



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 06:28 AM UTC

PDB ID : 8UXM / pdb_00008uxm
EMDB ID : EMD-42769
Title : Structure of PKA phosphorylated human RyR2-R420W in the open state in the presence of calcium and calmodulin
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.56 Å(reported)
Based on initial model : 7UA5

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

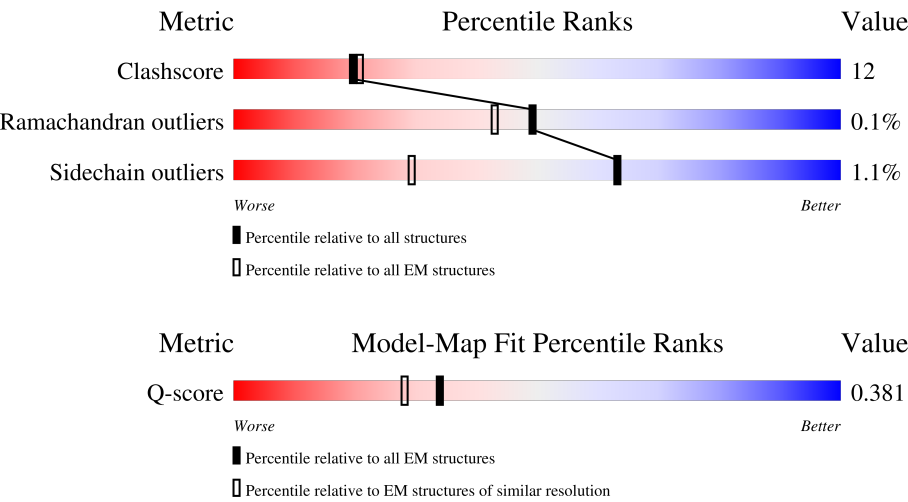
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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.



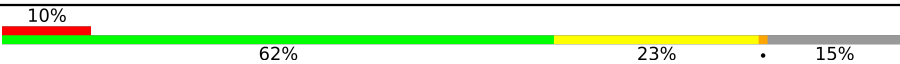
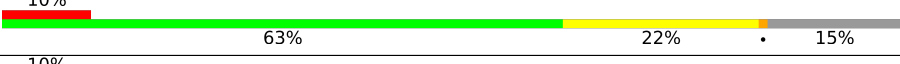
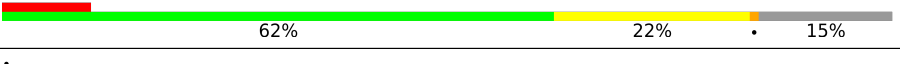
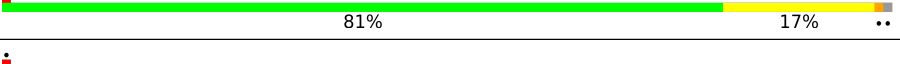
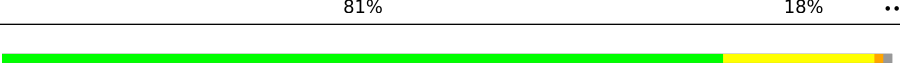
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12750 (3.06 - 4.06)

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	I	149	5% 50%42% ...
1	J	149	5% 54%37% ...
1	K	149	6% 54%38% ...
1	L	149	6% 54%38% ...

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Mol	Chain	Length	Quality of chain
2	A	4967	
2	B	4967	
2	C	4967	
2	D	4967	
3	E	108	
3	F	108	
3	G	108	
3	H	108	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 143464 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	J	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	L	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	K	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		

- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	B	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	C	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	D	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

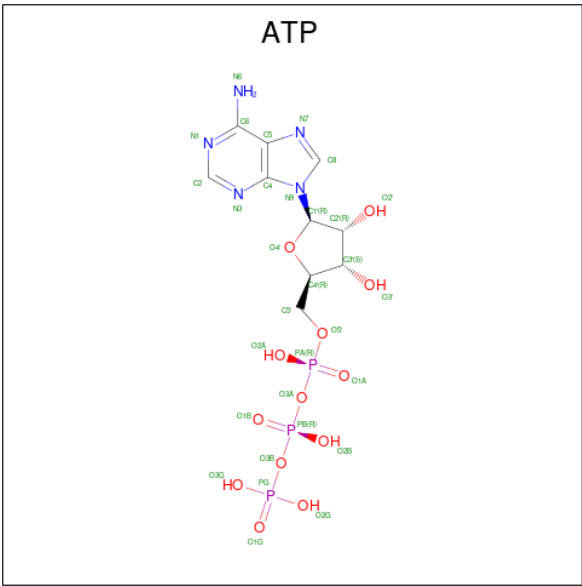
Mol	Chain	Residues	Atoms		AltConf
4	I	4	Total	Ca	0
			4	4	
4	A	1	Total	Ca	0
			1	1	
4	J	4	Total	Ca	0
			4	4	
4	L	4	Total	Ca	0
			4	4	
4	K	4	Total	Ca	0
			4	4	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃)

(labeled as "Ligand of Interest" by depositor).

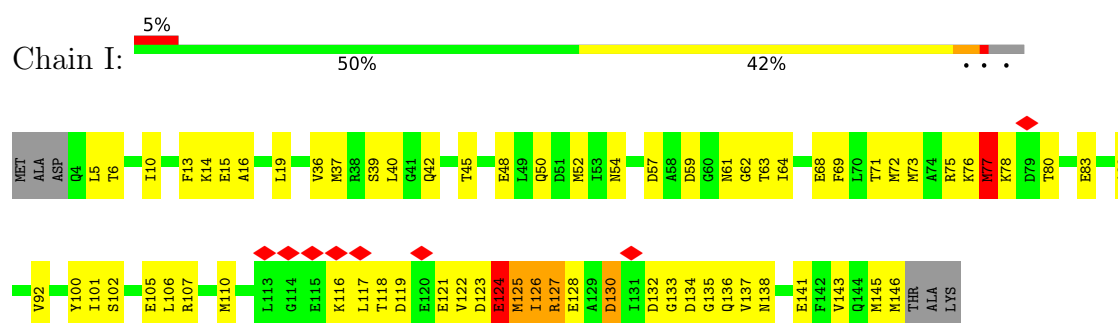


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10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

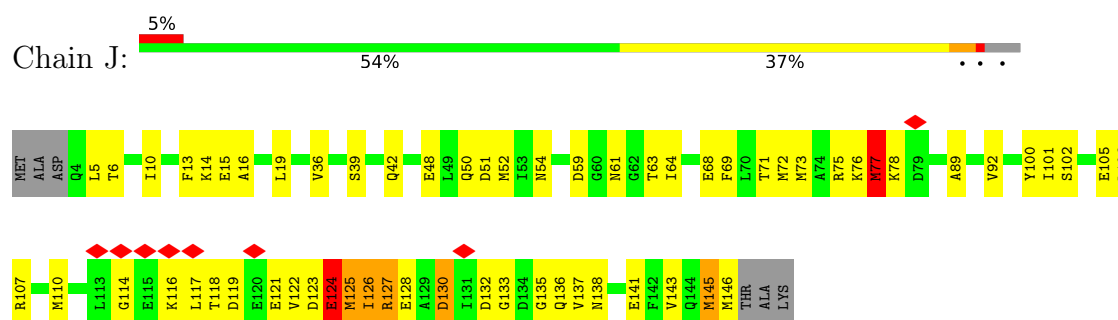
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

