



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:51 PM UTC

PDB ID : 8UXL / pdb_00008uxl
EMDB ID : EMD-42768
Title : Structure of PKA phosphorylated human RyR2-R420W in the primed state
in the presence of calcium and calmodulin
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.12 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:

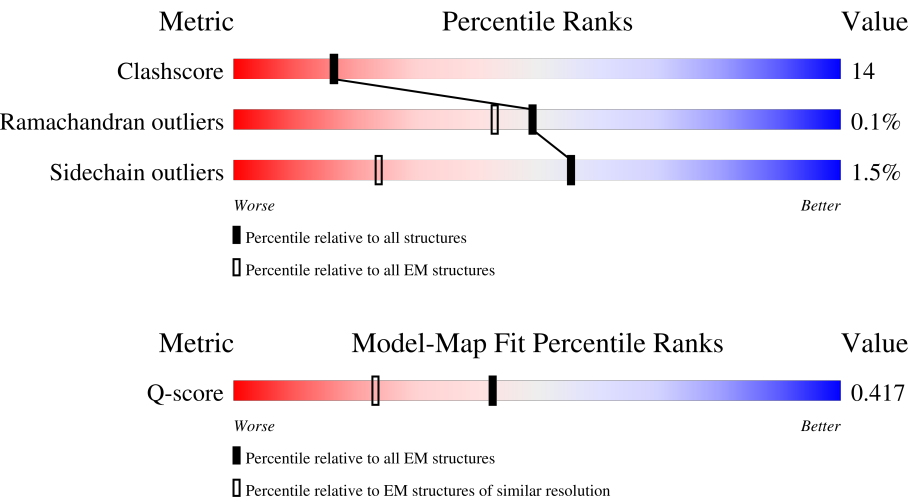
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.12 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	14478 (2.62 - 3.62)

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	7% 63% 22% • 15%
1	B	4967	7% 63% 22% • 15%
1	C	4967	7% 63% 21% • 15%
1	D	4967	7% 63% 21% • 15%

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Mol	Chain	Length	Quality of chain
2	E	108	
2	F	108	
2	G	108	
2	H	108	
3	I	149	
3	J	149	
3	K	149	
3	L	149	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 143500 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	4232	Total	C	N	O	S	2	0
			33858	21578	5766	6284	230		
1	B	4232	Total	C	N	O	S	2	0
			33858	21578	5766	6284	230		
1	C	4232	Total	C	N	O	S	2	0
			33858	21578	5766	6284	230		
1	D	4232	Total	C	N	O	S	2	0
			33858	21578	5766	6284	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 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		

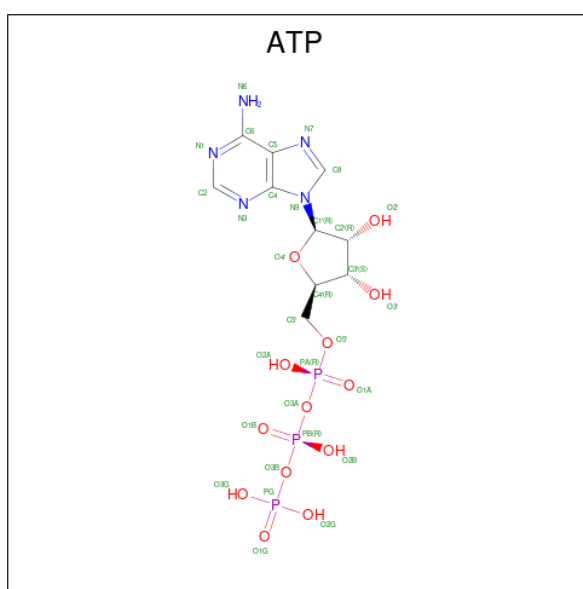
- Molecule 3 is a protein called Calmodulin-1.

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

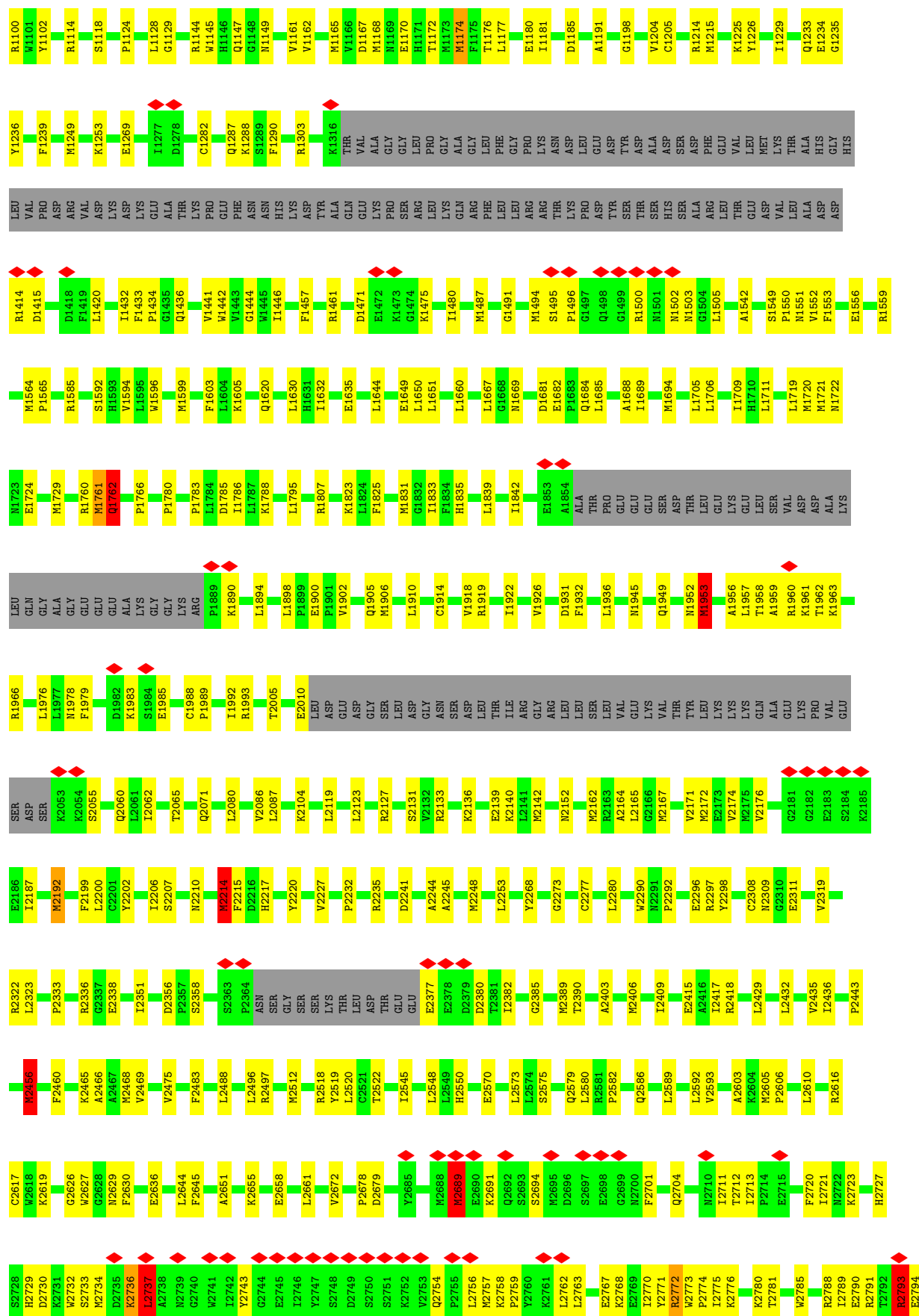
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	I	4	Total	Ca	0
			4	4	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	J	4	Total	Ca	0
			4	4	
6	L	4	Total	Ca	0
			4	4	
6	K	4	Total	Ca	0
			4	4	

3 Residue-property plots

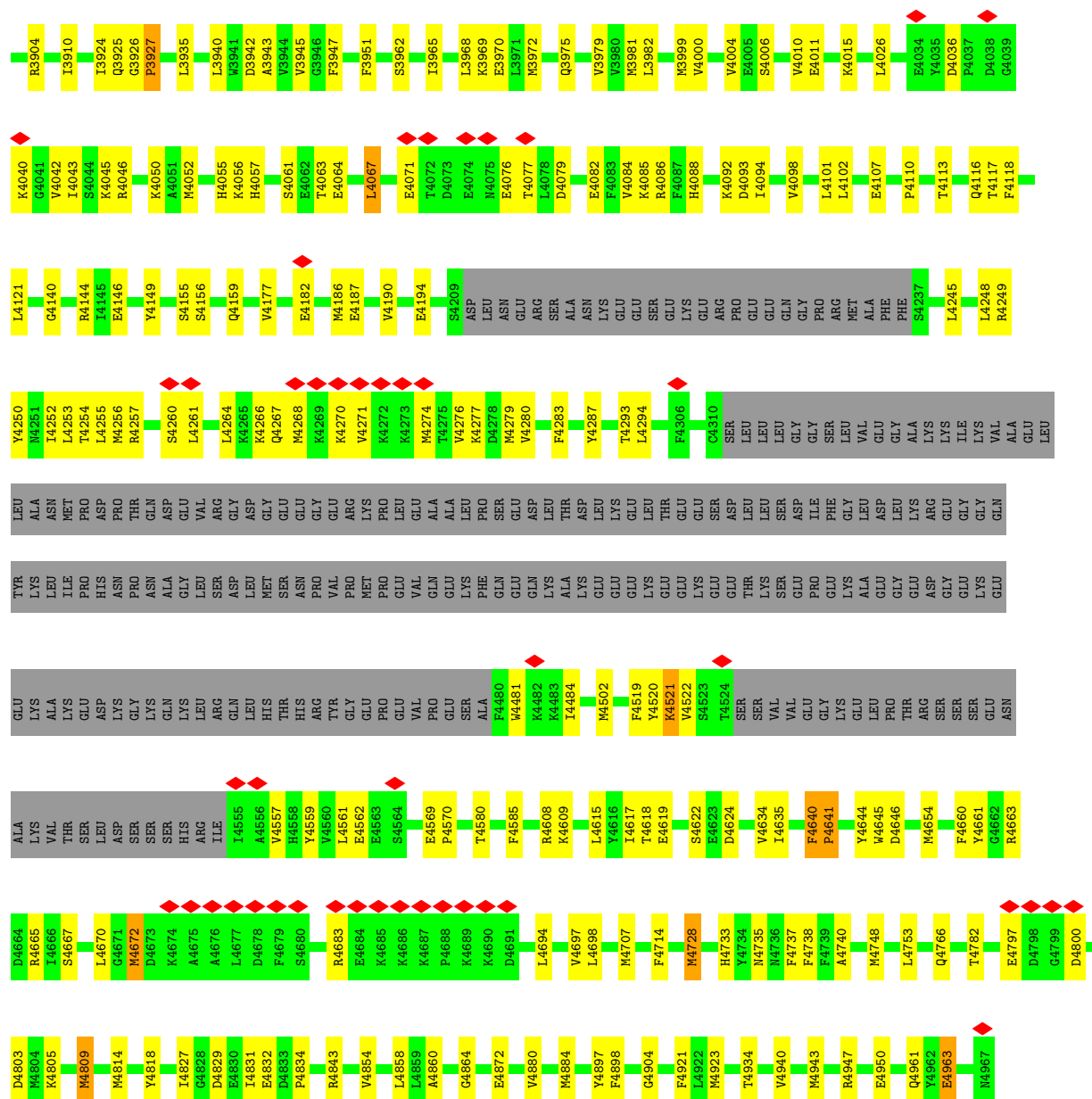
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

