



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 03:18 AM EDT

PDB ID : 5TAL
EMDB ID : EMD-8378
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1&2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 4.30 Å(reported)

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

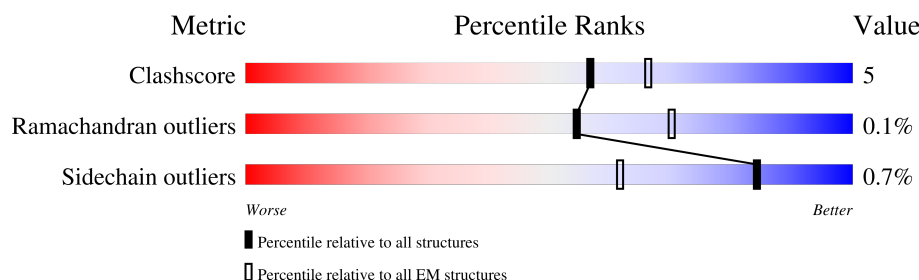
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	108	<div> <div>22%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	F	108	<div> <div>23%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	H	108	<div> <div>22%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	J	108	<div> <div>23%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	B	4416	<div> <div>37%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	E	4416	<div> <div>39%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	G	4416	<div> <div>38%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	I	4416	<div> <div>39%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	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		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

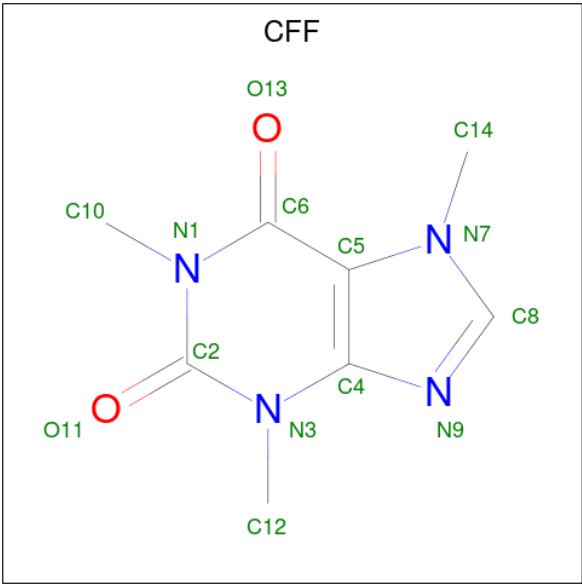
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

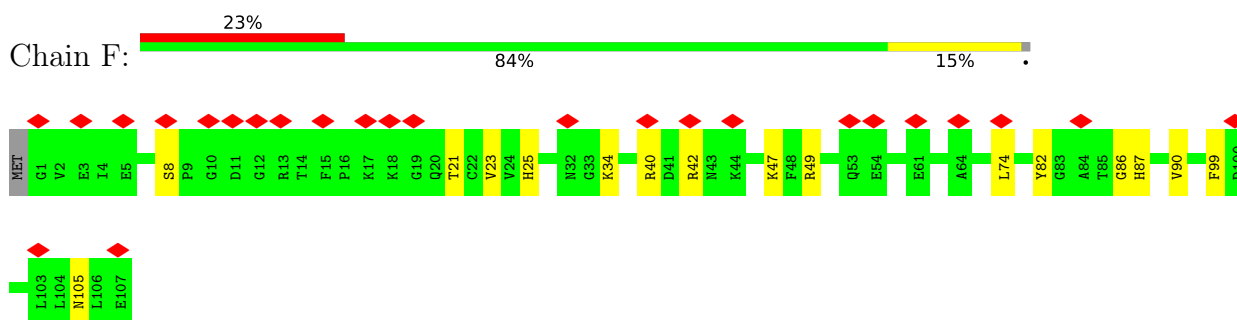
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

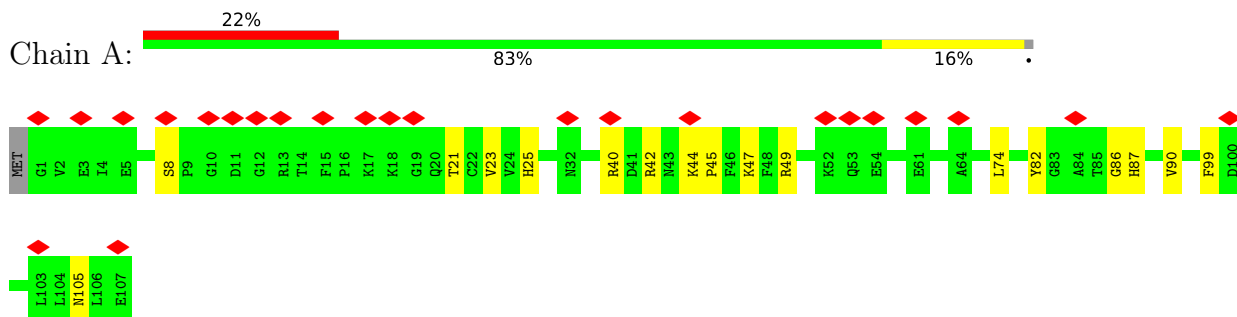
3 Residue-property plots [i](#)

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.

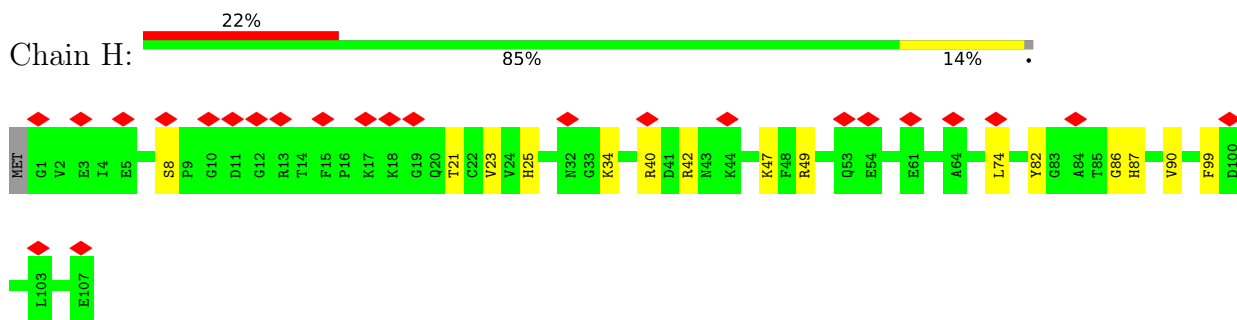
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



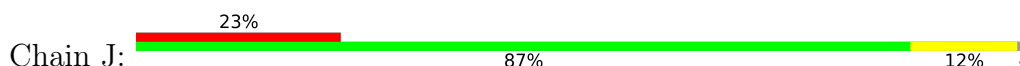
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

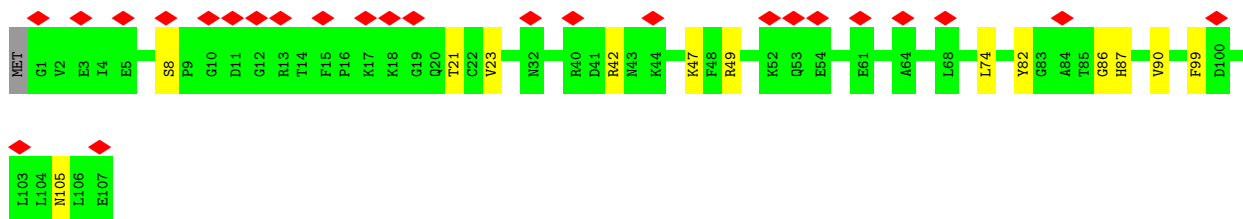


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



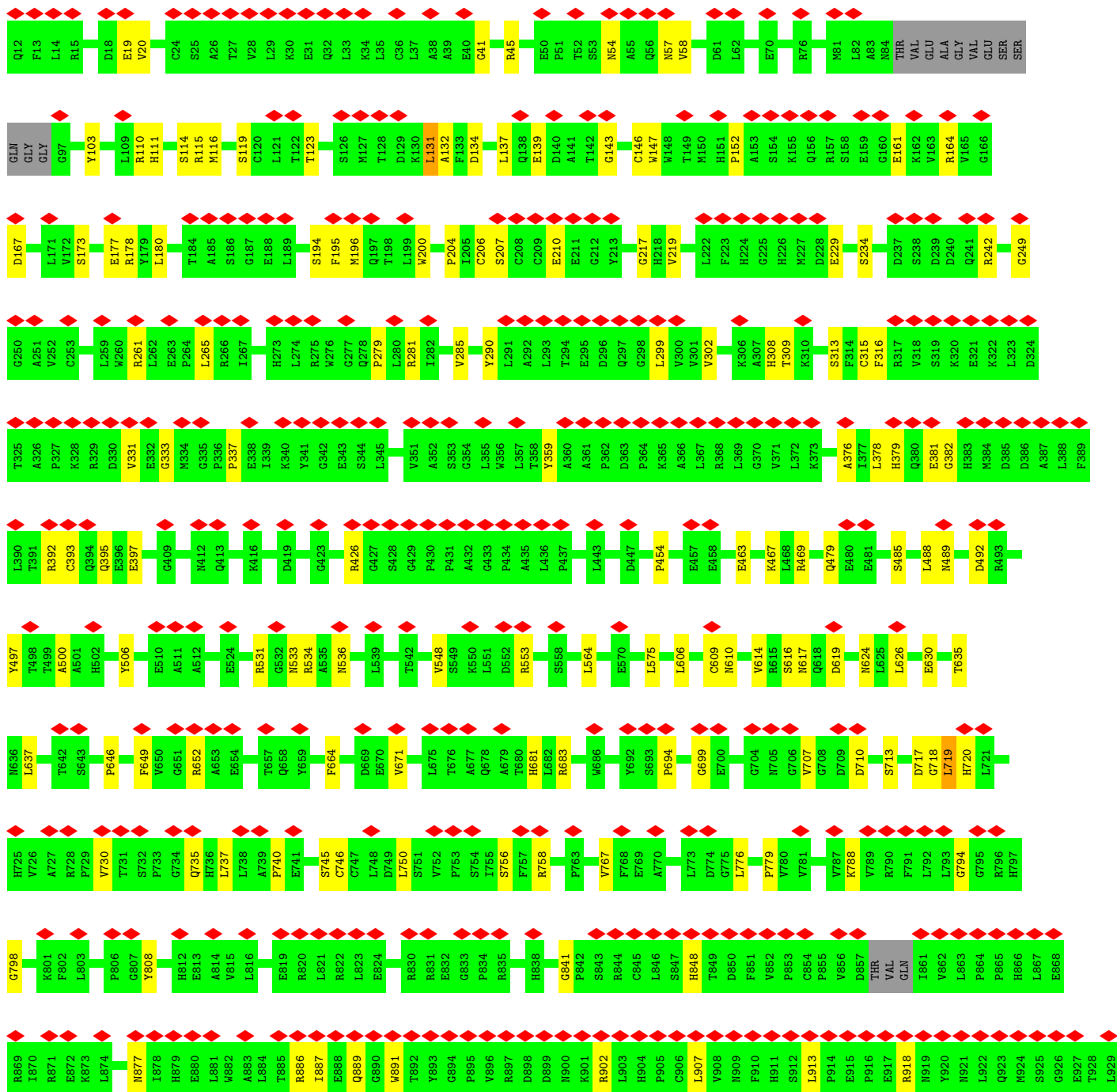
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: Ryanodine receptor 1

