



## wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 12:54 AM EST

PDB ID : 7UA4  
EMDB ID : EMD-26414  
Title : Structure of PKA phosphorylated human RyR2-R2474S in the open state in the presence of Calmodulin  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2022-03-11  
Resolution : 2.93 Å(reported)  
Based on initial model : 7UA3

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

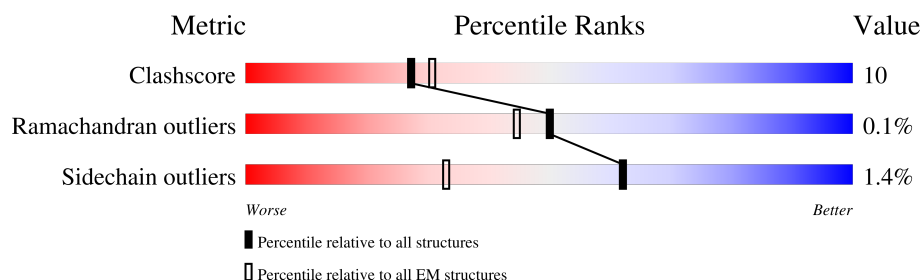
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	E	108	77% 20% ...
1	F	108	77% 20% ...
1	G	108	75% 22% ...
1	H	108	77% 20% ...
2	I	149	17% 48% 44% .. 5%
2	J	149	22% 49% 42% .. 5%
2	K	149	17% 51% 40% .. 5%
2	L	149	21% 49% 42% .. 5%

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Mol	Chain	Length	Quality of chain
3	A	4967	<div><div>6%</div><div><div></div><div>69%</div><div>18%</div><div>•</div><div>12%</div></div></div>
3	B	4967	<div><div>6%</div><div><div></div><div>69%</div><div>18%</div><div>•</div><div>12%</div></div></div>
3	C	4967	<div><div>7%</div><div><div></div><div>69%</div><div>19%</div><div></div><div>12%</div></div></div>
3	D	4967	<div><div>6%</div><div><div></div><div>69%</div><div>18%</div><div>•</div><div>12%</div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 147868 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
2	J	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
2	K	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
2	L	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		

- Molecule 3 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
3	B	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
3	C	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
3	D	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		

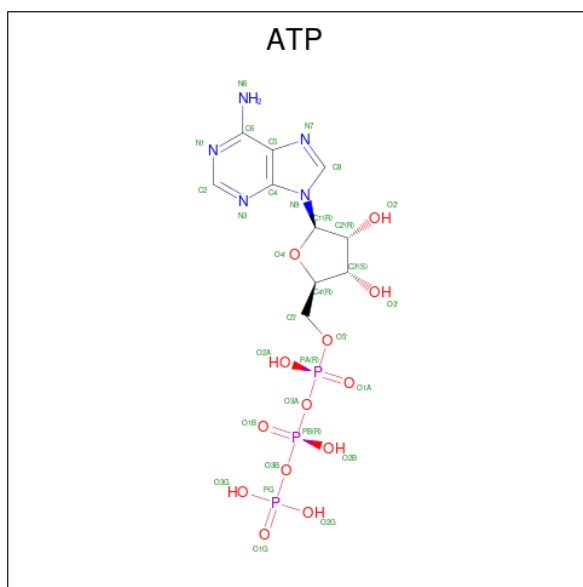
There are 4 discrepancies between the modelled and reference sequences:

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 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

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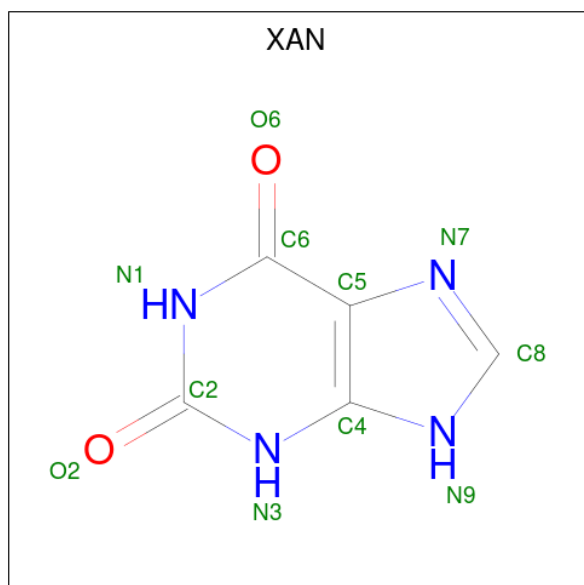
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Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is XANTHINE (three-letter code: XAN) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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


- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	3	Total	O	0
			3	3	
8	B	3	Total	O	0
			3	3	
8	C	3	Total	O	0
			3	3	
8	D	3	Total	O	0
			3	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: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 



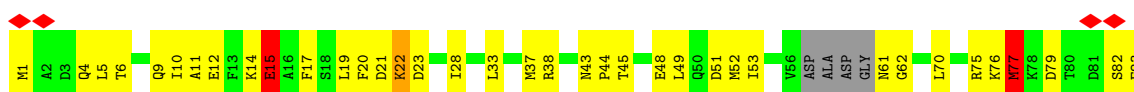
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 



- Molecule 2: Calmodulin-1

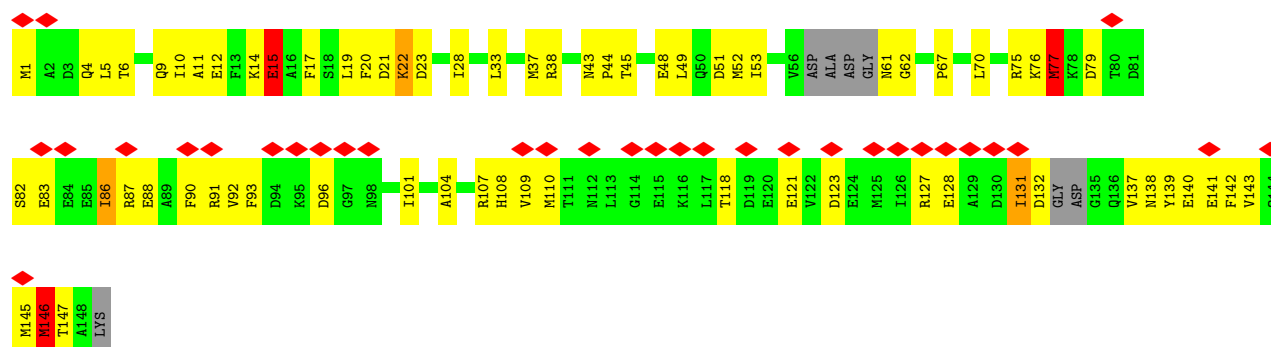
Chain I: 



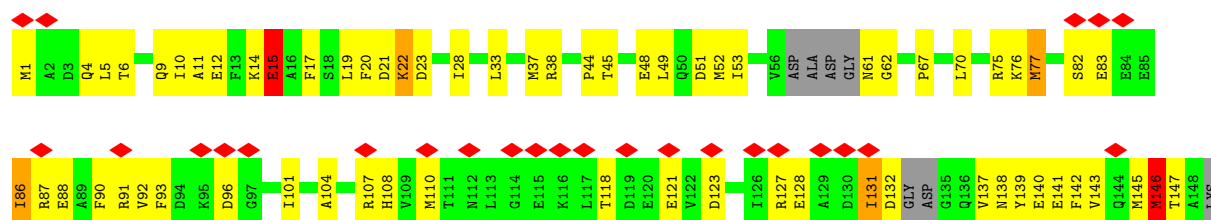




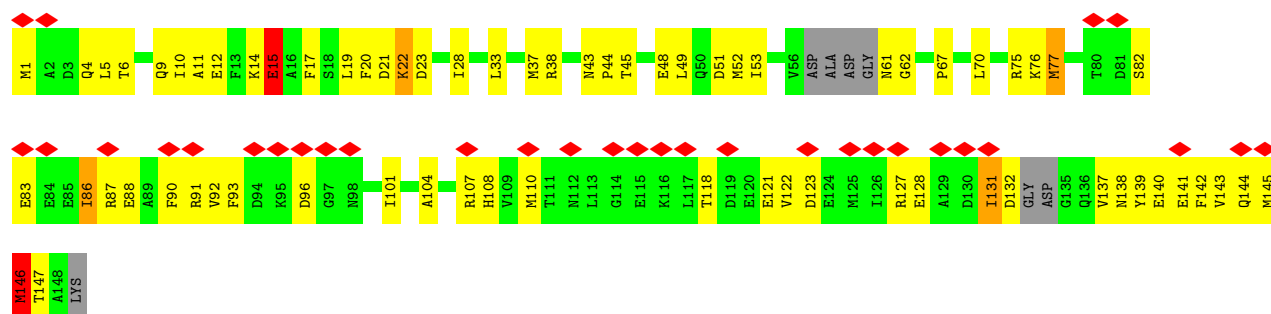
• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1

