



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:35 AM UTC

PDB ID : 7UA1 / pdb_00007ua1
EMDB ID : EMD-26412
Title : Structure of PKA phosphorylated human RyR2-R2474S in the closed state in the presence of ARM210
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 2.99 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:

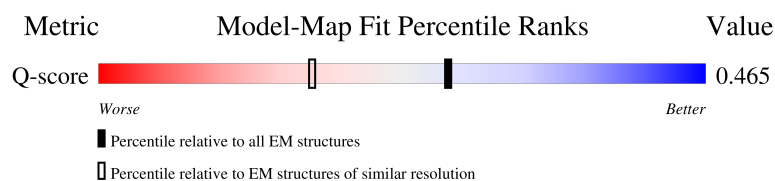
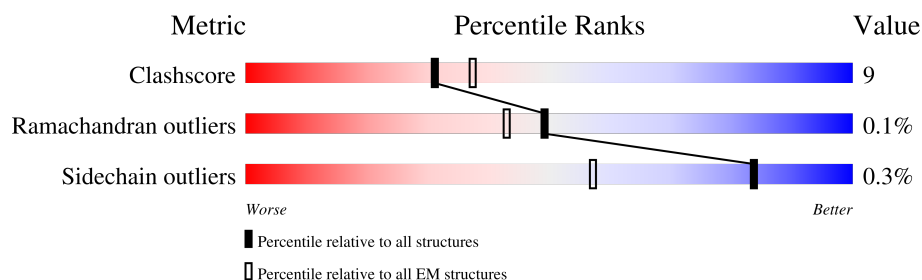
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.99 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	13287 (2.49 - 3.49)

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	 6% 66% 19% 15%
1	B	4967	 6% 66% 19% 15%
1	C	4967	 6% 66% 19% 15%
1	D	4967	 6% 66% 19% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	108	 78% 21% .
2	F	108	 78% 21% .
2	G	108	 78% 21% .
2	H	108	 78% 21% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	A	5003	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 138680 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	B	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	C	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	D	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		

There are 4 discrepancies between the modelled and reference sequences:

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

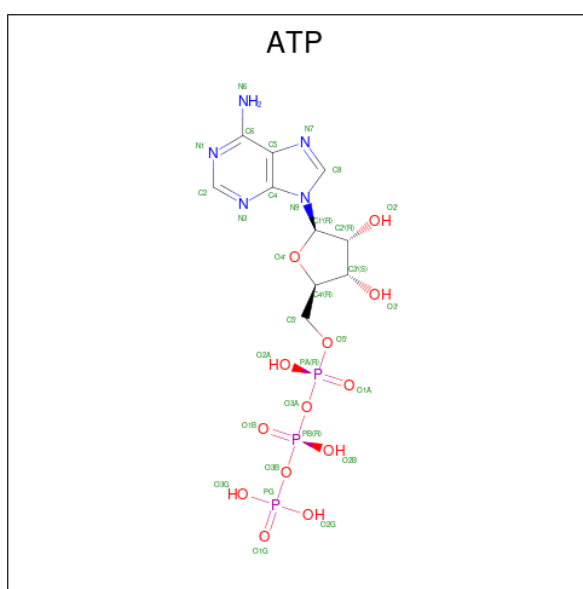
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 3 is ZINC ION (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).



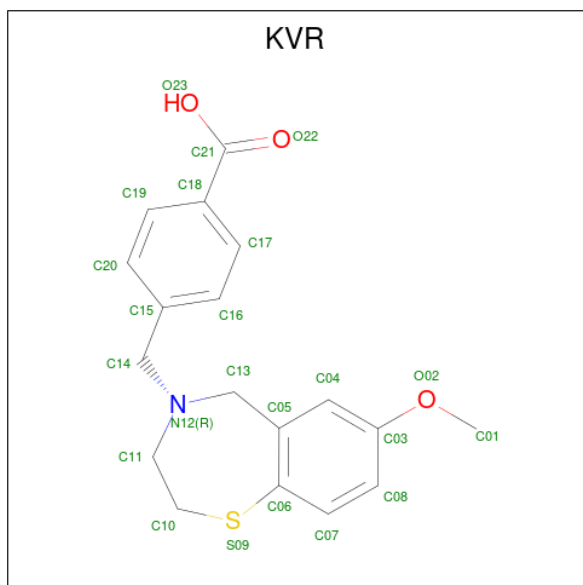
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10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

Continued on next page...

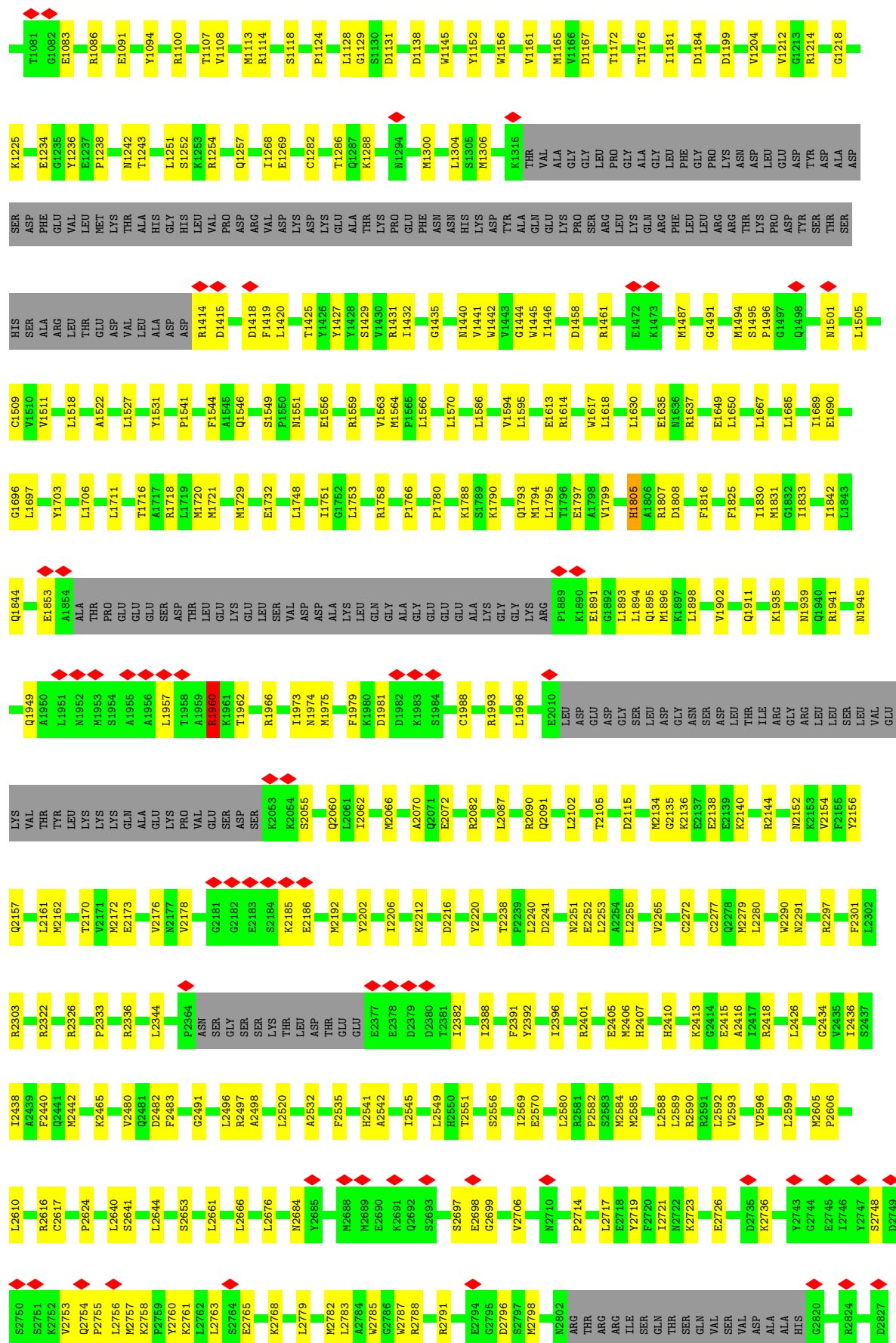
Continued from previous page...

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

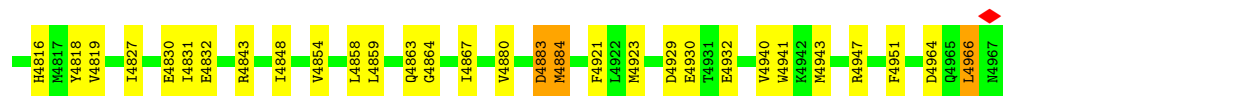
- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (CCD ID: KVR) (formula: C₁₈H₁₉NO₃S).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	A	1	23	18	1	3	1	0
5	B	1	23	18	1	3	1	0
5	C	1	23	18	1	3	1	0
5	D	1	23	18	1	3	1	0





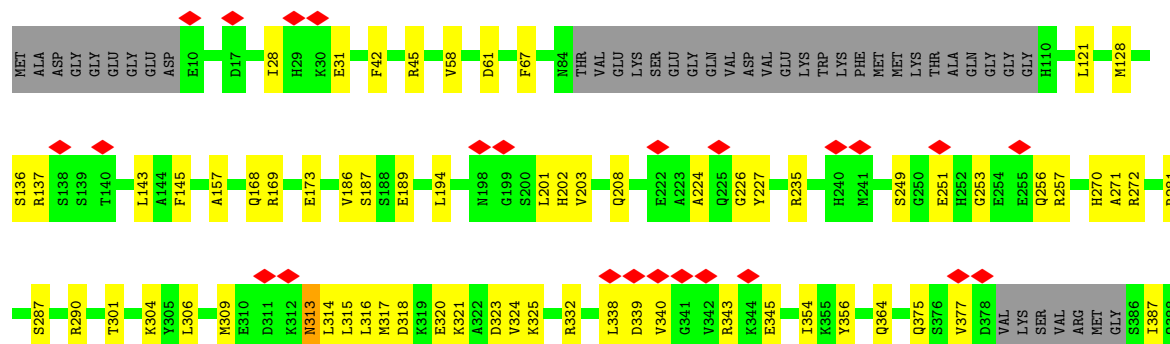


Chain B:



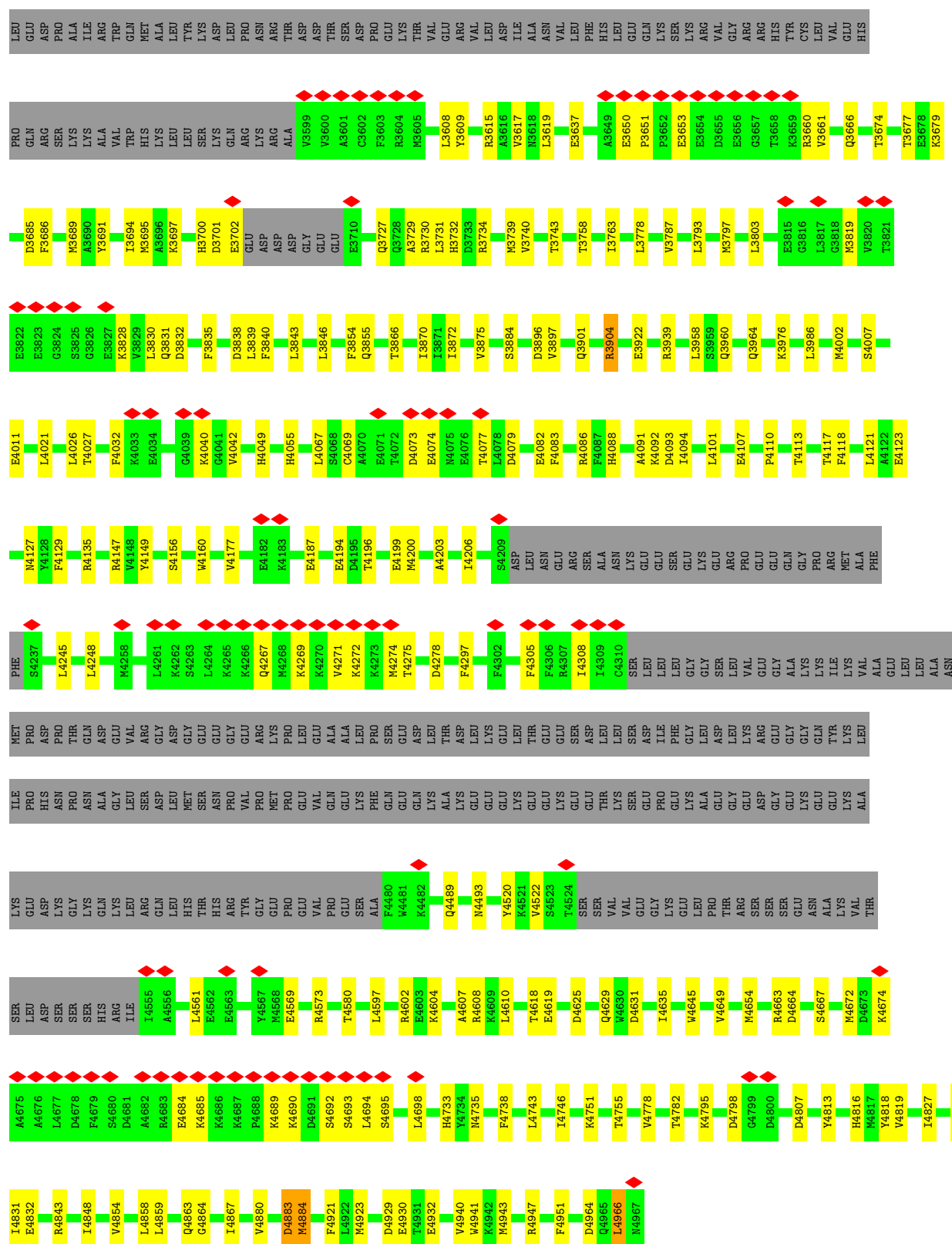


V3661	V3666	T3674	T3677	E3678	K3679	D3685	F3686	K3689	A3690	Y3691	L3694	K3695	A3696	K3697	H3700	D3701	E3702	GLU	ASP	ASP	GLY	GLU	E3710	V3711	Q3727	Q3728	R3730	L3731	H3732	H3733	R3734	M3739	V3740	T3743	T3758	I3763	L3778	K3784	V3787	L3793									
ARG	HIS	TYR	CYS	LEU	VAL	GLN	ARG	SER	GLN	TRP	HIS	LYS	LEU	LEU	LYS	GLN	ARG	ASP	ASP	ASP	GLY	GLU	E3710	V3711	Q3727	Q3728	R3730	L3731	H3732	H3733	R3734	M3739	V3740	T3743	A3649	E3650	P3651	P3652	E3653	E3654	D3655	E3656	T3658	R3659					
SER	ASN	ILE	HIS	LEU	VAL	GLN	GLY	ASP	PRO	GLN	MET	ALA	LEU	LEU	TYR	LYS	ARG	LEU	PRO	ASN	ARG	THR	ASP	GLU	GLY	THR	VAL	VAL	ARG	LEU	ASP	ILE	ALA	ASN	ALA	ASN	ASN	VAL	SER	ARG	VAL	GLY	ARG						
LYS	MET	LYS	ARG	LEU	PHE	GLY	ASP	ARG	TYR	SER	GLN	THR	SER	LEU	LEU	LYS	ARG	LEU	PRO	ASN	ARG	THR	ASP	GLY	GLN	ASP	GLY	ILE	ALA	LYS	THR	THR	THR	GLU	GLY	GLY	VAL	VAL	ASP	GLN	ILE	ARG							
GLU	ALA	GLU	GLU	LEU	PHE	GLY	ASP	ARG	MET	VAL	VAL	PHE	ILE	ALA	GLU	TYR	TRP	ALA	ALA	GLY	ASP	GLY	GLN	ASP	PRO	GLY	GLN	GLY	ILE	LYS	THR	THR	LEU	GLU	ALA	ALA	VAL	VAL	ASP	GLN	ILE	LYS							
H3178	N3179	I3180	N3185	T3186	K3187	S3188	S3189	R3190	R3191	R3192	A3193	A3194	P3198	T3199	T3200	N3201	V3202	L3203	D3204	C3205	I3208	L3211	M3215	V3219	E3220	S3224	G3225	I3226	R3227	Y3228	T3229	Q3230	H3233	V3234	M3235	E3236	V3237	P3240	M3241	L3242	Y3245	M3246	S3247	R3248	W3249	K3250	E3251	N3257	
GLN	PRO	K3088	G3089	V3090	L3102	P3103	M3104	L3108	L3112	Q3116	E3119	D3120	L3014	R3016	D3025	I3029	L3033	L3036	L3134	T3135	S3136	L3137	V3138	A3139	L3140	V3147	V3148	E3149	R3152	S3153	A3154	L3155	G3156	L3159	F3162	A3163	G3164	K3076	Q3077	G3078	Q3079	F3080	T3081	HIS	THR	ARG	ASN		
L2837	A2841	E2842	M2843	M2844	H2849	L2860	E2861	G2865	G2866	N2867	H2868	L2871	Y2874	D2875	T2876	L2877	K2882	R2886	D2891	L2892	L2893	K2894	R2905	G2906	D2909	L2910	E2911	L2912	D2913	T2914	P2915	H2937	I2940	L2941	D2944	G2945	G2946	S2947	R2948	G2949	K2950	G2951	E2952	H2953					
S2750	V2753	Q2754	P2755	L2756	M2757	K2758	P2759	V2760	K2761	L2762	L2763	S2764	E2765	K2768	L2779	M2782	L2783	A2784	V2785	G2786	R2787	R2788	R2791	D2796	S2797	M2798	N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	GLN	VAL	SER	VAL	ASP	ALA	ALA	HIS	G2820	R2824	V2831	T2832	L2833	
L2610	R2616	C2617	P2624	L2640	S2641	L2644	O2648	S2653	L2661	L2666	L2676	N2684	Y2685	M2688	M2689	E2690	K2691	Q2692	S2693	S2697	E2698	V2706	N2710	P2714	L2717	E2718	Y2719	F2720	N2721	N2722	L2723	Y2724	A2725	E2726	D2735	K2736	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749						



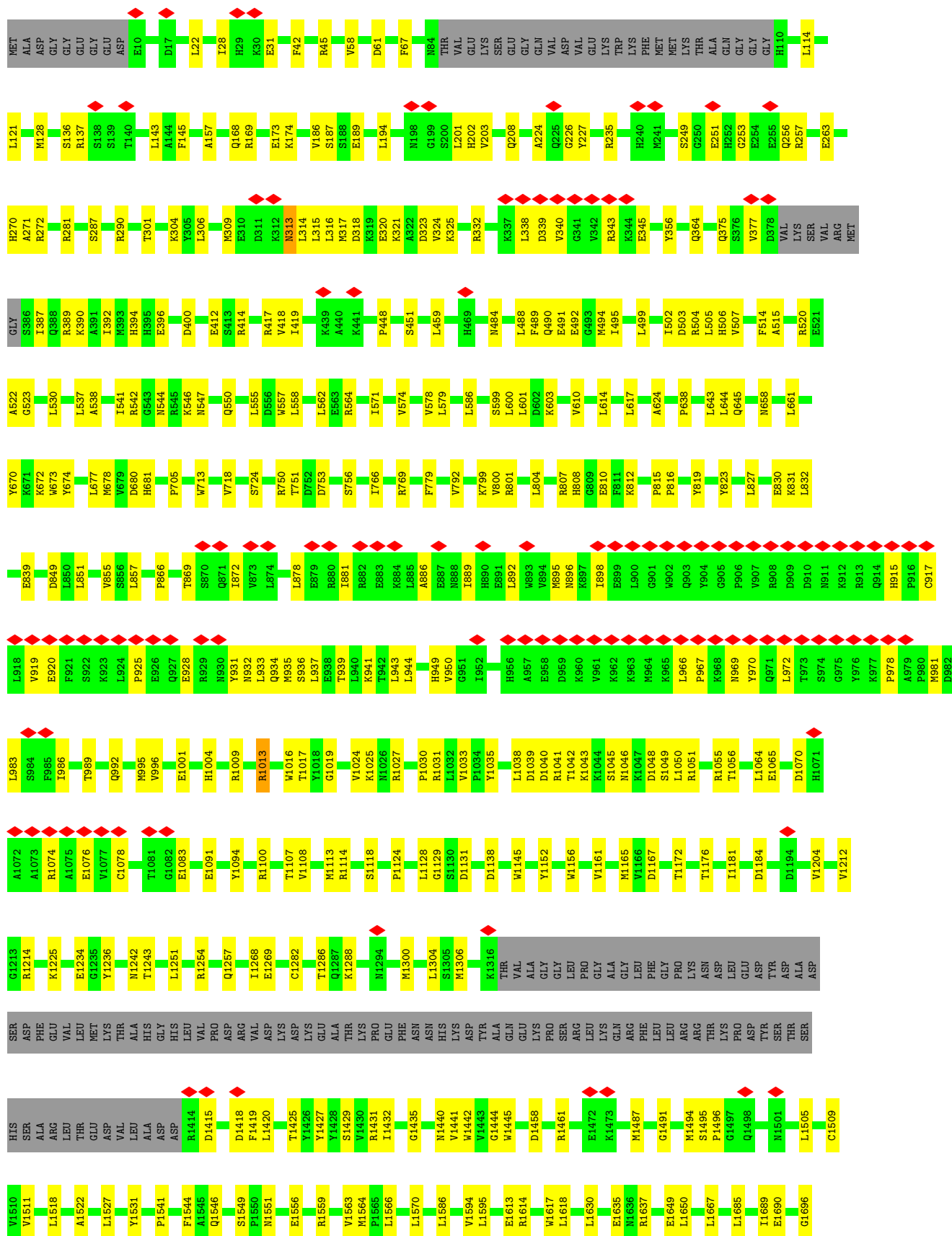


Tyr	Val	His	E3271	K3187	L3102	F2989	M2843	M2757	M2442	P2333	N2177	Tyr
Ser	Ala	Leu	H3272	S3188	L3103	S2992	M2844	K2758	K2465	R2336	V2178	Leu
Met	Val	Lys	M3273	S3189	M3104	S2992	H2849	P2769	K2465	G2337	G2180	Lys
Gln	Phe	Ala	N3274	R3190	L3108	H2995	H2849	K2761	V2480	E2338	G2181	Lys
Thr	Ile	Arg	E3277	E3191	I3112	H2996	L2860	L2762	Q2481	G2182	G2182	Gln
Leu	Tyr	Gly	G3278	A3193	I3112	S2997	E2861	L2763	D2482	E2183	G2183	Ala
Ile	Trp	Asp	N3279	A3194	I3116	N2998	E2765	L2661	F2483	L2344	E2184	Ala
Val	Ser	Met	G3280	P3198	Q3116	K3001	G2865	L2666	G2491	P2364	S2185	Lys
Ala	Ser	Thr	L3281	T3199	E3119	E3002	G2866	L2666	L2496	ASN	K2185	Pro
Leu	Asn	Glu	T3284	M3200	D3120	K3002	H2868	L2676	R2497	SER	E2186	Val
Arg	Phe	Ala	Y3285	V3201	L3121	G3012	L2871	L2676	A2498	SER	M2182	Ser
Leu	Leu	Glu	N3286	E3202	L3122	V3013	L2779	N2884	L2496	Lys	Y2202	Ser
Leu	Leu	Leu	N3287	D3203	L3123	L3015	M2782	L2783	L2520	Thr	L2206	Leu
Pro	Arg	Ile	L3288	V3204	L3124	V3016	L2784	L2783	A2532	Leu	S2207	Asp
Ile	Glu	Leu	C3205	C3205	D3125	R3016	W2785	W2785	F2535	Thr	R2208	Thr
Gly	Gln	Asp	G3289	I3208	D3126	D3025	G2786	G2786	F2535	Thr	K2212	Glu
Leu	Asn	Glu	I3290	I3208	Q3127	I3029	G2787	G2787	H2541	Glu	K2212	Glu
Asn	Phe	Thr	G3293	L3211	V3128	L3033	R2788	R2788	A2541	Leu	D2216	Thr
Val	Val	Thr	M3296	M3215	L3134	L3036	R2791	R2791	E2541	Thr	D2216	Thr
Leu	Gln	Leu	L3299	V3219	T3135	L3036	E2794	E2794	E2541	Thr	D2216	Thr
Ala	Asn	Ala	L3299	E3220	S3136	L3036	G2795	G2795	E2541	Thr	D2216	Thr
Gly	Glu	Arg	L3299	E3220	L3137	L3036	E2795	E2795	E2541	Thr	D2216	Thr
Asp	Ile	Asp	S3303	S3303	A3138	T3039	D2796	D2796	E2541	Thr	D2216	Thr
Gln	Asn	Leu	Q3304	E3220	Y3139	L3040	S2797	S2797	E2541	Thr	D2216	Thr
Leu	Asn	Tyr	P3305	S3224	L3140	L3040	M2798	M2798	E2541	Thr	D2216	Thr
Leu	Met	Ala	T3306	G3225	L3140	L3040	R2798	R2798	E2541	Thr	D2216	Thr
Leu	Ser	Phe	K3309	L3226	Y3147	L3043	R2798	R2798	E2541	Thr	D2216	Thr
Ala	Phe	Tyr	L3309	L3226	Y3147	L3043	R2798	R2798	E2541	Thr	D2216	Thr
Leu	Leu	Pro	V3310	R3227	V3148	M3046	E2799	E2799	E2541	Thr	D2216	Thr
Leu	Leu	Leu	V3311	L3228	E3149	M3046	E2799	E2799	E2541	Thr	D2216	Thr
Ala	Ile	Leu	P3312	T3229	L3152	L3050	E2799	E2799	E2541	Thr	D2216	Thr
Asn	Asp	Leu	Q3313	T3229	S3153	L3050	E2799	E2799	E2541	Thr	D2216	Thr
Asn	Asp	Leu	Q3313	T3229	S3153	L3050	E2799	E2799	E2541	Thr	D2216	Thr
Arg	Thr	Val	L3314	Q3233	A3154	L3054	E2799	E2799	E2541	Thr	D2216	Thr
Phe	Lys	Val	L3315	H3234	G3156	L3068	E2799	E2799	E2541	Thr	D2216	Thr
Ser	Ser	Val	L3316	M3235	G3156	L3068	E2799	E2799	E2541	Thr	D2216	Thr
Leu	Leu	Asp	T3317	E3236	L3159	L3068	E2799	E2799	E2541	Thr	D2216	Thr
Lys	Met	Tyr	K3318	V3237	F3162	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Asp	Ser	Asn	F3319	P3240	A3163	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Thr	Lys	Arg	L3320	M3241	G3164	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Ala	Ala	Ala	P3321	L3242	A3165	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Asp	Val	Trp	E3324	L3242	F3166	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Val	Val	Trp	K3325	Y3245	A3167	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Arg	Arg	Lys	L3326	M3246	F3167	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Asp	Asp	Glu	K3327	S3247	V3168	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Leu	Ile	Pro	K3328	R3248	A3169	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Arg	Arg	Asn	K3329	H3249	F3170	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Leu	Leu	Pro	A3330	W3250	L3171	L3070	E2799	E2799	E2541	Thr	D2216	Thr
Leu	Leu	Ala	A3331	E3251	D3176	L3081	E2799	E2799	E2541	Thr	D2216	Thr
Met	Met	Ala	T3332	N3256	N3179	HIS	E2799	E2799	E2541	Thr	D2216	Thr
Arg	Arg	Glu	V3333	N3257	I3180	THR	E2799	E2799	E2541	Thr	D2216	Thr
Lys	Lys	Leu	V3334	P3258	N3185	ARG	E2799	E2799	E2541	Thr	D2216	Thr
Gly	Gly	Leu	S3335	E3259	T3186	ASN	E2799	E2799	E2541	Thr	D2216	Thr
Arg	Arg	Met	E3336	R3260	L3268	PRO	E2799	E2799	E2541	Thr	D2216	Thr
			E3337	L3268								