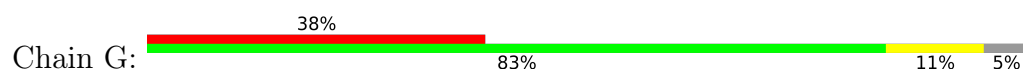
Chain B:



D2252	K2089	P2024	E1874	G1755	E1655	X1529	G1144	VAL	E990
Y2256	K2090	E2025	GLU	N1756	R1656	X1530	D1147	GLU	D999
N2260	Q2095	D2026	GLU	A1757	L1667	X1531	V1148	ASN	R1000
G2262	V2102	I2027	GLU	R1758	R1667	X1536	V1149	SER	V1001
I2263	R2104	Q2029	GLU	R1759	R1671	X1537	G1150	ARG	A934
L2264	Q2107	D2033	GLU	H1760	R1671	X1537	C1151	TRP	A1002
G2265	L2038	F2034	GLU	G1764	A1675	X1543	M1152	D1070	Q1003
L2124	L2265	L2038	GLU	L1771	L1676	X1544	L1155	R1071	A1009
H2125	H2041	L2038	GLU	R1772	M1679	X1545	T1156	V1072	VAL
R2126	C2042	L2038	GLU	H1776	R1680	X1546	E1157	R1073	GLN
Q2127	G2043	L2038	GLU	L1786	L1685	X1547	I1161	R1076	ASN
L2131	L2044	L2038	GLU	L1786	H1688	X1548	F1162	K1079	PRO
R2140	Q2045	L2038	ASP	P1787	H1688	X1549	T1163	E1091	ALA
A2277	L2046	L2038	GLU	P1787	V1689	X1549	T1163	F1092	ARG
	E2047	L2038	GLU	A1788	D1690	X1550	L1164	E1093	ARG
	G2048	L2038	GLU	ALA	Q1691	X1551	H1165	A1093	ASN
		L2038	LYS	GLY	L1695	M1573	H1165	A1094	PRO
		L2038	VAL	VAL	L1695	M1573	G1166	V1095	R1020
		L2038	GLU	ALA	L1698	P1593	L1169	L1021	A946
		L2038	GLU	ALA	L1698	P1593	L1169	L1021	E947
		L2038	ASP	E1793	L1698	P1593	M1170	E1099	D948
		L2038	GLU	A1794	E1699	L1600	S1171	M1100	N949
		L2038	GLU	P1795	D1700	L1600	D1172	L1026	L950
		L2038	GLU	A1796	A1701	S1604	G1174	V1102	K951
		L2038	GLU	R1797	L1707	W1605	S1173	G1103	D1028
		L2038	LYS	L1798	R1708	Q1614	E1029	W1104	K952
		L2038	GLU	L1802	A1709	V1615	S1175	A1105	E1029
		L2038	ASP	I1802	G1710	GLU	E1176	R1106	A1030
		L2038	ALA	R1808	Y1711	THR	T1177	T1031	K954
		L2038	LYS	D1809	Y1712	ARG	A1178	E1108	L955
		L2038	GLU	K1810	D1713	ARG	F1179	R1110	P956
		L2038	GLU	L1812	I1718	ALA	R1180	P1111	K957
		L2038	GLU	L1812	H1719	GLY	E1181	M1035	T958
		L2038	ALA	E1817	L1720	R1623	T1182	D1112	Y959
		L2038	PRO		E1721	L1624	E1183	R1036	M960
		L2038	GLU	D1821	R1725	G1625	G1195	D1037	M961
		L2038	GLY	R1827	R1728	W1626		S1038	S962
		L2038	LYS	D1828	R1731	A1627	V1199	L1039	N963
		L2038	ASP	D1828	L1731	V1628	G1200	C1040	G964
		L2038	ASP	P1840	P1737	Q1629	H1201	Q1041	Y965
		L2038	L1922	L1853	Q1631	D1632	D1207	E1119	K966
		L2038	E1923	L1853	D1632			L1120	P967
		L2038	E1924	A1744	D1632			V1123	A968
		L2038	G1925	I1745	I1745			F1124	P969
		L2038	L1926	T1746	T1746			N1125	L970
		L2038	L1926	K1860	L1747			G1126	L970
		L2038	L1931	Q1861				H1127	D971
		L2038	P1932	M1865				R1128	L972
		L2038	V1935	I1866	P1749			Y1049	S973
		L2038	D1948		P1750			G1050	H974
		L2038		E1869	G1751			Y1051	V975
		L2038	A2016	V1870	R1752			S1136	R976
		L2038	D2017	T1871	K1753			E1137	I1053
		L2038	E2018	T1872	G1754			I1053	T977
		L2038	E1873					E1054	T978
		L2038						PRO	P979
		L2038						ASP	A980
		L2038						GLN	Q981
		L2038						PRO	T982
		L2038						SER	T983
		L2038						GLN	L984
		L2038							V985
		L2038							D986
		L2038							R987
		L2038							L988
		L2038							A989

X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374																																																	
X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331																															
X3199	X3200	X3201	X3202			X3206	X3207	X3208											X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255																																
X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3005	X3006	X3007			X3010											X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024			X3027											X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048			X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059										
X3199	X3200	X3201	X3202			X3206	X3207	X3208											X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255			X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270																		
X3199	X3200	X3201	X3202			X3206	X3207	X3208											X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255			X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270																		
X3199	X3200	X3201	X3202			X3206	X3207	X3208											X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255			X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270																		
X3199	X3200	X3201	X3202			X3206	X3207	X3208											X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255			X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270																		
X3199	X3200	X3201	X3202			X3206	X3207	X3208											X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255			X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270																		
X3199	X3200	X3201	X3202			X3206	X3207	X3208											X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255			X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270																		
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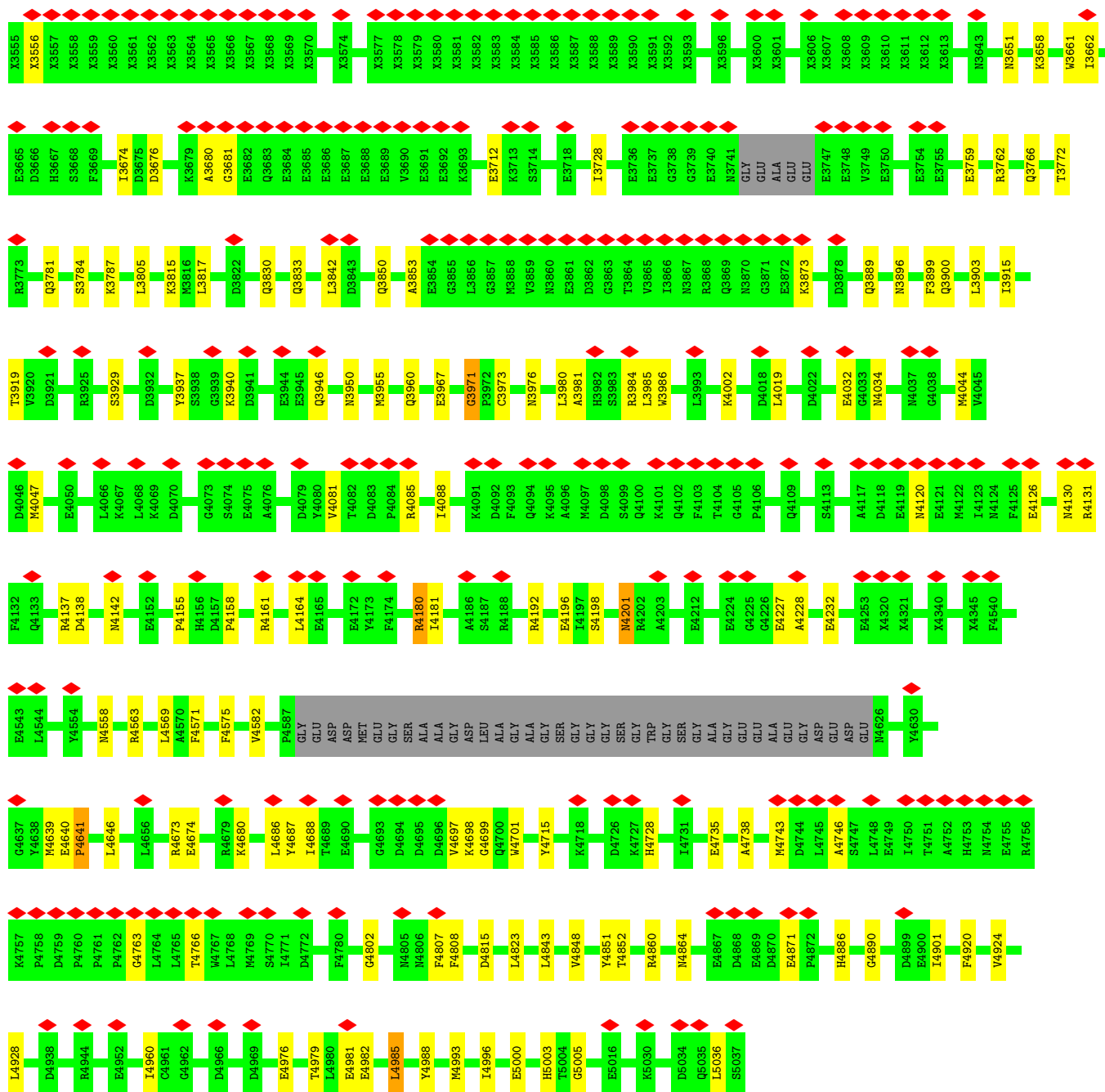
- Molecule 2: Ryanodine receptor 1



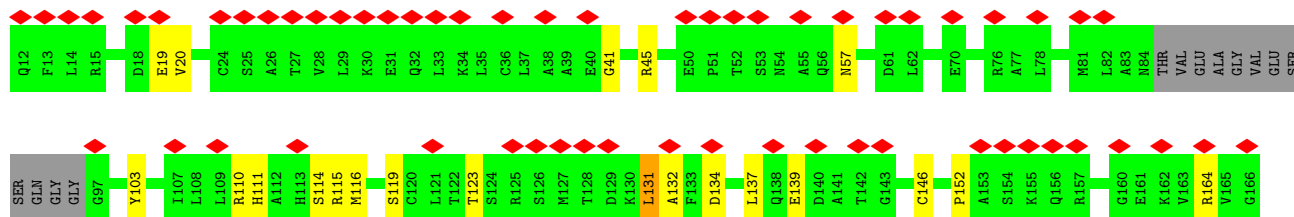
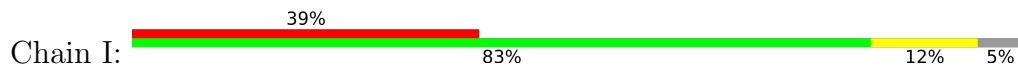