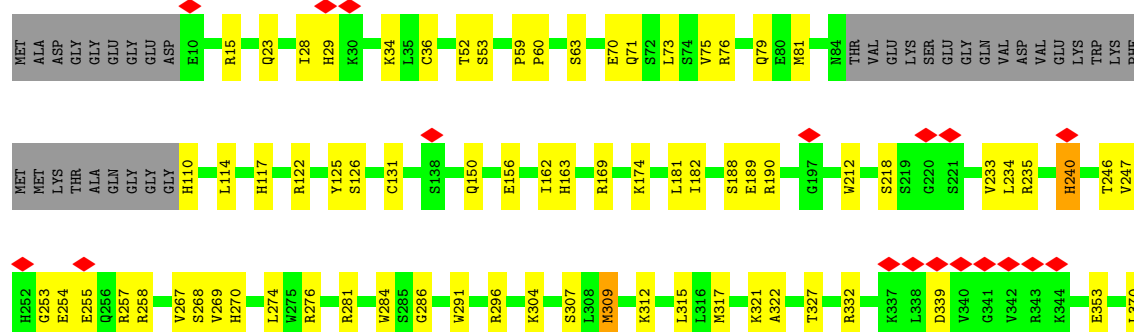




H3732	V3600	PRO	PRO	PRO	GLU	ILE	V3234	F3167	T3097	L3029	G2945	G2872	G2795
V3787	A3601	ASN	M3235	V3168	GLU	LEU	M3235	V3168	T3098	V3030	G2946	V2872	M2798
Q3791	F3603	THR	G3237	A3169	ASN	ASP	G3237	A3169	L3102	V3031	S2947	P2873	
L3796	R3604	ASP	L3238	F3170	PHE	THR	L3238	F3170	P3103	C3032	R2948	P2874	
K3797	M3605	THR	L3239	L3171	THR	THR	L3239	L3171	M3104	L3033	G2949	T2876	
	K3639	SER	P3240	E3172	LEU	THR	P3240	E3172	L3106	R3034	R2950	L2877	
	A3649	ASP	M3241	H3174	ALA	LEU	M3241	H3174	S3106	Q3038	G2951	R2886	
	P3650	PRO	C3242	L3175	ALA	ASP	C3242	L3175	S3107	T3039	E2952	R2887	
	P3651	GLY	C3243	D3176	ASP	THR	C3243	D3176	L3108	K2888	E2953	K2888	
	P3652	LYS	G3244	R3177	LEU	THR	G3244	R3177	F3109	A2889	R2954	A2889	
	E3653	VAL	M3246	H3178	ALA	THR	M3246	H3178	E3110	GLN	R2955	Q2890	
	E3654	GLU	R3247	L3180	PHE	THR	R3247	L3180	H3111	T3044	E2956	D2891	
	D3655	VAL	V3249	F3181	LEU	THR	V3249	F3181	G3112	L2892	E2957	L2892	
	E3656	LEU	E3251	T3182	ILE	THR	E3251	T3182	G3113	L2893	VAL	L2893	
	T3657	ASN	G3252	R3183	ASP	THR	G3252	R3183	H3114	K2894	SER	SER	
	K3658	LEU	H3253	N3184	VAL	THR	H3253	N3184	F3117	F2895	VAL	VAL	
	R3660	LEU	E3254	T3186	VAL	THR	E3254	T3186	G3118	E2958	SER	SER	
	V3661	THR	N3256	K3187	ASP	THR	N3256	K3187	L3121	E2959	ASP	ASP	
	L3664	HIS	N3257	S3188	THR	THR	N3257	S3188	L3122	L2960	ALA	ALA	
	H3665	LEU	F3258	S3189	ASN	THR	F3258	S3189	L3123	Y2901	ALA	ALA	
	G3666	GLU	G3259	R3190	ALA	THR	G3259	R3190	E3124	G2905	HIS	HIS	
	L3667	GLN	E3260	F3191	ALA	THR	E3260	F3191	D3125	G2906	G2820	G2820	
	L3668	LYS	R3261	R3192	THR	THR	R3261	R3192	G3126	P2823	G2821	G2821	
	E3678	LYS	A3261	A3193	LEU	THR	A3261	A3193	Q3127	A2825	A2825	A2825	
	L3687	ARG	E3262	A3194	GLY	THR	E3262	A3194	R3132	E2828	E2828	E2828	
	K3697	ARG	M3263	L3195	GLU	THR	M3263	L3195	D3067	E2829	E2829	E2829	
	S3698	THR	R3264	S3196	PRO	THR	R3264	S3196	L3061	N2830	N2830	N2830	
	H3700	TYR	C3265	L3197	ASN	THR	C3265	L3197	D3062	G2907	P2823	P2823	
	E3702	LEU	T3266	P3198	GLU	THR	T3266	P3198	K3063	K2908	R2824	R2824	
	D3701	LEU	G3267	V3201	LEU	THR	G3267	V3201	T3071	D2909	G2825	G2825	
	ASP	GLU	L3214	C3205	GLY	THR	L3214	C3205	M3072	E2918	E2828	E2828	
	ASP	GLY	M3215	E3216	VAL	THR	M3215	E3216	E3073	E2919	E2829	E2829	
	ASP	GLY	E3217	L3218	VAL	THR	E3217	L3218	N3074	E2918	E2830	E2830	
	ASP	GLY	L3219	V3219	VAL	THR	L3219	V3219	L3075	K2919	A2839	A2839	
	ASP	GLY	K3276	K3281	VAL	THR	K3276	K3281	K3076	E2840	E2840	E2840	
	ASP	GLY	L3277	L3282	VAL	THR	L3277	L3282	Q3077	R2920	A2841	A2841	
	ASP	GLY	G3278	L3283	VAL	THR	G3278	L3283	G3078	E2842	E2842	E2842	
	ASP	GLY	E3279	L3284	VAL	THR	E3279	L3284	Q3079	E2843	E2843	E2843	
	ASP	GLY	R3285	Y3285	VAL	THR	R3285	Y3285	E3080	A2844	A2844	A2844	
	ASP	GLY	N3286	E3286	VAL	THR	N3286	E3286	E3000	E2846	E2846	E2846	
	ASP	GLY	M3287	L3288	VAL	THR	M3287	L3288	K3001	E2847	E2847	E2847	
	ASP	GLY	G3289	G3289	VAL	THR	G3289	G3289	M3003	E2848	E2848	E2848	
	ASP	GLY	L3290	R3291	VAL	THR	L3290	R3291	T3004	E2849	E2849	E2849	
	ASP	GLY	E3292	E3292	VAL	THR	E3292	E3292	T3005	E2856	E2856	E2856	
	ASP	GLY	A3294	F3166	VAL	THR	A3294	F3166	F3008	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			C3009	E2856	E2856	E2856	
	ASP	GLY			VAL	THR			K3010	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			L3014	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			V3015	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			R3016	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			R3017	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			Q3092	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			L3018	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			L3019	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			D3025	E2857	E2857	E2857	
	ASP	GLY			VAL	THR			A3026	E2857	E2857	E2857	