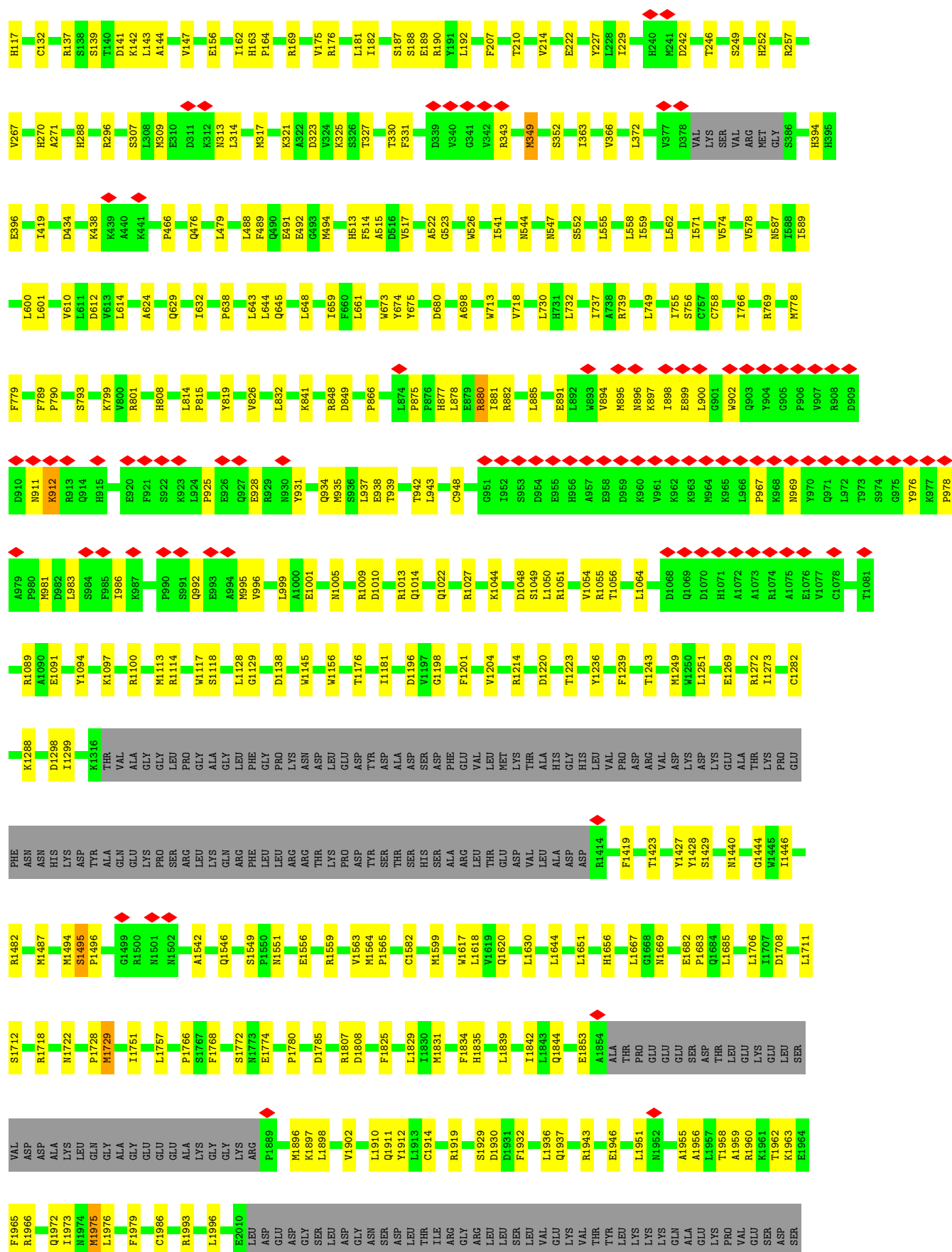


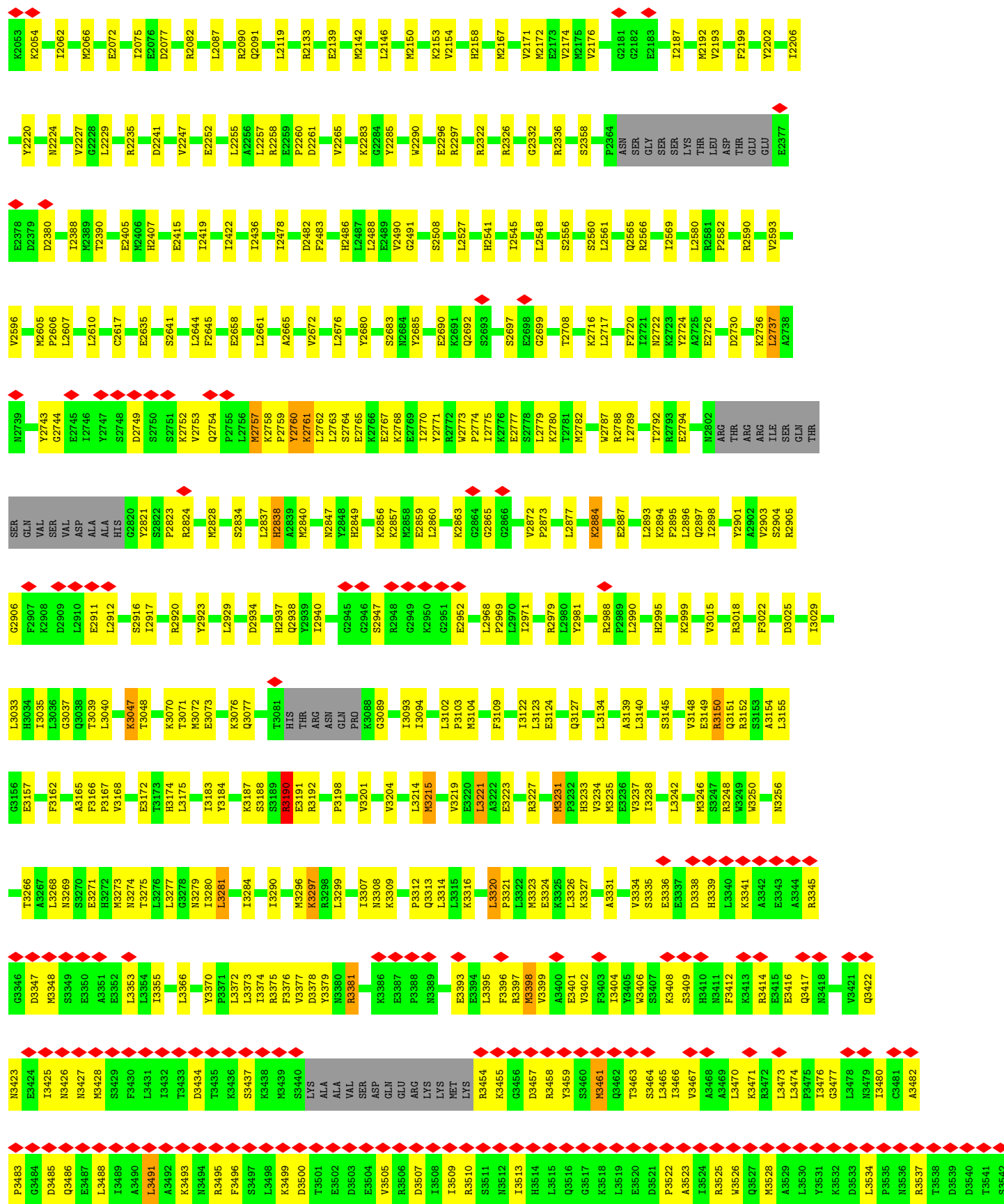
• Molecule 2: Calmodulin-1

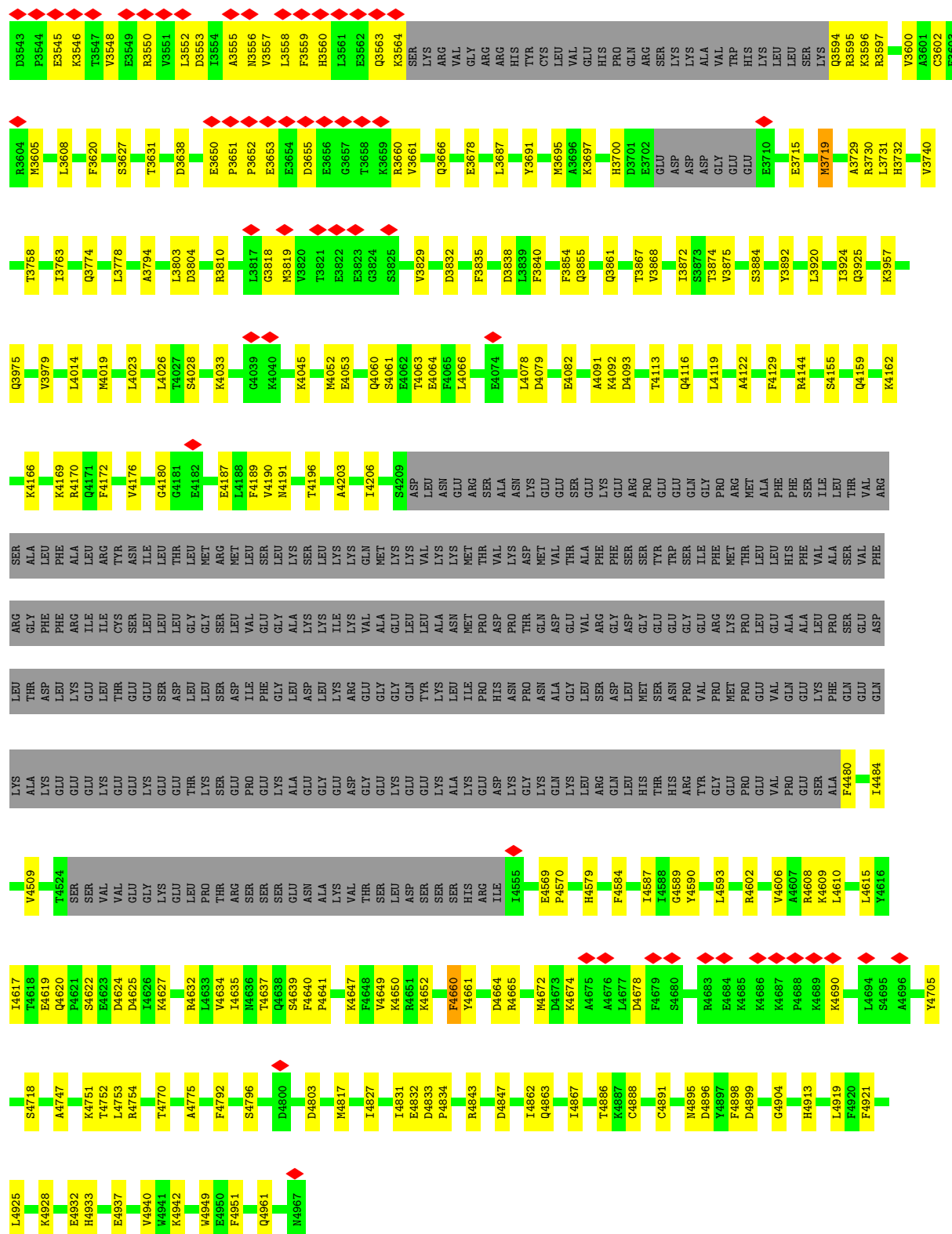


• Molecule 3: Ryanodine receptor 2









- Molecule 3: Ryanodine receptor 2





T3425	M3348	A3154	I3029	G2906	V2596	E2377	L2222	I1974
N3426	S3349	L3155	L3033	F2907	M2605	E2378	E2223	M1975
N3427	E3350	G3156	H3034	K2908	P2606	D2379	N2224	L1976
N3428	A3351	S3270	I3035	D2909	L2607	D2380	G2227	F1979
S3429	E3352	F3162	L3036	L2910	L2610	I2388	G2228	C1986
F3430	N3353	N3273	G3037	E2911	C2617	M2389	L2229	F1987
L3431	N3354	N3274	Q3038	L2912	S2641	T2390	R2235	C1988
L3432	L3355	F3167	L3040	S2916	E2405	E2406	E2076	P1989
T3433	L3366	L3277	K3047	R2920	H2407	V2407	D2077	R1993
D3434	N3279	G3278	T3048	Y2923	L2644	V2427	R2082	L1996
T3435	I3280	I3281	K3070	L2929	F2645	E2252	L2087	E2010
K3436	L3284	L3284	T3071	L2930	K2655	L2255	R2090	LEU
S3437	I3284	I3284	M3072	I2934	E2658	L2257	Q2091	ASP
K3438	I3290	I3290	E3073	D2934	L2661	R2258	L2119	GLU
M3439	M3296	M3296	K3076	H2937	A2665	E2259	R2133	ASP
S3440	K3297	K3297	Q3077	D2938	V2672	D2261	E2139	GLY
L3441	R3298	R3298	T3081	I2939	L2676	V2265	E2139	LEU
F3442	G3299	G3299	HIS	I2940	E2765	E2265	M2142	ASP
N3443	L3307	L3307	THR	G2945	K2766	D2482	M2142	GLY
N3444	N3308	N3308	ARG	G2946	E2767	F2483	L2146	ASN
N3445	K3309	K3309	ASN	G2947	K2768	H2486	L2146	SER
N3446	P3312	P3312	GLN	S2947	E2769	L2487	M2150	ASP
N3447	Q3313	Q3313	PRO	K2948	K2857	L2488	V2154	LEU
N3448	L3314	L3314	K3088	G2949	M2858	L2488	H2168	THR
N3449	L3315	L3315	G3089	K2950	E2859	E2489	M2167	ILE
N3450	K3316	K3316	I3093	G2951	L2860	V2490	G2171	ARG
N3451	F3319	F3319	I3094	E2952	K2863	G2491	M2175	ARG
N3452	L3320	L3320	L3102	Q2958	G2864	L2527	V2171	LEU
N3453	P3321	P3321	P3103	L2968	G2865	H2541	M2172	SER
N3454	E3323	E3323	M3104	P2969	G2866	G2699	E2173	LEU
N3455	E3324	E3324	F3109	L2970	V2872	L2779	M2174	VAL
N3456	K3327	K3327	I3122	L2971	P2873	K2780	V2176	LYS
N3457	A3331	A3331	L3123	R2979	L2877	L2782	G2181	VAL
N3458	T3332	T3332	E3124	L2980	K2884	K2716	G2182	THR
N3459	V3333	V3333	Q3127	Y2981	E2887	L2717	G2183	LEU
N3460	M3334	M3334	L3134	R2988	L2893	F2720	I2187	LYS
N3461	S3335	S3335	A3139	L2990	K2894	N2721	I2187	LYS
N3462	E3336	E3336	L3140	H2995	P2895	K2723	M2182	ALA
N3463	E3337	E3337	S3145	H2995	L2896	Y2724	M2182	GLY
N3464	D3338	D3338	V3148	H2995	L2897	A2725	V2193	LYS
N3465	H3339	H3339	E3149	H2995	Q2897	E2726	F2199	PRO
N3466	K3340	K3340	R3150	H2995	I2898	D2730	Y2202	VAL
N3467	K3341	K3341	R3151	H2995	Y2901	K2736	Y2202	GLU
N3468	A3342	A3342	Q3151	H2995	A2902	L2737	I2206	SER
N3469	E3343	E3343	R3152	H2995	S2903	A2738	I2206	ASP
N3470	E3344	E3344	R3152	H2995	S2904	N2739	Y2220	SER
N3471	R3345	R3345	S3153	H2995	R2905	V2593	L2221	SER
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N3637				H2995				
N3638								

D3485	E3545	F3620	A3794	M4019	F4172	ARG	ILE	LEU	LYS	VAL	P4621	L4753	K4928
Q3486	K3546	F3638	L3803	L4023	V4176	TYR	CYS	THR	GLU	VAL	S4622	R4754	E4932
E3487	T3547	D3638	D3804	L4023	G4180	ILE	LEU	GLU	LYS	GLY	E4623	T4770	H4933
L3488	V3548	E3650	R3810	L4026	G4181	THR	LEU	ASP	LYS	GLU	D4624	L4773	E4937
T3489	E3549	P3651	G3818	T4027	E4182	LEU	GLY	LEU	THR	LYS	L4626	L4774	V4940
A3490	R3550	P3652	M3819	S4028	G4187	MET	GLY	LEU	PRO	THR	K4627	A4775	K4941
L3491	V3551	P3652	G3818	K4033	E4187	ARG	GLY	LEU	LEU	LEU	R4632	F4792	V4942
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K3494	L3554	D3655	E3822	K4045	V4190	LEU	ALA	GLY	GLY	SER	N4636	A4796	E4950
A3555	A3555	E3656	E3822	K4045	T4196	LYS	LYS	ASP	LEU	GLU	T4637	D4800	E4950
R3495	N3556	G3657	E3822	M4052	F4199	SER	LYS	LEU	ASP	ASN	Q4638	D4803	F4951
F3496	V3557	G3658	G3824	E4053	V4191	LYS	ILE	LYS	LYS	LYS	P4640	M4817	Q4961
S3497	L3558	T3659	S3825	M4053	A4203	GLN	VAL	ARG	GLY	THR	N4642	Y4818	R4967
L3498	F3559	R3660	V3829	Q4060	L4206	MET	ALA	GLY	GLY	SER	M4643	R4822	
K3499	H3560	V3661	D3832	S4061	S4209	GLY	ALA	GLY	LYS	LEU	K4647	I4827	
D3500	L3561	Q3666	F3835	E4062	ASP	LYS	LEU	GLY	LYS	LEU	K4650	I4831	
T3501	E3562	E3678	F3838	T4063	LEU	THR	GLU	GLN	GLU	ASP	F4660	E4832	
E3502	Q3563	L3687	D3839	E4064	ASN	VAL	LEU	TYR	GLU	SER	Y4661	D4833	
D3503	K3564	L3687	F3840	F4065	GLU	LYS	ALA	LEU	GLU	SER		P4834	
E3504	SER	L3687	F3840	L4066	ARG	MET	ASN	LEU	LYS	THR		R4843	
V3505	LYS	Y3691	F3840	E4074	THR	THR	PRO	ILE	LYS	HIS		L4859	
R3506	ARG	Y3691	F3840	E4074	VAL	VAL	HIS	PRO	GLY	ARG		I4862	
D3507	VAL	M3695	F3840	E4074	LYS	LYS	ASN	PRO	GLY	ILE		Q4863	
T3508	GLY	M3695	F3840	E4074	ASN	ASN	ASN	PRO	GLY	ILE		R4867	
I3509	ARG	K3697	F3840	E4074	LYS	MET	GLN	ASP	GLY	ILE		T4886	
HIS	ARG	K3697	F3840	E4074	GLU	THR	ASP	ALA	LEU	ILE		C4888	
HIS	ARG	K3697	F3840	E4074	GLU	THR	ASP	ALA	LEU	ILE		C4891	
R3510	TYR	H3700	F3840	E4074	SER	THR	ASP	ALA	LEU	ILE		N4895	
S3511	CYS	D3701	F3840	E4074	GLU	ALA	PHE	VAL	LEU	ILE		D4896	
N3512	LEU	E3702	F3840	E4074	LYS	PHE	PHE	GLY	ASP	ILE		Y4897	
L3513	VAL	ASP	F3840	E4074	GLU	SER	GLY	GLY	LEU	ILE		F4898	
H3514	GLU	ASP	F3840	E4074	PRO	SER	GLY	GLY	LEU	ILE		D4899	
L3515	HIS	ASP	F3840	E4074	GLU	THR	GLY	GLY	LEU	ILE		H4903	
Q3516	PRO	ASP	F3840	E4074	GLU	THR	GLY	GLY	LEU	ILE		G4904	
G3517	GLN	GLY	F3840	E4074	GLN	ILE	GLY	VAL	VAL	ILE		H4913	
K3518	ARG	GLU	F3840	E4074	GLY	PHE	ARG	PRO	GLY	ILE		L4919	
L3519	LYS	E3710	F3840	E4074	PRO	MET	LYS	MET	GLU	ILE		F4920	
E3520	LYS	E3715	F3840	E4074	ARG	THR	THR	THR	GLU	ILE		F4921	
P3521	ALA	E3715	F3840	E4074	MET	LEU	PRO	PRO	GLU	ILE		L4925	
D3522	VAL	E3715	F3840	E4074	ALA	LEU	GLU	GLU	VAL	ILE			
L3524	TRP	M3719	F3840	E4074	PHE	HIS	ALA	ALA	VAL	ILE			
R3525	HIS	M3719	F3840	E4074	ALA	PHE	ALA	GLY	GLY	ILE			
K3526	LYS	M3719	F3840	E4074	SER	VAL	LEU	LYS	GLY	ILE			
Q3527	LYS	M3719	F3840	E4074	ARG	VAL	LEU	LYS	GLY	ILE			
K3528	R3595	M3719	F3840	E4074	ARG	VAL	LEU	LYS	GLY	ILE			
A3529	K3596	M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
L3530	R3597	M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
Y3531	F3603	M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
K3532	R3604	M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
D3533	M3605	M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
L3534	A3606	M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
P3535	P3607	M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
N3536	L3608	M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
R3537		M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
T3538		M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
D3539		M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
D3540		M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
T3541		M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
S3542		M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
D3543		M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			
P3544		M3719	F3840	E4074	ALA	VAL	LEU	LYS	GLY	ILE			