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H2902	P2903	L2904	L2905	P2906	P2907	P2908	P2909	P2910	L2911	T2912	A2913	A2914	E2915	K2916	A2917	D2918	D2919	R2920	E2921	A2922	Q2923	Q2924	E2925	L2926	L2927	K2928	P2929	L2930	Q2931	M2932	N2933	Q2934	V2935	A2936	V2937	T2938	R2939	H2940	N2941	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	K2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963																																																																														
ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	M2873	A2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	T2897	Q2898	G2899	Q2900	T2901																																																																																	
D2762	E2763	E2764	L2765	L2766	T2767	H2768	P2769	M2770	L2771	R2772	P2773	R2774	P2775	T2776	F2777	S2778	E2779	K2800	D2801	L2802	L2803	L2804	Y2805	R2806	V2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	A2819	E2820	R2821	T2822	E2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	N2775	S2776	V2777	E2778	G2779	N2780	V2781																																																																											
X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2660	X2661	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691																																																																				
X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2704	X2705	X2706	X2707	X2708	X2709	X2710	X2711	X2712	X2713	X2714	X2715	X2716	X2717	X2718	X2719	X2720	X2721	X2722	X2723	X2724	X2725	X2726	X2727	X2728	X2729	X2730	X2731	X2732	X2733	X2734	X2735	X2736	X2737	X2738	X2739	X2740	X2741	X2742	X2743	X2744	X2745	X2746	X2747	X2748	X2749	X2750	X2751	X2752	X2753	X2754	X2755	X2756	X2757	X2758	X2759	X2760	X2761	X2762	X2763	X2764	X2765	X2766	X2767	X2768	X2769	X2770	X2771	X2772	X2773	X2774	X2775	X2776	X2777	X2778	X2779	X2780	X2781																																																		



