



# wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 05:40 PM EDT

PDB ID : 7U9Q  
EMDB ID : EMD-26405  
Title : Structure of PKA phosphorylated human RyR2 in the closed state  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2022-03-11  
Resolution : 3.11 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](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

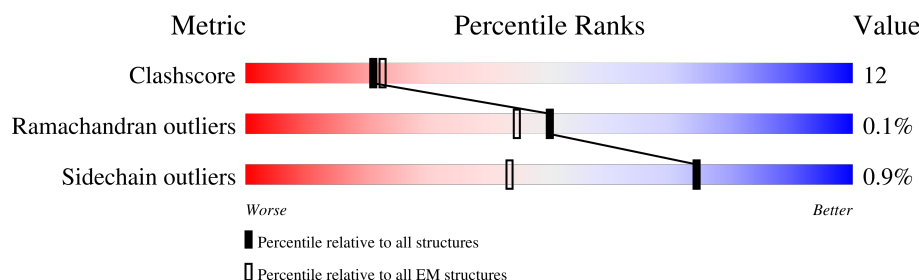
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.11 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	 80% 17% ...
1	F	108	 79% 19% ...
1	G	108	 79% 19% ...
1	H	108	 77% 20% ...
2	A	4967	 13% 62% 22% • 15%
2	B	4967	 13% 62% 22% • 15%
2	C	4967	 13% 62% 22% • 15%
2	D	4967	 13% 62% 22% • 15%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 138608 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	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
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		

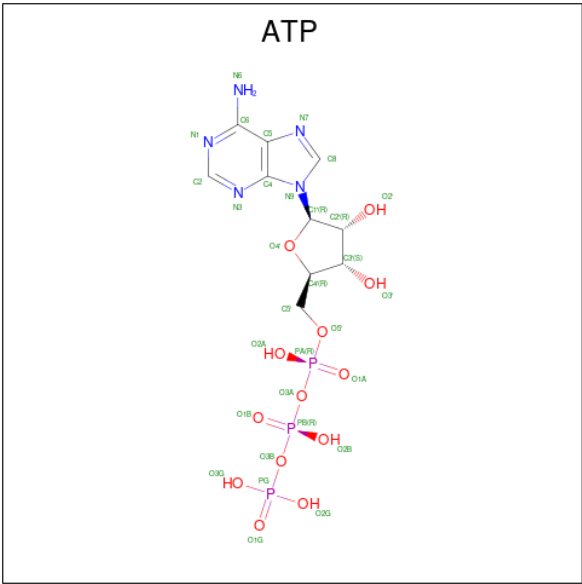
- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 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>) (labeled as "Ligand of Interest" by depositor).

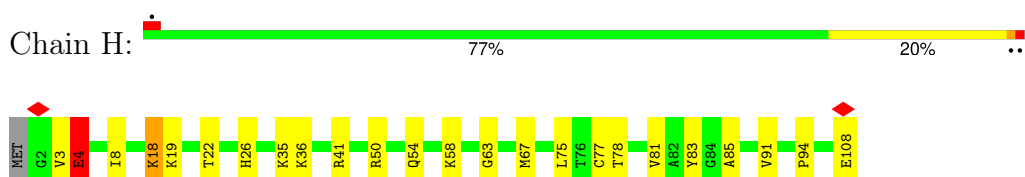


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10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

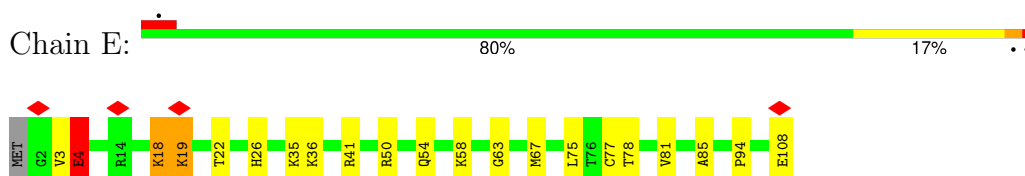
### 3 Residue-property plots [i](#)

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

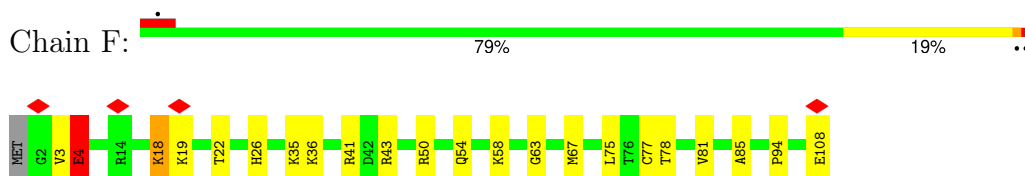
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



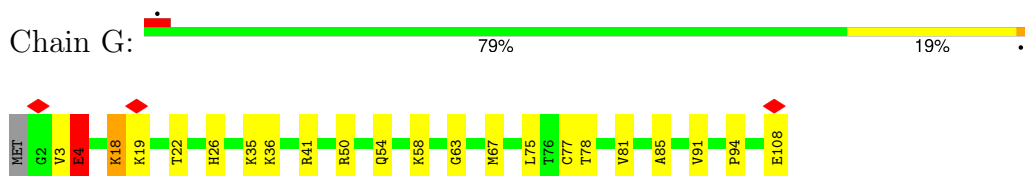
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



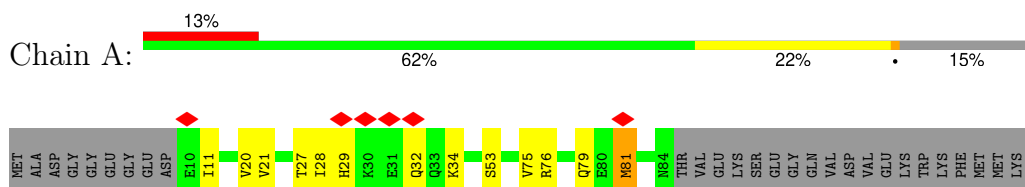
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



- Molecule 2: Ryanodine receptor 2



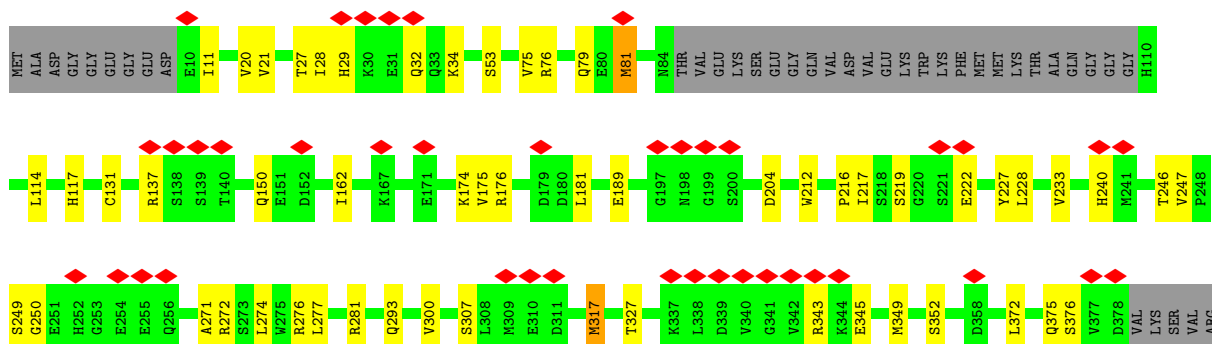
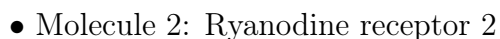