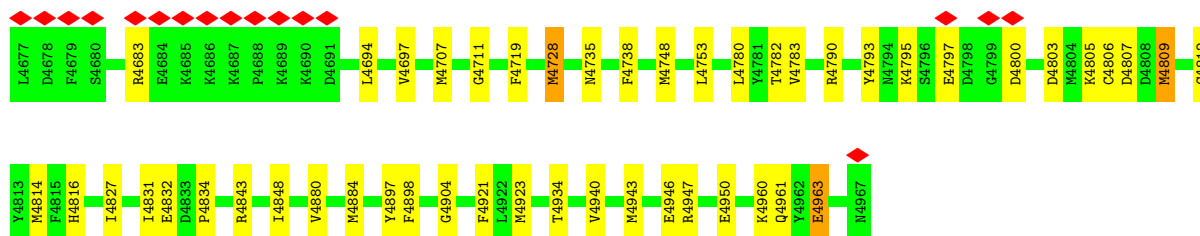
• Molecule 1: Ryanodine receptor 2



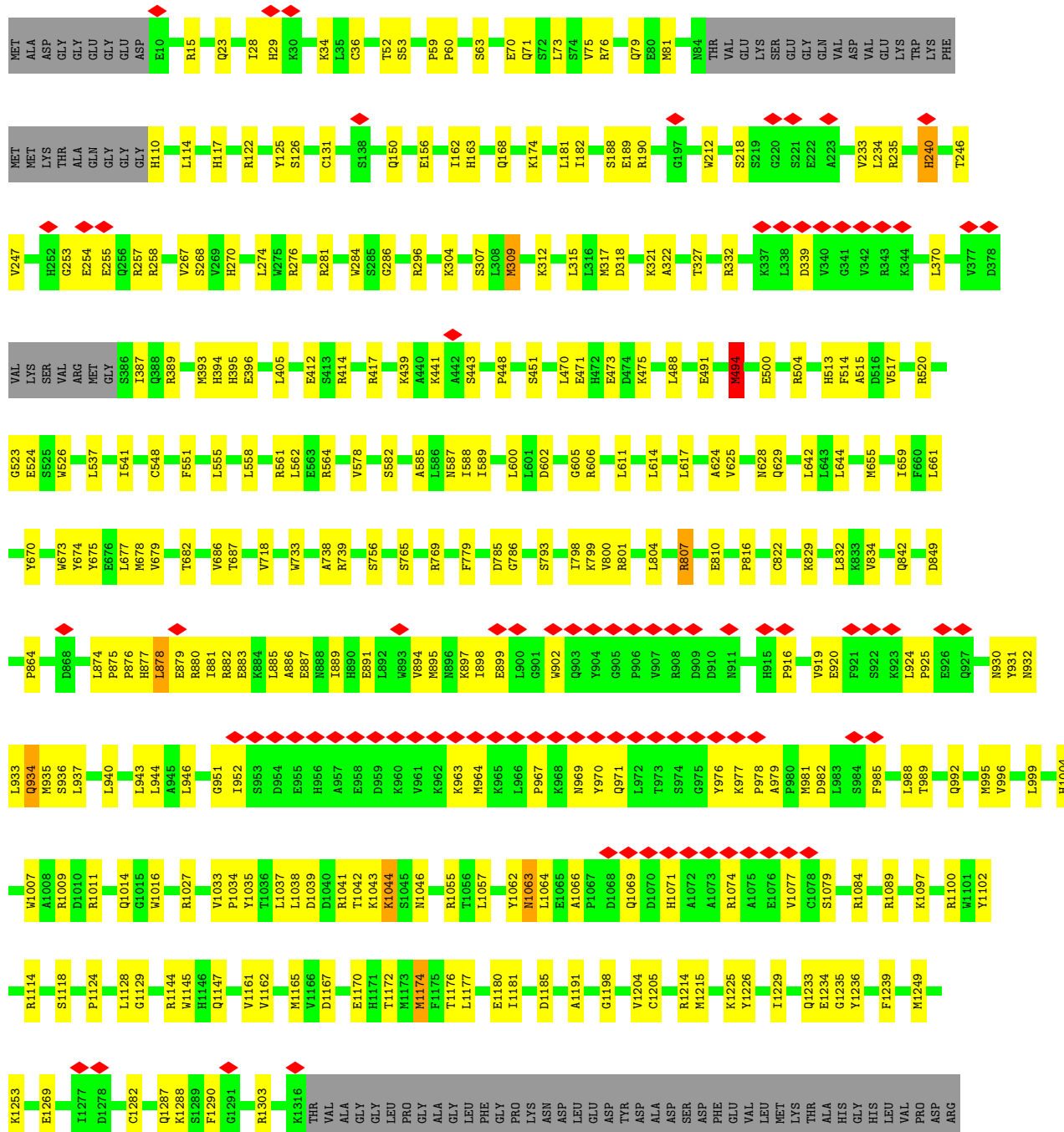




A4556	Y4559	Y4560	L4561	E4562	E4563	S4564	E4569	P4570	F4585	Y4591	R4608	K4609	L4615	L4616	L4617	E4619	S4622	F4623	D4624	D4625	I4626	V4634	I4635	F4640	P4641	Y4644	W4645	D4646	K4647	M4654	F4660	Y4661	G4662	D4663	D4664	R4665	I4666	S4667	L4670	G4671	D4672	D4673	K4674	A4675	A4676																																																																																																																																																																																																																																																																																																																																																																																																																					
HIS	ARG	TYR	GLY	GLY	PRO	VAL	PRO	GLN	GLY	SER	ALA	F4480	W4481	T4484	Y4487	L4491	M4502	L4518	F4519	Y4520	K4521	T4524	SER	SER	VAL	VAL	GLY	LYS	GLY	PRO	THR	SER	SER	GLY	ASN	LYS	THR	ARG	SER	SER	SER	HIS	ARG	ILE	L4555																																																																																																																																																																																																																																																																																																																																																																																																																					
ASN	PRO	VAL	PRO	MET	PRO	GLY	VAL	GLN	GLY	LYS	PHE	GLN	GLY	GLN	LYS	GLY	GLY	GLY	THR	LYS	GLY	GLY	GLY	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR																																																																																																																																																																																																																																																																																																																																																																																																																							
GLU	GLY	GLU	ARG	LYS	PRO	LEU	GLU	ALA	ALA	PRO	SER	GLU	GLU	ASP	THR	LYS	ASP	LEU	LEU	LEU	GLY	ILE	PHE	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																							
S4260	L4261	L4264	K4265	K4266	Q4267	M4268	K4269	K4270	Y4271	K4272	K4273	M4274	V4275	T4276	K4277	D4278	M4279	T4293	C4310	SER	LEU	LEU	LEU	LEU	GLY	VAL	GLY	GLY	ASP	GLY	LYS	ALA	LEU	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																						
G4140	R4144	I4145	E4146	Y4149	S4155	S4156	Q4159	V4177	M4186	E4187	V4190	E4194	S4209	ASP	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																							
G4041	V4042	I4043	K4045	R4046	K4050	A4051	M4052	H4055	K4056	H4057	S4061	E4062	T4063	E4064	L4067	E4071	T4072	D4073	E4074	H4075	E4076	T4077	L4078	D4079	E4082	F4083	V4084	K4085	R4086	F4087	H4088	K4092	D4093	I4094	V4098	L4101	L4102	E4107	P4110	T4113	Q4116	T4117	F4118	L4121																																																																																																																																																																																																																																																																																																																																																																																																																						
R3904	I3910	Q3925	G3926	P3927	L3935	L3940	D3942	A3943	V3945	G3946	F3947	F3951	S3962	I3965	L3968	K3969	E3970	L3971	M3972	Q3975	V3979	V3980	M3981	L3982	M3999	V4000	V4004	E4005	S4006	V4010	E4011	K4015	K4022	L4026	E4034	Y4035	D4036	K4040																																																																																																																																																																																																																																																																																																																																																																																																																												
L3731	H3732	V3787	Q3791	R3792	L3793	M3797	L3803	D3804	L3805	F3808	L3817	G3818	M3819	V3820	T3821	E3822	E3823	G3824	S3825	G3826	E3827	L3828	V3829	L3830	D3833	L3845	L3846	C3847	E3848	F3854	L3870	L3879	Q3882	E3883	S3884	D3887	F3888	Y3889	Y3891	Y3892	K3895	D3899	E3900																																																																																																																																																																																																																																																																																																																																																																																																																							
L3591	K3596	C3602	M3605	K3639	A3649	E3650	P3651	P3652	E3653	E3654	D3655	E3656	G3657	T3658	K3659	R3660	V3661	L3664	H3665	Q3666	L3667	I3668	E3678	L3687	K3697	S3698	C3699	H3700	D3701	E3702	GLU	ASP	ASP	GLY	GLY	GLY	E3710	V3711	K3717	E3718	M3719	Q3722	A3729	R3730																																																																																																																																																																																																																																																																																																																																																																																																																						
LEU	TYR	LYS	ASP	PRO	ASN	THR	ASP	THR	ASP	THR	THR	VAL	GLU	VAL	ASP	ILE	ALA	ASN	VAL	VAL	PHE	HIS	LEU	GLN	LYS	LYS	VAL	ARG	VAL	GLY	HIS	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																					
HIS	ASN	PHE	LYS	ARG	GLU	GLU	GLN	ASN	PHE	VAL	VAL	GLN	ASN	TYR	PHE	TYR	ILE	ASN	THR	LYS	THR	ILE	ALA	ASP	GLY	VAL	SER	LYS	MET	ASN	ASN	THR	LYS	ALA	LYS	GLN	GLY	ASP	THR	ILE	THR	TYR	TRP	GLN	VAL	LYS	ALA	ARG	GLY	ASP	MET	SER																																																																																																																																																																																																																																																																																																																																																																																																														
LEU	LYS	ARG	LEU	LEU	PRO	ILE	GLY	ASN	ASN	CYS	ALA	PRO	GLY	ASP	GLN	GLY	VAL	ASN	PHE	SER	LYS	ASN	PHE	GLY	ASP	VAL	SER	LYS	MET	ASN	THR	LYS	ALA	VAL	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY



• Molecule 1: Ryanodine receptor 2





Q3925	G3926	F3927	L3935	L3940	A3943	V3944	G3945	F3947	F3951	S3962	I3965	K3969	E3970	L3971	K3972	Q3975	V3979	V3980	K3981	L3982	K3999	V4000	V4004	E4005	S4006	V4010	E4011	K4015	L4026	T4027	E4034	V4035	D4036	F4037	D4038	G4039	K4040	G4041	V4042	I4043	S4044	K4045	R4046																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L3793	M3797	D3804	L3805	F3808	L3817	G3818	M3819	V3820	T3821	E3822	E3823	G3824	S3825	E3827	K3828	V3829	L3830	D3833	L3845	L3846	C3847	E3848	F3854	I3870	L3879	Q3882	E3883	S3884	D3887	F3888	V3889	Y3891	Y3892	K3895	D3899	E3900	R3904	K3908	A3909	I3910																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
R3604	M3605	K3639	A3649	E3650	P3651	P3652	E3653	E3654	D3655	E3656	T3658	K3659	R3660	V3661	L3664	H3665	Q3666	L3667	I3668	L3687	K3697	S3698	G3699	H3700	D3701	E3702	GLU	ASP	ASP	GLY	GLU	E3710	V3711	S3712	K3717	E3718	M3719	Q3722	A3729	R3730	L3731	H3732	V3787	Q3791	S3792																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
GLY	LEU	ASN	ILE	VAL	CYS	ALA	ASN	PRO	GLY	ASP	GLN	ASN	LEU	ILE	ALA	LEU	ASN	ASP	ARG	PHE	SER	THR	LEU	LEU	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
GLN	ASN	PHE	VAL	GLN	ASN	ALA	ASN	ALA	ILE	ASP	ASN	MET	ALA	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
ASP	GLU	PHE	THR	THR	LEU	ALA	ASP	ARG	ASP	ASP	ASP	THR	THR	PRO	PRO	LEU	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
K3297	K3298	L3299	A3300	V3234	M3235	E3236	V3237	L3238	L3239	P3240	M3241	C3242	L3243	S3244	Y3245	S3246	S3247	L3248	K3249	S3250	E3251	H3252	E3255	N3256	K3257	F3258	L3259	E3259	R3260	A3261	E3262	M3263	S3264	C3265	N3269	H3272	M3273	N3274	T3275	L3276	L3277	G3278	N3279	L3280	L3281	K3282	L3283	L3284	Y3285	N3286	N3287	L3288	G3289	L3290	D3291	E3292	L3293	L3294	L3295	L3296	T3297	L3298	Q3230																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR</





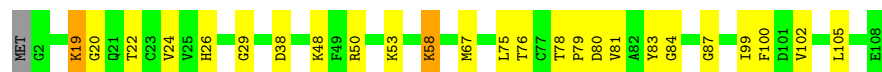


[illegible]



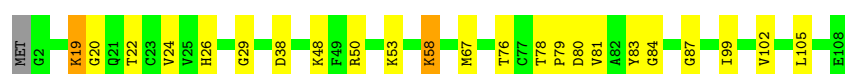
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 76% 21% ..



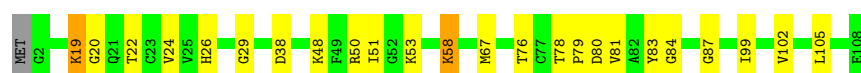
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 78% 19% ..



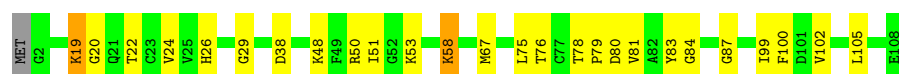
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 77% 20% ..



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

Chain H: 75% 22% ..



- Molecule 3: Calmodulin-1

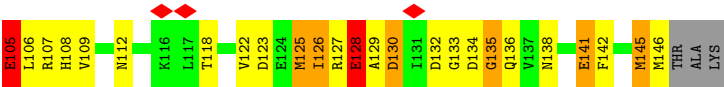
Chain I: 59% 31% 5% ..



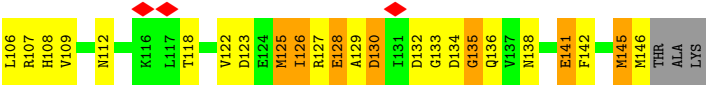
- Molecule 3: Calmodulin-1

Chain J: 56% 34% 5% ..

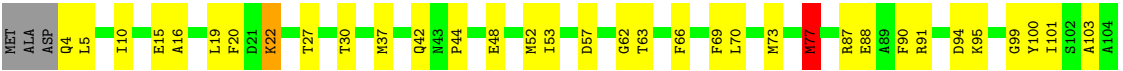




• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77625	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	0.637	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	A	0.23	9/34603 (0.0%)	0.50	28/46734 (0.1%)
1	B	0.23	9/34603 (0.0%)	0.50	27/46734 (0.1%)
1	C	0.23	9/34603 (0.0%)	0.50	28/46734 (0.1%)
1	D	0.23	9/34603 (0.0%)	0.50	28/46734 (0.1%)
2	E	0.17	0/834	0.46	0/1123
2	F	0.17	0/834	0.46	0/1123
2	G	0.17	0/834	0.46	0/1123
2	H	0.17	0/834	0.46	0/1123
3	I	0.35	0/1143	0.77	5/1534 (0.3%)
3	J	0.36	0/1143	0.76	5/1534 (0.3%)
3	K	0.36	0/1143	0.76	5/1534 (0.3%)
3	L	0.35	0/1143	0.77	5/1534 (0.3%)
All	All	0.24	36/146320 (0.0%)	0.51	131/197564 (0.1%)

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	8
1	B	0	8
1	C	0	8
1	D	0	8
All	All	0	32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3244	SER	CA-C	11.83	1.68	1.52
1	A	3244	SER	CA-C	11.79	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3244	SER	CA-C	11.78	1.68	1.52
1	B	3244	SER	CA-C	11.78	1.68	1.52
1	B	3164	GLY	CA-C	10.25	1.66	1.51

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3247	SER	CA-C-N	-14.93	100.28	120.28
1	D	3247	SER	C-N-CA	-14.93	100.28	120.28
1	A	3247	SER	CA-C-N	-14.91	100.30	120.28
1	A	3247	SER	C-N-CA	-14.91	100.30	120.28
1	B	3247	SER	CA-C-N	-14.90	100.31	120.28

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3058	ARG	Sidechain
1	A	3162	PHE	Peptide
1	A	3163	ALA	Peptide
1	A	3244	SER	Peptide,Mainchain
1	A	3247	SER	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	A	33858	0	33562	983	0
1	B	33858	0	33562	986	0
1	C	33858	0	33562	969	0
1	D	33858	0	33562	971	0
2	E	818	0	821	16	0
2	F	818	0	821	16	0
2	G	818	0	821	18	0
2	H	818	0	821	18	0
3	I	1131	0	1059	44	0
3	J	1131	0	1059	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1131	0	1059	50	0
3	L	1131	0	1059	49	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
5	A	62	0	24	0	0
5	B	62	0	24	0	0
5	C	62	0	24	0	0
5	D	62	0	24	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	4	0	0	2	0
6	J	4	0	0	2	0
6	K	4	0	0	2	0
6	L	4	0	0	2	0
All	All	143500	0	141864	4025	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 14.