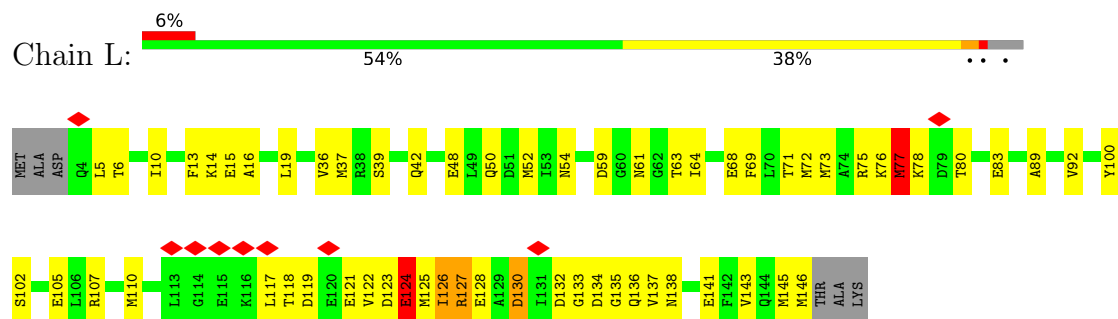
• Molecule 1: Calmodulin-1



• Molecule 1: Calmodulin-1

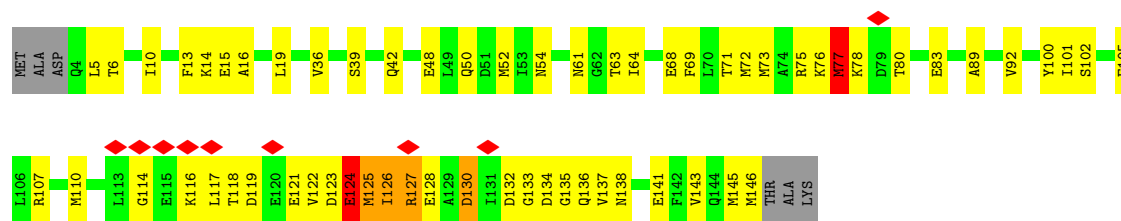


• Molecule 1: Calmodulin-1

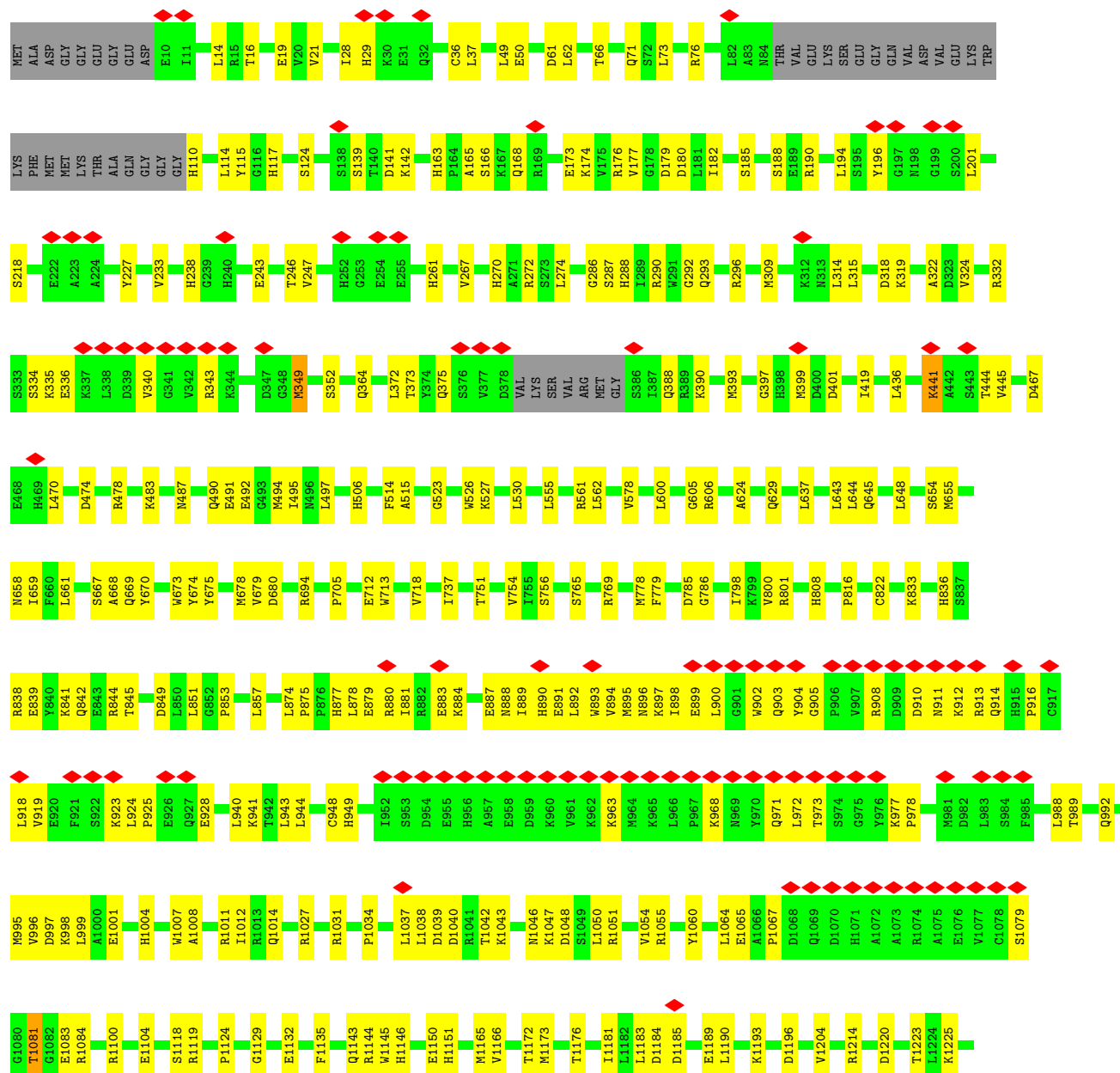


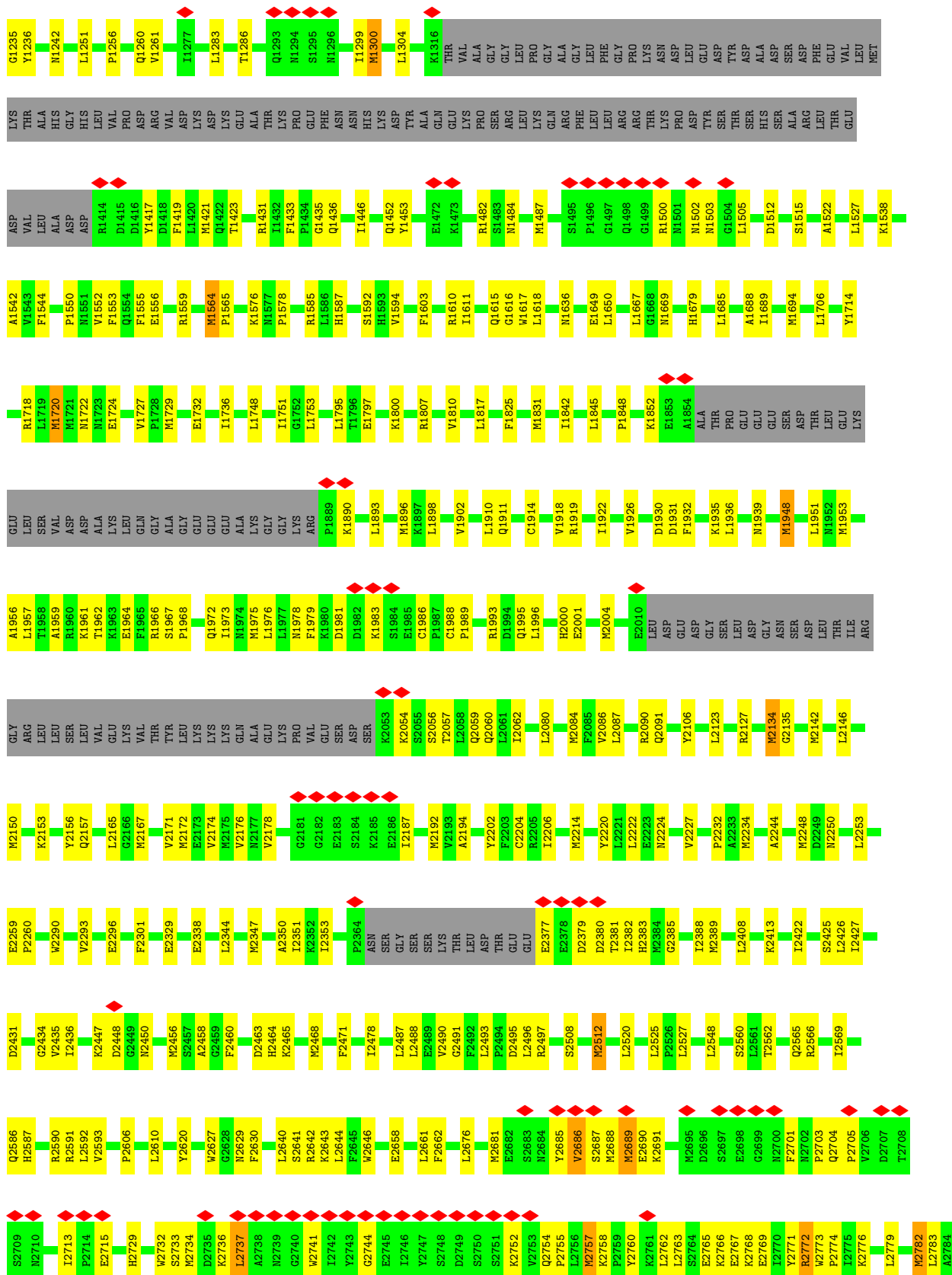
• Molecule 1: Calmodulin-1



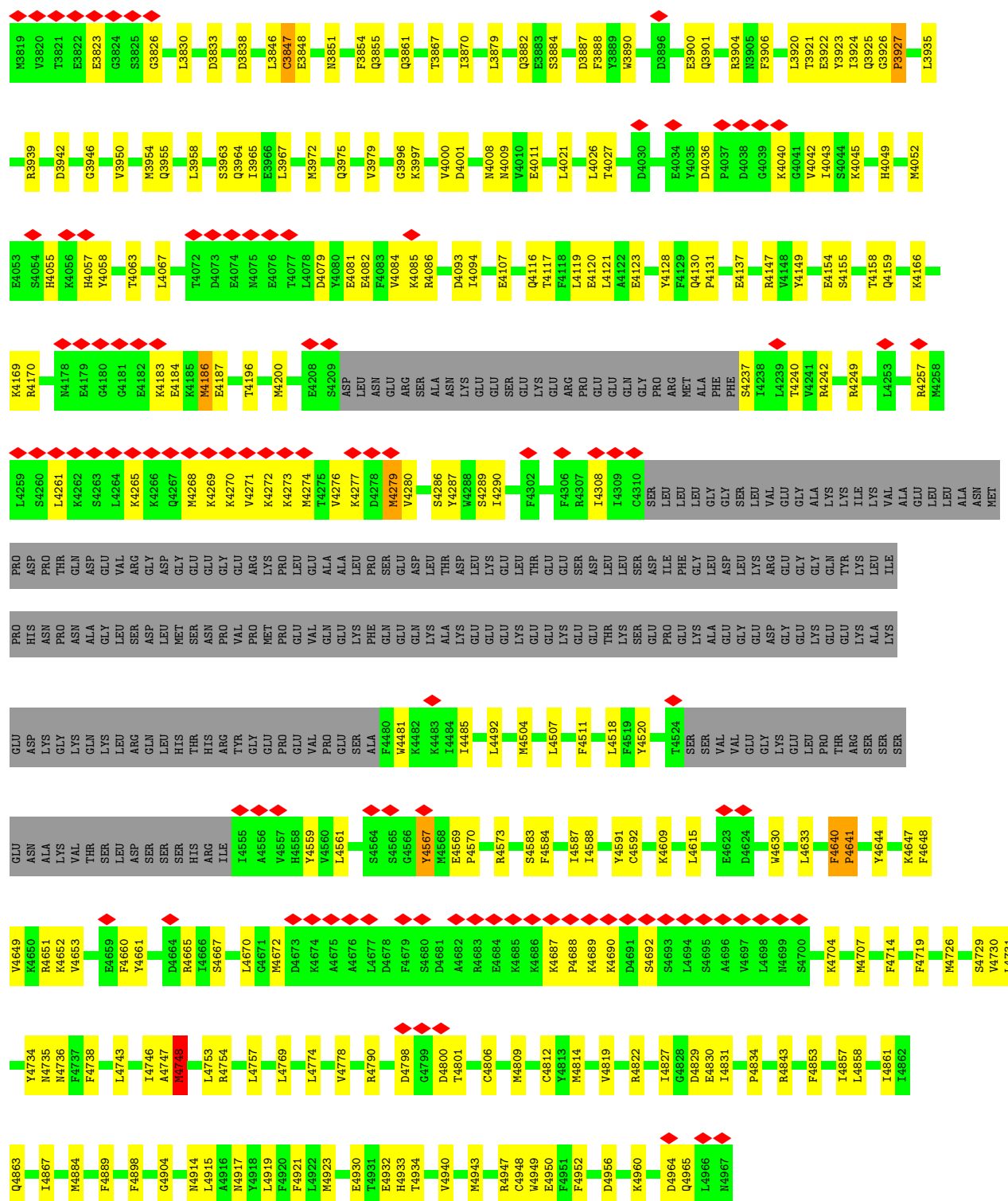


• Molecule 2: Ryanodine receptor 2

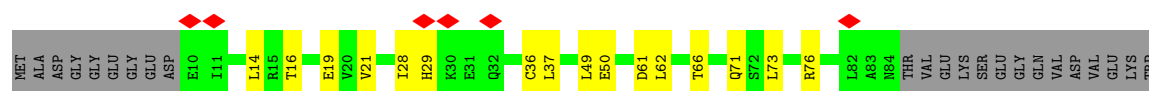


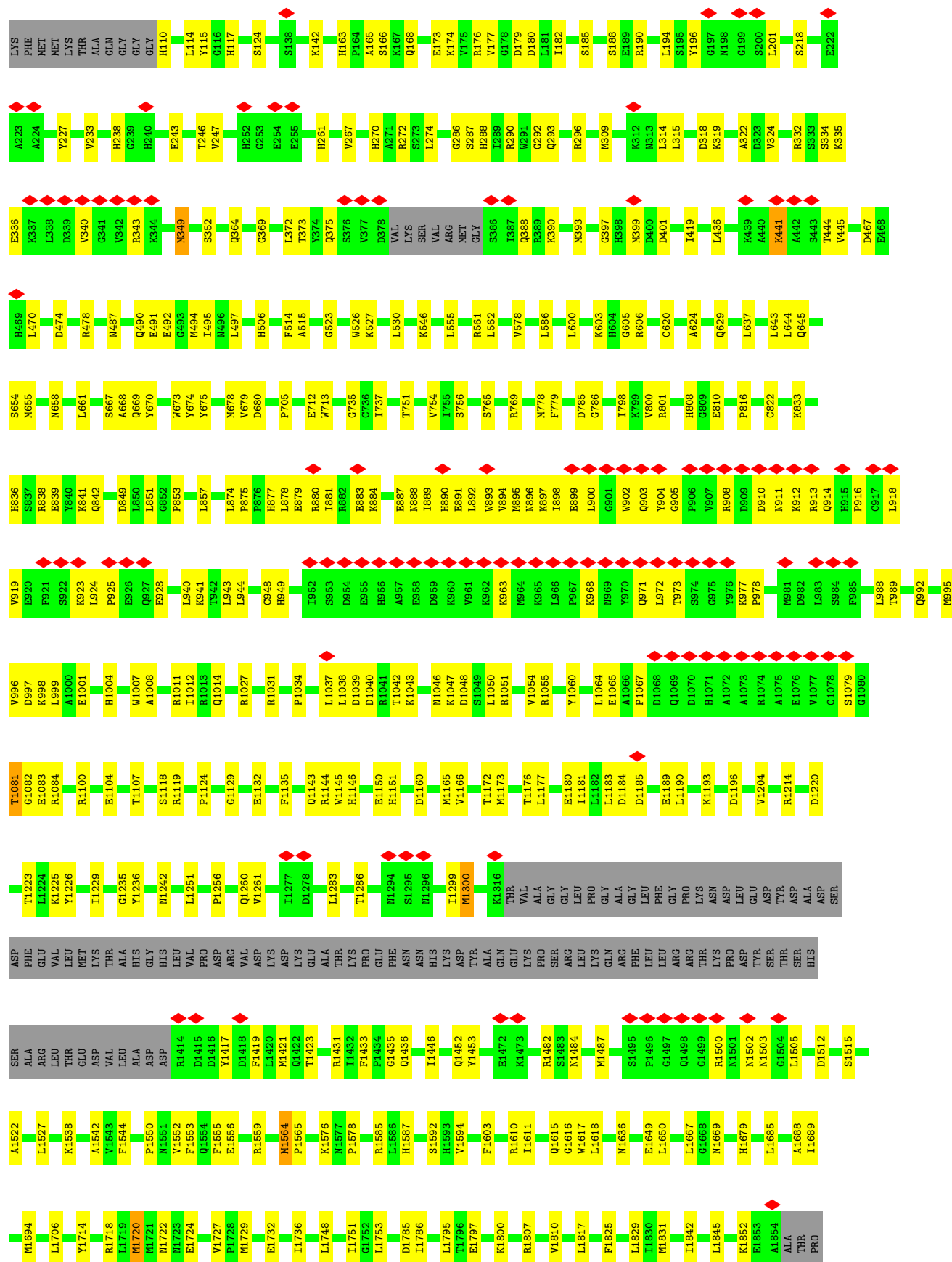


L3687	Y3688	M3689	D3693	K3697	H3700	D3701	E3702	GLU	ASP	ASP	ASP	GLY	GLU	E3710	V3711	E3715	M3719	A3729	H3732	T3743	I3744	S3747	P3753	M3754	T3758	I3763	E3783	K3784	M3797	L3803	D3804	L3805	N3806	R3810	Q3811	N3812	E3815	G3816	L3817	G3818																			
GLY	ARG	ARG	HIS	TRP	CYS	VAL	VAL	GLU	HIS	PRO	GLN	ARG	SER	K3584	V3587	H3588	K3589	L3590	L3591	S3592	R3595	K3596	A3601	C3602	F3603	R3604	M3605	L3608	R3615	A3649	E3650	P3651	P3652	E3653	E3654	D3655	E3656	G3657	T3658	K3659	R3660	V3661	L3664	H3665	Q3666	L3667	L3668	T3677	E3678	K3679									
ASN	PRO	GLU	ALA	THR	VAL	GLU	VAL	GLU	ASP	ARG	VAL	THR	PHE	ILE	ALA	TRP	ILE	TRP	SER	GLY	ASP	LYS	ARG	LEU	PRO	ASN	ARG	GLY	ASN	PRO	GLY	ASP	ILE	ASN	ASN	MET	GLU	ILE	SER	PHE	THR	LEU	LEU	ASP	ASN	LYS	THR	GLU	GLN	ASP	VAL	SER	VAL	ARG	GLN	GLU	ILE		
ILE	ARG	LYS	LYS	MET	ALA	TRP	VAL	ARG	ARG	ARG	VAL	THR	PHE	ILE	ALA	TRP	ILE	TRP	SER	GLY	ASP	LYS	ARG	LEU	PRO	ASN	ARG	GLY	ASN	PRO	GLY	ASP	ILE	ASN	ASN	MET	GLU	ILE	SER	PHE	THR	LEU	LEU	ASP	ASN	LYS	THR	GLU	GLN	ASP	VAL	SER	VAL	ARG	GLN	GLU	ILE		
GLY	ARG	ARG	HIS	TRP	CYS	VAL	VAL	GLU	HIS	PRO	GLN	ARG	SER	LYS	K3584	V3587	H3588	K3589	L3590	L3591	S3592	R3595	K3596	A3601	C3602	F3603	R3604	M3605	L3608	R3615	A3649	E3650	P3651	P3652	E3653	E3654	D3655	E3656	G3657	T3658	K3659	R3660	V3661	L3664	H3665	Q3666	L3667	L3668	T3677	E3678	K3679								
K3329	ALA	ALA	THR	VAL	VAL	GLU	VAL	GLU	ASP	HIS	LEU	LYS	VAL	ALA	ALA	TRP	ILE	TRP	SER	GLY	ASP	LYS	ARG	LEU	PRO	ASN	ARG	GLY	ASN	PRO	GLY	ASP	ILE	ASN	ASN	MET	GLU	ILE	SER	PHE	THR	LEU	LEU	ASP	ASN	LYS	THR	GLU	GLN	ASP	VAL	SER	VAL	ARG	GLN	GLU	ILE		
N3269	S3270	E3271	K3272	H3273	N3274	T3275	L3276	L3277	G3278	N3279	T3280	L3281	K3282	Y3283	T3284	Y3285	N3286	N3287	L3288	G3289	T3290	D3291	E3292	G3293	K3294	M3295	P3296	K3297	R3298	L3299	A3300	V3301	F3302	S3303	Q3304	P3305	T3306	I3307	N3308	K3309	V3310	K3311	P3312	Q3313	L3314	L3315	K3316	T3317	H3318	F3319	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328
V3204	C3205	N3206	I3207	N3208	F3209	S3210	L3211	E3212	K3213	L3214	M3215	E3216	E3217	I3218	Y3219	E3220	L3221	A3222	E3223	S3224	G3225	I3226	R3227	Y3228	T3229	Q3230	Q3231	H3232	P3233	V3234	M3235	I3238	L3239	P3240	M3241	Y3245	M3246	S3247	R3248	W3249	G3253	P3254	E3255	N3256	P3258	E3259	R3260	A3261	E3262	M3263	C3264	A3267	L3268						
T3142	S3143	K3144	S3145	T3146	T3147	V3148	E3149	E3150	Q3151	R3152	S3153	A3154	L3155	E3156	C3158	L3159	F3162	A3163	A3165	F3166	G3167	V3168	A3169	F3170	L3171	E3172	T3173	H3174	K3177	H3178	N3179	T3180	S3181	S3182	T3183	Y3184	N3185	T3186	K3187	S3188	S3189	R3190	E3191	R3192	A3193	A3194	L3195	S3196	L3197	F3198	T3199	N3200	V3201	E3202	D3203				
Q3079	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	G3089	V3090	T3091	Q3092	I3093	I3094	N3095	Y3096	T3097	T3098	V3099	A3100	L3101	L3102	P3103	M3104	S3105	S3106	S3107	L3108	F3109	E3110	H3111	I3112	G3113	Q3114	H3115	Q3116	F3117	G3118	E3119	D3120	L3121	I3122	L3123	E3124	D3125	V3126	Q3127	Y3131	R3132	I3133	L3134	T3135	Y3138	A3139	L3140	G3141		
C3009	K3010	V3013	R3016	H3017	R3018	I3019	S3020	L3021	F3022	D3025	A3026	I3029	H3034	T3035	L3036	G3037	Q3038	T3039	L3040	D3041	A3042	R3043	M3046	K3047	G3048	S3049	L3050	E3051	S3052	V3053	K3054	S3055	R3058	A3059	D3062	N3063	A3064	A3065	E3066	D3067	L3068	E3069	K3070	T3071	M3072	E3073	N3074	L3075	K3076	Q3077	G3078								
L2930	R2931	Y2932	F2943	D2944	G2945	G2946	S2947	R2948	G2949	K2950	G2951	E2952	H2953	F2954	P2955	Y2956	E2957	Q2958	E2959	K2961	F2962	R2965	V2966	V2967	L2968	P2969	L2970	L2971	D2972	Q2973	K2976	F2982	A2985	A2986	S2987	R2988	P2989	L2990	C2991	S2992	G2993	G2994	H2995	N2998	K2999	E3000	K3001	M3003	S3006										
K2854	K2857	M2858	E2859	L2860	R2861	S2862	K2863	G2864	G2865	G2866	N2867	H2868	L2871	D2875	T2876	L2877	E2881	R2886	E2887	K2888	A2889	Q2890	L2891	I2892	L2893	K2894	I2898	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	E2918	K2919	R2920	F2921	A2922	Y2923	S2924	F2925	L2926	Q2927	Q2928	L2929									
K2785	G2786	K2787	R2788	R2791	T2792	R2793	E2794	G2795	D2796	S2797	R2798	A2799	L2800	Y2801	N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA	HIS	G2820	Y2821	S2822	F2823	R2824	L2825	L2826	D2827	M2828	S2829	N2830	V2831	T2832	L2833	S2834	R2835	D2836	L2837	H2838	A2841	E2842	H2843	R2844	H2849				