WORLDWIDE  
PDB  
PROTEIN DATA BANK

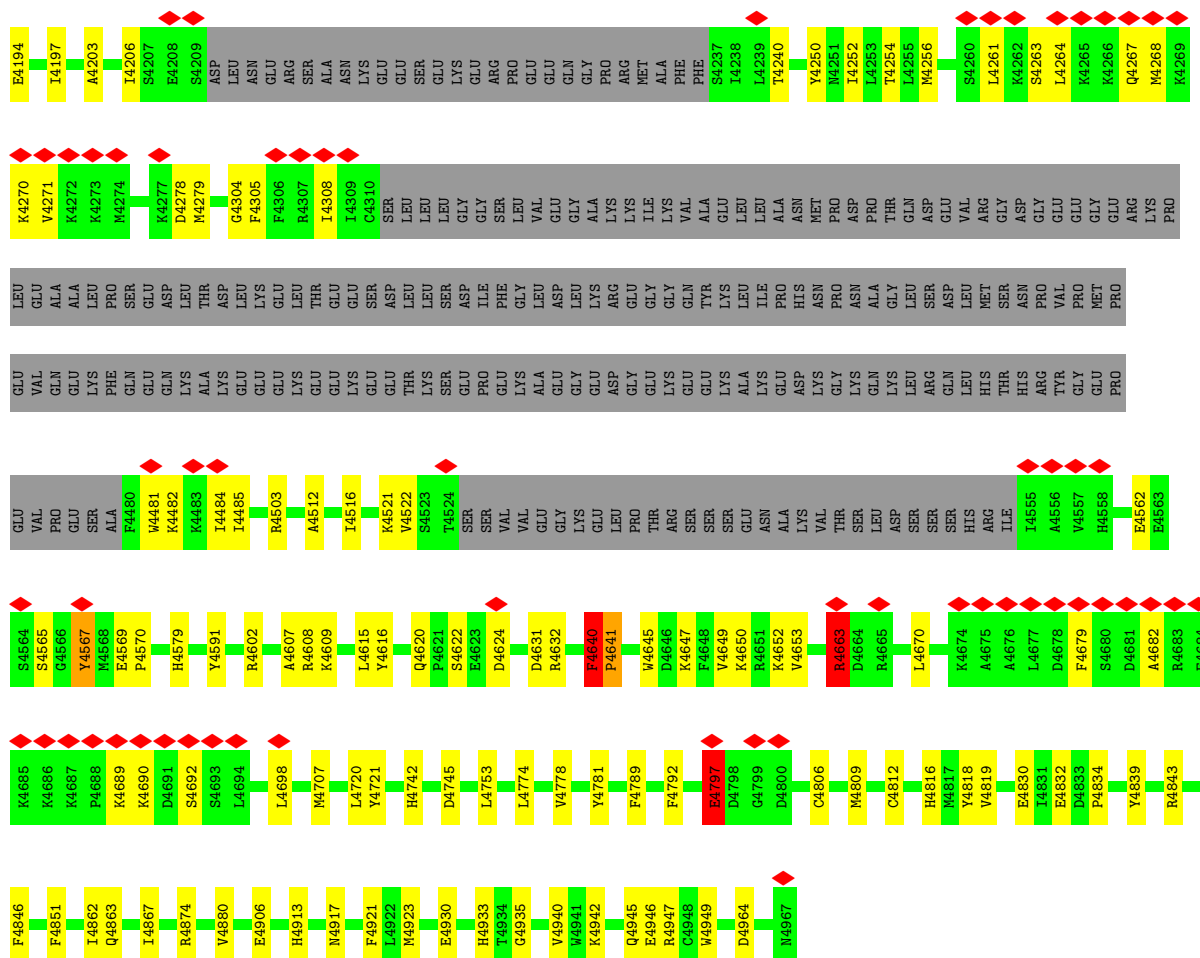




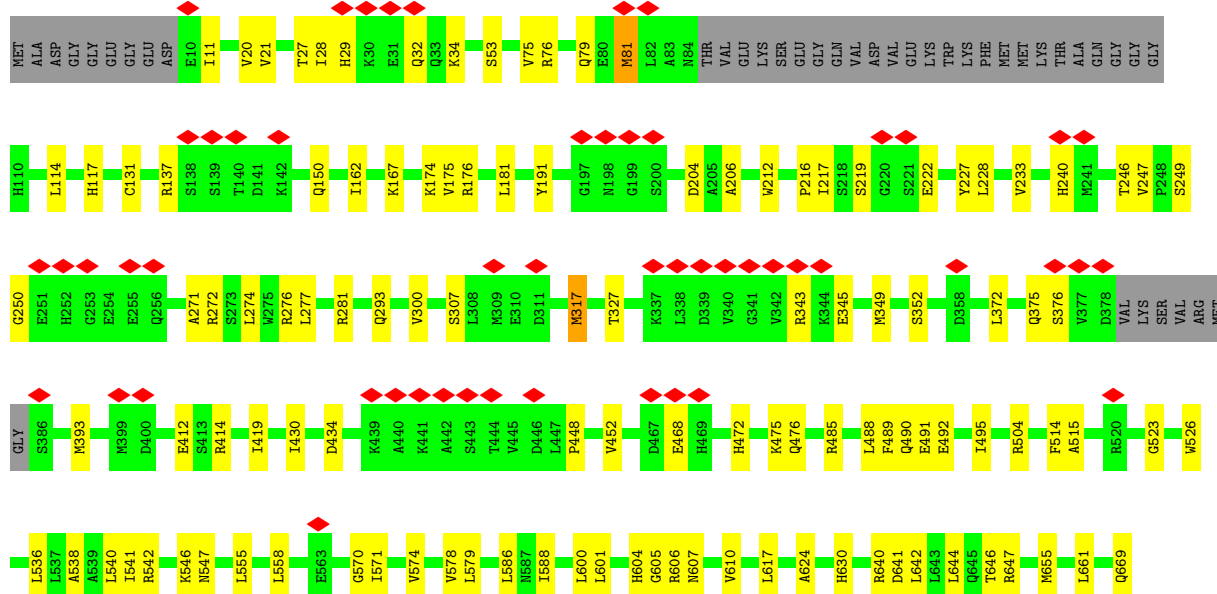




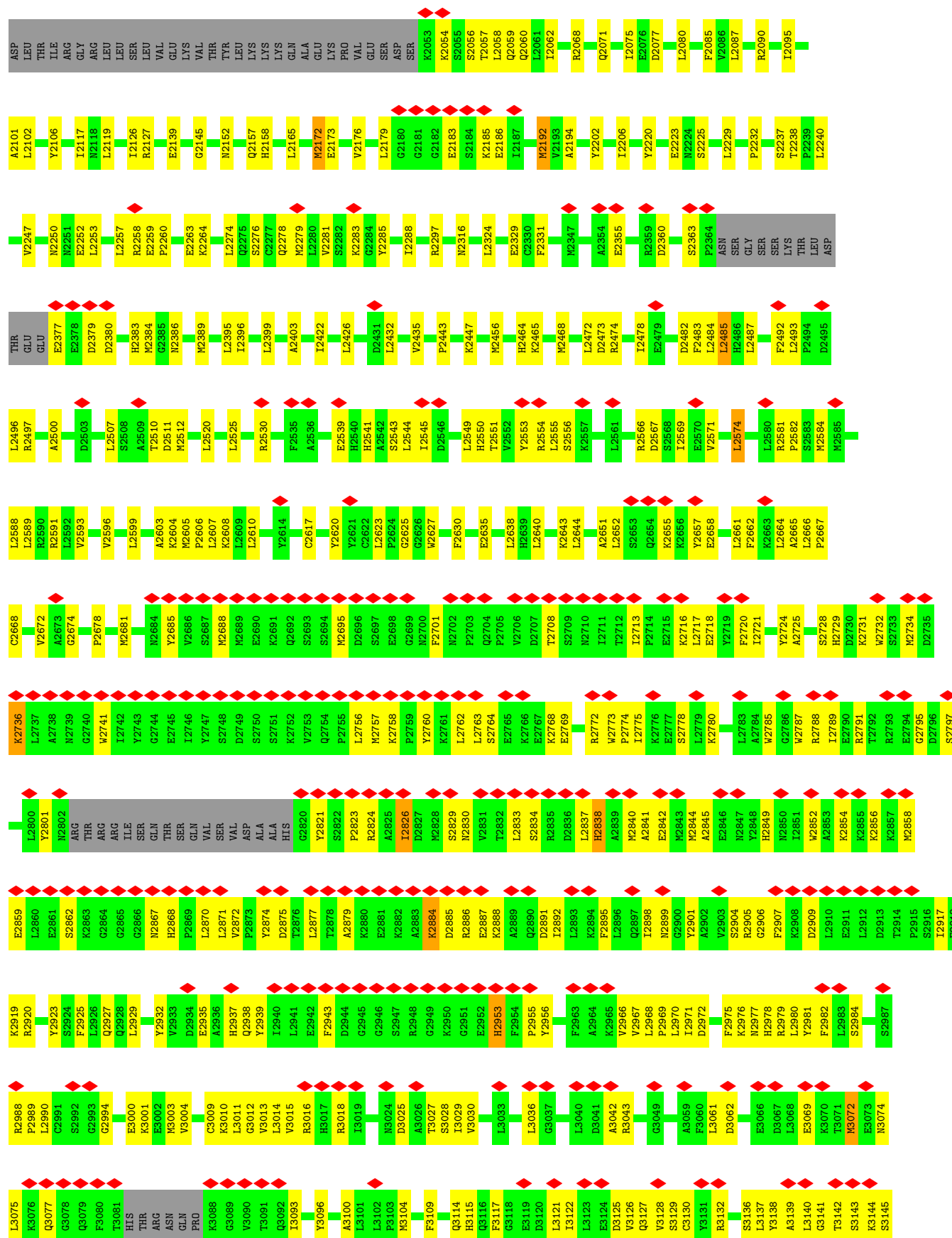
R4046	F9917	C3800	D3655	GLY	ILE	ARG	ASN	K3329	C3264	S3196	R3132	E3066	Y2981
D4047	N3918	L3805	E3656	ARG	ARG	LYS	PRO	A3330	C3265	L3197	S3136	D3067	F2982
F4048	T3919	N3806	G3657	ASN	ASN	MET	ALA	A3331	T3266	F3198	S3137	L3068	L2983
H4049	L3920		T3658	TYR	ILE	ARG	GLY	T3332	L3267	T3199	L3138	E3069	S2984
K4050	T3921		K3659	GLY	GLN	LYS	LEU	V3333	L3268	N3200	A3139	A2985	A2985
A4051	G3926		K3660	LEU	LEU	LEU	PHE	V3334	N3269	V3201	L3140	A2986	A2986
M4052			V3661	VAL	VAL	GLY	ASP	V3335	E3202	E3202	G3141	M3072	A2987
E4053	L3936		L3664	GLY	GLY	ARG	MET	E3336	D3203	D3203	T3142	N3074	R2988
S4054	L3940		H3665	PRO	PRO	TYR	VAL	E3337	S3270	V3204	L3143	P2989	P2989
H4055			I3668	GLN	ASP	GLY	ALA	ASP	E3271	C3205	S3143	K3075	L2990
K4056	V3945		E3684	SER	PRO	GLN	VAL	HIS	M3273	T3208	K3144	K3076	C2991
H4057			E3684	LYS	ALA	THR	VAL	LEU	L3276	P3209	S3145	Q3077	S2992
Q4060	Q3955		Y3691	LYS	ILE	SER	ILE	LYS	G3278	P3210	T3146	Q3078	G2993
E4064	K3957		K3697	ALA	ARG	LEU	TRP	ALA	N3279	E3210	Y3147	Q3079	G2994
F4065	L3958		H3700	VAL	GLN	TRP	ILE	ALA	L3280	L3211	E3148	F3080	H2995
E4071	D3961		D3701	TRP	GLN	VAL	SER	ALA	L3281	E3212	E3149	T3081	E3000
T4072	S3962		E3702	HIS	MET	ALA	LYS	ARG	K3282	K3213	Q3151	HIS	K3001
D4073	S3963		GLY	LYS	ALA	ALA	SER	GLY	I3283	L3214	R3152	THR	E3002
E4074	L3967		ASP	LEU	LEU	LEU	SER	ASP	I3284	M3215	S3153	ARG	K3003
M4075	L3968		ASP	LEU	LEU	LEU	ASN	MET	Y3285	E3216	A3154	ASN	V3004
E4076	K3969		GLY	LYS	LEU	LEU	PHE	SER	N3286	V3219	L3155	GLN	E3009
T4077	M3972		ASP	GLN	LEU	LEU	ARG	ALA	N3287	E3222	E3157	PRO	K3010
L4078	D3973		ASP	ARG	PRO	PRO	GLY	GLY	L3288	A3222	E3158	K3088	L3011
D4079	L3974		GLY	LYS	ARG	GLY	ILE	LEU	G3289	L3159	G3159	G3089	G3012
Y4080	Q3975		GLY	ALA	THR	THR	ASN	ILE	I3290	A3160	A3160	V3090	V3013
F4081	K3976		ASP	ASP	ASP	ASP	PHE	ASP	D3291	G3225	A3161	Q3091	L3014
E4082	D3977		GLY	ILE	THR	THR	VAL	ASP	G3292	I3226	F3162	Q3092	V3015
R4086	V3980		E3710	V3599	ASP	THR	VAL	GLU	G3293	R3227	A3163	I3083	R3016
D4093	M3985		E3711	V3600	THR	THR	GLN	LEU	A3294	Y3228	G3164	Y3096	H3017
I4094	S4006		E3716	A3601	SER	ASP	ALA	THR	M3295	T3229	A3165	Y3097	R3018
E4107	L4014		E3718	R3604	PRO	GLY	GLY	LEU	K3297	M3231	F3166	A3100	I3019
A4122	F4015		M3719	M3605	GLY	ILE	ILE	ALA	F3302	P3232	P3167	L3101	F3022
Y4128	F4016		Q3727	A3606	VAL	GLY	GLN	ASP	S3303	M3235	V3168	L3102	G3023
I4136	L4021		A3729	P3607	VAL	VAL	LEU	ALA	Q3304	E3236	A3169	P3103	G3024
R4147	F4032		H3732	L3608	ASP	LEU	LEU	PHE	P3306	V3237	F3170	M3104	N3024
F4150	E4034		A3736	P3612	ASP	LEU	ILE	THR	I3307	L3239	E3172	F3109	A3026
F4172	D4036		T3743	R3615	ILE	ASN	ASN	PRO	N3308	P3240	T3173	H3111	T3027
V4177	P4037		M3754	E3625	ALA	ARG	LYS	LEU	K3309	M3241	H3174	V3110	S3028
G4181	D4038		T3758	W3628	ALA	ASN	PHE	LEU	V3310	S3247	L3175	Q3114	I3029
E4182	G4039		I3765	I3629	VAL	VAL	SER	ILE	K3311	M3246	D3176	H3115	V3030
K4183	K4041		M3777	E3633	PHE	LEU	LEU	ARG	P3312	R3248	K3177	Q3116	L3036
E4187	I4043		L3778	D3638	LYS	LEU	THR	PHE	Q3313	W3249	H3178	F3117	Q3038
L4188	S4044		L3796	A3649	HIS	GLY	LYS	VAL	L3314	M3250	E3119	G3118	T3039
F4189	K4045			P3651	LEU	GLU	ALA	ASP	K3315	E3251	D3120	E3121	L3040
				P3652	GLN	GLY	ASN	ASP	K3316			D3121	L3041
				E3653	LYS	VAL	VAL	ALA	T3317	P3254	Y3184	I3122	A3042
				E3654	SER	ARG	SER	ASP	H3318	E3255	N3185	L3123	R3043
					LYS	ARG	GLN	TRP	F3319	N3256	T3186	E3124	
					VAL	ARG	GLY	LEU	L3320	M3257	K3187	D3125	T3048
									M3323	P3258	S3188	V3126	G3049
									K3324	E3259	S3189	Q3127	
									K3325	R3260	R3190	V3128	
									L3326	A3261	E3191	S3129	L3061
									K3327	E3262	R3192	C3130	D3062
									K3328	M3263	A3193	Y3131	A3065