The worst 5 of 4025 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3165:ALA:N	1:C:3244:SER:O	1.63	1.32
1:B:3165:ALA:N	1:B:3244:SER:O	1.63	1.31
1:A:3165:ALA:H	1:A:3244:SER:C	1.39	1.29
1:D:3165:ALA:N	1:D:3244:SER:O	1.63	1.29
1:B:3165:ALA:H	1:B:3244:SER:C	1.39	1.28

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	4206/4967 (85%)	4072 (97%)	130 (3%)	4 (0%)	48	77
1	B	4206/4967 (85%)	4072 (97%)	130 (3%)	4 (0%)	48	77
1	C	4206/4967 (85%)	4074 (97%)	128 (3%)	4 (0%)	48	77
1	D	4206/4967 (85%)	4073 (97%)	129 (3%)	4 (0%)	48	77
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
3	I	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
3	J	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
3	K	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
3	L	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
All	All	17808/20896 (85%)	17243 (97%)	549 (3%)	16 (0%)	49	77

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2793	ARG
1	A	2988	ARG
1	A	3927	PRO
1	A	4641	PRO
1	B	2793	ARG

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	3716/4358 (85%)	3667 (99%)	49 (1%)	61	75
1	B	3716/4358 (85%)	3667 (99%)	49 (1%)	61	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	3716/4358 (85%)	3667 (99%)	49 (1%)	61	75
1	D	3716/4358 (85%)	3667 (99%)	49 (1%)	61	75
2	E	88/89 (99%)	86 (98%)	2 (2%)	44	68
2	F	88/89 (99%)	86 (98%)	2 (2%)	44	68
2	G	88/89 (99%)	86 (98%)	2 (2%)	44	68
2	H	88/89 (99%)	86 (98%)	2 (2%)	44	68
3	I	123/127 (97%)	114 (93%)	9 (7%)	13	38
3	J	123/127 (97%)	114 (93%)	9 (7%)	13	38
3	K	123/127 (97%)	114 (93%)	9 (7%)	13	38
3	L	123/127 (97%)	114 (93%)	9 (7%)	13	38
All	All	15708/18296 (86%)	15468 (98%)	240 (2%)	55	73

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	81	MET
3	J	145	MET
1	C	2843	MET
3	J	128	GLU
3	K	126	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 182 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2978	HIS
1	D	1069	GLN
1	C	3318	HIS
1	C	4579	HIS
1	D	1615	GLN

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
5	ATP	D	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	A	5004	-	32,33,33	0.26	0	48,52,52	0.28	0
5	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	B	5004	-	32,33,33	0.25	0	48,52,52	0.29	0
5	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	C	5004	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	D	5004	-	32,33,33	0.26	0	48,52,52	0.28	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
5	ATP	D	5002	-	-	8/22/38/38	0/3/3/3
5	ATP	A	5004	-	-	11/22/38/38	0/3/3/3
5	ATP	C	5002	-	-	8/22/38/38	0/3/3/3
5	ATP	B	5004	-	-	11/22/38/38	0/3/3/3
5	ATP	A	5002	-	-	8/22/38/38	0/3/3/3
5	ATP	B	5002	-	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	C	5004	-	-	11/22/38/38	0/3/3/3
5	ATP	D	5004	-	-	11/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

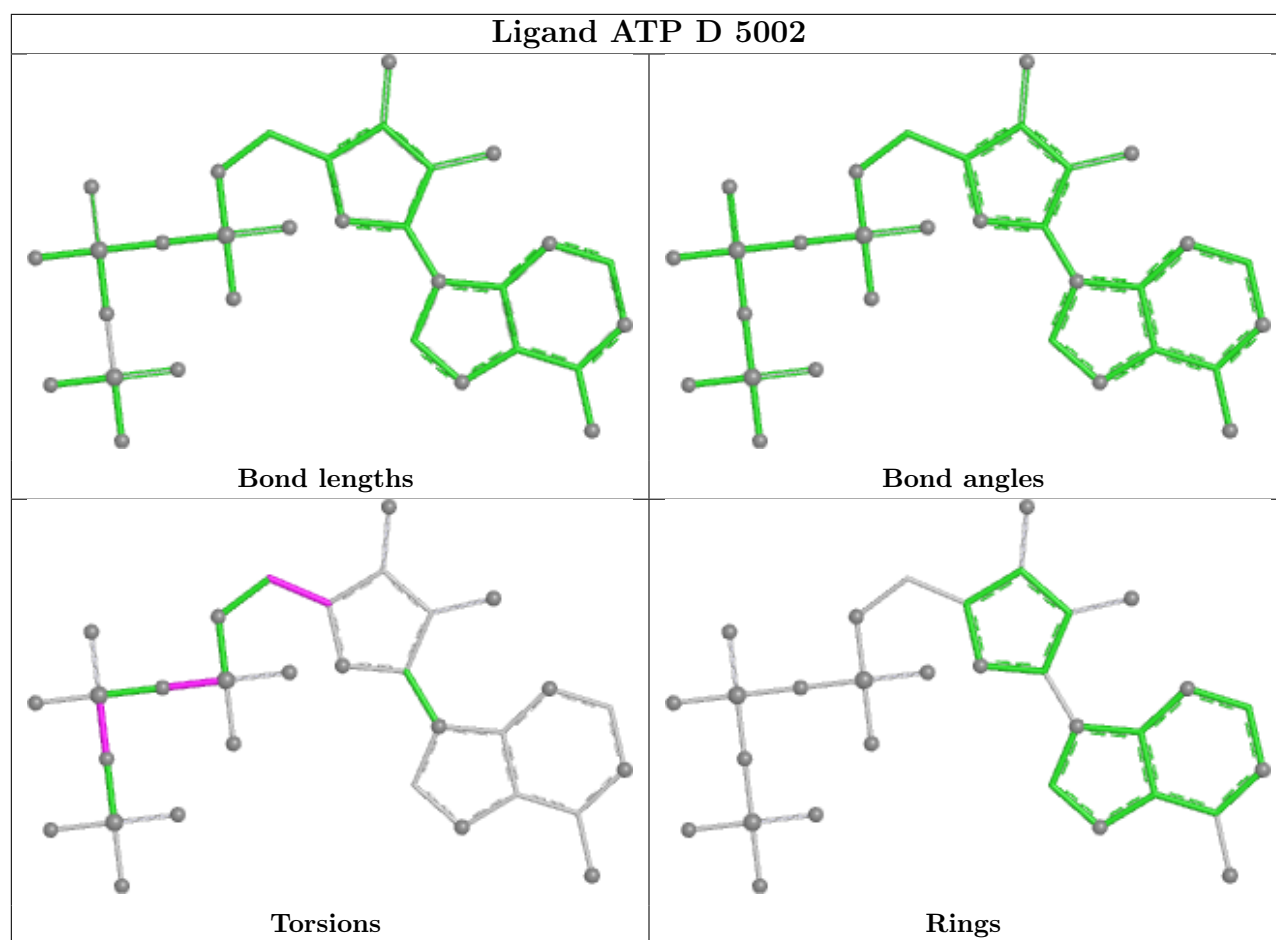
5 of 76 torsion outliers are listed below:

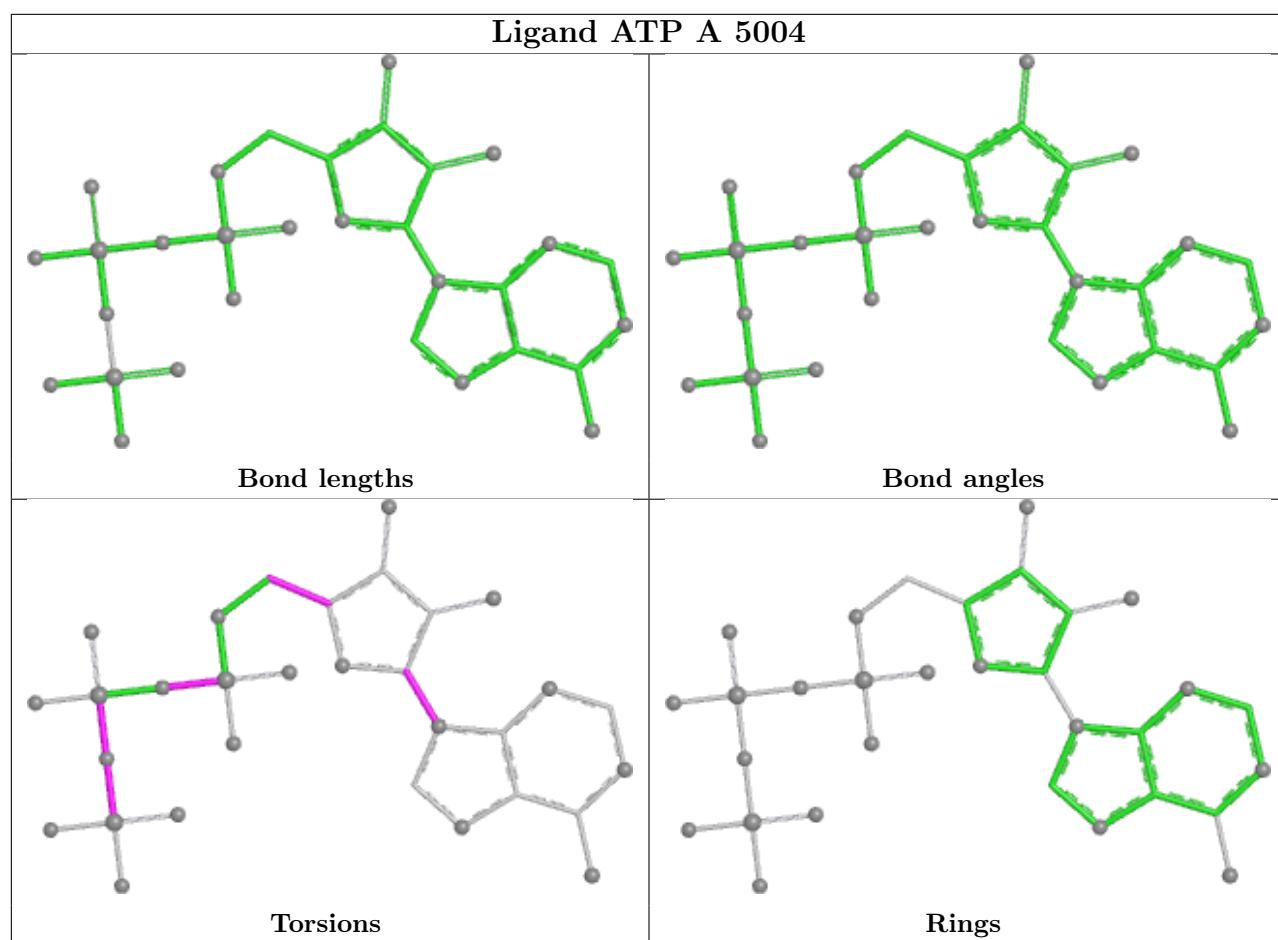
Mol	Chain	Res	Type	Atoms
5	A	5002	ATP	PB-O3A-PA-O5'
5	A	5004	ATP	PB-O3A-PA-O5'
5	B	5002	ATP	PB-O3A-PA-O5'
5	B	5004	ATP	PB-O3A-PA-O5'
5	C	5002	ATP	PB-O3A-PA-O5'

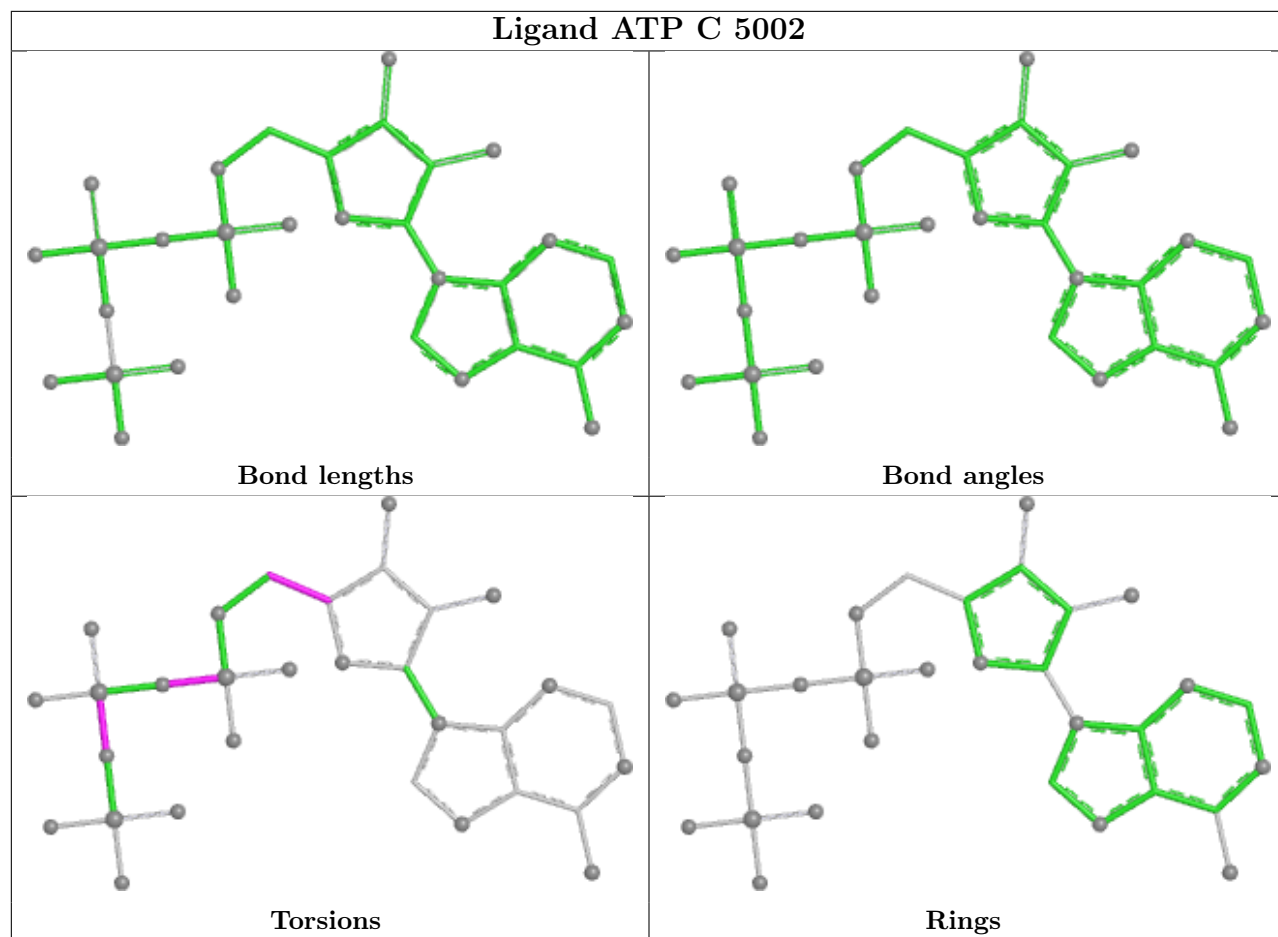
There are no ring outliers.