• Molecule 2: Ryanodine receptor 2



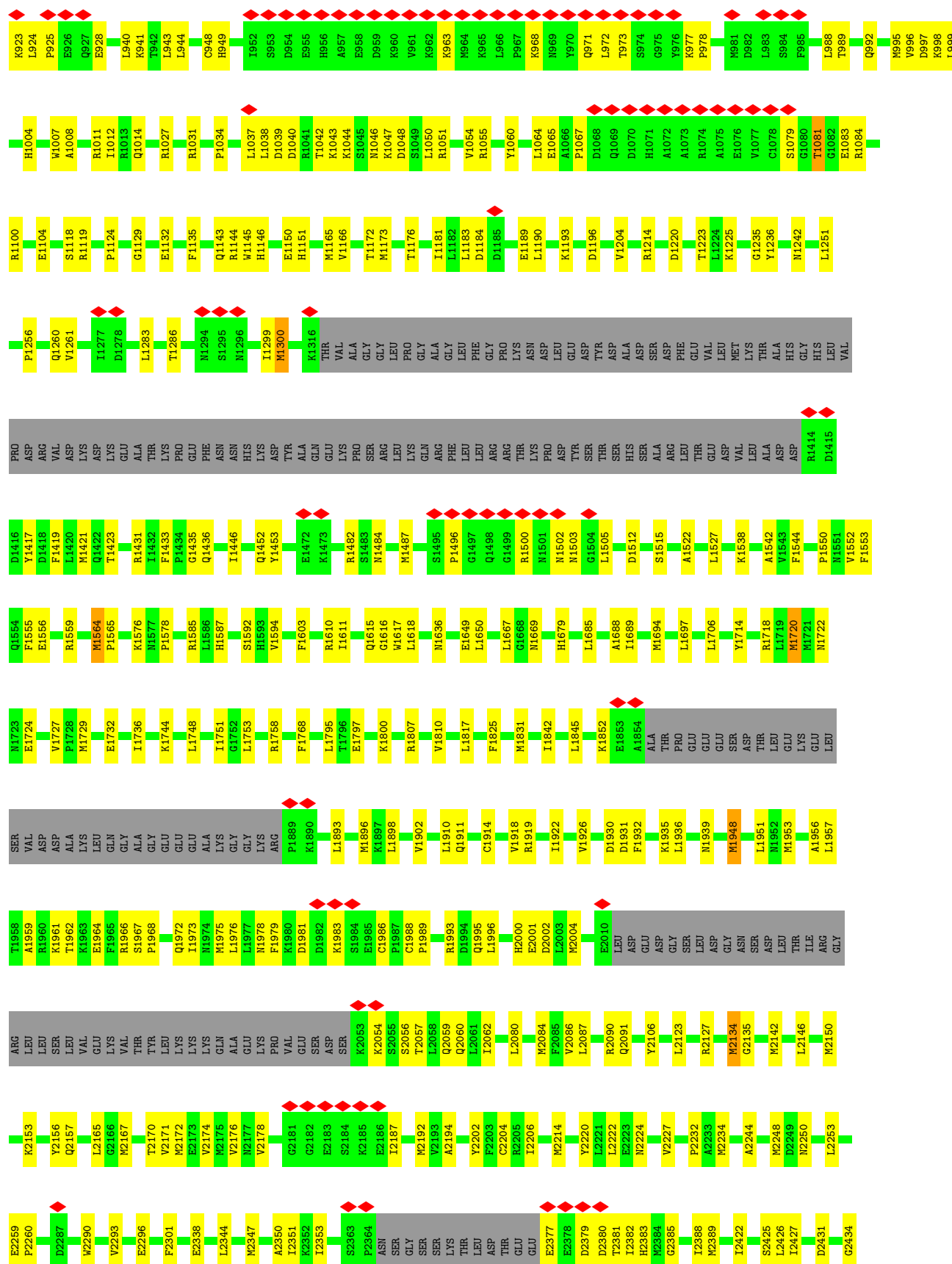




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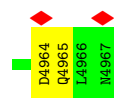


Y840	A688	K483	R343	V233	LYS	MET
K841	Q669	N487	K344	H238	PHE	ALA
Q842	Y670			G239	MET	ASP
D849	W673	Q490	D347	H240	LYS	GLY
L850	Y674	E491	G348		THR	GLU
L851	Y675	E492	K349	E243	ALA	GLY
G852	M678	G493	S352	T246	GLN	GLU
P853	W679	M494	I495	V247	GLY	ASP
L857	D680	N496	Q364		GLY	F10
		L497		H252	H110	F11
L874	R684	H506	L372	G253	L114	L14
P875	P705	H506	T373	E254	Y115	R15
R876	H877	F514	G375	E255	H116	T16
L877	E712	A515	S376		H117	
R878	W713	G523	V377	H261		E19
E879			D378	V267	S138	V20
R880	V718	W526	VAL		K142	V21
L881	G735	K527	LYS	H270		I28
R882	C736	L630	SER	A271	A165	H29
E883	I737	L630	VAL	R272	S166	K30
K884		L555	ARG	S273	K187	E31
	T751	L555	MET	L274	Q188	Q32
E887			GLY		R169	
R888	V754	R561	S386	G286		C36
L889	I755	L562	I387	G287	E173	L37
R890	S756	V578	Q388	H288	K174	L49
L891		K390	R389	I289	V175	E50
R893	S765	L600	K393	G292	R176	D61
V894	R769	K603	G397	Q293	V177	L62
R896	M778	H604	H398		G178	
K897	F779	R605	K399	R296	D179	
L898		R606	D400	K309	D180	
E899	D785	L900	D401	L314	S185	T66
	G786	A624		L315	S188	Q71
L900		Q629	T419	L318	E189	S72
	I798	L637	L436	D318	R190	L73
W902	K799	R801	K319		L194	R76
Q903	R900	L643	K439		S195	
Q905	Y904	L644	A440	A322	Y196	L82
	H808	Q645	A441	D323	G197	A83
P906	G809	E810	K441	V324	I198	H84
Y907		L648	A442		G199	
R908	P816	S654	S443	R332	S200	THR
D909	C822	M655	V445	S332	L201	VAL
D910		N658	D467	S333		GLU
N911	K833	L659	E468	S334	G218	LYS
K912	H836	F660	H469	K335		SER
R913	S837	L661	L470	E336		GLY
Q914	R838		D474	K337	E222	GLN
H915	E839	S667	R478	L338	A223	ASP
P916				D339	A224	VAL
				V340		GLU
G917				G341	Y227	LYS
L918				V342		TRP
V919						
E920						
F921						
S922						