• Molecule 2: Ryanodine receptor 2



Y670	K671	K672	W673	Y674	Y675	E676	L677	W678	D680	H682	V695	A698	Y703	G709	W713	G717	V718	F723	F727	I737	D752	I755	S756	F768	R769	P774	V775	M778	F779	E780	F788	F789	P790	V791	V792	S793	V800	R801	F802	L803																		
H808	L814	P815	P816	Y819	E824	L832	H836	E839	Y840	K841	Q842	E843	R844	L851	G852	P853	S856	L857	T858	Q859	A860	P866	T869	L874	P875	P876	H877	L878	E879	R880	I881	R882	E883	K884	E887	N888	I889	H890	E891	L892	W893	V894	M895	H896	K897	I898	E899											
W902	Q903	Y904	G905	P906	V907	R908	D909	N910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	N931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960
V961	K962	M963	K964	K965	L966	P967	K968	N969	Y970	Q971	L972	T973	S974	G975	K976	P978	A979	D982	L983	I986	Q992	V996	D997	K998	L999	N1002	V1006	W1007	A1008	R1009	D1010	R1011	Q1014	G1015	W1016	T1020	Q1021	Q1022	R1027	R1028	N1029	P1030	R1031	I1035	T1036	L1037	L1038	D1039										
D1040	R1041	T1042	K1043	K1044	S1045	M1046	D1047	S1049	L1050	R1051	E1052	R1055	Y1062	L1063	L1064	E1065	A1066	D1067	Q1069	D1070	H1071	A1072	A1073	R1074	A1075	E1076	V1077	C1078	S1079	G1080	T1081	G1082	E1083	R1086	R1100	W1101	Y1102	E1106	R1114	S1118	R1119	L1128	G1129	A1134	K1141	A1142	Q1143											
R1144	W1145	E1150	R1154	M1165	E1180	L1181	L1182	L1183	D1184	D1185	S1188	A1191	D1194	F1195	D1196	D1199	V1204	R1214	E1234	F1239	N1242	M1249	W1250	L1251	P1262	H1265	E1266	H1267	I1268	R1272	L1273	I1277	D1278	C1282	L1283	G1291	S1292	Q1293	N1294																			
S1295	N1296	R1303	K1316	THR	VAL	ALA	GLY	GLY	PRO	GLY	ALA	GLY	LEU	PHE	GLY	PRO	LYS	ASN	ASP	GLU	ASP	TYR	ASP	ALA	ASP	ASP	PHE	GLU	VAL	LEU	MET	LYS	THR	THR	ALA	HIS	HIS	GLY	HIS	LEU	VAL	PRO	ASP	ARG	VAL	ASP	LYS	LYS	GLU	ALA	LYS	PRO	GLU	PHE				
ASN	ASN	HIS	LYS	ASP	TYR	ALA	GLN	GLU	PRO	LYS	SER	ARG	LEU	GLN	PHE	LEU	ARG	THR	LYS	PRO	ASP	TYR	THR	SER	HIS	SER	ALA	ARG	LEU	THR	ASP	R1414	D1415	D1416	Y1417	D1418	F1419	L1420	M1421	Q1422	Y1427	Y1428	R1431	Q1436														
M1440	G1444	I1446	R1461	D1471	E1472	K1473	K1474	K1475	M1487	E1492	S1493	M1494	S1495	P1496	G1497	Q1498	G1499	R1500	M1501	N1502	N1503	G1504	L1505	S1515	Q1532	W1533	E1534	A1542	Q1546	S1549	P1550	M1551	V1552	F1553	G1554	F1555	E1556	R1559	M1562	V1563	M1564	P1565	K1576	P1578														
C1582	R1585	F1590	L1591	S1592	M1599	P1600	E1602	F1603	V1608	I1611	R1614	Q1615	L1618	L1630	P1633	E1634	L1644	E1649	L1650	L1651	S1662	L1667	R1671	S1678	D1681	E1682	L1685	M1694	P1695	G1696	L1697	L1698	R1699	Y1702	Y1703	M1664	P1665	K1676	P1677	L1706	I1707																	
D1708	S1712	A1717	R1718	L1719	M1720	N1722	Y1725	E1731	N1743	K1744	K1745	L1757	P1766	S1767	F1768	E1774	P1780	K1788	L1795	L1804	H1805	A1806	R1807	V1810	E1815	L1817	F1818	V1819	L1821	L1824	T1827	L1828	L1829	I1830	I1833	F1834	L1839																					
I1842	Q1843	L1844	I1845	I1846	E1847	V1850	F1851	L1852	E1853	A1854	THR	PRO	GLU	GLU	SER	THR	LEU	GLU	LYS	GLU	LEU	GLN	GLY	ALA	GLY	GLY	GLU	GLU	GLU	LYS	GLY	ARG	P1889	K1890	Q1895	L1898	V1902	L1910	D1915	F1932																		
Q1937	R1943	H1946	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	L1956	T1957	T1958	A1959	R1960	K1961	T1962	K1963	E1964	F1965	R1966	S1967	P1968	Q1972	I1973	F1979	D1982	K1983	S1984	E1985	E1990	E1991	I1992	R1993	D1994	Q1995	L1996	L2003	M2004	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	SER								





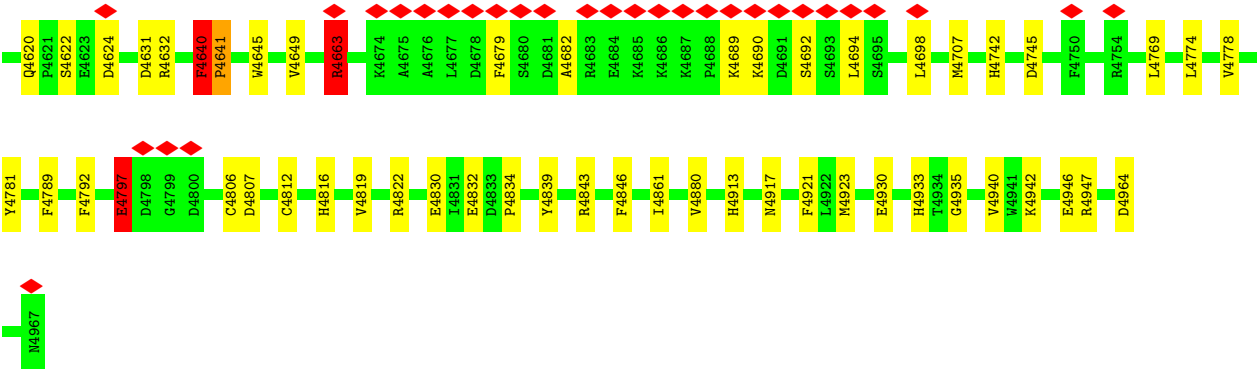






V3204	K3144	E3073	S2984	I2917	K2857	G2795	S2733	L2666	M2585	H2486	L2487	L26250
C3205	S3145	N3074	S2987	E2918	M2858	D2796	M2734	P2667	L2588	L2487	L2487	M2250
I3208	I3147	K3076	R2888	R2920	E2859	S2797	D2735	C2668	L2589	F2492	F2492	M2251
P3209	V3148	Q3077	P2889	R2920	L2860	L2800	K2736	V2672	R2590	L2493	L2493	L2253
S3210	E3149	G3078	L2990	S2994	E2861	Y2801	L2737	A2673	R2591	P2494	P2494	L2257
L3211	R3150	Q3079	C2991	F2925	K2862	N2802	L2738	G2674	R2592	D2495	D2495	R2258
E3212	Q3151	F3080	G2992	Q2927	K2863	ARG	M2739	A2675	V2593	L2496	L2496	P2260
K3213	S3152	F3081	G2993	Q2928	D2864	THR	Q2740	P2678	V2596	R2497	R2497	E2259
M3215	A3154	T3081	G2994	L2929	G2865	ARG	M2741	M2681	L2599	A2500	A2500	E2263
E3216	L3155	HIS	E3000	Y2932	G2866	ILE	L2742		L2589			K2264
V3219	K3001	THR	K3001	Y2932	N2867	SER	Y2743		A2603	D2503	D2503	L2274
A3222	E3002	ARG	E3002	E2935	H2868	GLN	Q2744		M2604	L2507	L2507	Q2275
E3223	M3003	GLN	M3003	E2935	P2869	THR	E2745		M2605	S2508	S2508	S2276
S3224	V3004	PRO	V3004	A2936	L2870	SER	L2746		P2606	L2509	L2509	C2277
G3225	C3009	K3088	C3009	H2937	L2871	GLN	Q2747		L2607	T2510	T2510	Q2278
G3226	K3010	G3089	K3010	Q2938	P2872	VAL	S2748		M2608	D2511	D2511	R2279
I3227	L3011	V3090	L3011	Y2939	P2873	VAL	Q2749		M2689	L2609	L2609	V2281
A3163	G3012	T3091	G3012	I2940	Y2874	ASP	S2750		K2691	M2512	M2512	S2282
G3164	V3013	Q3092	V3013	L2941	D2875	ALA	S2751		Q2692	L2520	L2520	K2283
A3165	L3014	I3093	L3014	E2942	T2876	ALA	Q2752		S2693	L2525	L2525	G2284
F3166	V3015	Y3096	V3015	F2943	L2877	HIS	P2753		S2694	R2530	R2530	Y2285
F3167	R3016	T3097	R3016	D2944	T2878		Q2754		M2695	A2536	A2536	P2286
V3168	H3017	G2945	H3017	G2945	K2879		P2755		Y2620	L2426	L2426	D2287
A3169	R3018	G2946	R3018	G2946	A2880		L2756		Y2621	D2431	D2431	L2288
F3170	I3019	S2947	I3019	S2947	E2881		K2757		P2694	L2432	L2432	R2297
L3171	N3024	R2948	N3024	R2948	K2882		K2758		H2540	V2436	V2436	N2316
E3172	D3025	G2949	D3025	G2949	A2883		P2759		G2625	L2542	L2542	R2302
T3173	K3026	K2950	K3026	K2950	K2884		Y2760		M2627	S2543	S2543	L2323
H3174	A3026	G2951	A3026	G2951	D2885		Q2761		F2630	L2544	L2544	L2324
L3175	T3027	E2952	T3027	E2952	R2886		L2762		E2635	L2545	L2545	E2329
D3176	S3028	H2953	S3028	H2953	K2887		P2703		L2638	D2546	D2546	C2330
K3177	I3029	F2954	I3029	F2954	E2887		Q2705		H2639	L2549	L2549	F2331
N3178	V3030	P2955	V3030	P2955	L2832		S2764		L2640	T2551	T2551	E2336
I3179	L3036	Y2956	L3036	Y2956	Y2833		E2765		M2456	Y2552	Y2552	Q2337
I3180	L3040	E2957	L3040	E2957	L2833		K2766		H2464	R2554	R2554	E2338
Y3181	D3041	K2961	D3041	K2961	R2835		E2767		K2465	L2555	L2555	V2347
D3182	A3042	A2964	A3042	A2964	D2836		E2769		M2468	L2556	L2556	A2354
I3183	R3043	K2965	R3043	K2965	L2837		R2772		L2472	D2566	D2566	E2355
N3185	M3046	V2966	M3046	V2966	H2838		Q2773		R2567	L2569	L2569	R2359
K3187	G3049	V2967	G3049	V2967	A2839		P2774		R2564	E2570	E2570	D2360
S3188	S3129	L2968	S3129	L2968	M2840		L2775		Q2654	L2571	L2571	S2363
S3189	C3130	P2969	C3130	P2969	A2841		K2776		K2655	L2574	L2574	P2364
R3190	A3059	L2970	A3059	L2970	E2842		E2777		L2473	R2568	R2568	ASN
E3191	F3060	L2971	F3060	L2971	M2844		S2778		R2474	S2569	S2569	GLY
R3192	L3061	D2972	L3061	D2972	A2845		L2779		T2478	V2571	V2571	SER
A3193	D3062	F2975	D3062	F2975	E2846		K2780		E2479	L2574	L2574	
I3194	E3066	K2976	E3066	K2976	N2847		L2783		D2482	R2581	R2581	
L3195	D3067	N2977	D3067	N2977	Y2848		A2784		F2483	L2484	L2484	
S3196	L3068	H2978	L3068	H2978	H2849		Q2785		L2664	S2582	S2582	
L3197	E3069	R2979	E3069	R2979	Y2852		Q2786		S2583	M2584	M2584	
P3198	K3070	L2980	K3070	L2980	A2853		K2787					
T3199	Y2981	Y2981	Y2981	Y2981	K2854		R2788					
N3200	F2982	L2982	F2982	L2982	K2855		I2789					
E3201	S3071	P2982	S3071	P2982	K2856		E2790					
E3202	M3072	L2983	M3072	L2983			K2791					
D3203							L2792					
							K2793					
							E2794					





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94476	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	0.590	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.028	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	E	0.31	0/834	0.59	1/1123 (0.1%)
1	F	0.31	0/834	0.60	1/1123 (0.1%)
1	G	0.30	0/834	0.59	1/1123 (0.1%)
1	H	0.31	0/834	0.59	1/1123 (0.1%)
2	A	0.26	0/34511	0.53	15/46614 (0.0%)
2	B	0.26	0/34511	0.53	15/46614 (0.0%)
2	C	0.26	0/34511	0.53	15/46614 (0.0%)
2	D	0.26	0/34511	0.53	14/46614 (0.0%)
All	All	0.26	0/141380	0.53	63/190948 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4	GLU	CA-CB-CG	8.33	131.72	113.40
1	G	4	GLU	CA-CB-CG	8.31	131.68	113.40
1	H	4	GLU	CA-CB-CG	8.31	131.68	113.40
1	E	4	GLU	CA-CB-CG	8.30	131.66	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2736	LYS	CD-CE-NZ	-7.74	93.90	111.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1009	ARG	Sidechain
2	A	4640	PHE	Peptide
2	B	1009	ARG	Sidechain
2	D	1009	ARG	Sidechain
2	D	4640	PHE	Peptide