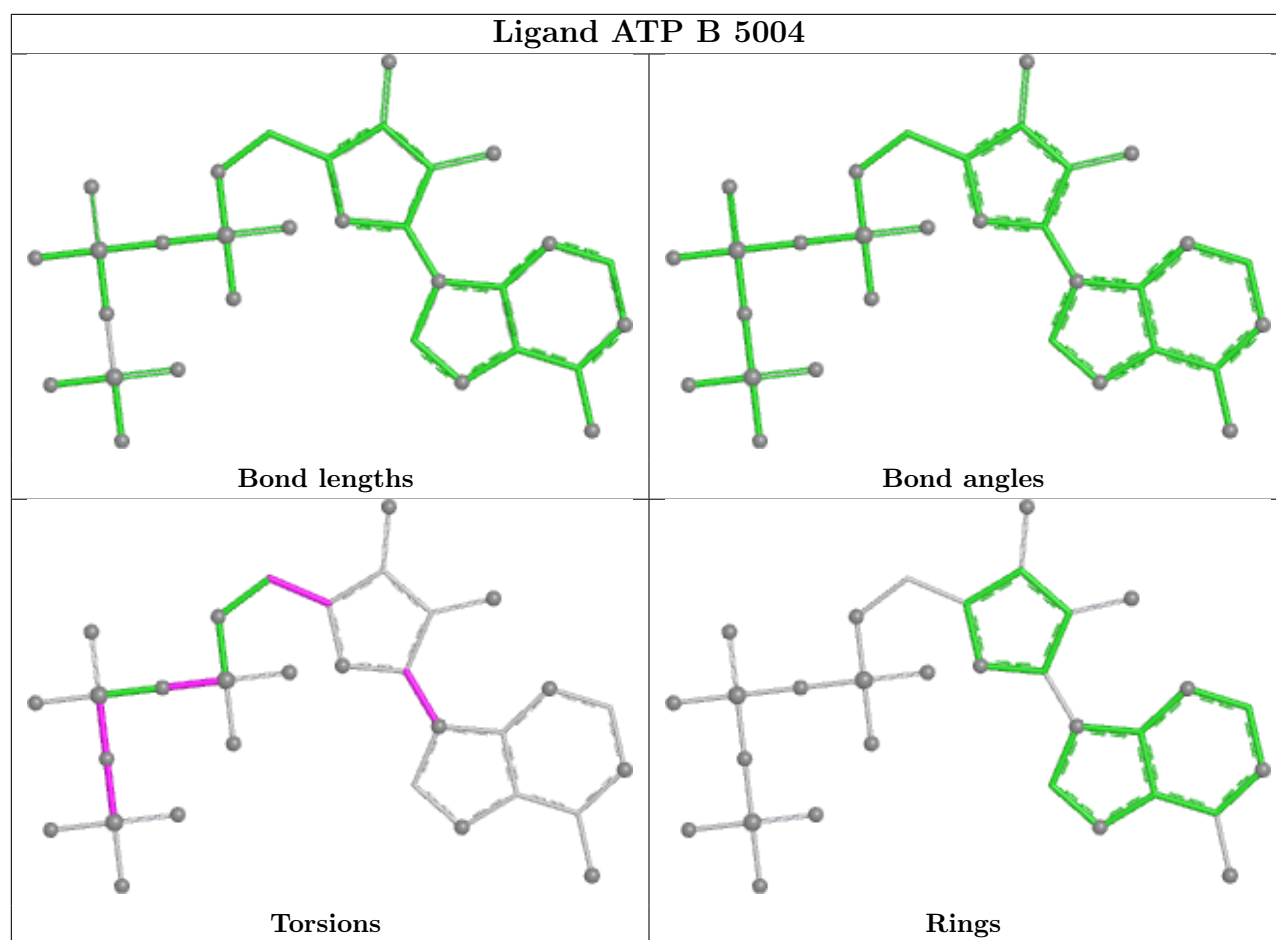
No monomer is involved in short contacts.

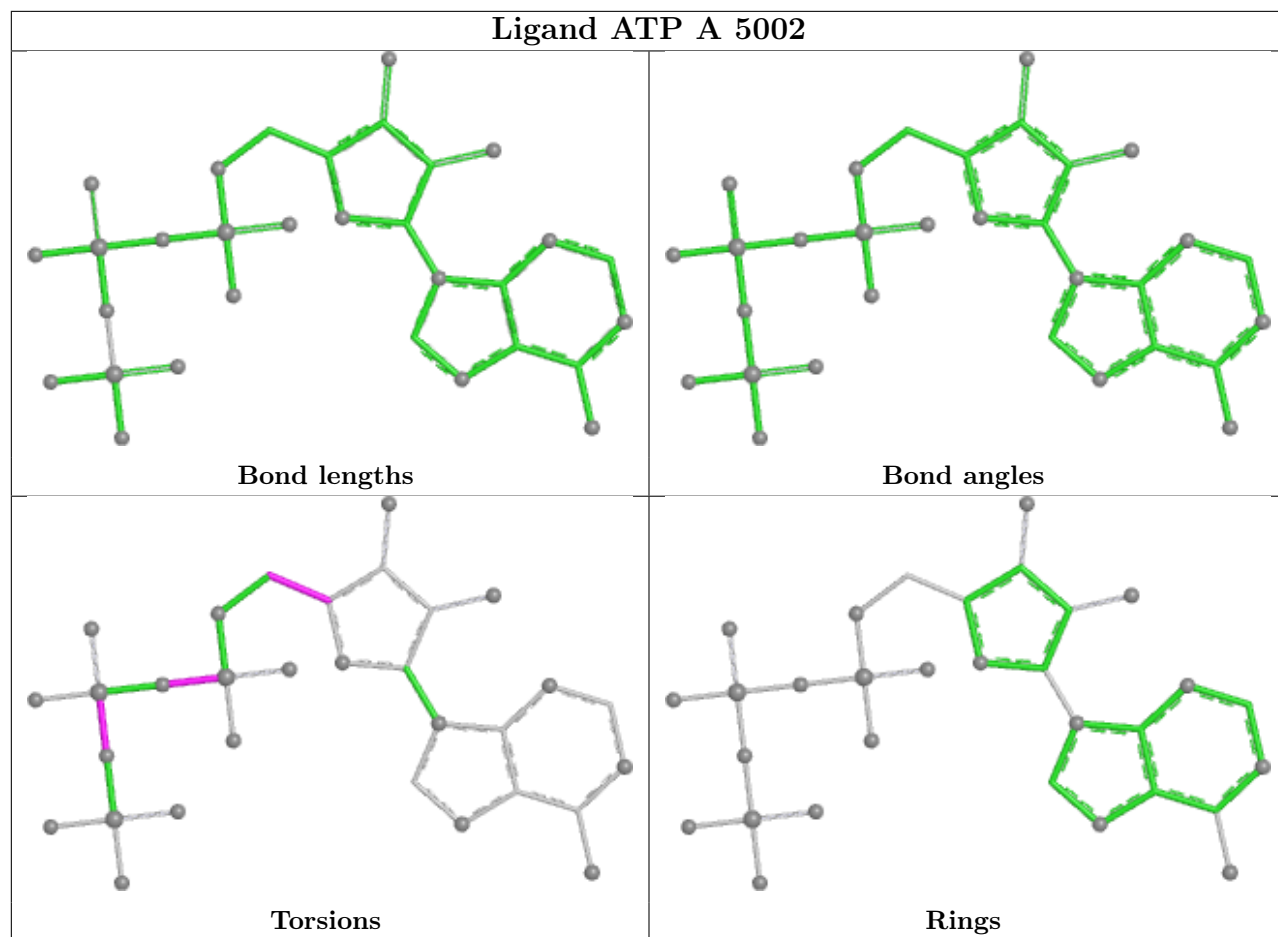
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