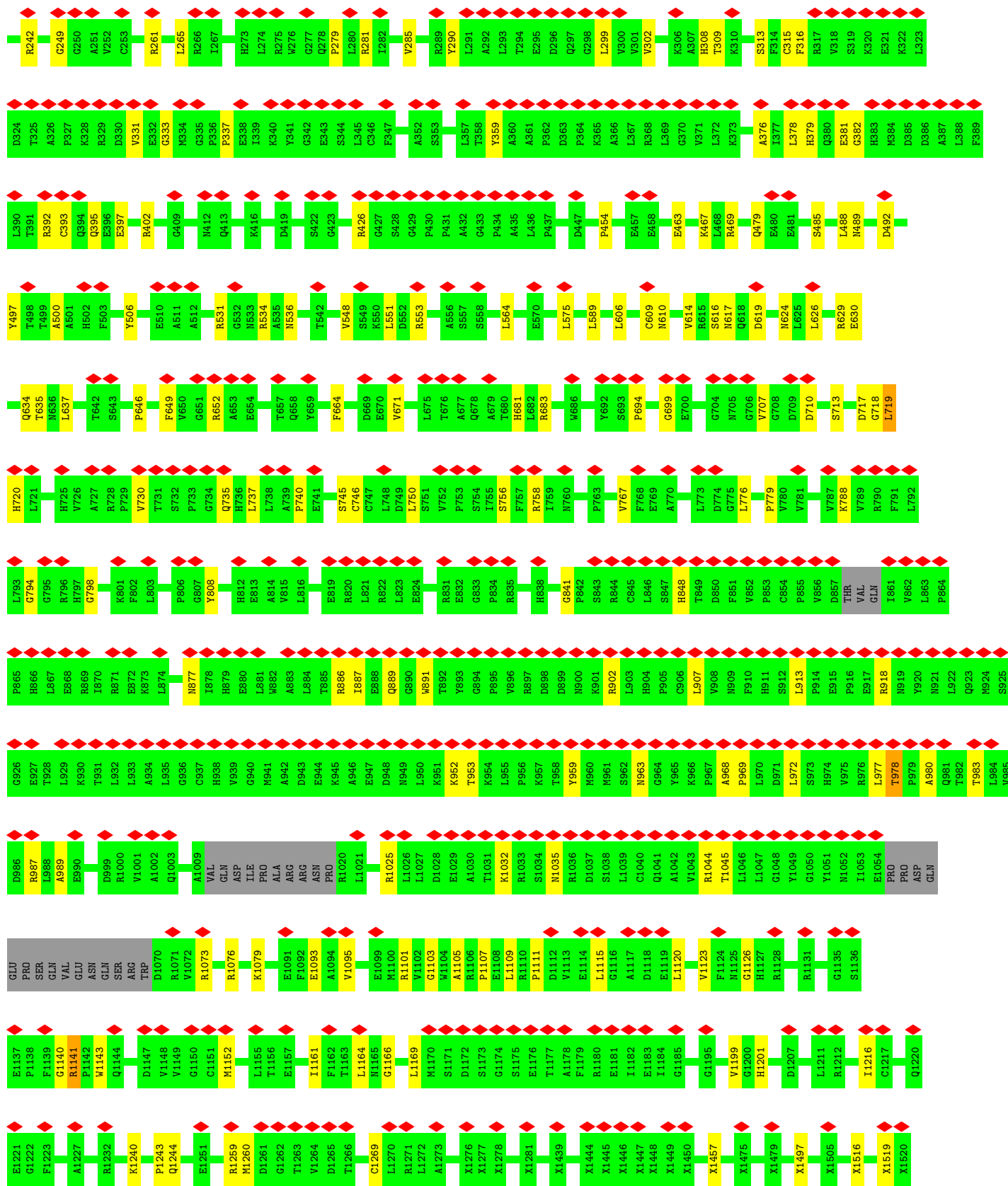
• Molecule 2: Ryanodine receptor 1





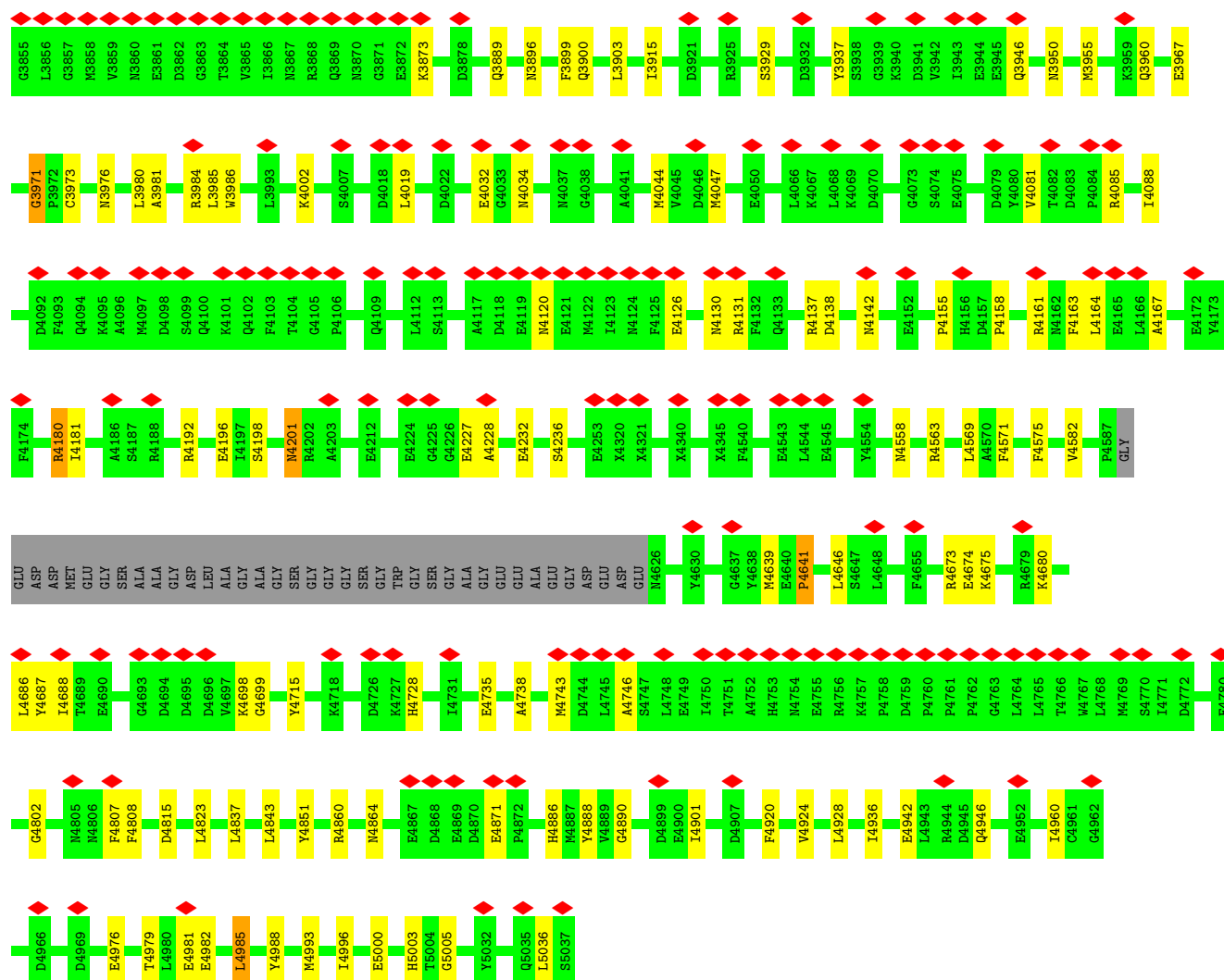








E2760	E2761	T2762	H2763	E2764	K2765	K2766	K2767	F2768	K2769	K2770	L2771	Q2772	K2773	K2774	K2775	S2776	V2777	G2778	E2779	K2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	T2789	K2790	L2791	R2792	T2793	K2794	K2795	T2796	T2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	T2805	K2806	K2807	F2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	K2816	L2817	A2818	K2819																																																																				
E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879																																																																						
E2880	N2881	Y2882	H2883	N2884	T2885	K2886	K2887	K2888	K2889	K2890	K2891	K2892	K2893	L2894	E2895	A2896	K2897	G2898	G2899	T2900	G2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	T2909	T2910	L2911	T2912	A2913	K2914	E2915	A2916	A2917	R2918	D2919	K2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	P2929	L2930	Q2931	M2932	N2933	G2934	V2935	Y2936	V2937	T2938	R2939																																																																				
K2942	K2943	K2944	K2945	K2946	K2947	K2948	K2949	K2950	K2951	K2952	K2953	K2954	K2955	K2956	K2957	K2960	K2961	K2962	K2963	K2964	K2965	K2966	K2967	K2968	K2969	K2970	K2971	K2972	K2973	K2974	K2975	K2976	K2977	K2978	K2979	K2980	K2981	K2982	K2983	K2984	K2985	K2986	K2987	K2988	K2989	K2990	K2991	K2992	K2993	K2994	K2995	K2996	K2997	K2998	K2999	K3000	K3001	K3002	K3003	K3004	K3005	K3006	K3007	K3008	K3009	K3010	K3013	K3014	K3015	K3016	K3017	K3018	K3019	K3020	K3021																																																				
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K3156	K3157	K3158	K3159	K3160	K3161	K3162	K3163	K3170	K3171	K3172	K3173	K3174	K3175	K3176	K3177	K3178	K3179	K3180	K3181	K3182	K3186	K3187	K3188	K3189	K3190	K3191	K3192	K3193	K3194	K3195	K3196	K3197	K3198	K3199	K3200	K3201	K3202	K3203	K3204	K3207	K3208	K3211	K3212	K3213	K3214	K3215	K3216	K3217	K3218	K3219	K3220	K3221	K3222	K3223	K3224	K3225																																																																							
K3226	K3227	K3228	K3229	K3230	K3231	K3232	K3233	K3234	K3235	K3236	K3241	K3242	K3243	K3244	K3245	K3246	K3247	K3248	K3249	K3250	K3251	K3252	K3253	K3254	K3261	K3262	K3263	K3264	K3265	K3266	K3267	K3268	K3269	K3270	K3271	K3272	K3273	K3274	K3275	K3276	K3277	K3278	K3279	K3280	K3281	K3282	K3283	K3284	K3285	K3286	K3287	K3288	K3289	K3290	K3291	K3292	K3293	K3294	K3295																																																																				
K3296	K3297	K3298	K3299	K3300	K3301	K3302	K3303	K3304	K3308	K3309	K3310	K3311	K3312	K3313	K3314	K3315	K3316	K3317	K3318	K3319	K3320	K3321	K3322	K3323	K3324	K3325	K3326	K3327	K3328	K3329	K3330	K3331	K3332	K3333	K3334	K3335	K3336	K3337	K3338	K3339	K3340	K3341	K3342	K3343	K3344	K3345	K3346	K3347	K3348	K3349	K3350	K3351	K3352	K3353	K3354	K3355	K3356	K3357																																																																					
K3358	K3359	K3360	K3361	K3362	K3363	K3364	K3365	K3366	K3367	K3368	K3369	K3370	K3371	K3372	K3373	K3374	K3377	K3378	K3379	K3380	K3381	K3382	K3383	K3384	K3385	K3386	K3387	K3388	K3389	K3390	K3391	K3392	K3393	K3394	K3395	K3396	K3397	K3398	K3399	K3400	K3401	K3402	K3403	K3404	K3405	K3406	K3407	K3408	K3409	K3410	K3411	K3412	K3413	K3414	K3416	K3417	K3418																																																																						
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K3527	K3528	K3529	K3530	K3531	K3532	K3533	K3534	K3538	K3539	K3540	K3541	K3542	K3543	K3544	K3545	K3546	K3547	K3548	K3549	K3550	K3551	K3552	K3553	K3554	K3555	K3556	K3557	K3558	K3559	K3560	K3561	K3562	K3563	K3564	K3565	K3566	K3567	K3568	K3569	K3570	K3574	K3577	K3578	K3579	K3580	K3581	K3582	K3583	K3584	K3585	K3586	K3587	K3588	K3589	K3590	K3591																																																																							
K3592	K3593	K3596	K3597	K3600	K3601	K3604	K3608	K3609	K3610	K3611	K3612	K3613	K3643	K3644	N3651	M3652	F3653	K3658	V3661	I3662	E3665	D3666	H3667	S3668	F3669	I3674	D3675	D3676	K3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	R3707	E3712	K3713																																																																																	
S3714	E3718	D3719	V3720	I3728	E3736	E3737	G3738	G3739	E3740	N3741	GLY	ALA	GLU	GLU	E3747	E3748	V3749	E3750	E3754	E3755	E3759	R3762	Q3766	T3772	R3773	Q3781	S3784	K3787	L3805	K3815	K3816	L3817	Q3830	Q3833	L3842	D3843	K3849	Q3850	K3853	E3854																																																																																							



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (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	F	0	1
1	H	0	1
1	J	0	1
2	B	0	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	7.51	132.57	115.30
2	G	131	LEU	CA-CB-CG	7.51	132.56	115.30
2	I	131	LEU	CA-CB-CG	7.51	132.56	115.30
2	B	131	LEU	CA-CB-CG	7.49	132.53	115.30
2	B	1676	LEU	CA-CB-CG	6.38	129.96	115.30

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	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	A	818	0	824	10	0
1	F	818	0	824	11	0
1	H	818	0	824	8	0
1	J	818	0	824	7	0
2	B	29499	0	24746	286	0
2	E	29499	0	24747	282	0
2	G	29499	0	24747	279	0
2	I	29499	0	24747	284	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102371	1145	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 5.

The worst 5 of 1145 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:E:2318:TYR:HH	2:E:2414:ASN:N	1.86	0.74
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.86	0.72
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.86	0.71
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.87	0.71
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.56	0.70

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	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2886 (89%)	345 (11%)	4 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	51	85
2	G	3235/4416 (73%)	2889 (89%)	341 (10%)	5 (0%)	47	81
2	I	3235/4416 (73%)	2888 (89%)	342 (11%)	5 (0%)	47	81
All	All	13360/18096 (74%)	11935 (89%)	1407 (10%)	18 (0%)	54	85

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	4641	PRO
2	G	1708	ARG
2	G	4641	PRO
2	I	1708	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	84	90

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	131	LEU

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Mol	Chain	Res	Type
2	E	4085	ARG
2	E	553	ARG
2	E	1676	LEU
2	E	4201	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	582	HIS
2	E	1679	ASN
2	E	3946	GLN
2	G	725	HIS
2	G	582	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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
3	ATP	E	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.63	5 (16%)
3	ATP	B	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.64	5 (16%)
4	CFF	I	5102	-	8,15,15	2.54	3 (37%)	8,23,23	1.26	1 (12%)
3	ATP	I	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.64	5 (16%)
3	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.64	5 (16%)
4	CFF	B	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.26	1 (12%)
4	CFF	E	5102	-	8,15,15	2.55	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	G	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.25	1 (12%)

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
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-4.60	1.33	1.39
4	B	5102	CFF	C5-C4	-4.57	1.33	1.39
4	I	5102	CFF	C5-C4	-4.55	1.33	1.39
4	G	5102	CFF	C5-C4	-4.54	1.33	1.39
4	G	5102	CFF	C6-N1	-4.23	1.32	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	PB-O3B-PG	-3.66	120.26	132.83
3	E	5101	ATP	PB-O3B-PG	-3.66	120.27	132.83
3	G	5101	ATP	PB-O3B-PG	-3.64	120.32	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	ATP	PB-O3B-PG	-3.63	120.36	132.83
3	I	5101	ATP	PA-O3A-PB	-3.50	120.80	132.83

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

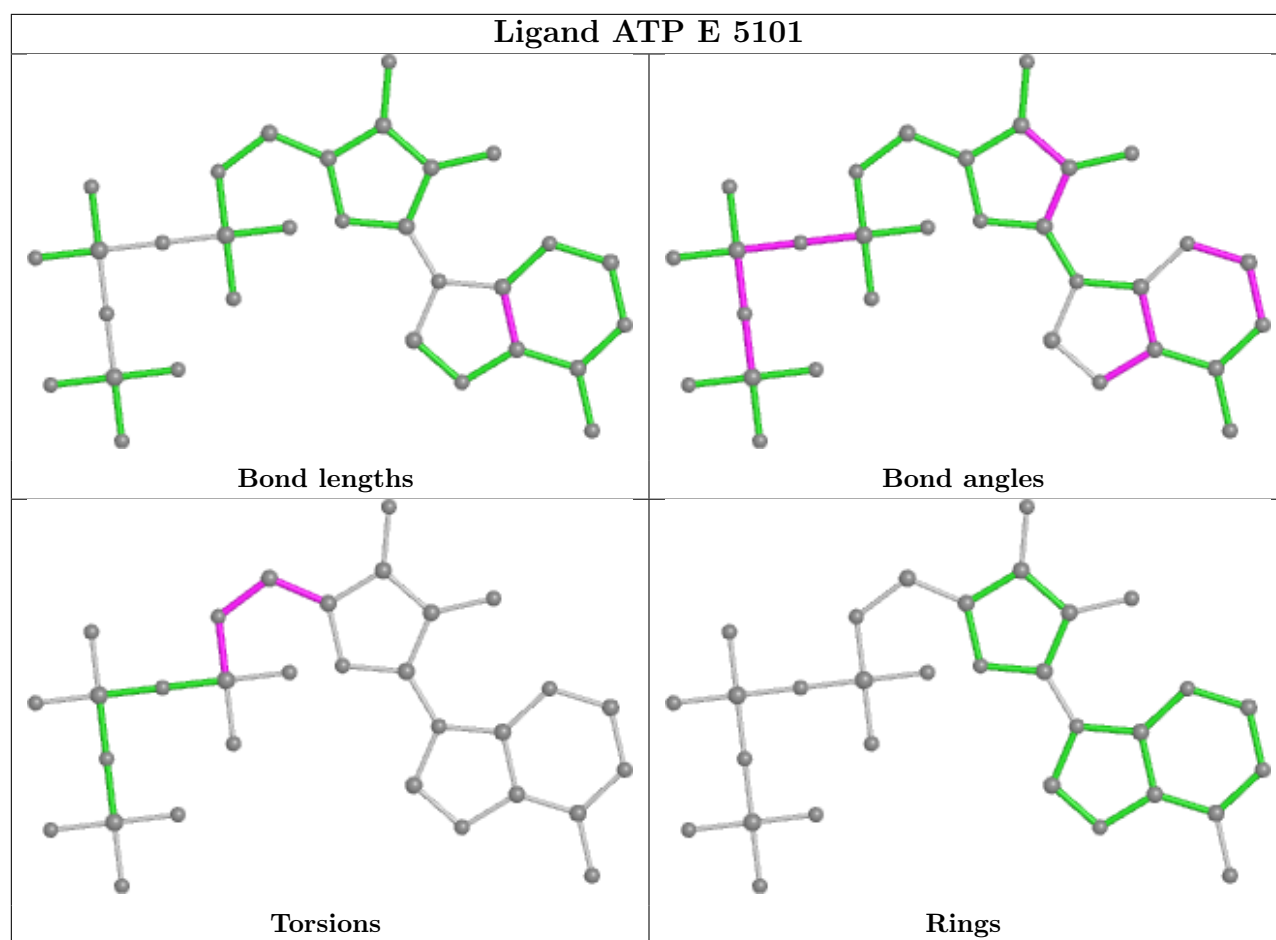
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O2A

