



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 05:21 PM UTC

PDB ID : 7UA4 / pdb_00007ua4
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

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

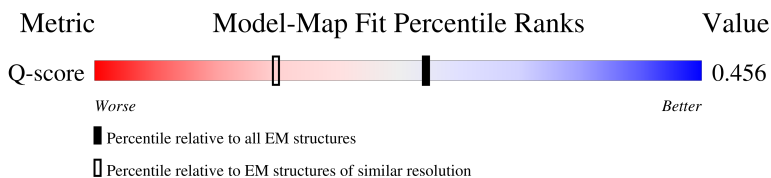
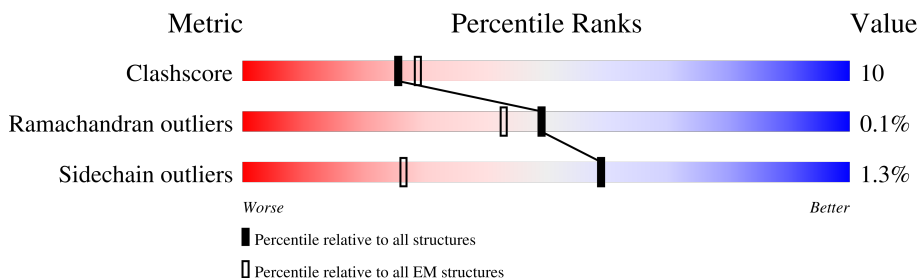
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



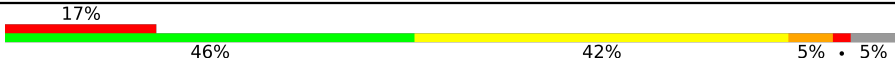
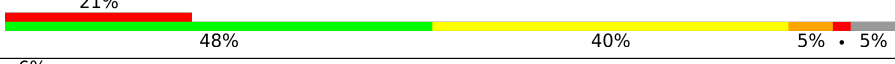
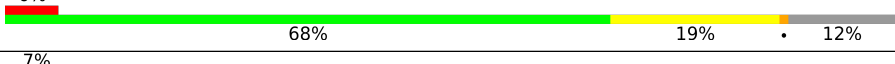
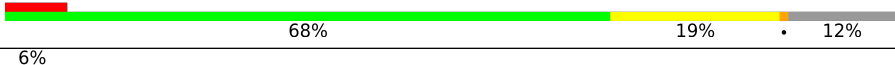
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13037 (2.43 - 3.43)

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	E	108	 76% 21% ...
1	F	108	 77% 20% ...
1	G	108	 75% 22% ...
1	H	108	 77% 20% ...

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Mol	Chain	Length	Quality of chain
2	I	149	
2	J	149	
2	K	149	
2	L	149	
3	A	4967	
3	B	4967	
3	C	4967	
3	D	4967	

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		

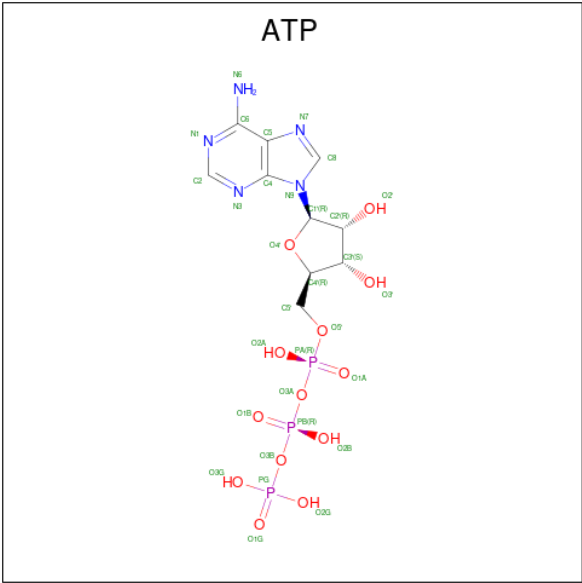
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



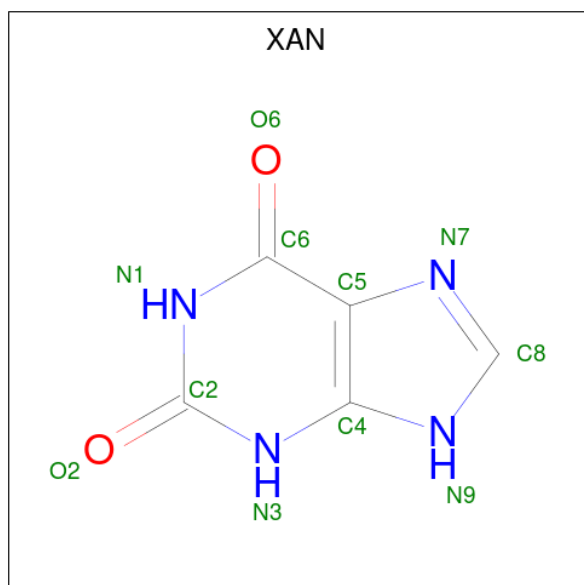
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Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CALCIUM ION (CCD ID: 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 (CCD ID: XAN) (formula: C₅H₄N₄O₂) (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.

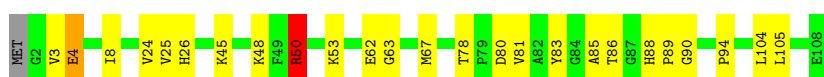
Mol	Chain	Residues	Atoms		AltConf
8	A	3	Total	O	0
			3	3	
8	B	3	Total	O	0
			3	3	
8	C	3	Total	O	0
			3	3	
8	D	3	Total	O	0
			3	3	

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: 



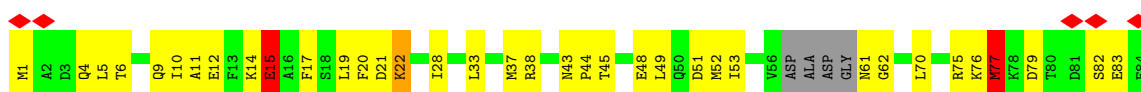
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

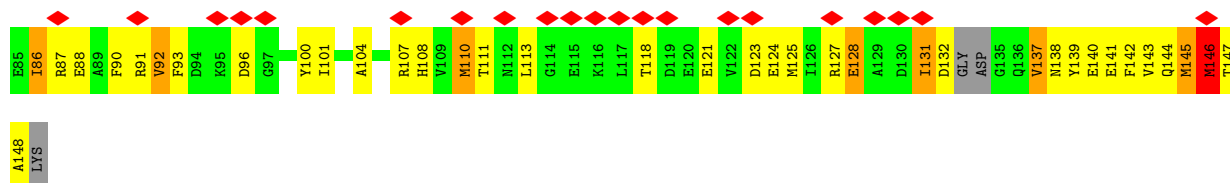
Chain H: 



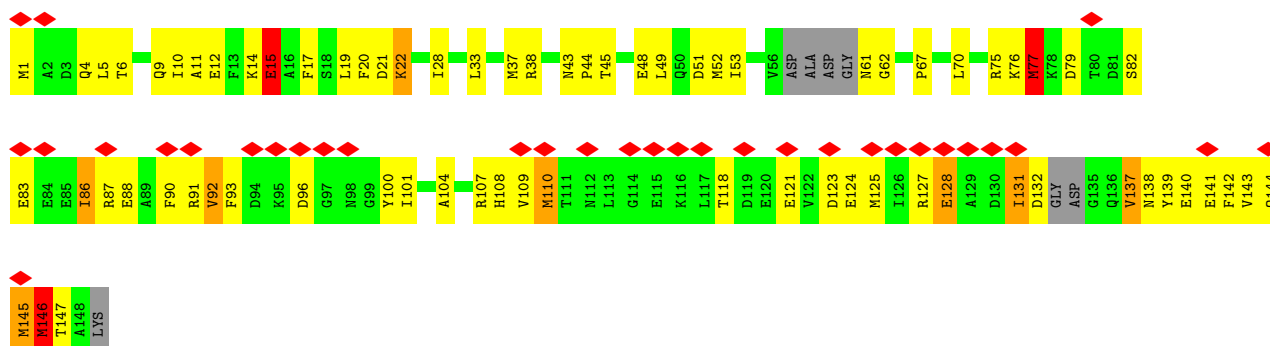
- Molecule 2: Calmodulin-1

Chain I: 