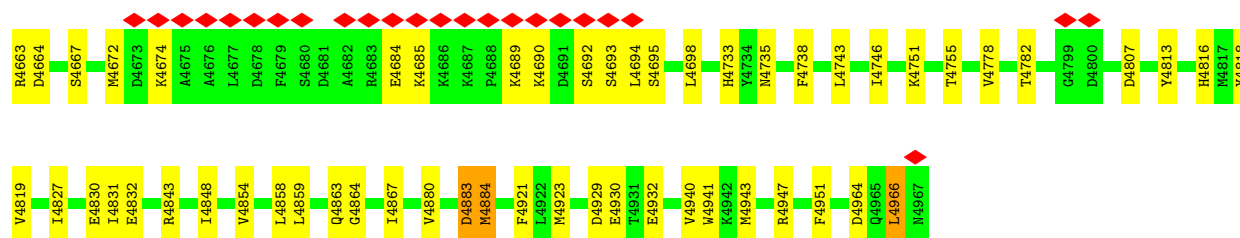
- Molecule 1: Ryanodine receptor 2





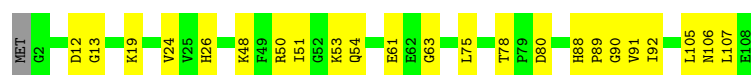
D3176	N3179	I3180	N3185	T3186	K3187	S3188	S3189	K3190	E3191	R3192	A3193	K3194	P3198	T3199	N3200	V3201	E3202	D3203	V3204	C3205	I3208	L3211	K3215	V3219	E3220	S3224	G3225	I3226	K3227	Y3228	T3229	Q3230	H3233	V3234	K3235	E3236	V3237	P3240	K3241	L3242	Y3245	K3246	S3247	K3248	K3249	K3250	E3251																
ARG	ASN	GLN	PRO	K3088	L3102	P3103	M3104	L3108	T3112	Q3116	E3119	D3120	L3121	L3122	L3123	E3124	D3125	V3126	Q3127	V3128	L3134	T3135	S3136	L3137	Y3138	A3139	L3140	S3145	T3146	Y3147	V3148	E3149	R3152	S3153	A3154	L3155	G3156	L3159	F3162	A3163	G3164	A3165	F3166	F3167	V3168	A3169	F3170	L3171															
R2979	P2989	S2992	H2995	A2996	S2997	N2998	K3001	E3002	G3012	V3013	L3014	V3015	R3016	D3025	I3029	L3033	L3036	T3039	L3040	D3041	A3042	R3043	M3046	L3050	E3051	S3052	V3053	K3054	R3058	L3068	S3069	K3070	T3071	M3072	E3073	N3074	L3075	G3078	Q3079	F3080	T3081	HIS	THR																				
A2841	E2842	M2843	N2844	H2849	L2860	E2861	G2865	G2866	N2867	H2868	L2871	Y2874	D2875	T2876	L2877	K2882	R2886	L2893	K2894	R2905	G2906	D2909	L2910	E2911	D2913	T2914	P2915	H2937	I2940	L2941	D2944	G2945	G2946	S2947	R2948	G2949	K2950	G2951	E2952	H2953	Q2958	F2969																					
M2757	K2758	P2759	Y2760	K2761	L2762	L2763	L2764	E2765	K2768	L2779	M2782	L2783	A2784	W2785	G2786	W2787	R2788	R2791	E2794	G2795	D2796	S2797	M2798	N2802	THR	ARG	ILE	GLN	THR	SER	GLN	VAL	SER	ASP	ALA	ALA	HIS	G2820	R2824	A2825	I2826	D2827	V2831	T2832	L2833	L2837																	
L2644	S2653	L2661	L2666	L2676	N2684	L2685	N2688	M2689	E2690	K2691	Q2692	S2697	E2698	G2699	V2706	N2710	P2714	L2717	E2718	Y2719	F2720	L2721	N2722	K2723	E2726	D2735	K2736	N2739	Y2743	G2744	E2745	I2746	Y2747	S2748	D2749	S2750	K2751	Y2752	Q2753	Q2754	P2755	L2756																					
V2480	Q2481	D2482	F2483	G2491	L2496	R2497	A2498	L2520	A2532	F2535	H2541	A2542	I2545	L2549	S2556	I2569	E2570	L2580	R2581	S2583	M2584	M2585	L2588	L2589	R2590	R2591	L2592	V2593	V2596	L2599	M2605	P2606	L2610	R2616	C2617	P2624	L2640	S2641																									
ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLU	E2377	E2378	D2379	D2380	T2381	L2382	I2388	F2391	Y2392	I2396	R2401	E2405	H2406	H2407	H2410	K2413	G2414	E2415	A2416	I2417	R2418	R2424	S2425	L2426	G2434	V2435	I2438	S2437	A2439	F2440	Q2441	N2442	M2446	C2461	K2465																		
V2176	N2177	V2178	G2181	G2182	E2183	S2184	K2185	E2186	M2192	Y2202	K2053	K2054	S2055	Q2060	L2061	I2062	M2066	E2072	R2082	L2087	Q2090	R2091	L2102	T2105	D2115	C2272	C2277	Q2278	M2279	L2280	W2290	N2291	R2297	R2303	Y2156	Q2157	L2161	M2162	W2172	E2173																							
TYR	LEU	LYS	GLN	ALA	GLU	LYS	PRO	VAL	GLU	SER	ASP	SER	K2053	K2054	S2055	Q2060	L2061	I2062	M2066	E2072	R2082	L2087	Q2090	R2091	L2102	T2105	D2115	C2272	C2277	Q2278	M2279	L2280	W2290	N2291	R2297	R2303	Y2156	Q2157	L2161	M2162	W2172	E2173																					
E1853	A1854	ALA	THR	PRO	GLU	GLU	GLU	GLU	GLU	GLU	LYS	LYS	LEU	SER	VAL	ASP	ASP	ALA	LYS	LEU	GLN	GLY	ALA	GLY	GLU	GLU	GLU	ALA	LYS	LYS	GLY	GLY	LYS	ARG	P1889	K1890	E1891	A1798	L1893	L1894	A1895	Q1895	M1896	K1897	L1898	F1816	V1902	Q1911	K1935	I1830	M1831	G1832	I1833	Q1940	N1939	Q1940	LEU	F1941	F1942	L1843	R1943	Q1844	N1945





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

Chain E: 78% 21%



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

Chain F: 78% 21%



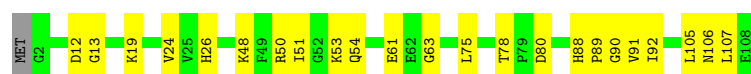
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 78% 21%



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

Chain H: 78% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113172	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	1.040	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.036	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: KVR, ATP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/34506	0.34	5/46608 (0.0%)
1	B	0.13	0/34506	0.34	5/46608 (0.0%)
1	C	0.13	0/34506	0.34	5/46608 (0.0%)
1	D	0.13	0/34506	0.34	5/46608 (0.0%)
2	E	0.16	0/834	0.40	0/1123
2	F	0.16	0/834	0.40	0/1123
2	G	0.16	0/834	0.40	0/1123
2	H	0.16	0/834	0.40	0/1123
All	All	0.13	0/141360	0.34	20/190924 (0.0%)

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

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

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1960	ARG	CA-CB-CG	7.20	128.50	114.10
1	B	1960	ARG	CA-CB-CG	7.20	128.50	114.10
1	D	1960	ARG	CA-CB-CG	7.20	128.49	114.10
1	C	1960	ARG	CA-CB-CG	7.18	128.46	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1960	ARG	CG-CD-NE	-6.77	97.11	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3187	LYS	Peptide
1	B	3187	LYS	Peptide
1	C	3187	LYS	Peptide
1	D	3187	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33766	0	33444	617	0
1	B	33766	0	33444	603	0
1	C	33766	0	33444	603	0
1	D	33766	0	33444	606	0
2	E	818	0	821	12	0
2	F	818	0	821	12	0
2	G	818	0	821	12	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	9	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
5	A	23	0	0	3	0
5	B	23	0	0	0	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
All	All	138680	0	137156	2428	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 2428 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:931:TYR:HD2	4:A:5003:ATP:N6	0.96	1.44
1:A:931:TYR:CD2	4:A:5003:ATP:N6	1.86	1.41
4:A:5003:ATP:H5'1	5:A:5004:KVR:C19	1.97	0.95
1:C:3149:GLU:HA	1:C:3152:ARG:HG2	1.52	0.92
1:A:3149:GLU:HA	1:A:3152:ARG:HG2	1.52	0.91

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%)	4053 (96%)	140 (3%)	5 (0%)	48	80
1	B	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	48	80
1	C	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	48	80
1	D	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	48	80
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%)	16620 (97%)	572 (3%)	20 (0%)	49	80

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1495	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2915	PRO
1	A	4884	MET
1	B	1495	SER
1	B	2915	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%)	3699 (100%)	9 (0%)	87	92
1	B	3708/4358 (85%)	3699 (100%)	9 (0%)	87	92
1	C	3708/4358 (85%)	3699 (100%)	9 (0%)	87	92
1	D	3708/4358 (85%)	3699 (100%)	9 (0%)	87	92
2	E	88/89 (99%)	86 (98%)	2 (2%)	44	74
2	F	88/89 (99%)	86 (98%)	2 (2%)	44	74
2	G	88/89 (99%)	86 (98%)	2 (2%)	44	74
2	H	88/89 (99%)	86 (98%)	2 (2%)	44	74
All	All	15184/17788 (85%)	15140 (100%)	44 (0%)	84	91