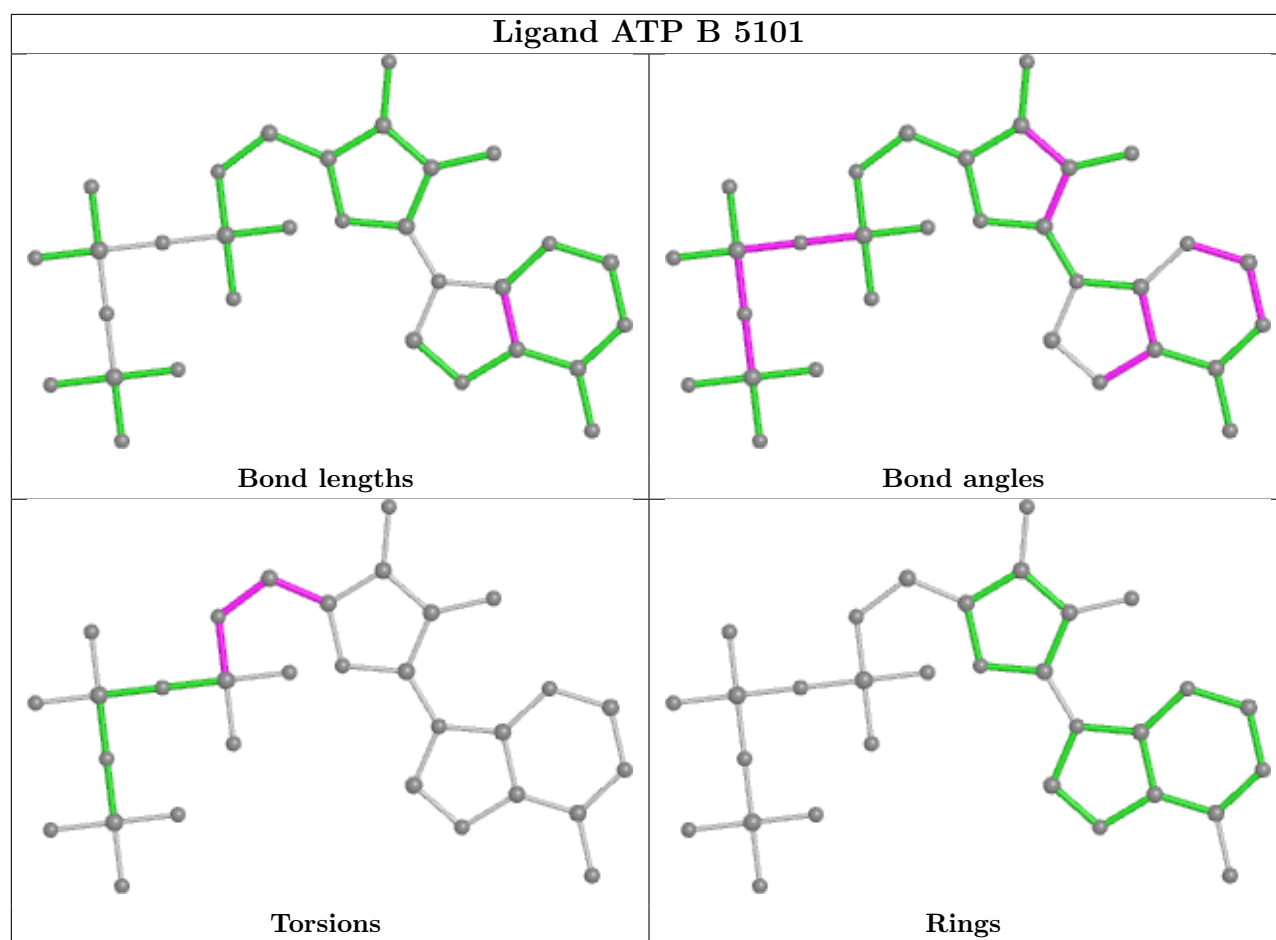
There are no ring outliers.

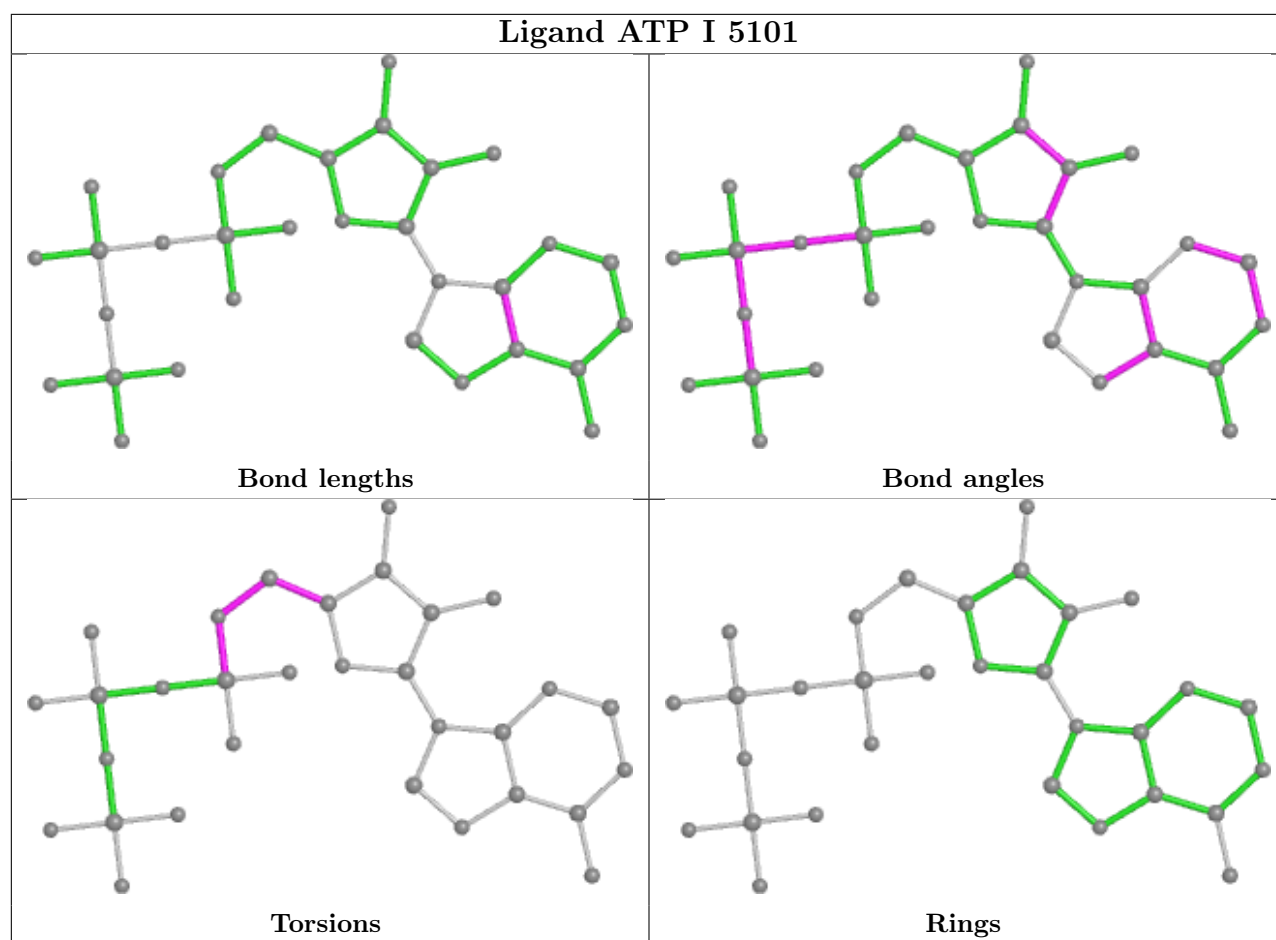
4 monomers are involved in 4 short contacts:

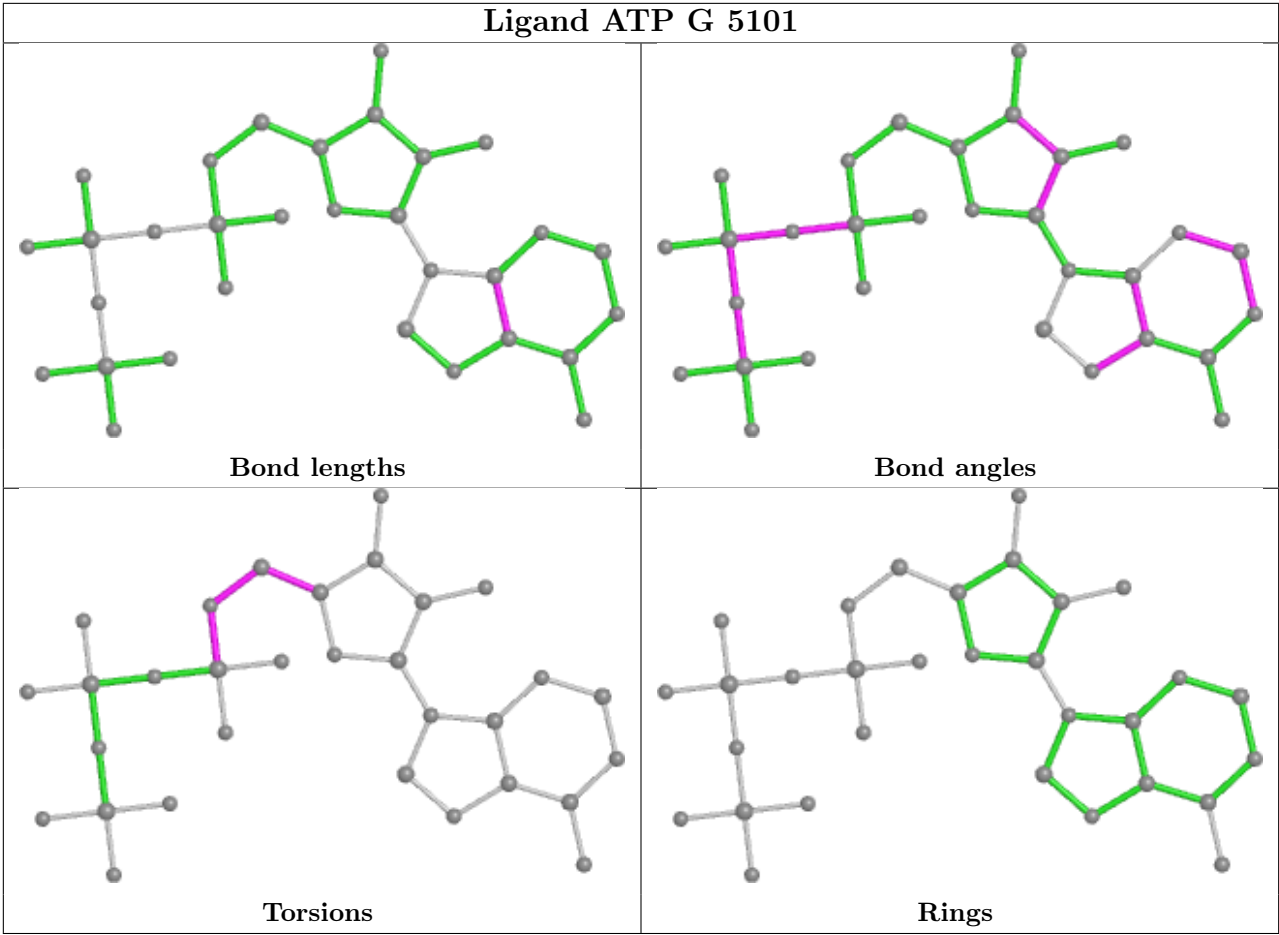
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	1	0
3	B	5101	ATP	1	0
3	I	5101	ATP	1	0
3	G	5101	ATP	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	G	14
2	I	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.32
1	G	4345:UNK	C	4540:PHE	N	73.24

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.23
1	E	4345:UNK	C	4540:PHE	N	73.22
1	E	3613:UNK	C	3639:THR	N	45.34

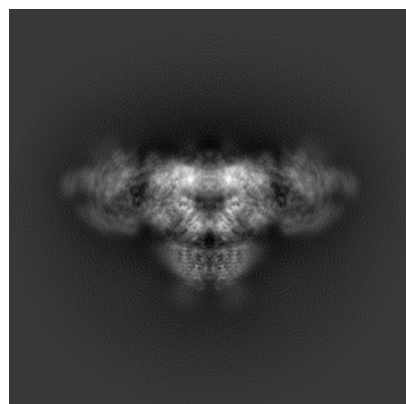
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8378. These allow visual inspection of the internal detail of the map and identification of artifacts.