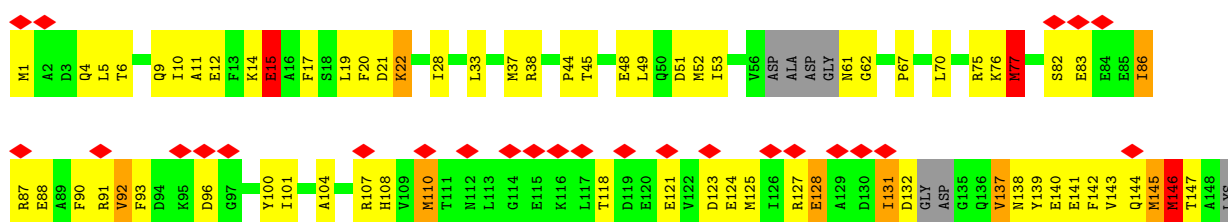




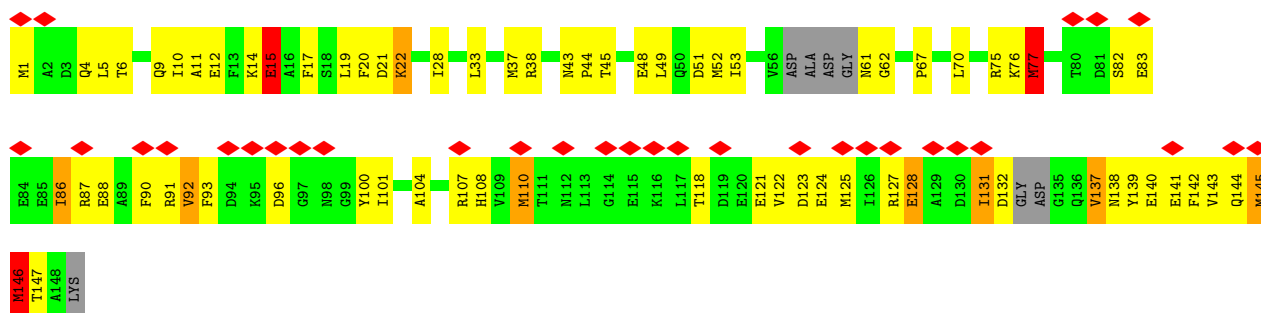
- Molecule 2: Calmodulin-1



- Molecule 2: Calmodulin-1

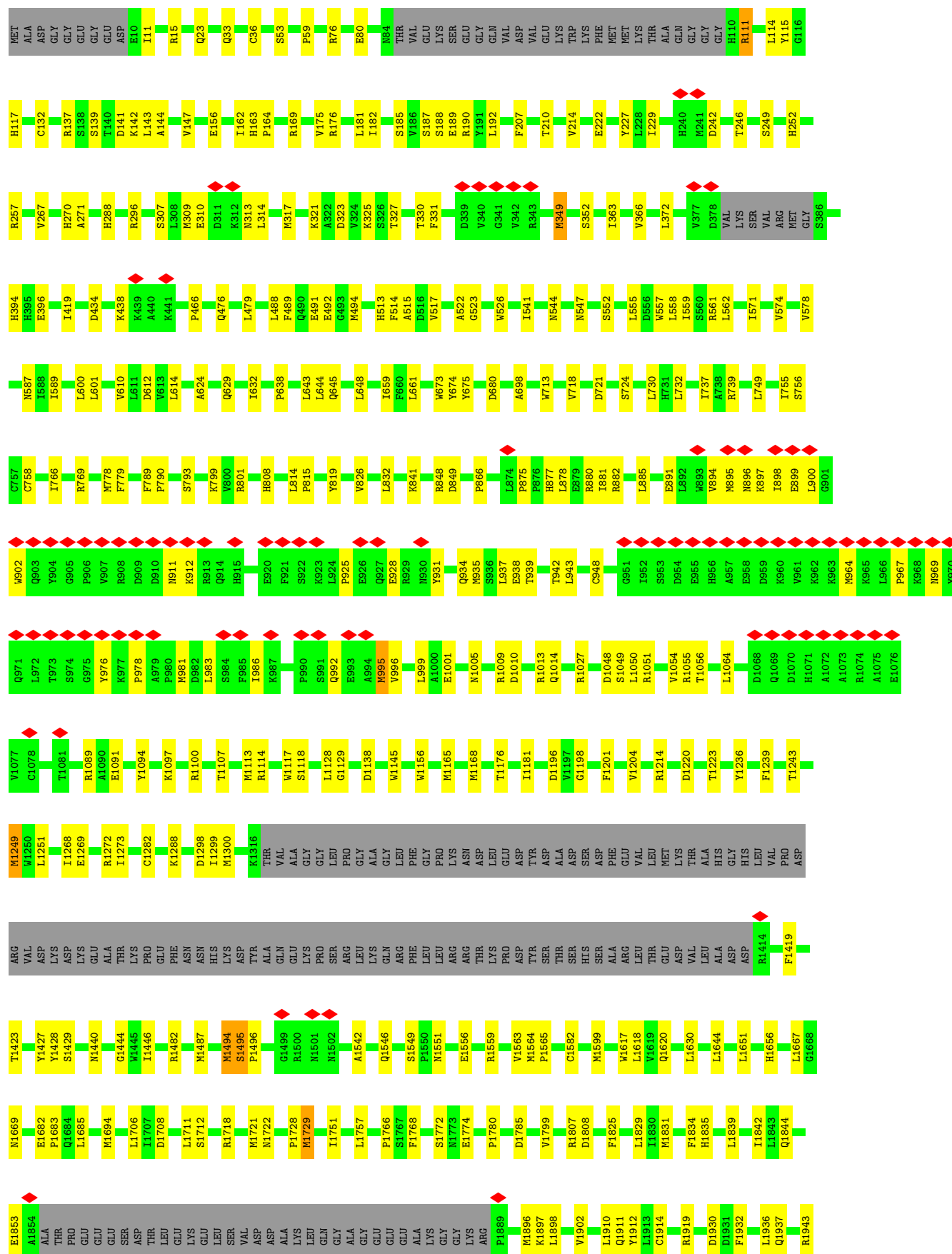


- Molecule 2: Calmodulin-1



- Molecule 3: Ryanodine receptor 2





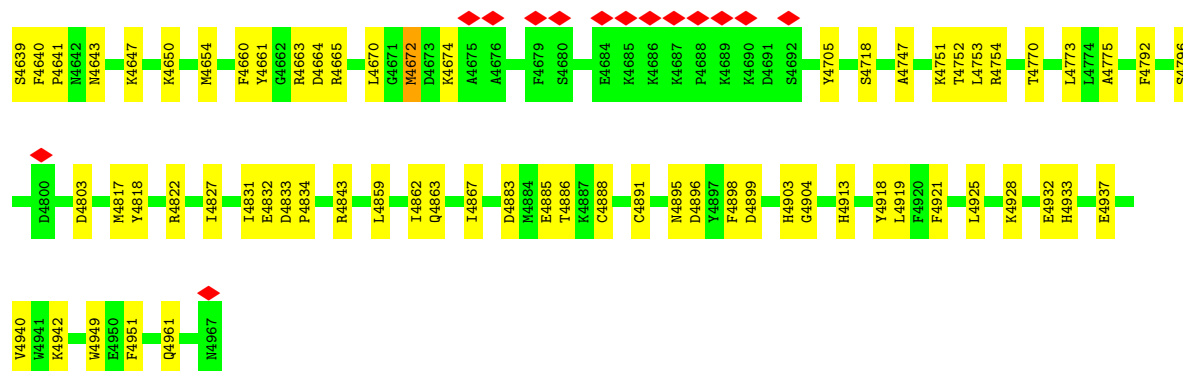




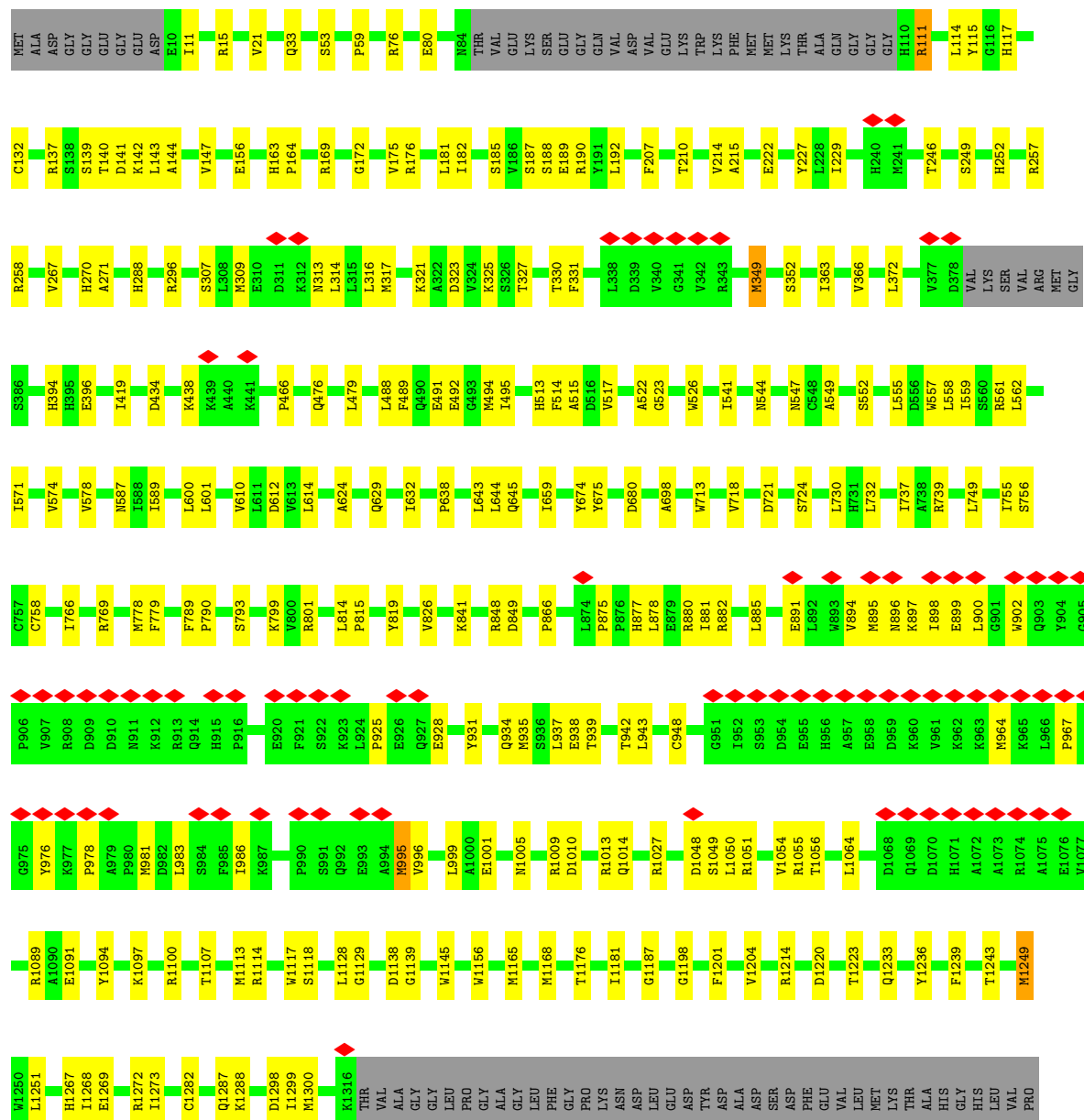


E3223	F3109	I2971	G2866	M2782	K2716	I2569	THR	Y2202	ALA	A1959	ASP	M1694
R3227	I3121	R2979	V2872	W2785	L2717	L2580	LEU	I2206	GLU	R1960	THR	L1706
M3231	I3122	R2981	G2786	W2787	F2720	P2581	ASP	Y2220	PRO	L1961	GLU	I1707
P3232	L3123	Y2981	R2787	R2788	L2721	P2582	GLU	L2221	VAL	D1708	LYS	D1708
H3233	E3124	R2988	L2877	I2789	W2722	S2583	GLU	L2222	GLU	F1965	GLU	L1711
V3234		P2989	K2884	I2789	K2723	M2584	THR	L2223	SER	R1966	LEU	S1712
M3235		L2990	E2887	T2792	K2724	R2590	ASP	M2224	ASP	S1967	SER	
E3236		H2995	E2887	E2794	A2725	V2593	GLU	V2227	SER	Q1972	VAL	R1718
V3237		V3015	E2887	E2794	K2726	V2593	GLU	G2228	ASP	I1973	ASP	M1721
I3238		F3022	V2802	E2794	A2726	V2593	GLU	L2229	ALA	M1974	LYS	M1722
L3242		F3022	ARG	E2794	D2730	V2593	GLU	R2235	LEU	M1975	GLN	M1729
M3246		F3022	THR	E2794	M2734	V2596	GLU	R2235	GLY	Q1972	GLY	
G3247		D3025	ARG	E2794	D2735	A2603	GLY	D2241	ALA	I1973	ALA	I1761
R3248		Y3149	ARG	E2794	K2736	M2604	GLY	E2072	GLY	M1974	GLY	
W3249		R3150	ILE	E2794	L2737	M2605	GLY	I2075	GLU	M1975	GLY	P1766
W3250		I3029	SER	E2794	H2407	P2606	GLU	E2076	GLU	M1976	GLU	S1767
N3256		I3033	GLN	E2794	E2415	L2607	GLU	D2077	ALA	F1979	ALA	F1768
L3268		L3033	THR	E2794	I2419	L2610	GLU	R2082	LYS	Q1972	LYS	S1772
N3269		H3034	SER	E2794	I2422	C2617	GLU	R2082	GLY	I1973	GLY	N1773
G3270		R3035	VAL	E2794	I2422	S2641	GLU	L2087	LYS	M1974	GLY	E1774
E3271		L3036	ASP	E2794	S2425	L2644	GLU	R2090	ARG	M1975	LYS	P1780
H3272		G3037	ASP	E2794	I2436	F2645	GLU	Q2091	ASP	I1976	ARG	
M3273		Q3038	ASP	E2794	I2436	L2645	GLU	R2133	GLU	F1979	ASP	
N3274		T3039	ASP	E2794	I2436	L2645	GLU	E2139	ASP	M1896	ASP	I1792
T3275		L3040	ASP	E2794	I2436	L2645	GLU	M2142	GLY	K1897	GLY	V1799
L3276		M3046	ASP	E2794	I2436	L2645	GLU	L2146	LEU	D1807	LEU	R1807
G3277		K3047	ASP	E2794	I2436	L2645	GLU	M2150	ASP	D1808	LEU	D1808
N3278		T3070	ASP	E2794	I2436	L2645	GLU	E2285	ASP	V1902	GLY	F1825
I3280		M3072	ASP	E2794	I2436	L2645	GLU	R2290	ASN	L1910	GLY	L1829
L3281		E3073	ASP	E2794	I2436	L2645	GLU	E2296	SER	Q1911	LYS	Y1912
I3284		K3076	ASP	E2794	I2436	L2645	GLU	R2297	ASP	L1913	GLY	I1830
I3290		Q3077	ASP	E2794	I2436	L2645	GLU	E2285	LEU	C1914	GLY	M1831
W3295		T3081	ASP	E2794	I2436	L2645	GLU	R2322	THR	THR	ILE	F1834
M3296		HIS	ASP	E2794	I2436	L2645	GLU	H2158	ARG	H1835	ARG	H1835
K3297		THR	ASP	E2794	I2436	L2645	GLU	V2171	GLY	D1930	GLY	D1838
R3298		THR	ASP	E2794	I2436	L2645	GLU	R2306	ARG	D1931	ARG	D1838
L3299		GLN	ASP	E2794	I2436	L2645	GLU	G2332	LEU	F1932	LEU	L1839
I3307		PRO	ASP	E2794	I2436	L2645	GLU	R2336	SER	L1936	SER	I1842
N3308		K3088	ASP	E2794	I2436	L2645	GLU	G2337	VAL	Q1937	VAL	L1843
K3309		G3089	ASP	E2794	I2436	L2645	GLU	E2338	GLY	R1943	GLY	Q1844
P3312		I3093	ASP	E2794	I2436	L2645	GLU	S2368	THR	E1946	THR	E1853
Q3313		I3094	ASP	E2794	I2436	L2645	GLU	P2364	THR	A1854	ALA	A1854
L3314		A3100	ASP	E2794	I2436	L2645	GLU	ASN	TYR	L1951	TYR	THR
M3215		L3214	ASP	E2794	I2436	L2645	GLU	SER	LEU	N1952	LEU	PRO
V3219		L3101	ASP	E2794	I2436	L2645	GLU	GLY	LYS	N1952	LYS	GLU
E3220		L3102	ASP	E2794	I2436	L2645	GLU	SER	LYS	A1955	LYS	GLU
L3221		P3103	ASP	E2794	I2436	L2645	GLU	LYS	GLN	T1958	GLN	SER
A3222		M3104	ASP	E2794	I2436	L2645	GLU	LYS	GLN			