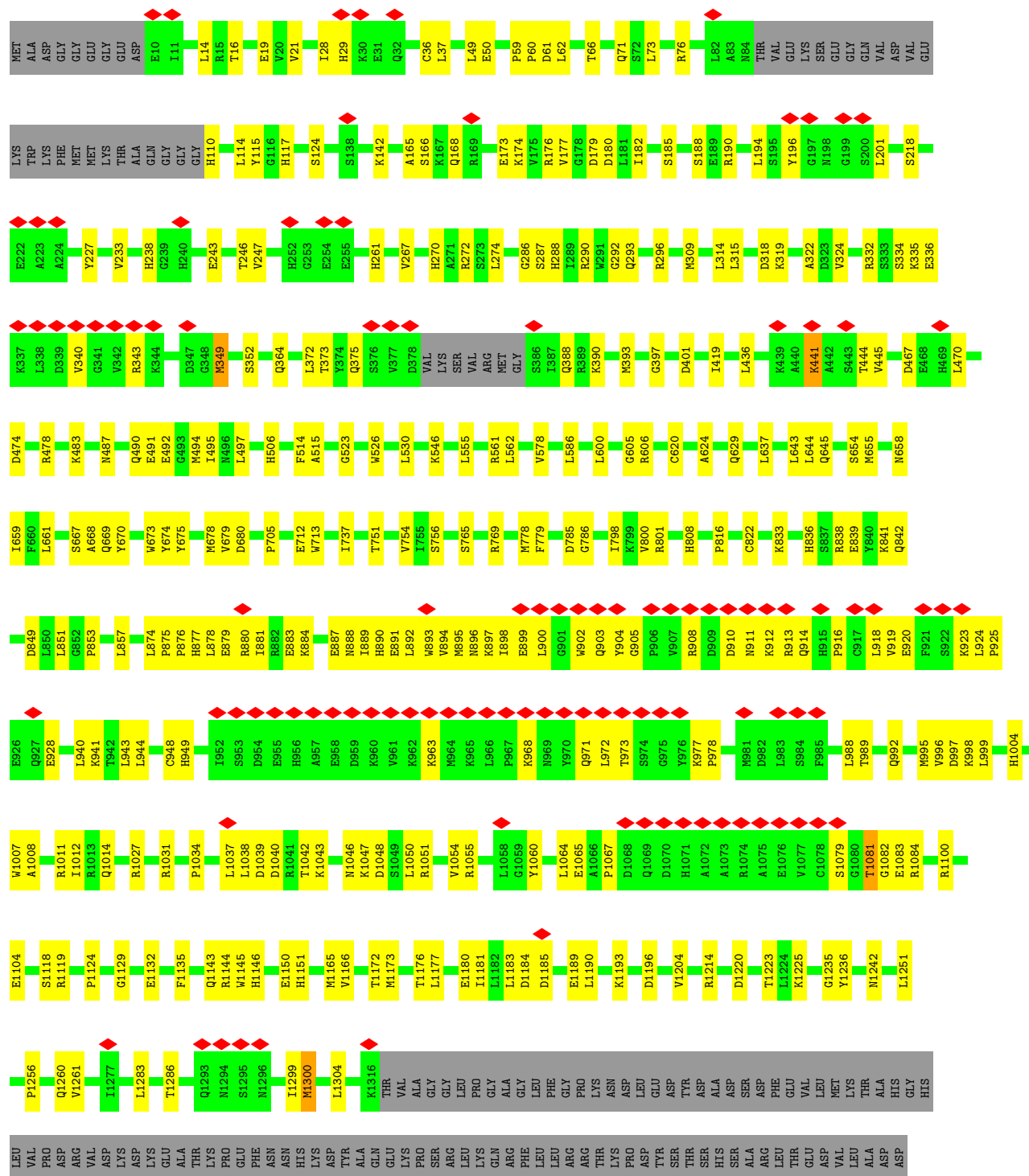


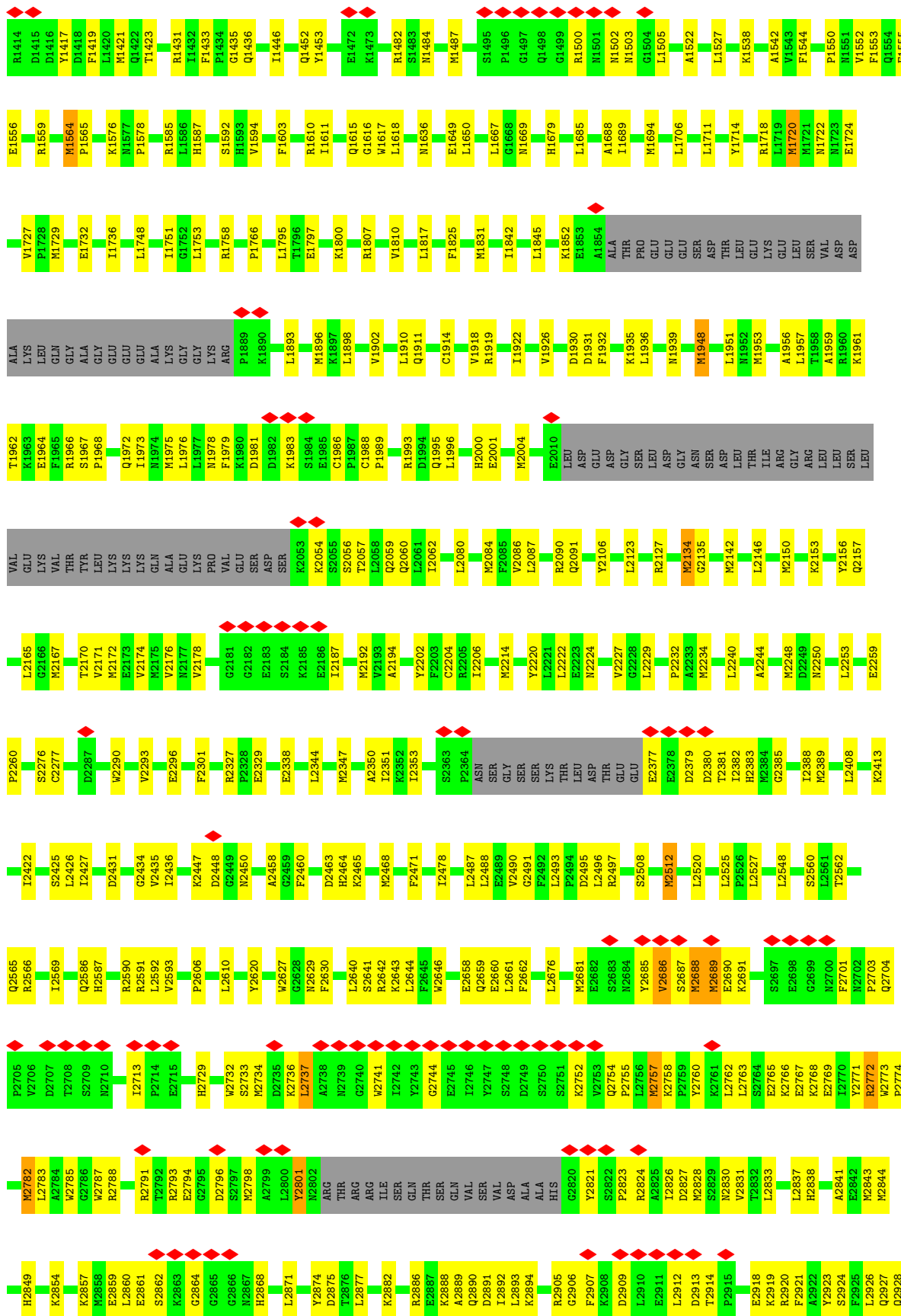


C4812	E4684	E4569	ALA	PRO	PHE	GLN	GLU	V4084	V3979	F3854	M3719	L3590	GLN
T4813	K4685	P4570	F4480	SER	GLN	ARG	ARG	K4085	V3979	Q3855	M3719	L3590	GLN
M4814	K4686	R4573	K4483	GLU	GLN	SER	SER	R4086	G3996	Q3861	A3729	L3591	ALA
Y4818	K4687	S4583	L4492	LEU	LYS	ALA	ALA	D4093	K3997	T3867	H3732	S3592	LEU
V4819	P4688	F4584	M4502	THR	LYS	ASP	LYS	E4107	V4000	I3870	T3743	R3595	LYS
T4827	K4689	F4585	R4503	ASP	GLU	LEU	GLU	E4107	D4001	I3870	T3743	K3596	ASP
E4830	K4690	C4586	M4504	LEU	GLU	LEU	SER	T4117	M4008	L3879	I3744	A3601	LEU
L4831	D4691	L4587	M4504	GLU	GLU	LEU	LYS	T4117	N4009	L3879	I3744	R3604	PRO
L4831	S4692	L4588	L4507	THR	GLU	THR	GLU	F4118	V4010	Q3882	S3747	M3605	ARG
P4834	S4693	C4592	C4310	GLU	GLU	GLU	ARG	F4119	E4011	Q3882	P3753	M3605	THR
R4843	L4694	K4609	F4511	LEU	LYS	PRO	PRO	L4121	L4021	D3887	M3754	L3608	ASP
F4853	S4695	L4615	Y4520	SER	GLU	GLU	GLN	E4122	L4026	F3888	T3758	R3615	THR
T4857	A4696	E4623	T4524	LEU	THR	GLY	GLY	E4123	T4027	Y3889	I3763	R3615	SER
L4858	L4698	D4624	T4524	LEU	LEU	GLY	ARG	Y4128	D4030	W3890	L3778	A3649	PRO
I4861	S4700	L4633	T4524	PRO	GLY	PRO	GLY	F4129	D4030	E3900	L3778	E3650	GLU
Q4863	K4704	F4640	T4524	ILE	SER	MET	MET	Q4130	E4034	Q3901	E3783	P3651	LYS
T4867	M4707	P4641	T4524	VAL	PHE	ALA	PHE	P4131	F4035	Q3901	K3784	P3652	VAL
M4884	M4726	Y4644	T4524	GLY	GLY	GLY	GLY	E4137	P4037	R3904	M3797	E3654	ARG
F4889	S4729	K4647	T4524	LEU	GLU	LEU	LEU	R4147	P4037	F3906	L3803	D3655	LEU
M4914	V4730	F4648	T4524	LYS	GLU	LYS	LYS	Y4148	D4038	L3920	L3803	E3656	ASP
L4915	L4731	V4649	T4524	ARG	GLY	ARG	ILE	Y4149	G4039	T3921	D3804	G3657	ILE
A4916	K4650	K4650	T4524	GLY	GLY	GLY	LYS	E4154	K4040	E3922	L3805	T3668	ALA
N4917	K4652	K4652	T4524	VAL	VAL	VAL	LYS	S4155	V4042	I3923	N3806	T3668	ASN
Y4918	V4653	V4653	T4524	ALA	ALA	ALA	ALA	T4158	V4042	I3923	R3810	K3659	VAL
L4919	F4737	V4653	T4524	GLN	GLN	GLN	GLN	Q4159	V4042	I3923	Q3810	R3660	LEU
F4920	F4738	V4653	T4524	TYR	TYR	TYR	TYR	K4166	V4042	I3923	Q3810	R3660	PHE
F4921	L4743	P4660	T4524	LYS	LYS	LYS	LYS	Q4167	V4042	I3923	Q3810	R3660	HIS
E4930	I4746	P4660	T4524	ILE	ILE	ILE	ILE	K4167	V4042	I3923	Q3810	R3660	LEU
T4931	A4747	P4660	T4524	PRO	PRO	PRO	PRO	E4168	V4042	I3923	Q3810	R3660	GLY
E4932	M4748	P4660	T4524	ASN	ASN	ASN	ASN	K4169	V4042	I3923	Q3810	R3660	LYS
H4933	R4663	P4660	T4524	THR	THR	THR	THR	R4170	V4042	I3923	Q3810	R3660	LYS
T4934	R4664	P4660	T4524	ALA	ALA	ALA	ALA	Q4171	V4042	I3923	Q3810	R3660	ARG
V4940	R4665	P4660	T4524	GLY	GLY	GLY	GLY	M4178	V4042	I3923	Q3810	R3660	VAL
M4943	S4667	P4660	T4524	LEU	LEU	LEU	LEU	E4179	V4042	I3923	Q3810	R3660	GLY
R4947	L4670	P4660	T4524	ASP	ASP	ASP	ASP	G4180	V4042	I3923	Q3810	R3660	ARG
C4948	M4671	P4660	T4524	GLN	GLN	GLN	GLN	E4182	V4042	I3923	Q3810	R3660	ARG
N4949	D4672	P4660	T4524	LEU	LEU	LEU	LEU	K4183	V4042	I3923	Q3810	R3660	HIS
E4950	M4673	P4660	T4524	THR	THR	THR	THR	E4184	V4042	I3923	Q3810	R3660	VAL
F4951	D4674	P4660	T4524	ASN	ASN	ASN	ASN	K4185	V4042	I3923	Q3810	R3660	LEU
F4952	A4675	P4660	T4524	PRO	PRO	PRO	PRO	M4186	V4042	I3923	Q3810	R3660	GLU
D4956	A4676	P4660	T4524	VAL	VAL	VAL	VAL	E4187	V4042	I3923	Q3810	R3660	PRO
K4960	L4677	P4660	T4524	GLU	GLU	GLU	GLU	T4196	V4042	I3923	Q3810	R3660	GLN
	G4798	P4660	T4524	LEU	LEU	LEU	LEU	E4208	V4042	I3923	Q3810	R3660	ARG
	G4799	P4660	T4524	ALA	ALA	ALA	ALA	S4209	V4042	I3923	Q3810	R3660	SER
	T4801	P4660	T4524	LEU	LEU	LEU	LEU	ASP	V4042	I3923	Q3810	R3660	LYS
	C4806	P4660	T4524	ALA	ALA	ALA	ALA	LEU	V4042	I3923	Q3810	R3660	K3584
	M4809	P4660	T4524	LEU	LEU	LEU	LEU	ASN	V4042	I3923	Q3810	R3660	W3587
		P4660	T4524						V4042	I3923	Q3810	R3660	E3710
		P4660	T4524						V4042	I3923	Q3810	R3660	V3711
		P4660	T4524						V4042	I3923	Q3810	R3660	E3715

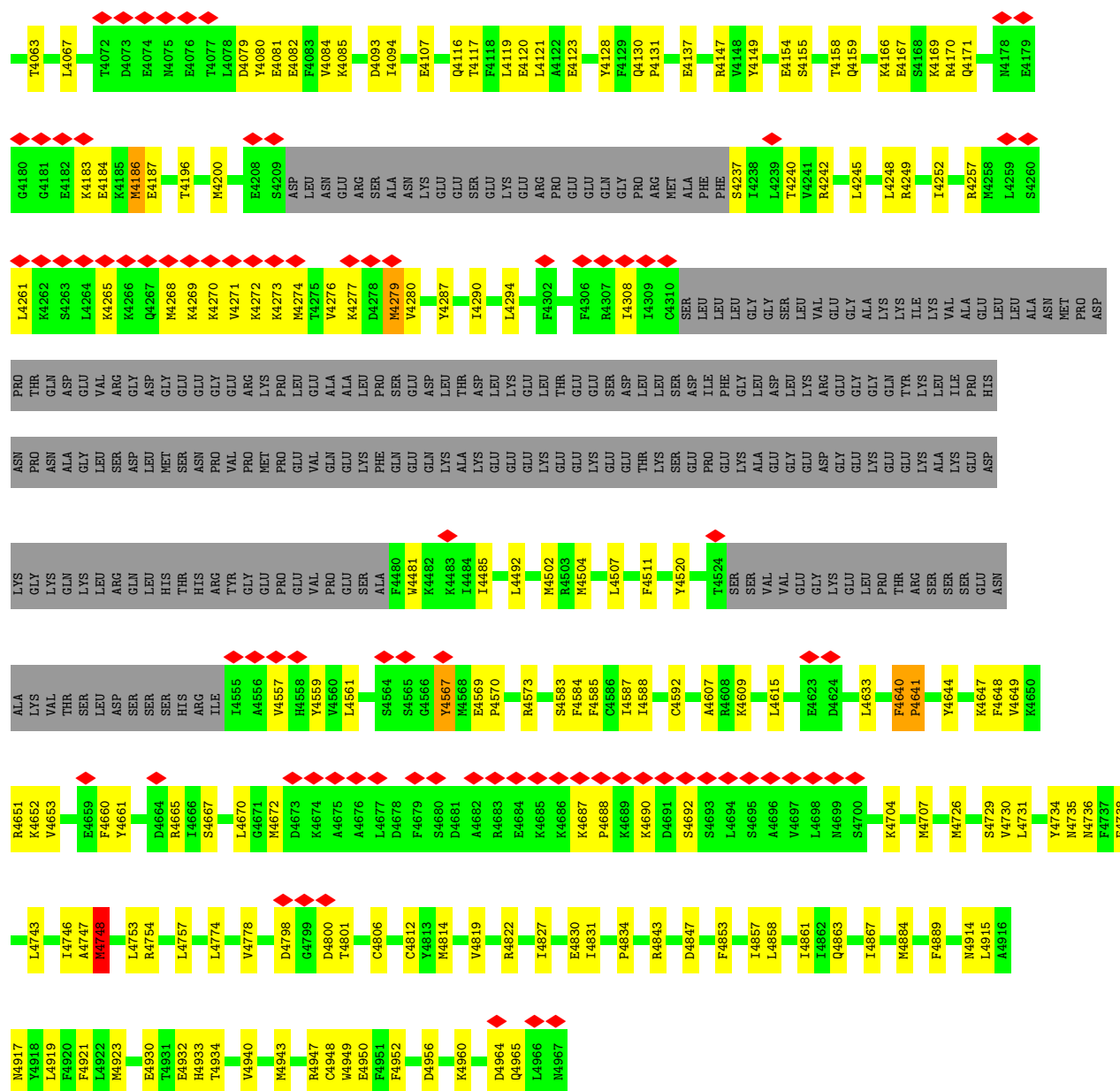


• Molecule 2: Ryanodine receptor 2





[illegible]



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 81% 17%



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 81% 18%



- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:  81% 18% ..



- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:  81% 17% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49606	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	0.594	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, 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	I	0.29	0/1143	0.68	3/1534 (0.2%)
1	J	0.29	0/1143	0.68	3/1534 (0.2%)
1	K	0.29	0/1143	0.68	3/1534 (0.2%)
1	L	0.29	0/1143	0.68	3/1534 (0.2%)
2	A	0.37	7/34594 (0.0%)	0.45	6/46723 (0.0%)
2	B	0.37	7/34594 (0.0%)	0.45	6/46723 (0.0%)
2	C	0.37	7/34594 (0.0%)	0.45	6/46723 (0.0%)
2	D	0.37	7/34594 (0.0%)	0.45	6/46723 (0.0%)
3	E	0.16	0/834	0.41	0/1123
3	F	0.16	0/834	0.41	0/1123
3	G	0.16	0/834	0.41	0/1123
3	H	0.16	0/834	0.41	0/1123
All	All	0.37	28/146284 (0.0%)	0.46	36/197520 (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
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	2
All	All	0	8

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3205	CYS	CB-SG	54.55	3.61	1.81
2	A	3205	CYS	CB-SG	54.53	3.61	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3205	CYS	CB-SG	54.53	3.61	1.81
2	C	3205	CYS	CB-SG	54.50	3.61	1.81
2	B	3131	TYR	CD2-CE2	15.06	1.83	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3205	CYS	CA-CB-SG	9.28	135.73	114.40
2	A	3205	CYS	CA-CB-SG	9.27	135.71	114.40
2	B	3205	CYS	CA-CB-SG	9.25	135.68	114.40
2	D	3205	CYS	CA-CB-SG	9.25	135.68	114.40
1	K	124	GLU	N-CA-C	-7.28	102.52	111.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2801	TYR	Peptide
2	A	4640	PHE	Peptide
2	B	2801	TYR	Peptide
2	B	4640	PHE	Peptide
2	C	2801	TYR	Peptide

5.2 Too-close contacts [i](#)

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	I	1131	0	1058	56	0
1	J	1131	0	1058	52	0
1	K	1131	0	1058	51	0
1	L	1131	0	1058	49	0
2	A	33849	0	33549	855	0
2	B	33849	0	33549	849	0
2	C	33849	0	33549	830	0
2	D	33849	0	33549	850	0
3	E	818	0	821	10	0
3	F	818	0	821	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	818	0	821	13	0
3	H	818	0	821	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	62	0	24	1	0
6	B	62	0	24	1	0
6	C	62	0	24	1	0
6	D	62	0	24	1	0
All	All	143464	0	141808	3551	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 12.