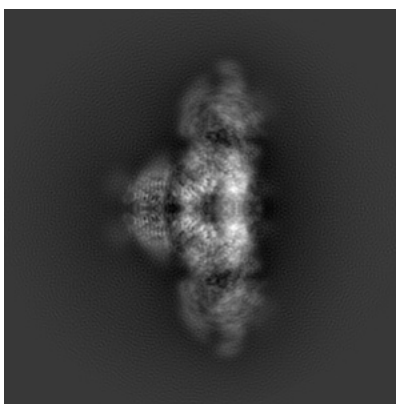
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

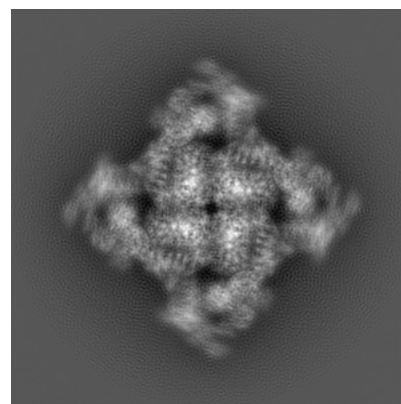
6.1.1 Primary map



X

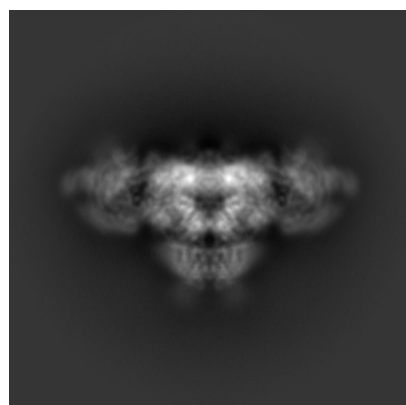


Y

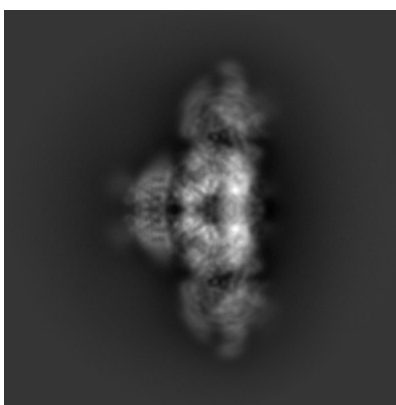


Z

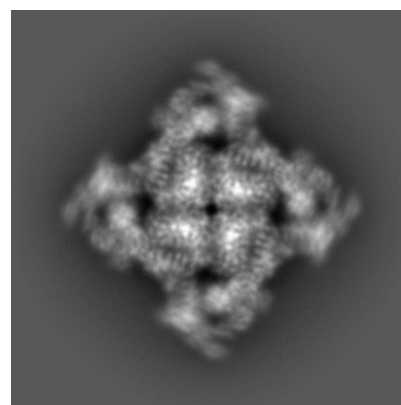
6.1.2 Raw map



X



Y

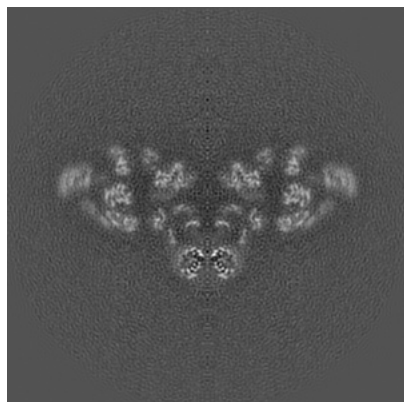


Z

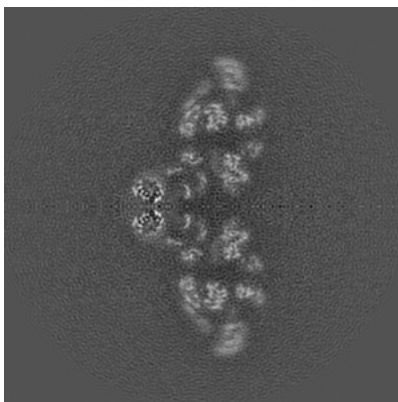
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

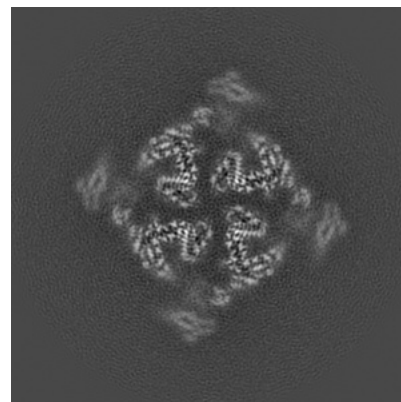
6.2.1 Primary map



X Index: 200

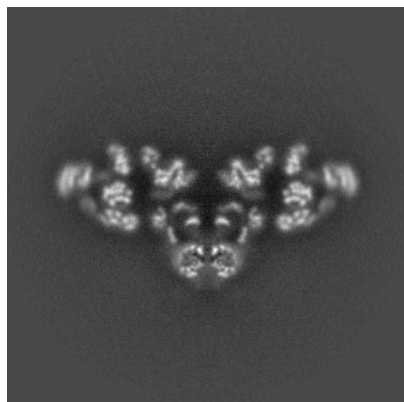


Y Index: 200

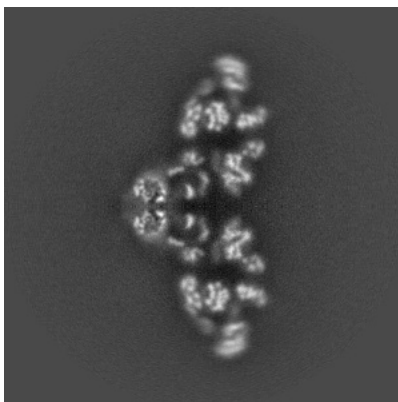


Z Index: 200

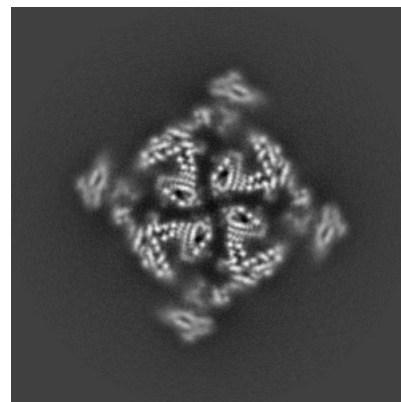
6.2.2 Raw map



X Index: 200



Y Index: 200

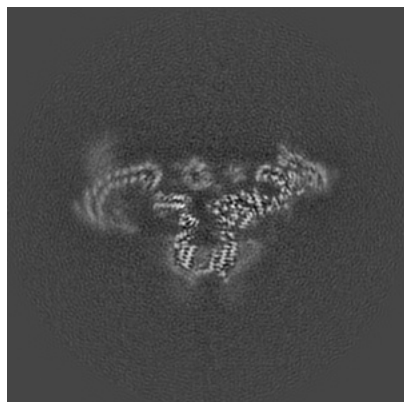


Z Index: 200

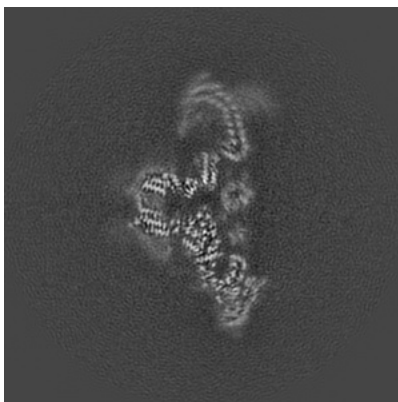
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