• Molecule 3: Ryanodine receptor 2





THR	GLU	GLU	SER	CYS	TYR	V4176	G4039	V3820	R3660	Q3563	D3503	ALA	D3378	K3297	E3191	ARG
LEU	LEU	SER	LEU	SER	ILE	E4182	K4040	T3821	V3661	K3564	E3504	VAL	Y3379	R3298	R3192	ASN
LEU	LEU	LEU	LEU	LEU	THR	K4183	K4045	E3822	Q3666	SER	V3505	ASP	R3381	L3299	P3198	GLN
LEU	GLY	LEU	GLY	LEU	THR	M4186	M4052	E3823	E3678	VAL	R3506	GLU	K3386	N3307	V3201	G3088
LEU	GLY	LEU	GLY	LEU	THR	E4187	E4053	E3824	E3684	ARG	D3507	ARG	E3387	K3309	V3204	I3093
LEU	GLY	LEU	GLY	LEU	THR	L4188	M4062	E3825	E3685	ARG	I3508	GLY	E3388	P3312	V3204	I3093
LEU	GLY	LEU	GLY	LEU	THR	F4189	S4061	E3826	F3686	ARG	I3509	LYS	E3389	K3310	V3204	I3093
LEU	GLY	LEU	GLY	LEU	THR	V4190	T4063	E3827	L3687	ARG	R3510	LYS	E3390	L3313	L3214	I3094
LEU	GLY	LEU	GLY	LEU	THR	M4191	T4064	E3828	Y3688	TYR	R3511	LYS	E3391	L3314	M3215	A3100
LEU	GLY	LEU	GLY	LEU	THR	T4196	E4065	E3829	K3689	CYS	S3512	LYS	E3392	L3315	M3215	L3101
LEU	GLY	LEU	GLY	LEU	THR	A4203	L4066	E3830	K3690	VAL	T3513	LYS	E3393	K3316	E3220	L3102
LEU	GLY	LEU	GLY	LEU	THR	T4206	E4074	E3831	Y3691	VAL	H3514	LYS	E3394	L3317	L3221	F3103
LEU	GLY	LEU	GLY	LEU	THR	S4209	L4078	E3832	K3695	GLY	H3515	LYS	E3395	F3319	E3221	K3104
LEU	GLY	LEU	GLY	LEU	THR	ASP	D4079	E3833	F3696	GLY	Q3516	LYS	E3396	L3320	L3222	F3103
LEU	GLY	LEU	GLY	LEU	THR	ASN	D4082	E3834	K3697	GLY	Q3517	LYS	E3397	P3321	E3223	K3104
LEU	GLY	LEU	GLY	LEU	THR	ASN	E4091	E3835	H3700	ALA	K3518	LYS	E3400	K3323	F3109	F3109
LEU	GLY	LEU	GLY	LEU	THR	LEU	L4092	E3836	D3701	LYS	R3519	LYS	E3401	E3324	L3121	L3121
LEU	GLY	LEU	GLY	LEU	THR	LEU	K4093	E3837	E3702	LYS	E3520	LYS	E3402	L3325	L3122	L3122
LEU	GLY	LEU	GLY	LEU	THR	LEU	T3867	E3838	ASP	TRP	E3521	LYS	E3403	K3326	E3124	E3124
LEU	GLY	LEU	GLY	LEU	THR	LEU	V3868	E3839	ASP	TRP	P3522	LYS	E3404	L3327	Q3127	Q3127
LEU	GLY	LEU	GLY	LEU	THR	LEU	I3872	E3840	ASP	HIS	A3523	LYS	E3405	E3236	L3134	L3134
LEU	GLY	LEU	GLY	LEU	THR	LEU	S3873	E3841	ASP	HIS	I3524	LYS	E3406	V3237	A3139	A3139
LEU	GLY	LEU	GLY	LEU	THR	LEU	T3874	E3842	GLY	LEU	R3525	LYS	E3407	L3238	L3140	L3140
LEU	GLY	LEU	GLY	LEU	THR	LEU	V3875	E3843	GLY	LEU	Q3526	LYS	E3408	M3235	L3242	S3145
LEU	GLY	LEU	GLY	LEU	THR	LEU	H4108	E3844	GLY	LEU	W3526	LYS	E3409	E3336	L3242	S3145
LEU	GLY	LEU	GLY	LEU	THR	LEU	M4109	E3845	E3710	LYS	Q3527	LYS	E3410	E3337	M3246	M3246
LEU	GLY	LEU	GLY	LEU	THR	LEU	S3884	E3846	E3711	LYS	M3528	LYS	E3411	P3338	S3247	V3148
LEU	GLY	LEU	GLY	LEU	THR	LEU	T4113	E3847	E3715	LYS	A3529	LYS	E3412	H3339	R3149	R3149
LEU	GLY	LEU	GLY	LEU	THR	LEU	Q4116	E3848	K3719	LYS	L3530	LYS	E3413	L3340	R3248	R3248
LEU	GLY	LEU	GLY	LEU	THR	LEU	L4119	E3849	E3729	LYS	Y3531	LYS	E3414	H3341	Q3151	Q3151
LEU	GLY	LEU	GLY	LEU	THR	LEU	A4122	E3850	R3730	LYS	K3532	LYS	E3415	A3342	R3152	R3152
LEU	GLY	LEU	GLY	LEU	THR	LEU	I3924	E3851	L3731	LYS	D3533	LYS	E3416	E3343	S3153	S3153
LEU	GLY	LEU	GLY	LEU	THR	LEU	Q3925	E3852	H3732	LYS	L3534	LYS	E3417	A3344	A3154	A3154
LEU	GLY	LEU	GLY	LEU	THR	LEU	K3957	E3853	V3740	LYS	F3535	LYS	E3418	R3345	G3156	G3156
LEU	GLY	LEU	GLY	LEU	THR	LEU	Q3975	E3854	E3758	LYS	N3536	LYS	E3419	E3346	E3157	E3157
LEU	GLY	LEU	GLY	LEU	THR	LEU	V3979	E3855	T3763	LYS	R3537	LYS	E3420	D3347	F3162	F3162
LEU	GLY	LEU	GLY	LEU	THR	LEU	K3997	E3856	I3763	LYS	T3538	LYS	E3421	M3273	A3165	A3165
LEU	GLY	LEU	GLY	LEU	THR	LEU	S4155	E3857	Q3774	LYS	D3539	LYS	E3422	N3274	F3166	F3166
LEU	GLY	LEU	GLY	LEU	THR	LEU	L4014	E3858	E3778	LYS	T3541	LYS	E3423	T3275	P3167	P3167
LEU	GLY	LEU	GLY	LEU	THR	LEU	M4019	E3859	A3794	LYS	S3542	LYS	E3424	L3276	G3276	G3276
LEU	GLY	LEU	GLY	LEU	THR	LEU	L4023	E3860	L3803	LYS	P3544	LYS	E3425	A3351	V3168	V3168
LEU	GLY	LEU	GLY	LEU	THR	LEU	K4166	E3861	D3804	LYS	E3545	LYS	E3426	E3352	N3279	N3279
LEU	GLY	LEU	GLY	LEU	THR	LEU	L4026	E3862	R3810	LYS	S3546	LYS	E3427	L3353	L3174	L3174
LEU	GLY	LEU	GLY	LEU	THR	LEU	T4027	E3863	E3818	LYS	T3547	LYS	E3428	E3354	L3175	L3175
LEU	GLY	LEU	GLY	LEU	THR	LEU	S4028	E3864	G3818	LYS	V3548	LYS	E3429	L3355	I3183	I3183
LEU	GLY	LEU	GLY	LEU	THR	LEU	Q4171	E3865	N3819	LYS	E3549	LYS	E3430	I3284	Y3184	Y3184
LEU	GLY	LEU	GLY	LEU	THR	LEU	F4172	E3866	E3819	LYS	R3551	LYS	E3431	E3356	K3187	K3187
LEU	GLY	LEU	GLY	LEU	THR	LEU	K4033	E3867	E3819	LYS	L3552	LYS	E3432	L3357	S3188	S3188
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3868	E3819	LYS	L3553	LYS	E3433	M3296	M3296	M3296
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3869	E3819	LYS	I3554	LYS	E3434	E3357	E3357	E3357
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3870	E3819	LYS	A3555	LYS	E3435	L3372	S3189	S3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3871	E3819	LYS	N3556	LYS	E3436	L3373	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3872	E3819	LYS	V3557	LYS	E3437	L3374	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3873	E3819	LYS	L3560	LYS	E3438	F3376	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3874	E3819	LYS	E3561	LYS	E3439	V3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3875	E3819	LYS	E3562	LYS	E3440	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3876	E3819	LYS	E3563	LYS	E3441	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3877	E3819	LYS	E3564	LYS	E3442	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3878	E3819	LYS	E3565	LYS	E3443	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3879	E3819	LYS	E3566	LYS	E3444	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3880	E3819	LYS	E3567	LYS	E3445	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3881	E3819	LYS	E3568	LYS	E3446	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3882	E3819	LYS	E3569	LYS	E3447	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3883	E3819	LYS	E3570	LYS	E3448	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3884	E3819	LYS	E3571	LYS	E3449	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3885	E3819	LYS	E3572	LYS	E3450	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3886	E3819	LYS	E3573	LYS	E3451	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3887	E3819	LYS	E3574	LYS	E3452	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3888	E3819	LYS	E3575	LYS	E3453	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3889	E3819	LYS	E3576	LYS	E3454	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3890	E3819	LYS	E3577	LYS	E3455	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3891	E3819	LYS	E3578	LYS	E3456	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3892	E3819	LYS	E3579	LYS	E3457	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3893	E3819	LYS	E3580	LYS	E3458	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3894	E3819	LYS	E3581	LYS	E3459	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3895	E3819	LYS	E3582	LYS	E3460	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3896	E3819	LYS	E3583	LYS	E3461	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3897	E3819	LYS	E3584	LYS	E3462	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3898	E3819	LYS	E3585	LYS	E3463	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3899	E3819	LYS	E3586	LYS	E3464	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3900	E3819	LYS	E3587	LYS	E3465	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3901	E3819	LYS	E3588	LYS	E3466	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3902	E3819	LYS	E3589	LYS	E3467	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3903	E3819	LYS	E3590	LYS	E3468	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3904	E3819	LYS	E3591	LYS	E3469	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3905	E3819	LYS	E3592	LYS	E3470	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3906	E3819	LYS	E3593	LYS	E3471	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3907	E3819	LYS	E3594	LYS	E3472	E3377	R3189	R3189
LEU	GLY	LEU	GLY	LEU	THR	LEU	E4033	E3908	E3819	LYS	E3595	LYS				



• Molecule 3: Ryanodine receptor 2







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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, XAN, ATP, 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	E	0.16	0/834	0.46	2/1123 (0.2%)
1	F	0.16	0/834	0.46	2/1123 (0.2%)
1	G	0.16	0/834	0.46	2/1123 (0.2%)
1	H	0.16	0/834	0.46	2/1123 (0.2%)
2	I	0.31	0/1122	0.79	4/1504 (0.3%)
2	J	0.31	0/1122	0.79	4/1504 (0.3%)
2	K	0.31	0/1122	0.79	4/1504 (0.3%)
2	L	0.32	0/1122	0.79	4/1504 (0.3%)
3	A	0.16	0/35720	0.37	7/48254 (0.0%)
3	B	0.16	0/35720	0.37	5/48254 (0.0%)
3	C	0.16	0/35720	0.37	7/48254 (0.0%)
3	D	0.16	0/35720	0.37	5/48254 (0.0%)
All	All	0.17	0/150704	0.39	48/203524 (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

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	77	MET	CB-CG-SD	8.34	137.71	112.70
2	K	77	MET	CB-CG-SD	8.34	137.72	112.70
2	L	77	MET	CB-CG-SD	8.33	137.69	112.70
2	I	77	MET	CB-CG-SD	8.33	137.68	112.70
3	C	1729	MET	CB-CG-SD	-8.22	88.05	112.70

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

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	17	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	92	0
2	J	1112	0	1053	78	0
2	K	1112	0	1053	79	0
2	L	1112	0	1053	80	0
3	A	34959	0	34588	673	0
3	B	34959	0	34588	667	0
3	C	34959	0	34588	682	0
3	D	34959	0	34588	669	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	4	0
5	B	62	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3014	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 3014 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	71
3	B	4343/4967 (87%)	4191 (96%)	148 (3%)	4 (0%)	48	71
3	C	4343/4967 (87%)	4192 (96%)	147 (3%)	4 (0%)	48	71
3	D	4343/4967 (87%)	4191 (96%)	148 (3%)	4 (0%)	48	71
All	All	18336/20896 (88%)	17666 (96%)	654 (4%)	16 (0%)	49	71

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	58
1	F	88/89 (99%)	85 (97%)	3 (3%)	32	58
1	G	88/89 (99%)	85 (97%)	3 (3%)	32	58
1	H	88/89 (99%)	85 (97%)	3 (3%)	32	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	119/127 (94%)	105 (88%)	14 (12%)	5	14
2	J	119/127 (94%)	105 (88%)	14 (12%)	5	14
2	K	119/127 (94%)	105 (88%)	14 (12%)	5	14
2	L	119/127 (94%)	105 (88%)	14 (12%)	5	14
3	A	3836/4358 (88%)	3799 (99%)	37 (1%)	68	81
3	B	3836/4358 (88%)	3799 (99%)	37 (1%)	68	81
3	C	3836/4358 (88%)	3799 (99%)	37 (1%)	68	81
3	D	3836/4358 (88%)	3799 (99%)	37 (1%)	68	81
All	All	16172/18296 (88%)	15956 (99%)	216 (1%)	59	77

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	2737	LEU
3	C	309	MET
3	D	3231	MET
3	B	2838[A]	HIS
3	B	3398	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1805	HIS
3	D	2998	ASN
3	D	3775	GLN
3	B	2754	GLN
3	B	2550	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
7	XAN	A	5004	-	12,12,12	0.92	1 (8%)	14,17,17	0.93	0
5	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	C	5005	-	32,33,33	0.54	0	48,52,52	0.57	0
7	XAN	D	5004	-	12,12,12	0.91	1 (8%)	14,17,17	0.92	0
7	XAN	C	5004	-	12,12,12	0.92	1 (8%)	14,17,17	0.92	0
5	ATP	D	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	D	5005	-	32,33,33	0.53	0	48,52,52	0.57	0
5	ATP	A	5005	-	32,33,33	0.53	0	48,52,52	0.57	0
5	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	B	5005	-	32,33,33	0.54	0	48,52,52	0.57	0
7	XAN	B	5004	-	12,12,12	0.92	1 (8%)	14,17,17	0.92	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
7	XAN	A	5004	-	-	-	0/2/2/2
5	ATP	B	5002	-	-	4/22/38/38	0/3/3/3
5	ATP	C	5005	-	-	4/22/38/38	0/3/3/3
7	XAN	D	5004	-	-	-	0/2/2/2
7	XAN	C	5004	-	-	-	0/2/2/2
5	ATP	D	5002	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	A	5002	-	-	4/22/38/38	0/3/3/3
5	ATP	D	5005	-	-	4/22/38/38	0/3/3/3
5	ATP	A	5005	-	-	4/22/38/38	0/3/3/3
5	ATP	C	5002	-	-	4/22/38/38	0/3/3/3
5	ATP	B	5005	-	-	4/22/38/38	0/3/3/3
7	XAN	B	5004	-	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5004	XAN	C4-N3	-2.59	1.33	1.37
7	B	5004	XAN	C4-N3	-2.58	1.33	1.37
7	C	5004	XAN	C4-N3	-2.56	1.33	1.37
7	D	5004	XAN	C4-N3	-2.55	1.33	1.37

There are no bond angle outliers.

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

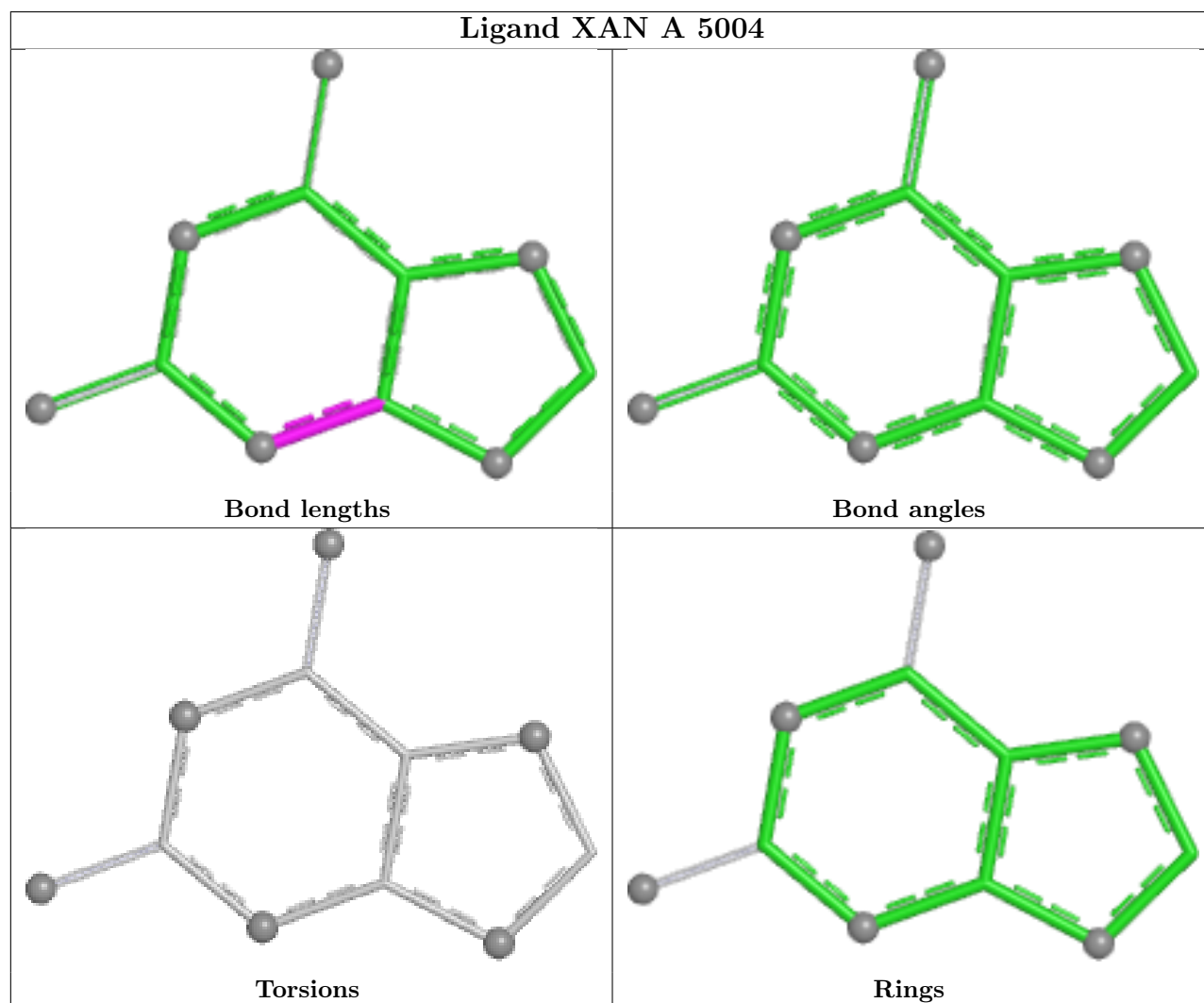
There are no ring outliers.