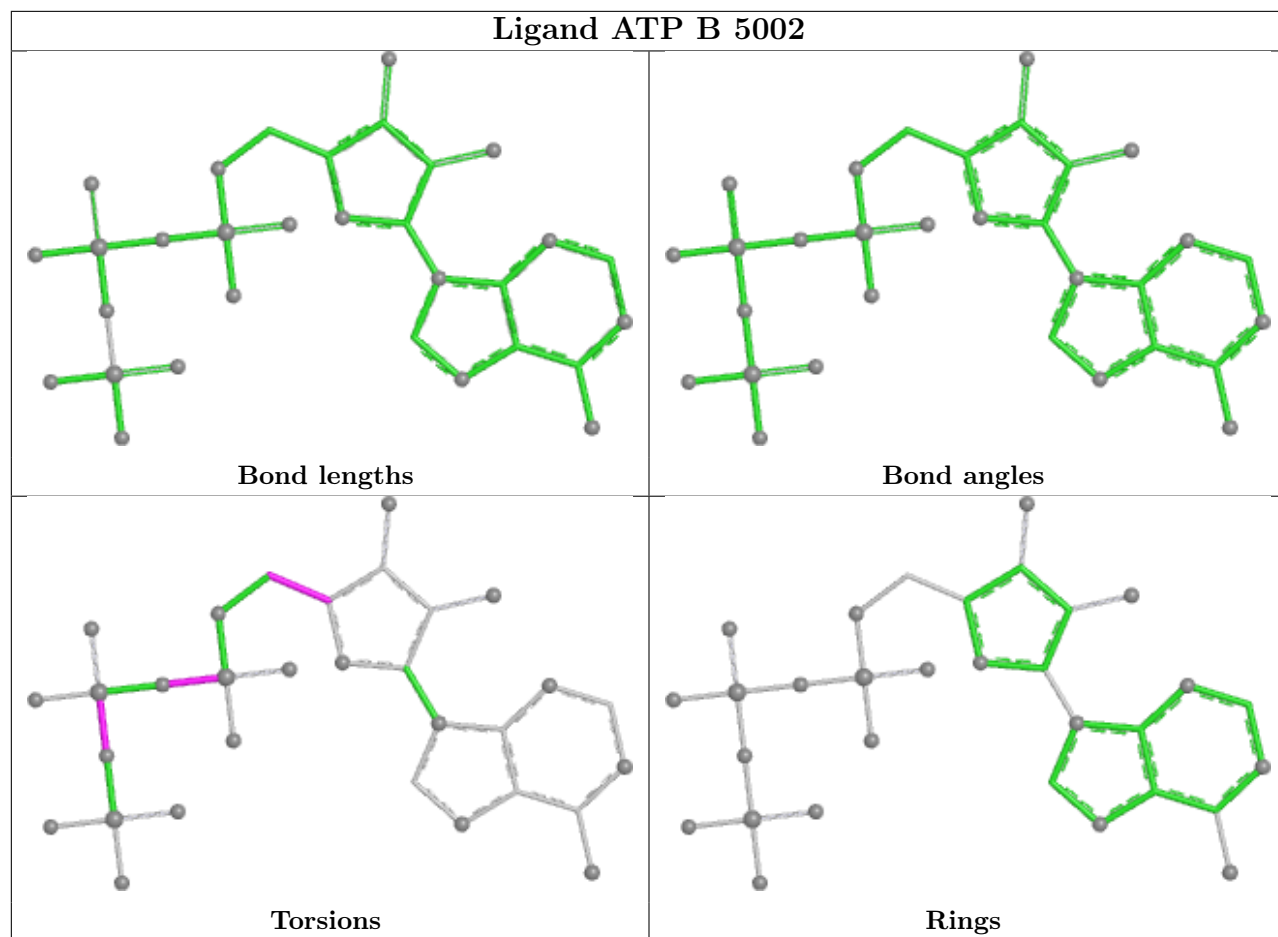


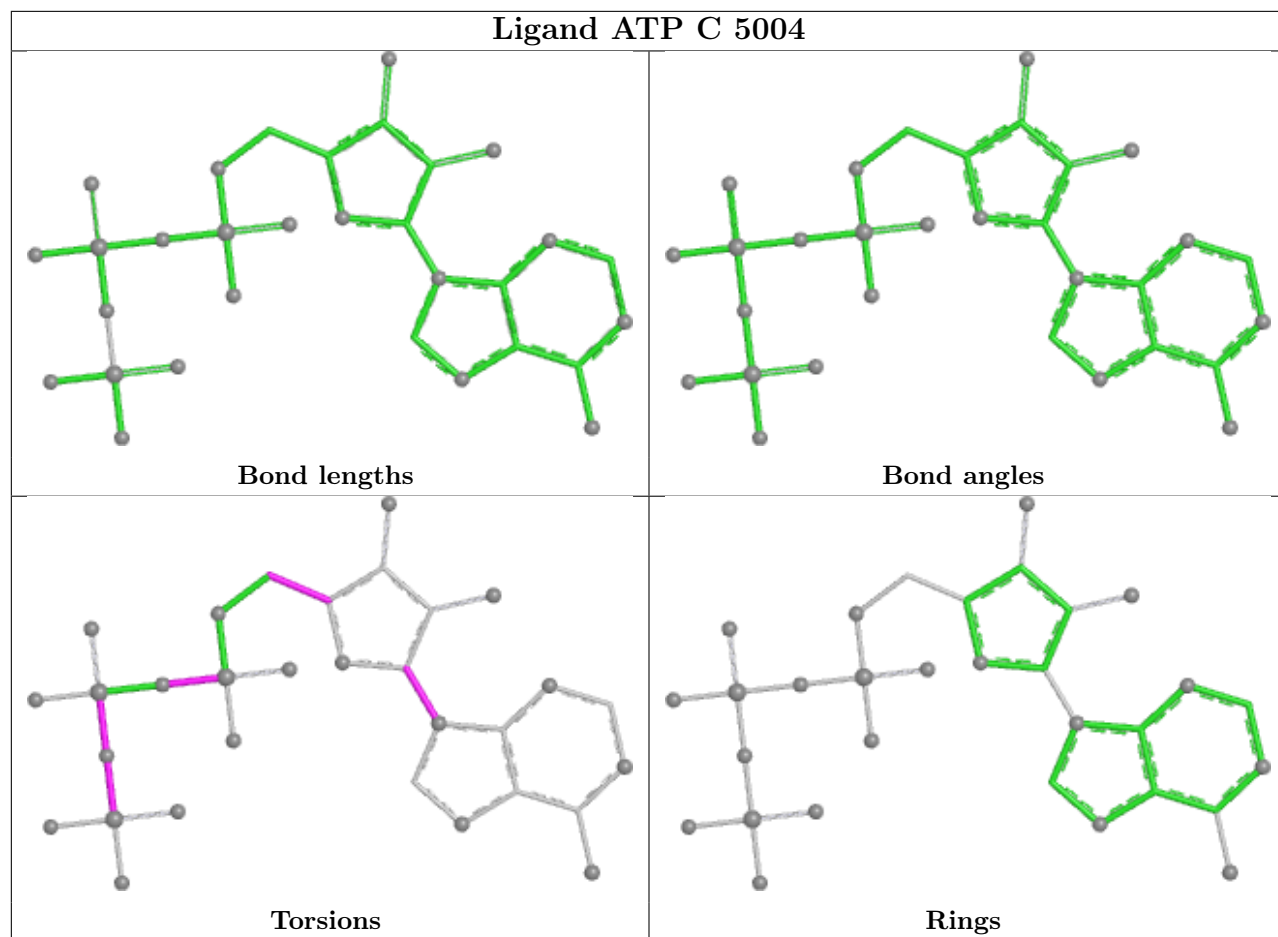


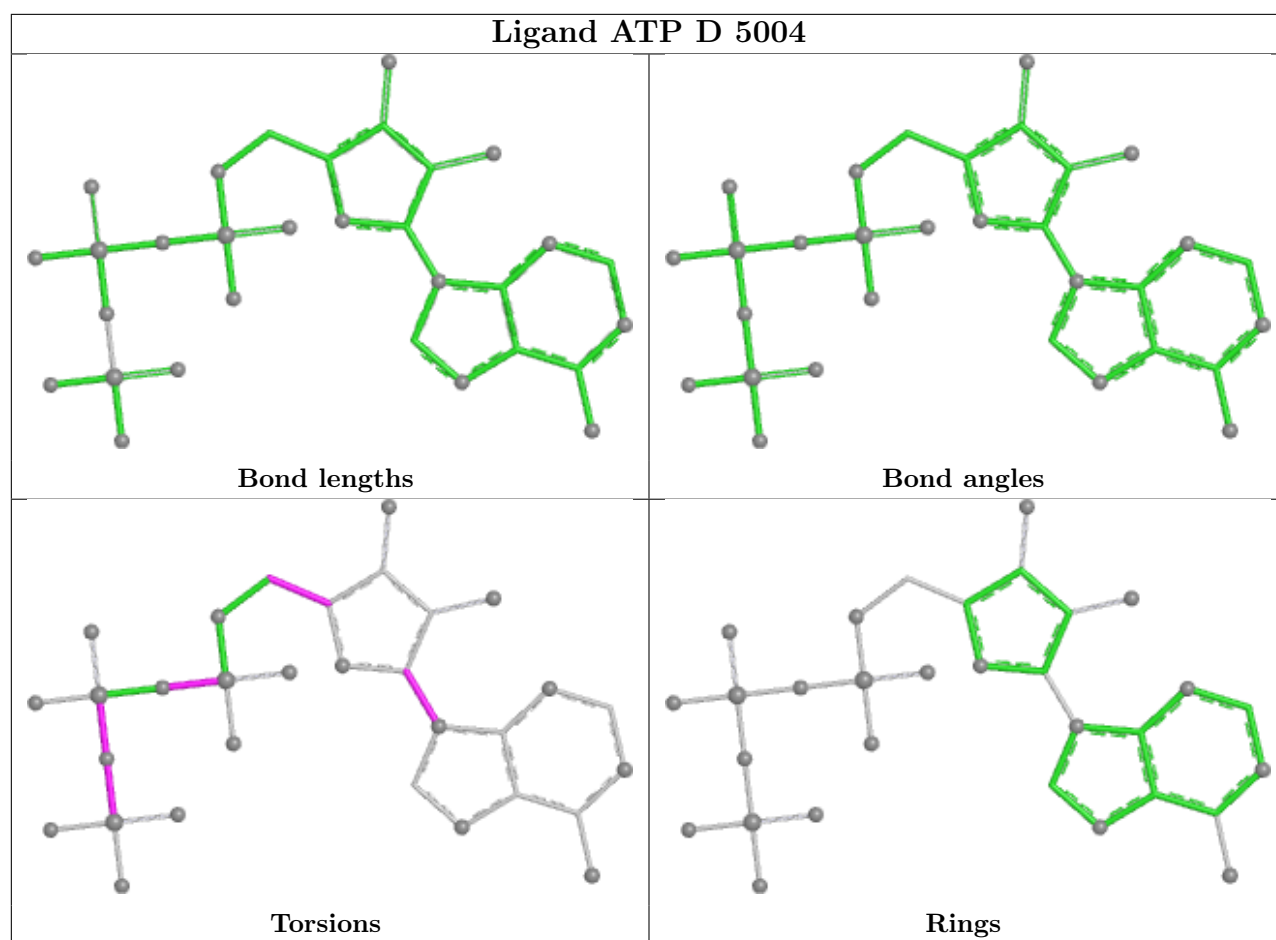












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

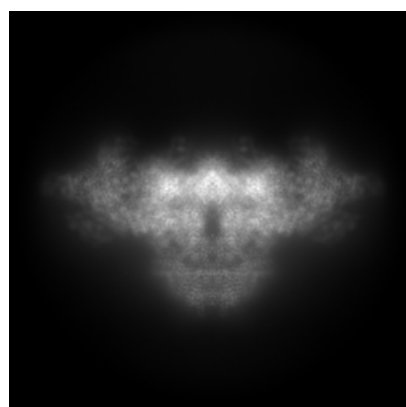
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42768. These allow visual inspection of the internal detail of the map and identification of artifacts.

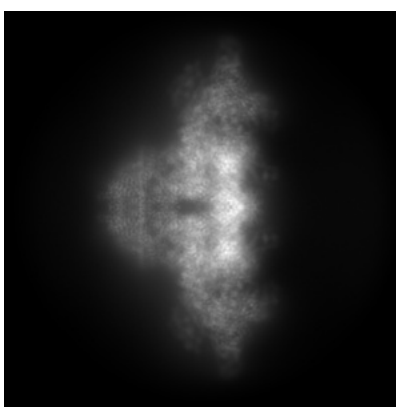
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

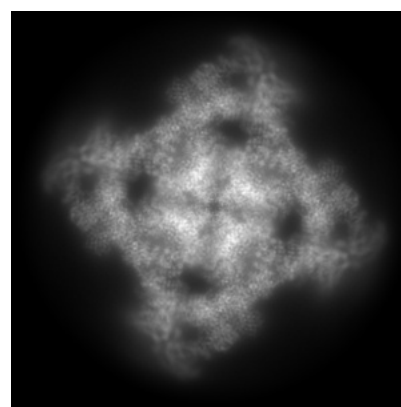
6.1.1 Primary map



X



Y



Z

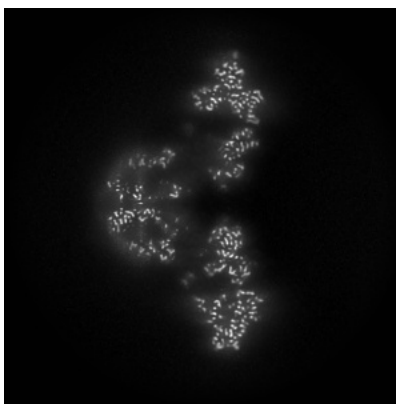
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

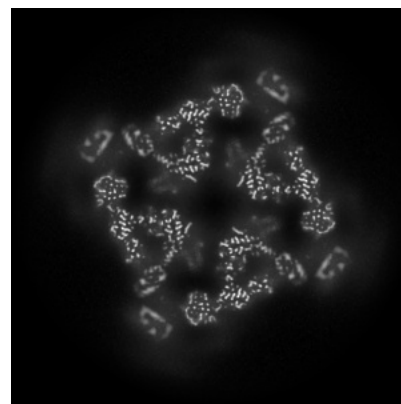
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

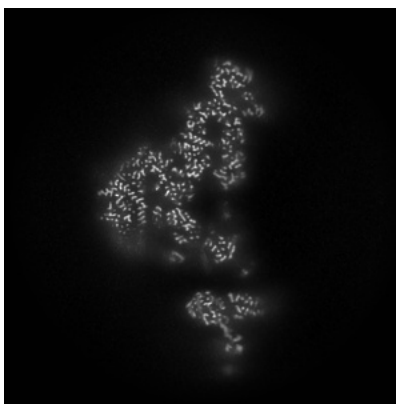
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

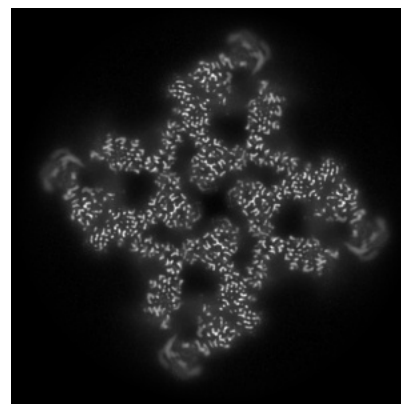
6.3.1 Primary map



X Index: 278



Y Index: 278

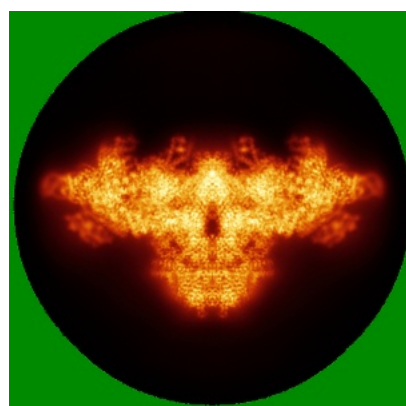


Z Index: 285

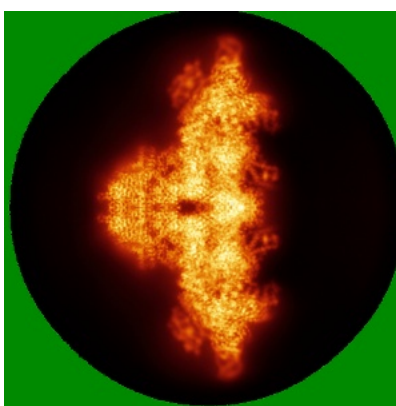
The images above show the largest variance slices of the map in three orthogonal directions.