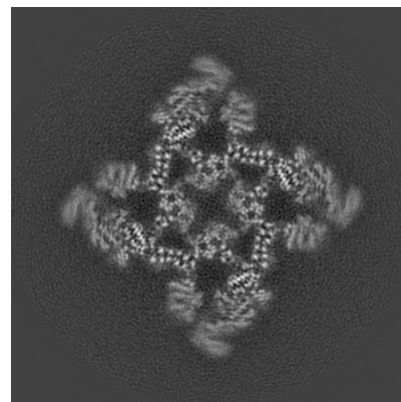
6.3.1 Primary map



X Index: 175

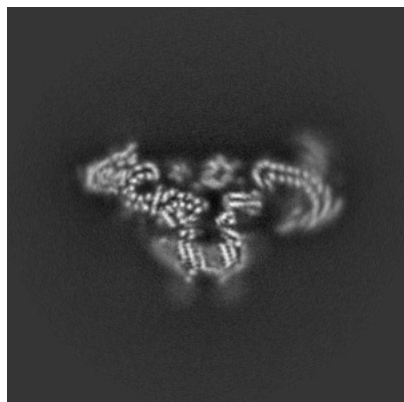


Y Index: 175

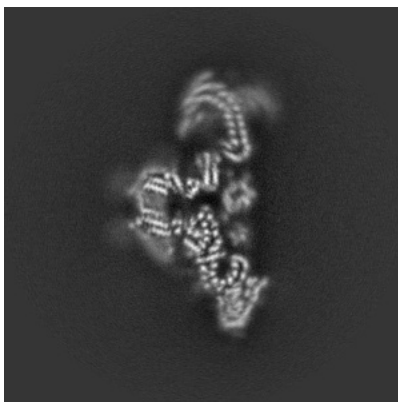


Z Index: 225

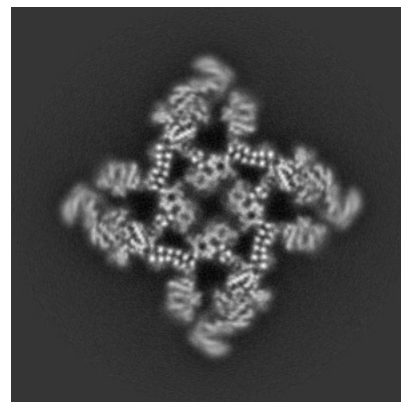
6.3.2 Raw map



X Index: 225



Y Index: 175

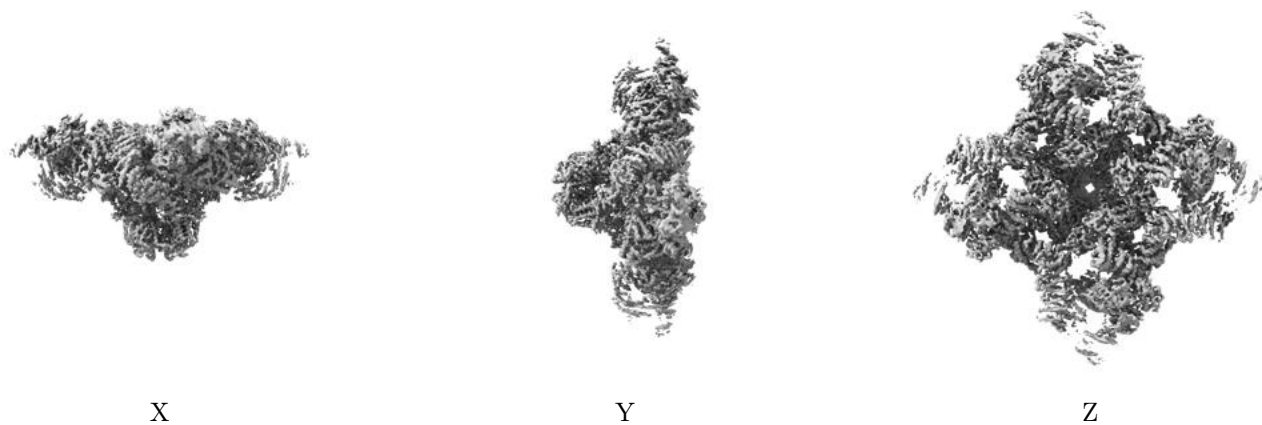


Z Index: 227

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

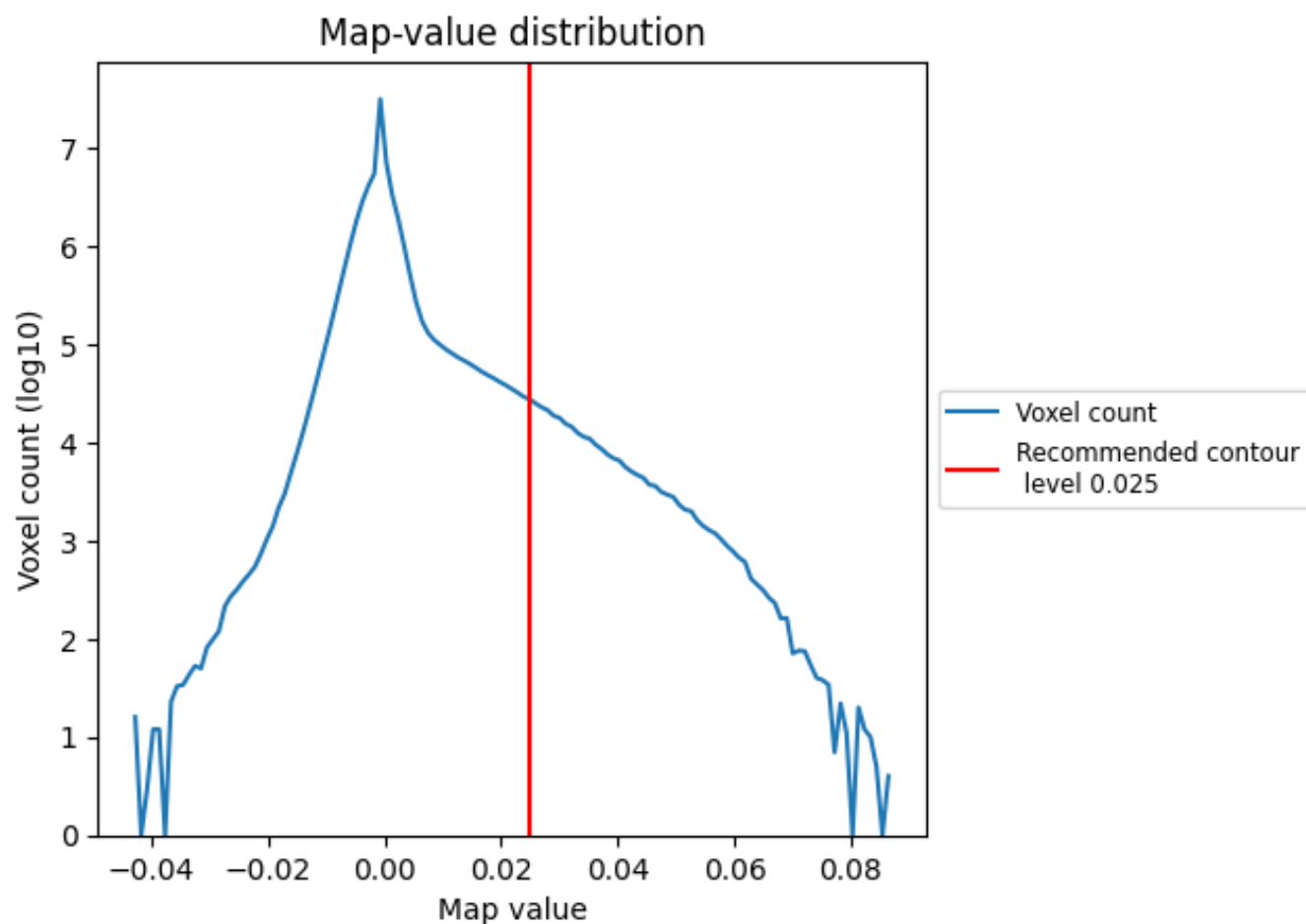
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

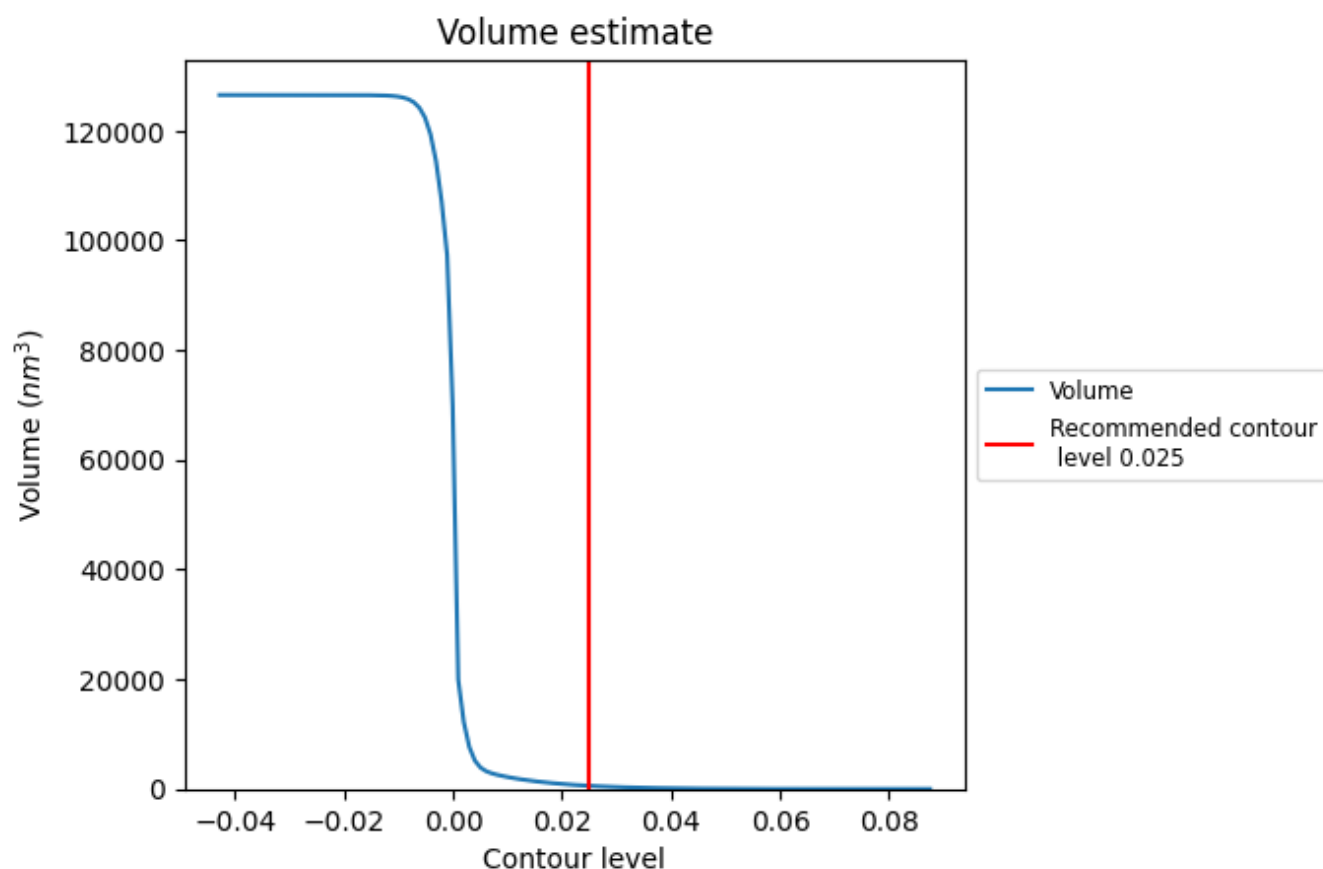
This section contains the results of statistical analysis of the map.

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.

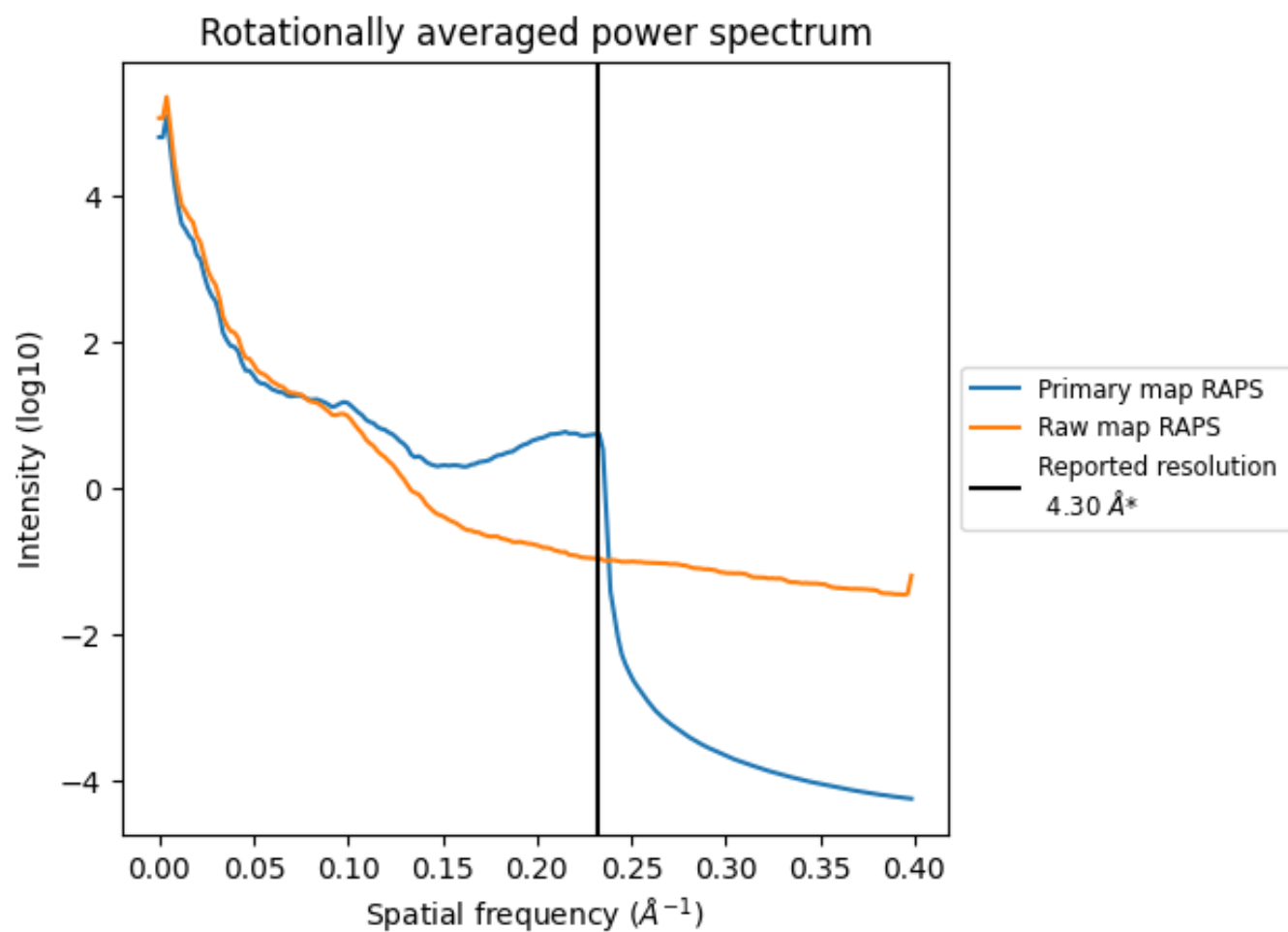
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 572 nm³; this corresponds to an approximate mass of 517 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 ⓘ