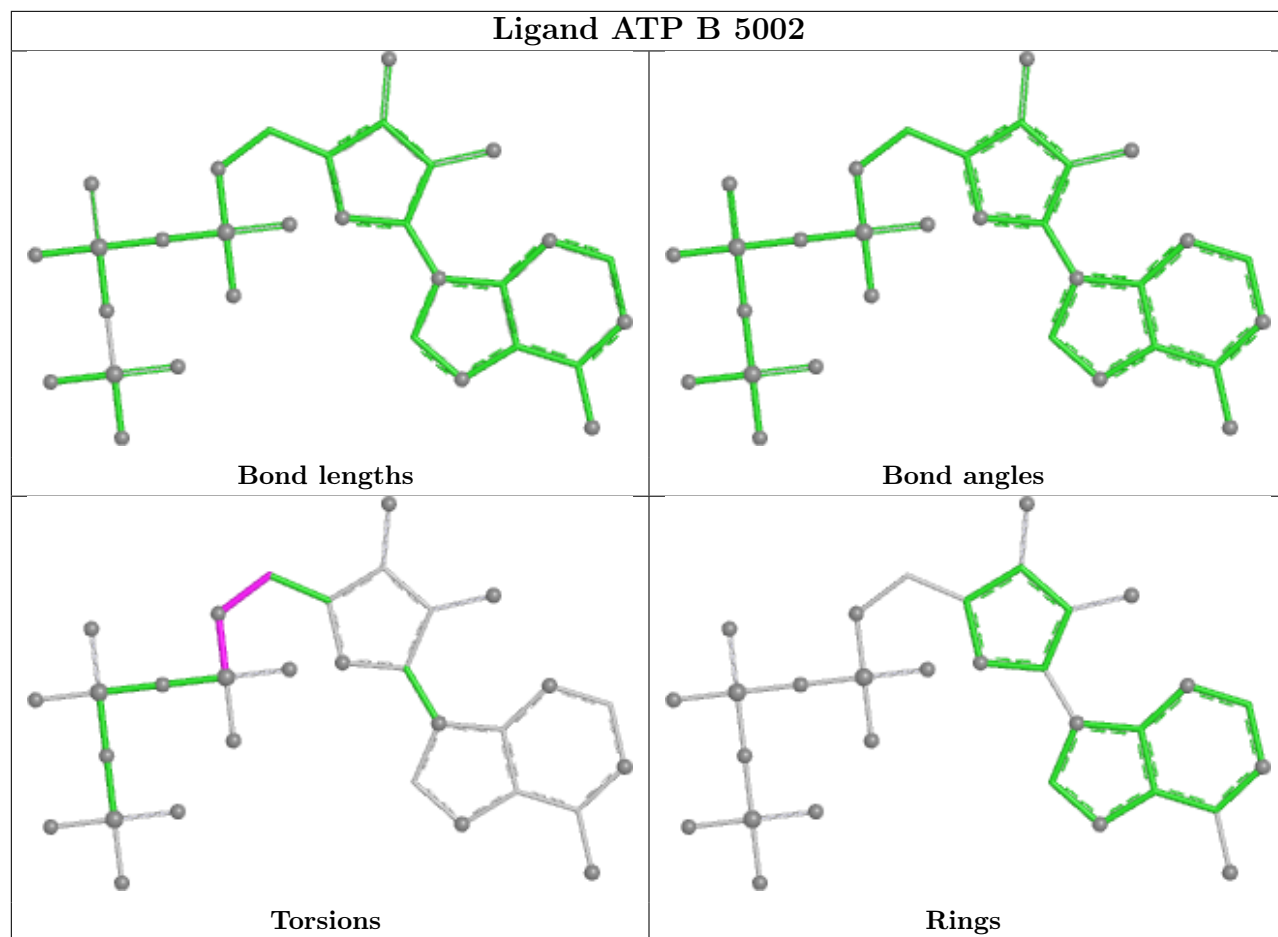
8 monomers are involved in 16 short contacts:

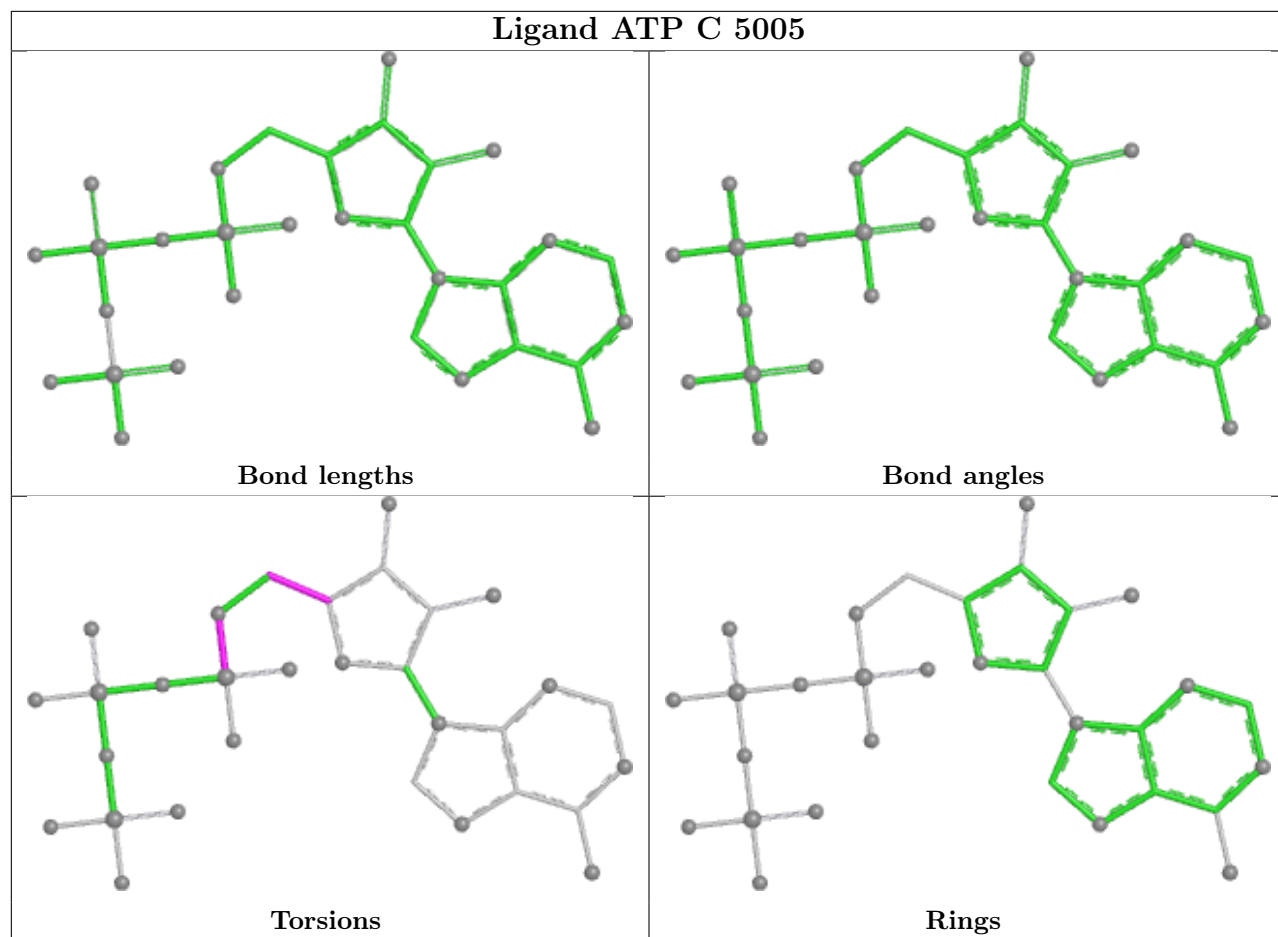
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5002	ATP	3	0
5	C	5005	ATP	1	0
5	D	5002	ATP	3	0
5	A	5002	ATP	3	0
5	D	5005	ATP	1	0
5	A	5005	ATP	1	0
5	C	5002	ATP	3	0
5	B	5005	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

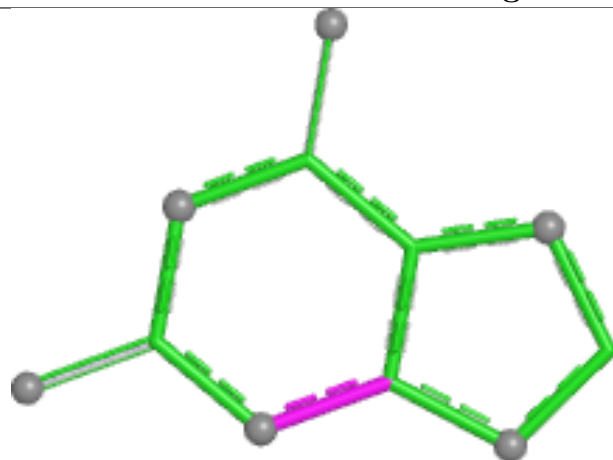
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



