



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:06 PM UTC

PDB ID : 7UA3 / pdb_00007ua3
EMDB ID : EMD-26413
Title : Structure of PKA phosphorylated human RyR2-R2474S in the closed state in the presence of Calmodulin
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 2.97 Å(reported)
Based on initial model : 7U9X

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

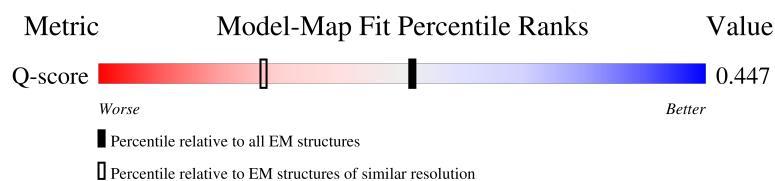
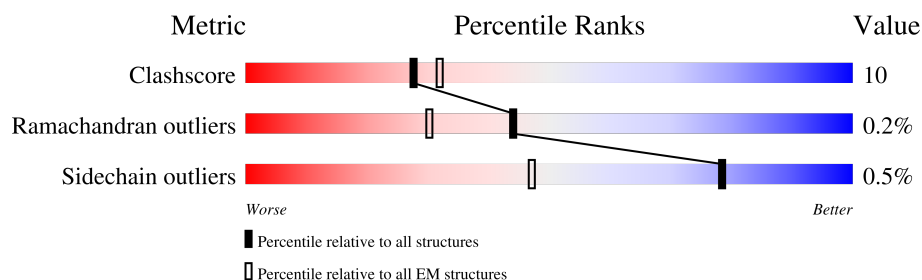
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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	 11% 70% 20% 11%
1	B	4967	 11% 69% 20% 11%
1	C	4967	 11% 69% 20% 11%
1	D	4967	 11% 69% 20% 11%

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Mol	Chain	Length	Quality of chain
2	E	108	 73% 24% ...
2	F	108	 70% 27% ...
2	G	108	 73% 24% ...
2	H	108	 73% 24% ...
3	I	149	 64% 57% 33% 5% • 5%
3	J	149	 64% 56% 33% 5% • 5%
3	K	149	 63% 57% 32% 6% 5%
3	L	149	 66% 58% 32% 5% • 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 150252 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	4443	Total	C	N	O	S	2	0
			35570	22656	6059	6618	237		
1	B	4443	Total	C	N	O	S	2	0
			35570	22656	6059	6618	237		
1	C	4443	Total	C	N	O	S	2	0
			35570	22656	6059	6618	237		
1	D	4443	Total	C	N	O	S	2	0
			35570	22656	6059	6618	237		

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

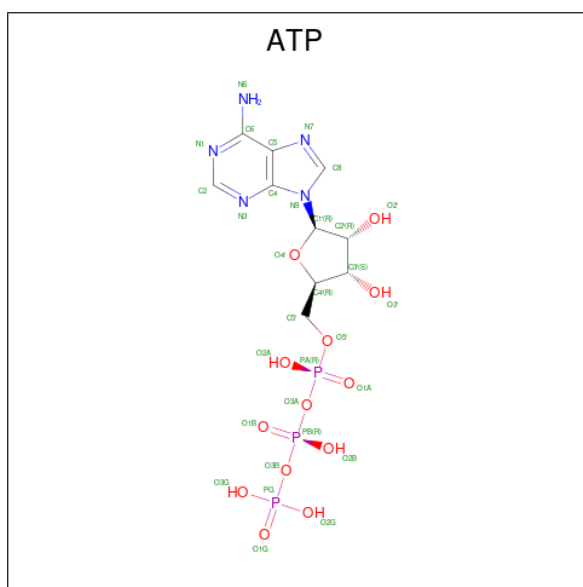
- Molecule 3 is a protein called Calmodulin-1.

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

- 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	

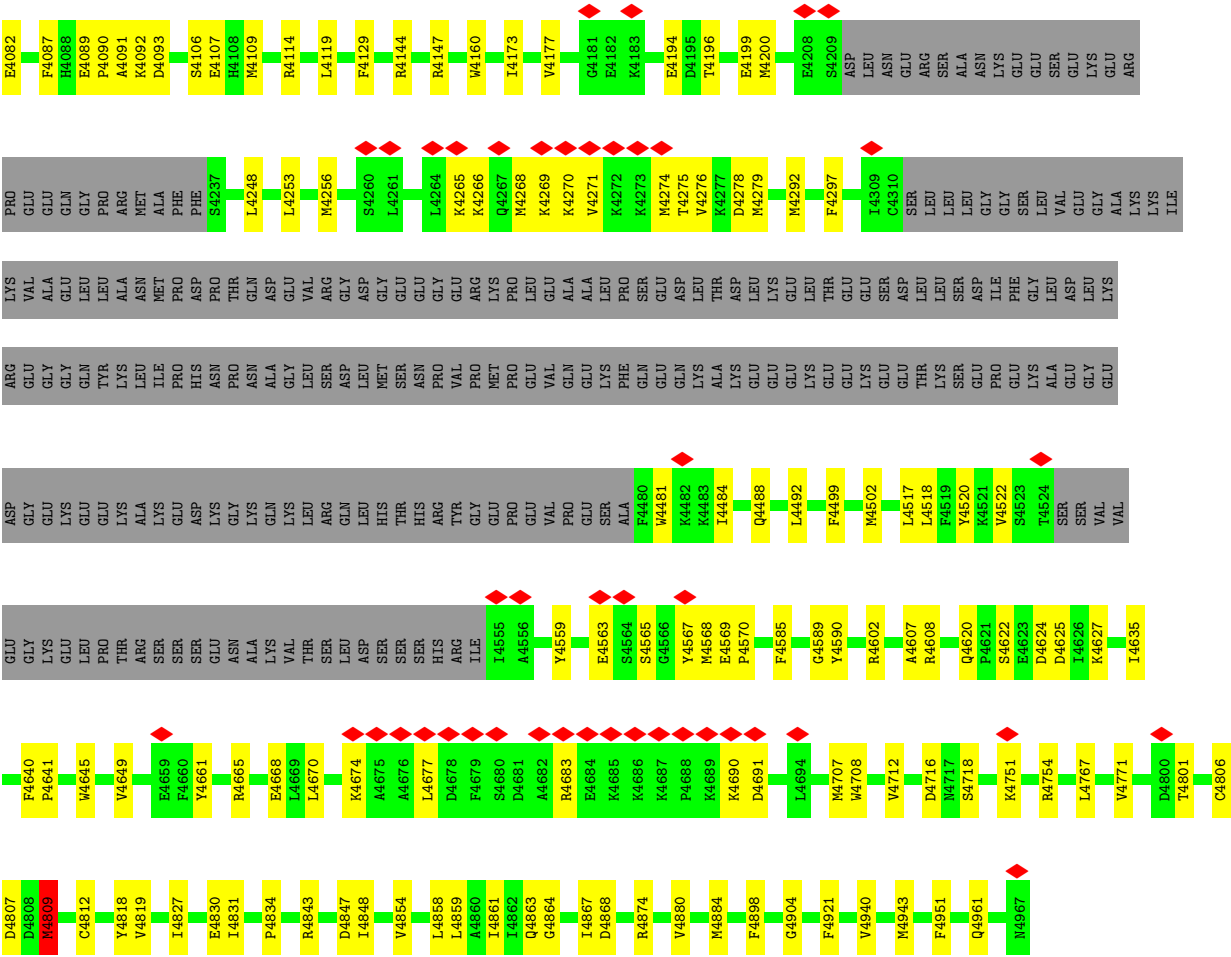
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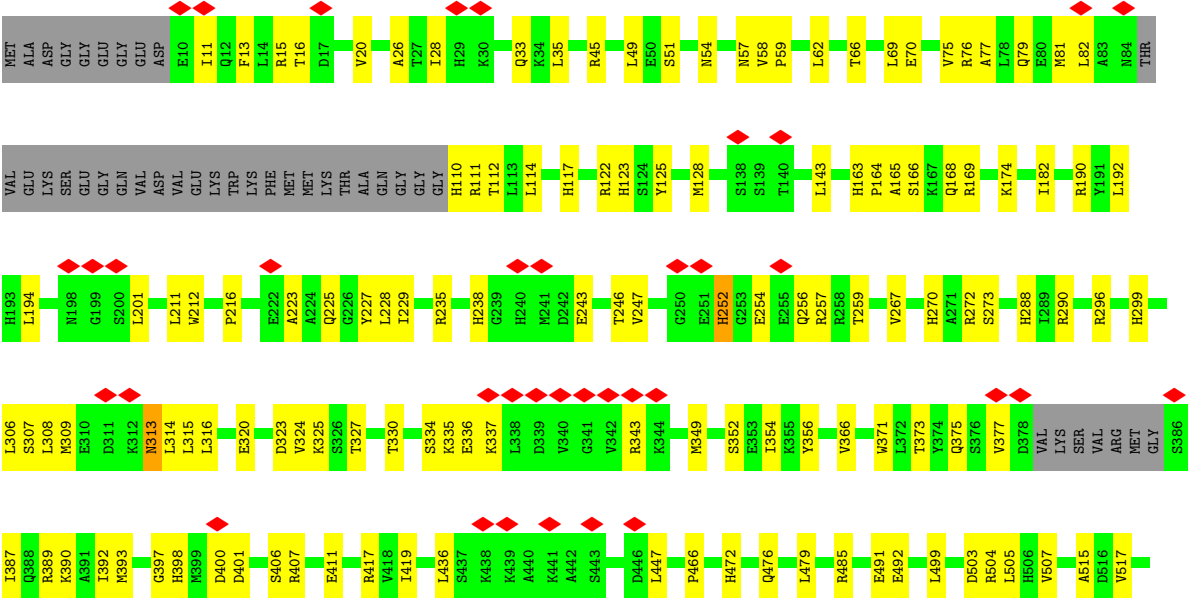
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10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

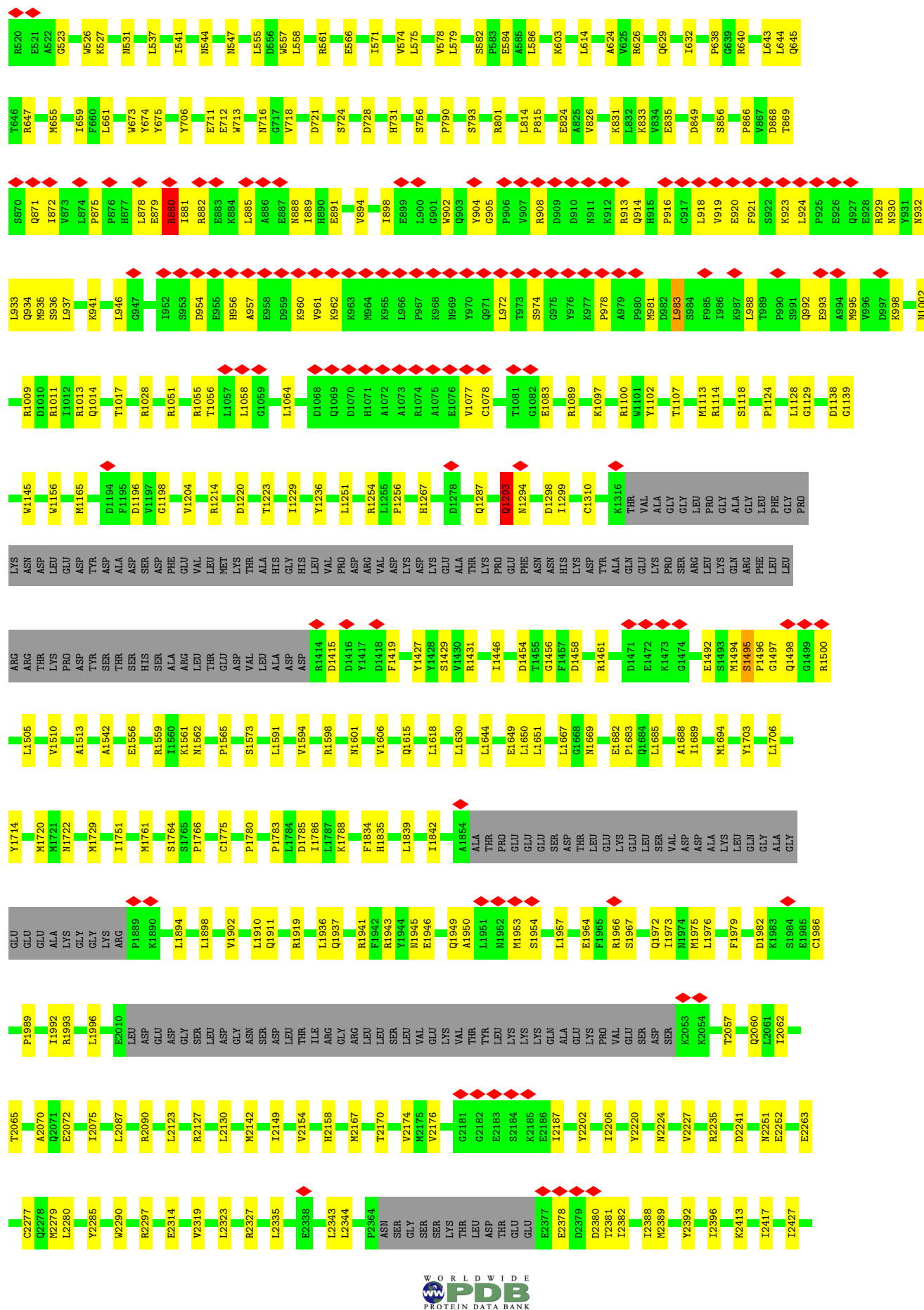
L2742	L2609	E2453	L2280	E2072	P1989	ALA	M1721	A1513	SER	ASP	G1198	R1051
Y2743	L2610	F2460	Y2285	L2087	I1992	LYS	N1722	A1542	HIS	SER	V1204	R1055
E2745	C2617	H2464	W2290	R2087	R1993	GLY	M1729	E1556	ALA	ASP	R1214	T1056
L2746	K2465	K2465	R2297	R2090	L1996	LYS	I1751	R1559	LEU	GLU	D1220	L1057
Y2747	F2630	W2468	E2314	L2123	E2010	ARG	M1761	T1560	THR	LEU	L1058	L1059
S2748	L2640	Y2476	E2314	I2126	L1894	P1989	S1764	K1561	GLU	MET	T1223	L1064
D2749	L2644	G2477	L2324	R2127	L1898	L1894	P1766	N1562	VAL	THR	I1229	
S2750	L2644	I2478	F2331	L2130	V1902	V1902	C1775	P1565	ALA	HIS	Y1236	
S2751	E2658	D2482	L2335	M2142	L1910	L1910	P1780	S1573	ASP	HIS	L1251	D1068
Q2752	Q2659	F2483	L2335	M2142	Q1911	Q1911	P1780	L1591	LEU	VAL	L1251	Q1069
Q2754	E2660	L2484	E2338	I2149	ASN	ASN	P1783	V1594	ASP	PRO	R1254	D1070
P2755	F2662	L2488	L2343	V2154	SER	SER	L1784	R1598	VAL	ARG	P1256	H1071
L2756	L2664	L2496	L2344	H2159	ASP	ASP	D1785	R1598	VAL	ASP	H1267	A1072
M2757	L2665	S2508	P2364	M2167	THR	THR	I1787	N1601	LYS	ASP	D1267	A1073
Y2760	L2666	T2510	ASN	T2170	ILE	ILE	K1788	V1606	LYS	ASP	D1278	R1074
L2763	P2678	L2520	SER	T2170	GLY	GLY	F1834	Q1615	GLU	ASP	Q1287	A1075
E2767	Y2685	C2521	GLY	V2174	ARG	ARG	H1835	L1618	ALA	LYS	D1287	V1077
S2778	M2688	L2525	GLY	M2175	THR	THR	L1839	V1619	THR	THR	G1291	T1081
L2779	M2689	L2525	THR	V2176	LEU	LEU	I1842	L1630	LYS	PRO	S1292	G1082
K2780	E2690	L2545	LEU	E2181	VAL	VAL	A1854	L1644	ASN	GLU	Q1293	E1083
T2781	K2691	L2548	ASP	G2181	GLU	GLU	ALA	L1644	ASN	ASN	R1089	R1089
M2782	Y2692	L2556	THR	E2182	LYS	LYS	THR	E1649	LYS	HIS	K1097	K1097
V2785	Q2693	S2560	GLU	G2183	VAL	VAL	PR0	T1455	LYS	LYS	C1310	R1100
G2786	S2697	S2560	E2377	S2184	THR	THR	THR	L1650	ASP	ASP	K1316	Y1101
W2787	E2698	L2569	E2378	K2185	LYS	LYS	GLU	L1651	THR	ALA	THR	T1107
R2788	G2699	L2574	D2379	E2186	LYS	LYS	ASP	L1667	GLN	GLN	VAL	T1107
G2789	G2706	L2577	T2381	I2187	GLN	GLN	THR	G1668	LYS	LYS	ALA	T1107
E2790	D2707	C2577	T2382	Y2202	ALA	ALA	LEU	N1669	PRO	PRO	GLY	M1113
R2793	T2708	L2580	T2388	I2206	GLU	GLU	GLU	D1681	ARG	ARG	GLY	R1114
E2794	S2709	R2581	M2389	Y2220	LYS	LYS	LYS	E1682	LEU	LEU	PRO	S1118
G2795	R2710	P2582	V2392	L2221	VAL	VAL	GLU	P1683	LEU	LYS	GLY	P1124
D2796	L2711	S2583	T2396	L2222	GLU	GLU	SER	Q1684	ARG	ARG	ALA	L1128
S2797	T2712	M2584	K2413	E2223	SER	SER	VAL	L1685	THR	ASN	GLY	G1129
M2798	T2716	M2585	R2413	N2224	ASP	ASP	ASP	A1688	LEU	LEU	LEU	W1145
Y2801	L2717	L2589	I2417	V2227	SER	SER	ASP	I1689	LEU	LEU	PHE	W1156
M2802	F2720	R2590	I2417	R2235	K2053	K2054	ALA	M1694	ARG	ARG	GLY	W1156
ARG	T2721	R2591	T2427	R2235	M1974	M1975	LYS	P1496	THR	THR	GLY	M1165
THR	I2721	L2592	T2427	D2241	L1976	L1976	LEU	G1497	LYS	LYS	ASP	D1194
ARG	W2732	V2593	Q2434	N2251	F1979	F1979	GLN	Q1498	PRO	PRO	LEU	F1195
ILE	K2736	K2604	V2435	D1982	D1982	D1982	ALA	G1499	ASP	ASP	GLU	V1196
GLN	L2737	M2605	I2436	K1983	K1983	K1983	GLY	R1500	TYR	TYR	TYR	W1197
THR	A2738	P2606	S2437	S1984	S1984	S1984	GLU	L1505	THR	THR	ASP	
SER	N2739		I2438	E1985	E1985	E1985	GLU	V1510			ALA	
GLN	K2740			C1986	C1986	C1986	GLU					
VAL	V2741											
SER												
VAL												
ASP												