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1960	ARG
1	D	1013	ARG
1	C	3180	ILE
1	C	3319	PHE
1	D	1960	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	202	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2937	HIS
1	D	3092	GLN
1	C	409	GLN
1	C	1743	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 16 ligands modelled in this entry, 4 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	C	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	A	5003	-	32,33,33	1.31	4 (12%)	48,52,52	1.86	10 (20%)
4	ATP	B	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	C	5002	-	32,33,33	0.28	0	48,52,52	0.40	0
5	KVR	D	5004	-	24,25,25	1.65	3 (12%)	31,34,34	2.07	5 (16%)
5	KVR	B	5004	-	24,25,25	1.63	3 (12%)	31,34,34	2.07	5 (16%)
5	KVR	A	5004	-	24,25,25	0.51	0	31,34,34	0.97	2 (6%)
4	ATP	D	5002	-	32,33,33	0.29	0	48,52,52	0.40	0
4	ATP	B	5002	-	32,33,33	0.28	0	48,52,52	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	KVR	C	5004	-	24,25,25	1.63	3 (12%)	31,34,34	2.07	5 (16%)
4	ATP	A	5002	-	32,33,33	0.28	0	48,52,52	0.40	0
4	ATP	D	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	C	5003	-	-	10/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	8/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	10/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/22/38/38	0/3/3/3
5	KVR	D	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	B	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	A	5004	-	-	8/10/20/20	0/2/3/3
4	ATP	D	5002	-	-	10/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	9/22/38/38	0/3/3/3
5	KVR	C	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	A	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	11/22/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5004	KVR	C06-S09	6.15	1.83	1.77
5	D	5004	KVR	C06-S09	6.15	1.83	1.77
5	C	5004	KVR	C06-S09	6.11	1.83	1.77
4	A	5003	ATP	C5-C4	4.38	1.46	1.39
5	D	5004	KVR	C13-N12	-2.66	1.45	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5004	KVR	C10-S09-C06	8.54	114.81	102.71
5	B	5004	KVR	C10-S09-C06	8.52	114.78	102.71
5	D	5004	KVR	C10-S09-C06	8.51	114.77	102.71
4	A	5003	ATP	C5-C4-N3	-6.31	118.03	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5003	ATP	N3-C4-N9	5.25	136.10	127.17

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

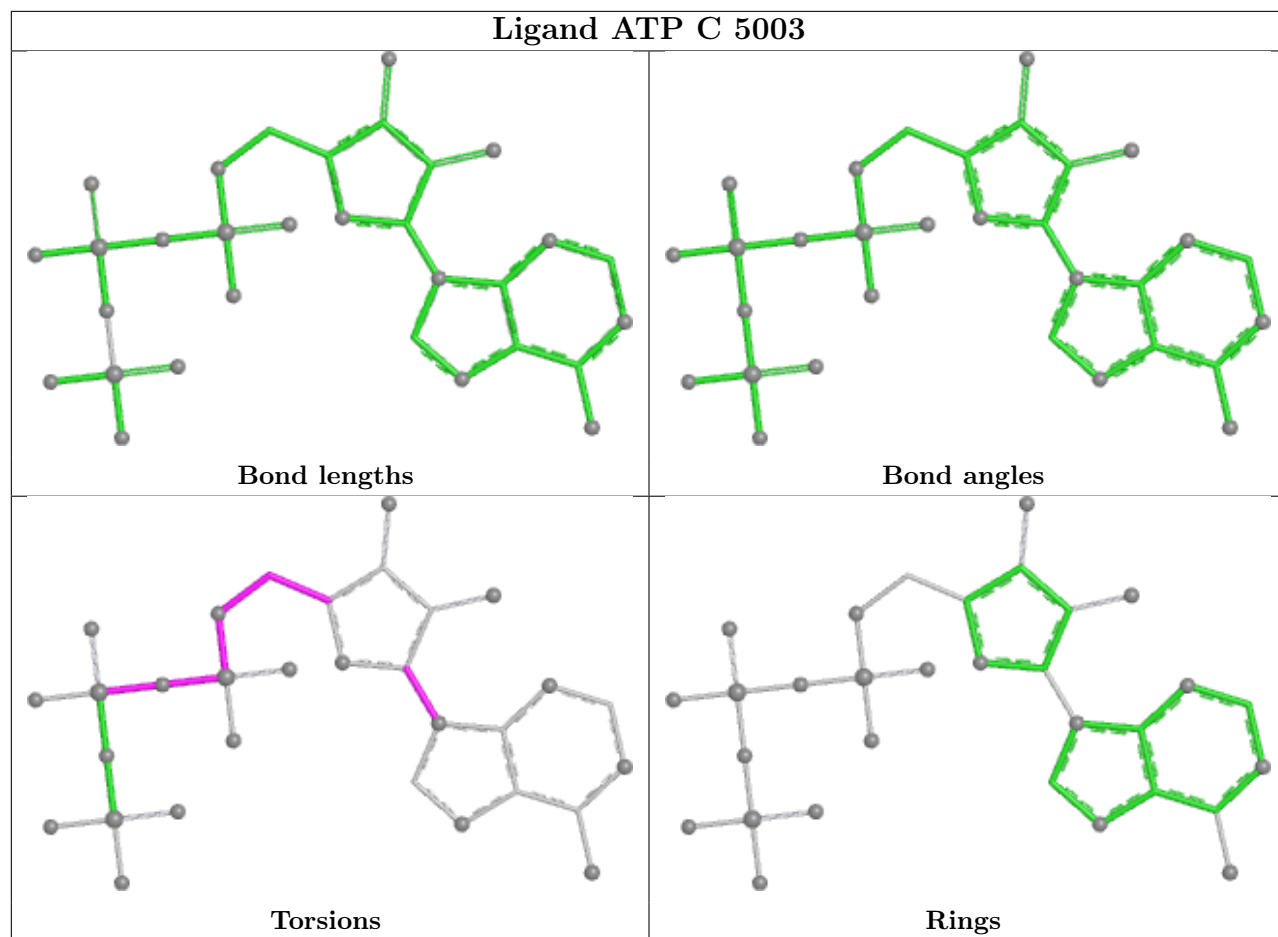
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5002	ATP	O4'-C4'-C5'-O5'
4	A	5002	ATP	C3'-C4'-C5'-O5'
4	A	5003	ATP	C5'-O5'-PA-O1A

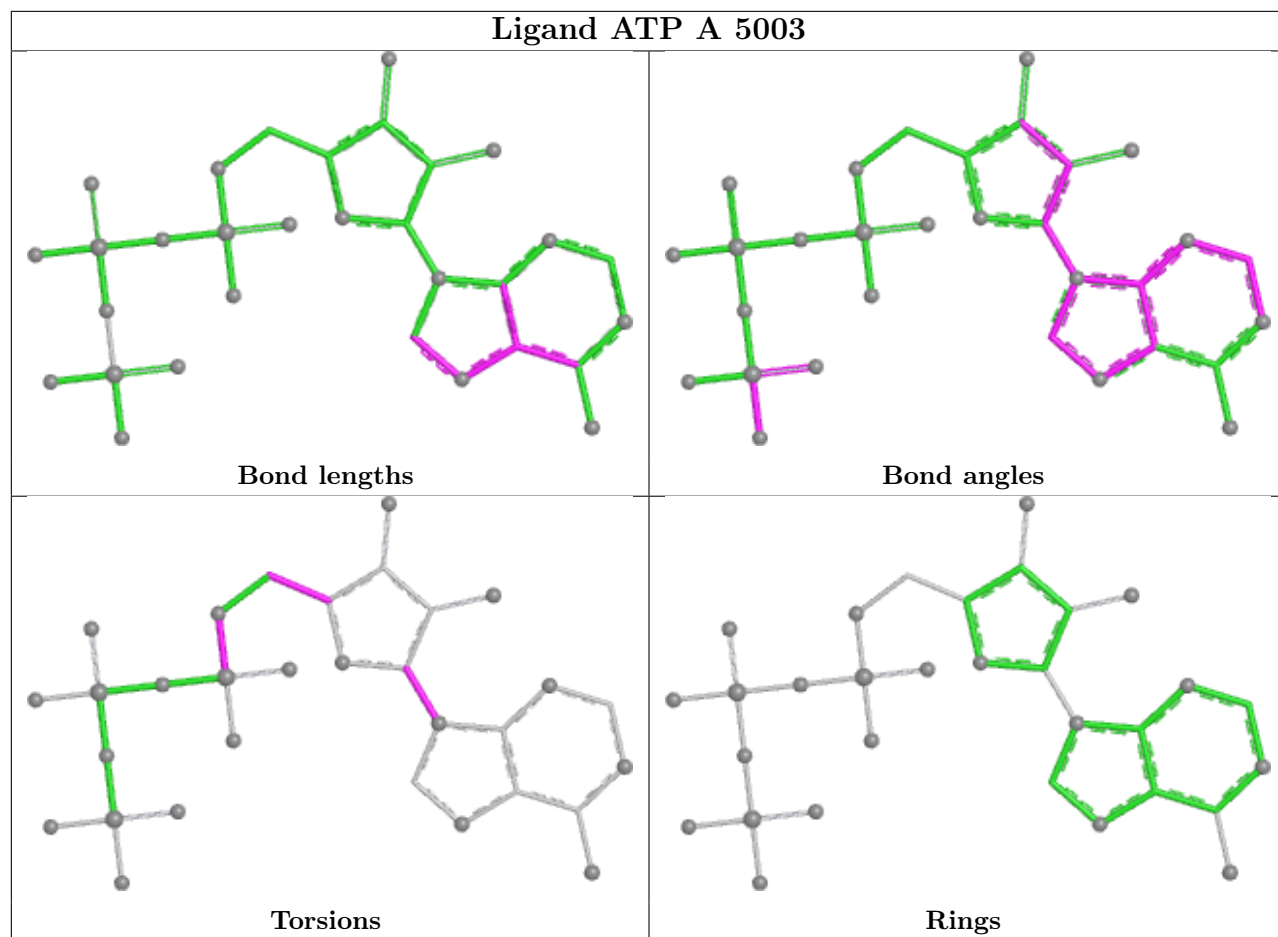
There are no ring outliers.

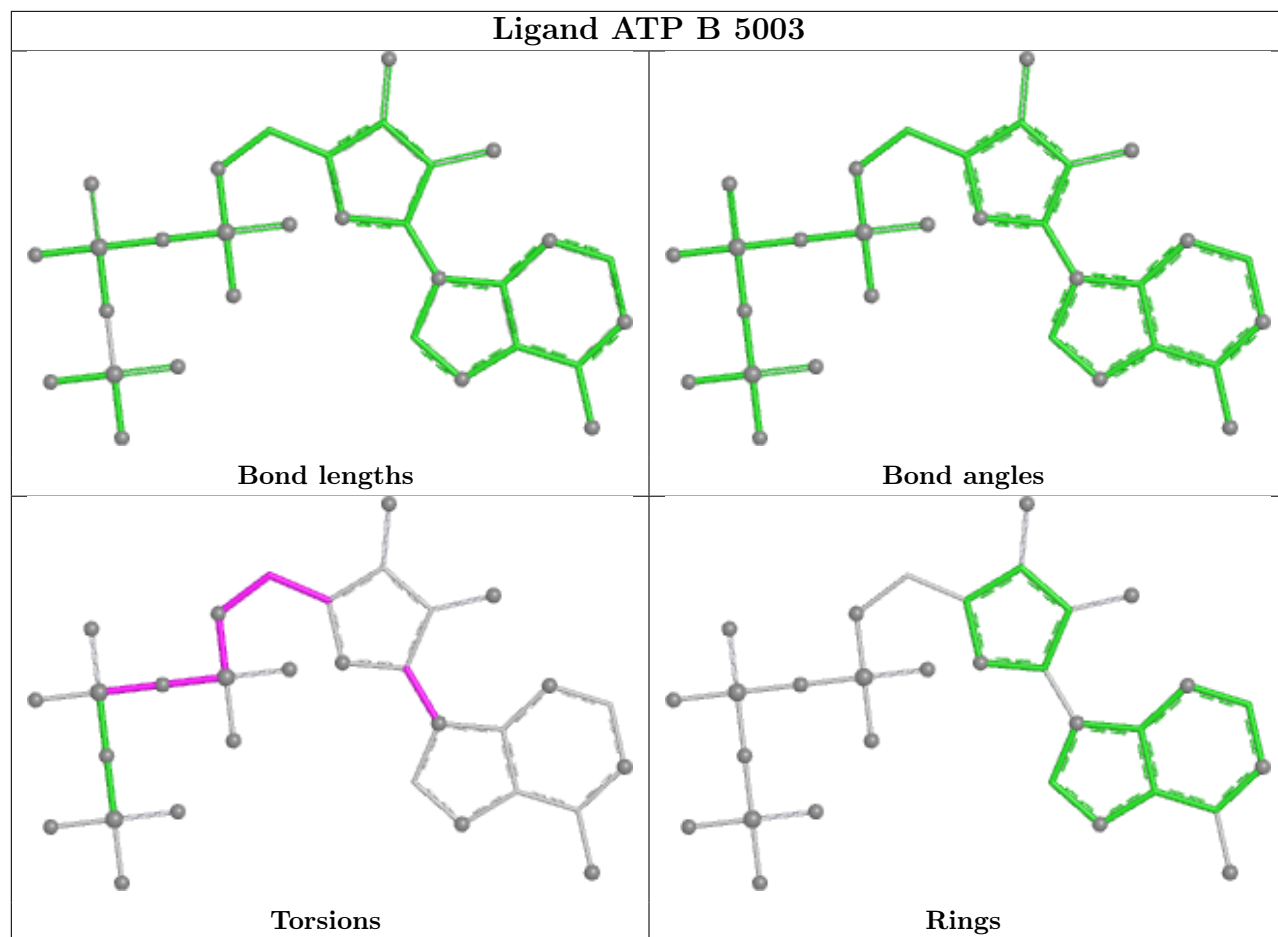
2 monomers are involved in 9 short contacts:

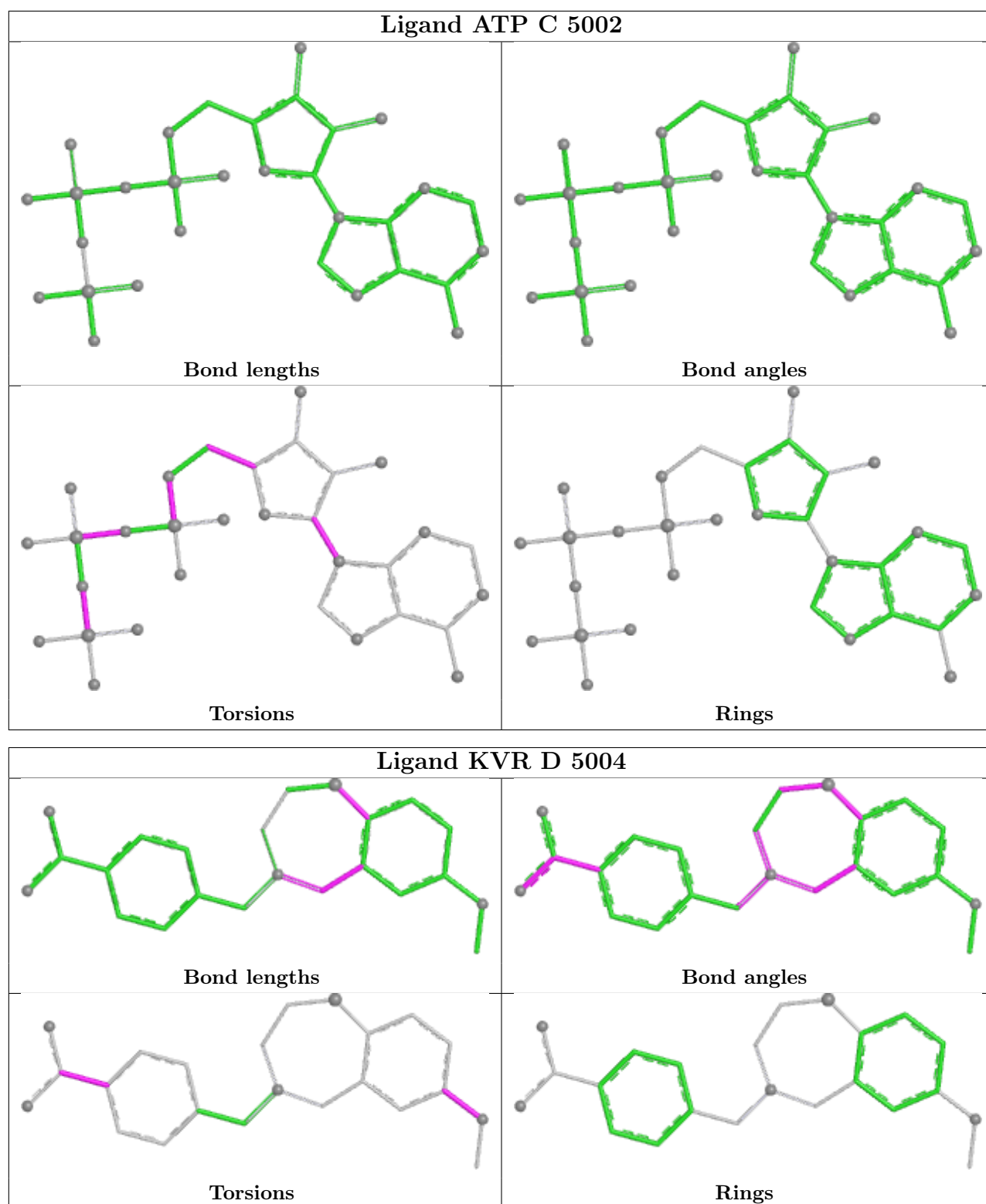
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5003	ATP	9	0
5	A	5004	KVR	3	0

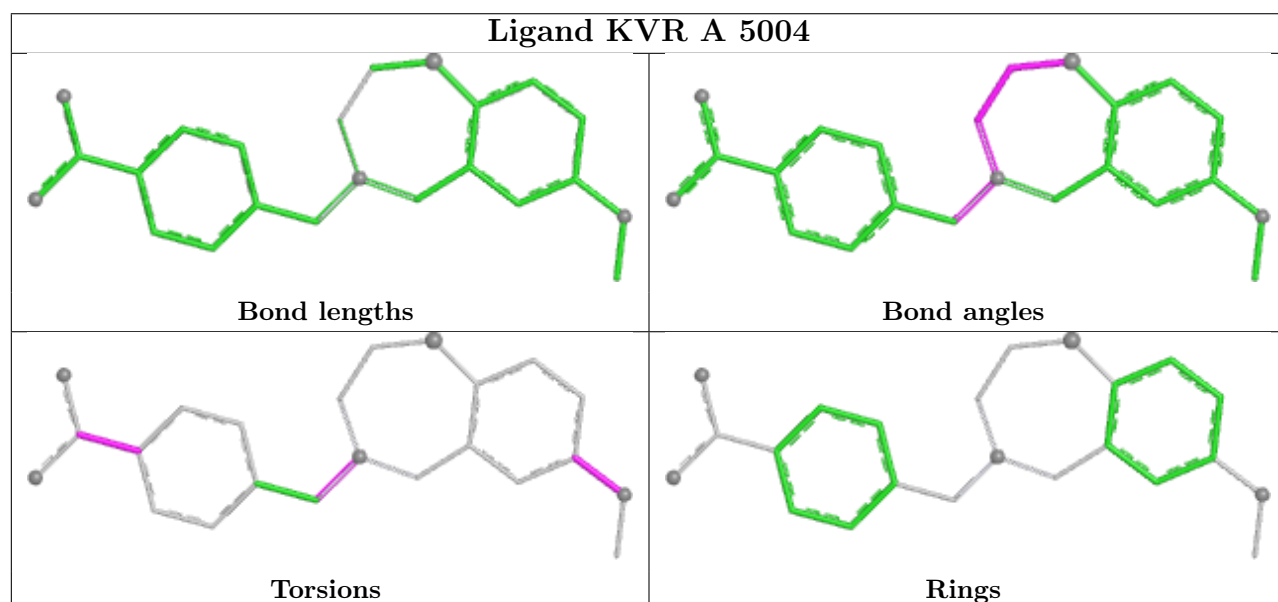
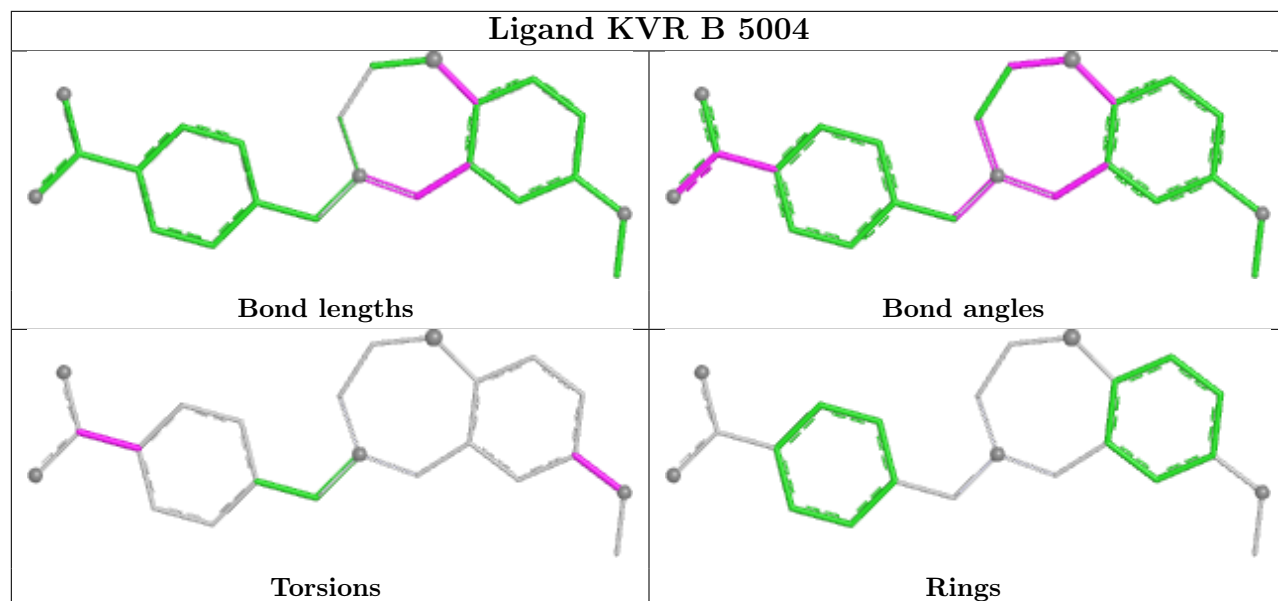
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