## 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	15	0
1	F	818	0	821	16	0
1	G	818	0	821	16	0
1	H	818	0	821	17	0
2	A	33771	0	33455	816	0
2	B	33771	0	33455	808	0
2	C	33771	0	33455	811	0
2	D	33771	0	33455	819	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
All	All	138608	0	137200	3223	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 3223 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:C:4663:ARG:HG2	2:C:4663:ARG:HH11	1.37	0.90
2:D:4797:GLU:N	2:D:4797:GLU:OE1	2.07	0.88
2:B:2830:ASN:HB3	2:C:1549:SER:HB2	1.55	0.88
2:C:4797:GLU:OE1	2:C:4797:GLU:N	2.07	0.88
2:B:4797:GLU:OE1	2:B:4797:GLU:N	2.07	0.88

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%)	103 (98%)	2 (2%)	0	100	100
1	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	A	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	48	78
2	B	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	48	78
2	C	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	48	78
2	D	4198/4967 (84%)	4050 (96%)	144 (3%)	4 (0%)	48	78
All	All	17212/20300 (85%)	16618 (96%)	578 (3%)	16 (0%)	50	78

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2988	ARG
2	A	3292	GLU
2	A	4641	PRO
2	D	2988	ARG

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Mol	Chain	Res	Type
2	D	3292	GLU

### 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	60
1	F	88/89 (99%)	85 (97%)	3 (3%)	32	60
1	G	88/89 (99%)	85 (97%)	3 (3%)	32	60
1	H	88/89 (99%)	85 (97%)	3 (3%)	32	60
2	A	3708/4358 (85%)	3675 (99%)	33 (1%)	75	87
2	B	3708/4358 (85%)	3675 (99%)	33 (1%)	75	87
2	C	3708/4358 (85%)	3675 (99%)	33 (1%)	75	87
2	D	3708/4358 (85%)	3675 (99%)	33 (1%)	75	87
All	All	15184/17788 (85%)	15040 (99%)	144 (1%)	74	87

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	929	ARG
2	C	4797	GLU
2	C	1421	MET
2	C	2838[B]	HIS
2	D	844	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	4936	GLN
2	C	4936	GLN
2	B	2540	HIS
2	C	4579	HIS

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Mol	Chain	Res	Type
2	C	2830	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	$\# Z  > 2$
4	ATP	C	5003	-	28,33,33	0.61	0	34,52,52	0.59	1 (2%)
4	ATP	D	5002	-	28,33,33	0.62	0	34,52,52	0.67	1 (2%)
4	ATP	C	5002	-	28,33,33	0.63	0	34,52,52	0.67	1 (2%)
4	ATP	A	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	B	5003	-	28,33,33	0.61	0	34,52,52	0.60	1 (2%)
4	ATP	B	5002	-	28,33,33	0.63	0	34,52,52	0.67	1 (2%)
4	ATP	A	5002	-	28,33,33	0.62	0	34,52,52	0.67	1 (2%)
4	ATP	D	5003	-	28,33,33	0.61	0	34,52,52	0.59	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
4	ATP	C	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	9/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5002	ATP	C5-C6-N6	2.34	123.88	120.31
4	A	5002	ATP	C5-C6-N6	2.34	123.87	120.31
4	C	5003	ATP	C5-C6-N6	2.33	123.86	120.31
4	B	5002	ATP	C5-C6-N6	2.32	123.84	120.31
4	B	5003	ATP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	O4'-C4'-C5'-O5'
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	O4'-C4'-C5'-O5'
4	D	5003	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

8 monomers are involved in 8 short contacts:

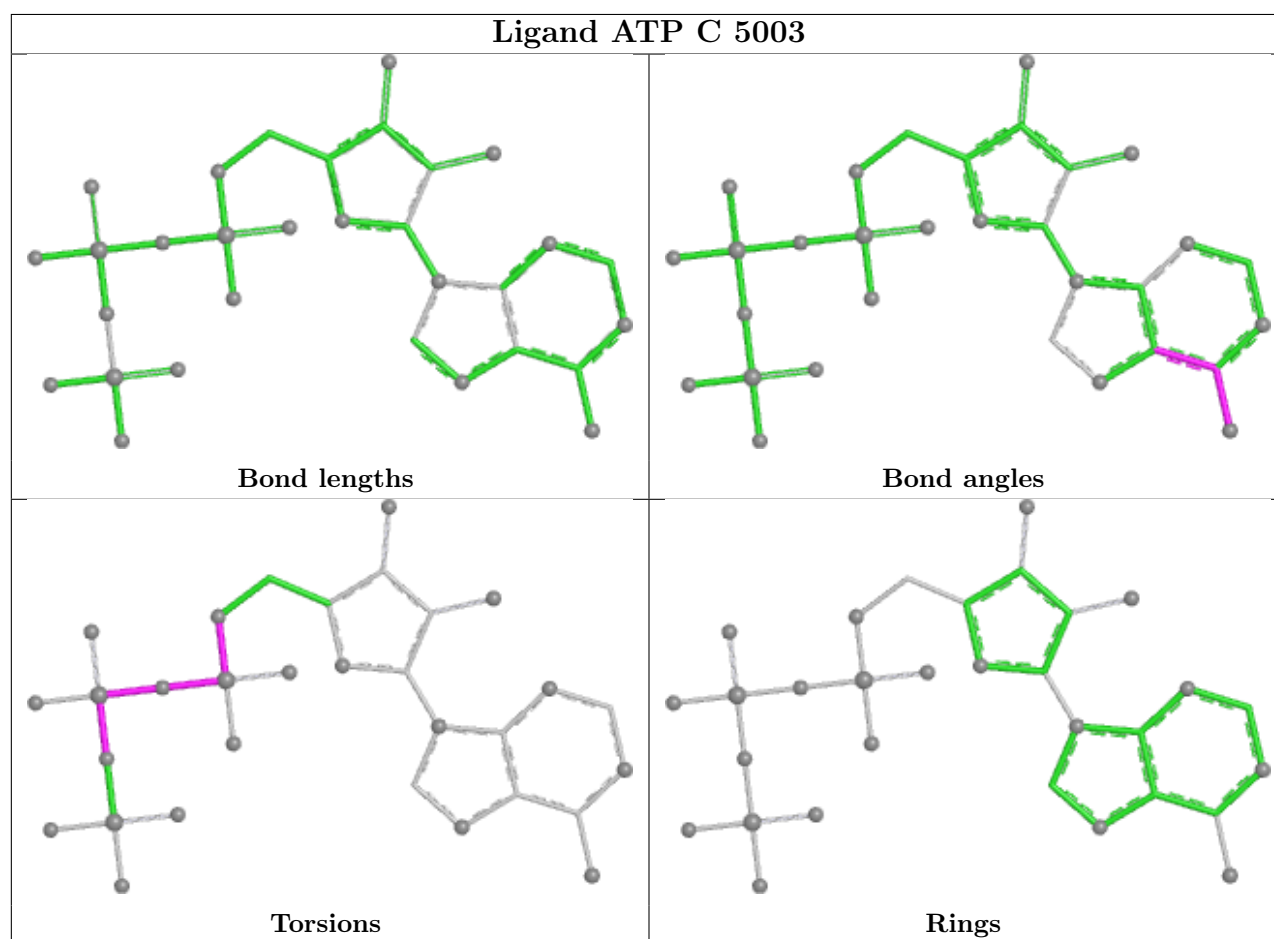
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5003	ATP	1	0
4	D	5002	ATP	1	0
4	C	5002	ATP	1	0
4	A	5003	ATP	1	0