A3729	K3890	A3729	A3468	K3408	M3528	HIS	K3594	N3770	A3729	A3468	K3408	D3347	M3274	A3194	Y3096	C2991	L2898	ALA
R3730	Y3891	R3730	A3469	S3409	A3529	LYS	R3595	N3770	A3469	K3469	S3409	M3348	T3275	L3197	L3102	K2999	Y2901	ALA
H3732	Y3892	H3732	K3470	H3410	L3530	LEU	R3596	L3778	L3470	K3471	H3410	S3349	L3276	P3198	M3104	E3000	A2902	HIS
M3739	I3898	M3739	R3472	N3411	K3531	SER	R3597	D3779	K3471	R3472	N3411	E3350	T3284	V3201	H3115	K3001	S2904	
	E3922		L3473	K3413	D3532	LYS	K3598	N3536	L3473	L3473	K3413	E3352	Y3285	E3202		K3002	R2905	
	P3927		L3474	R3414	D3533		R3599	R3537	F3475	L3474	R3414	E3353		D3203		G2906	G2906	
	L3958		F3477	E3416	L3534		A3598	R3537	N3476	L3476	E3416	L3355	D3291	V3204	E3119	V3004	F2907	
	K3784		G3477	Q3417	R3535		V3599	R3537	G3477	Q3417	Q3417	T3355		C3205		V3013	F2907	
	M3972		L3478	N3418	T3538		V3600	T3538	L3478	N3418	F3419	L3356	M3296	I3208		R3016	K2908	
	V3787		N3479	F3419	D3539		A3601	D3539	N3479	F3419	F3419	D3357	K3297	P3209		H3017	D2909	
	E3987		I3480	V3420	D3540		C3602	D3540	I3480	V3420	V3420	E3358	R3298	S3210		R3018	L2910	
	N3992		C3481	V3421	T3541		F3603	T3541	C3481	V3421	V3421	F3359	L3299	E3212		I3019	E2911	
	K3997		A3482	Q3422	S3542		F3603	T3541	A3482	Q3422	Q3422	T3360	F3302	K3213		S3020	L2912	
	D4001		F3483	N3423	D3543		R3604	R3544	F3483	N3423	N3423	T3361	S3303	L3214		L3021	D2913	
			G3484	E3424	P3544			P3544	G3484	E3424	E3424	L3362	Q3304	E3216		G3023	T2914	
			D3485	T3425	R3545			R3544	D3485	T3425	T3425	A3363	Q3305	K3215		D3025	S2916	
			Q3486	I3426	E3545			P3544	Q3486	I3426	I3426	R3364	P3306	E3217		L3137	L2926	
			E3487	N3426	K3546			E3545	E3487	N3426	N3426	D3365	I3307	E3220		A3139	L2929	
			T3547	N3427	T3547			K3546	E3487	N3427	N3427	L3366	N3308	A3222		L3140	H2937	
			V3548	M3428	V3548			T3547	L3488	M3428	M3428	Y3367	K3309	E3223		G3141		
			E3549	S3429	E3549			V3548	I3489	S3429	S3429	A3368	V3310	E3223		K3144		
			R3550	F3430	R3550			V3549	A3490	F3430	F3430	F3369	P3312	S3224		S3145	L2940	
			V3551	L3431	V3551			R3550	L3491	L3431	L3431	Y3370	Q3313	G3225		I3146	L2941	
			L3552	K3493	L3552			V3551	A3492	K3493	K3493	L3372	L3314	R3226		E3149		
			D3553	N3494	D3553			L3552	K3493	N3494	N3494	L3373	L3315	R3227		L3050	D2944	
			I3554	R3495	I3554			D3553	N3494	R3495	N3495	L3374	K3325	Y3228		K3051	G2945	
			A3555	F3496	A3555			I3554	R3495	F3496	F3496	I3375	K3326	T3229		S3052	G2946	
			V3556	S3497	V3556			A3555	F3496	S3497	S3497	R3381	L3326	R3152		E2859	S2947	
			V3557	L3498	V3557			V3556	S3497	L3498	L3498	R3382	L3327	Q3230		L3057	R2948	
			L3558	K3499	L3558			V3557	L3498	K3499	K3499	F3377	P3321	M3231		L3155		
			F3559	D3500	F3559			L3558	K3499	D3500	D3500	D3378	L3322	V3234		L3159		
			H3560	T3501	H3560			F3559	D3500	T3501	T3501	Y3379	M3323	M3235		F3162	K2950	
			L3561	E3502	L3561			H3560	T3501	E3502	E3502	N3380	E3324	E3236		F3166	G2951	
			E3562	D3503	E3562			L3561	E3502	D3503	D3503	R3381	K3325	V3237		P3167	E2952	
			K3563	E3504	K3563			E3562	D3503	E3504	S3440	A3382	L3326	L3239		V3168	H2953	
			SER	V3505	SER			K3564	V3505	SER	ALA	K3383	K3327	P3240		E3172	F2954	
			LYS	R3506	LYS			E3678	R3506	GLN	VAL	W3384	K3328	C3243			E2957	
			ARG	D3507	ARG			M3695	D3507	GLU	SER	E3387	V3333	M3246		L3175	L2960	
			VAL	I3508	VAL				ARG	GLU	VAL	E3387	V3333	S3247		D3176	K2961	
			GLY	T3509	GLY				VAL	GLY	VAL	N3389	E3336	R3248		H3178		
			ARG	I3510	ARG				GLY	LYS	LYS	P3390	E3337	W3250		T3183	V2967	
			ASP	R3511	ASP				ARG	LYS	LYS	E3391	E3337	K3250		ARG	L2968	
			ASP	N3512	ASP				GLY	LYS	LYS	A3392	E3337	K3250		ASN	P2969	
			ASP	I3871	ASP				GLY	LYS	LYS	E3392	E3337	K3250		GLN	L2970	
			GLY	H3514	GLY				VAL	VAL	VAL	E3393	E3337	K3250		PRO	L2971	
			GLU	L3515	GLU				VAL	VAL	VAL	E3394	E3337	K3250				
			GLU	Q3516	GLU				HIS	R3458	R3458	E3394	E3337	K3250				
			PRO	G3517	PRO				PRO	PRO	PRO	E3394	E3337	K3250				
			ARG	K3518	ARG				ARG	ARG	ARG	E3394	E3337	K3250				
			SER	L3519	SER				SER	SER	SER	E3394	E3337	K3250				
			LYS	E3520	LYS				LYS	LYS	LYS	E3394	E3337	K3250				
			ALA	D3521	ALA				ALA	ALA	ALA	E3394	E3337	K3250				
			TRP	I3524	TRP				TRP	TRP	TRP	E3394	E3337	K3250				
				R3525								E3394	E3337	K3250				
				Q3527								E3394	E3337	K3250				
												E3394	E3337	K3250				
												E3394	E3337	K3250				
												E3394	E3337	K3250				
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												E3394	E3337	K3250				
												E						