The worst 5 of 3551 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)
2:D:3131:TYR:CD1	2:D:3131:TYR:CE1	1.82	1.68
2:A:3131:TYR:CD1	2:A:3131:TYR:CE1	1.82	1.63
2:C:3131:TYR:CD2	2:C:3131:TYR:CE2	1.83	1.61
2:C:3131:TYR:CE1	2:C:3131:TYR:CD1	1.82	1.61
2:D:3131:TYR:CE2	2:D:3131:TYR:CD2	1.83	1.61

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	J	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	K	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	L	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	A	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	48	79
2	B	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	48	79
2	C	4205/4967 (85%)	4082 (97%)	118 (3%)	5 (0%)	48	79
2	D	4205/4967 (85%)	4080 (97%)	120 (3%)	5 (0%)	48	79
3	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
All	All	17804/20896 (85%)	17292 (97%)	492 (3%)	20 (0%)	49	79

5 of 20 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	123/127 (97%)	113 (92%)	10 (8%)	11	36
1	J	123/127 (97%)	113 (92%)	10 (8%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	123/127 (97%)	113 (92%)	10 (8%)	11	36
1	L	123/127 (97%)	113 (92%)	10 (8%)	11	36
2	A	3715/4358 (85%)	3684 (99%)	31 (1%)	73	77
2	B	3715/4358 (85%)	3684 (99%)	31 (1%)	73	77
2	C	3715/4358 (85%)	3684 (99%)	31 (1%)	73	77
2	D	3715/4358 (85%)	3684 (99%)	31 (1%)	73	77
3	E	88/89 (99%)	87 (99%)	1 (1%)	65	74
3	F	88/89 (99%)	87 (99%)	1 (1%)	65	74
3	G	88/89 (99%)	87 (99%)	1 (1%)	65	74
3	H	88/89 (99%)	87 (99%)	1 (1%)	65	74
All	All	15704/18296 (86%)	15536 (99%)	168 (1%)	63	74

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1953	MET
2	D	1564	MET
2	C	2689	MET
2	C	3847	CYS
2	D	2689	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 225 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	4706	GLN
2	D	4879	GLN
2	C	2850	ASN
2	D	4742	HIS
2	D	3017	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 24 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	$\# Z > 2$
6	ATP	A	5002	-	32,33,33	0.54	0	48,52,52	0.56	0
6	ATP	B	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
6	ATP	A	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
6	ATP	B	5002	-	32,33,33	0.54	0	48,52,52	0.56	0
6	ATP	C	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
6	ATP	D	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
6	ATP	C	5002	-	32,33,33	0.54	0	48,52,52	0.56	0
6	ATP	D	5002	-	32,33,33	0.53	0	48,52,52	0.55	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
6	ATP	A	5002	-	-	8/22/38/38	0/3/3/3
6	ATP	B	5004	-	-	11/22/38/38	0/3/3/3
6	ATP	A	5004	-	-	11/22/38/38	0/3/3/3
6	ATP	B	5002	-	-	8/22/38/38	0/3/3/3
6	ATP	C	5004	-	-	11/22/38/38	0/3/3/3
6	ATP	D	5004	-	-	11/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	C	5002	-	-	8/22/38/38	0/3/3/3
6	ATP	D	5002	-	-	8/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

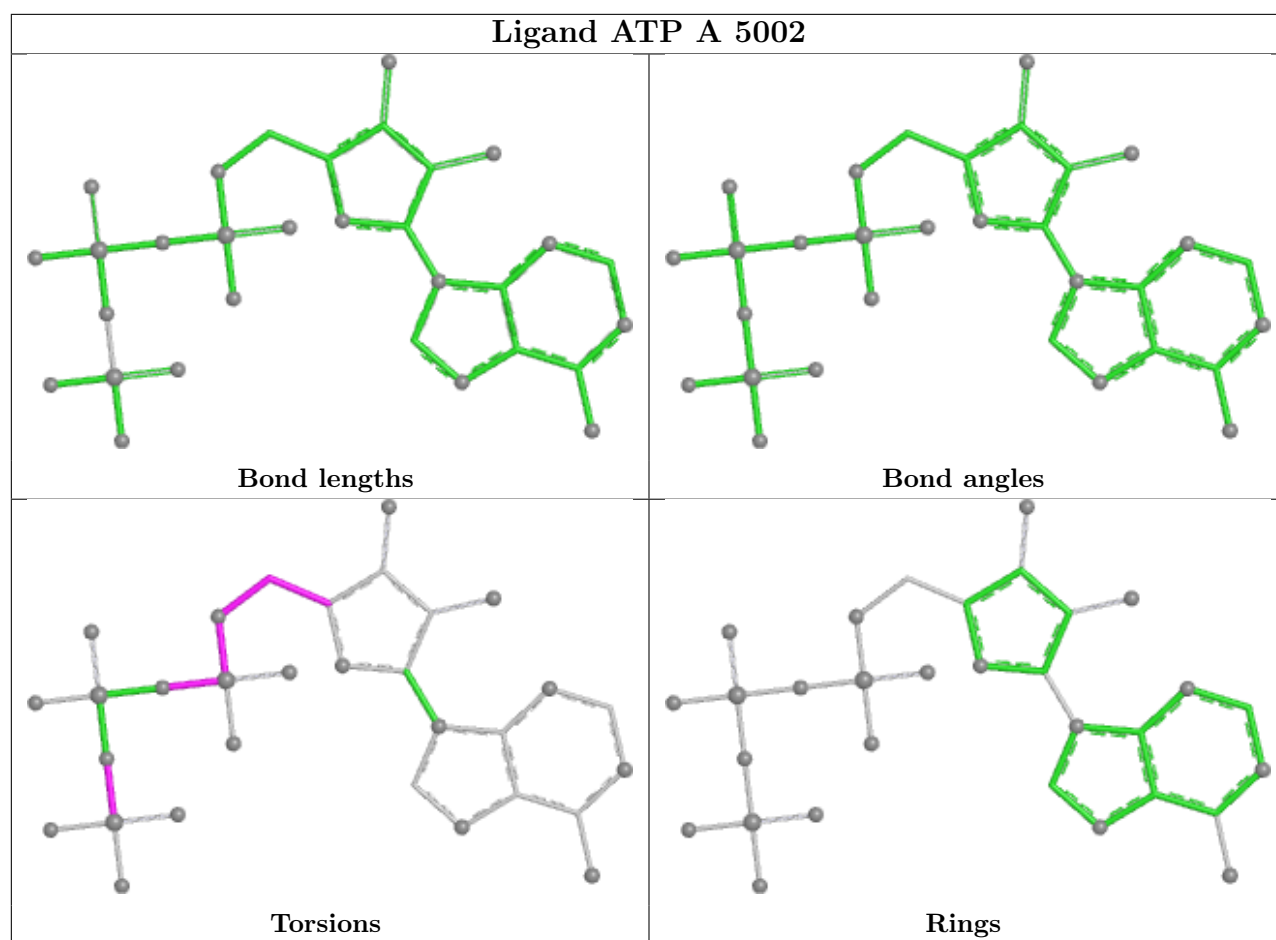
Mol	Chain	Res	Type	Atoms
6	A	5002	ATP	C5'-O5'-PA-O1A
6	A	5002	ATP	C5'-O5'-PA-O2A
6	A	5002	ATP	C5'-O5'-PA-O3A
6	A	5004	ATP	PB-O3A-PA-O5'
6	A	5004	ATP	C5'-O5'-PA-O1A

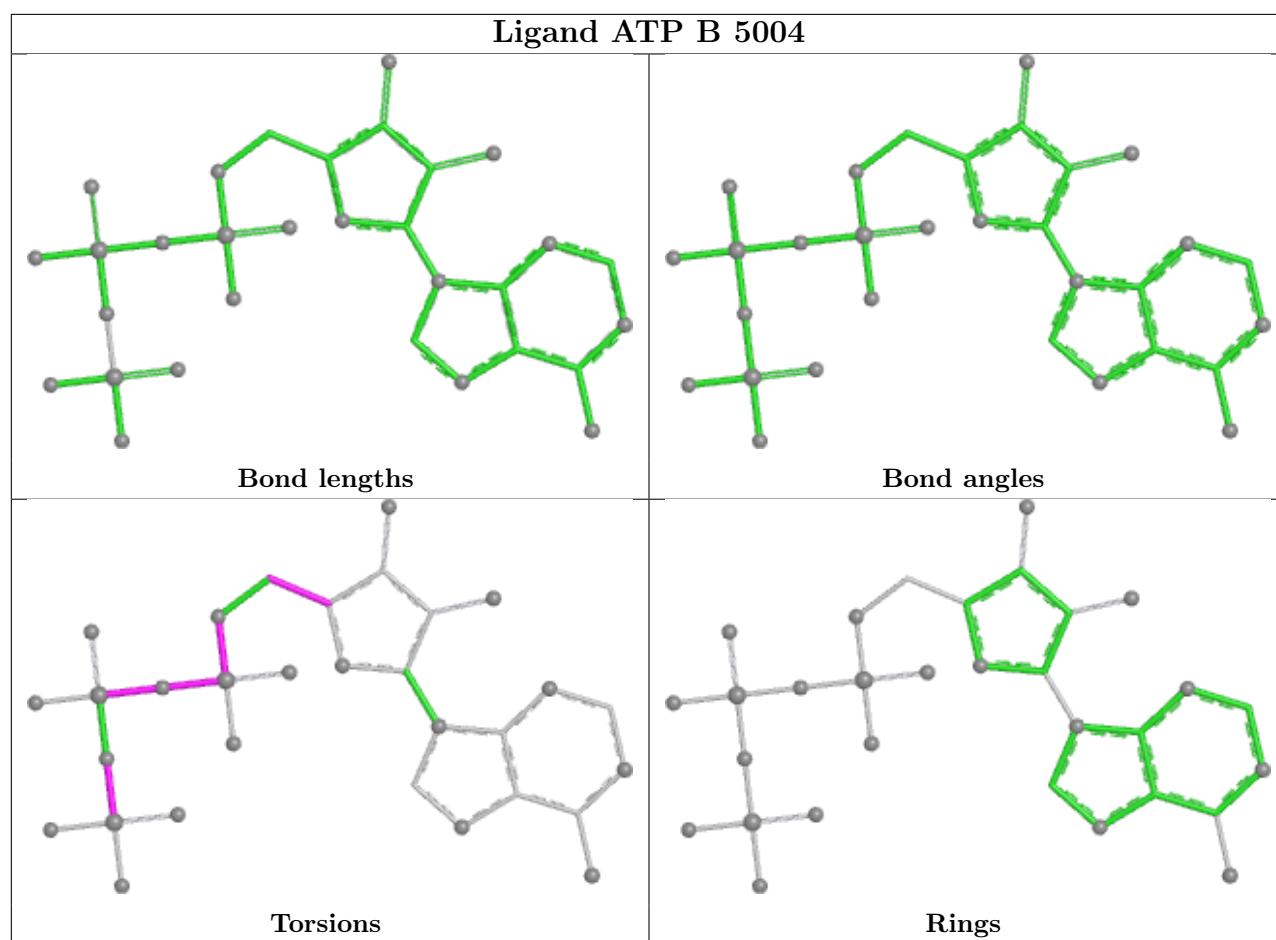
There are no ring outliers.

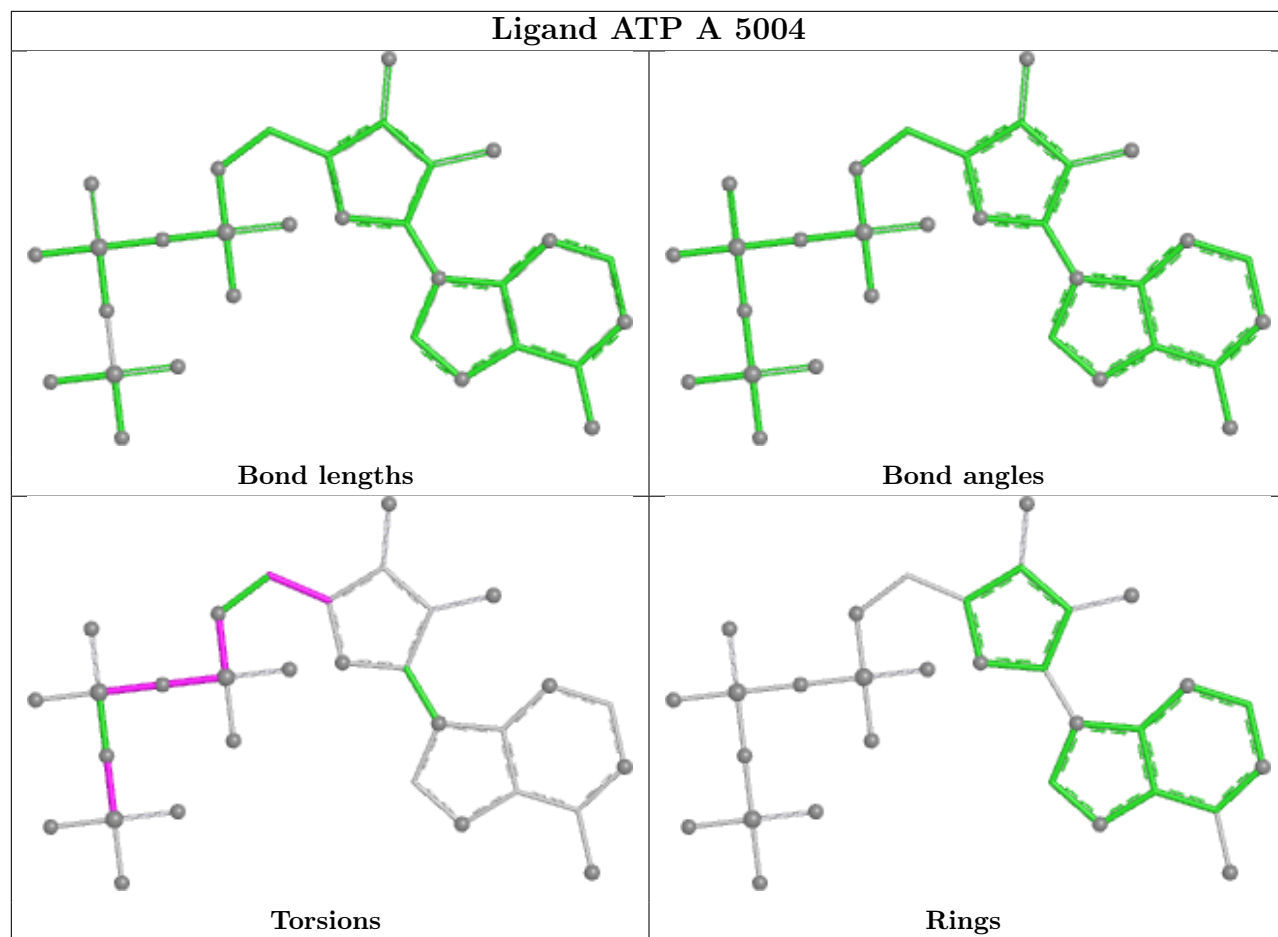
4 monomers are involved in 4 short contacts:

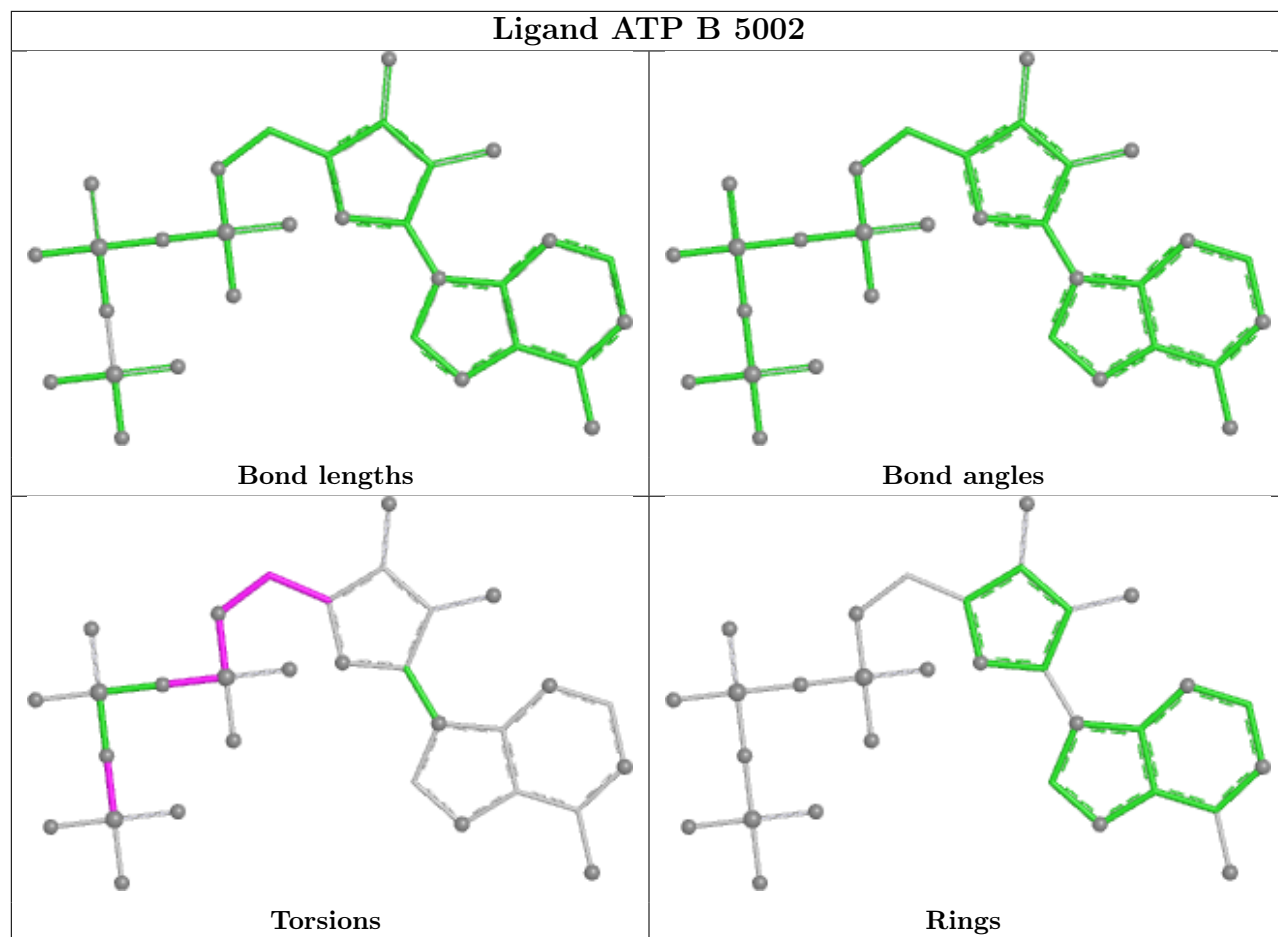
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	5004	ATP	1	0
6	A	5004	ATP	1	0
6	C	5004	ATP	1	0
6	D	5004	ATP	1	0