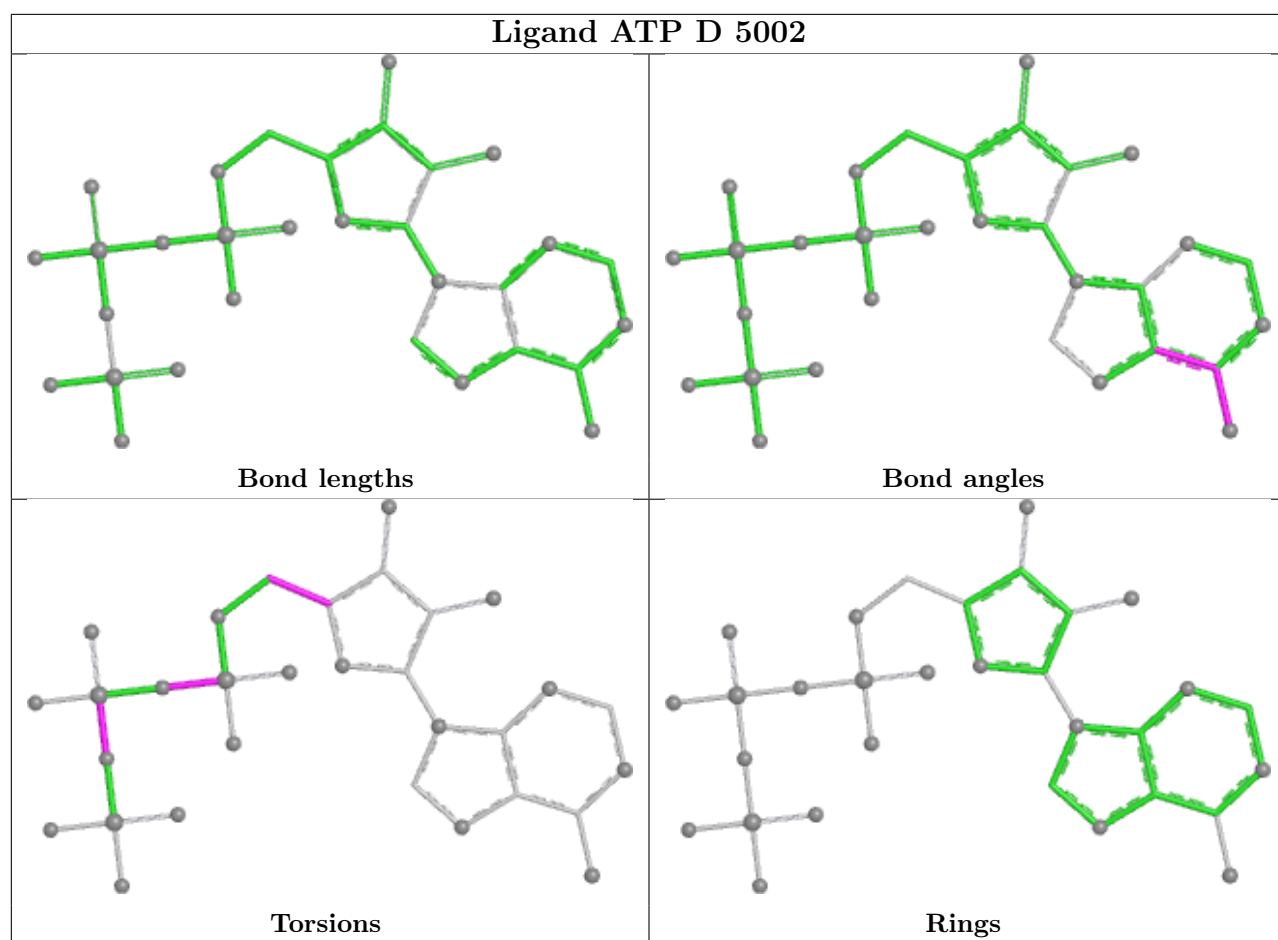
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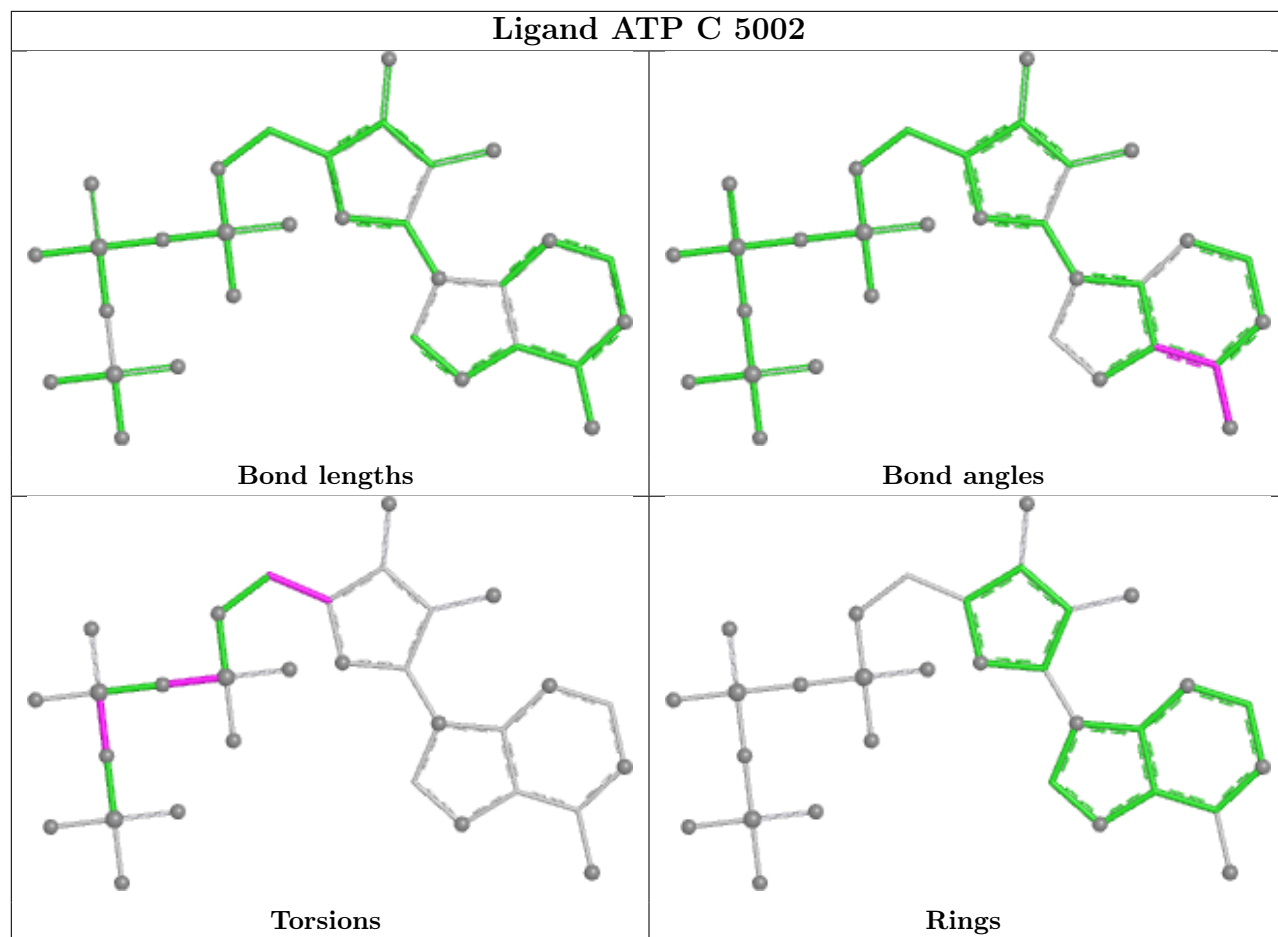
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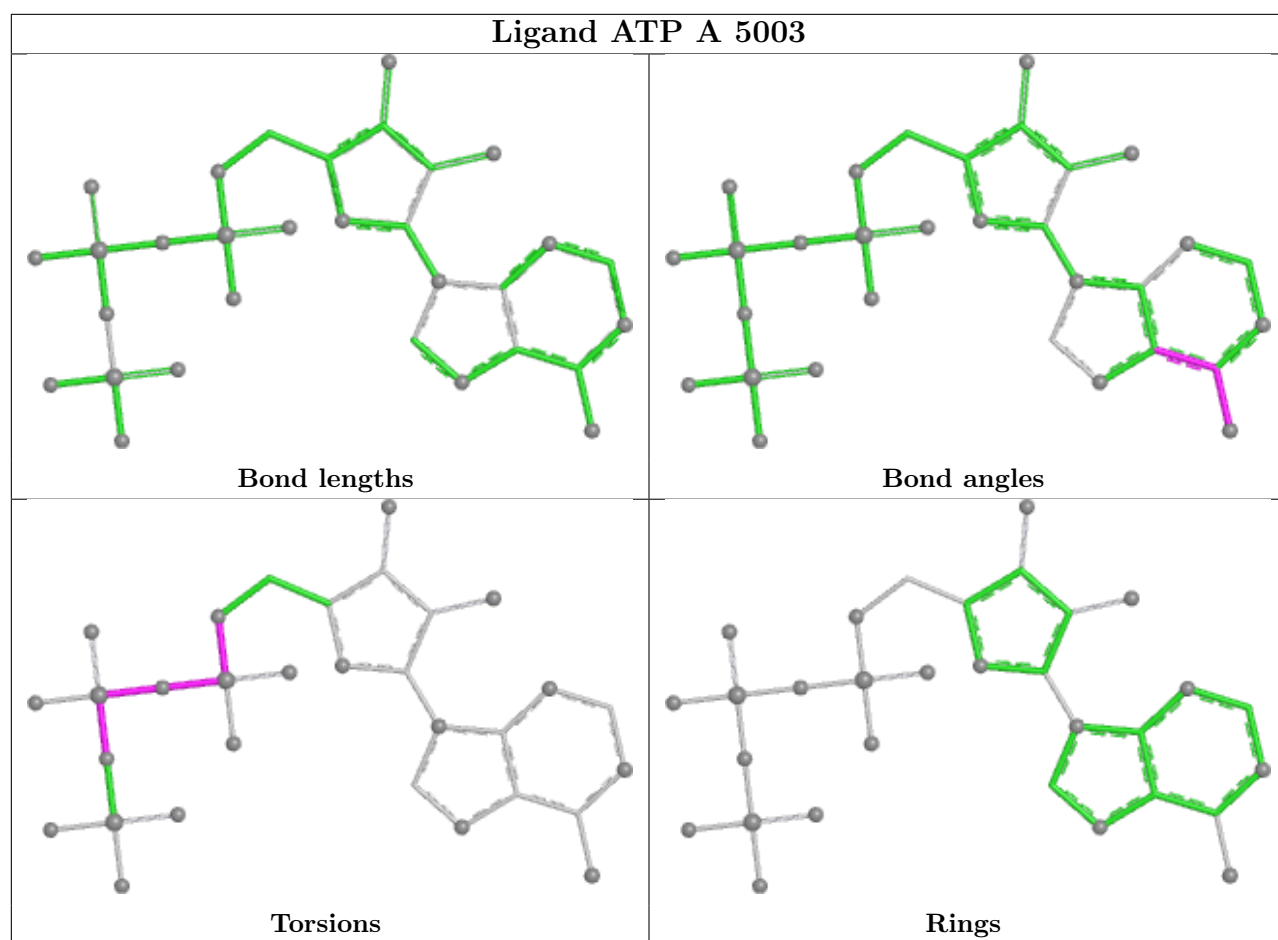
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5003	ATP	1	0
4	B	5002	ATP	1	0
4	A	5002	ATP	1	0
4	D	5003	ATP	1	0