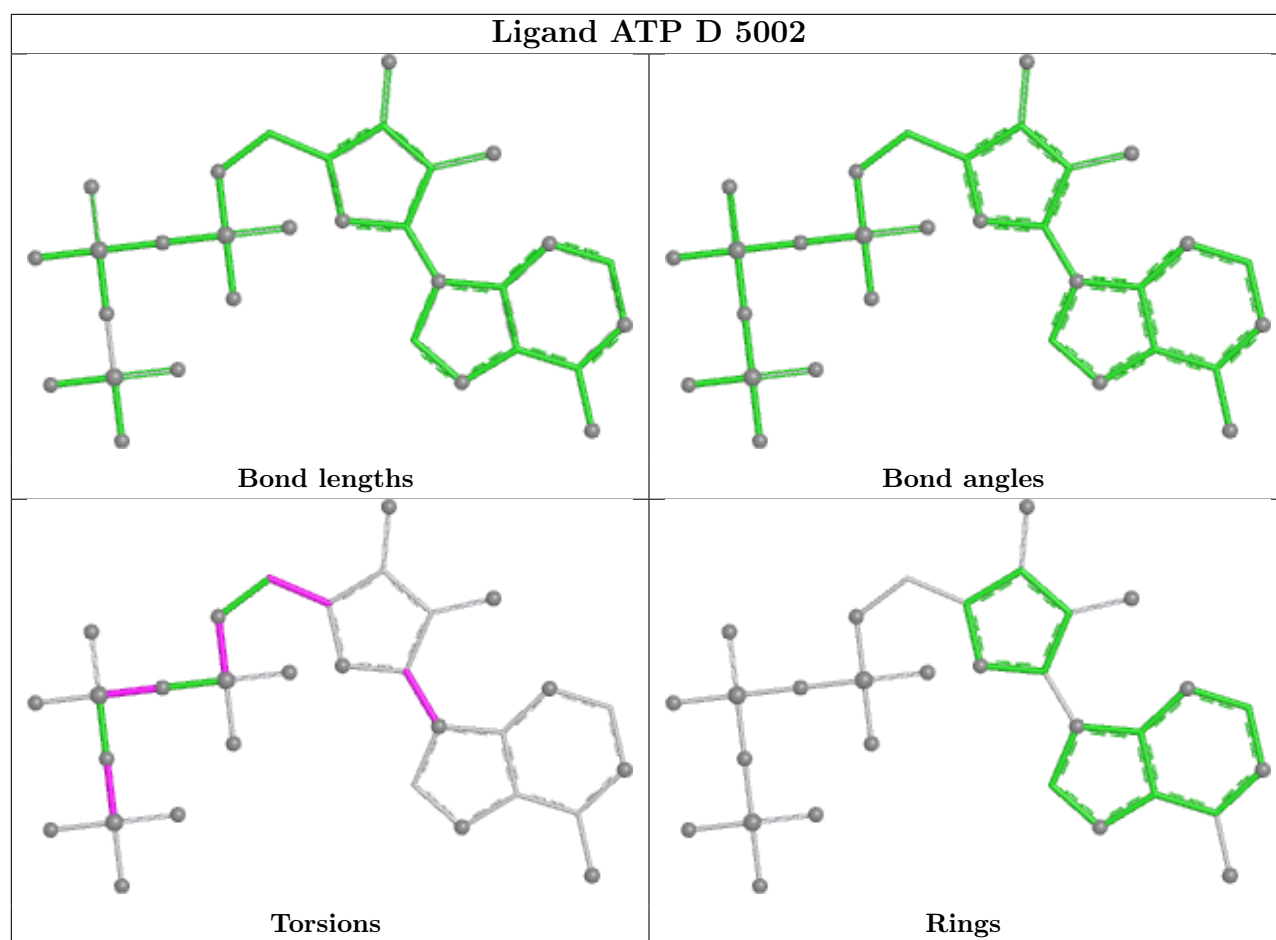


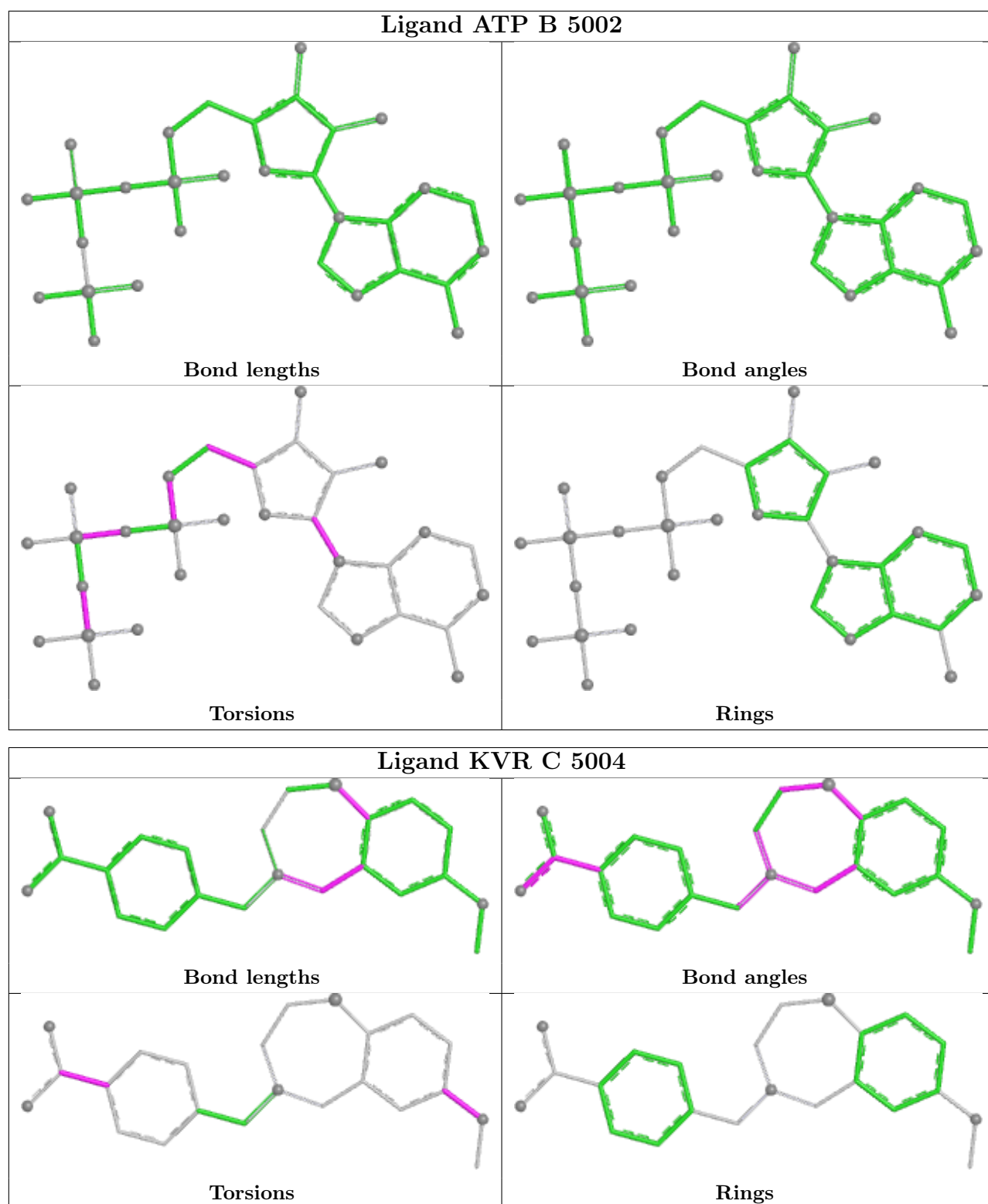


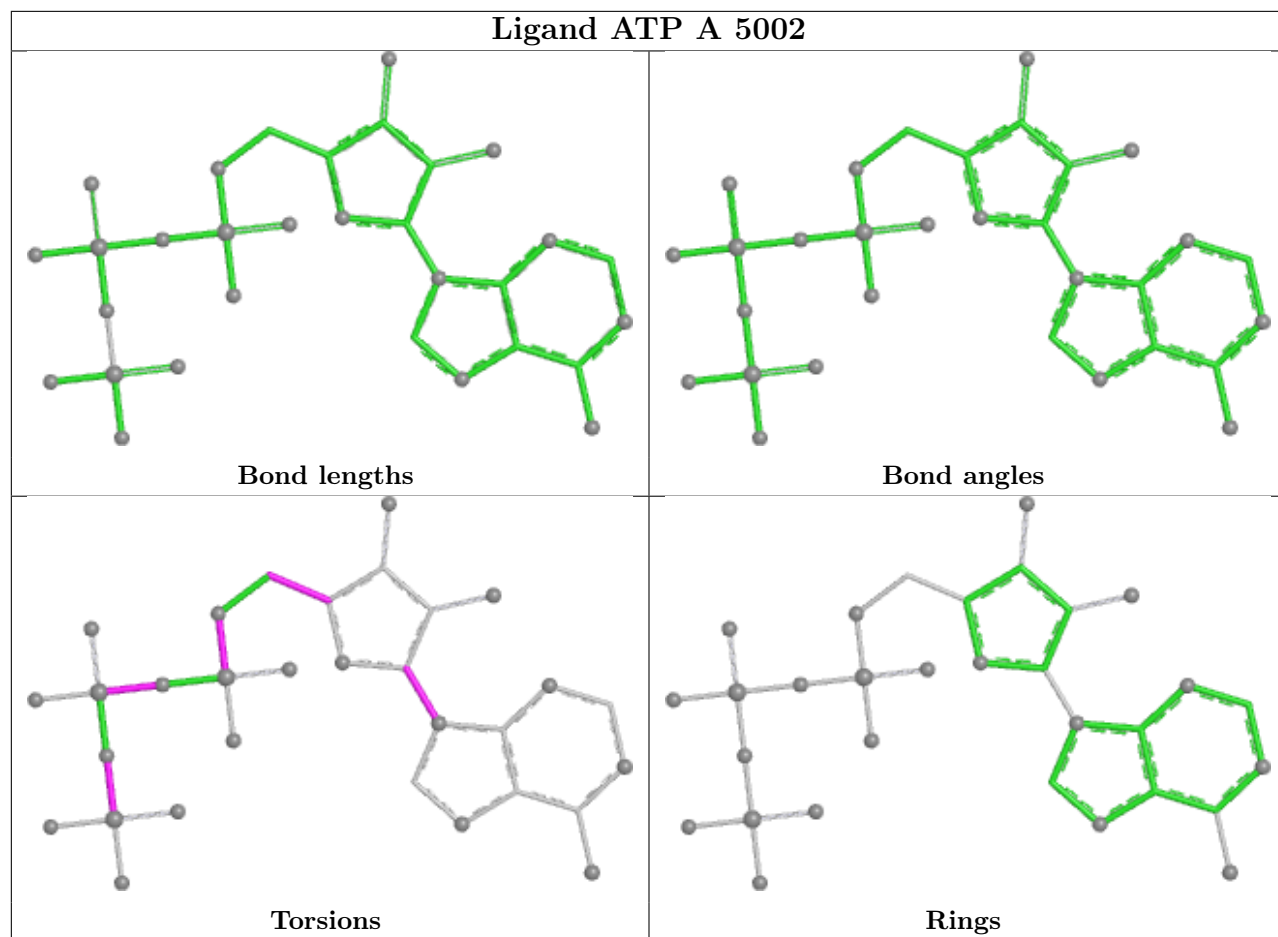


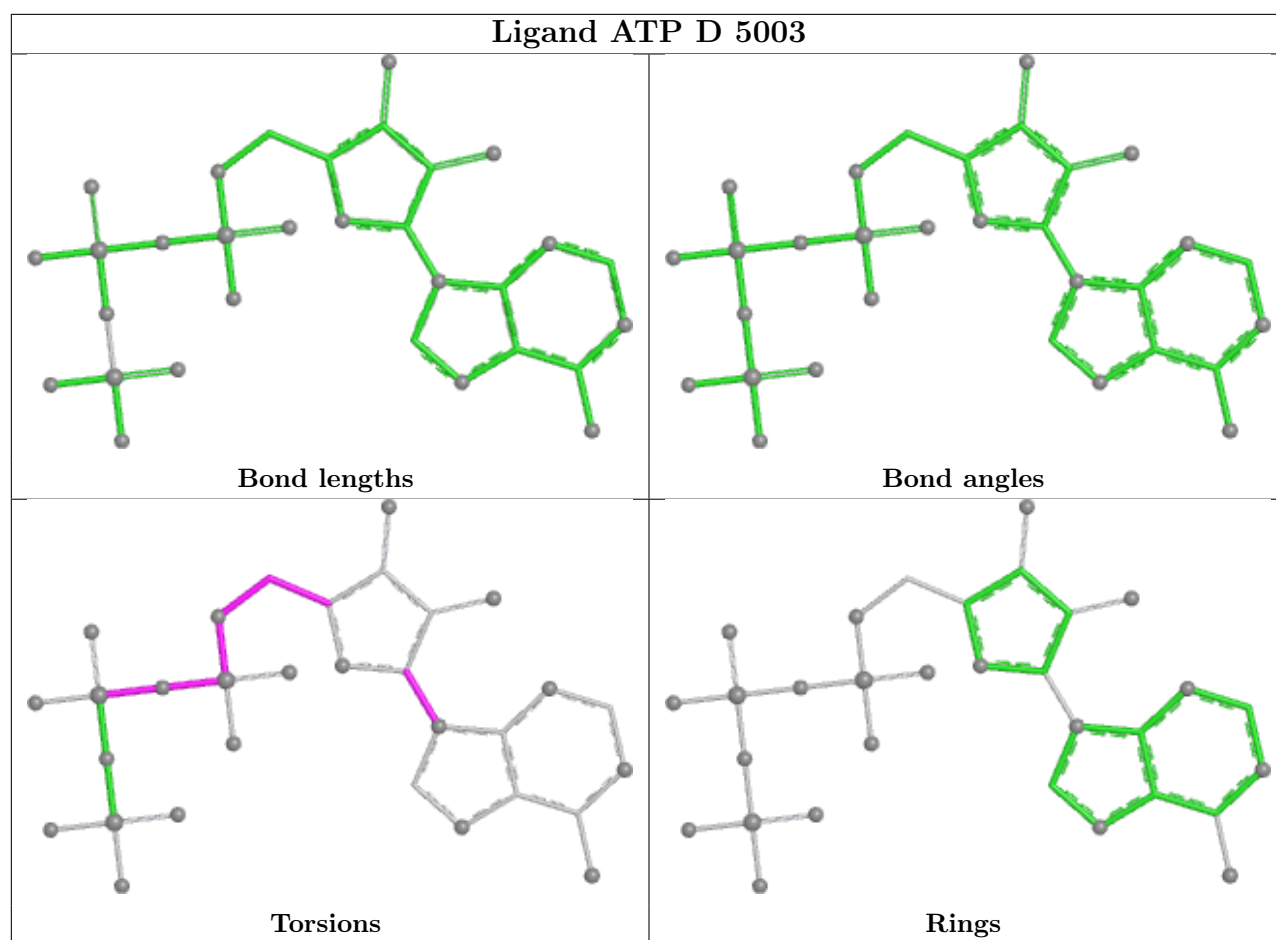












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

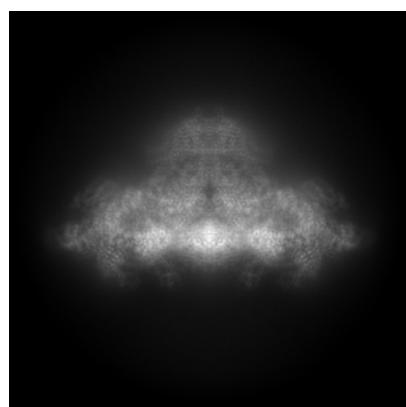
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26412. These allow visual inspection of the internal detail of the map and identification of artifacts.