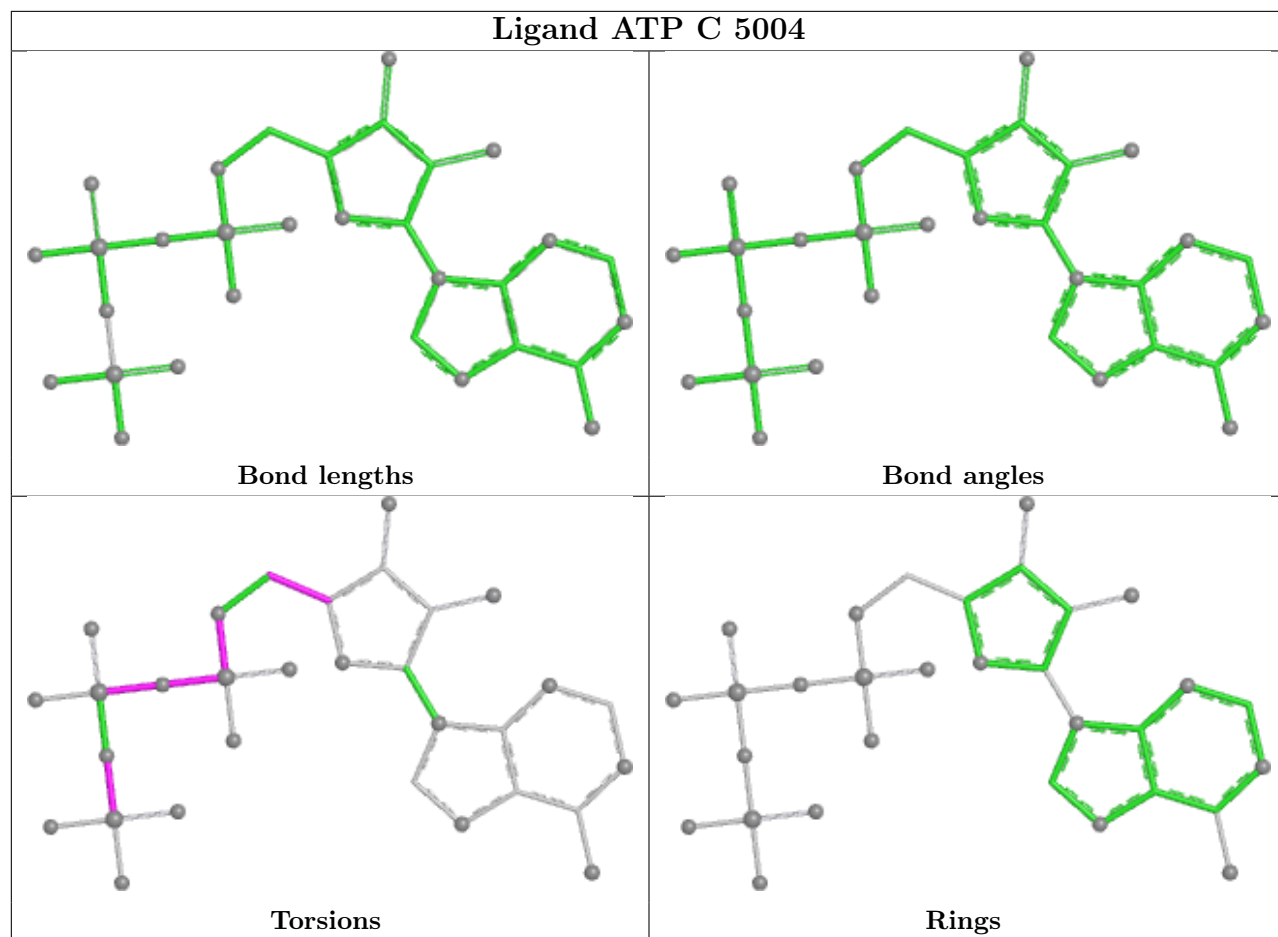
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