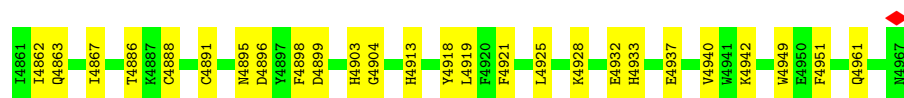
• Molecule 3: Ryanodine receptor 2



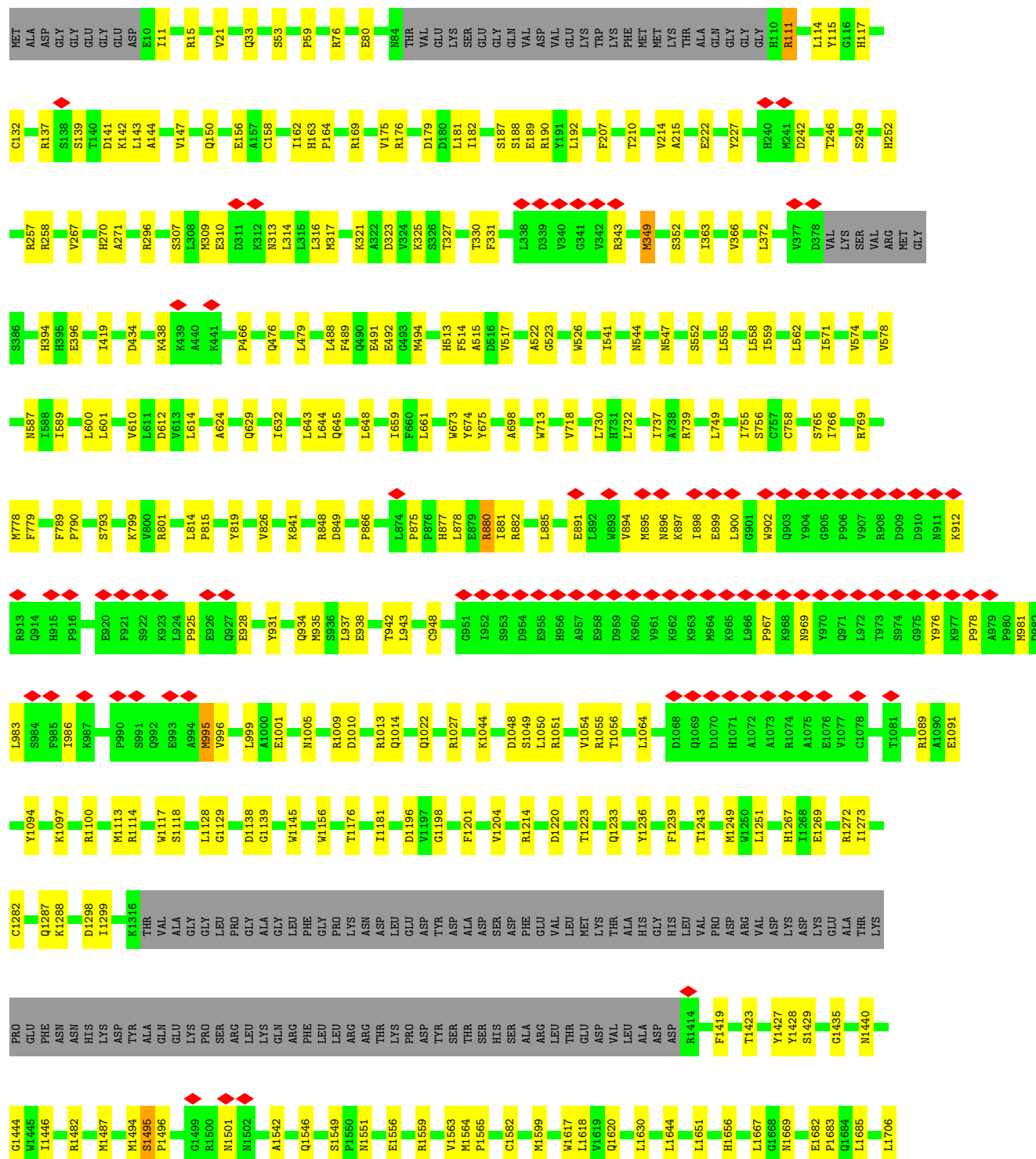






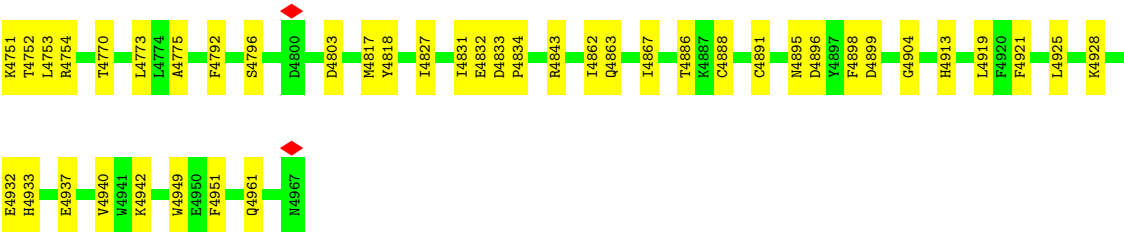


### • Molecule 3: Ryanodine receptor 2



W3249	R3152	D3025	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	S2916	L2917	R2920	Y2923	L2929	H2937	K3076	Q3077	S3187	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	V3332	V3333	V3334	S3335	E3336	E3337	M3246	S3247	R3248	L3340
N3256	G3156	L3033	G3156	E3157	G3158	L3036	G3037	Q3038	T3039	L3040	K3047	T3048	K3048	K3070	T3071	M3072	E3073	K3076	Q3077	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	V3332	V3333	V3334	S3335	E3336	E3337	M3246	S3247	R3248	L3340
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N3269	E3157	L3033	G3156	E3157	G3158	L3036	G3037	Q3038	T3039	L3040	K3047	T3048	K3048	K3070	T3071	M3072	E3073	K3076	Q3077	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	V3332	V3333	V3334	S3335	E3336	E3337	M3246	S3247	R3248	L3340
S3270	E3157	L3033	G3156	E3157	G3158	L3036	G3037	Q3038	T3039	L3040	K3047	T3048	K3048	K3070	T3071	M3072	E3073	K3076	Q3077	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	V3332	V3333	V3334	S3335	E3336	E3337	M3246	S3247	R3248	L3340
E3271	E3157	L3033	G3156	E3157	G3158	L3036	G3037	Q3038	T3039	L3040	K3047	T3048	K3048	K3070	T3071	M3072	E3073	K3076	Q3077	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	V3332	V3333	V3334	S3335	E3336	E3337	M3246	S3247	R3248	L3340
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L3281	E3157	L3033	G3156	E3157	G3158	L3036	G3037	Q3038	T3039	L3040	K3047	T3048	K3048	K3070	T3071	M3072	E3073	K3076	Q3077	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	V3332	V3333	V3334	S3335	E3336	E3337	M3246	S3247	R3248	L3340
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L3290	E3157	L3033	G3156	E3157	G3158	L3036	G3037	Q3038	T3039	L3040	K3047	T3048	K3048	K3070	T3071	M3072	E3073	K3076	Q3077	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	V3332	V3333	V3334	S3335	E3336	E3337	M3246	S3247	R3248	L3340
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L3314	E3157	L3033	G3156	E3157	G3158	L3036	G3037	Q3038	T3039	L3040	K3047	T3048	K3048	K3070	T3071	M3072	E3073	K3076	Q3077	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3323	E3324	K3325	L3326	K3327	K3328	K3329	A3330	A3331	V3332	V3333	V3334	S3335	E3336	E3337	M3246	S3247	R3248	L3340
L3315	E3157	L3033	G3156	E3157	G3158	L3036	G3037	Q3038	T3039	L3040	K3047	T3048	K3048	K3070	T3071	M3072	E3073	K3076	Q3077	S3188	S3189	R3190	R3191	R3192	P3198	N3308	K3309	P3312	Q3313	L3314	L3315	K3316	L3320	P3321	L3322	M3																		





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.728	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, XAN, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	E	0.30	0/834	0.61	2/1123 (0.2%)
1	F	0.31	0/834	0.61	2/1123 (0.2%)
1	G	0.31	0/834	0.61	2/1123 (0.2%)
1	H	0.31	0/834	0.61	2/1123 (0.2%)
2	I	0.38	0/1122	0.80	6/1504 (0.4%)
2	J	0.38	0/1122	0.79	6/1504 (0.4%)
2	K	0.38	1/1122 (0.1%)	0.80	6/1504 (0.4%)
2	L	0.38	0/1122	0.80	6/1504 (0.4%)
3	A	0.26	0/35720	0.50	7/48254 (0.0%)
3	B	0.26	0/35720	0.50	7/48254 (0.0%)
3	C	0.26	0/35720	0.50	7/48254 (0.0%)
3	D	0.26	0/35720	0.50	7/48254 (0.0%)
All	All	0.27	1/150704 (0.0%)	0.51	60/203524 (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
3	A	0	2
3	B	0	2
3	C	0	2
3	D	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	15	GLU	CG-CD	-5.00	1.44	1.51



The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	77	MET	CB-CG-SD	8.44	137.71	112.40
2	K	77	MET	CB-CG-SD	8.44	137.72	112.40
2	L	77	MET	CB-CG-SD	8.43	137.69	112.40
2	I	77	MET	CB-CG-SD	8.43	137.68	112.40
3	C	1729	MET	CB-CG-SD	-8.12	88.05	112.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	3190	ARG	Sidechain
3	A	3381	ARG	Sidechain
3	B	3190	ARG	Sidechain
3	B	3381	ARG	Sidechain
3	C	3190	ARG	Sidechain

## 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	E	818	0	821	16	0
1	F	818	0	821	15	0
1	G	818	0	821	18	0
1	H	818	0	821	15	0
2	I	1112	0	1053	84	0
2	J	1112	0	1053	69	0
2	K	1112	0	1053	70	0
2	L	1112	0	1053	72	0
3	A	34959	0	34588	632	0
3	B	34959	0	34588	632	0
3	C	34959	0	34588	644	0
3	D	34959	0	34588	627	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	62	0	24	4	0
5	B	62	0	24	4	0
5	C	62	0	24	4	0
5	D	62	0	24	4	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
7	A	11	0	4	0	0
7	B	11	0	4	0	0
7	C	11	0	4	0	0
7	D	11	0	4	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	3	0	0	0	0
All	All	147868	0	145960	2823	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 10.

The worst 5 of 2823 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:L:128:GLU:CB	2:L:131:ILE:CD1	1.83	1.57
2:L:128:GLU:HB3	2:L:131:ILE:CD1	1.11	1.56
2:J:128:GLU:HB3	2:J:131:ILE:CD1	1.11	1.55
2:I:128:GLU:HB3	2:I:131:ILE:CD1	1.11	1.54
2:K:128:GLU:HB3	2:K:131:ILE:CD1	1.11	1.54

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	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	I	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
2	J	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
2	K	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
2	L	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
3	A	4343/4967 (87%)	4192 (96%)	147 (3%)	4 (0%)	48	72
3	B	4343/4967 (87%)	4191 (96%)	148 (3%)	4 (0%)	48	72
3	C	4343/4967 (87%)	4192 (96%)	147 (3%)	4 (0%)	48	72
3	D	4343/4967 (87%)	4191 (96%)	148 (3%)	4 (0%)	48	72
All	All	18336/20896 (88%)	17666 (96%)	654 (4%)	16 (0%)	50	72

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1495	SER
3	A	2358	SER
3	B	1495	SER
3	B	2358	SER
3	C	1495	SER

### 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	E	88/89 (99%)	85 (97%)	3 (3%)	32	56
1	F	88/89 (99%)	85 (97%)	3 (3%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	88/89 (99%)	85 (97%)	3 (3%)	32	56
1	H	88/89 (99%)	85 (97%)	3 (3%)	32	56
2	I	119/127 (94%)	108 (91%)	11 (9%)	7	19
2	J	119/127 (94%)	108 (91%)	11 (9%)	7	19
2	K	119/127 (94%)	108 (91%)	11 (9%)	7	19
2	L	119/127 (94%)	108 (91%)	11 (9%)	7	19
3	A	3836/4358 (88%)	3792 (99%)	44 (1%)	70	82
3	B	3836/4358 (88%)	3792 (99%)	44 (1%)	70	82
3	C	3836/4358 (88%)	3792 (99%)	44 (1%)	70	82
3	D	3836/4358 (88%)	3792 (99%)	44 (1%)	70	82
All	All	16172/18296 (88%)	15940 (99%)	232 (1%)	62	79

5 of 232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	2757	MET
3	D	3381	ARG
3	B	4951	PHE
3	D	3296	MET
3	D	1975	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	2754	GLN
3	C	3426	ASN
3	C	3256	ASN
3	C	3563	GLN
3	A	3256	ASN

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	ATP	A	5005	-	28,33,33	0.74	0	34,52,52	0.76	1 (2%)
5	ATP	D	5005	-	28,33,33	0.74	0	34,52,52	0.76	1 (2%)
5	ATP	A	5002	-	28,33,33	0.62	0	34,52,52	0.62	1 (2%)
5	ATP	B	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
5	ATP	D	5002	-	28,33,33	0.62	0	34,52,52	0.62	1 (2%)
7	XAN	C	5004	-	7,12,12	1.56	1 (14%)	6,17,17	5.21	3 (50%)
5	ATP	C	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
7	XAN	B	5004	-	7,12,12	1.56	1 (14%)	6,17,17	5.20	2 (33%)
5	ATP	B	5005	-	28,33,33	0.74	0	34,52,52	0.76	1 (2%)
7	XAN	D	5004	-	7,12,12	1.56	1 (14%)	6,17,17	5.23	3 (50%)
7	XAN	A	5004	-	7,12,12	1.56	1 (14%)	6,17,17	5.20	3 (50%)
5	ATP	C	5005	-	28,33,33	0.74	0	34,52,52	0.76	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	A	5005	-	-	4/18/38/38	0/3/3/3
5	ATP	D	5005	-	-	4/18/38/38	0/3/3/3
5	ATP	A	5002	-	-	4/18/38/38	0/3/3/3
5	ATP	B	5002	-	-	4/18/38/38	0/3/3/3
5	ATP	D	5002	-	-	4/18/38/38	0/3/3/3
7	XAN	C	5004	-	-	-	0/2/2/2
5	ATP	C	5002	-	-	4/18/38/38	0/3/3/3
7	XAN	B	5004	-	-	-	0/2/2/2
5	ATP	B	5005	-	-	4/18/38/38	0/3/3/3
7	XAN	D	5004	-	-	-	0/2/2/2
7	XAN	A	5004	-	-	-	0/2/2/2
5	ATP	C	5005	-	-	4/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	5004	XAN	C6-N1	3.70	1.39	1.33
7	C	5004	XAN	C6-N1	3.69	1.39	1.33
7	A	5004	XAN	C6-N1	3.68	1.39	1.33
7	B	5004	XAN	C6-N1	3.68	1.39	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	5004	XAN	C2-N1-C6	10.45	123.91	115.09
7	C	5004	XAN	C2-N1-C6	10.41	123.88	115.09
7	A	5004	XAN	C2-N1-C6	10.40	123.87	115.09
7	B	5004	XAN	C2-N1-C6	10.39	123.87	115.09
7	D	5004	XAN	C5-C6-N1	-6.91	114.18	123.42