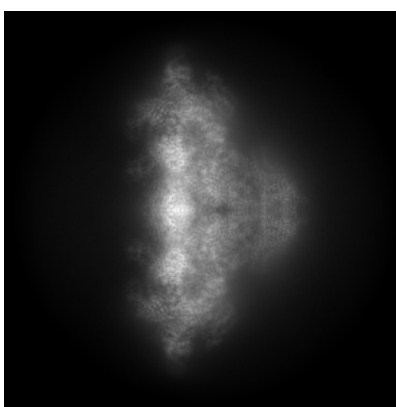
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

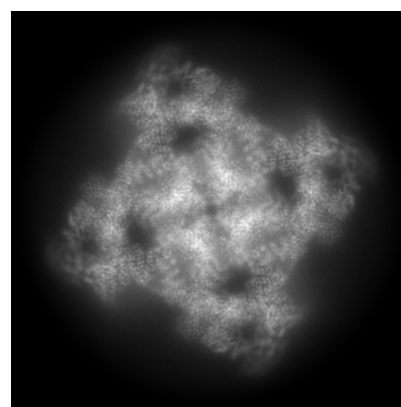
6.1.1 Primary map



X



Y

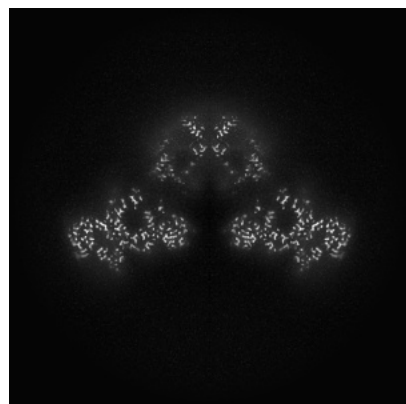


Z

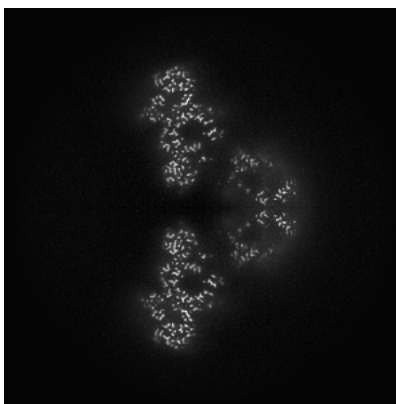
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

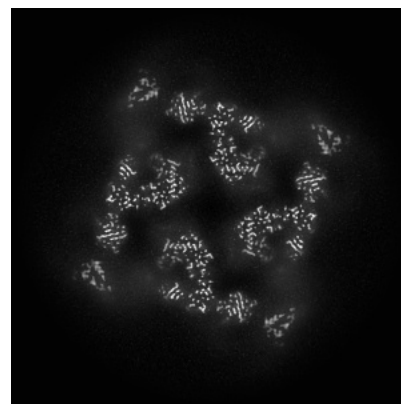
6.2.1 Primary map



X Index: 256



Y Index: 256

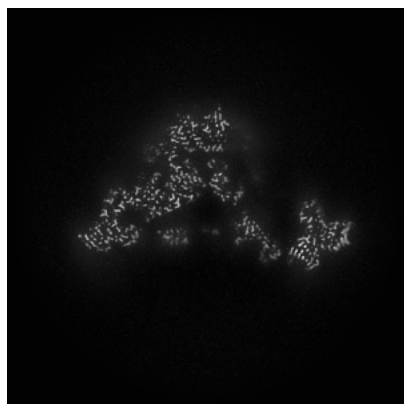


Z Index: 256

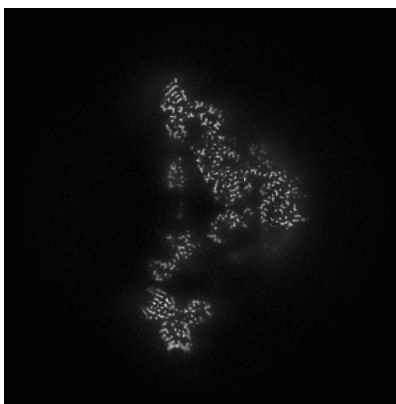
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

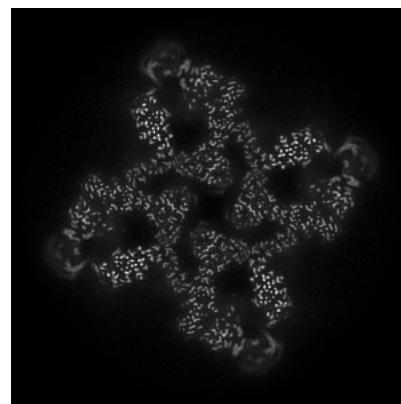
6.3.1 Primary map



X Index: 237



Y Index: 238

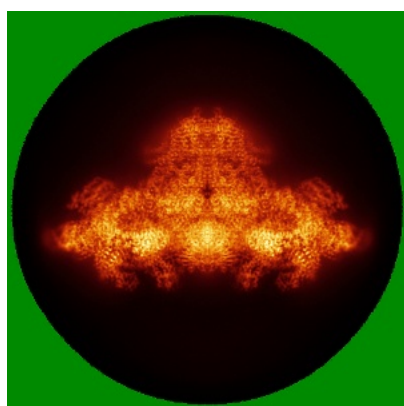


Z Index: 223

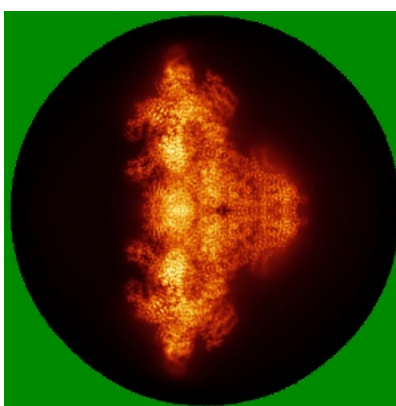
The images above show the largest variance slices of the map in three orthogonal directions.

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

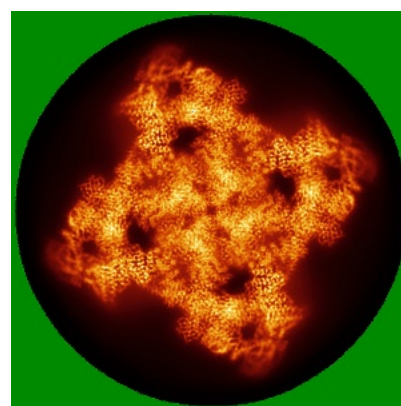
6.4.1 Primary map



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

This section was not generated.