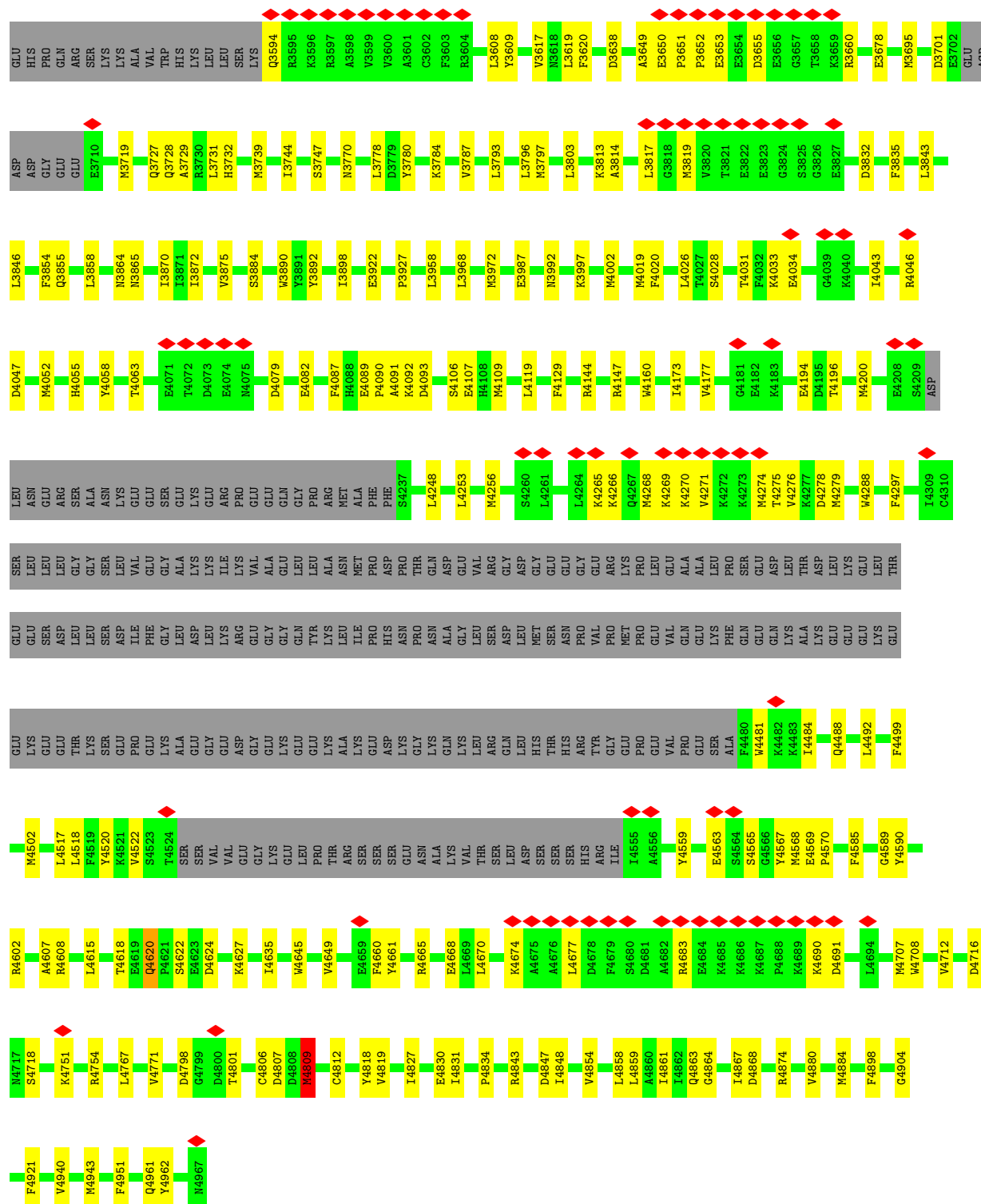


● Molecule 1: Ryanodine receptor 2

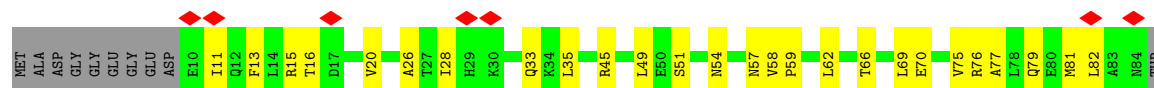


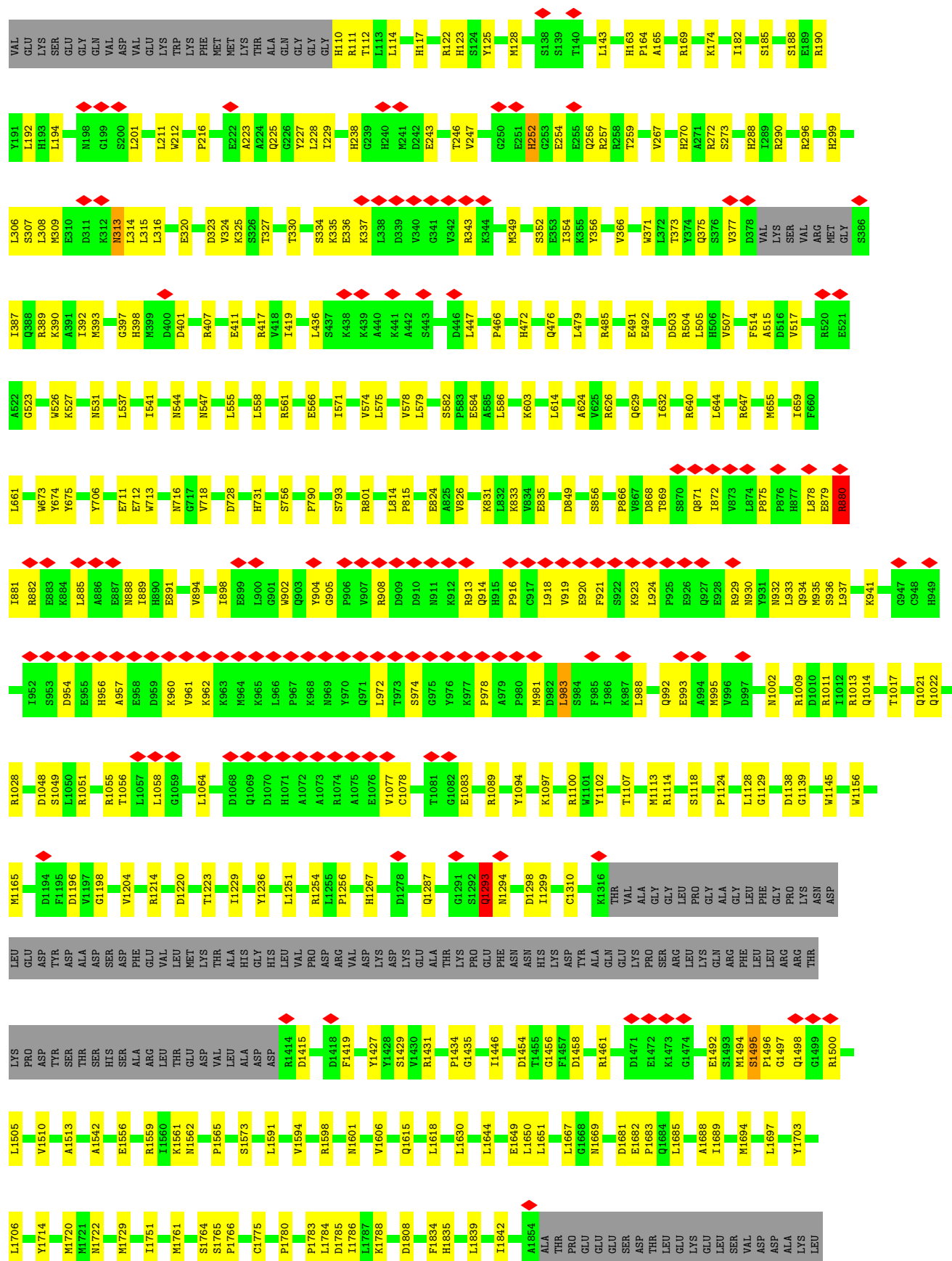


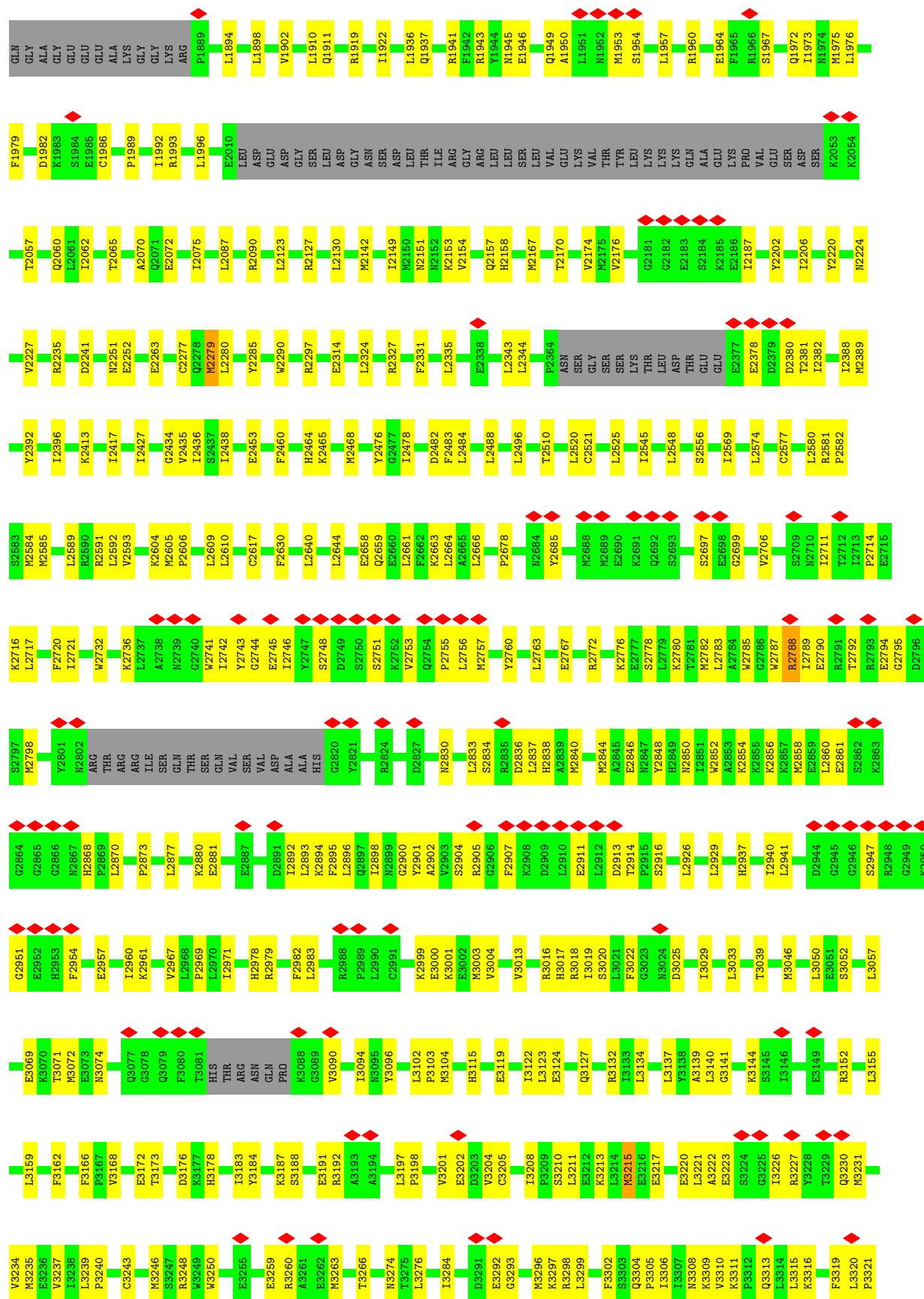




• Molecule 1: Ryanodine receptor 2









G2740	N2605	V2435	R2235	SER	I1973	A1688	M1487	LYS	ALA	G1129	H1002
V2741	P2606	I2436	R2241	ASP	N1974	I1689	E1492	GLN	GLY	G1138	R1009
I2742	L2609	S2437	D2241	SER	M1975	M1694	S1493	ARG	LEU	D1138	D1010
G2743	L2610	I2438	N2251	ALA	L1976	M1694	M1494	PHE	GLY	R1011	R1011
E2745	C2617	E2453	E2252	LYS	F1979	Y1703	S1495	LEU	PRO	W1145	I1012
I2746	F2630	F2460	C2277	GLN	D1982	L1706	P1496	ARG	LYS	W1166	R1013
S2748	L2640	K2465	Q2278	GLY	K1983	Y1714	Q1498	THR	ASP	M1165	Q1014
D2749	L2644	M2468	L2279	GLY	E1984	M1721	G1499	PRO	LEU	D1194	T1017
S2750	L2644	M2468	L2280	GLU	F1985	M1721	R1500	ASP	GLU	F1195	R1028
S2751	L2644	M2468	L2280	GLU	C1986	M1722	L1505	THR	TYR	D1194	D1048
K2752	E2658	I2478	Y2285	GLU	P1989	M1722	V1510	ASP	ASP	F1195	S1049
V2753	Q2659	D2482	W2290	ALA	I1992	M1729	V1510	THR	ALA	G1197	L1050
Q2754	F2483	F2483	R2297	GLY	R1993	M1729	A1513	HIS	ASP	V1198	R1051
P2755	L2484	L2484	L2297	GLY	L1996	I1751	A1513	SER	ASP	V1204	R1055
L2756	L2488	L2488	E2314	LYS	L1996	M1761	A1542	ALA	PHE	R1214	T1056
N2757	L2496	L2496	L2335	ARG	E2010	S1764	E1556	LEU	VAL	L1057	L1058
Y2760	S2508	A2509	E2338	P1889	LEU	P1766	R1559	THR	LYS	D1220	G1059
L2763	L2510	T2510	L2343	L1894	ASP	C1775	K1561	VAL	THR	T1223	L1064
E2767	L2520	C2521	L2344	L1898	GLY	P1780	N1562	ALA	ASP	I1229	L1064
I2770	L2525	L2525	P2364	V1902	ASP	P1780	P1565	ASP	ASP	Y1236	D1068
R2771	L2525	L2525	ASN	Q1911	GLY	P1783	S1573	LEU	GLY	L1281	Q1069
R2772	L2525	L2525	SER	Y1912	ASN	L1784	L1591	VAL	HIS	L1281	L1070
K2776	I2545	I2545	GLY	R1919	SER	D1785	L1594	PRO	LEU	R1284	H1071
E2777	L2548	L2548	SER	R1936	ASP	I1786	V1594	ASP	ARG	L1285	A1072
S2778	L2548	L2548	THR	L1937	THR	L1787	R1598	VAL	ASP	P1256	A1073
L2779	S2556	S2556	THR	Q1937	THR	K1788	R1598	ASP	LYS	H1287	R1074
K2780	S2556	S2556	THR	R1941	THR	L1829	R1598	LYS	ASP	D1278	A1075
T2781	S2560	S2560	THR	R1942	GLY	F1884	M1601	ASP	LYS	G1287	A1075
H2782	I2569	I2569	GLU	R1943	ARG	H1835	V1606	GLY	ALA	Q1287	Y1077
V2785	L2574	L2574	GLU	N1945	SER	L1839	Q1615	ALA	THR	G1287	C1078
Q2786	C2577	C2577	E2377	E1946	VAL	I1842	Q1615	LYS	THR	G1291	T1081
V2787	L2574	L2574	E2378	Q1949	LYS	I1842	L1618	GLU	PRO	S1292	G1082
D2788	L2574	L2574	E2378	A1950	LYS	A1854	L1618	THR	GLU	Q1283	E1083
I2789	L2580	L2580	D2379	L1951	VAL	ALA	L1630	PRO	PHE	N1294	R1089
R2791	R2581	R2581	T2381	N1952	THR	THR	L1644	LYS	ASN	D1298	K1097
T2792	P2582	P2582	T2382	M1953	THR	PRO	L1644	LYS	ASN	I1299	R1100
R2793	S2583	S2583	T2382	M1954	THR	GLU	L1651	ASP	LYS	C1310	Y1101
E2794	M2584	M2584	T2388	S1954	LYS	GLU	L1667	TYR	ASP	K1316	Y1102
C2795	M2585	M2585	M2389	A1955	LYS	GLU	G1668	ALA	ALA	THR	T1107
D2796	M2585	M2585	M2389	A1956	LYS	ASP	G1668	GLN	GLN	K1316	Y1102
S2797	L2589	L2589	Y2392	L1957	GLN	THR	N1669	VAL	GLU	THR	T1107
M2798	R2590	R2590	I2206	L1957	ALA	LEU	E1682	LYS	LYS	ALA	M1113
Y2799	L2592	L2592	Y2220	F1965	LYS	GLU	P1683	PRO	PRO	ALA	M113
K2799	V2593	V2593	N2224	R1966	VAL	GLU	Q1684	ARG	ARG	GLY	R1114
D2799	K2604	K2604	V2227	S1967	GLU	LEU	L1685	LEU	LEU	PRO	S1118
Y2801	Y2801	Y2801	Y2227	Q1972	GLU	LEU	L1685	GLY	GLY	GLY	P124
N2802	Y2801	Y2801	Y2227	Q1972	GLU	LEU	L1685	GLY	GLY	GLY	L1128
ARG	ARG	ARG	Y2227	Q1972	GLU	LEU	L1685	GLY	GLY	GLY	L1128
THR	THR	THR	Y2227	Q1972	GLU	LEU	L1685	GLY	GLY	GLY	L1128
ARG	ARG	ARG	Y2227	Q1972	GLU	LEU	L1685	GLY	GLY	GLY	L1128
ARG	ARG	ARG	Y2227	Q1972	GLU	LEU	L1685	GLY	GLY	GLY	L1128
ILE	ILE	ILE	Y2227	Q1972	GLU	LEU	L1685	GLY	GLY	GLY	L1128
SER	SER	SER	Y2227	Q1972	GLU	LEU	L1685	GLY	GLY	GLY	L1128



Chain G:  73% 24% ...