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

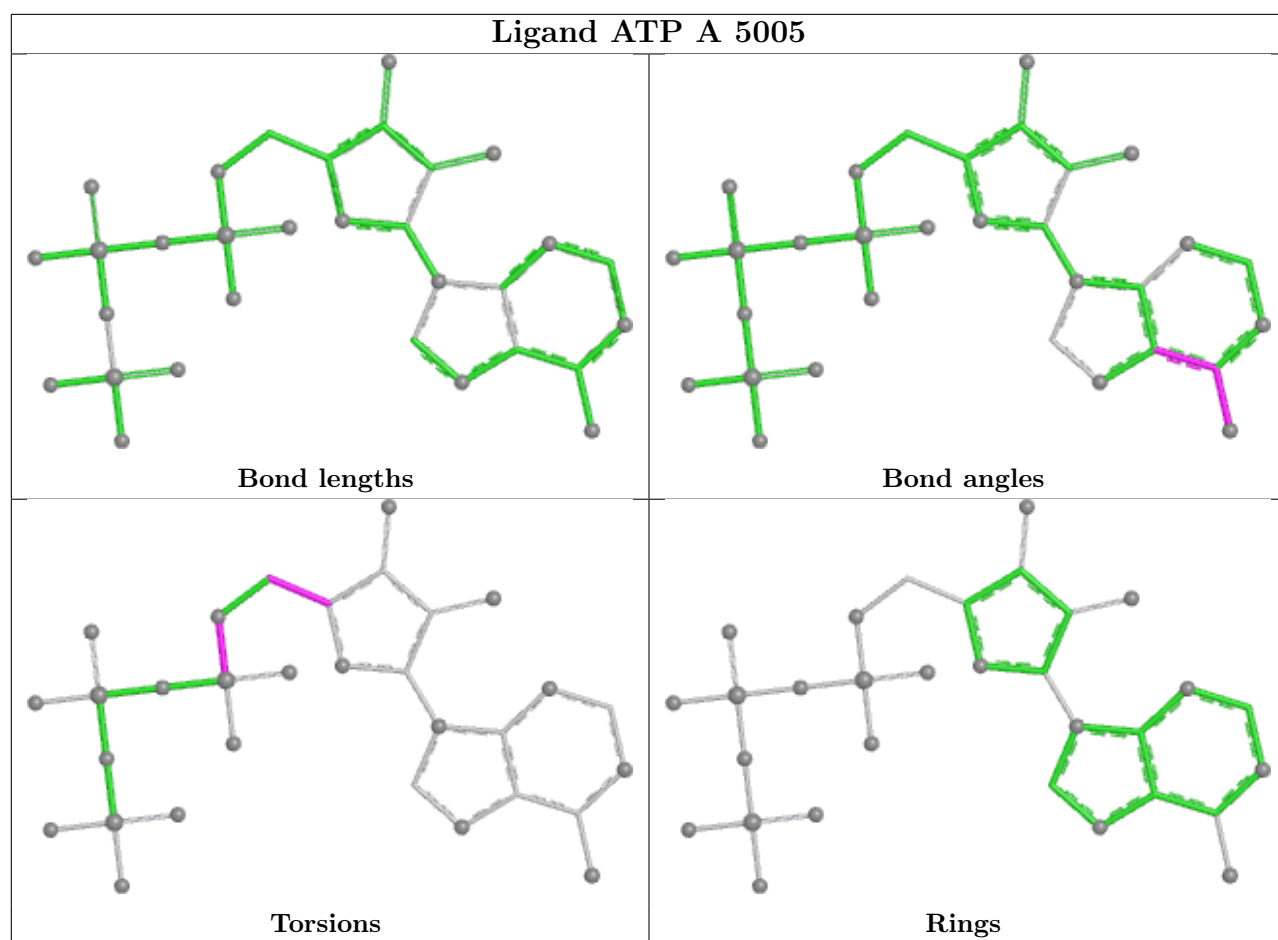
Mol	Chain	Res	Type	Atoms
5	A	5002	ATP	C5'-O5'-PA-O1A
5	A	5002	ATP	C5'-O5'-PA-O3A
5	A	5005	ATP	C5'-O5'-PA-O3A
5	A	5005	ATP	O4'-C4'-C5'-O5'
5	B	5002	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

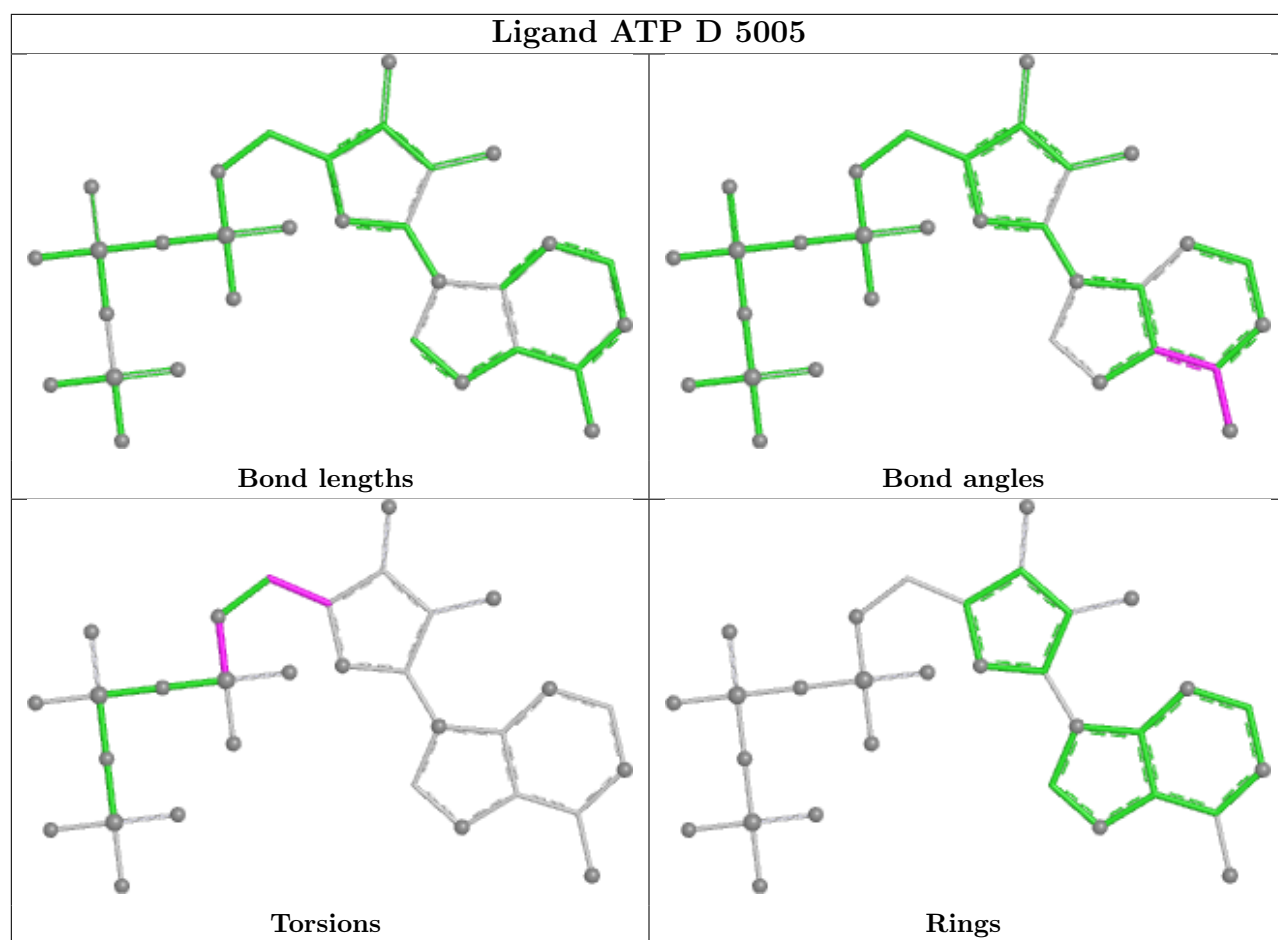
8 monomers are involved in 16 short contacts:

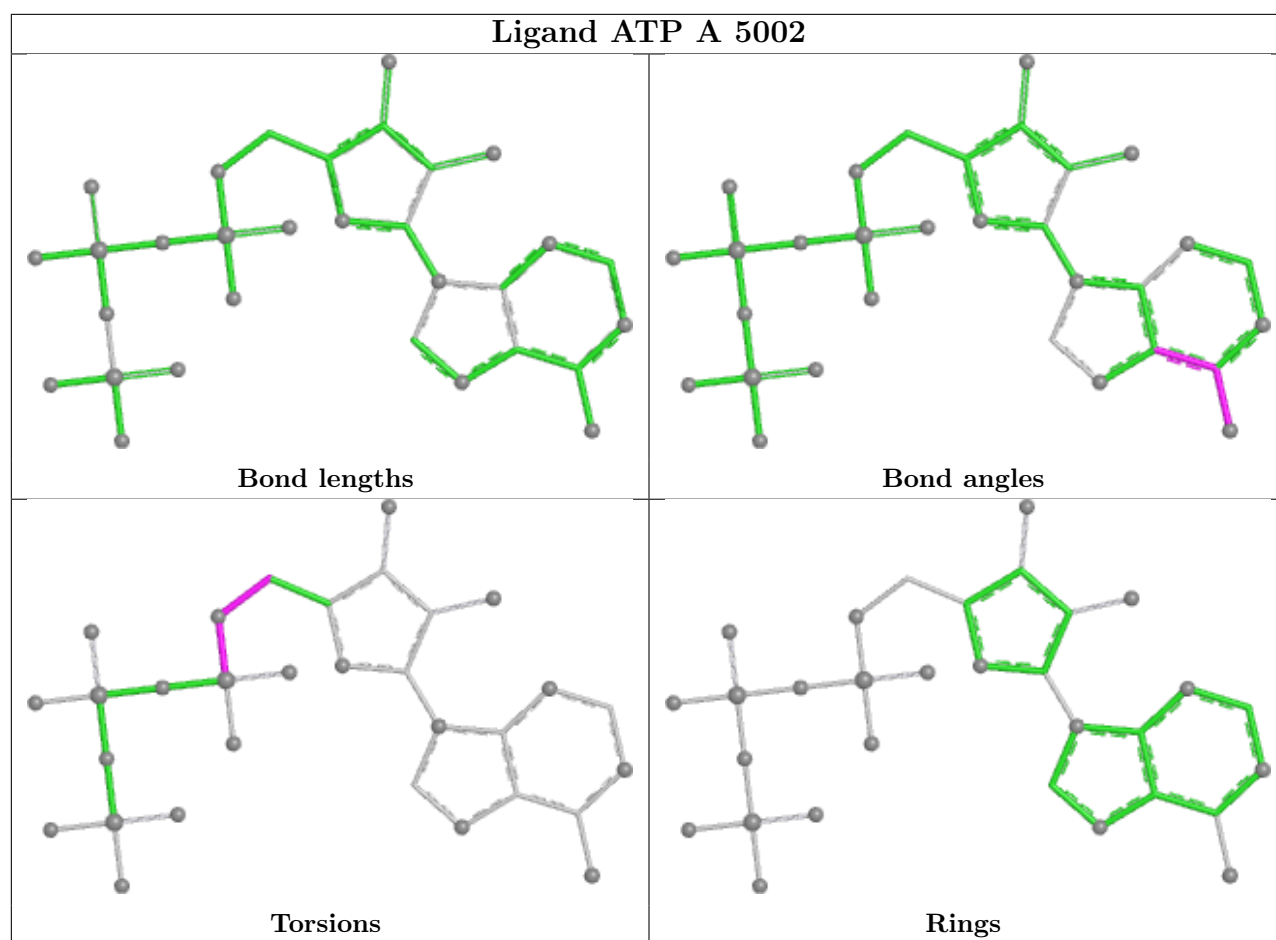
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5005	ATP	1	0
5	D	5005	ATP	1	0
5	A	5002	ATP	3	0
5	B	5002	ATP	3	0
5	D	5002	ATP	3	0
5	C	5002	ATP	3	0
5	B	5005	ATP	1	0
5	C	5005	ATP	1	0

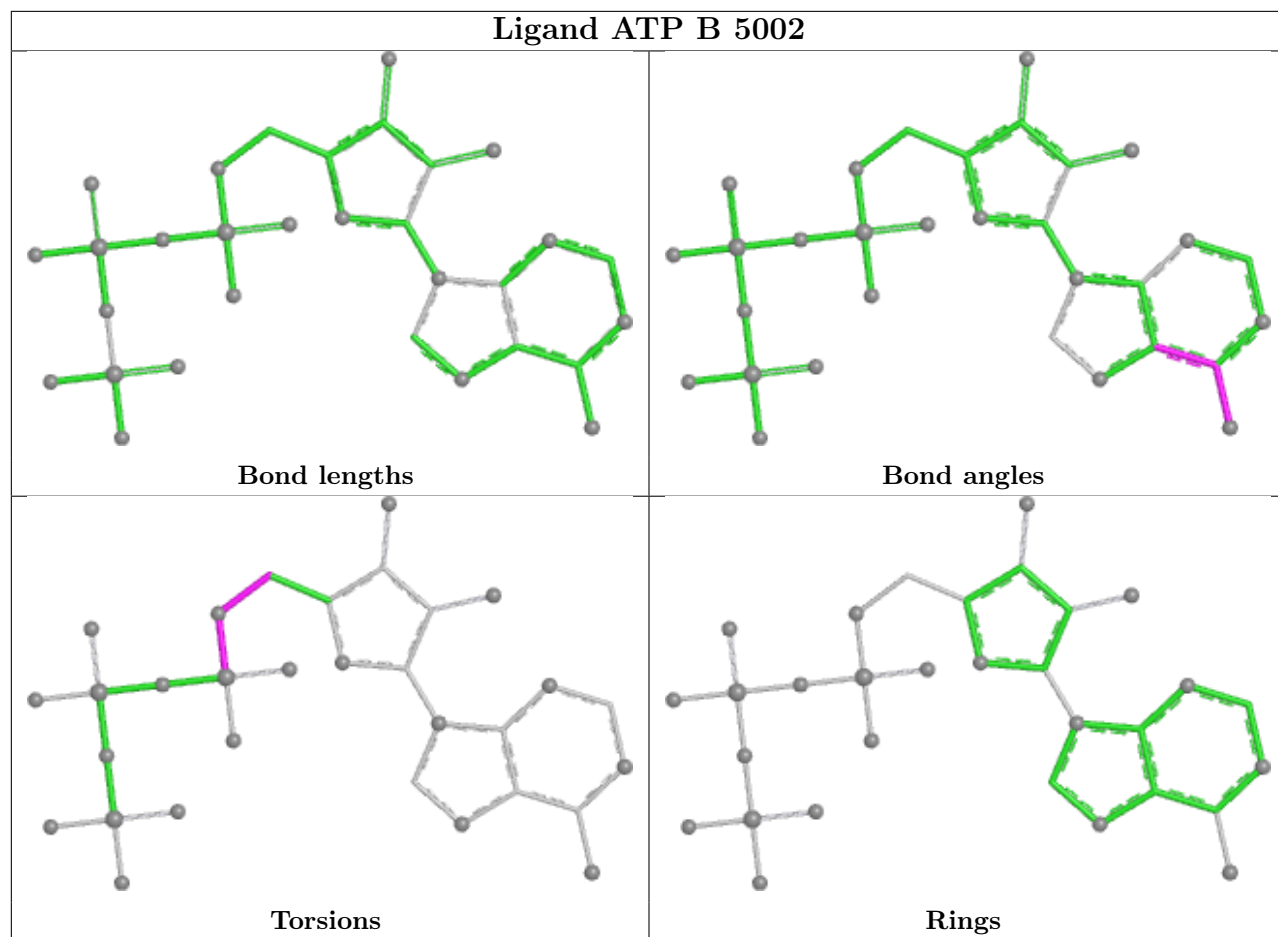
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