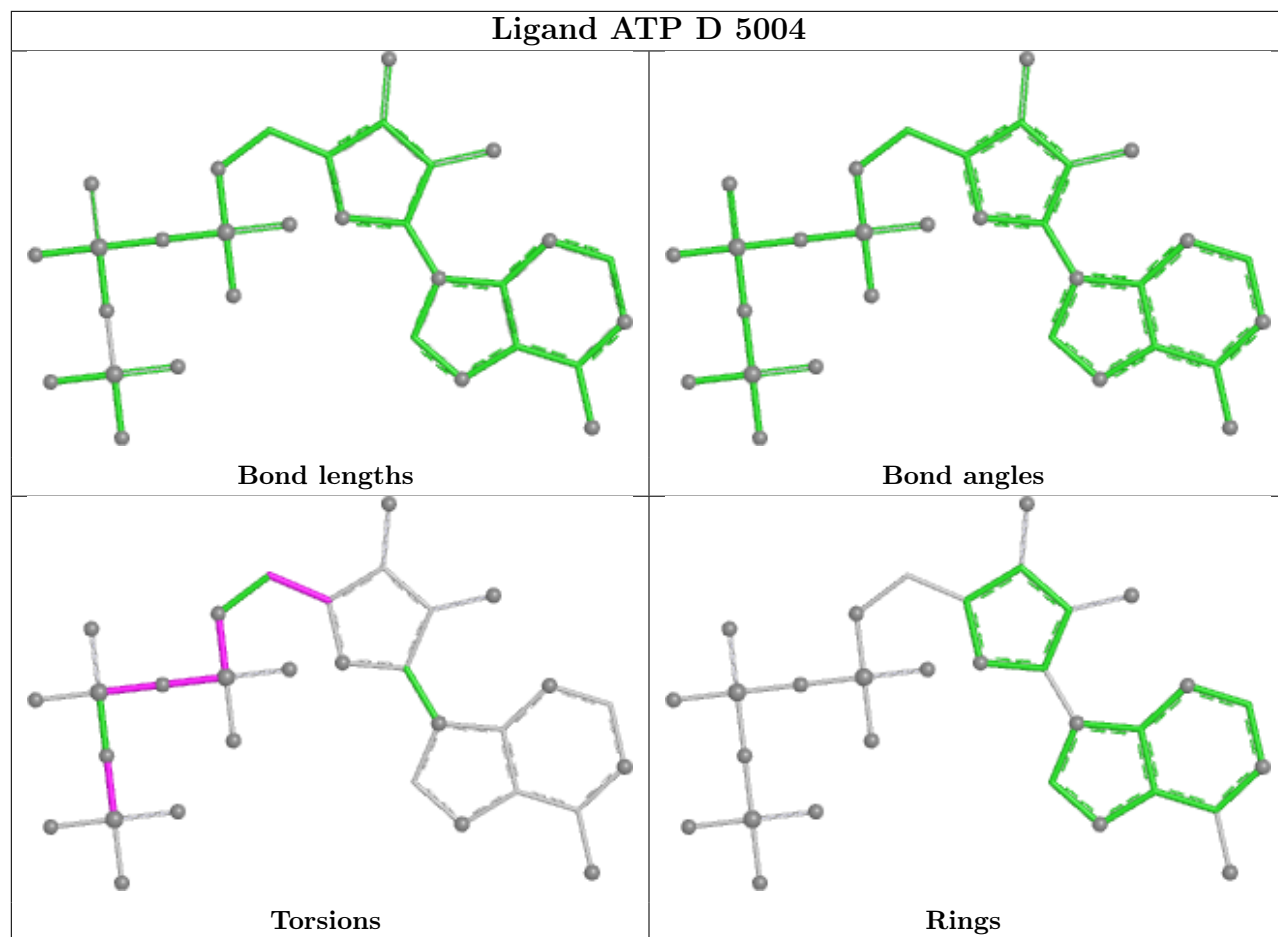


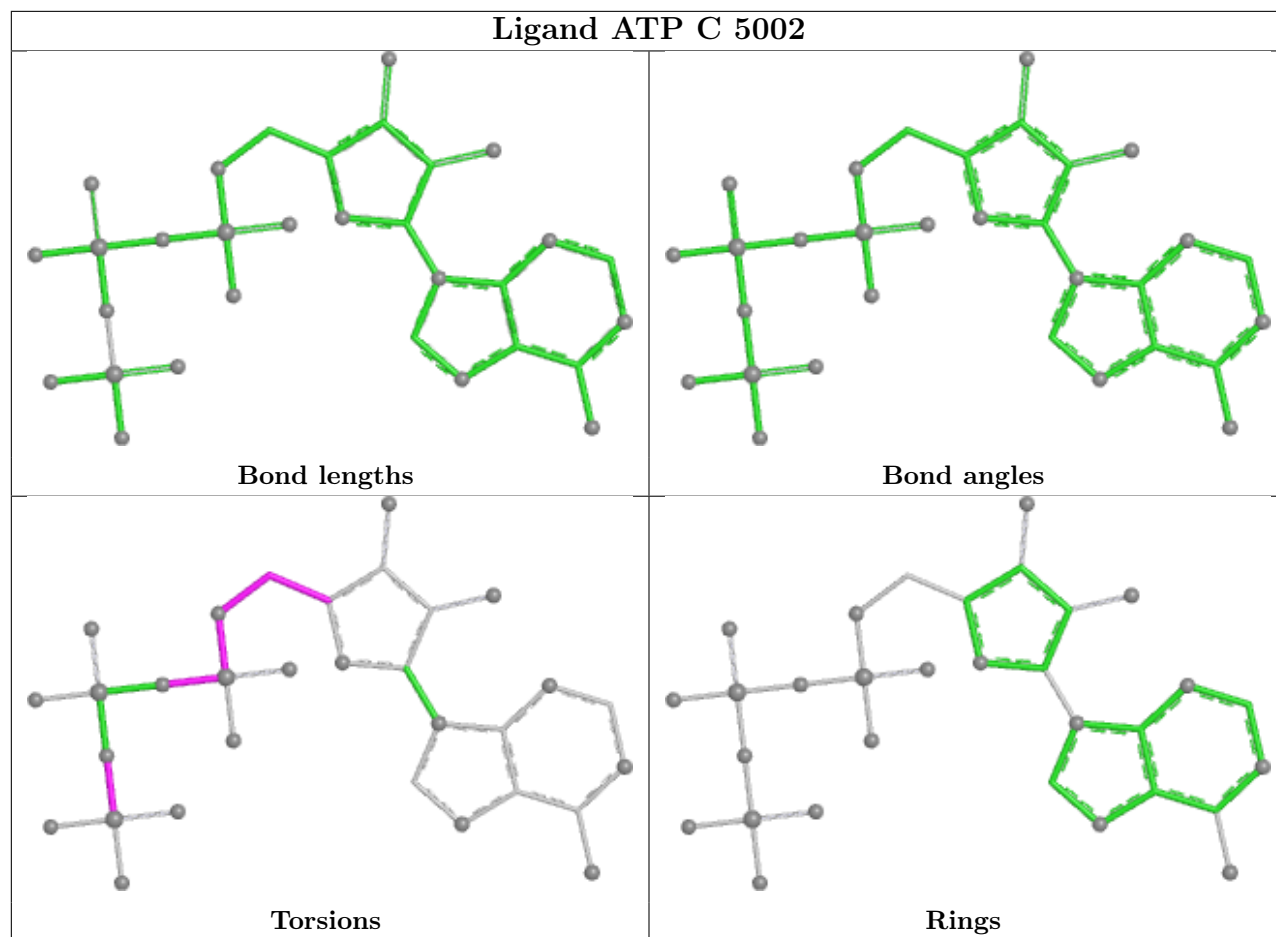


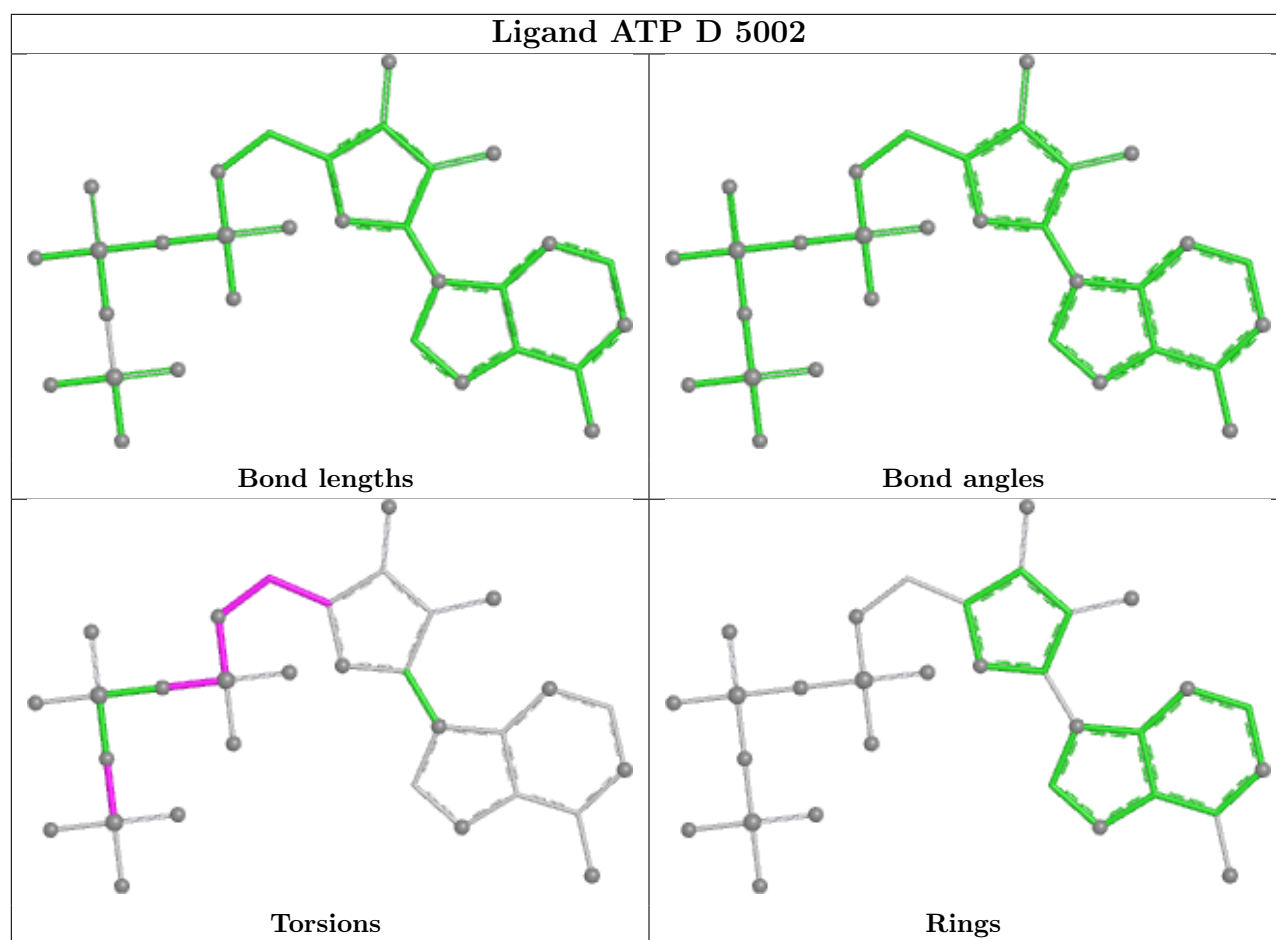












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

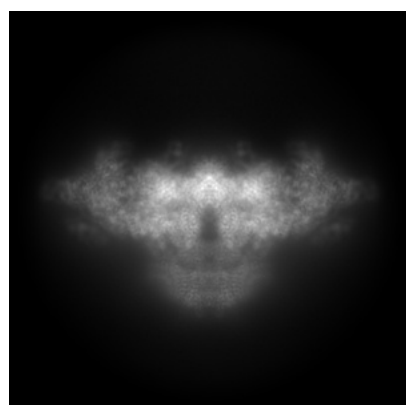
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42769. These allow visual inspection of the internal detail of the map and identification of artifacts.

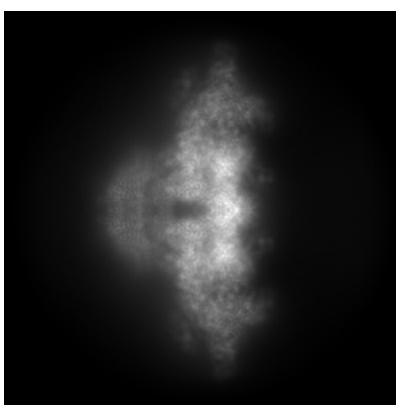
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

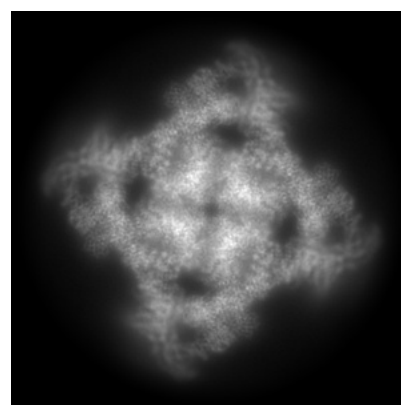
6.1.1 Primary map



X



Y



Z

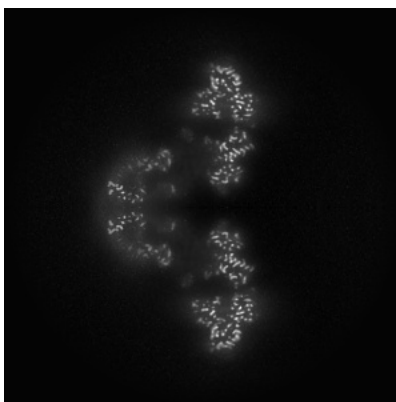
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

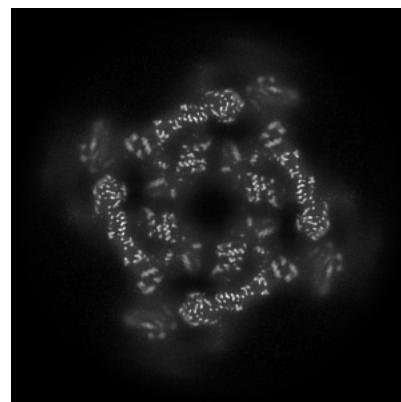
6.2.1 Primary map



X Index: 256



Y Index: 256

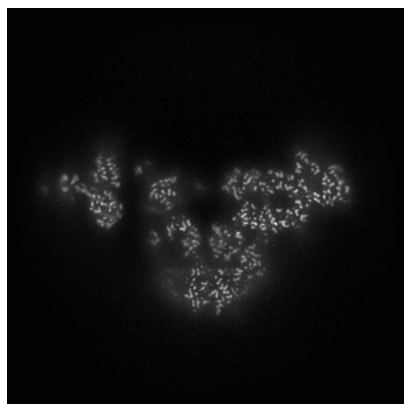


Z Index: 256

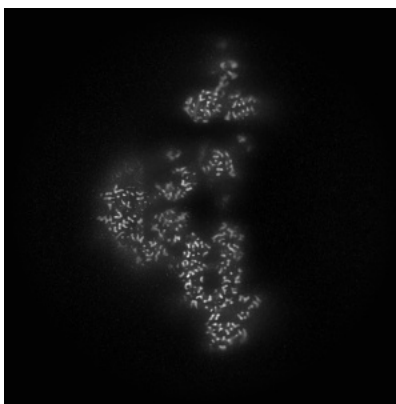
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

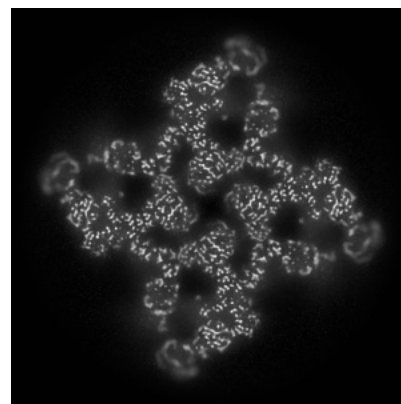
6.3.1 Primary map



X Index: 239



Y Index: 239



Z Index: 283

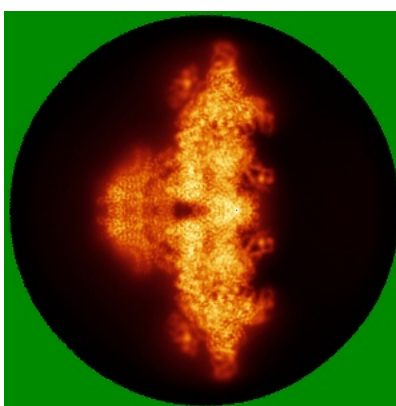
The images above show the largest variance slices of the map in three orthogonal directions.

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

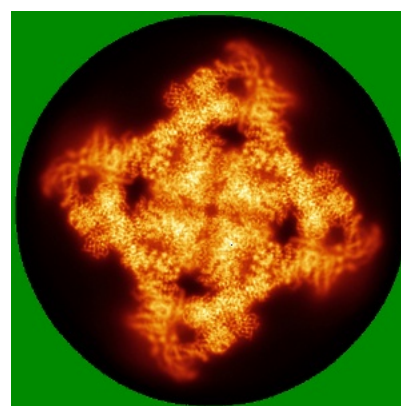
6.4.1 Primary map



X



Y

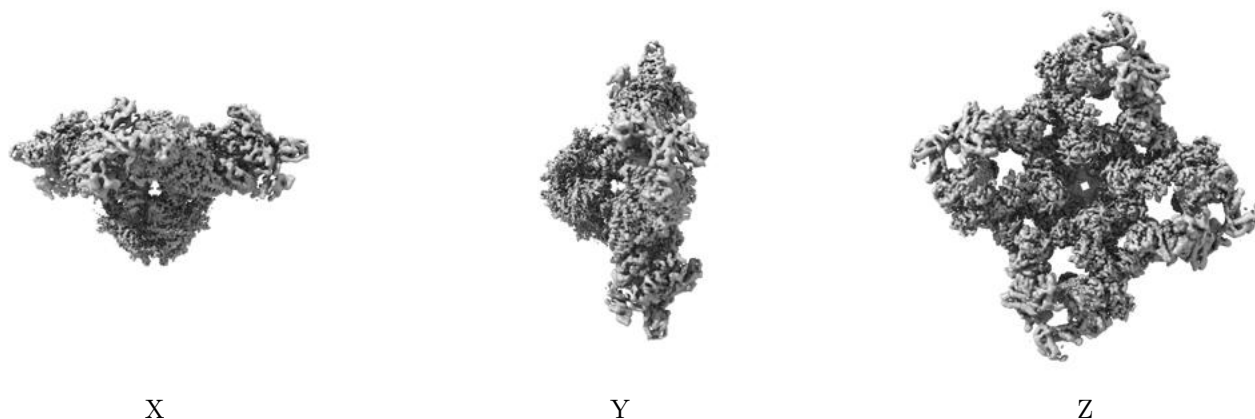


Z

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

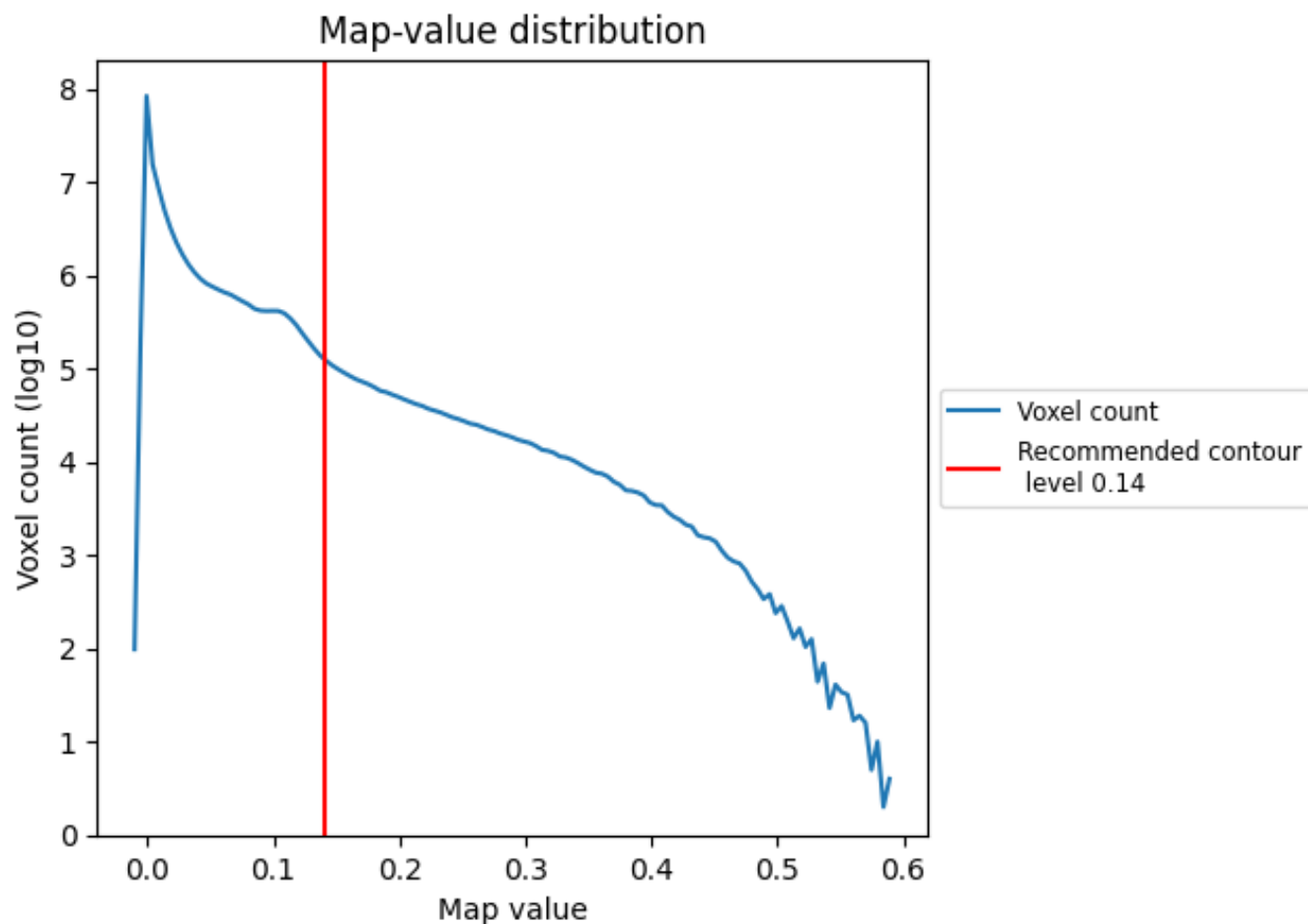
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

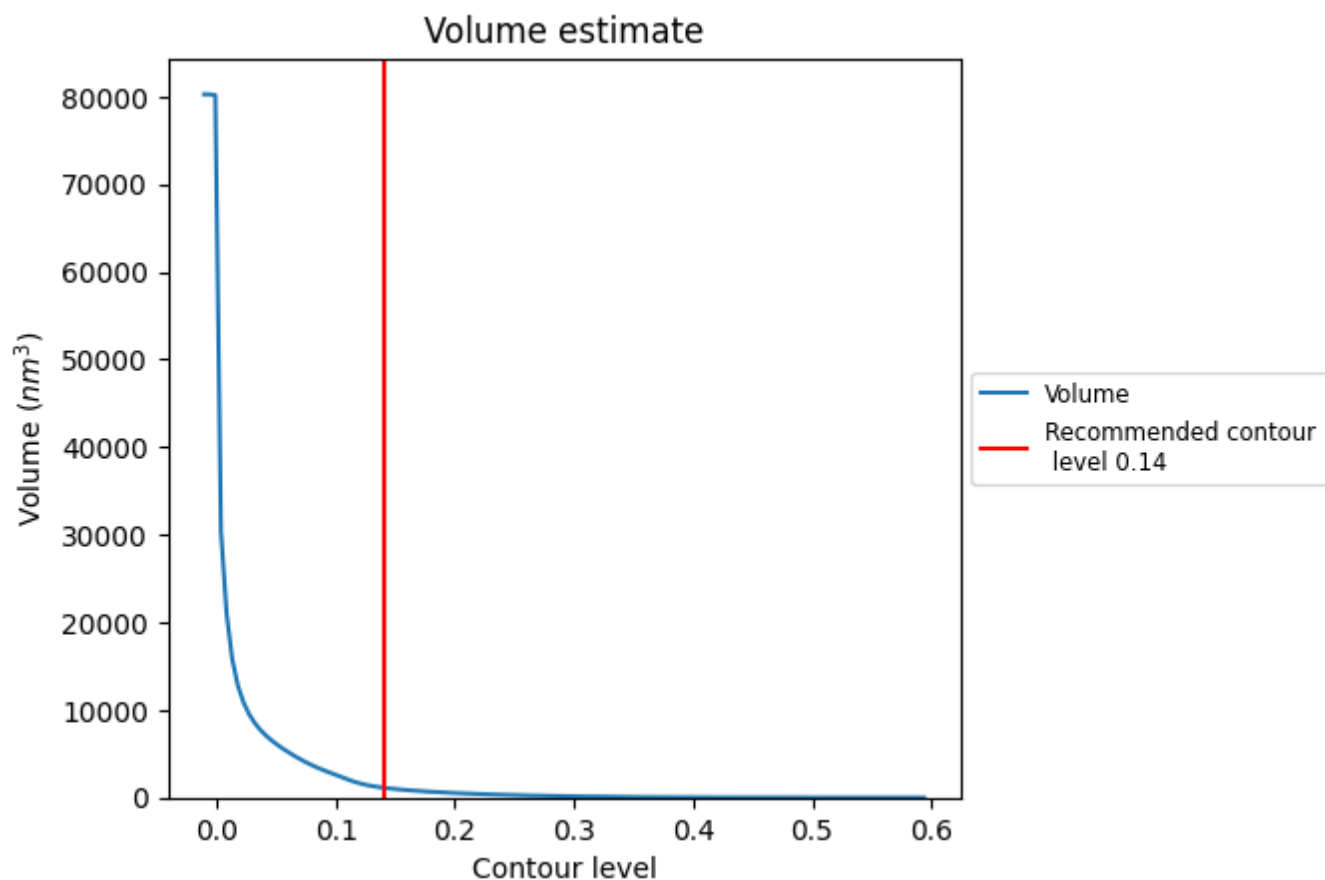
This section contains the results of statistical analysis of the map.