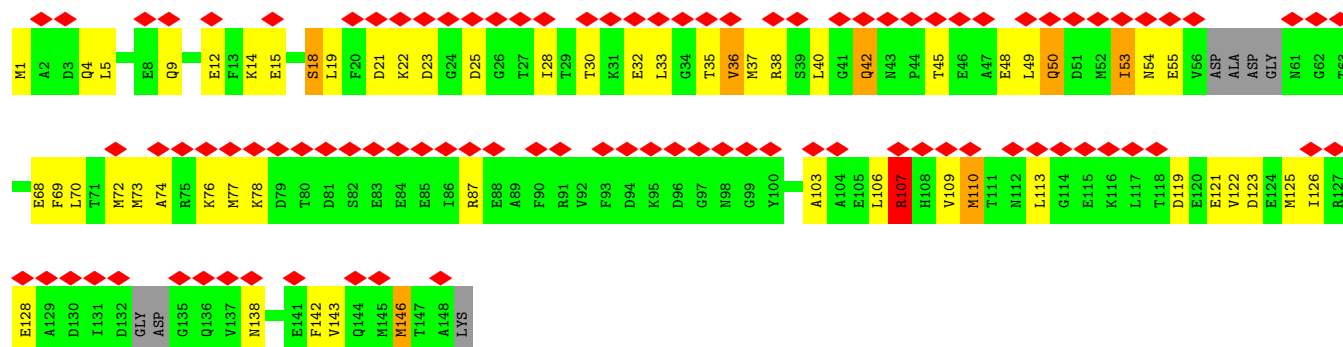
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:  73% 24% ...



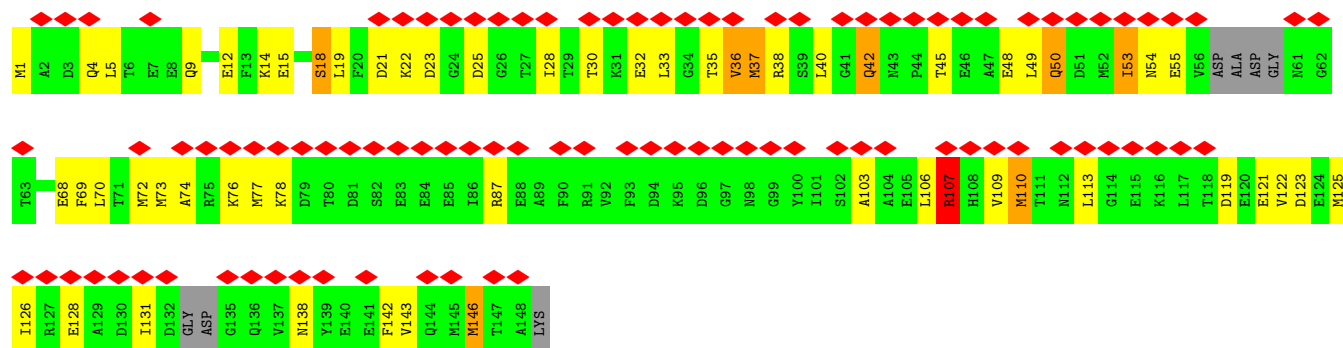
- Molecule 3: Calmodulin-1

Chain I:  64% 57% 33% 5% • 5%



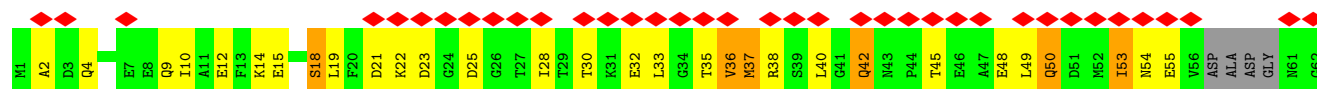
- Molecule 3: Calmodulin-1

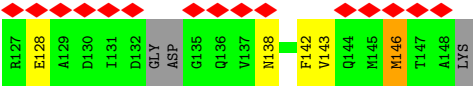
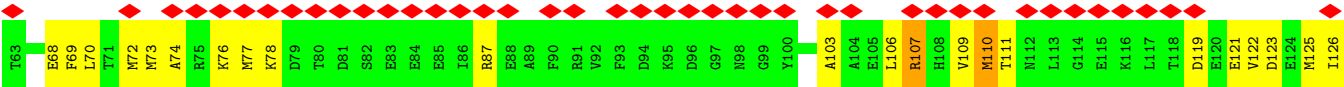
Chain J:  64% 56% 33% 5% • 5%



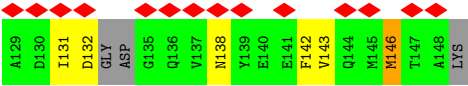
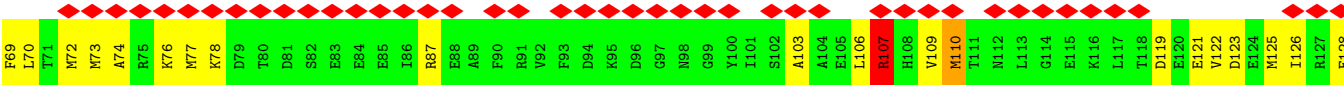
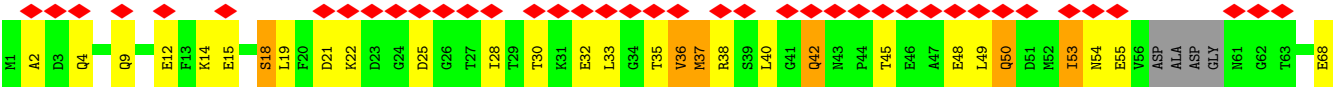
- Molecule 3: Calmodulin-1

Chain K:  63% 57% 32% 6% 5%





• 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	73052	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.746	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/36343	0.36	8/49085 (0.0%)
1	B	0.14	0/36343	0.36	8/49085 (0.0%)
1	C	0.14	0/36343	0.36	8/49085 (0.0%)
1	D	0.14	0/36343	0.36	8/49085 (0.0%)
2	E	0.16	0/834	0.45	0/1123
2	F	0.16	0/834	0.45	0/1123
2	G	0.16	0/834	0.45	0/1123
2	H	0.16	0/834	0.45	0/1123
3	I	0.27	0/1122	0.80	1/1504 (0.1%)
3	J	0.27	0/1122	0.79	1/1504 (0.1%)
3	K	0.27	0/1122	0.80	1/1504 (0.1%)
3	L	0.27	0/1122	0.79	1/1504 (0.1%)
All	All	0.14	0/153196	0.38	36/206848 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
3	I	0	1
3	J	0	1
3	K	0	1
3	L	0	1
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1293	GLN	CA-CB-CG	7.96	130.02	114.10
1	A	1293	GLN	CA-CB-CG	7.94	129.98	114.10
1	B	1293	GLN	CA-CB-CG	7.93	129.96	114.10
1	C	1293	GLN	CA-CB-CG	7.92	129.94	114.10
1	D	4046	ARG	CG-CD-NE	6.38	126.04	112.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3520	GLU	Peptide
3	I	107	ARG	Sidechain
3	J	107	ARG	Sidechain
3	K	107	ARG	Sidechain
3	L	107	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	A	35570	0	35258	681	0
1	B	35570	0	35258	684	0
1	C	35570	0	35258	695	0
1	D	35570	0	35258	689	0
2	E	818	0	821	20	0
2	F	818	0	821	22	0
2	G	818	0	821	20	0
2	H	818	0	821	20	0
3	I	1112	0	1053	35	0
3	J	1112	0	1053	37	0
3	K	1112	0	1053	41	0
3	L	1112	0	1053	36	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	0	0
5	B	62	0	24	0	0
5	C	62	0	24	0	0
5	D	62	0	24	0	0
All	All	150252	0	148624	2895	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 2895 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:2905:ARG:NH1	1:C:2907:PHE:O	1.97	0.98
1:D:2905:ARG:NH1	1:D:2907:PHE:O	1.97	0.97
1:B:2905:ARG:NH1	1:B:2907:PHE:O	1.97	0.97
1:A:2905:ARG:NH1	1:A:2907:PHE:O	1.97	0.97
3:I:138:ASN:O	3:I:142:PHE:HB2	1.64	0.96

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	4415/4967 (89%)	4241 (96%)	168 (4%)	6 (0%)	48	78
1	B	4415/4967 (89%)	4240 (96%)	169 (4%)	6 (0%)	48	78
1	C	4415/4967 (89%)	4241 (96%)	168 (4%)	6 (0%)	48	78
1	D	4415/4967 (89%)	4241 (96%)	168 (4%)	6 (0%)	48	78
2	E	105/108 (97%)	101 (96%)	3 (3%)	1 (1%)	12	42
2	F	105/108 (97%)	100 (95%)	4 (4%)	1 (1%)	12	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	105/108 (97%)	99 (94%)	5 (5%)	1 (1%)	12	42
2	H	105/108 (97%)	100 (95%)	4 (4%)	1 (1%)	12	42
3	I	136/149 (91%)	126 (93%)	10 (7%)	0	100	100
3	J	136/149 (91%)	126 (93%)	10 (7%)	0	100	100
3	K	136/149 (91%)	126 (93%)	10 (7%)	0	100	100
3	L	136/149 (91%)	126 (93%)	10 (7%)	0	100	100
All	All	18624/20896 (89%)	17867 (96%)	729 (4%)	28 (0%)	44	73

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	VAL
1	A	1495	SER
2	E	3	VAL
2	F	3	VAL
2	G	3	VAL

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	3905/4358 (90%)	3898 (100%)	7 (0%)	87	92
1	B	3905/4358 (90%)	3896 (100%)	9 (0%)	87	92
1	C	3905/4358 (90%)	3896 (100%)	9 (0%)	87	92
1	D	3905/4358 (90%)	3896 (100%)	9 (0%)	87	92
2	E	88/89 (99%)	85 (97%)	3 (3%)	32	64
2	F	88/89 (99%)	85 (97%)	3 (3%)	32	64
2	G	88/89 (99%)	85 (97%)	3 (3%)	32	64
2	H	88/89 (99%)	85 (97%)	3 (3%)	32	64
3	I	119/127 (94%)	109 (92%)	10 (8%)	10	35
3	J	119/127 (94%)	109 (92%)	10 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	119/127 (94%)	109 (92%)	10 (8%)	10	35
3	L	119/127 (94%)	109 (92%)	10 (8%)	10	35
All	All	16448/18296 (90%)	16362 (100%)	86 (0%)	78	89

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	110	MET
1	C	2279	MET
1	B	880	ARG
1	B	2838[B]	HIS
1	C	3215	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4636	ASN
1	D	3850	HIS
1	D	79	GLN
1	D	1615	GLN
1	D	4493	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	C	5002	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	A	5003	-	32,33,33	0.26	0	48,52,52	0.28	0
5	ATP	D	5002	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	B	5003	-	32,33,33	0.26	0	48,52,52	0.28	0
5	ATP	D	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
5	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	C	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
5	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.29	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	C	5002	-	-	7/22/38/38	0/3/3/3
5	ATP	A	5003	-	-	5/22/38/38	0/3/3/3
5	ATP	D	5002	-	-	7/22/38/38	0/3/3/3
5	ATP	B	5003	-	-	5/22/38/38	0/3/3/3
5	ATP	D	5003	-	-	5/22/38/38	0/3/3/3
5	ATP	B	5002	-	-	7/22/38/38	0/3/3/3
5	ATP	C	5003	-	-	5/22/38/38	0/3/3/3
5	ATP	A	5002	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5002	ATP	C5'-O5'-PA-O1A