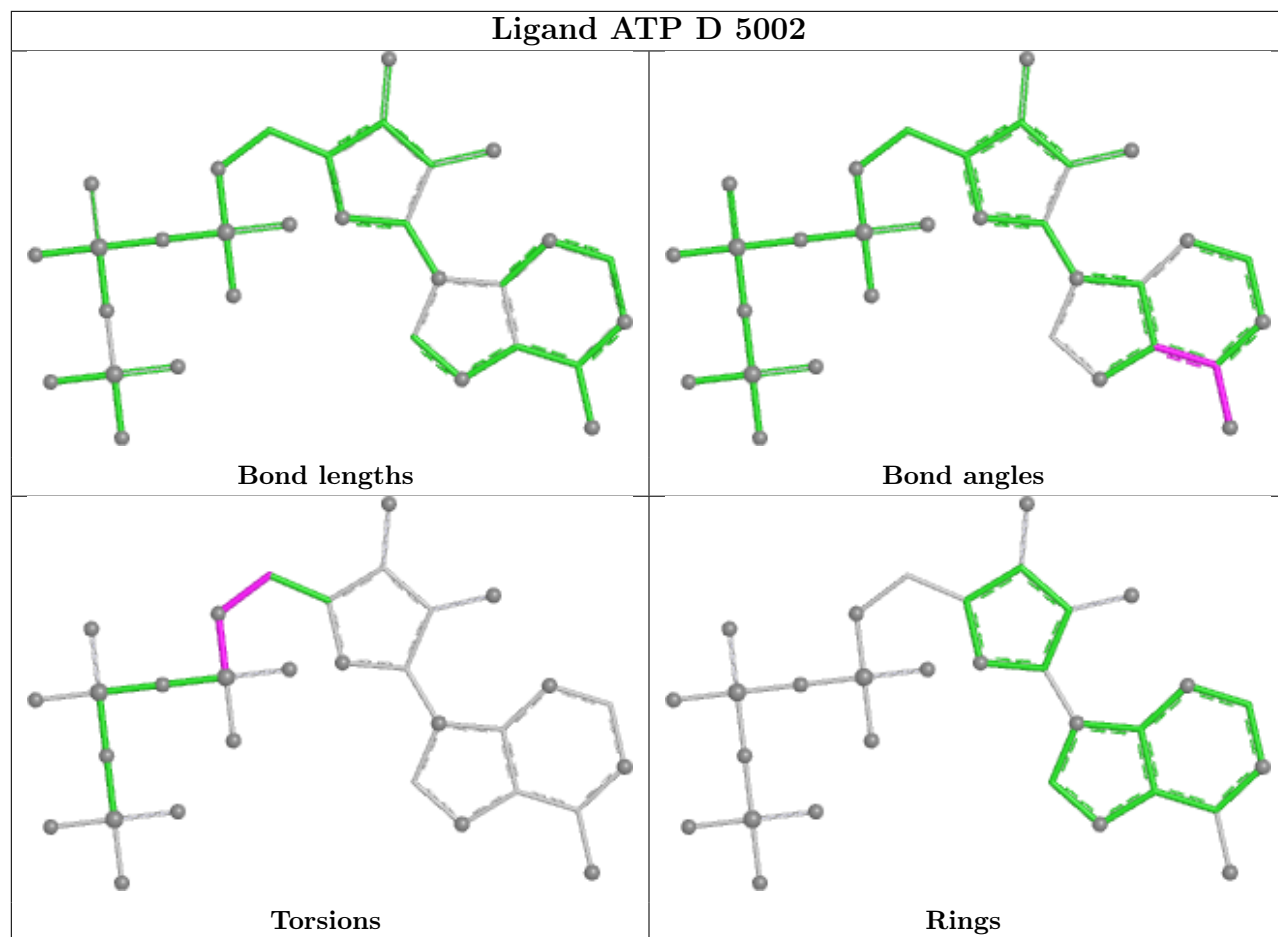




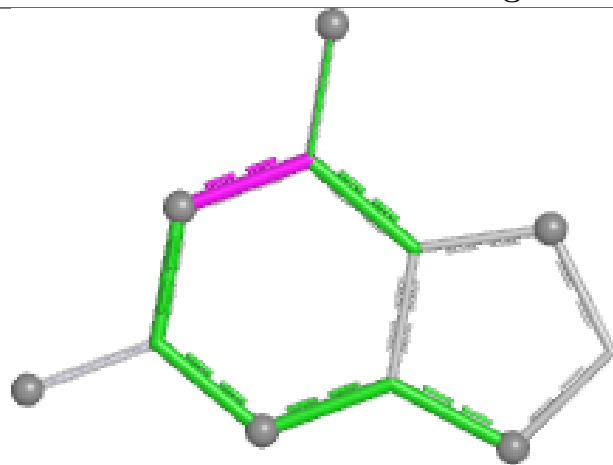




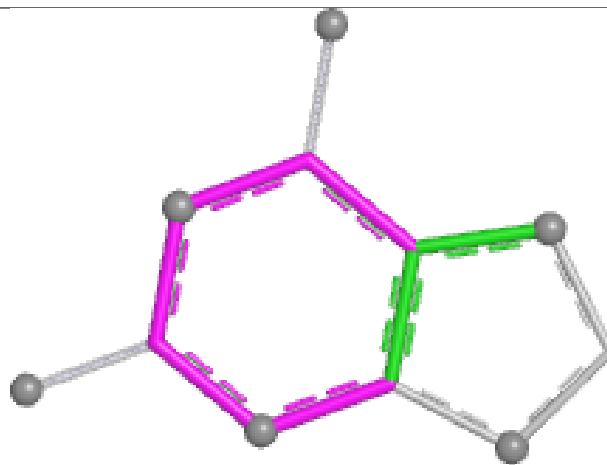




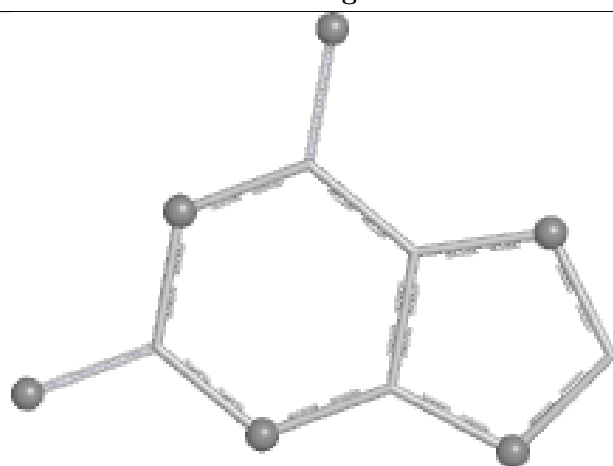
## Ligand XAN C 5004



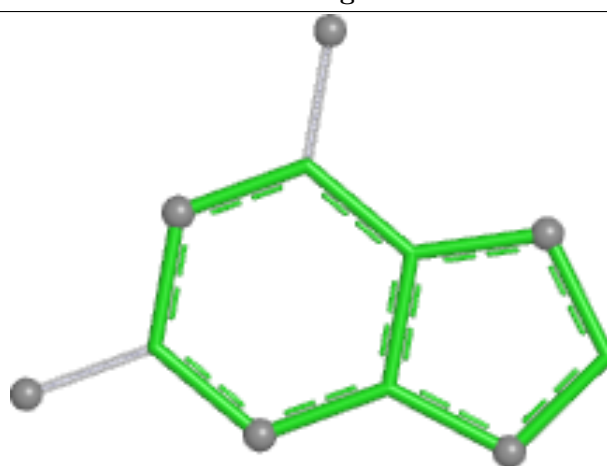
Bond lengths



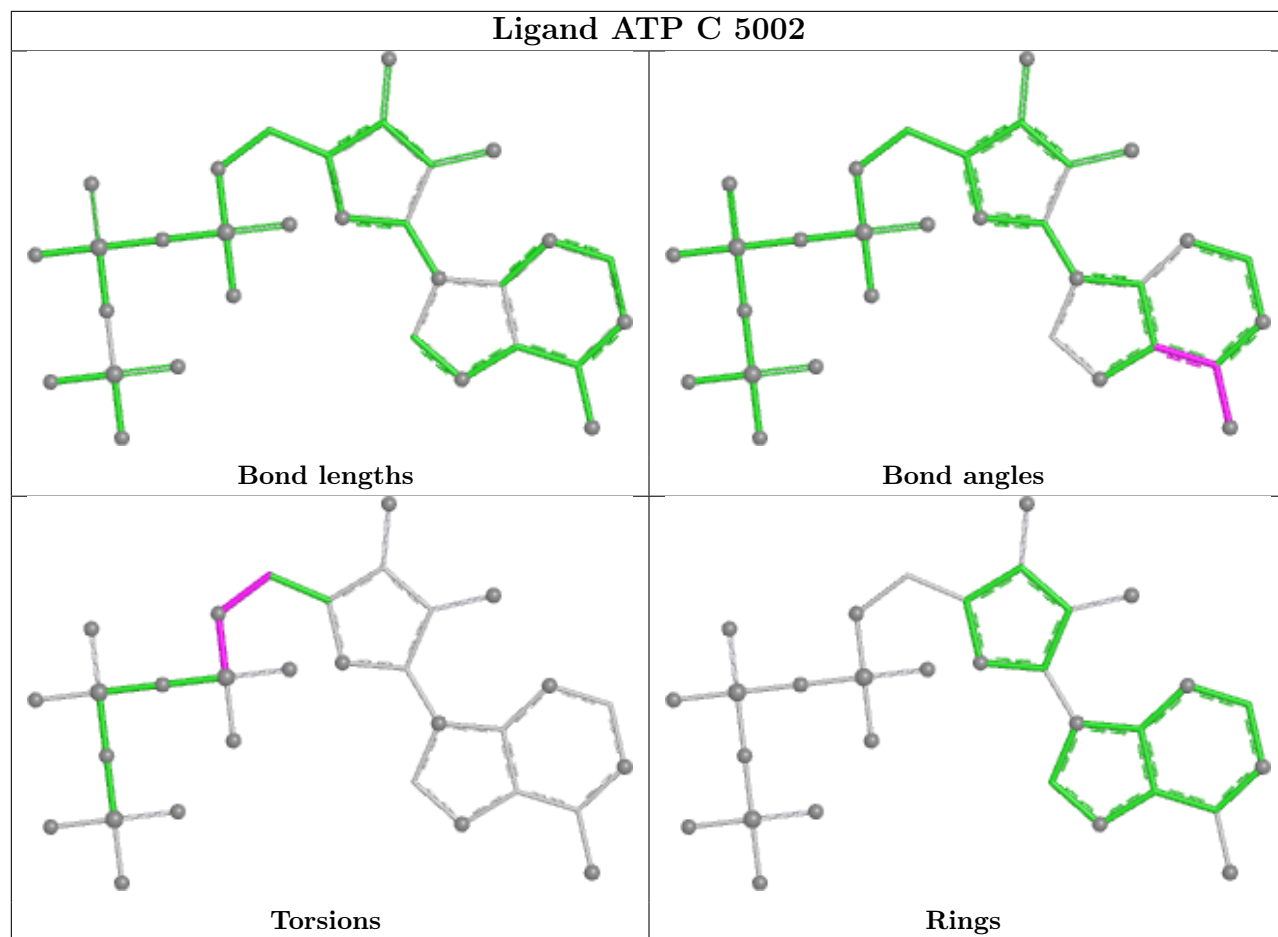
Bond angles



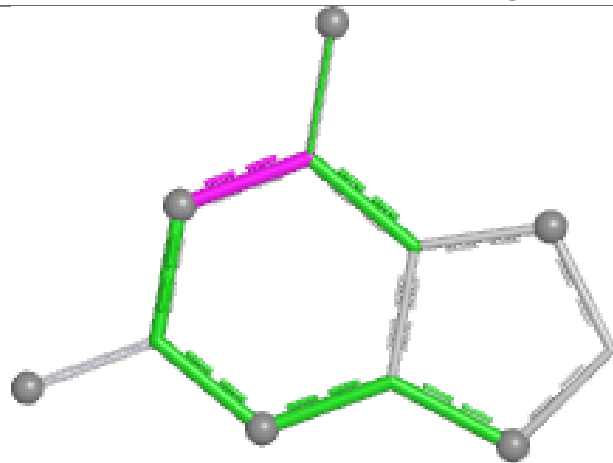
Torsions



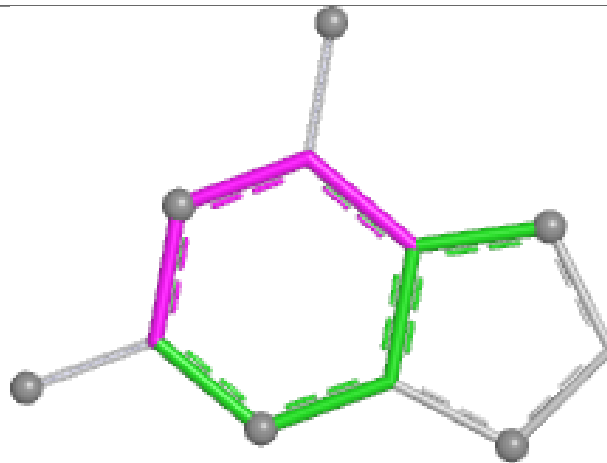
Rings



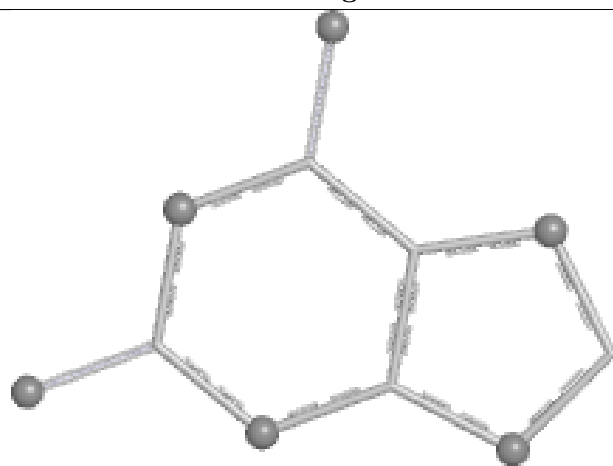
## Ligand XAN B 5004



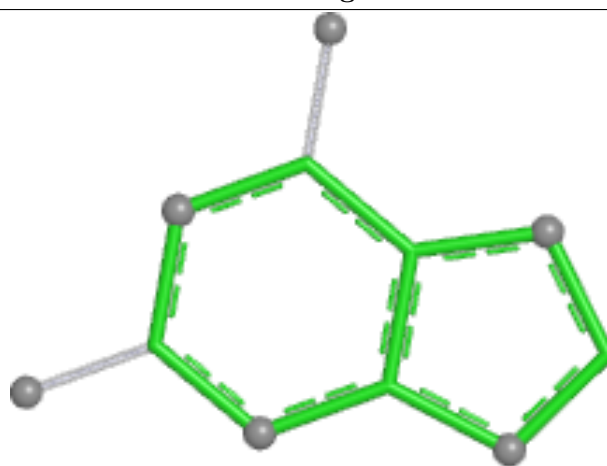
Bond lengths



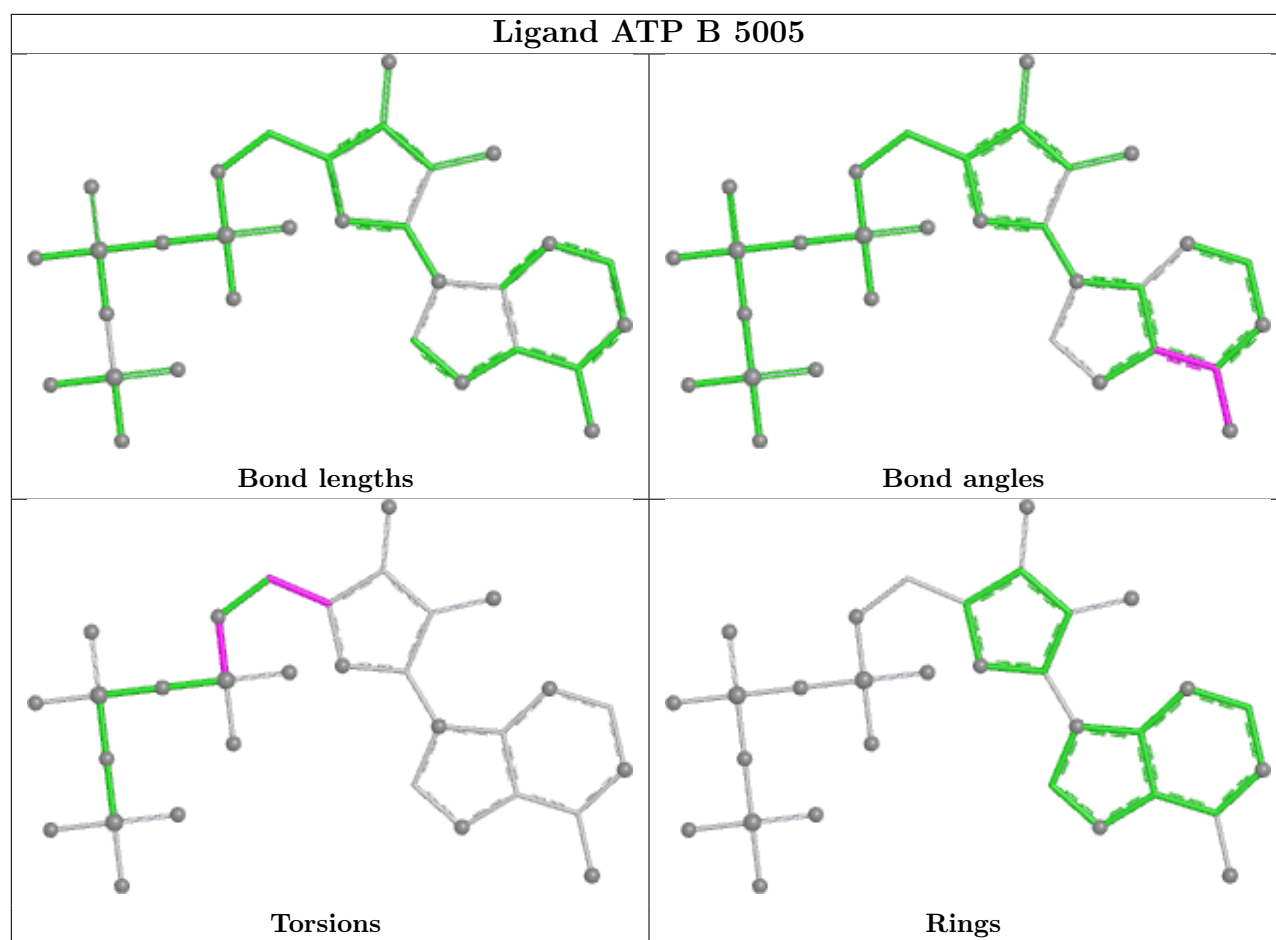
Bond angles



Torsions