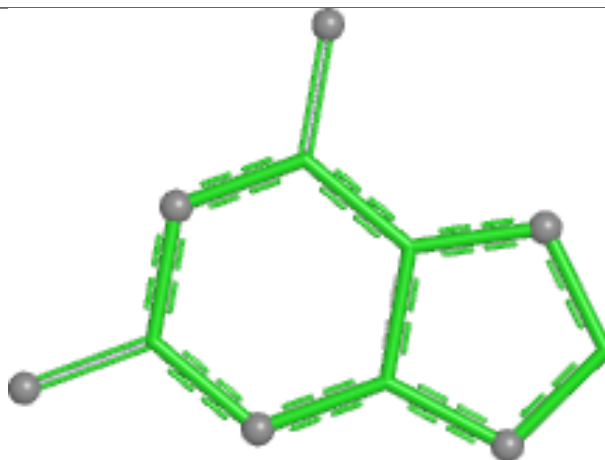




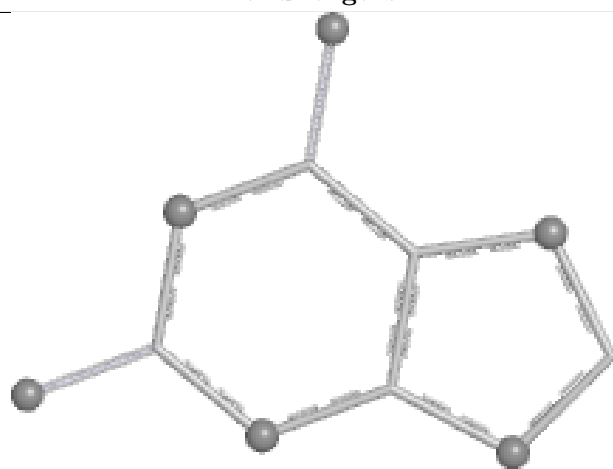
Ligand XAN D 5004



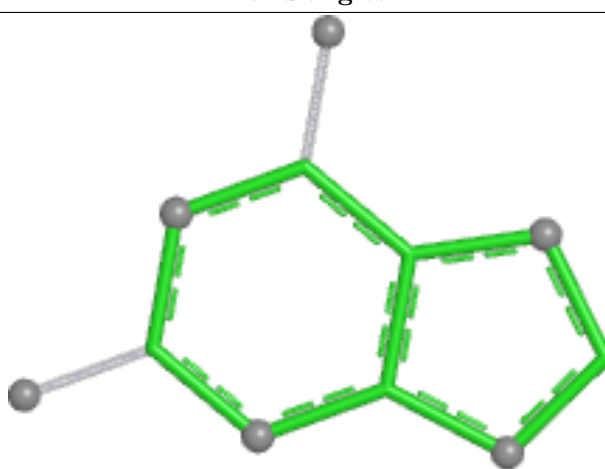
Bond lengths



Bond angles

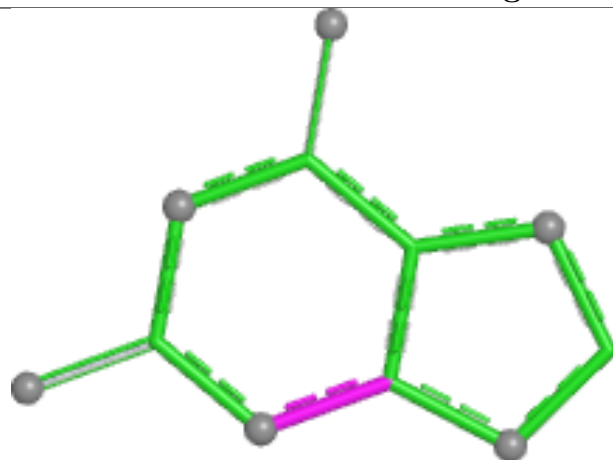


Torsions

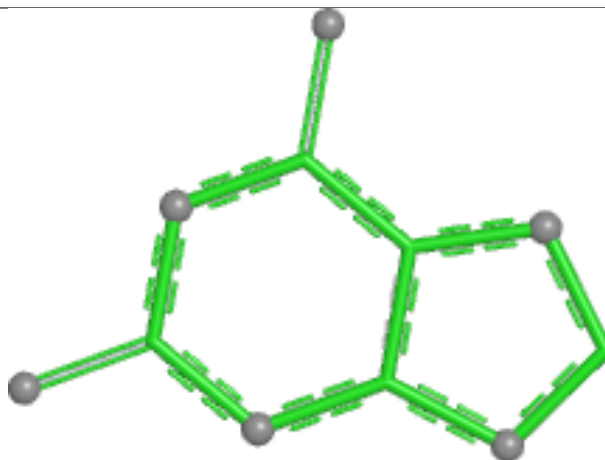


Rings

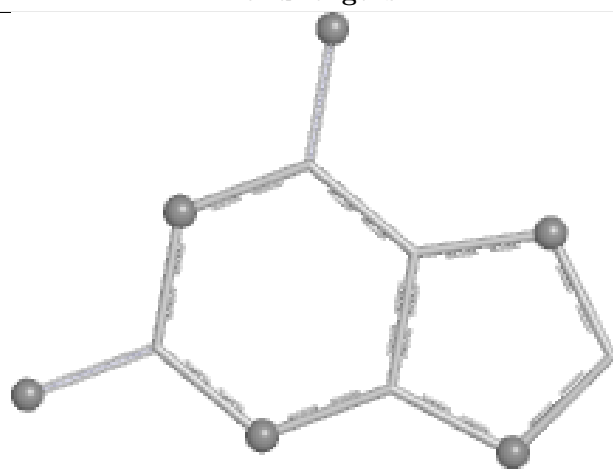
Ligand XAN C 5004



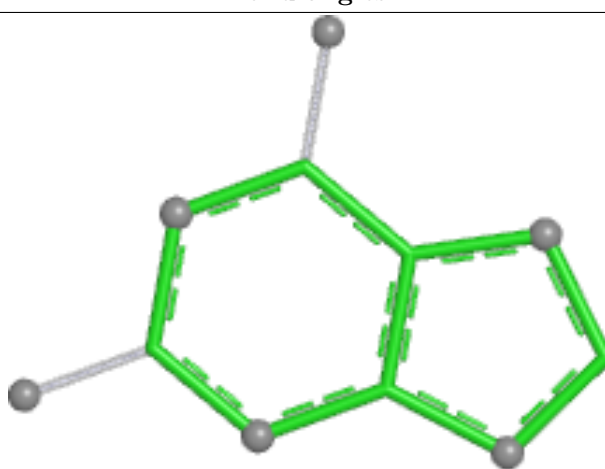
Bond lengths



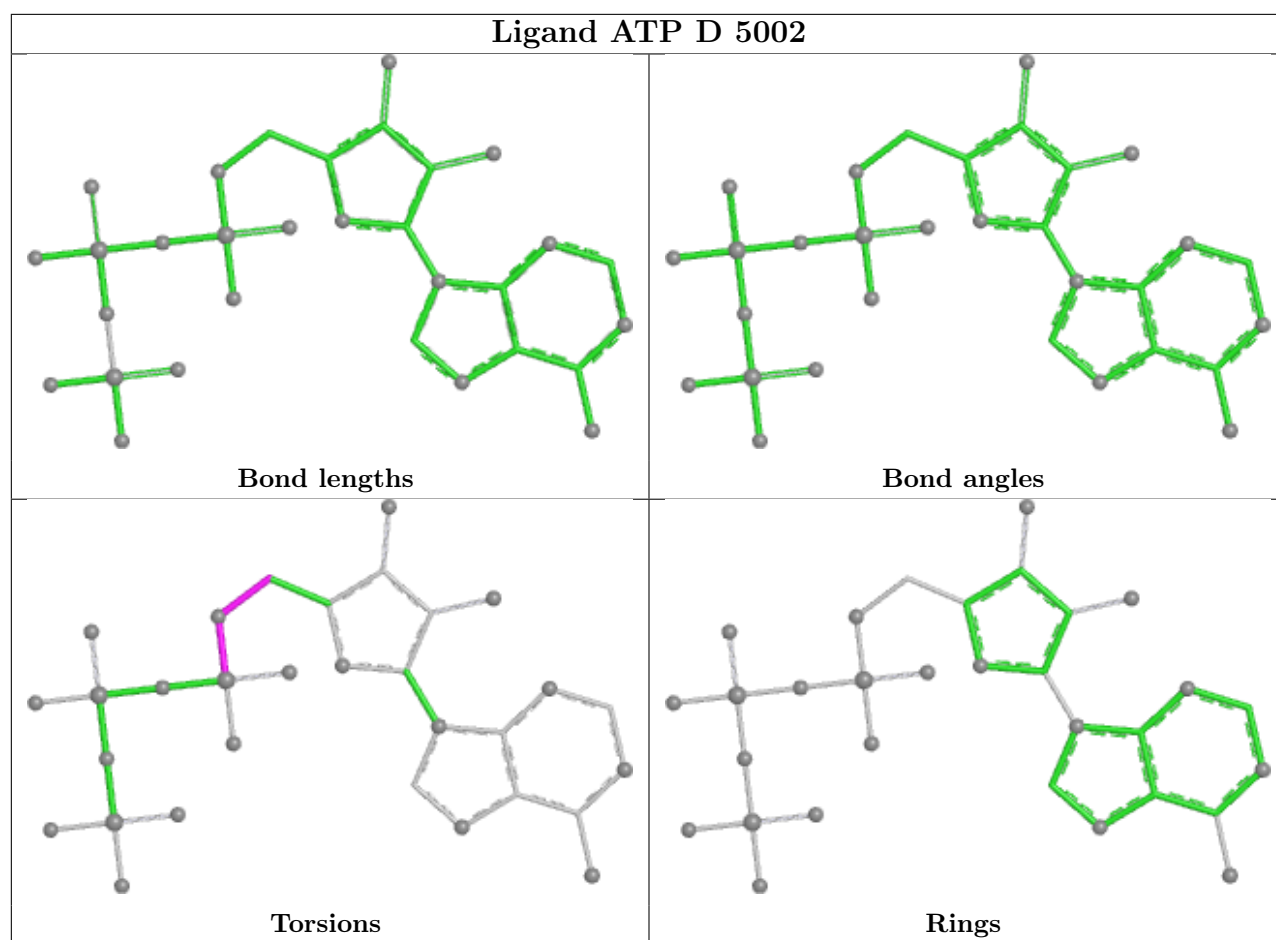
Bond angles