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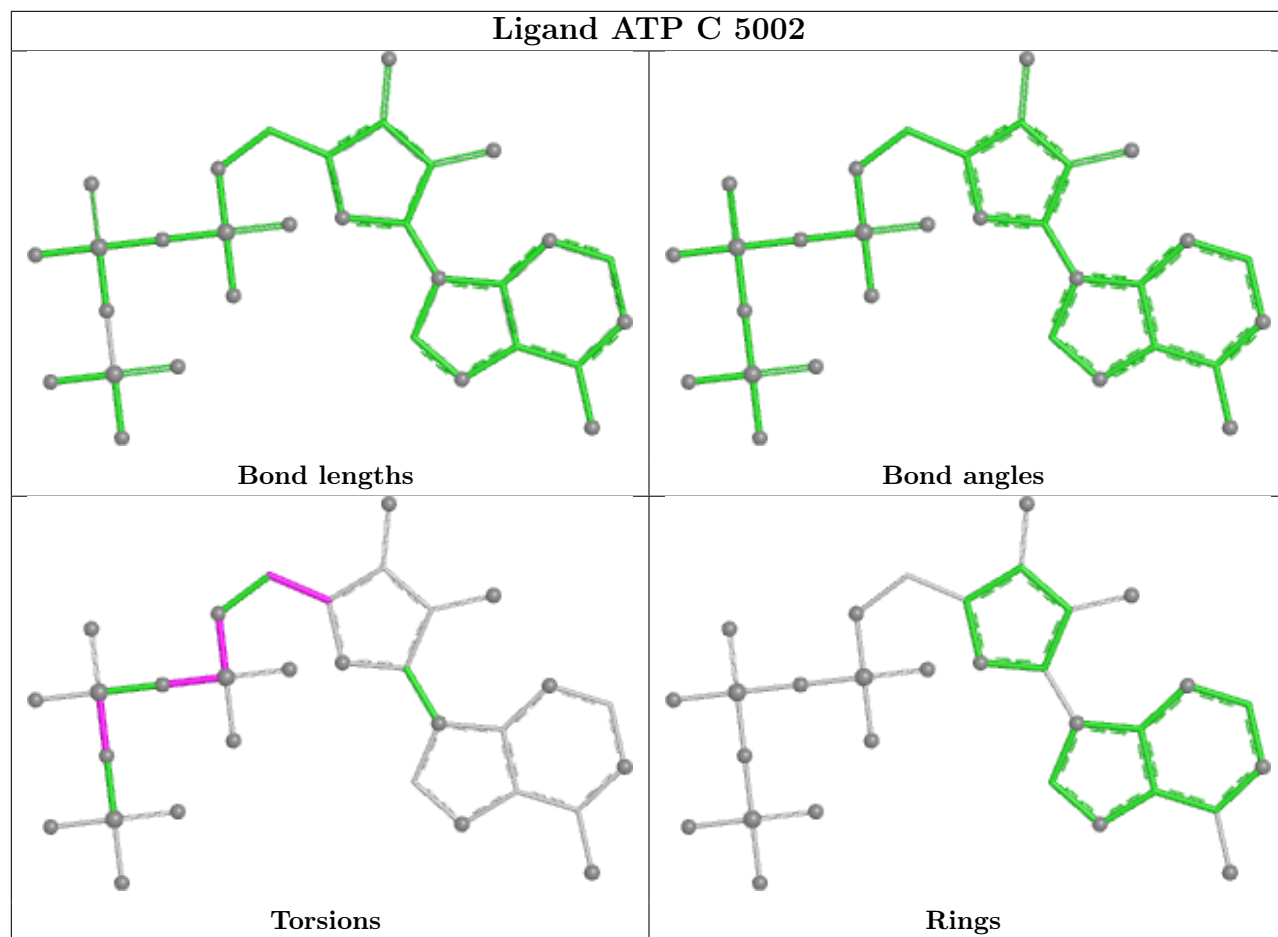
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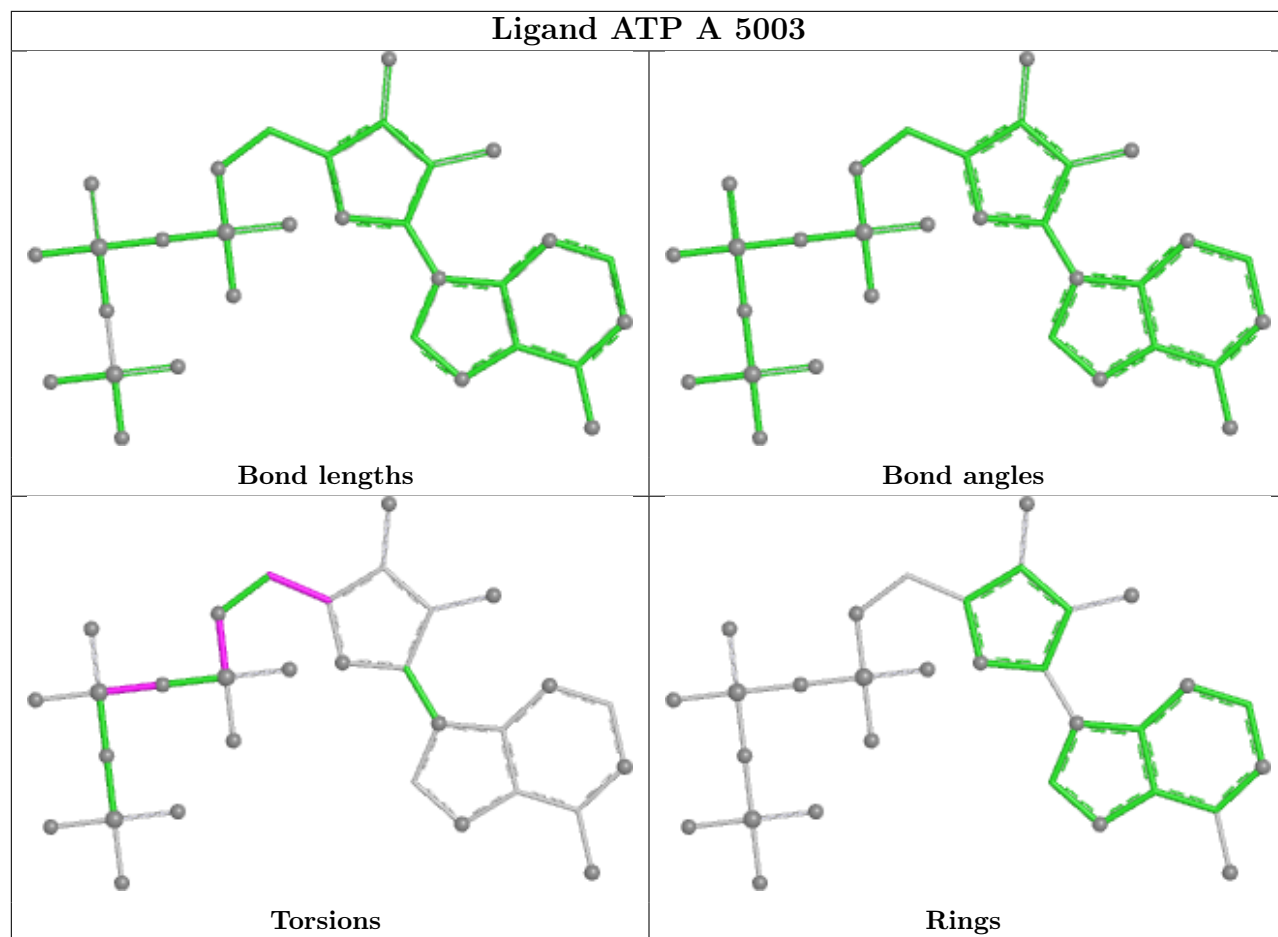
Mol	Chain	Res	Type	Atoms
5	A	5002	ATP	C5'-O5'-PA-O2A
5	A	5002	ATP	C5'-O5'-PA-O3A
5	A	5003	ATP	C5'-O5'-PA-O1A
5	A	5003	ATP	C5'-O5'-PA-O2A

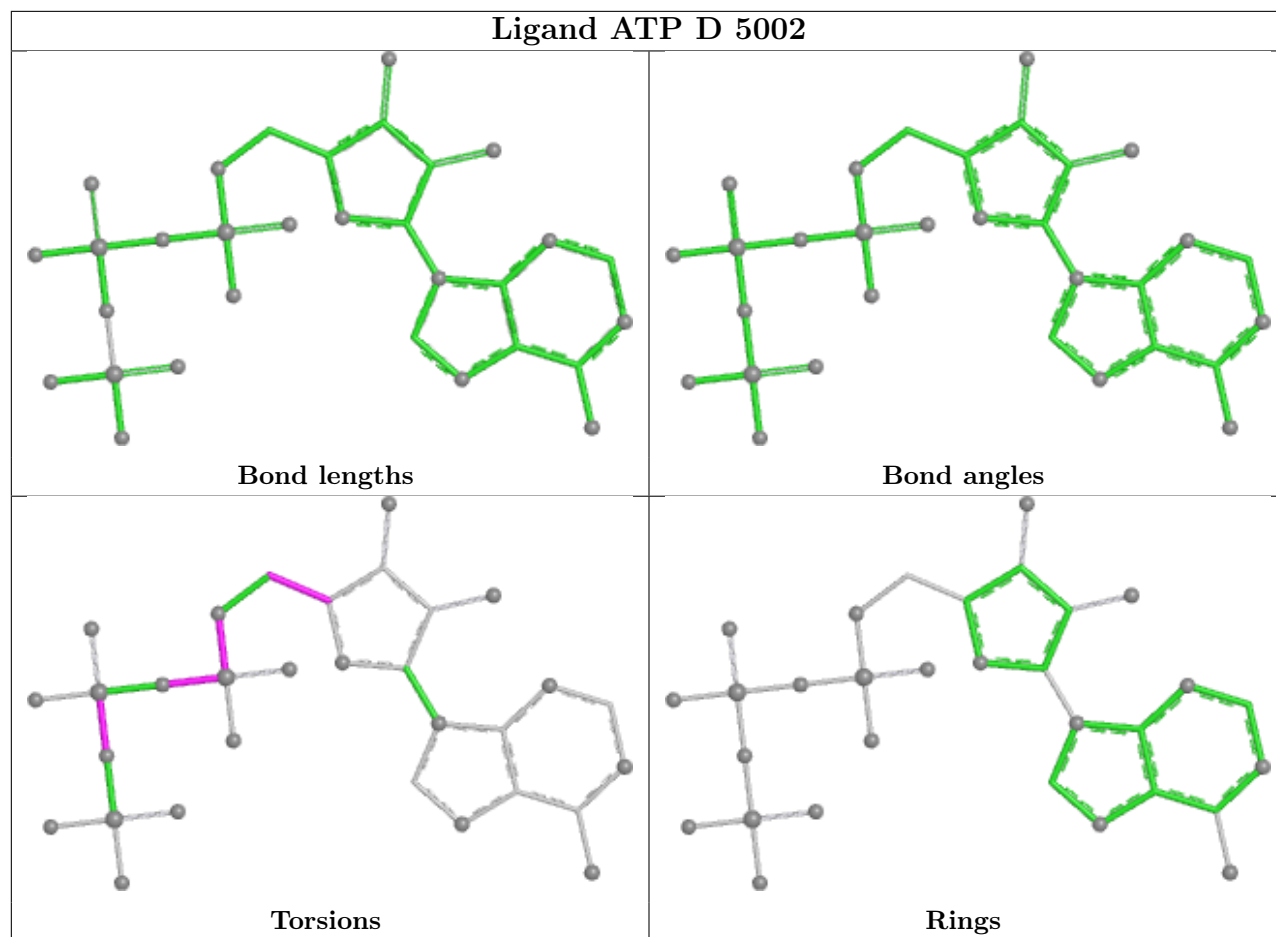
There are no ring outliers.

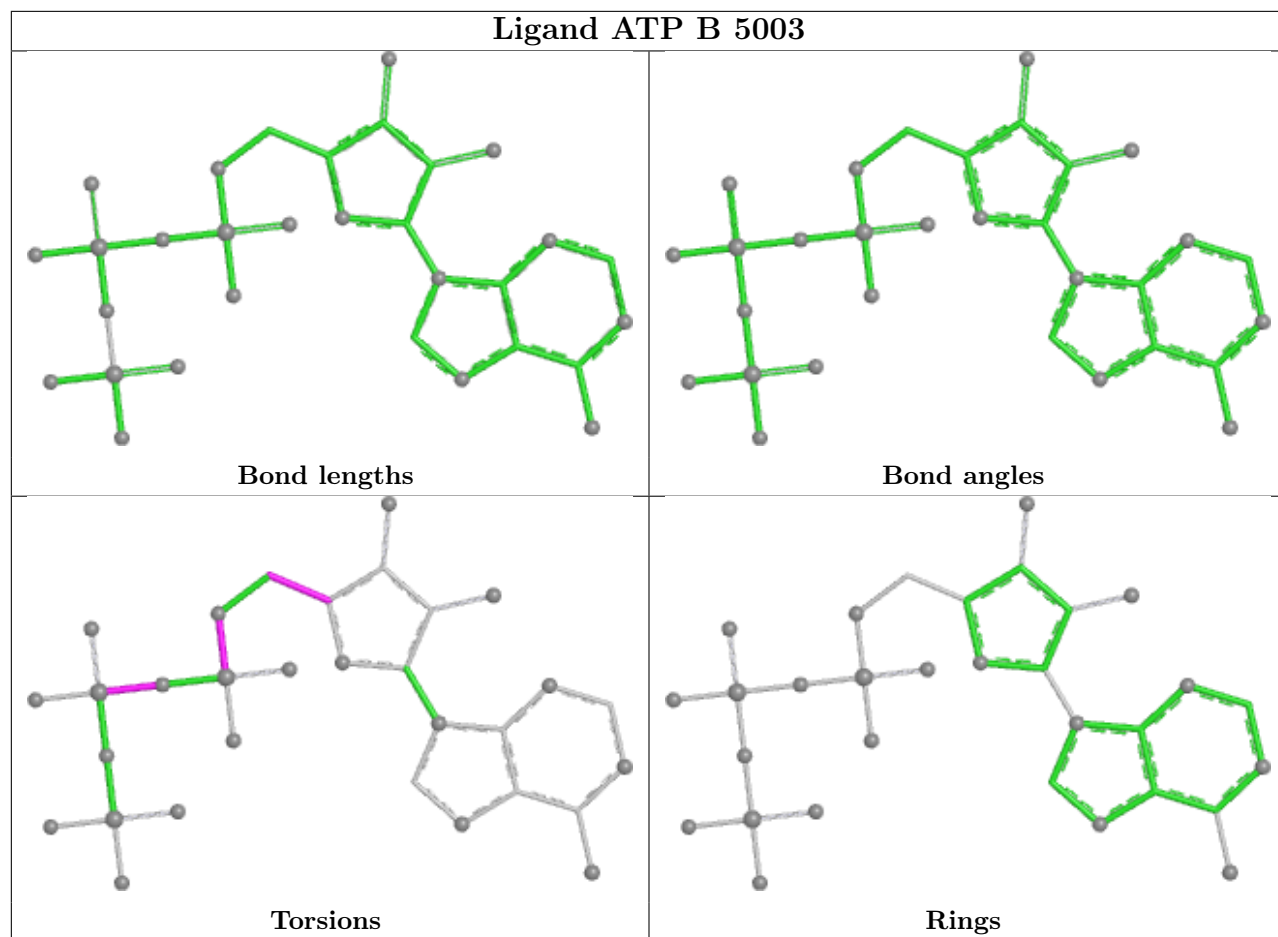
No monomer is involved in short contacts.