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

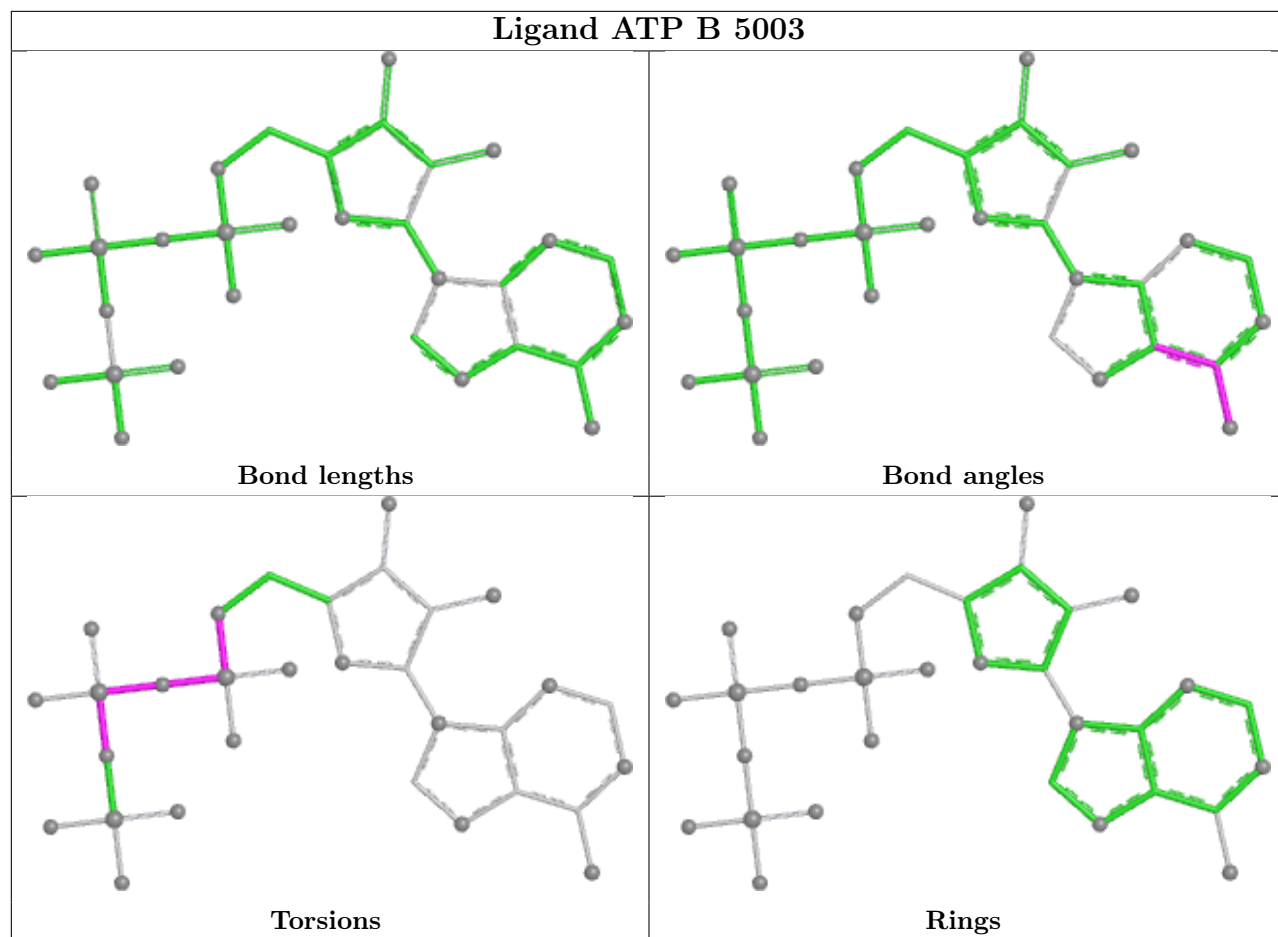


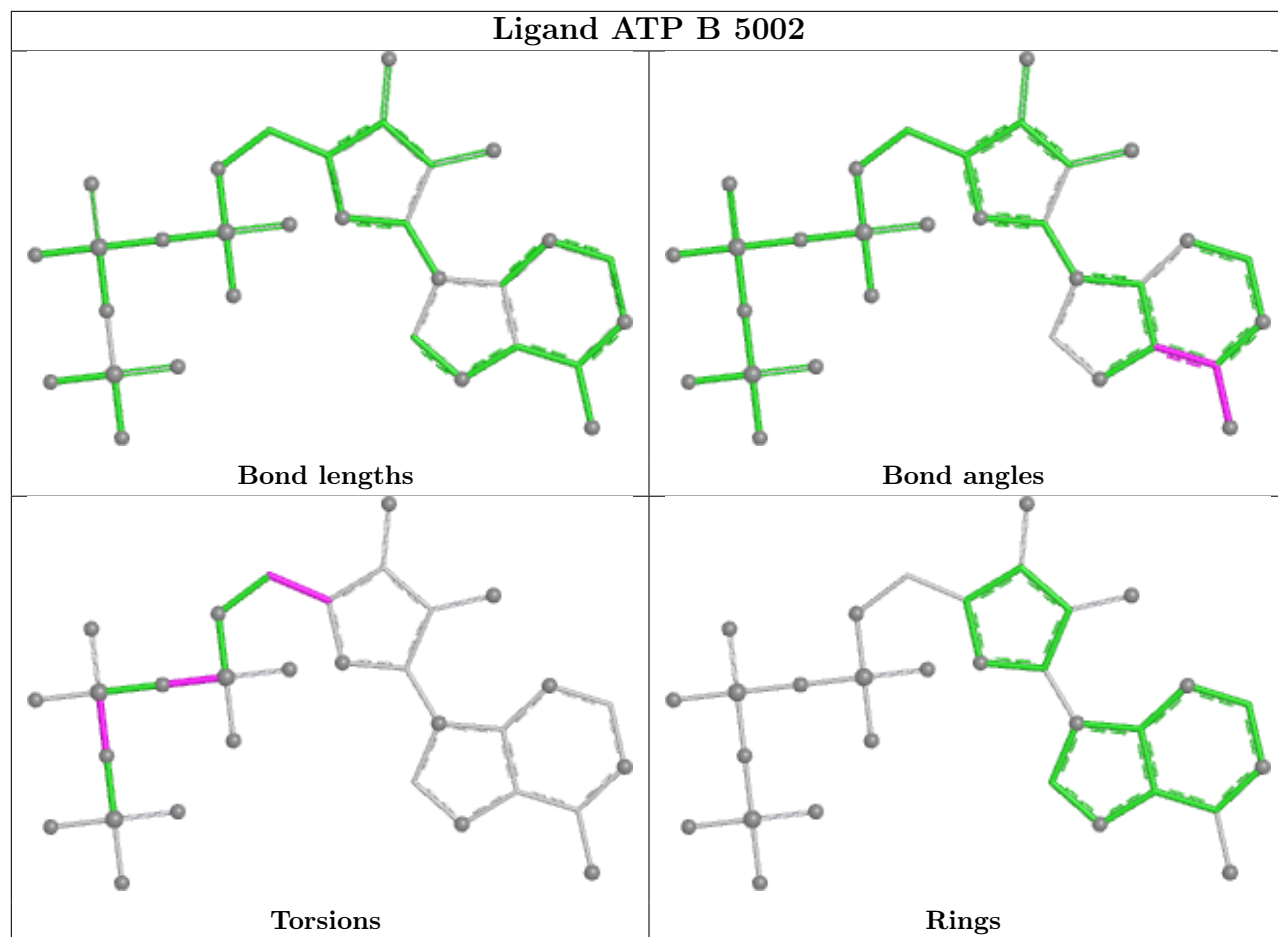


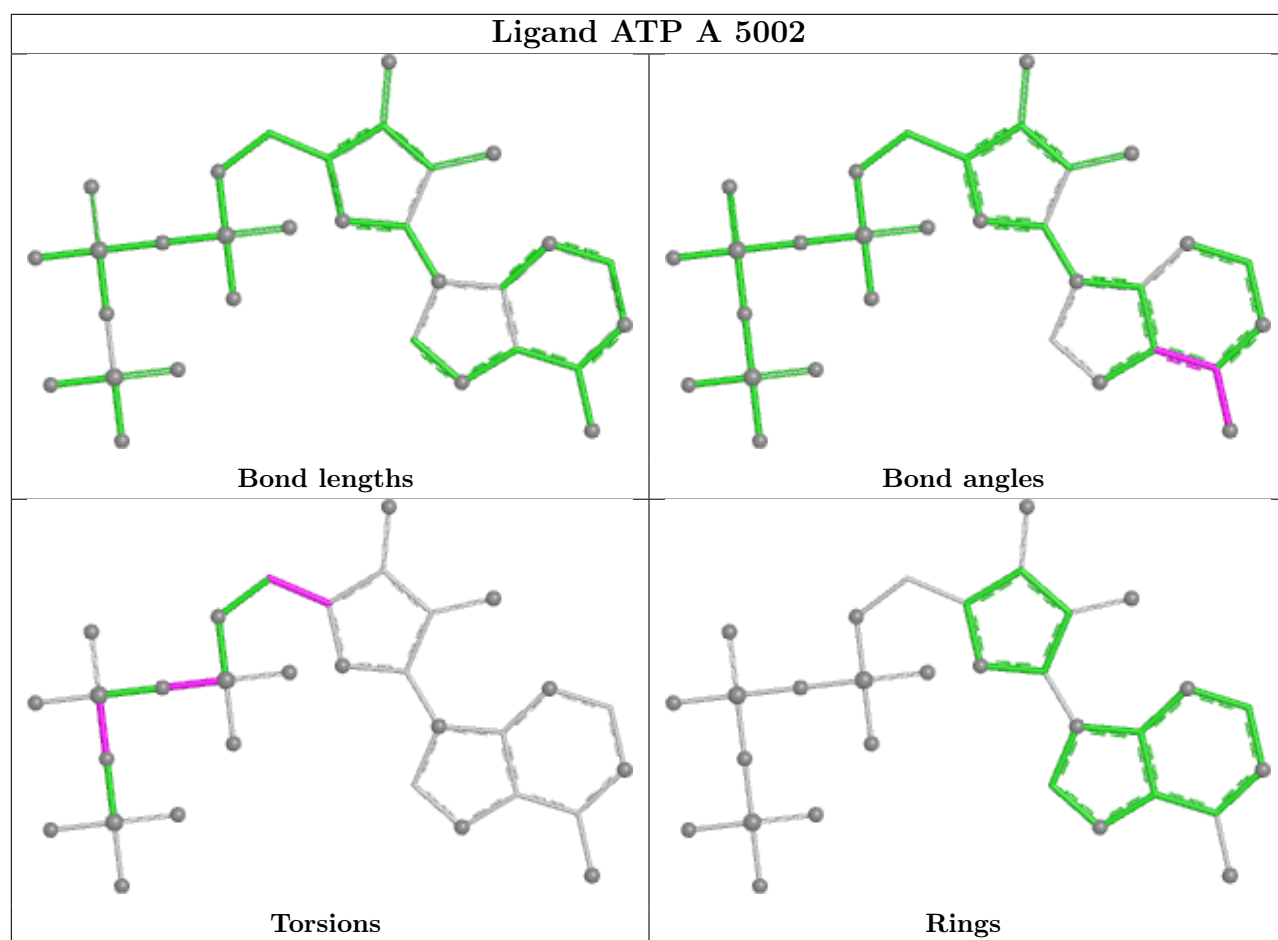


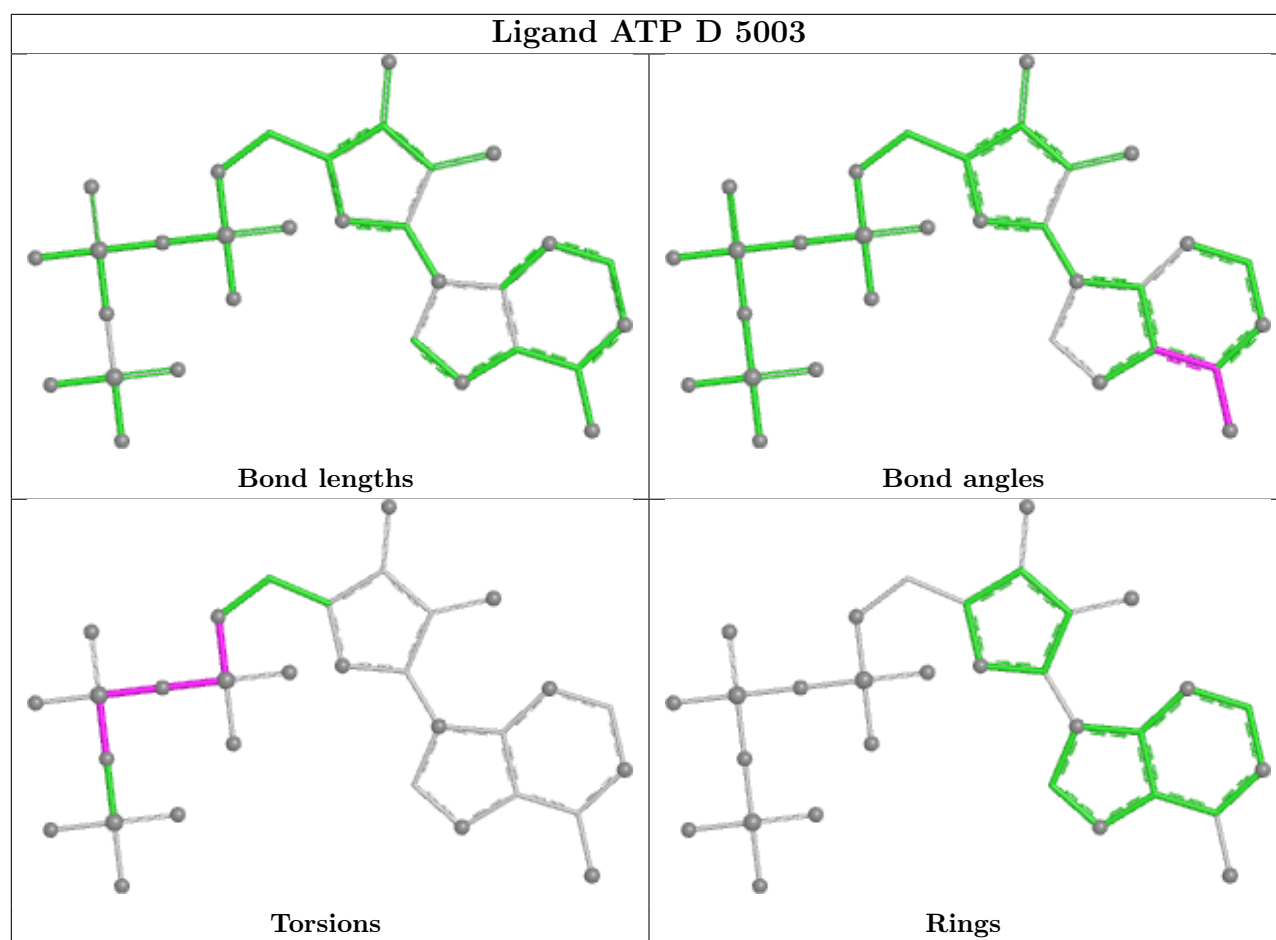












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

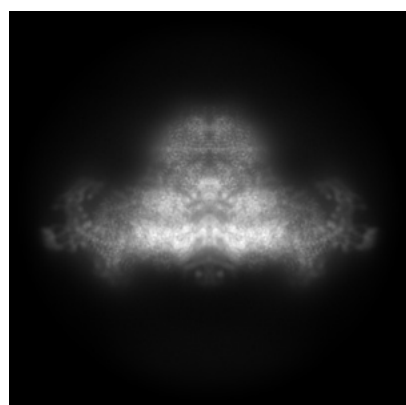
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26405. These allow visual inspection of the internal detail of the map and identification of artifacts.

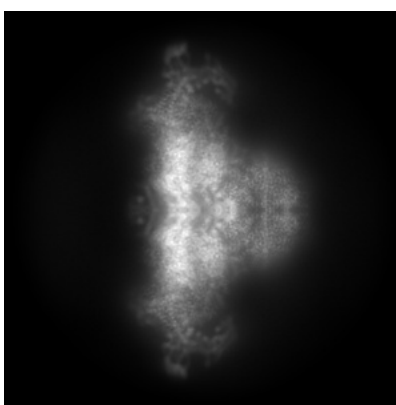
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

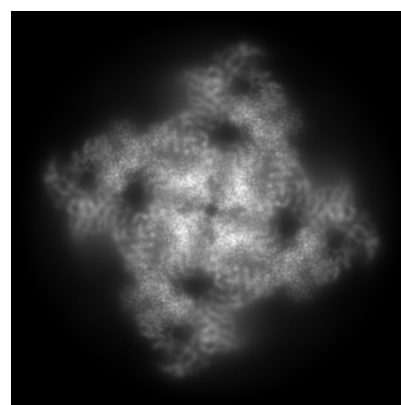
#### 6.1.1 Primary map



X



Y

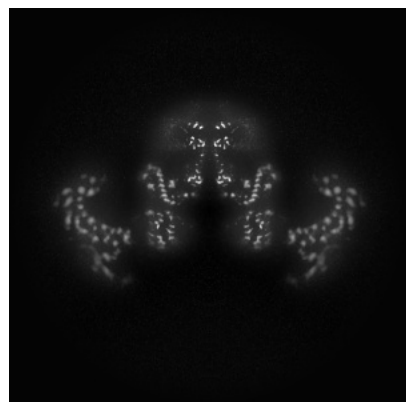


Z

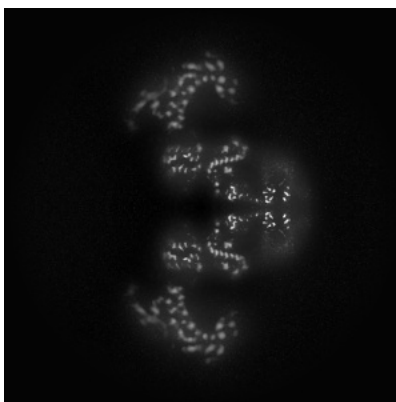
The images above show the map projected in three orthogonal directions.