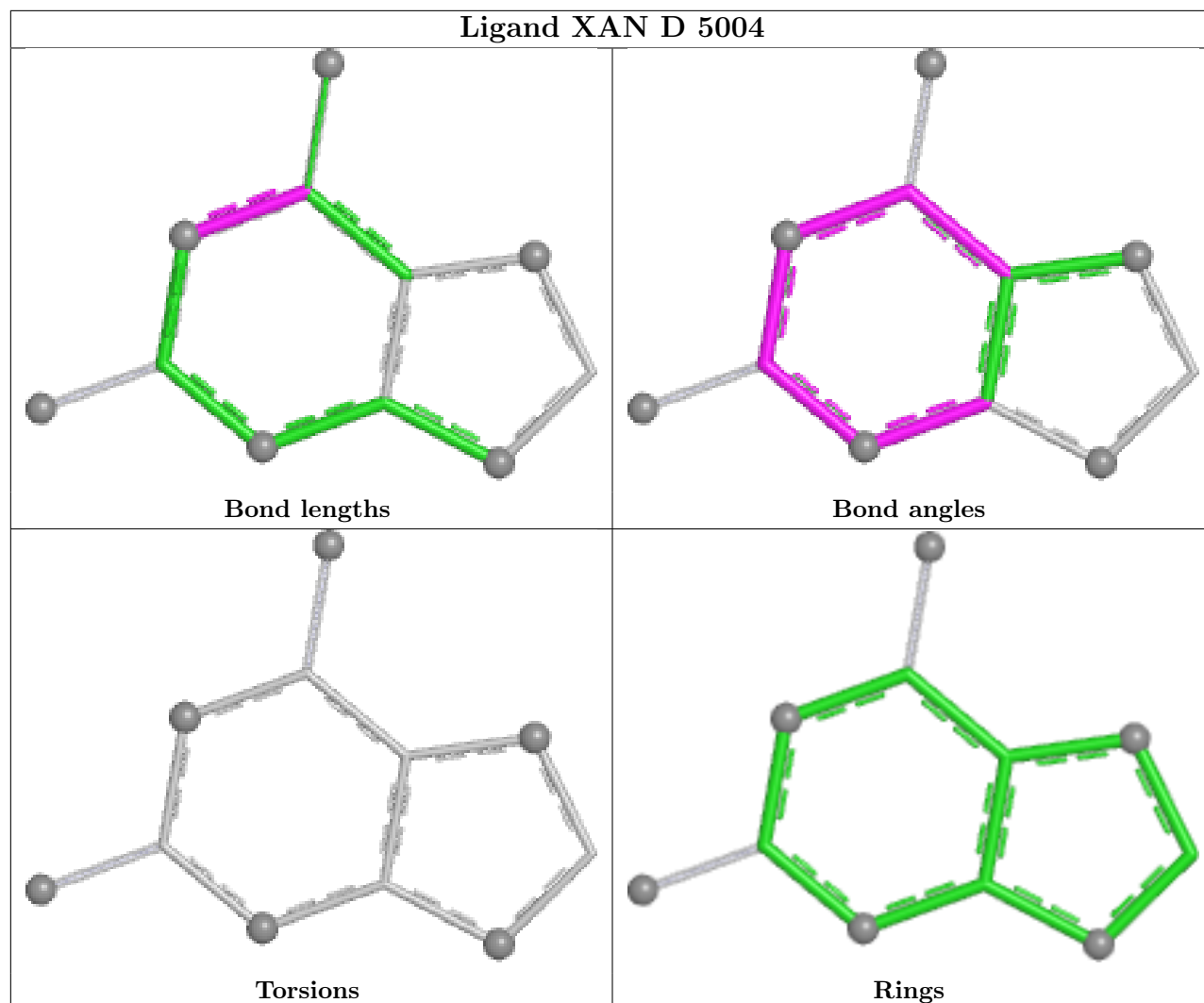


Rings

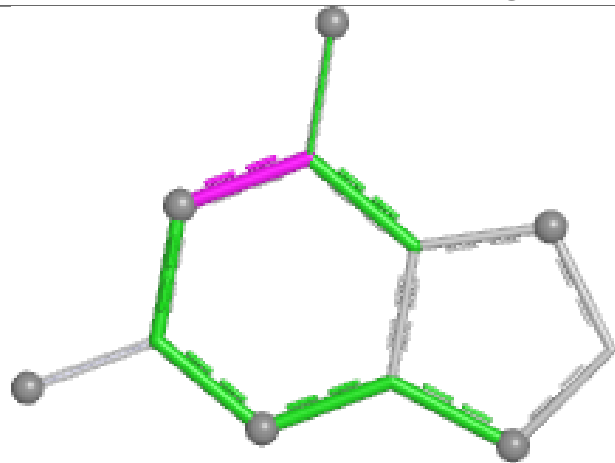




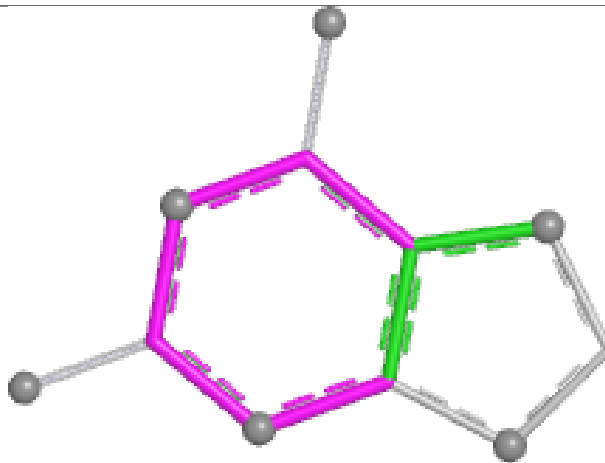
## Ligand XAN D 5004



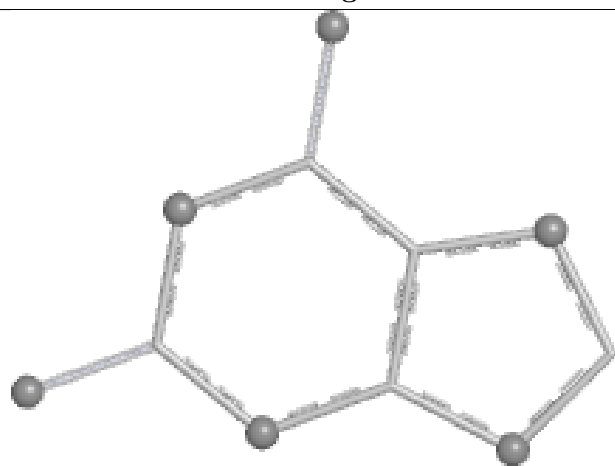
## Ligand XAN A 5004



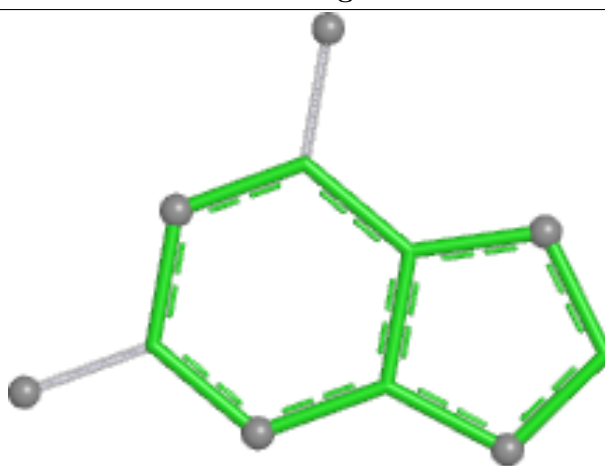
Bond lengths



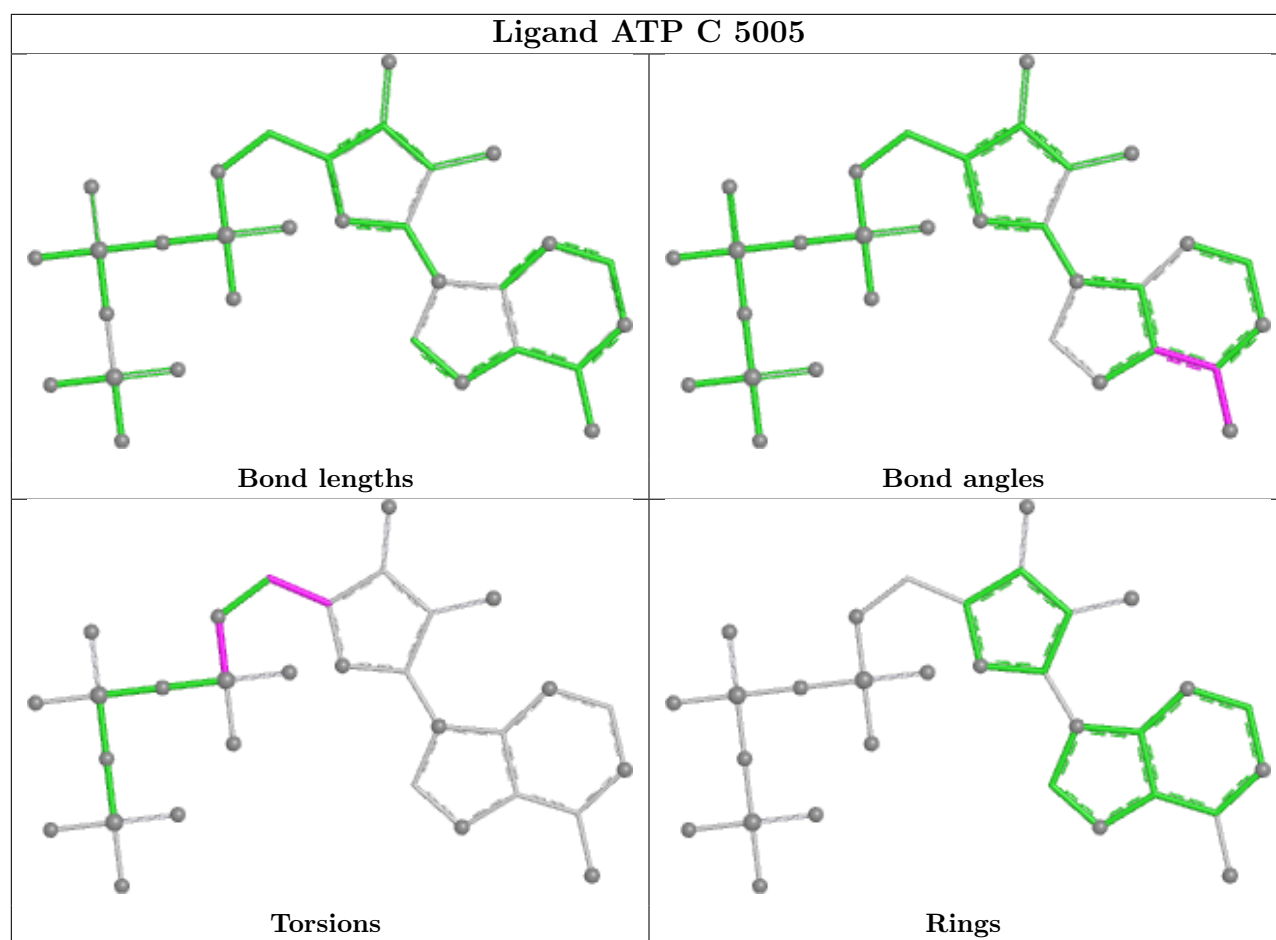
Bond angles



Torsions



Rings



## 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.

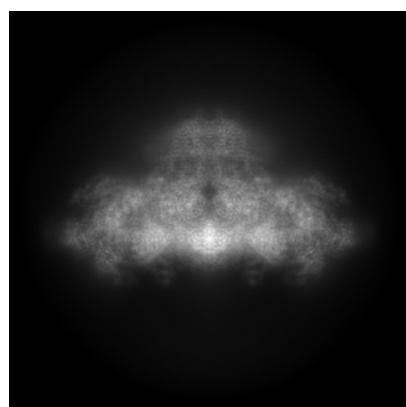
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26414. These allow visual inspection of the internal detail of the map and identification of artifacts.