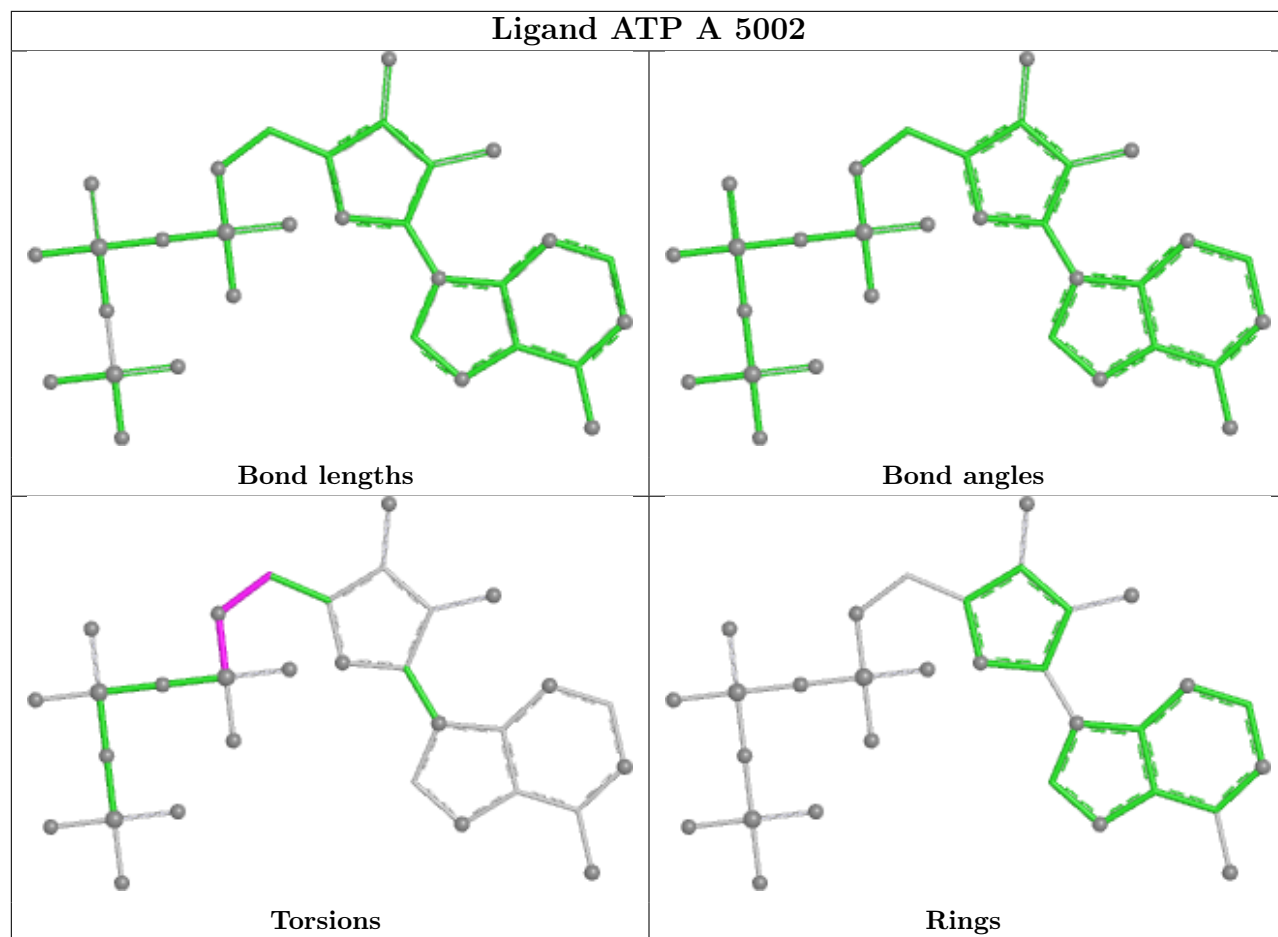


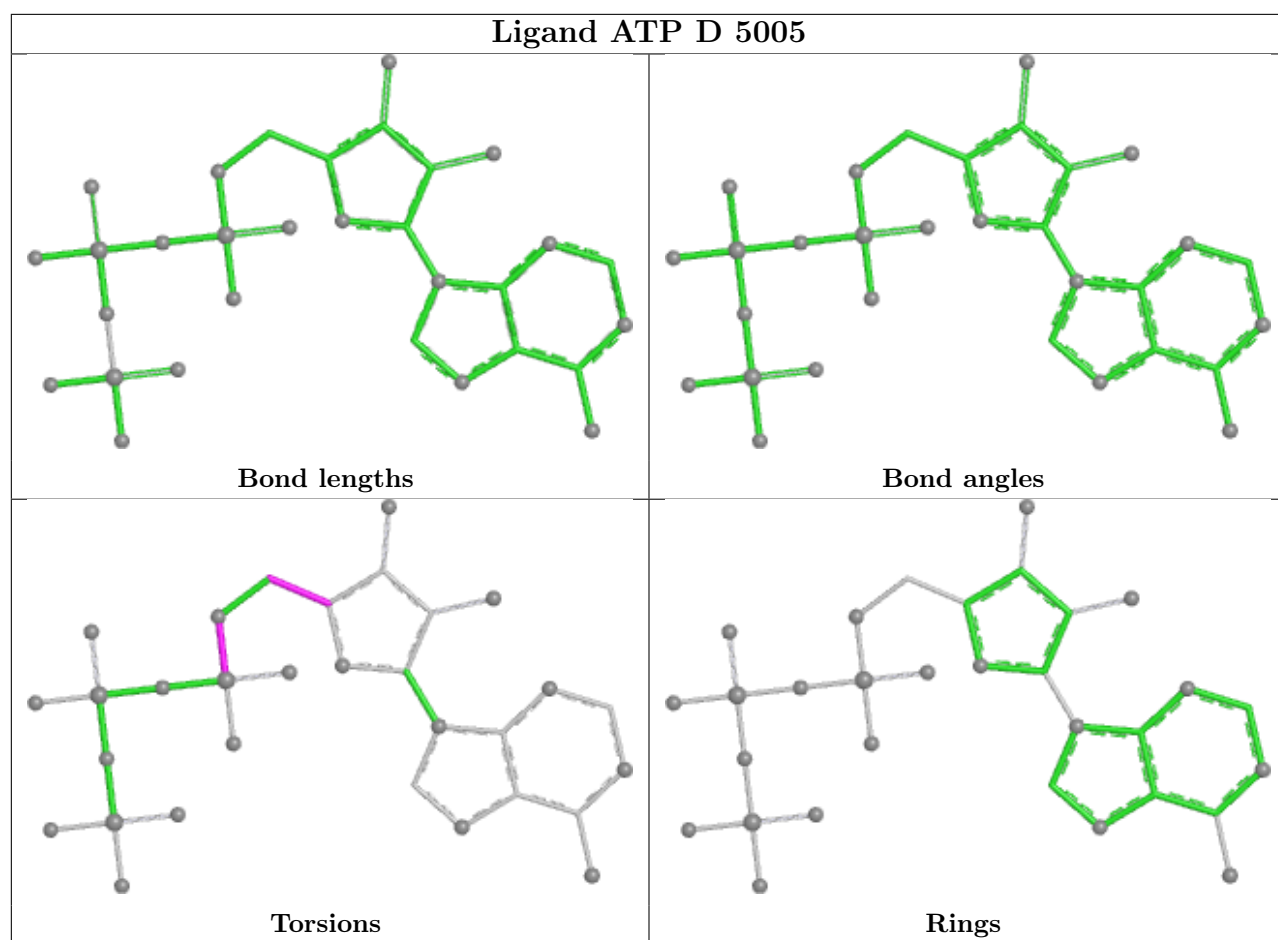
Torsions

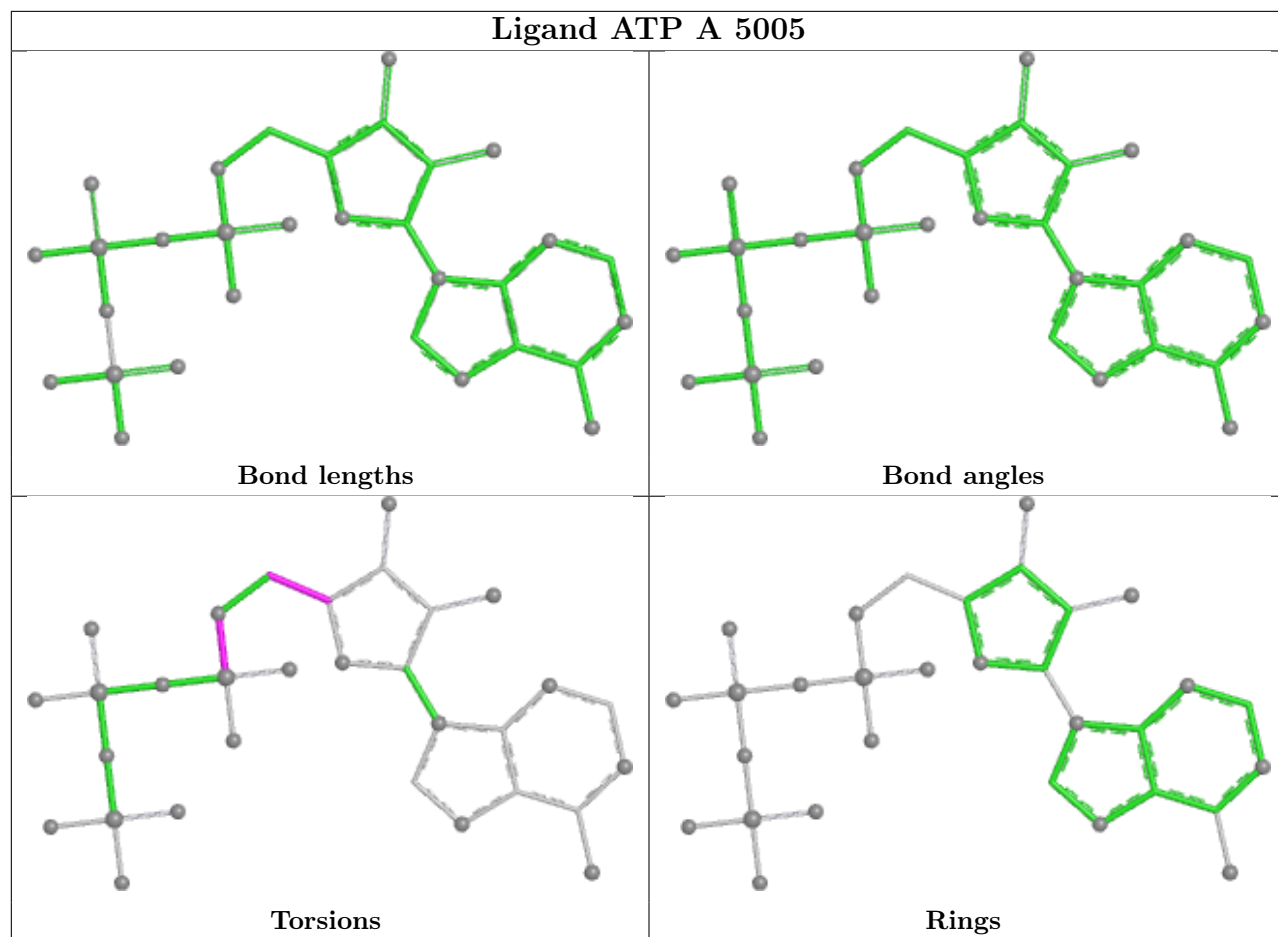


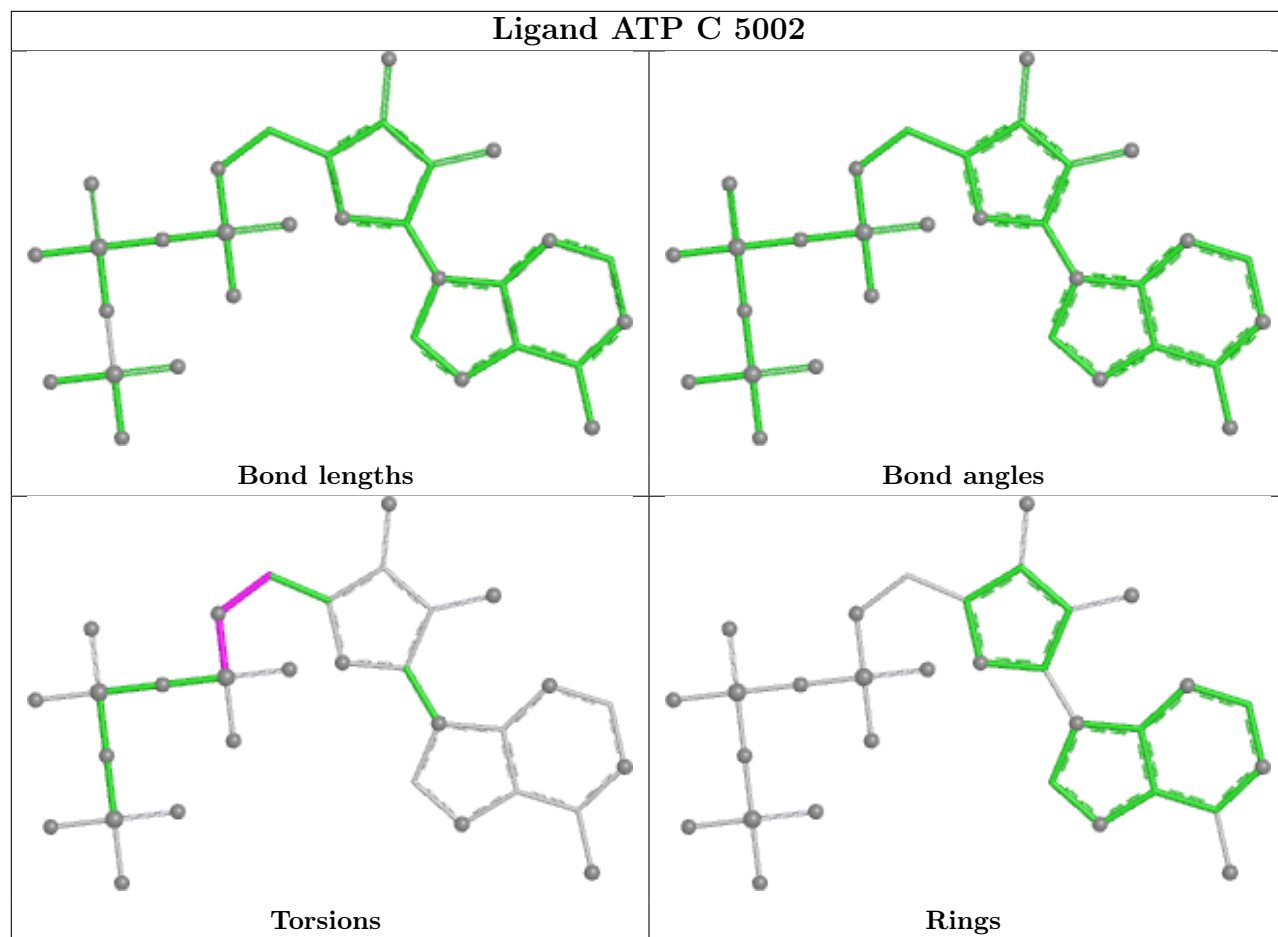
Rings

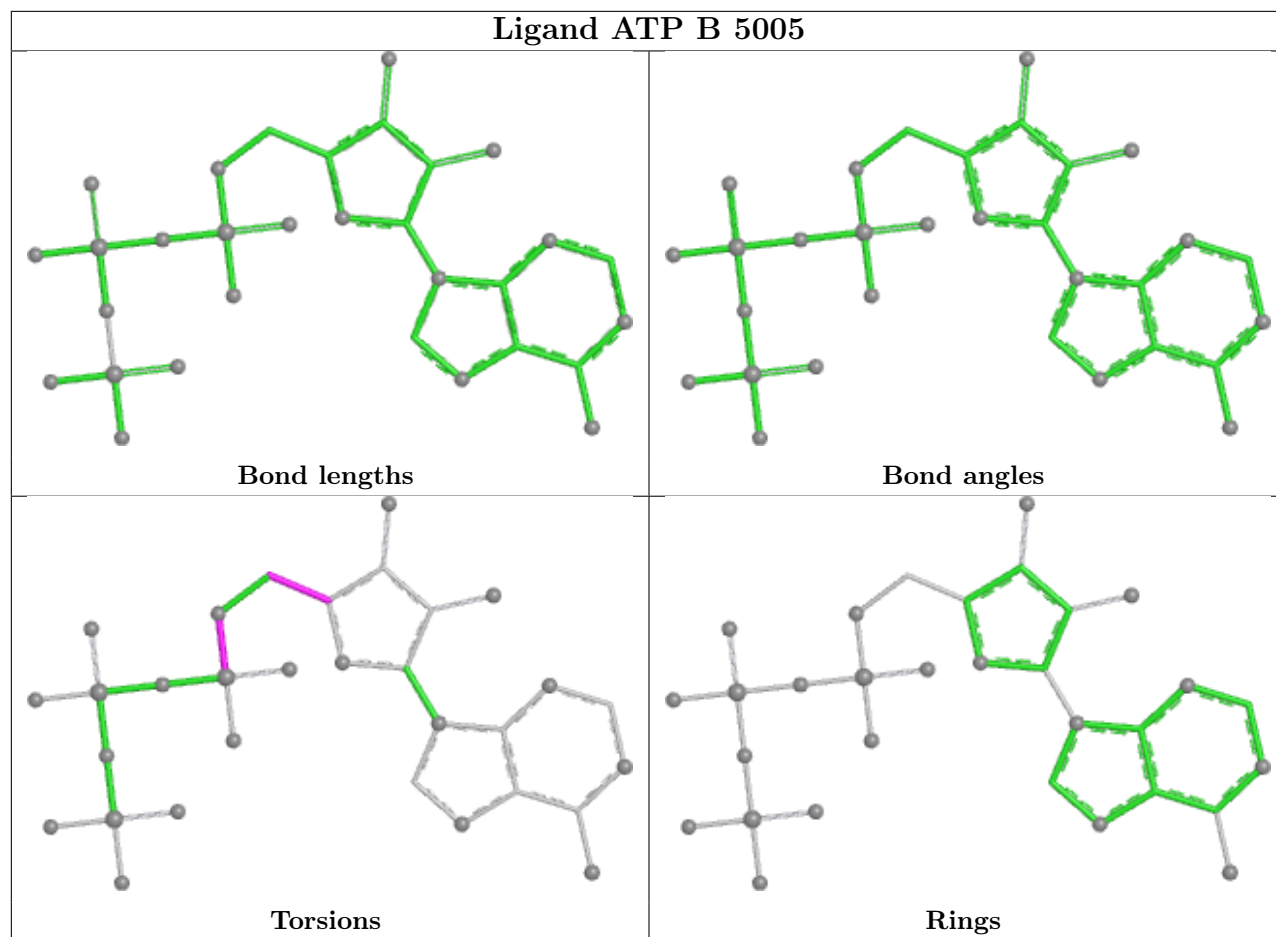


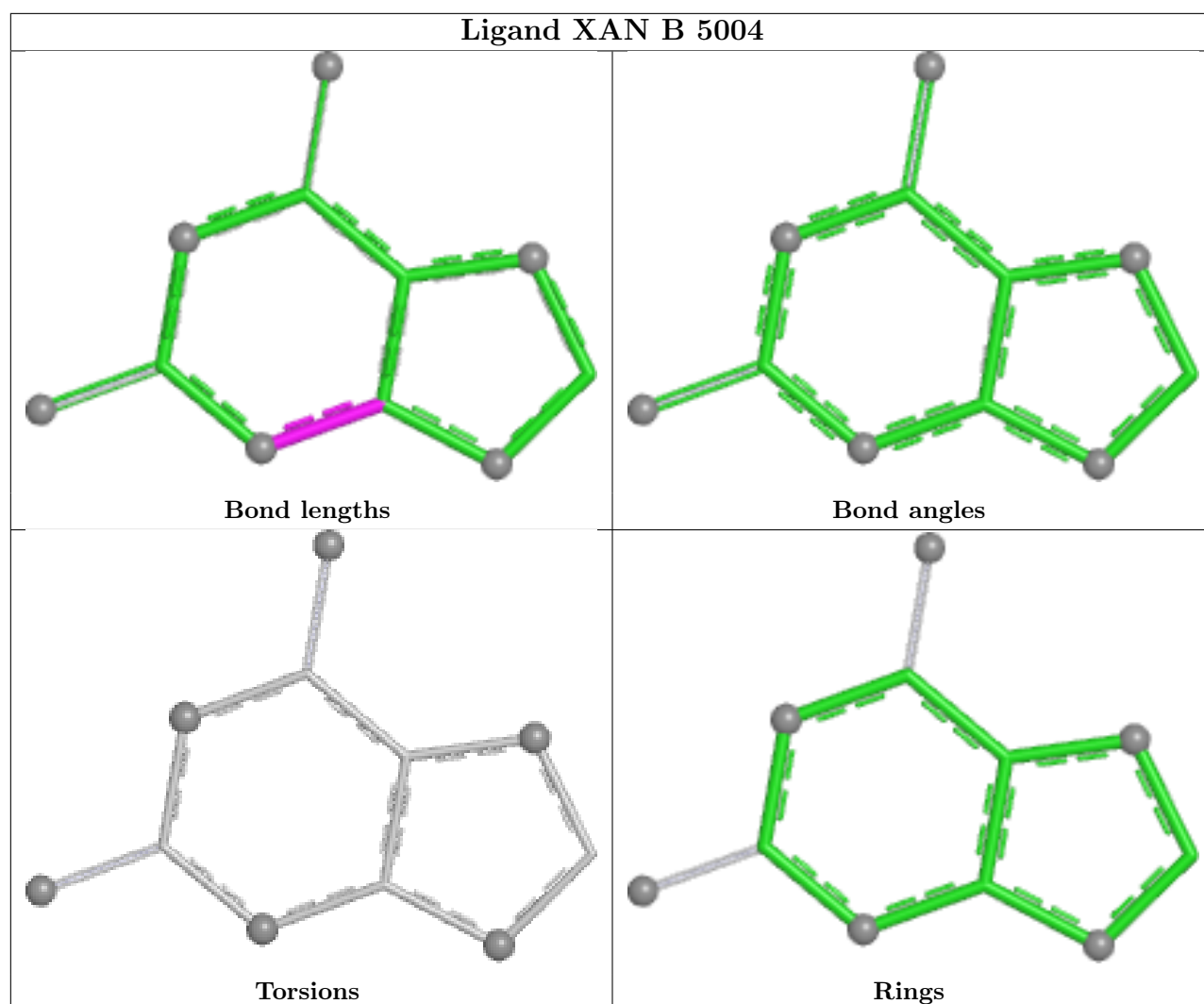












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

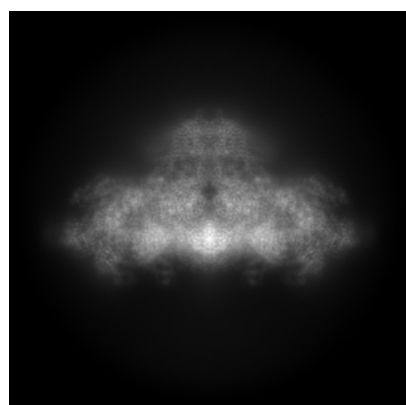
6 Map visualisation [i](#)

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.