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.

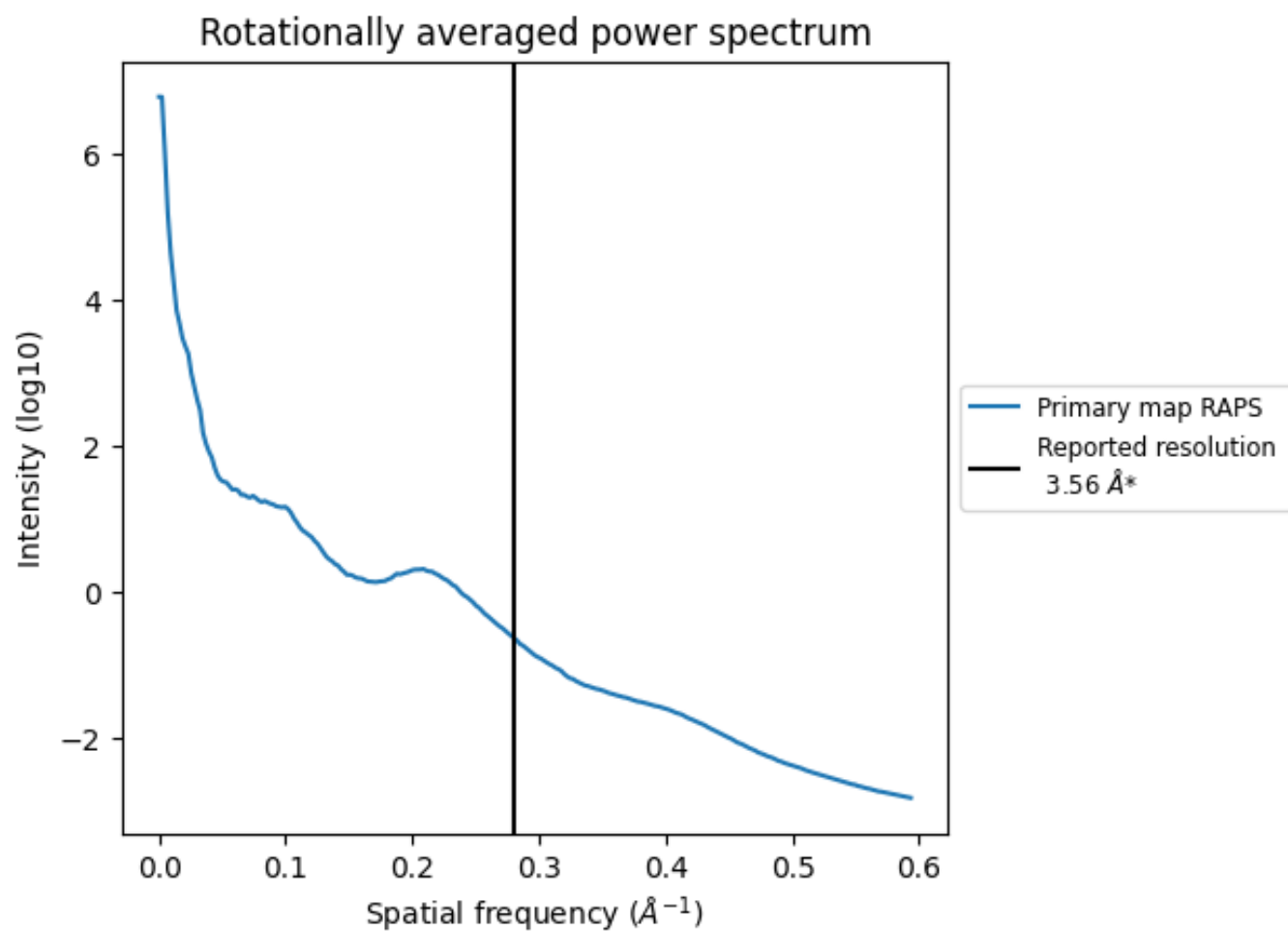
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1122 nm^3 ; this corresponds to an approximate mass of 1014 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 0.281 Å⁻¹

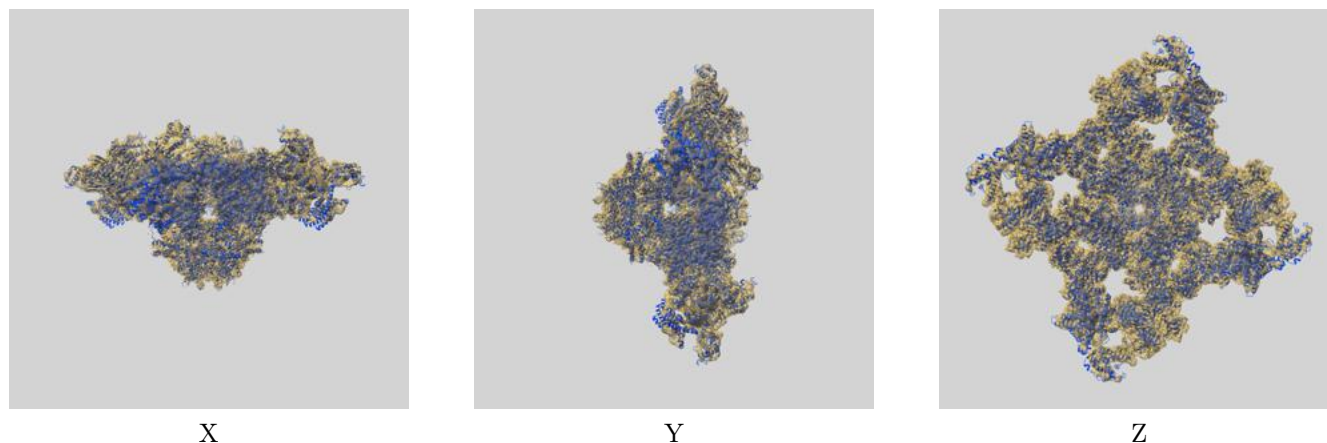
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

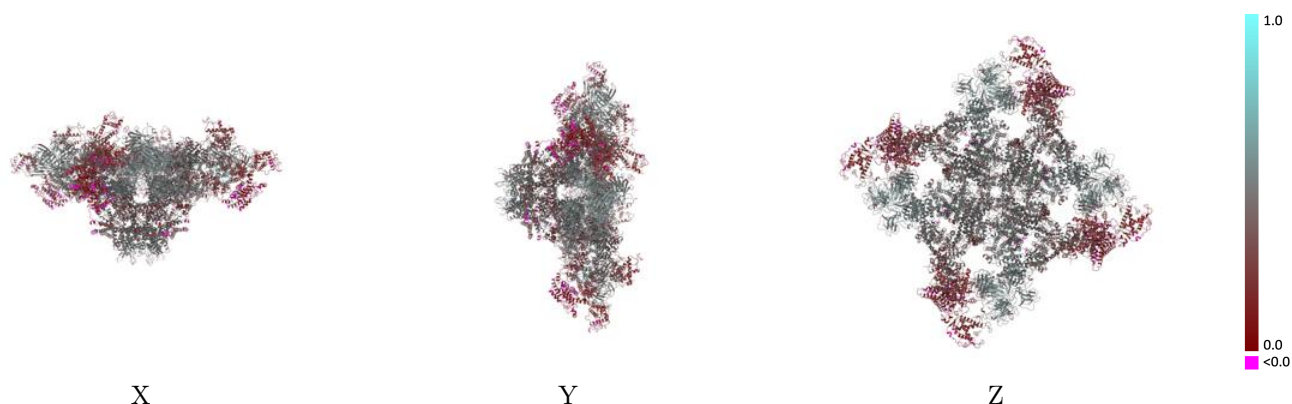
This section contains information regarding the fit between EMDB map EMD-42769 and PDB model 8UXM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



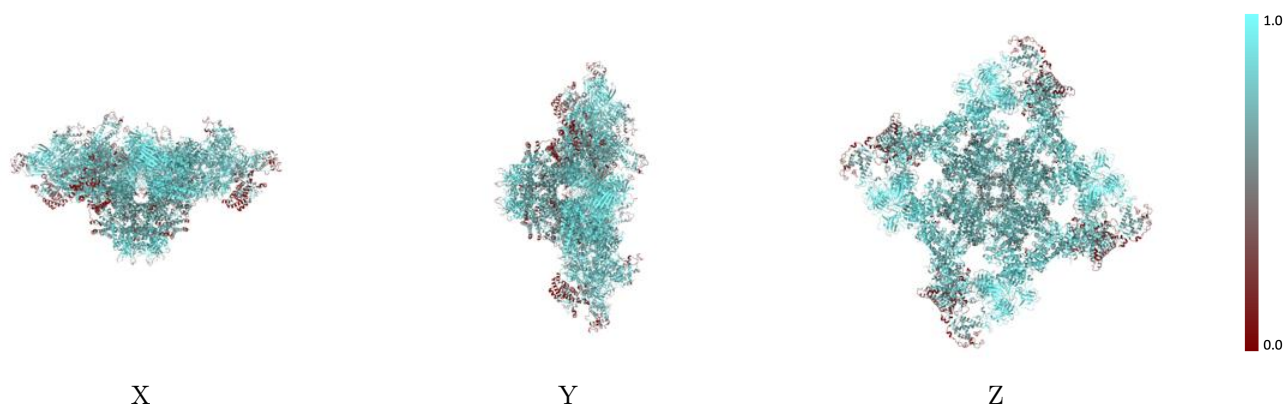
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



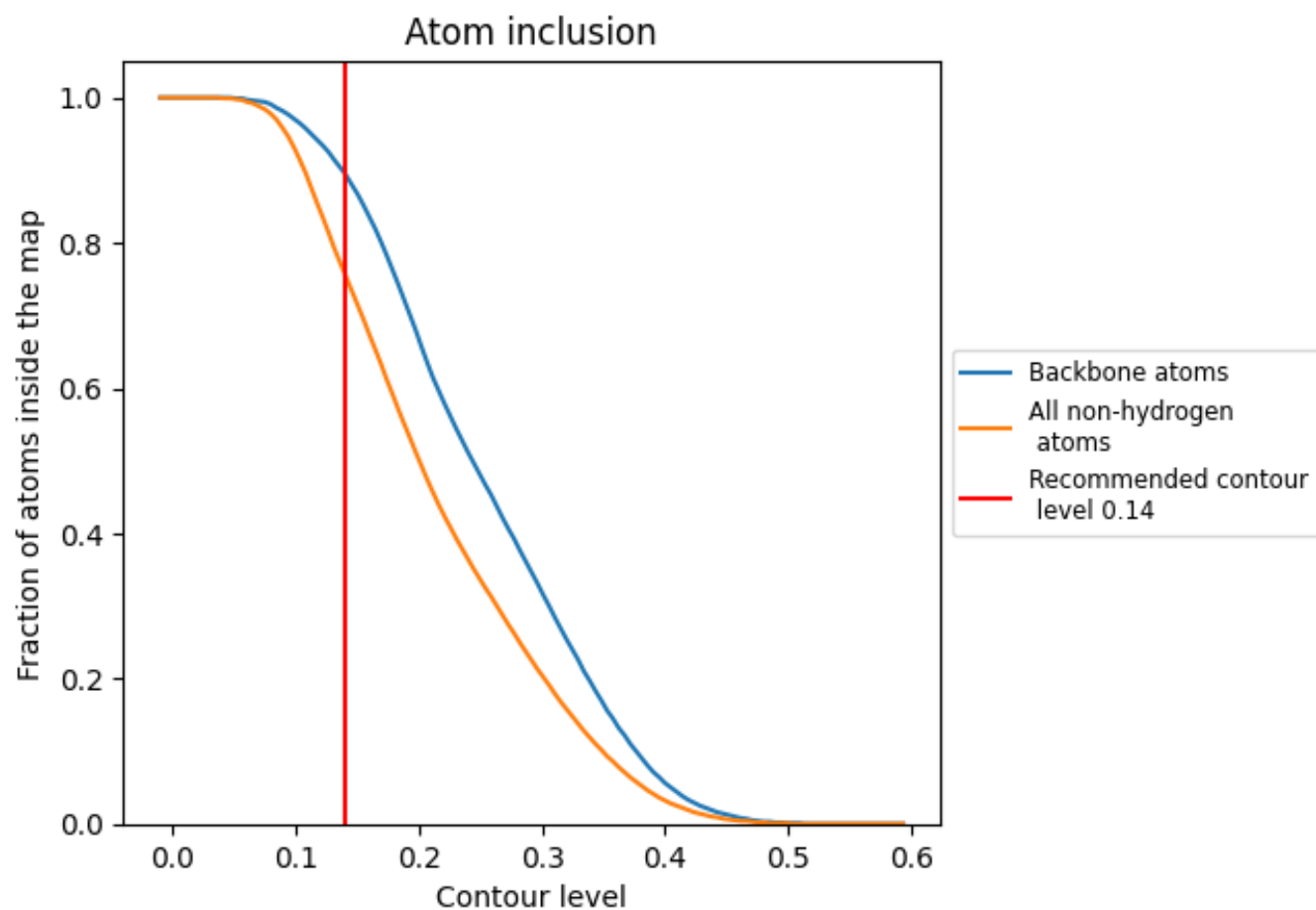
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.3810
A	0.7540	0.3840
B	0.7560	0.3860
C	0.7520	0.3800
D	0.7540	0.3820
E	0.8920	0.5130
F	0.8910	0.5110
G	0.8960	0.5120
H	0.8970	0.5110
I	0.7240	0.2220
J	0.7320	0.2220
K	0.7240	0.2220
L	0.7310	0.2190

1.0

0.0

<0.0