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

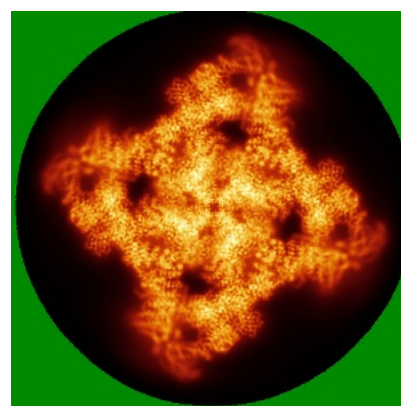
6.4.1 Primary map



X



Y

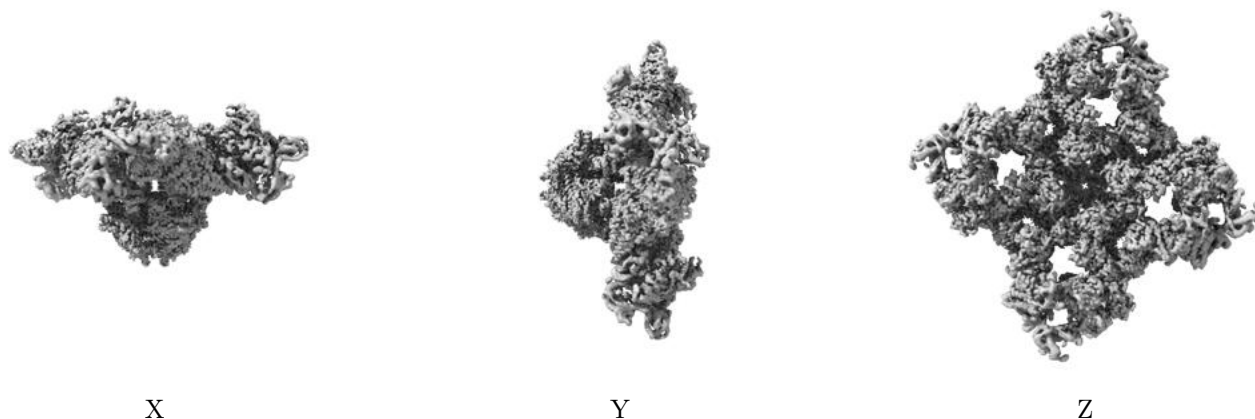


Z

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.

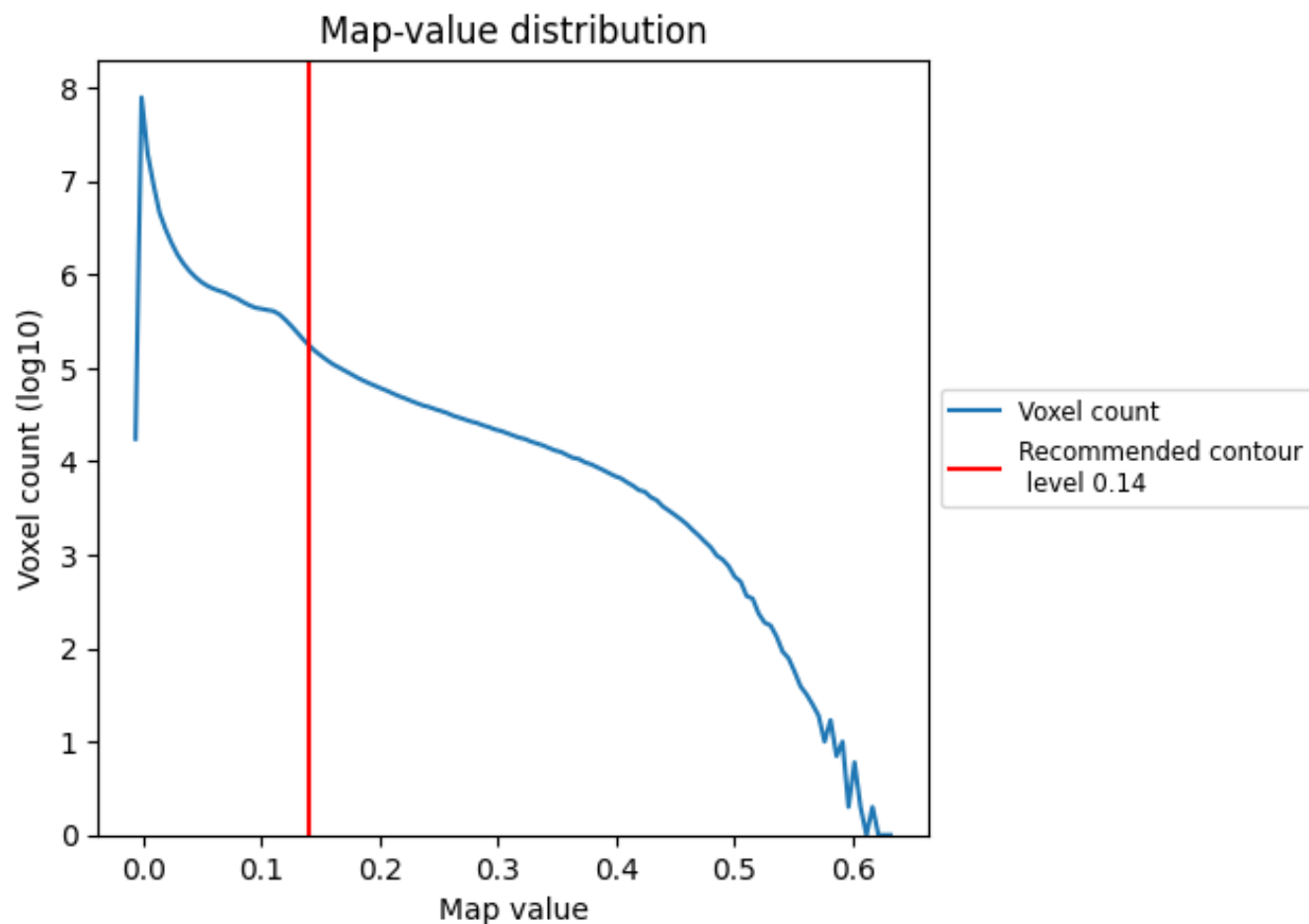
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

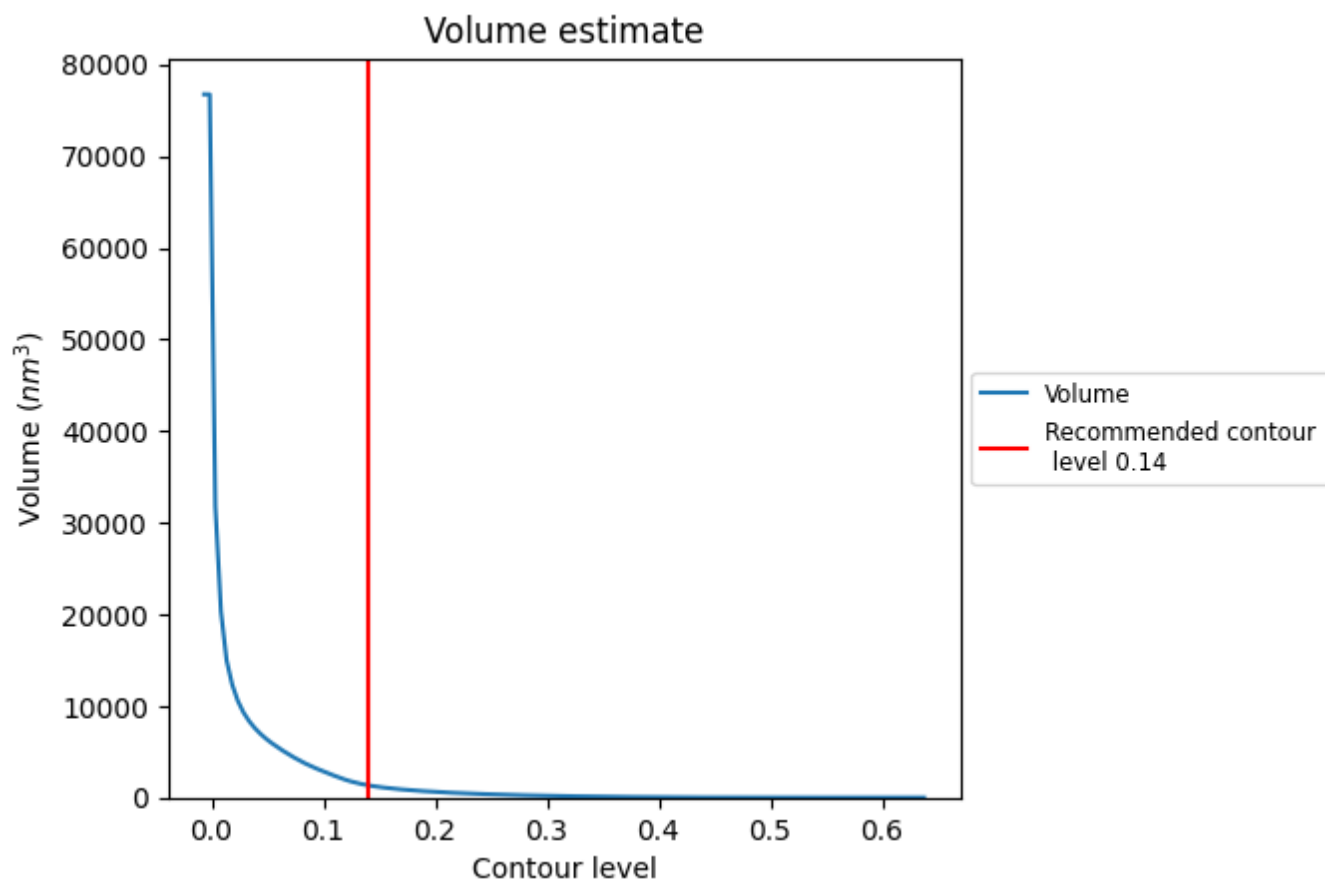
This section contains the results of statistical analysis of the map.

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.