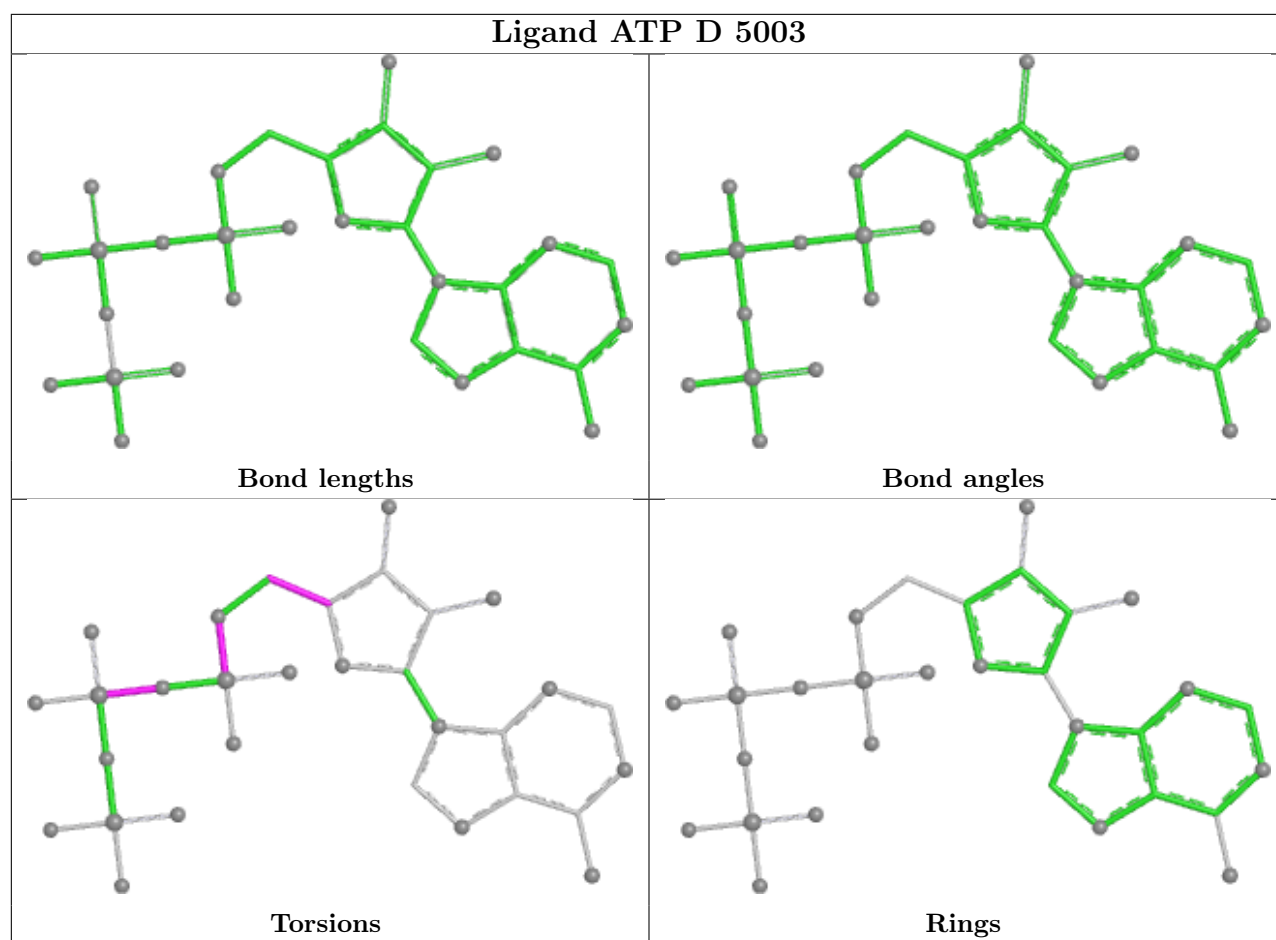
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

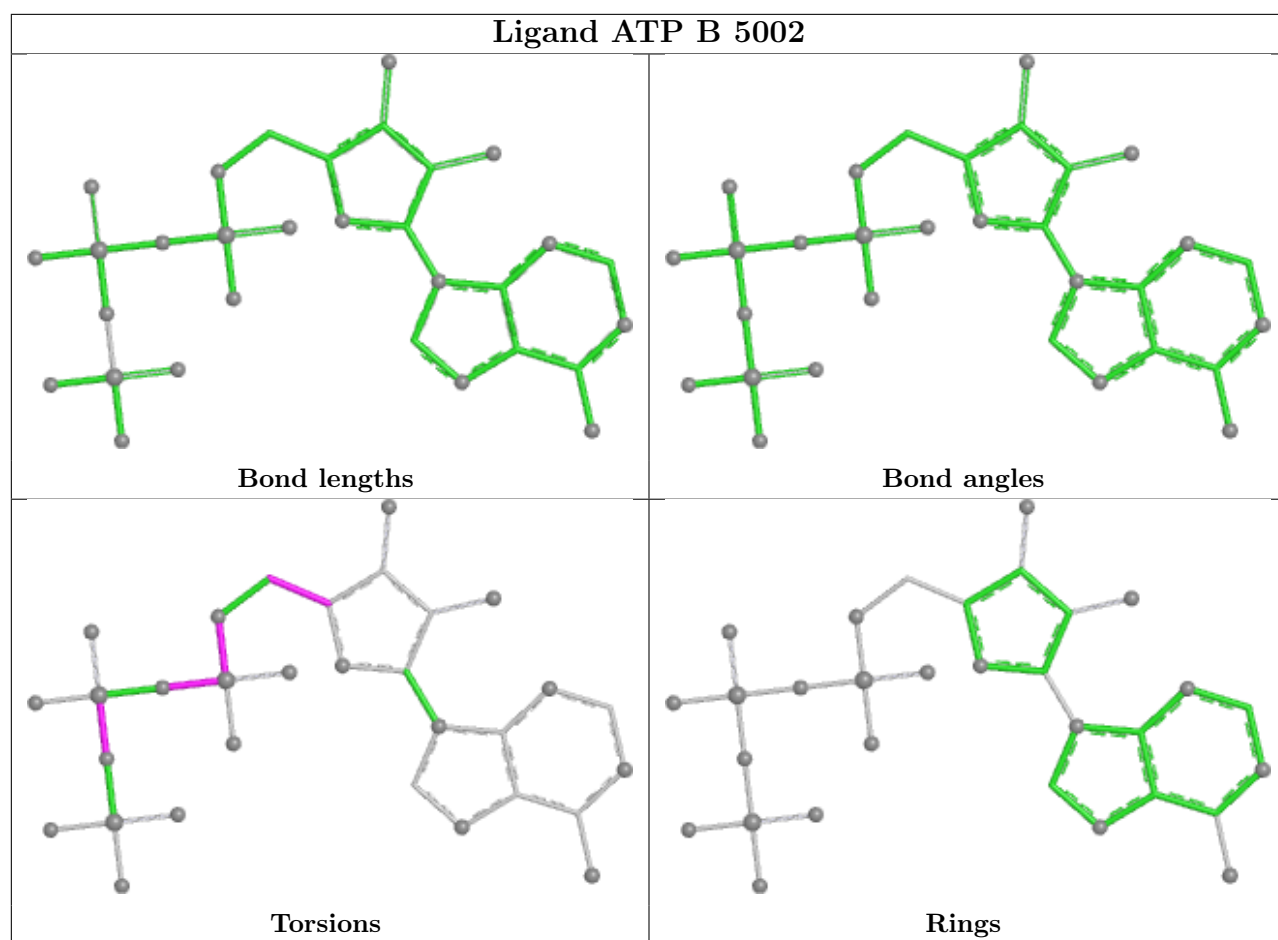


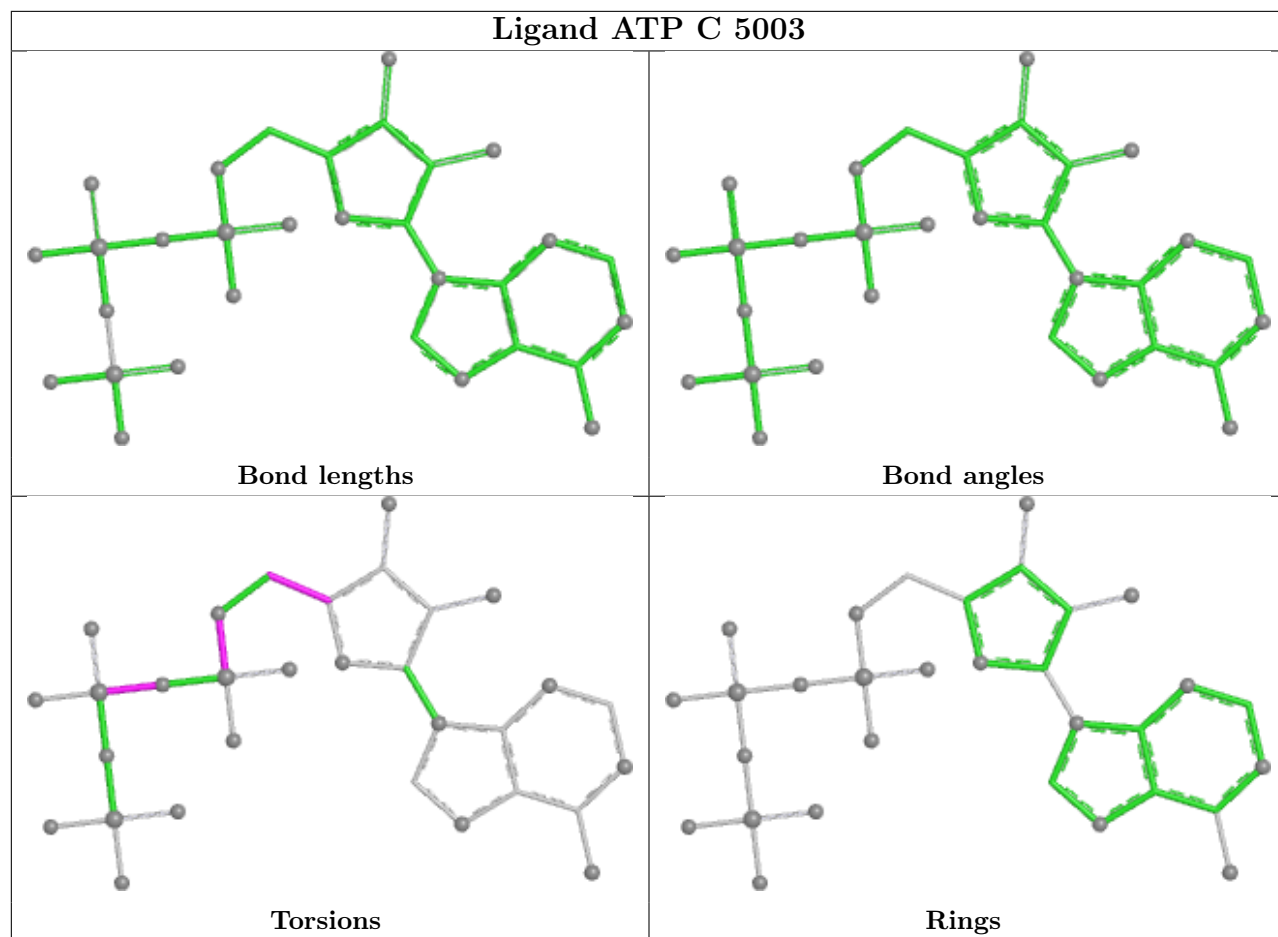


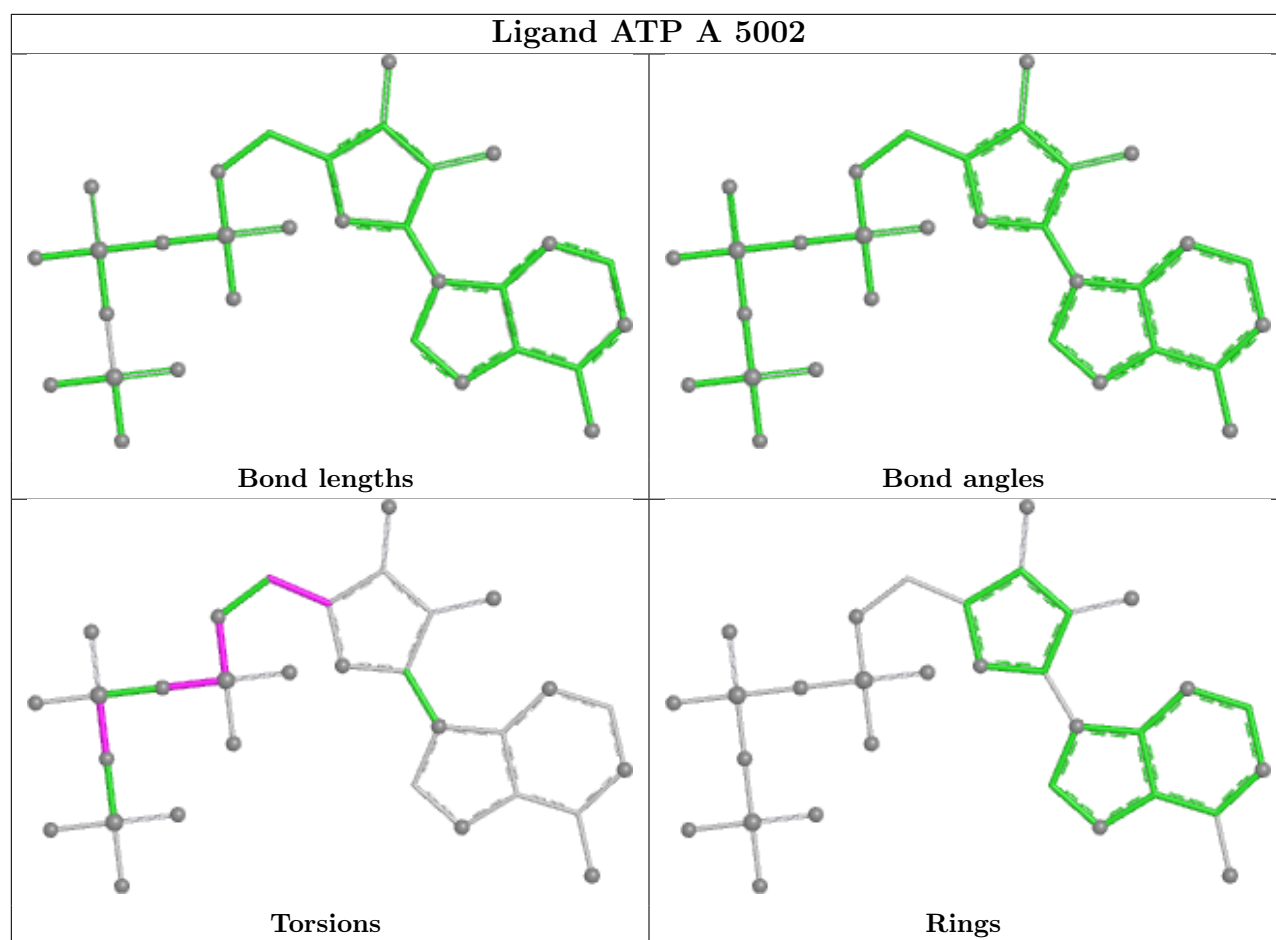












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

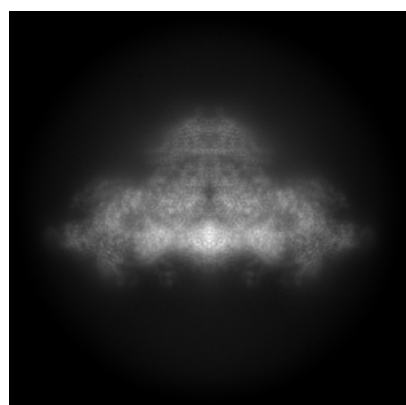
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26413. These allow visual inspection of the internal detail of the map and identification of artifacts.