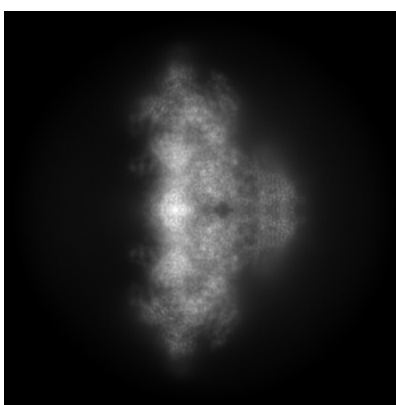
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

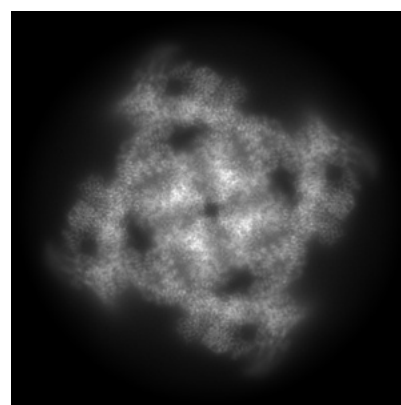
6.1.1 Primary map



X



Y

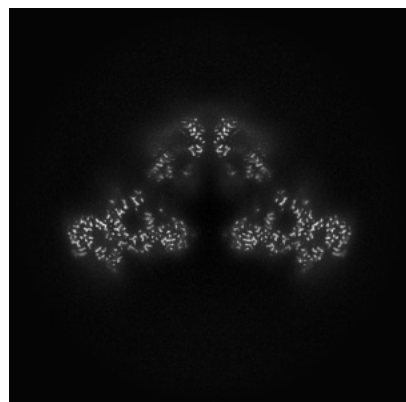


Z

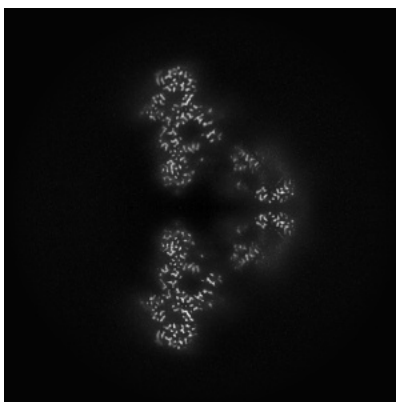
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

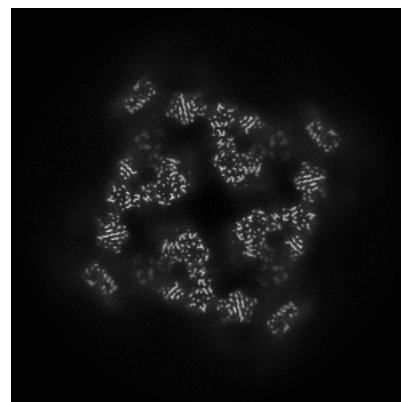
6.2.1 Primary map



X Index: 256



Y Index: 256

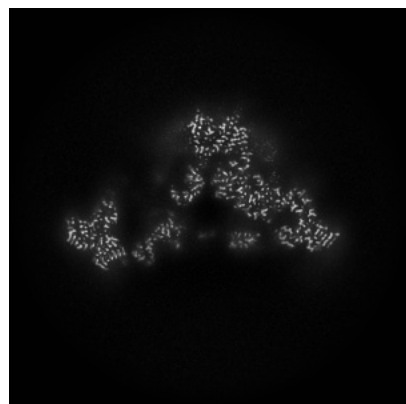


Z Index: 256

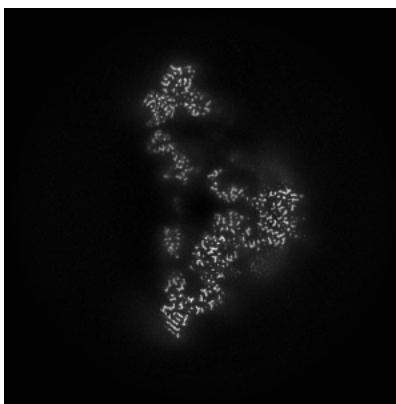
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

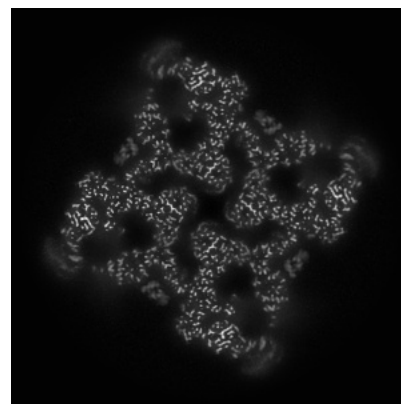
6.3.1 Primary map



X Index: 275



Y Index: 274

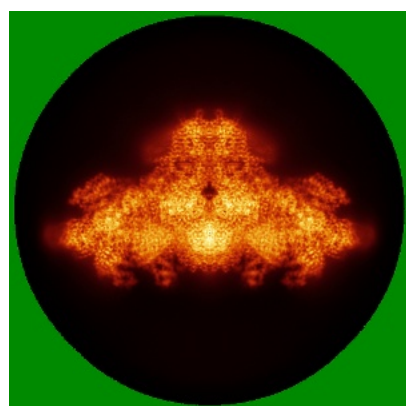


Z Index: 220

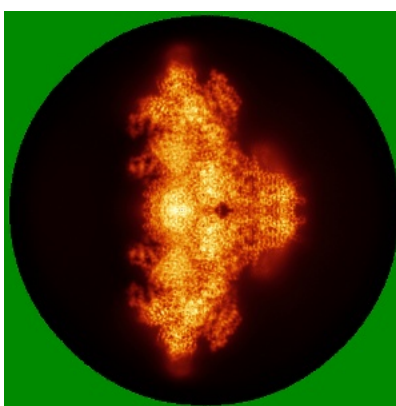
The images above show the largest variance slices of the map in three orthogonal directions.

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

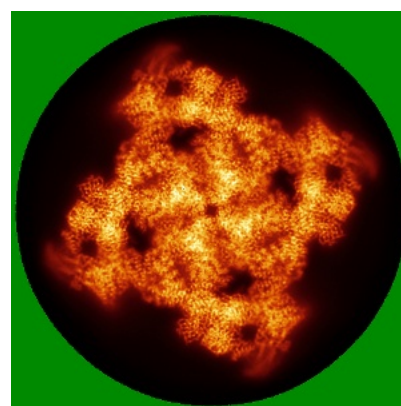
6.4.1 Primary map



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.

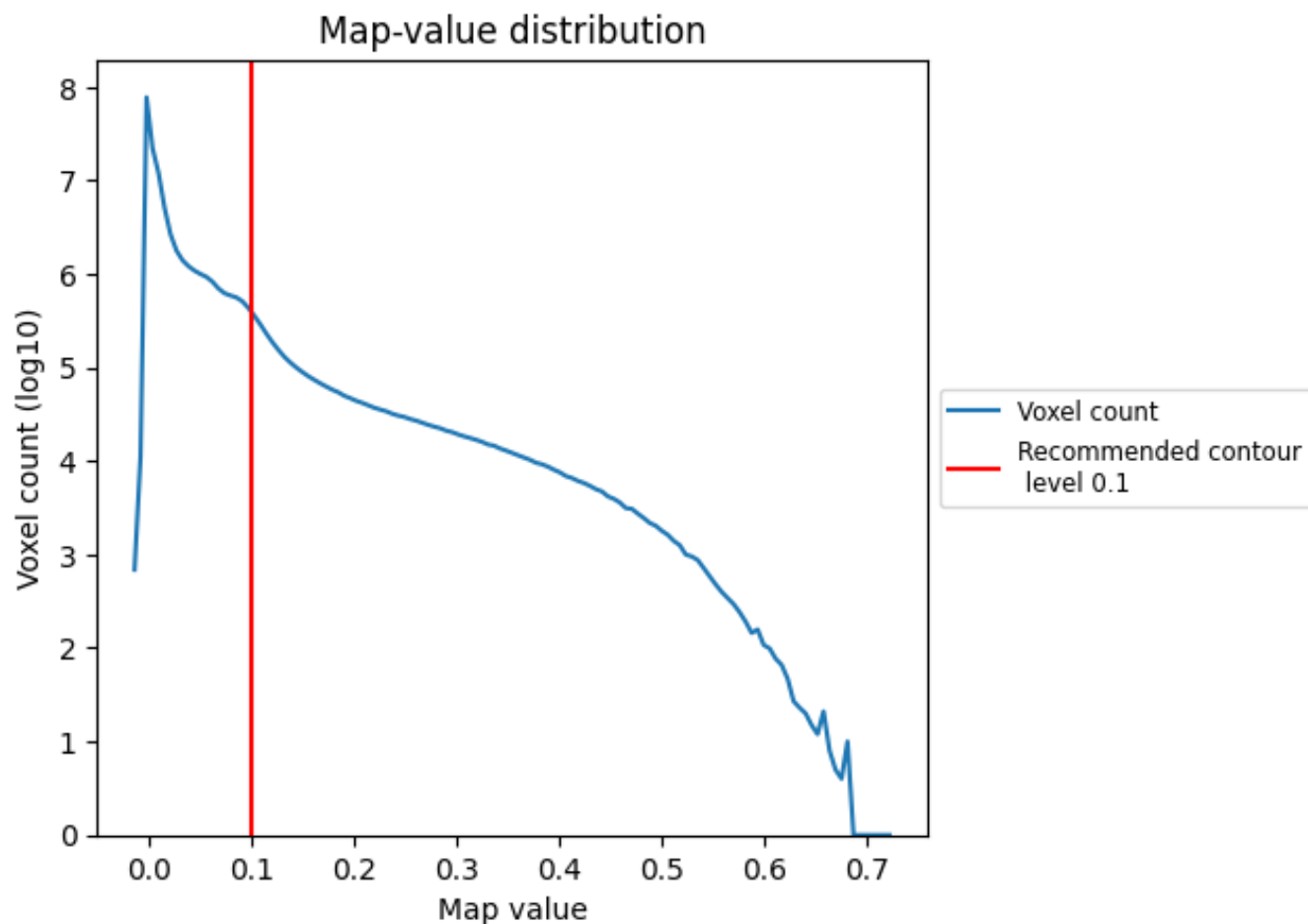
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

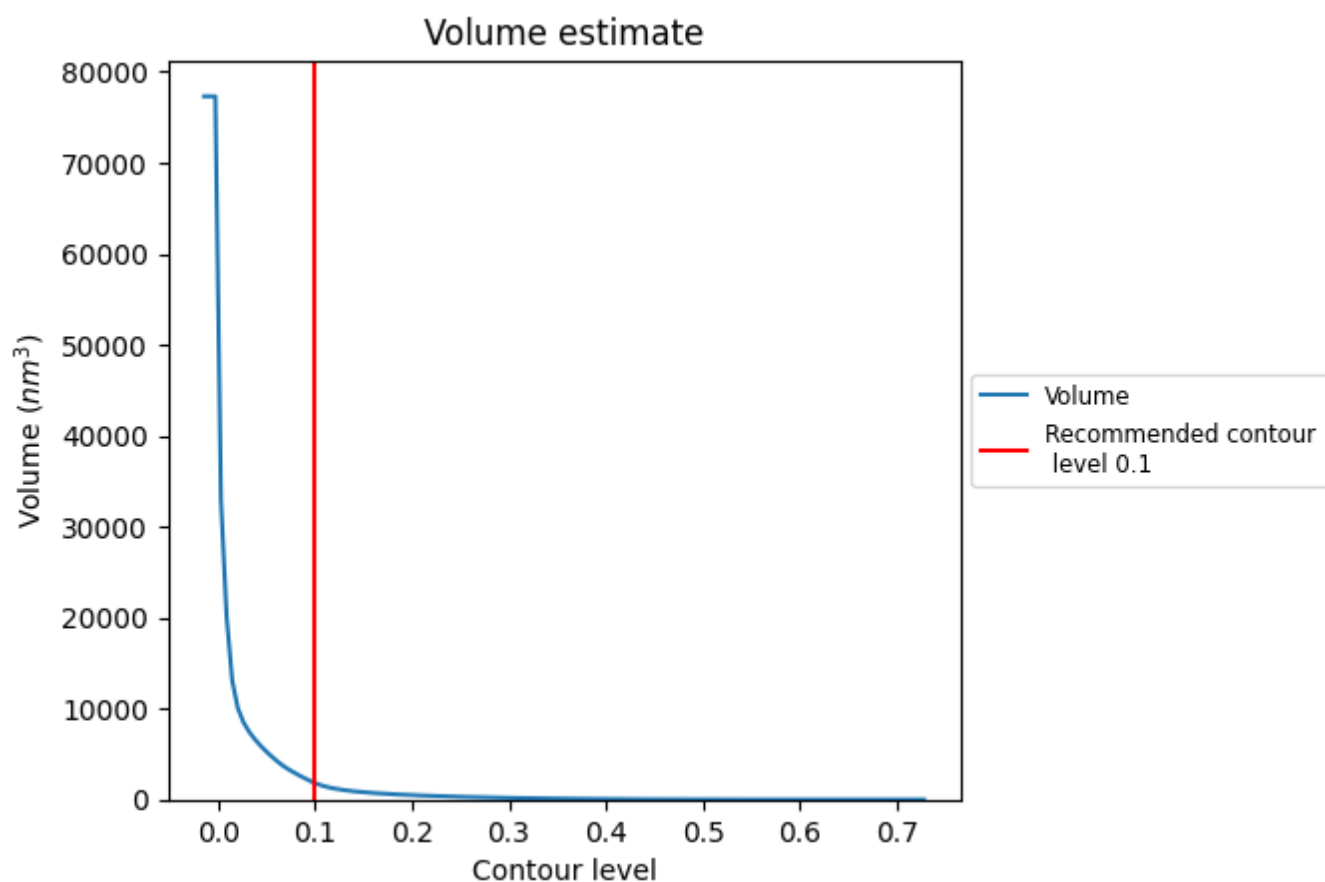
This section contains the results of statistical analysis of the map.