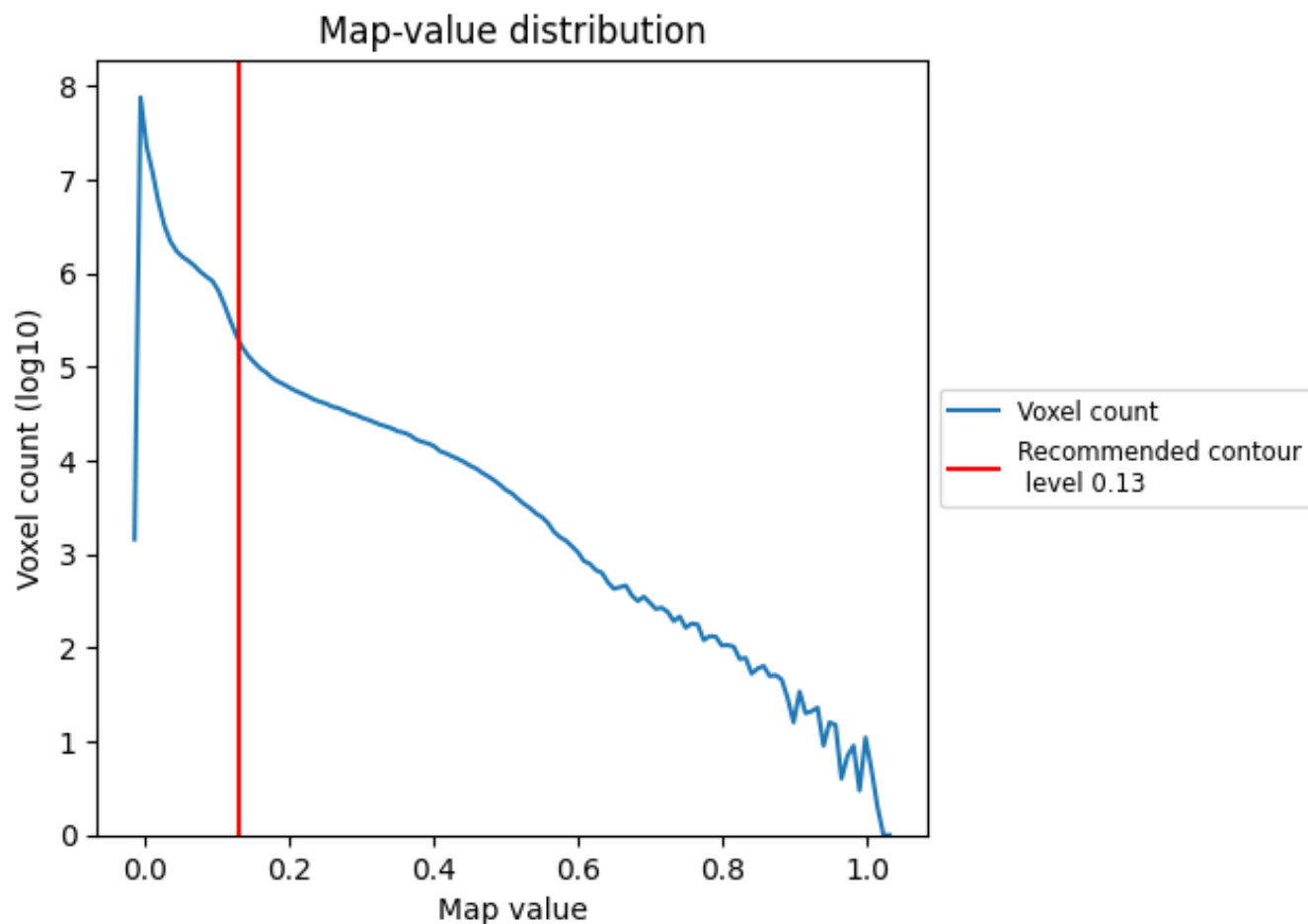
6.6 Mask visualisation

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

7 Map analysis [i](#)

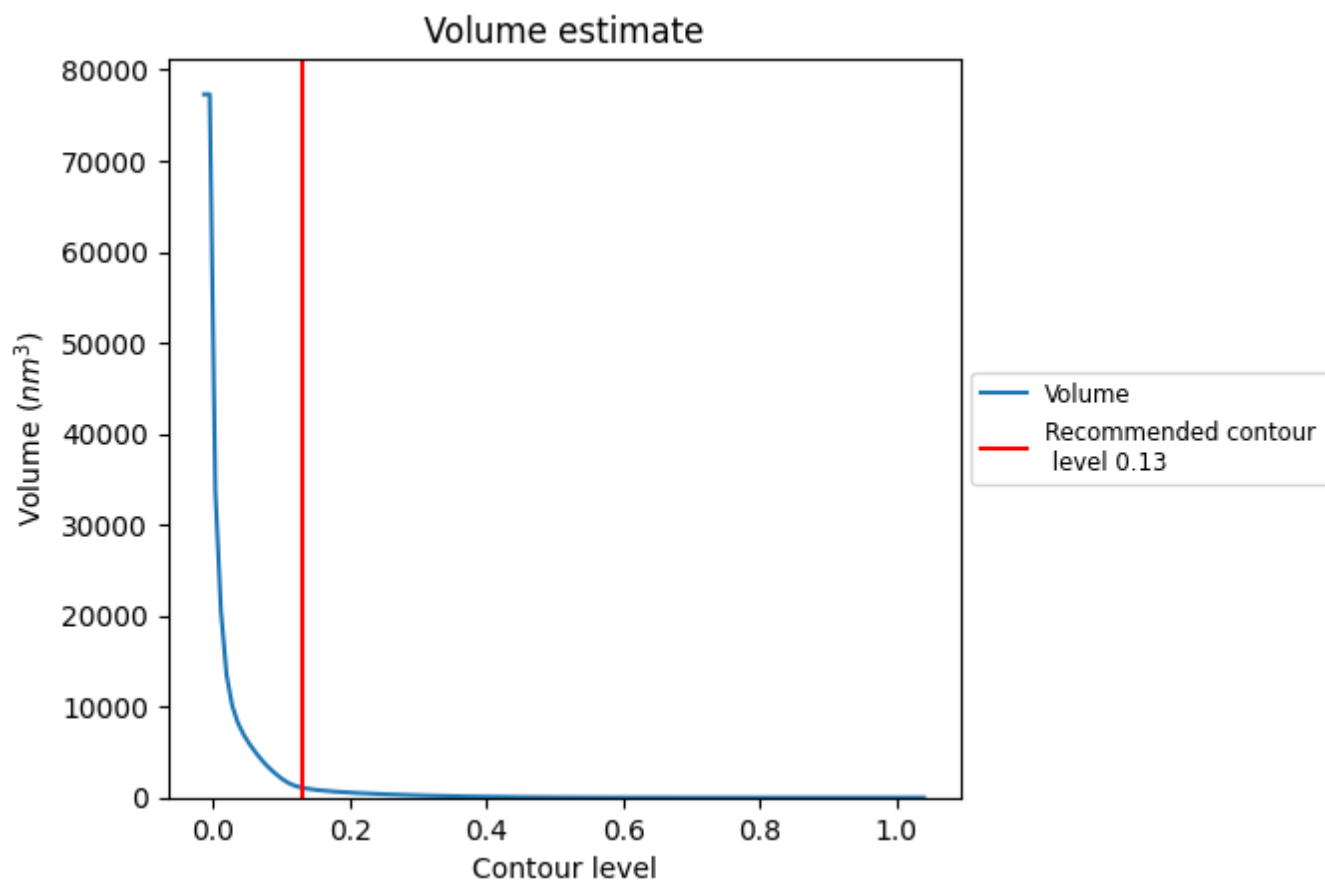
This section contains the results of statistical analysis of the map.

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.

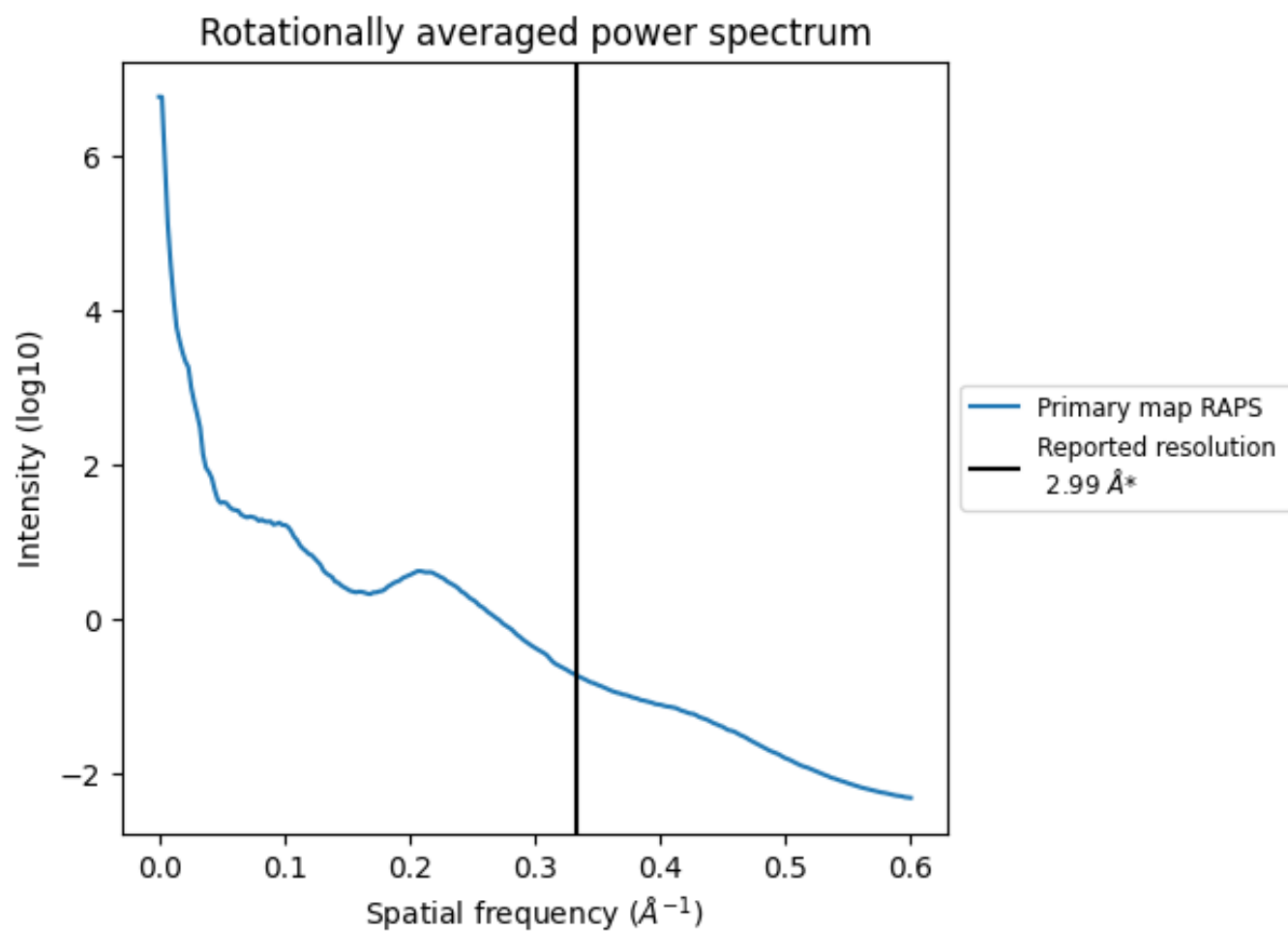
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1081 nm³; this corresponds to an approximate mass of 977 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 0.334 Å⁻¹

8 Fourier-Shell correlation

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

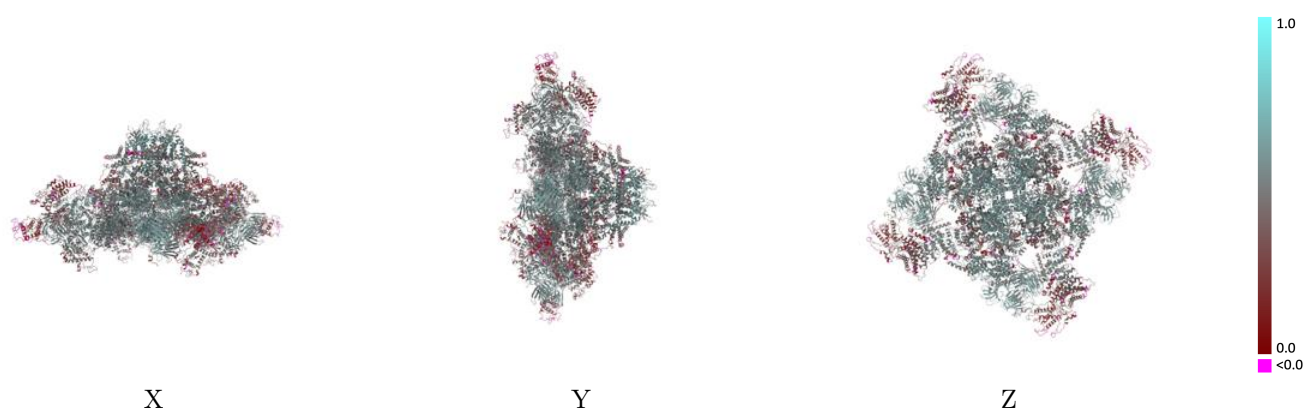
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26412 and PDB model 7UA1. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

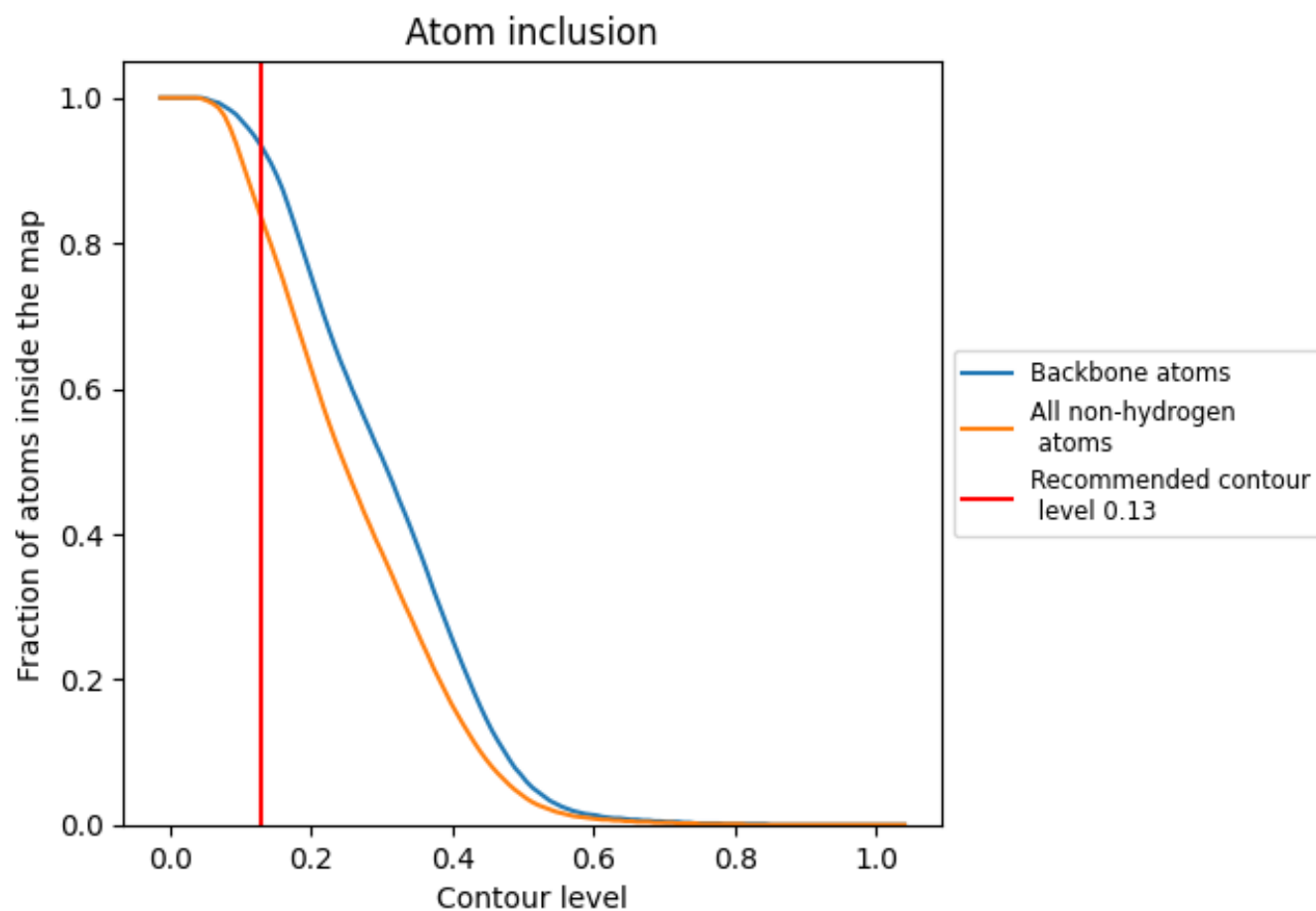


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 83% 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	0.8320	0.4650
A	0.8310	0.4660
B	0.8280	0.4580
C	0.8300	0.4630
D	0.8310	0.4660
E	0.9300	0.5600
F	0.9240	0.5540
G	0.9280	0.5570
H	0.9330	0.5720

1.0

0.0

<0.0