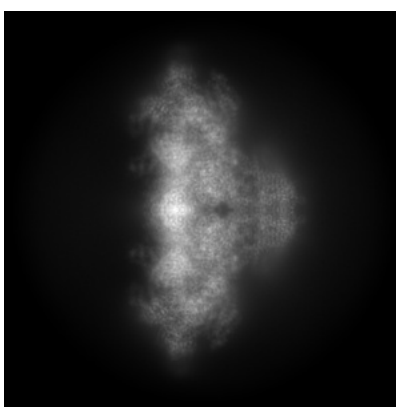
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

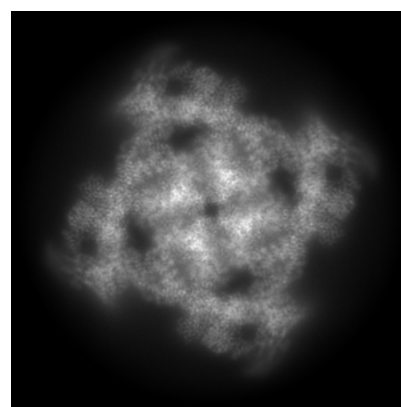
#### 6.1.1 Primary map



X



Y

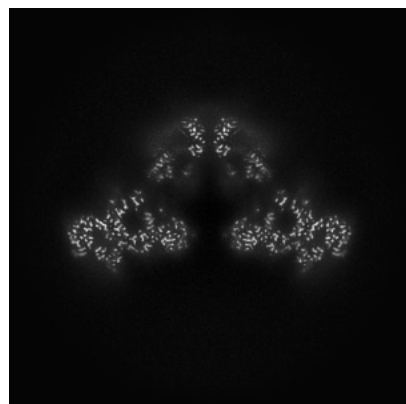


Z

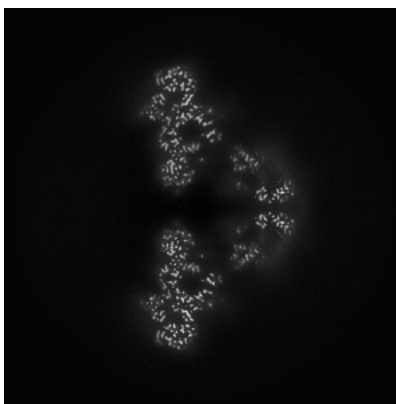
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

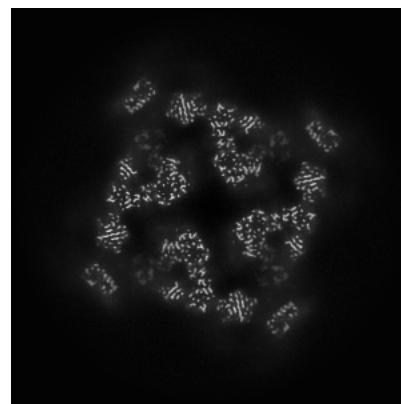
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

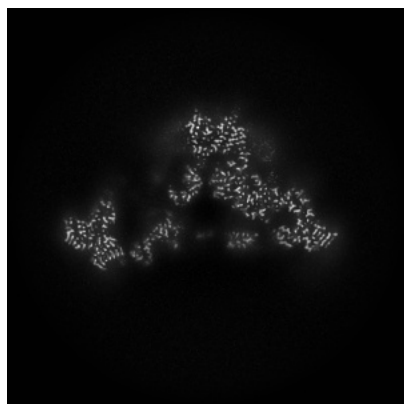


Z Index: 256

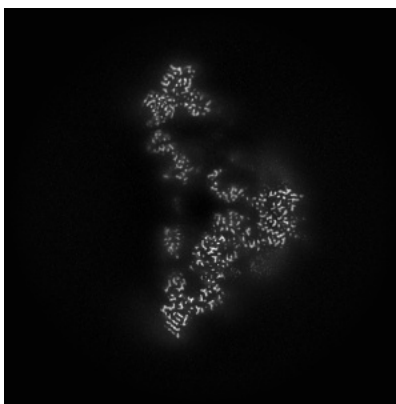
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

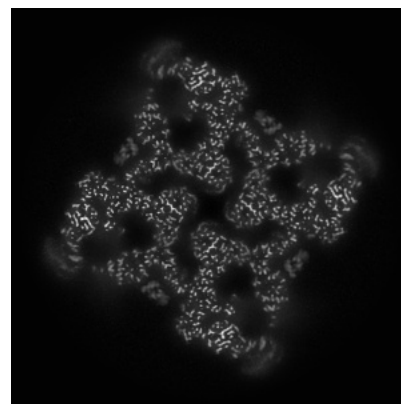
### 6.3.1 Primary map



X Index: 275



Y Index: 274

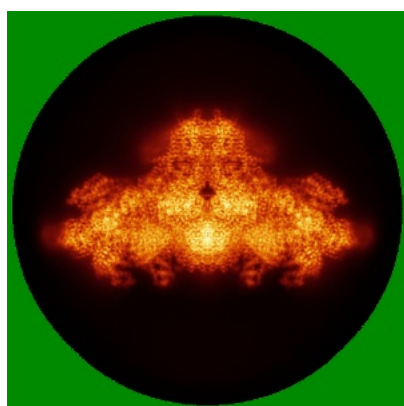


Z Index: 220

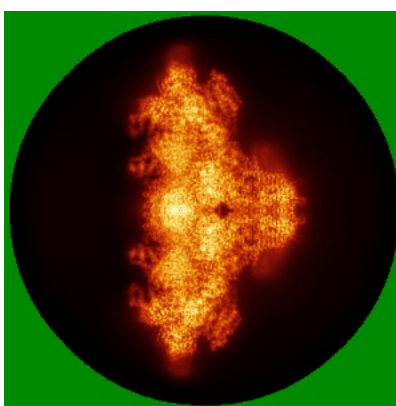
The images above show the largest variance slices of the map in three orthogonal directions.

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

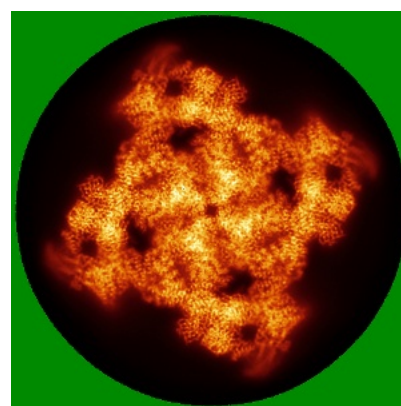
### 6.4.1 Primary map



X



Y

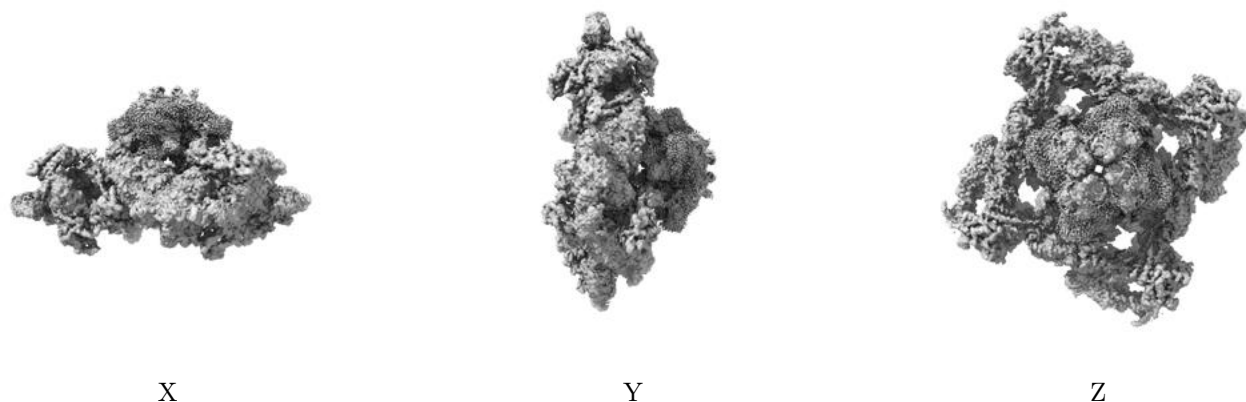


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

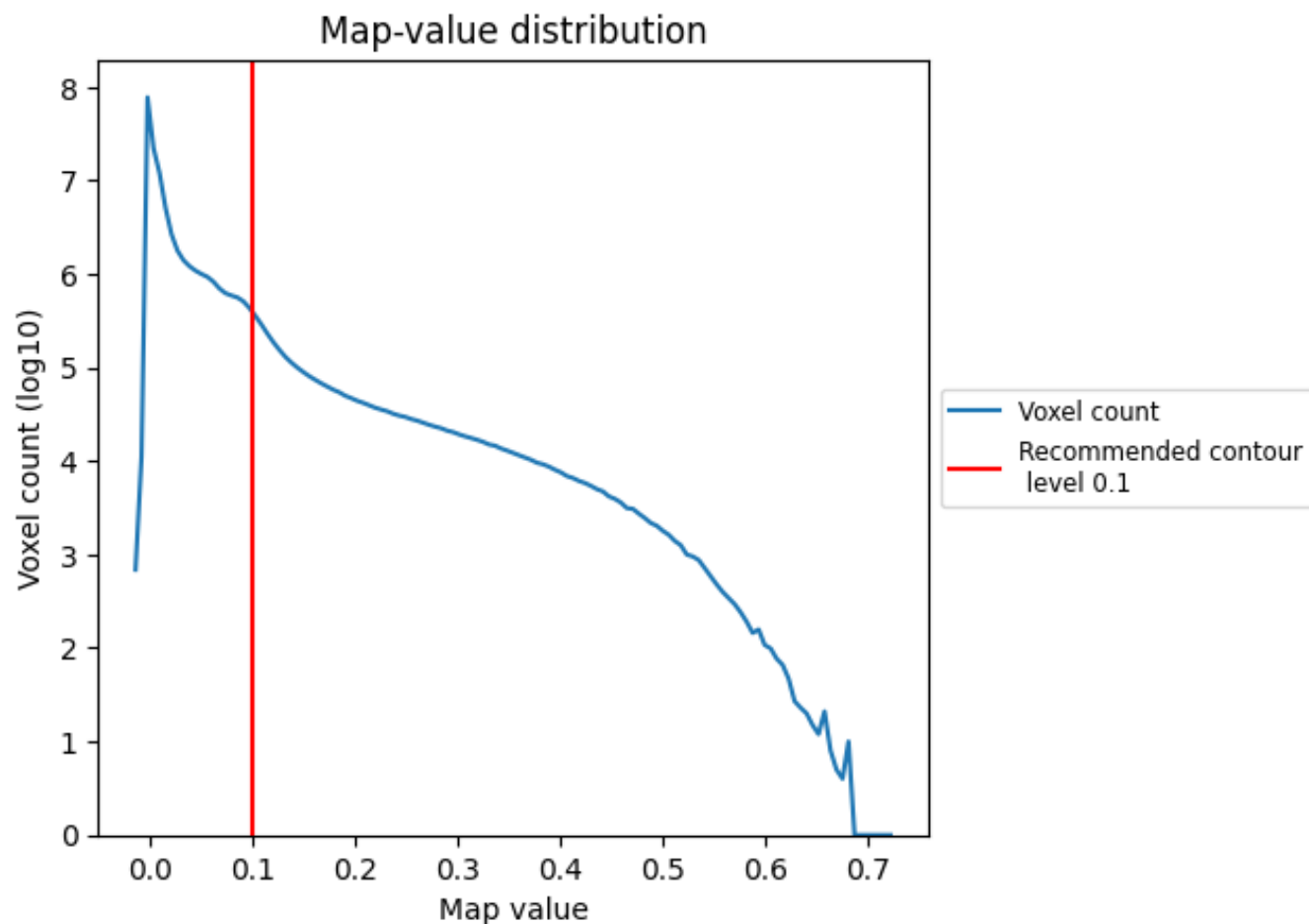
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

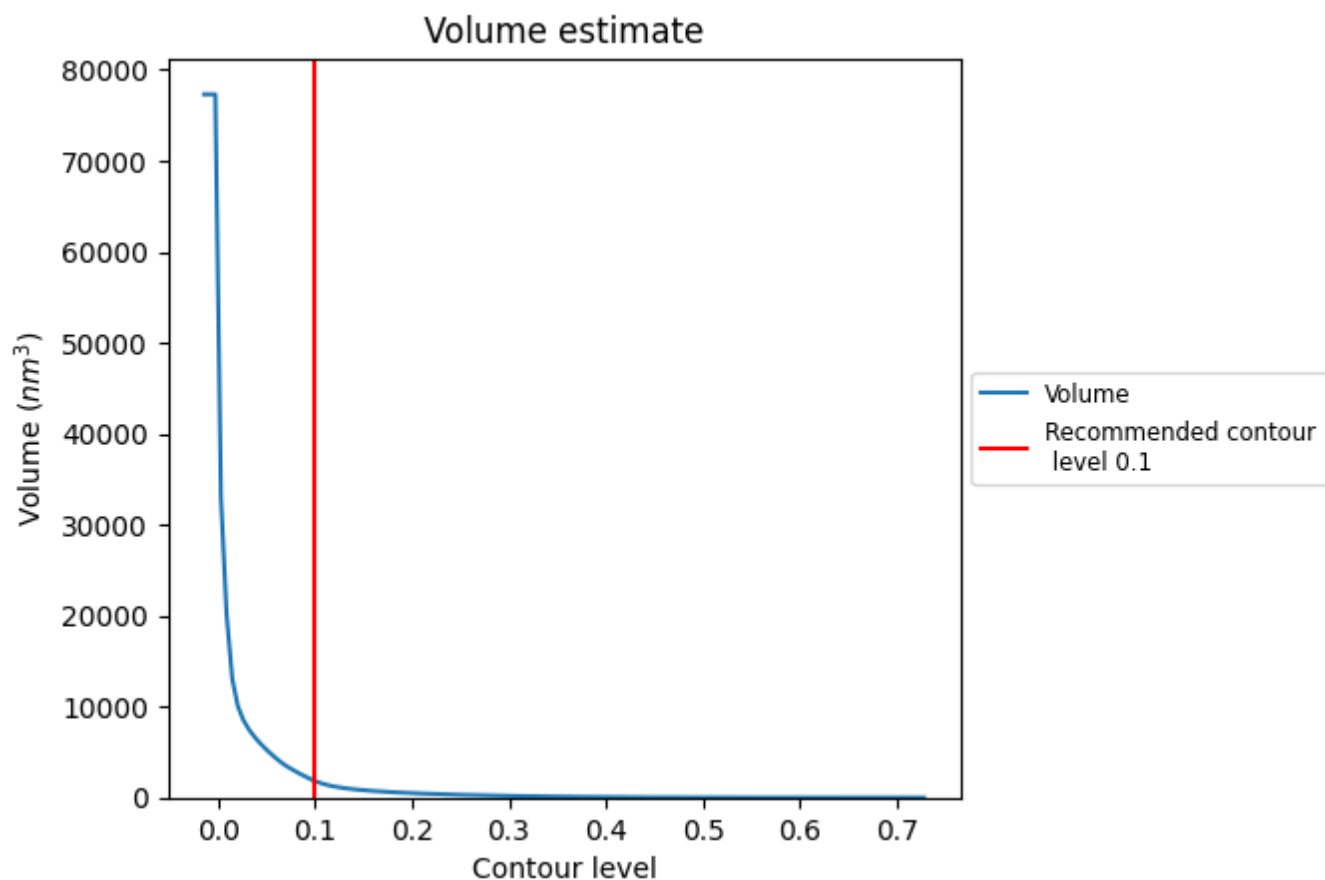
This section contains the results of statistical analysis of the map.