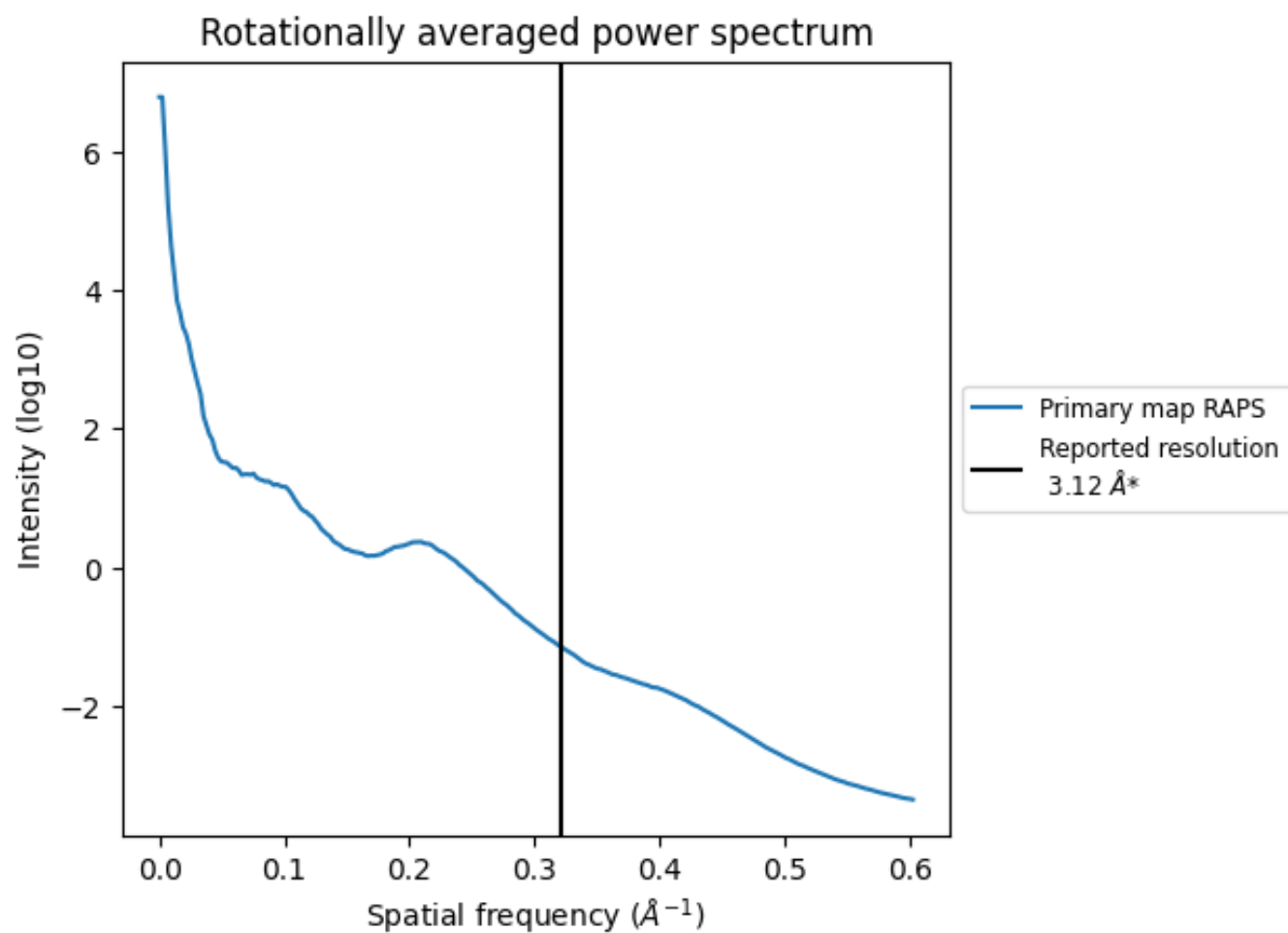
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1339 nm³; this corresponds to an approximate mass of 1210 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 0.321 Å⁻¹

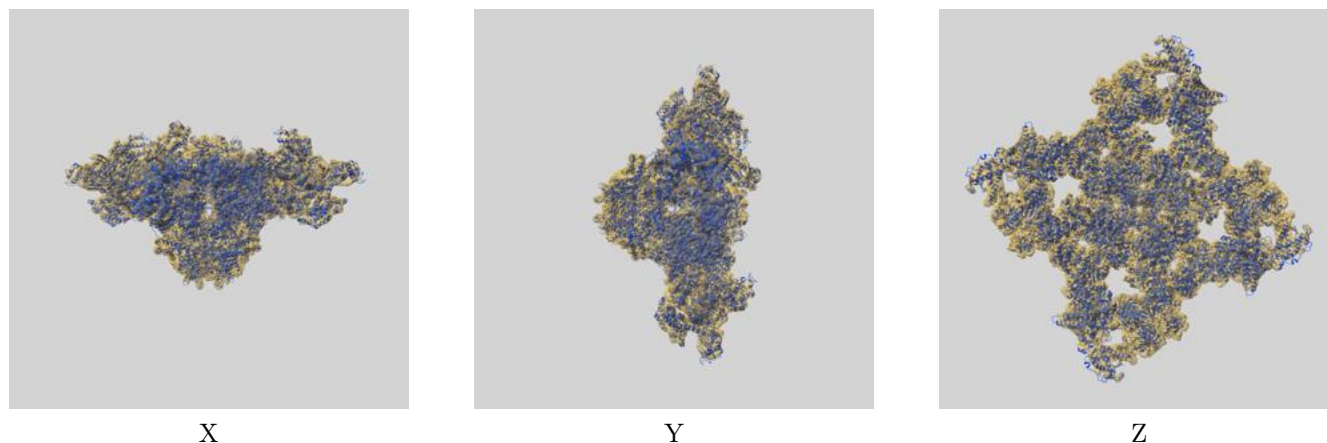
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

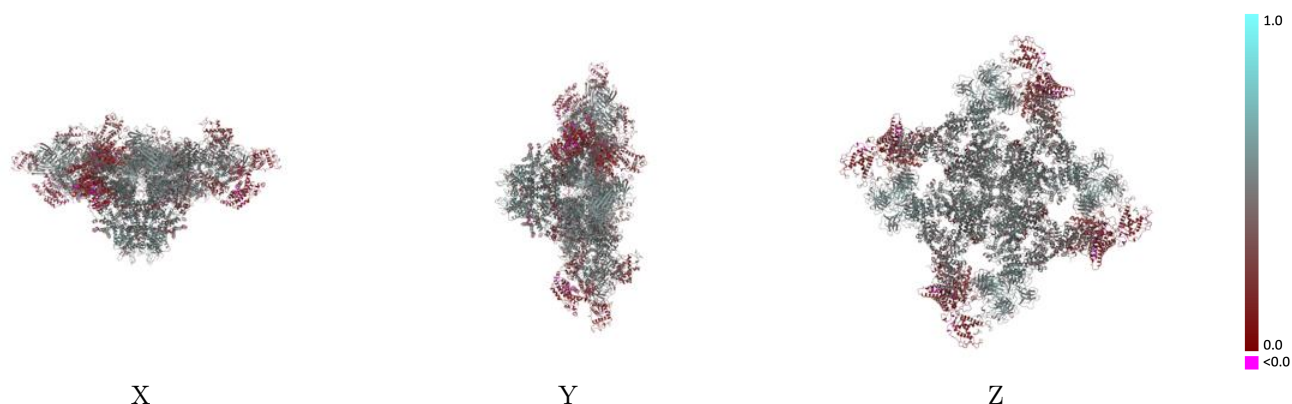
This section contains information regarding the fit between EMDB map EMD-42768 and PDB model 8UXL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



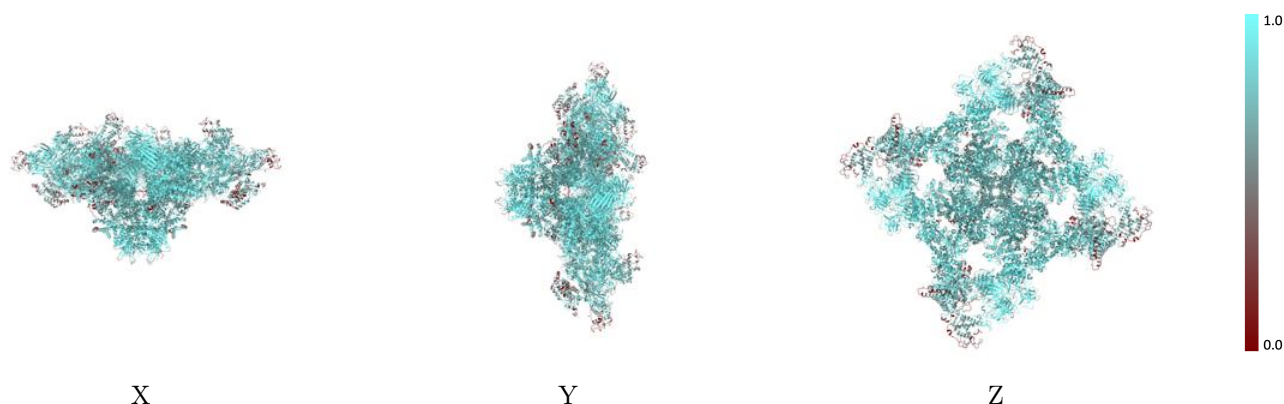
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



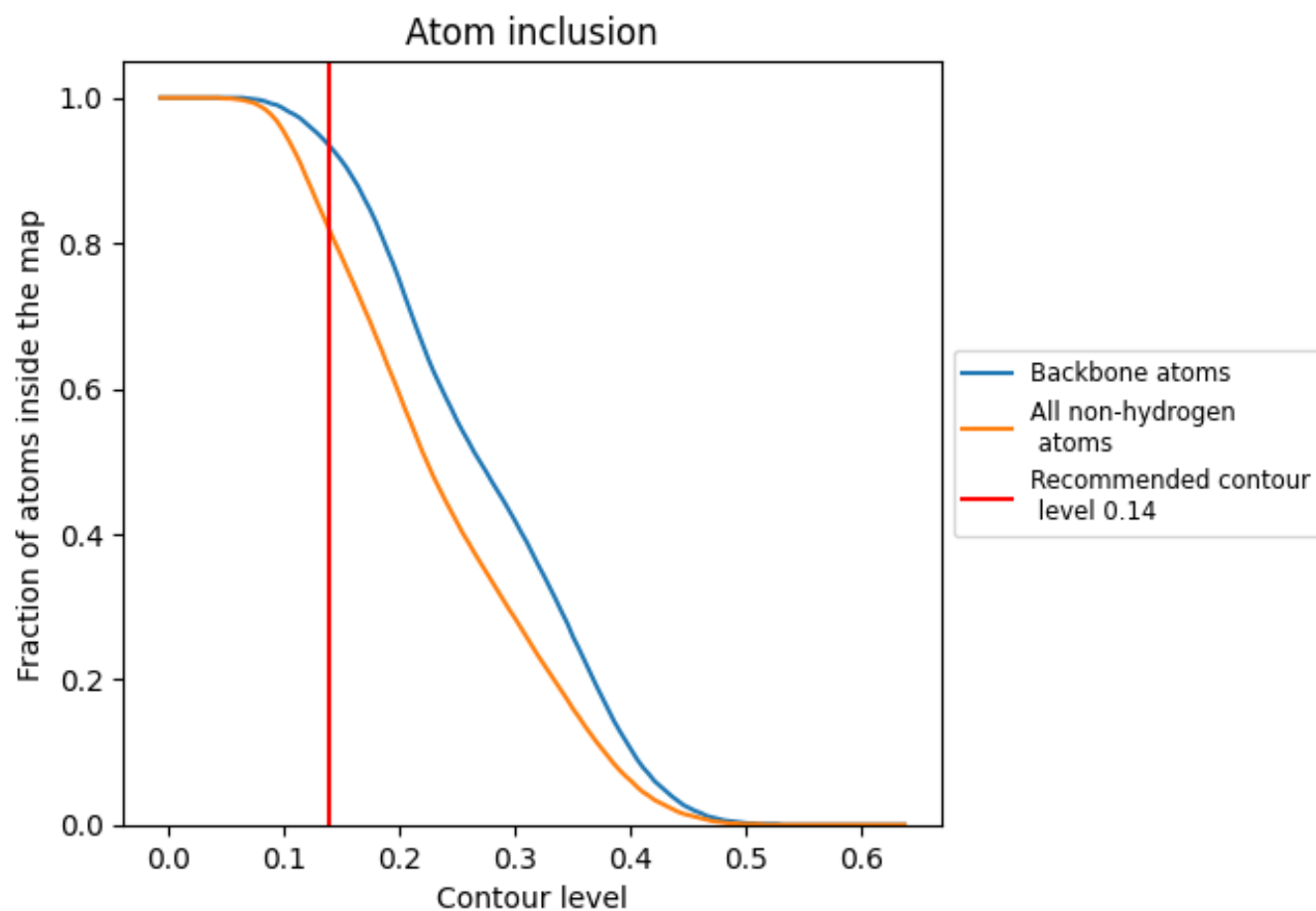
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% of all backbone atoms, 82% 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	0.8160	0.4170
A	0.8150	0.4190
B	0.8170	0.4250
C	0.8150	0.4210
D	0.8110	0.4130
E	0.9130	0.5170
F	0.9130	0.5160
G	0.9130	0.5190
H	0.9160	0.5180
I	0.7920	0.2590
J	0.7920	0.2600
K	0.7950	0.2600
L	0.7890	0.2530

1.0

0.0

<0.0