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.

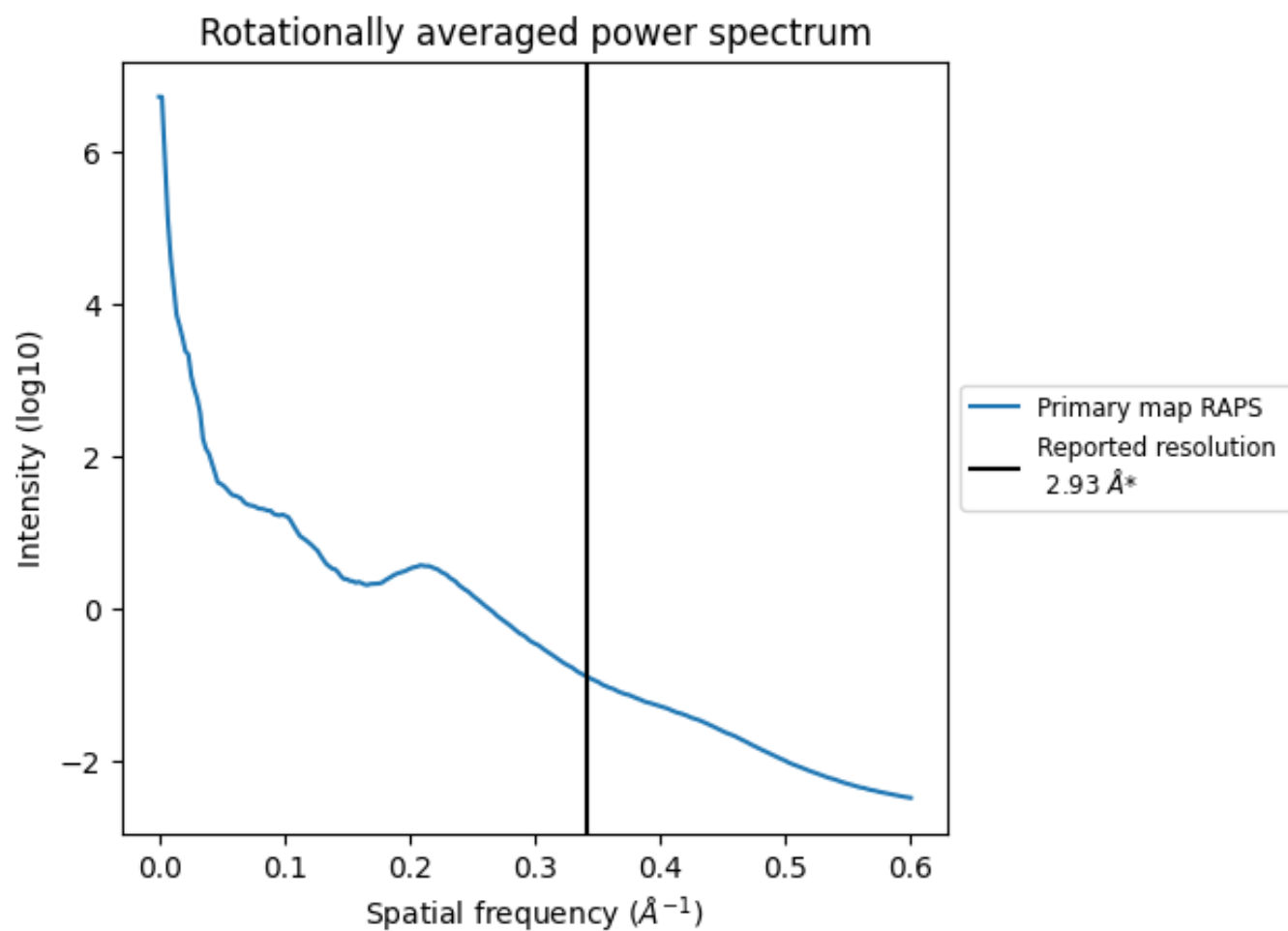
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1824 nm³; 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⁻¹

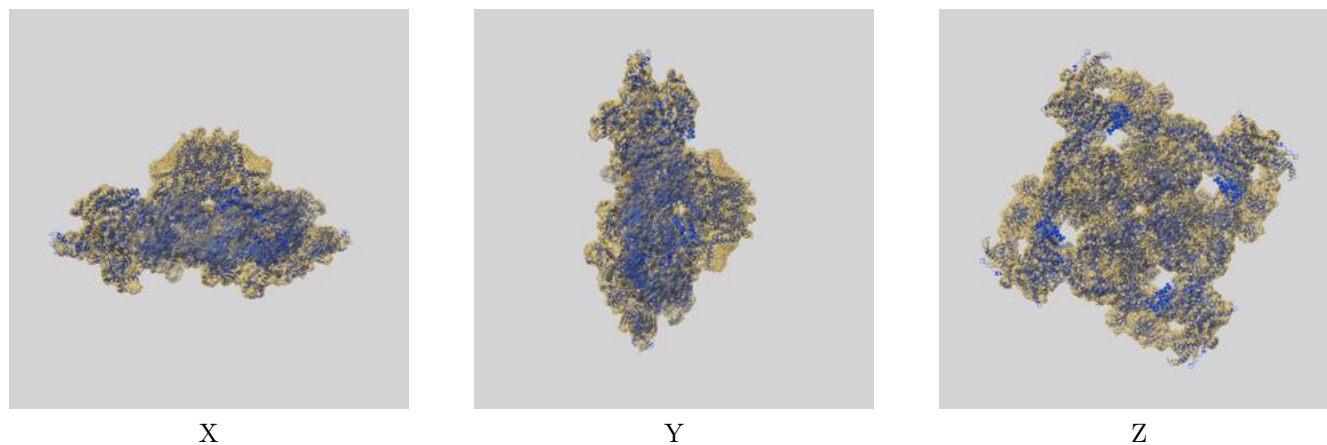
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

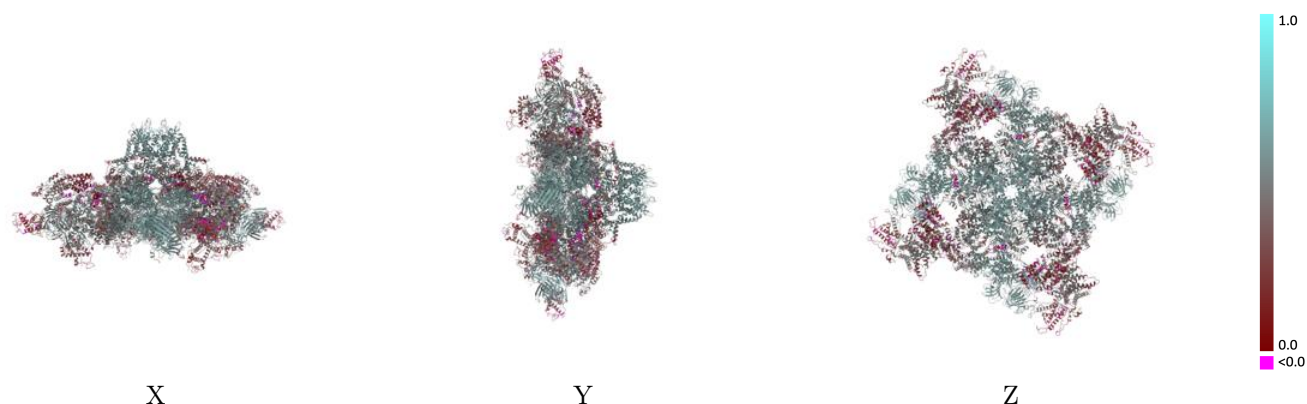
This section contains information regarding the fit between EMDB map EMD-26414 and PDB model 7UA4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



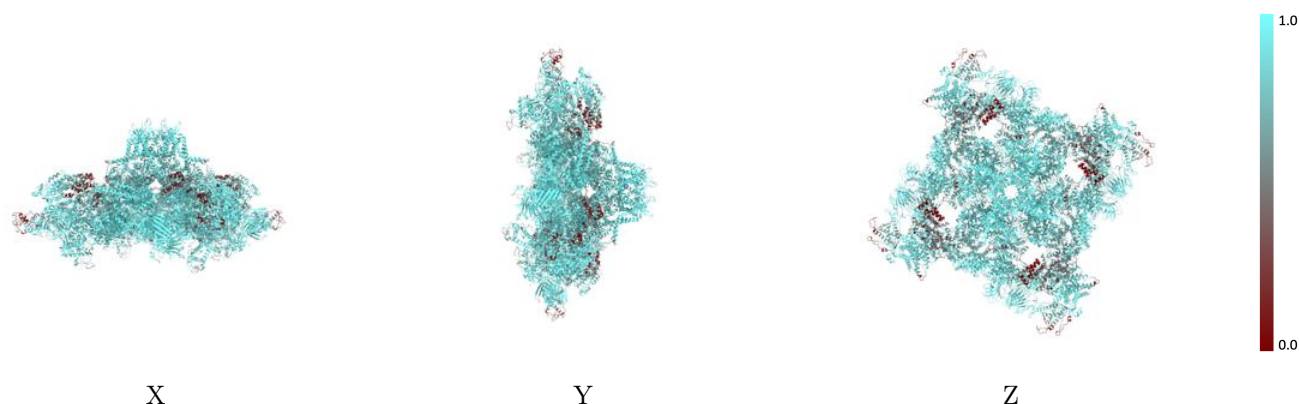
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



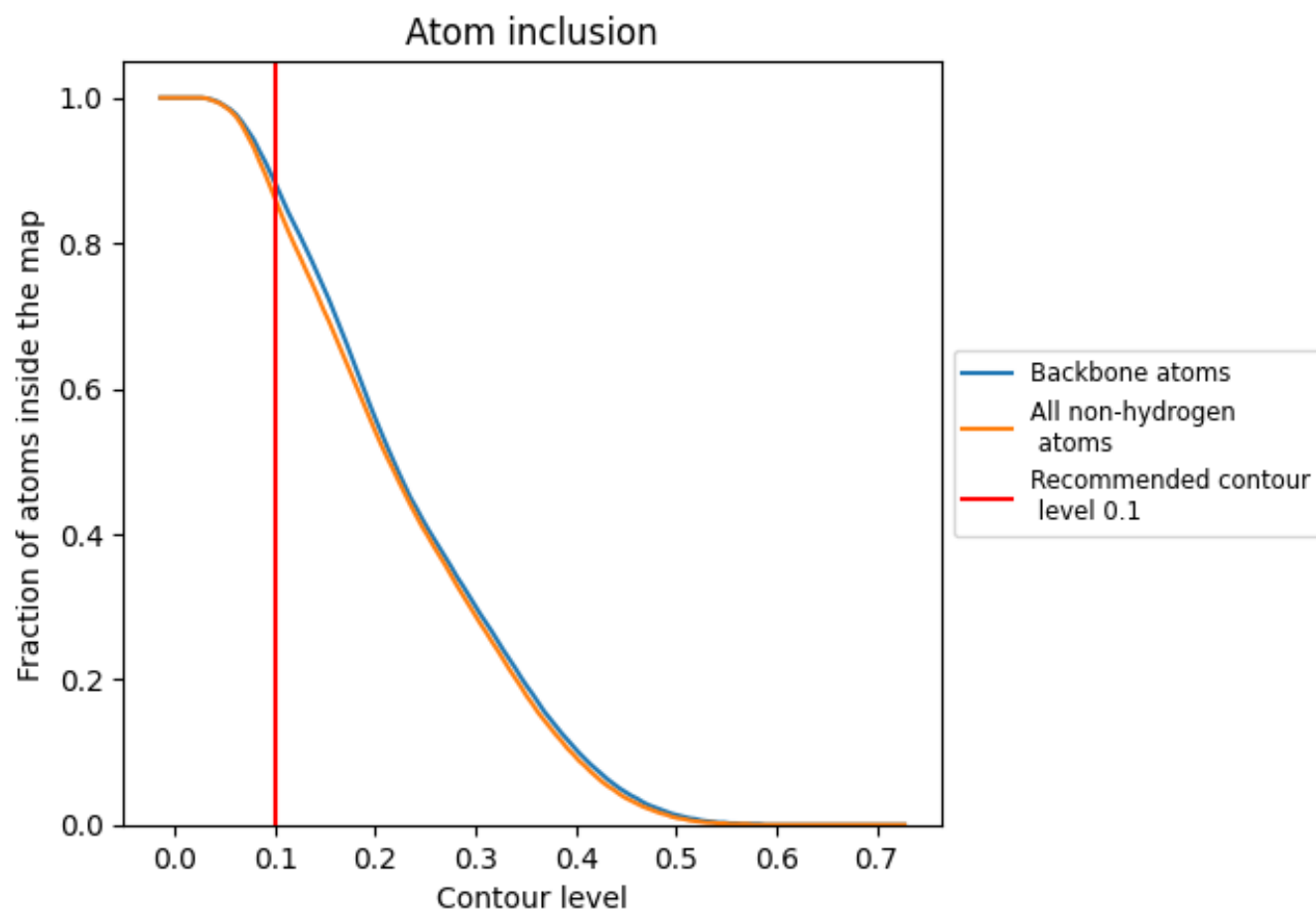
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.8610	0.4560
A	0.8680	0.4670
B	0.8670	0.4580
C	0.8660	0.4570
D	0.8660	0.4610
E	0.9670	0.5880
F	0.9720	0.5700
G	0.9720	0.5710
H	0.9690	0.5730
I	0.6900	0.2200
J	0.6640	0.2040
K	0.6880	0.2240
L	0.6650	0.2110

1.0

0.0

<0.0