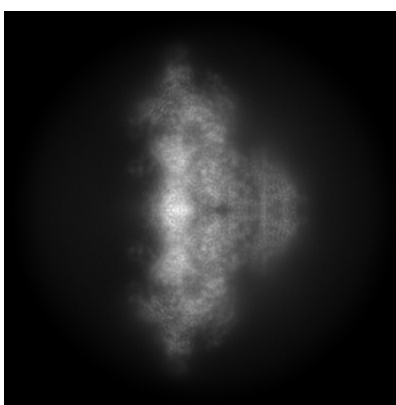
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

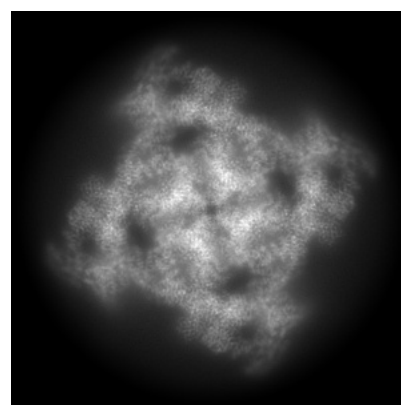
6.1.1 Primary map



X



Y

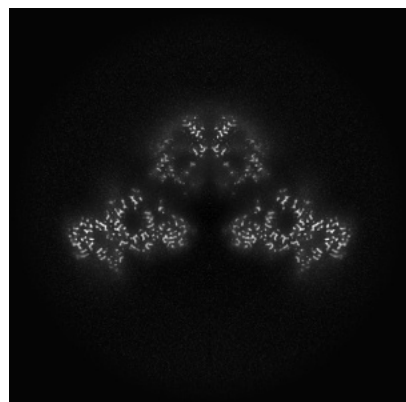


Z

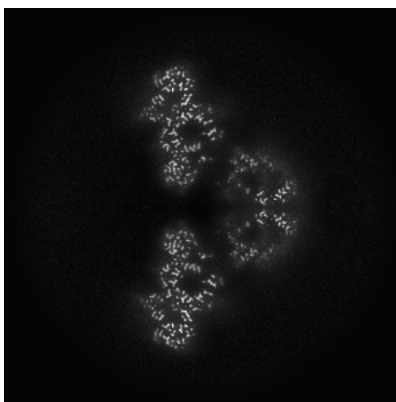
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

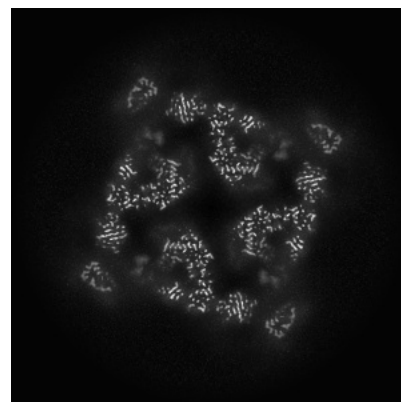
6.2.1 Primary map



X Index: 256



Y Index: 256

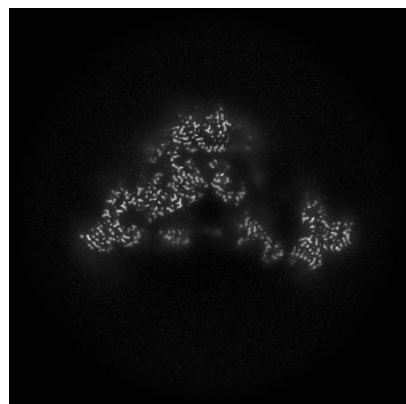


Z Index: 256

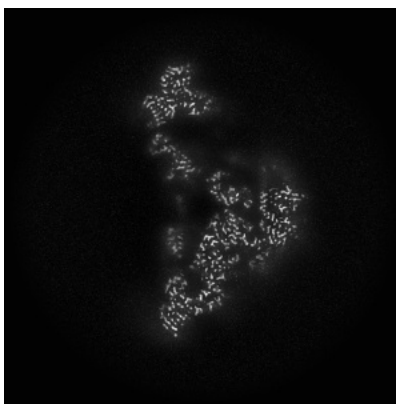
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

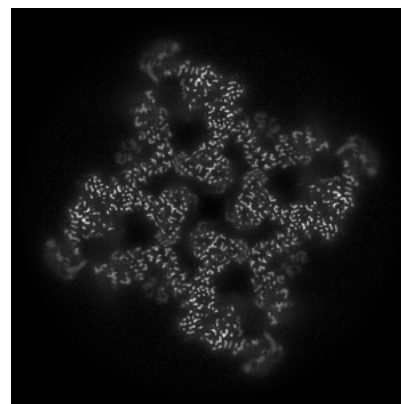
6.3.1 Primary map



X Index: 237



Y Index: 275

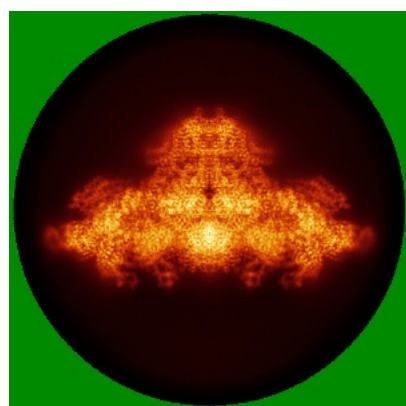


Z Index: 223

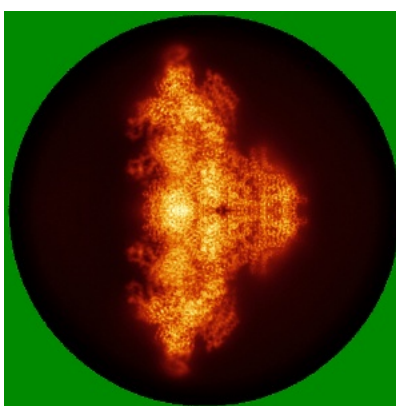
The images above show the largest variance slices of the map in three orthogonal directions.

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

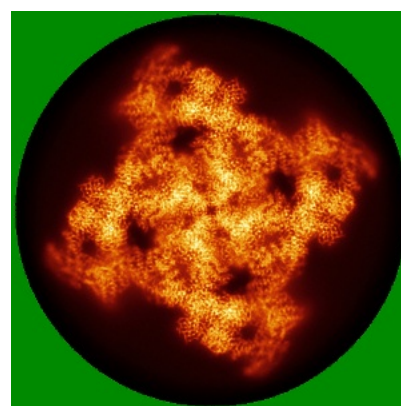
6.4.1 Primary map



X



Y

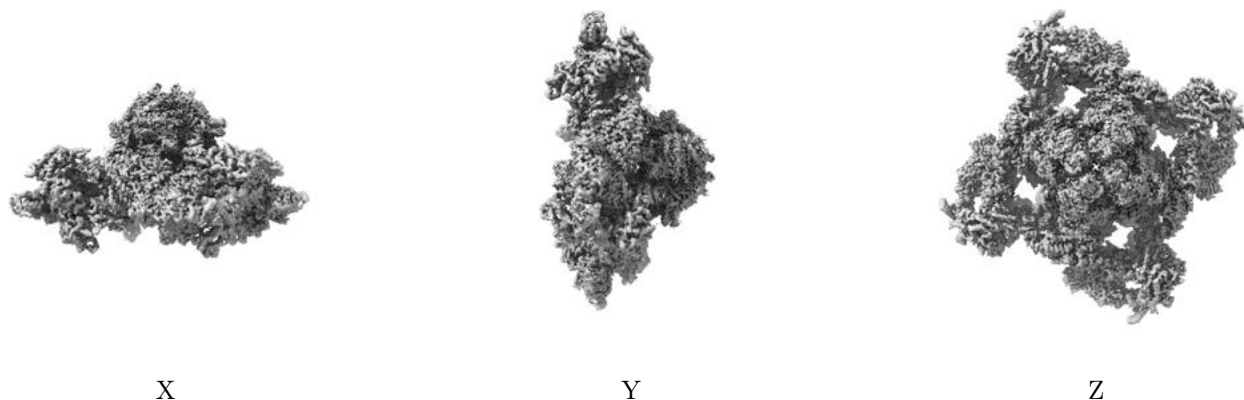


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

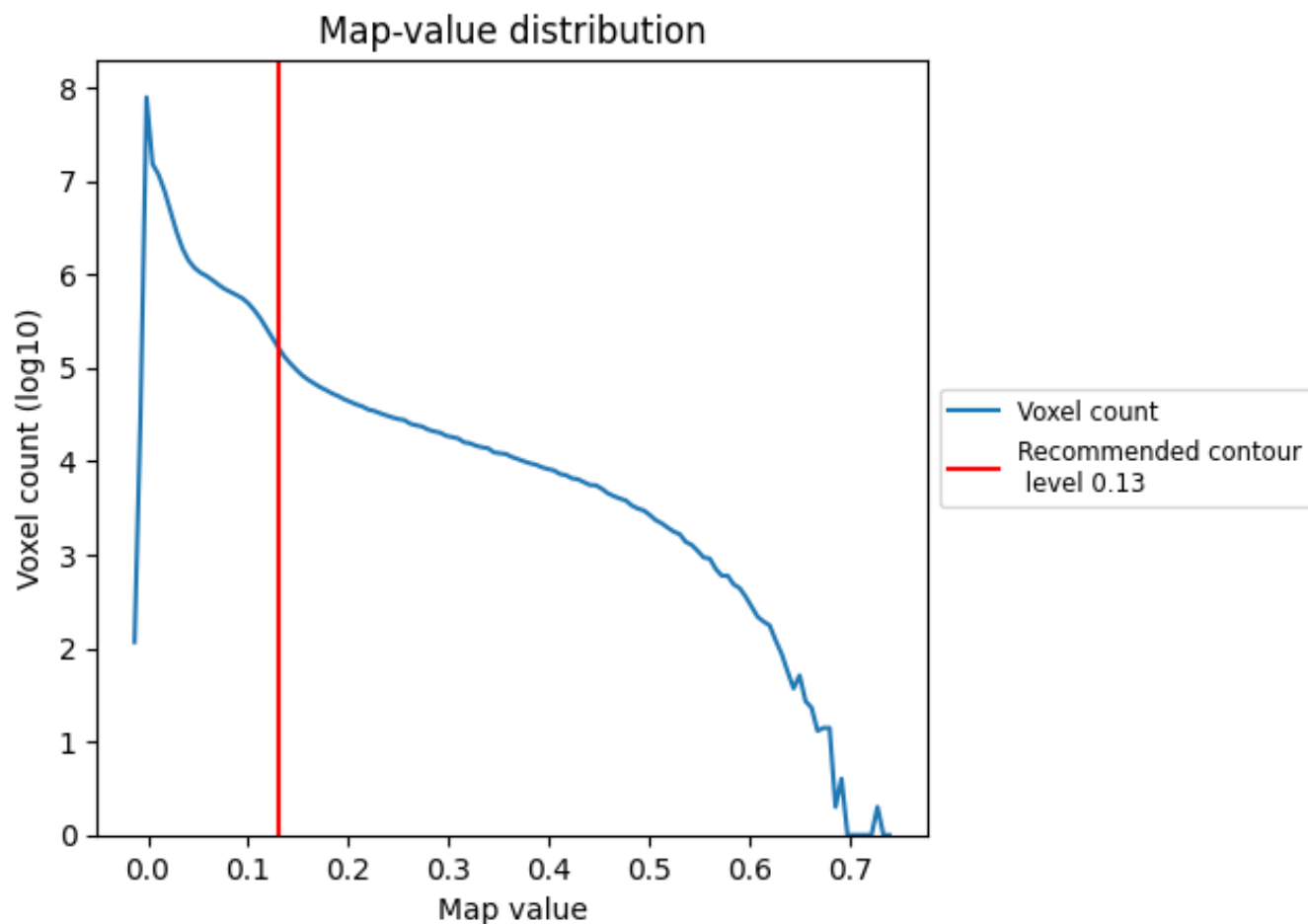
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

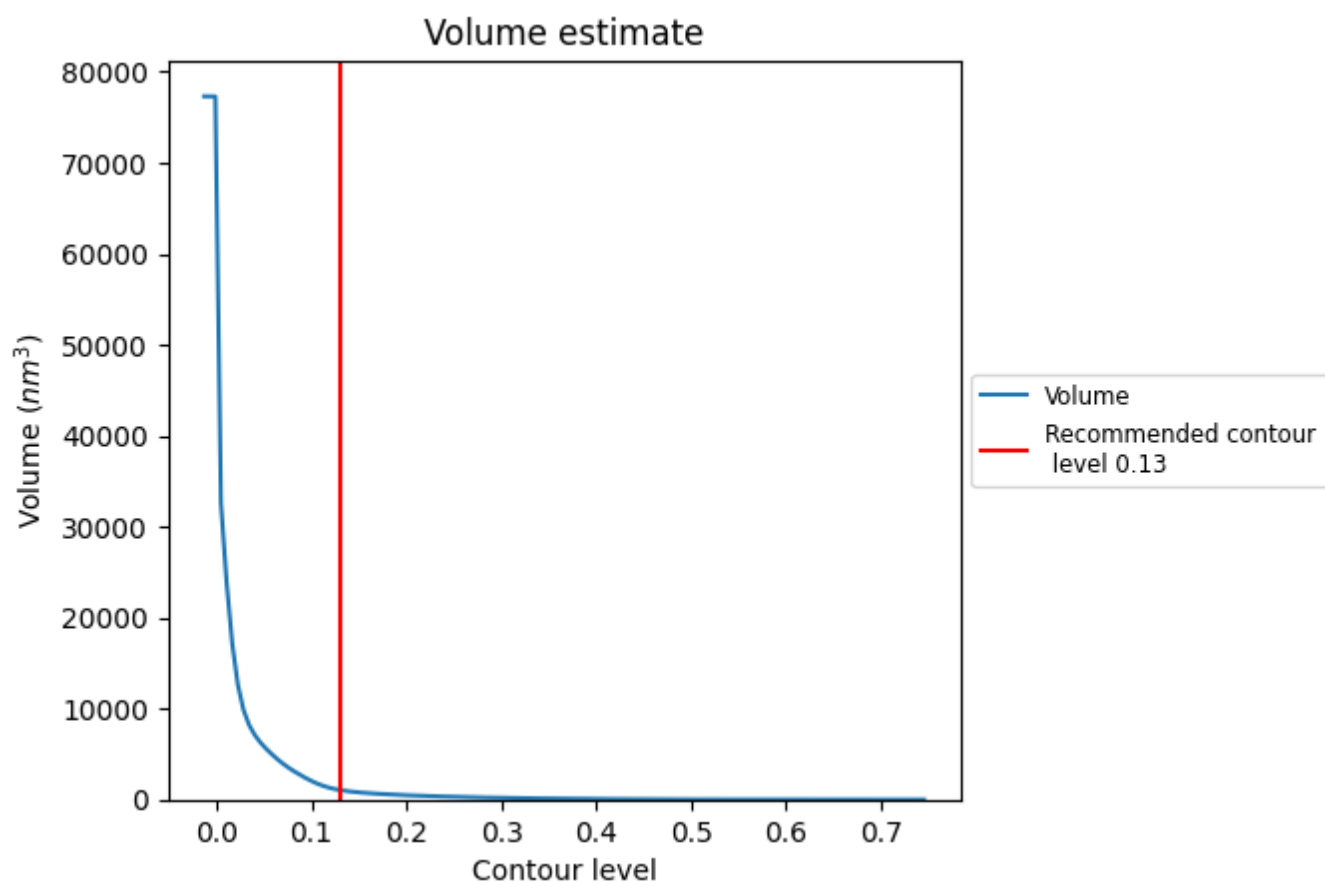
This section contains the results of statistical analysis of the map.