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

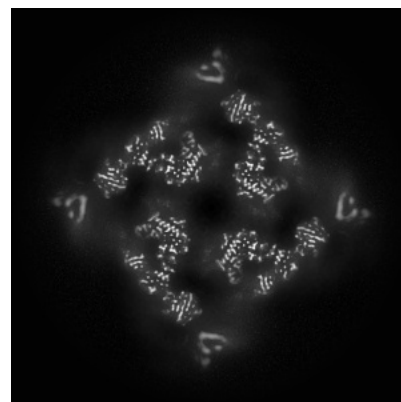
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

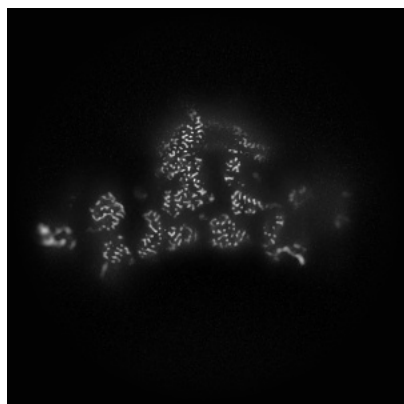


Z Index: 256

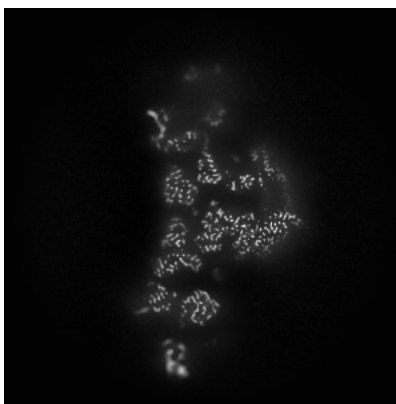
The images above show central slices of the map in three orthogonal directions.

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

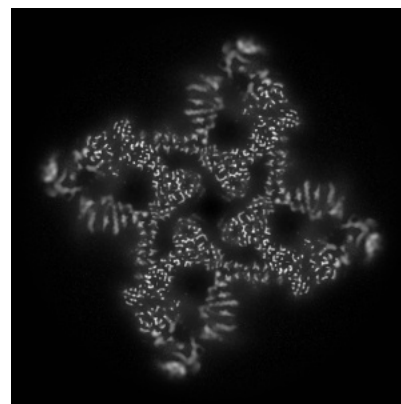
### 6.3.1 Primary map



X Index: 219



Y Index: 293

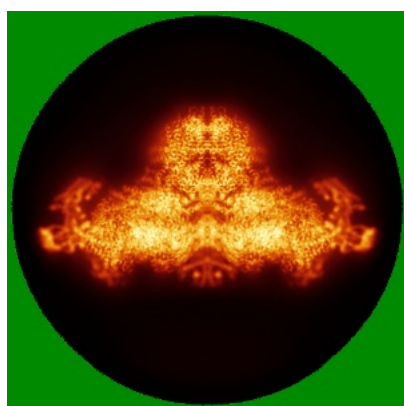


Z Index: 224

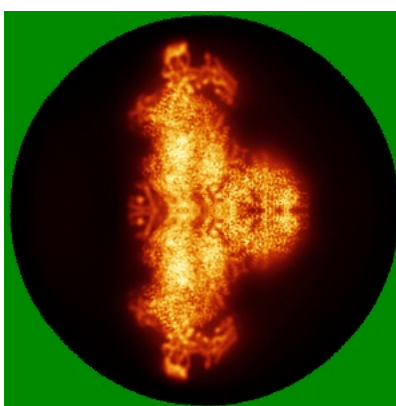
The images above show the largest variance slices of the map in three orthogonal directions.

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

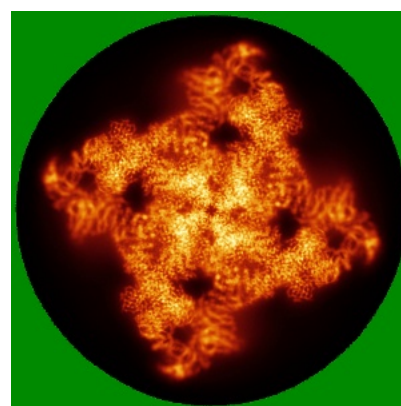
### 6.4.1 Primary map



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.

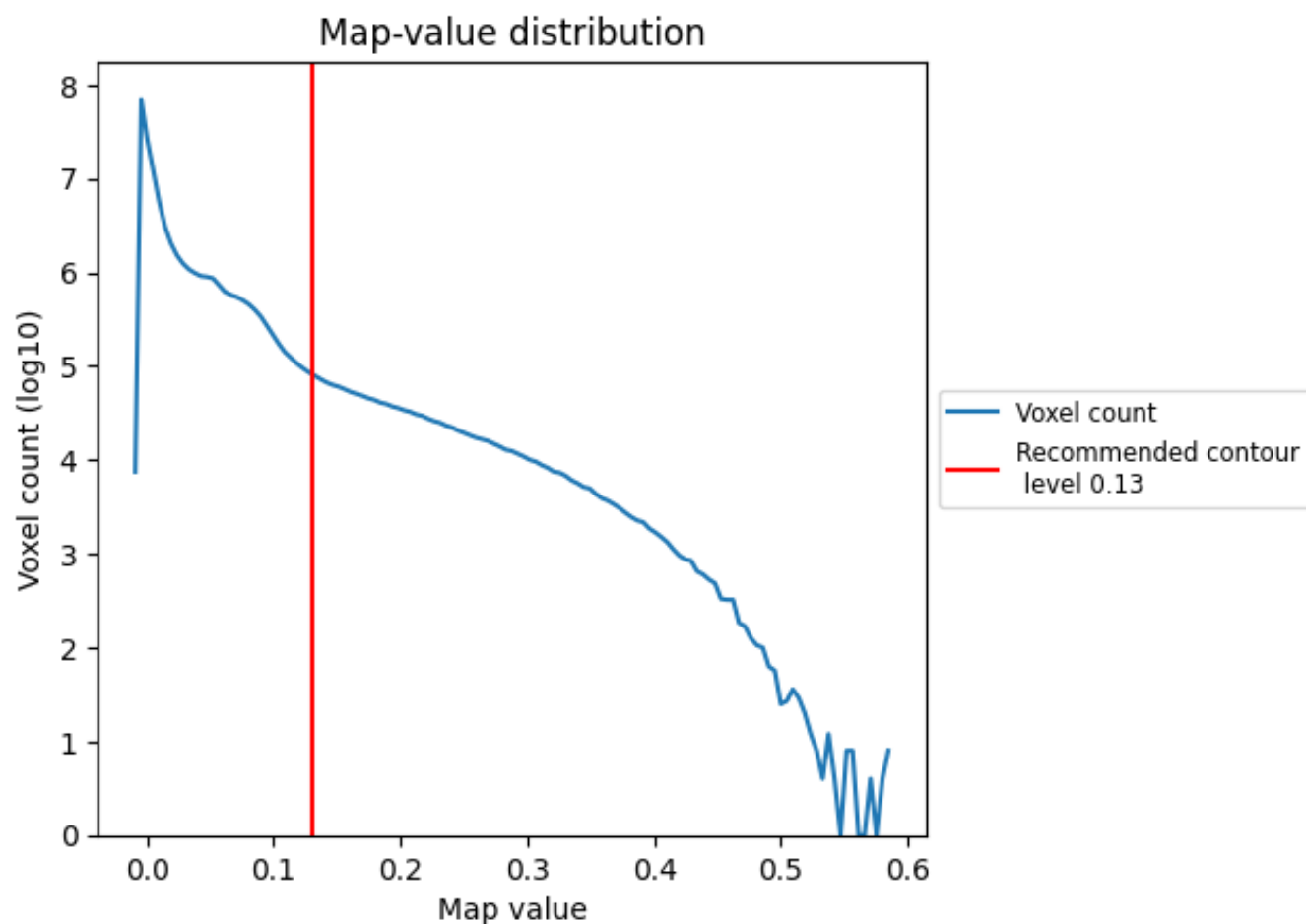
## 6.6 Mask visualisation [i](#)

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.

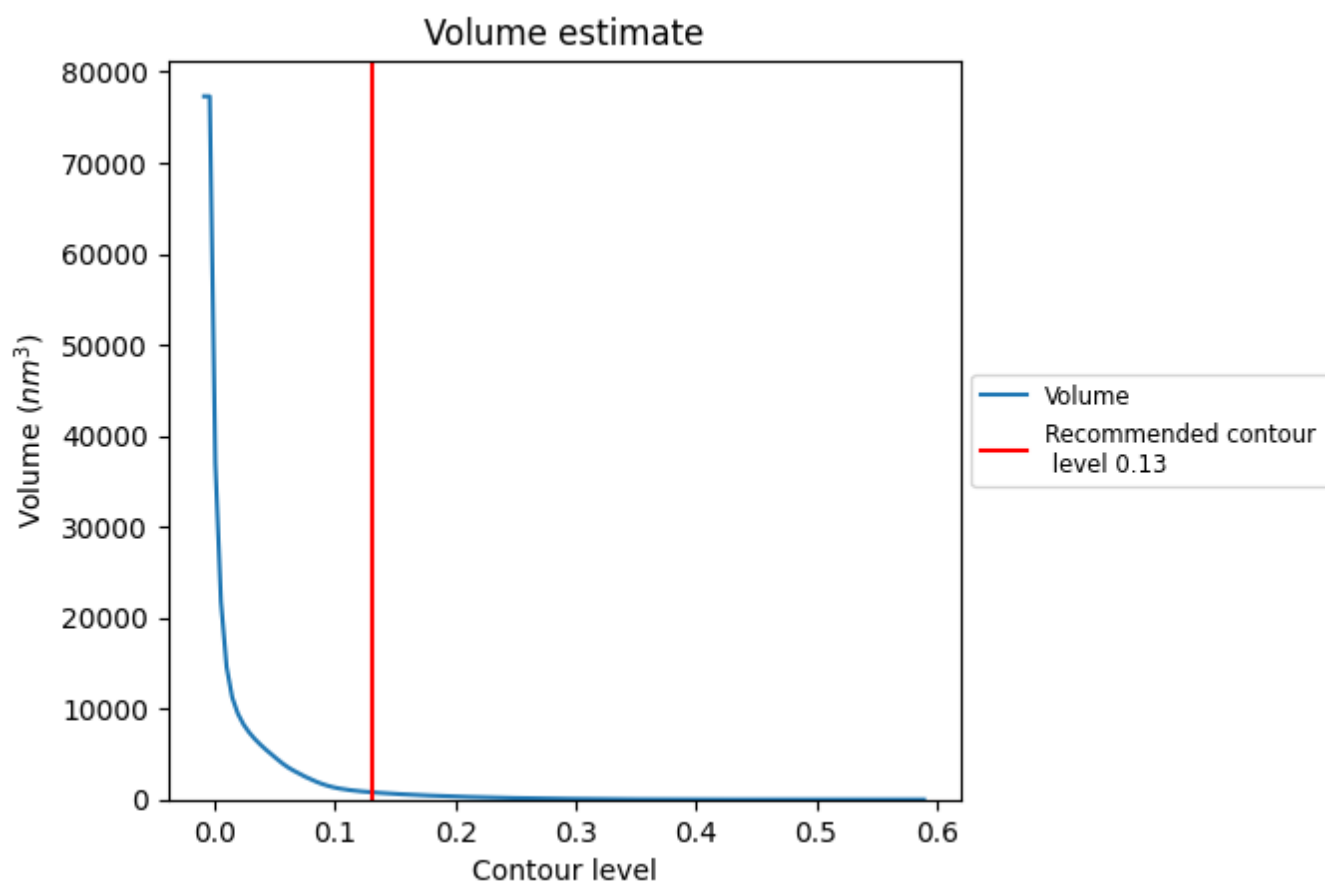
### 7.1 Map-value distribution [i](#)



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.



