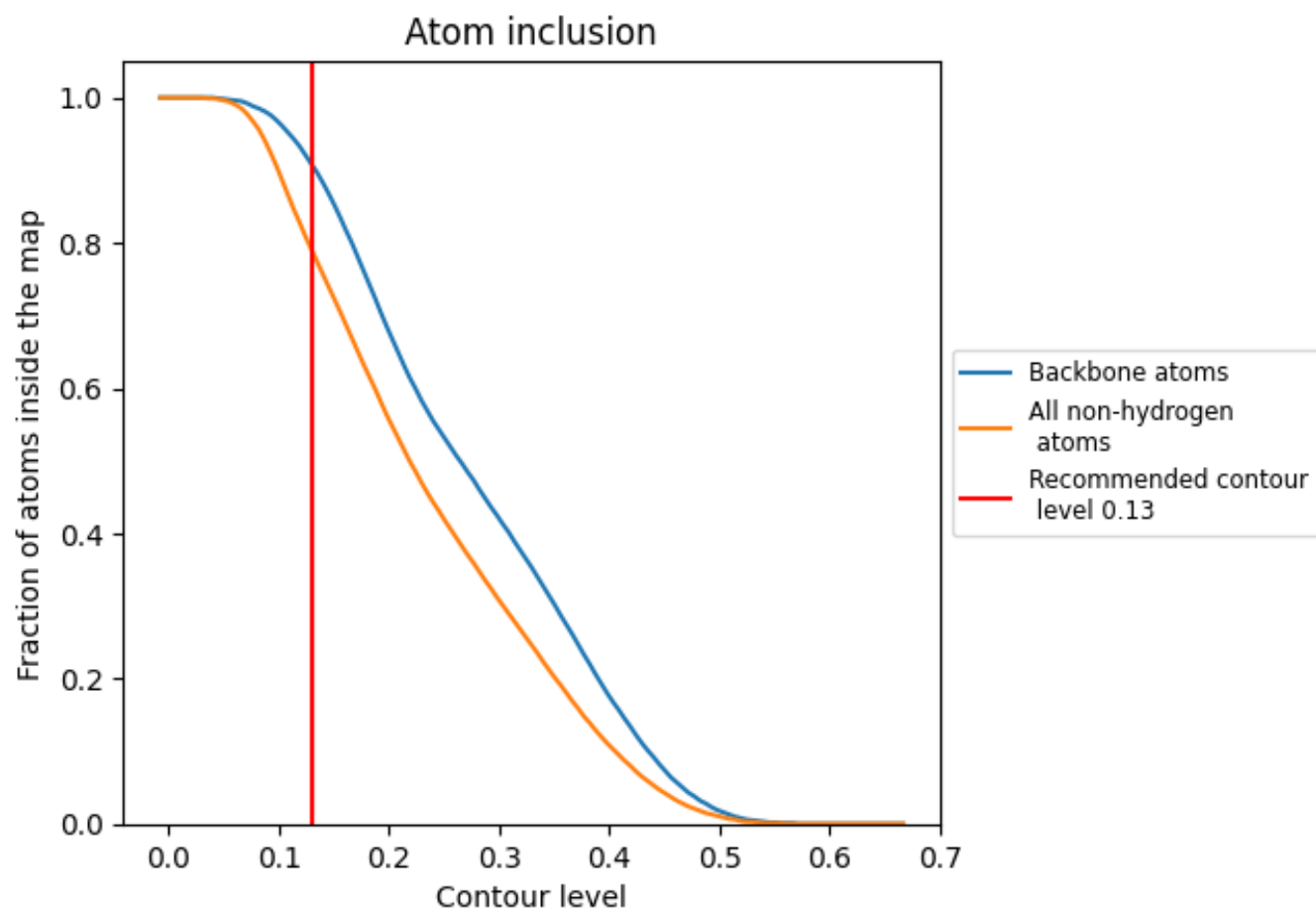
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 79% 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	0.7910	0.4480
A	0.7880	0.4490
B	0.7880	0.4480
C	0.7880	0.4470
D	0.7850	0.4380
E	0.9220	0.5670
F	0.9260	0.5600
G	0.9220	0.5650
H	0.9230	0.5640

1.0

0.0

<0.0