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.

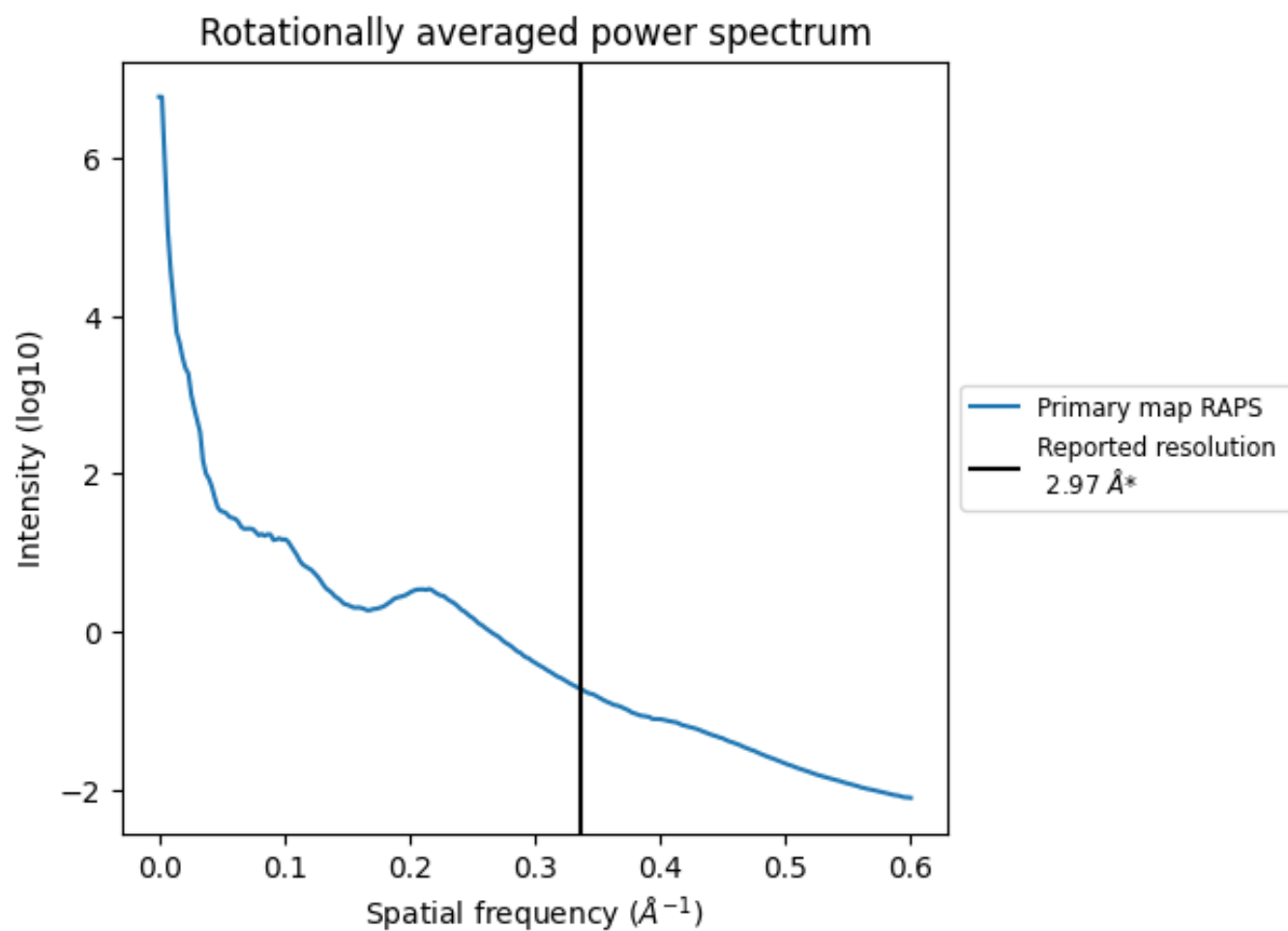
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1047 nm³; this corresponds to an approximate mass of 946 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 0.337 Å⁻¹

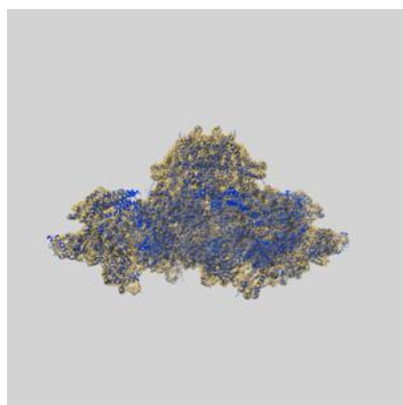
8 Fourier-Shell correlation

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

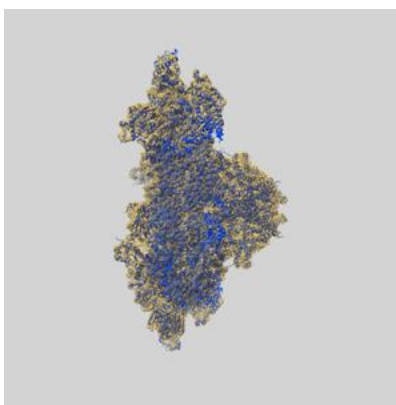
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26413 and PDB model 7UA3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

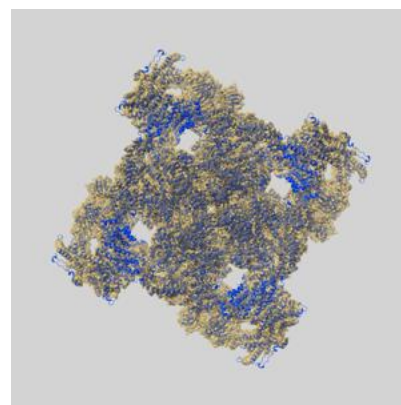
9.1 Map-model overlay [i](#)



X



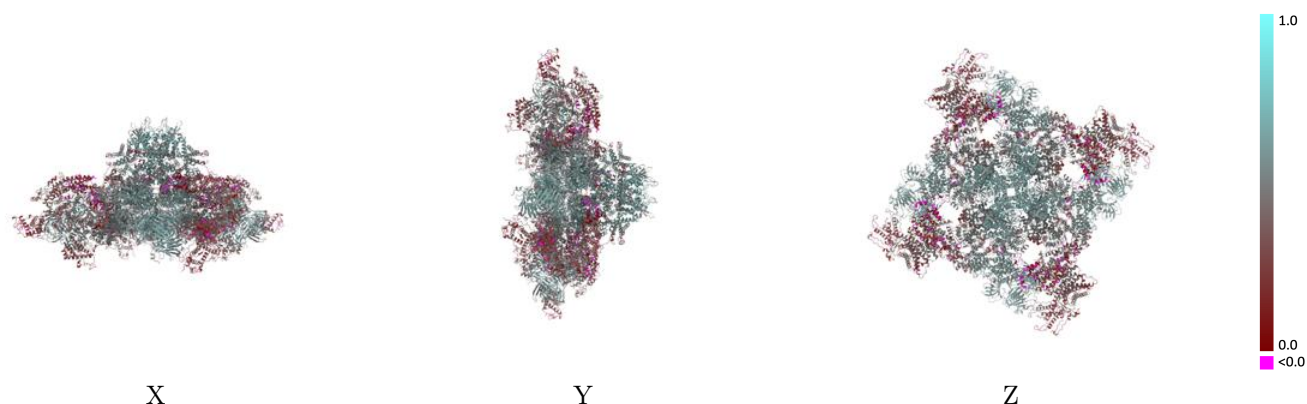
Y



Z

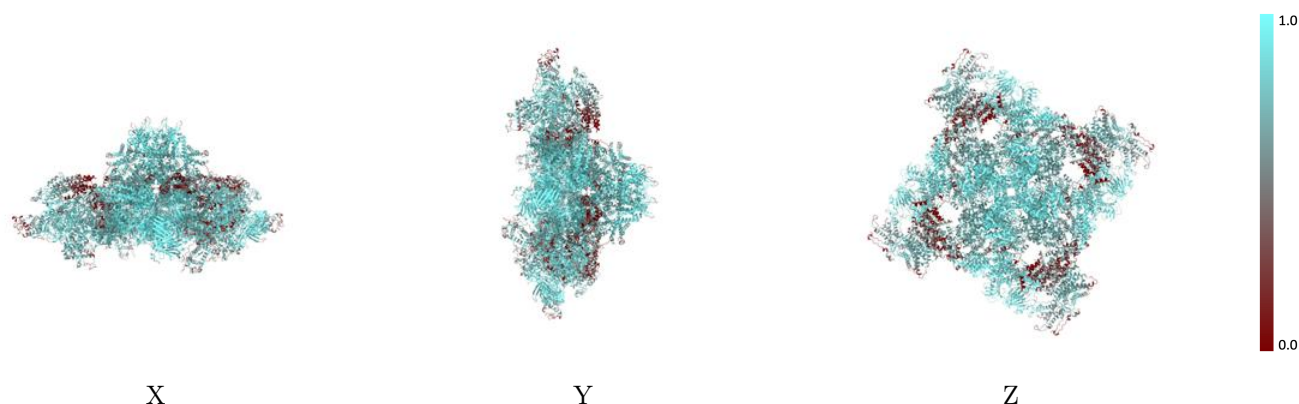
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



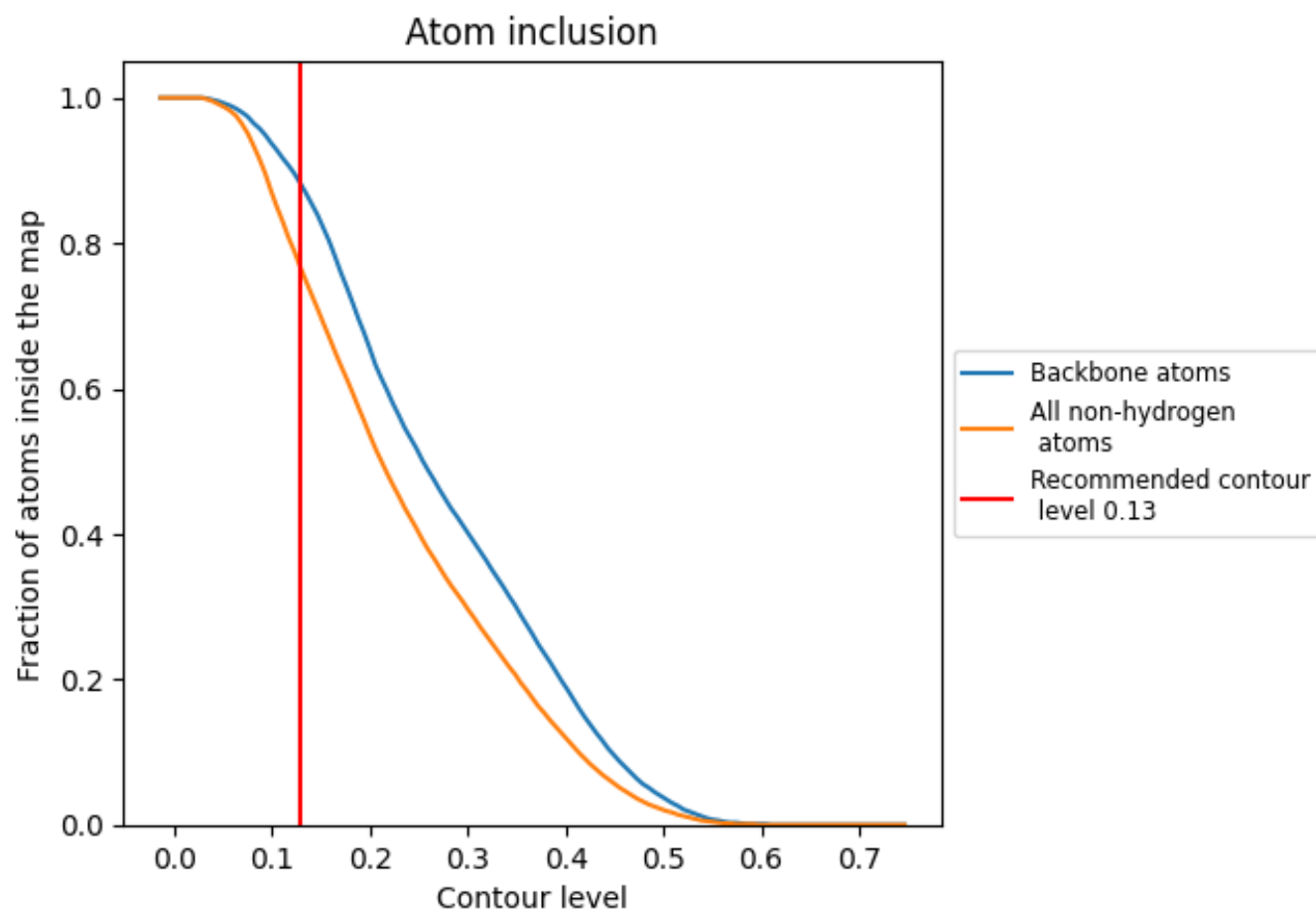
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.4470
A	0.7770	0.4530
B	0.7760	0.4520
C	0.7760	0.4520
D	0.7760	0.4520
E	0.9270	0.5680
F	0.9290	0.5710
G	0.9330	0.5700
H	0.9300	0.5710
I	0.2810	0.1610
J	0.2820	0.1670
K	0.2950	0.1660
L	0.2820	0.1640

1.0

0.0

<0.0