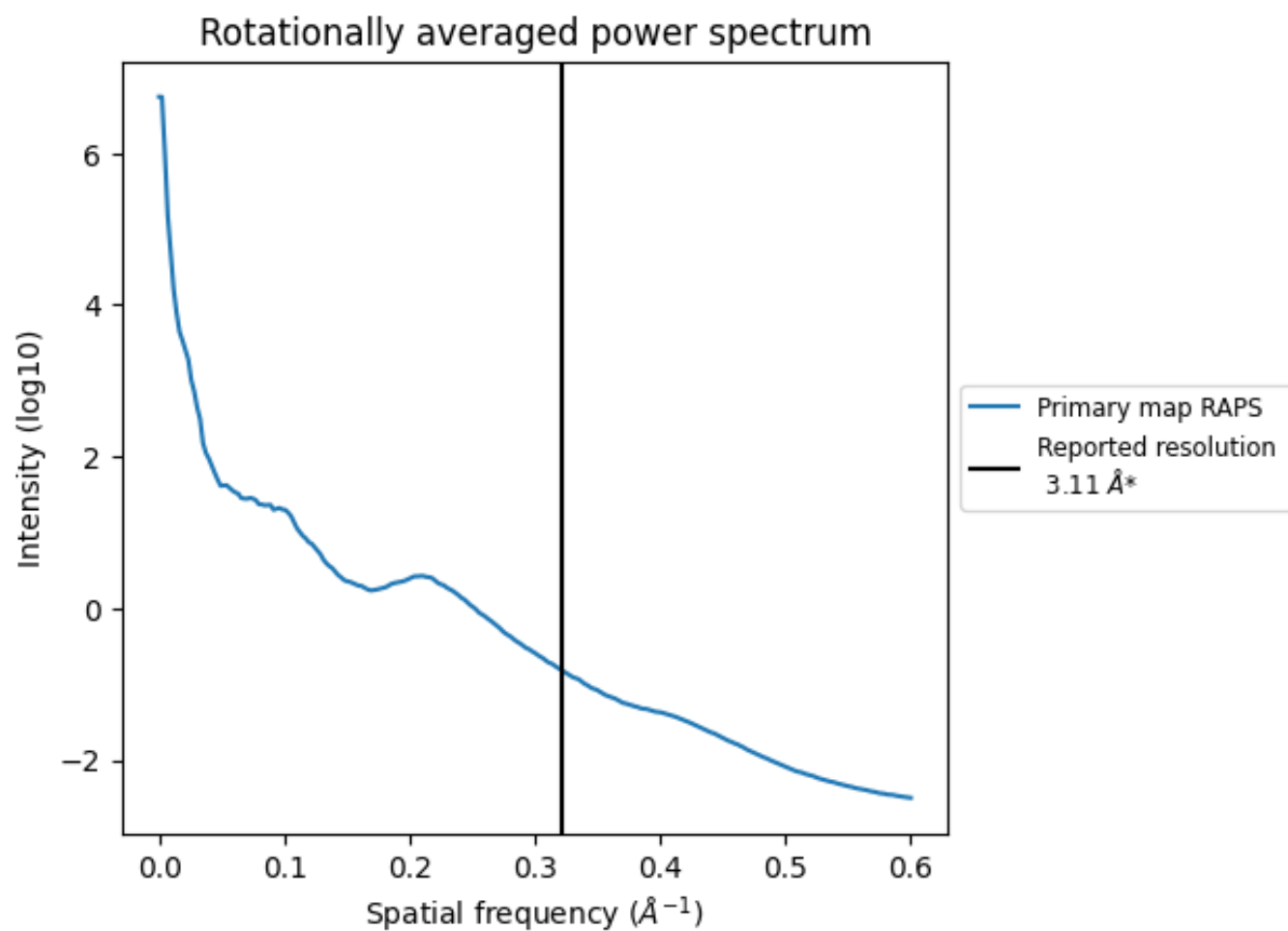
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 805  $\text{nm}^3$ ; this corresponds to an approximate mass of 728 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 0.322 Å<sup>-1</sup>

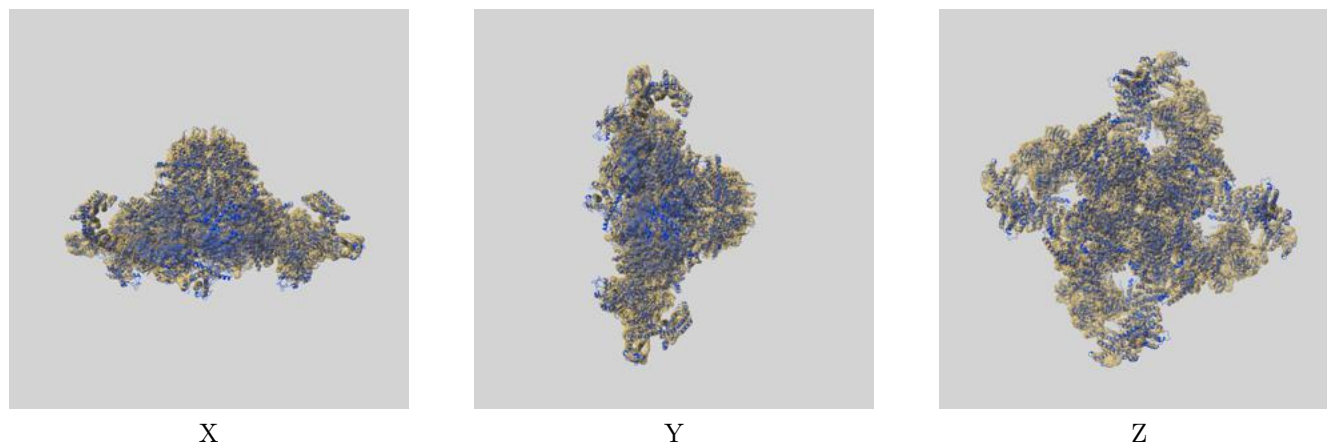
## 8 Fourier-Shell correlation

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

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

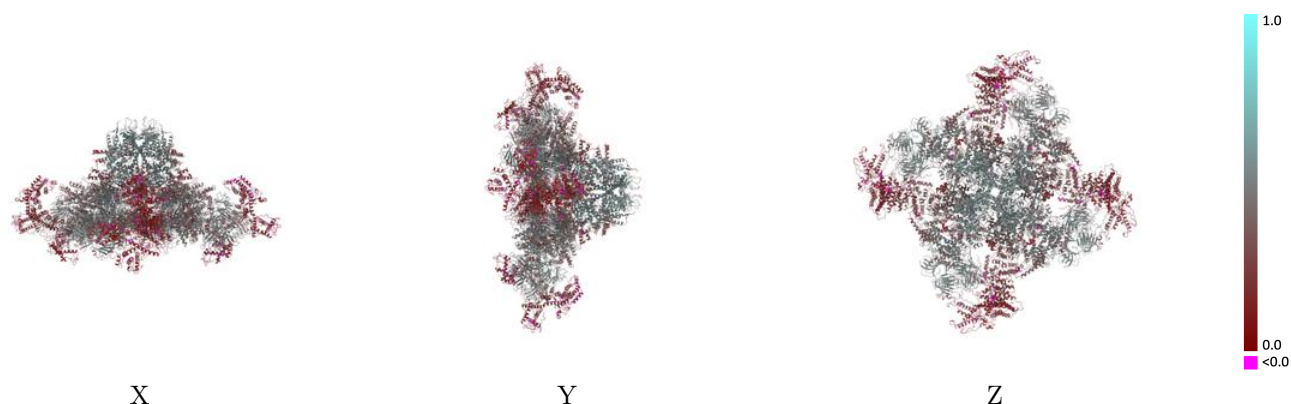
This section contains information regarding the fit between EMDB map EMD-26405 and PDB model 7U9Q. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



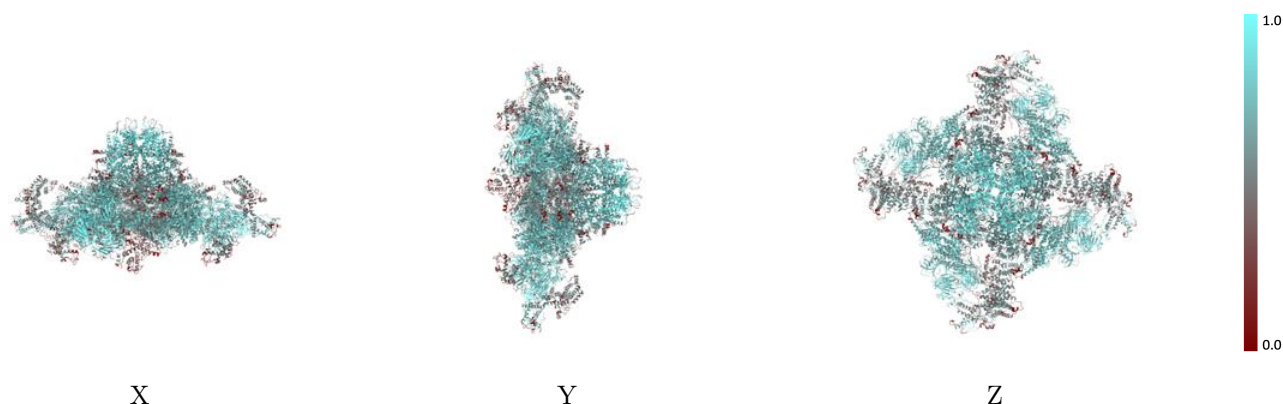
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



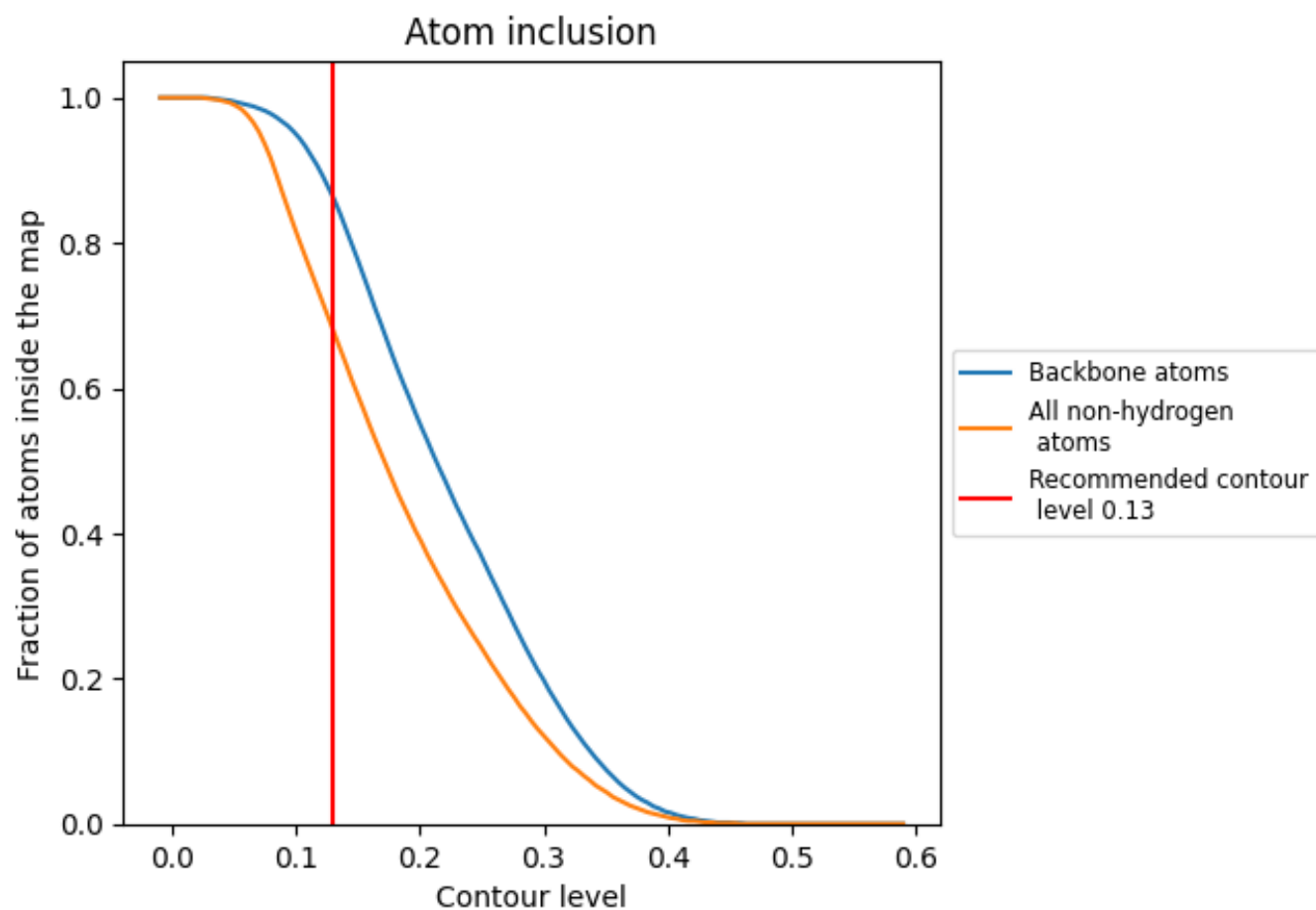
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 68% 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	<div></div> 0.6810	<div></div> 0.3770
A	<div></div> 0.6830	<div></div> 0.3810
B	<div></div> 0.6700	<div></div> 0.3640
C	<div></div> 0.6810	<div></div> 0.3790
D	<div></div> 0.6780	<div></div> 0.3740
E	<div></div> 0.7980	<div></div> 0.4950
F	<div></div> 0.7870	<div></div> 0.4900
G	<div></div> 0.7890	<div></div> 0.5020
H	<div></div> 0.8090	<div></div> 0.5130

1.0

0.0

<0.0