### 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](#)

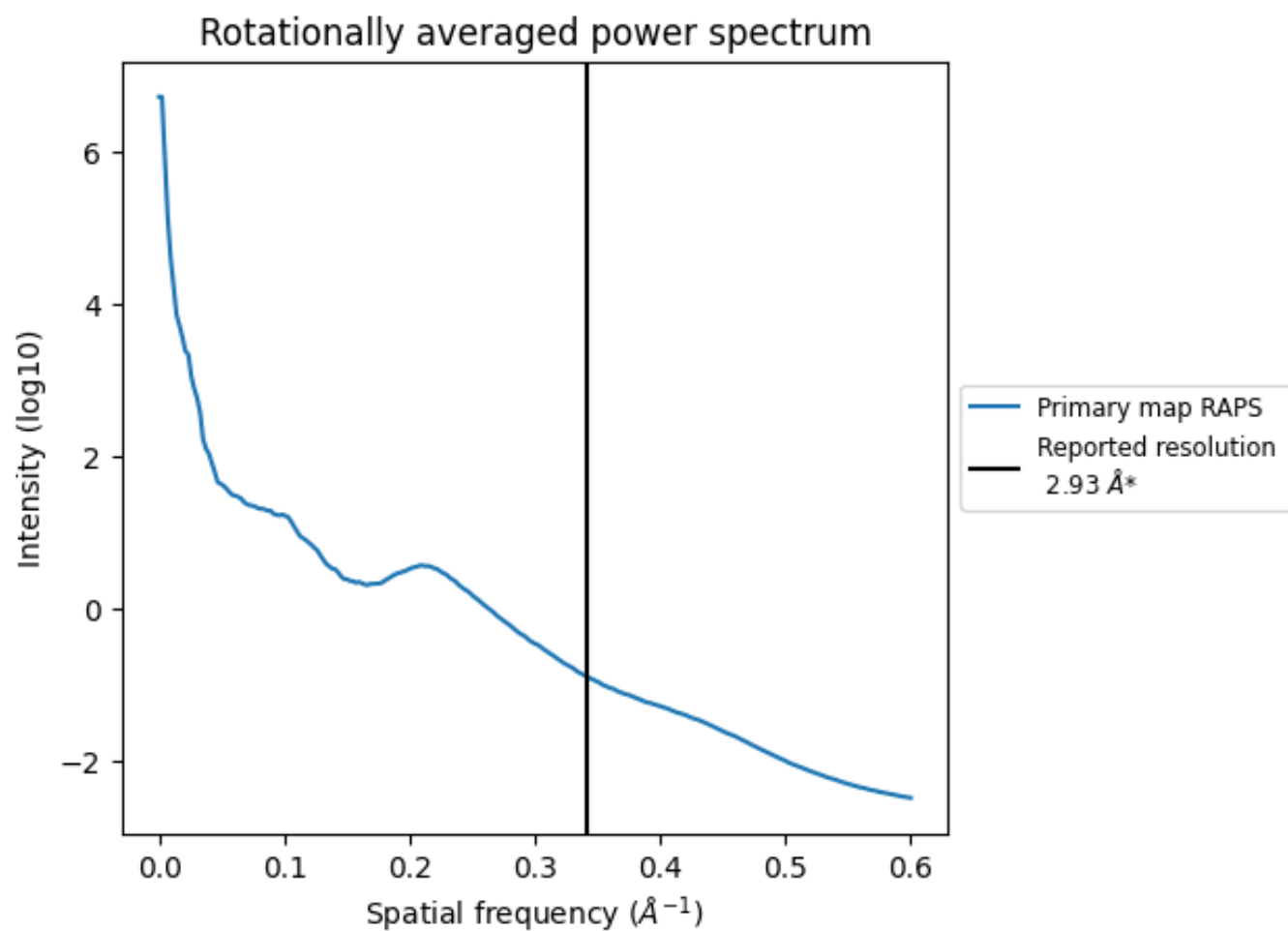


The volume at the recommended contour level is 1824 nm<sup>3</sup>; this corresponds to an approximate mass of 1648 kDa.

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 0.341 Å<sup>-1</sup>

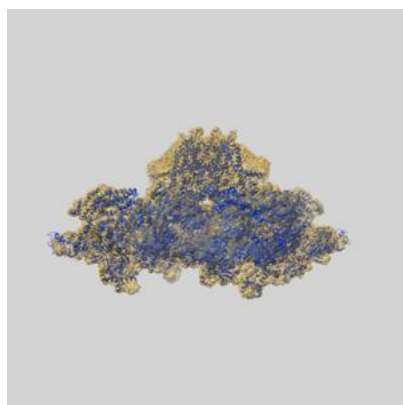
## 8 Fourier-Shell correlation

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

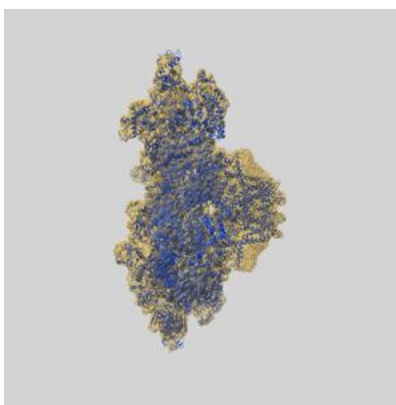
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26414 and PDB model 7UA4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

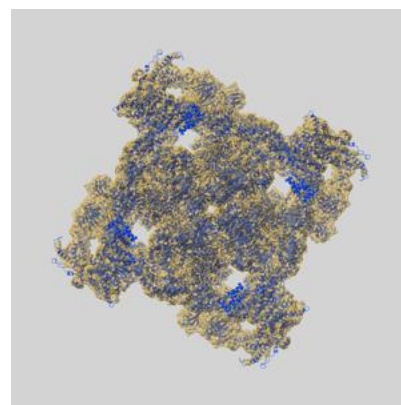
### 9.1 Map-model overlay [i](#)



X



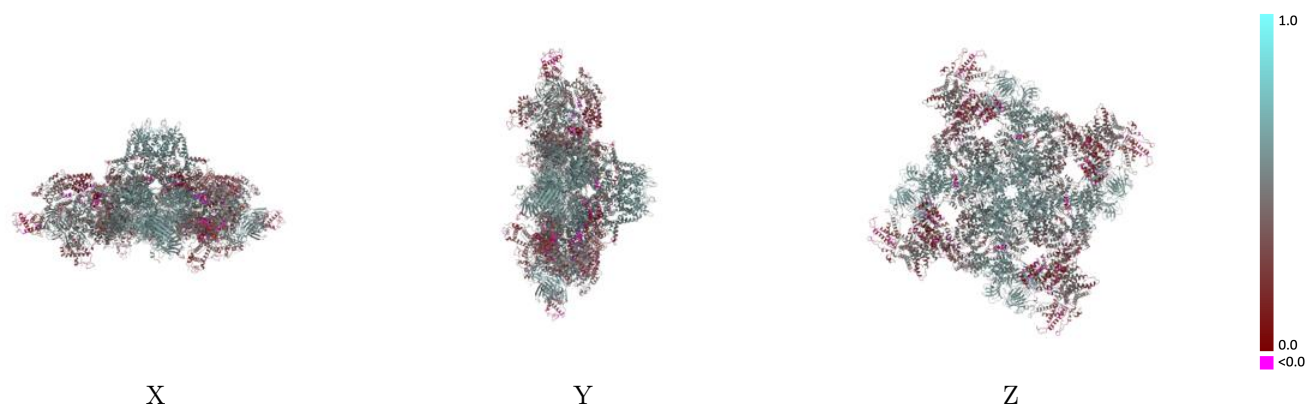
Y



Z

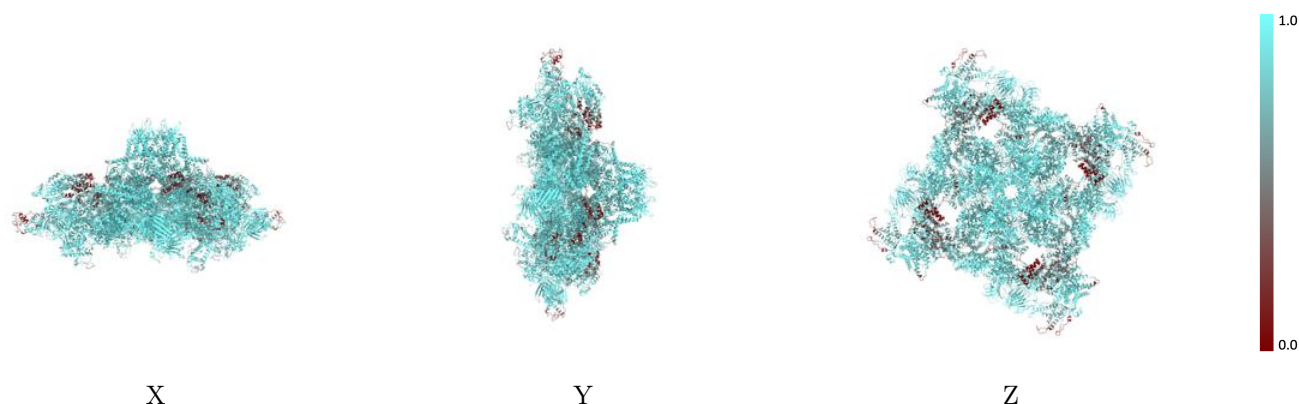
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



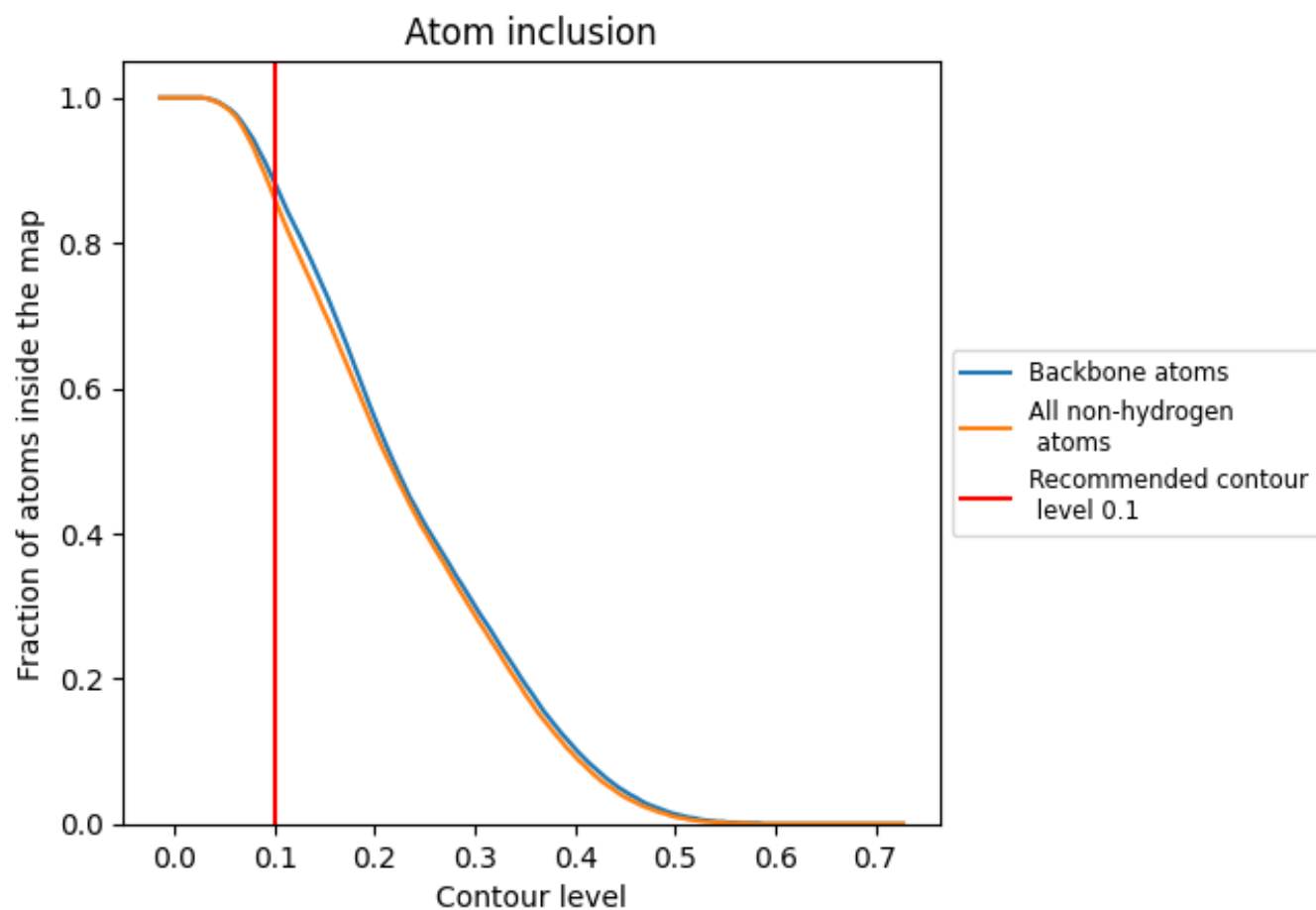
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8610	<div></div> 0.4560
A	<div></div> 0.8680	<div></div> 0.4670
B	<div></div> 0.8670	<div></div> 0.4580
C	<div></div> 0.8660	<div></div> 0.4570
D	<div></div> 0.8660	<div></div> 0.4610
E	<div></div> 0.9670	<div></div> 0.5880
F	<div></div> 0.9720	<div></div> 0.5700
G	<div></div> 0.9720	<div></div> 0.5710
H	<div></div> 0.9690	<div></div> 0.5730
I	<div></div> 0.6900	<div></div> 0.2200
J	<div></div> 0.6640	<div></div> 0.2040
K	<div></div> 0.6880	<div></div> 0.2240
L	<div></div> 0.6650	<div></div> 0.2110