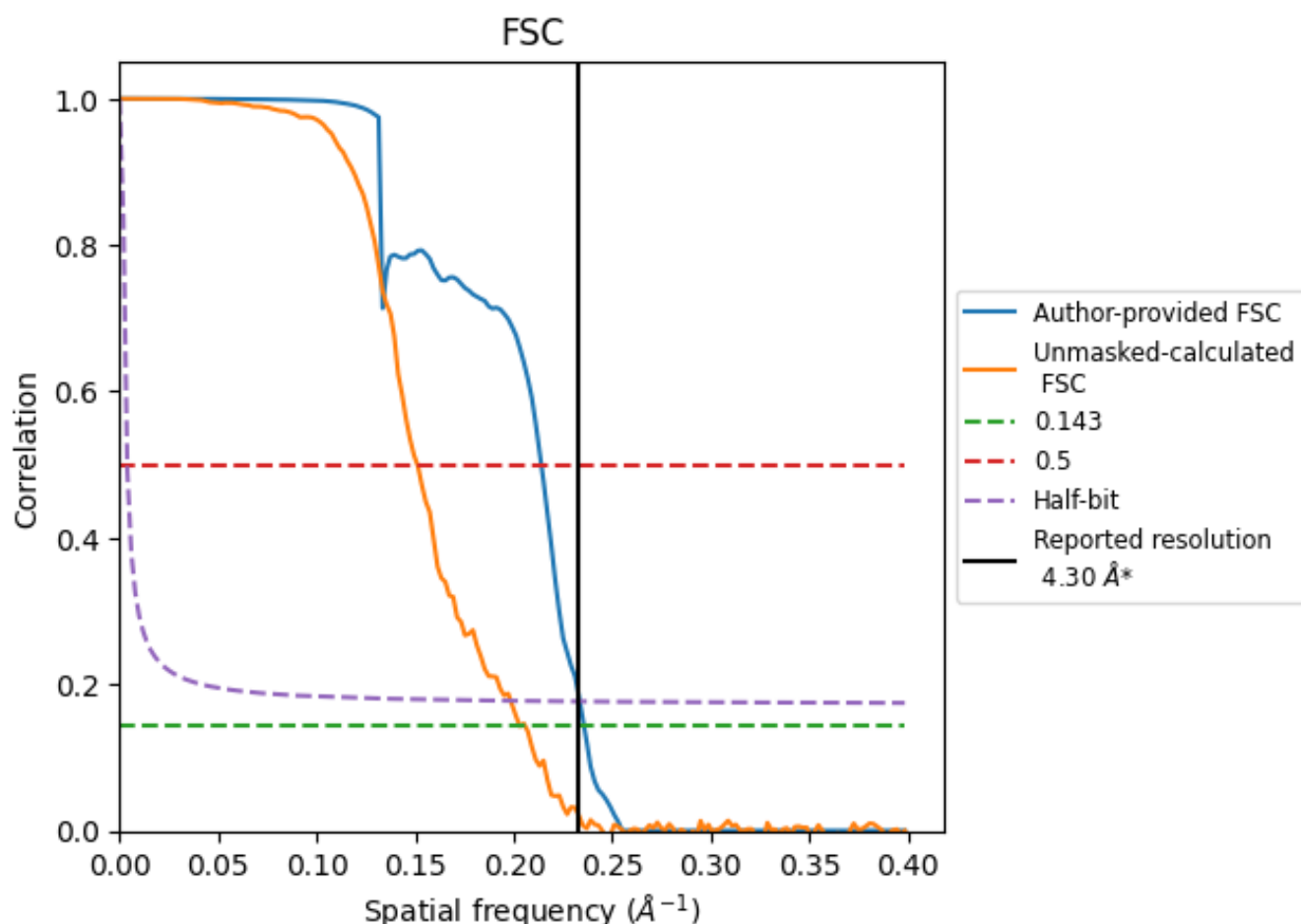


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

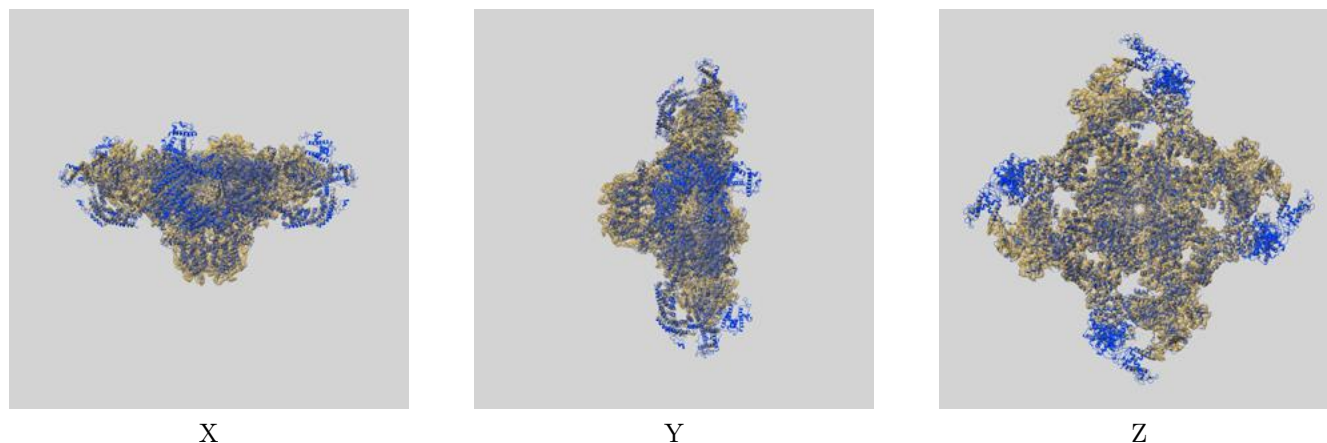
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.24	4.67	4.28
Unmasked-calculated*	4.92	6.61	5.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.92 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

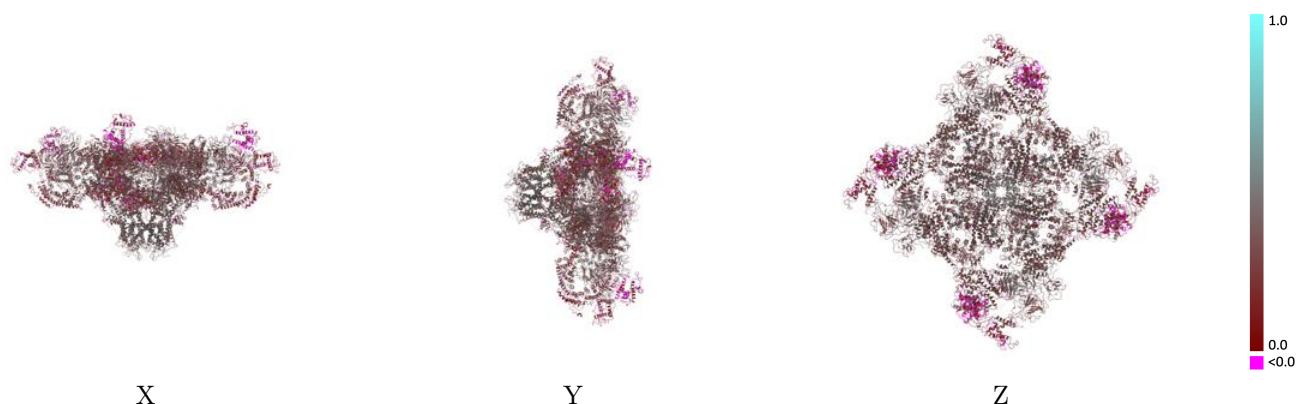
This section contains information regarding the fit between EMDB map EMD-8378 and PDB model 5TAL. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



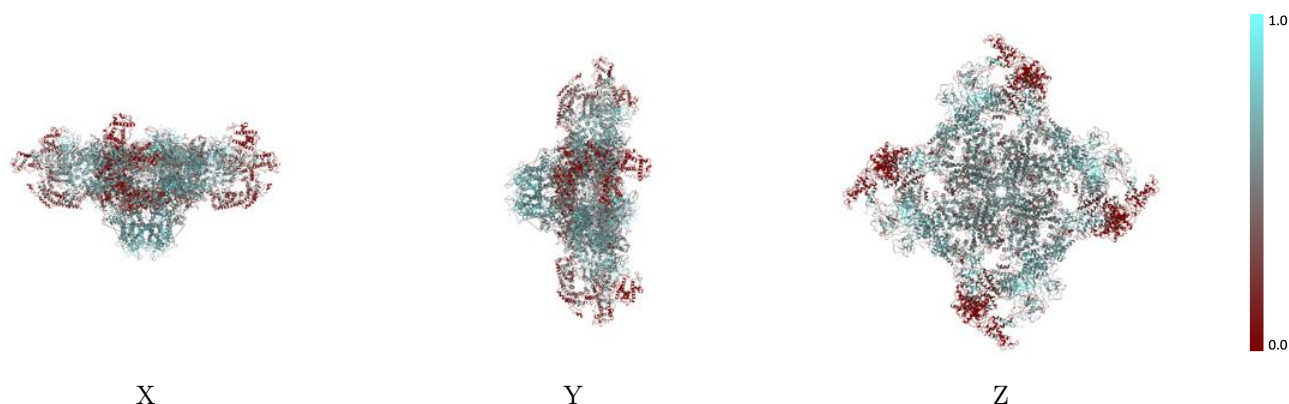
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



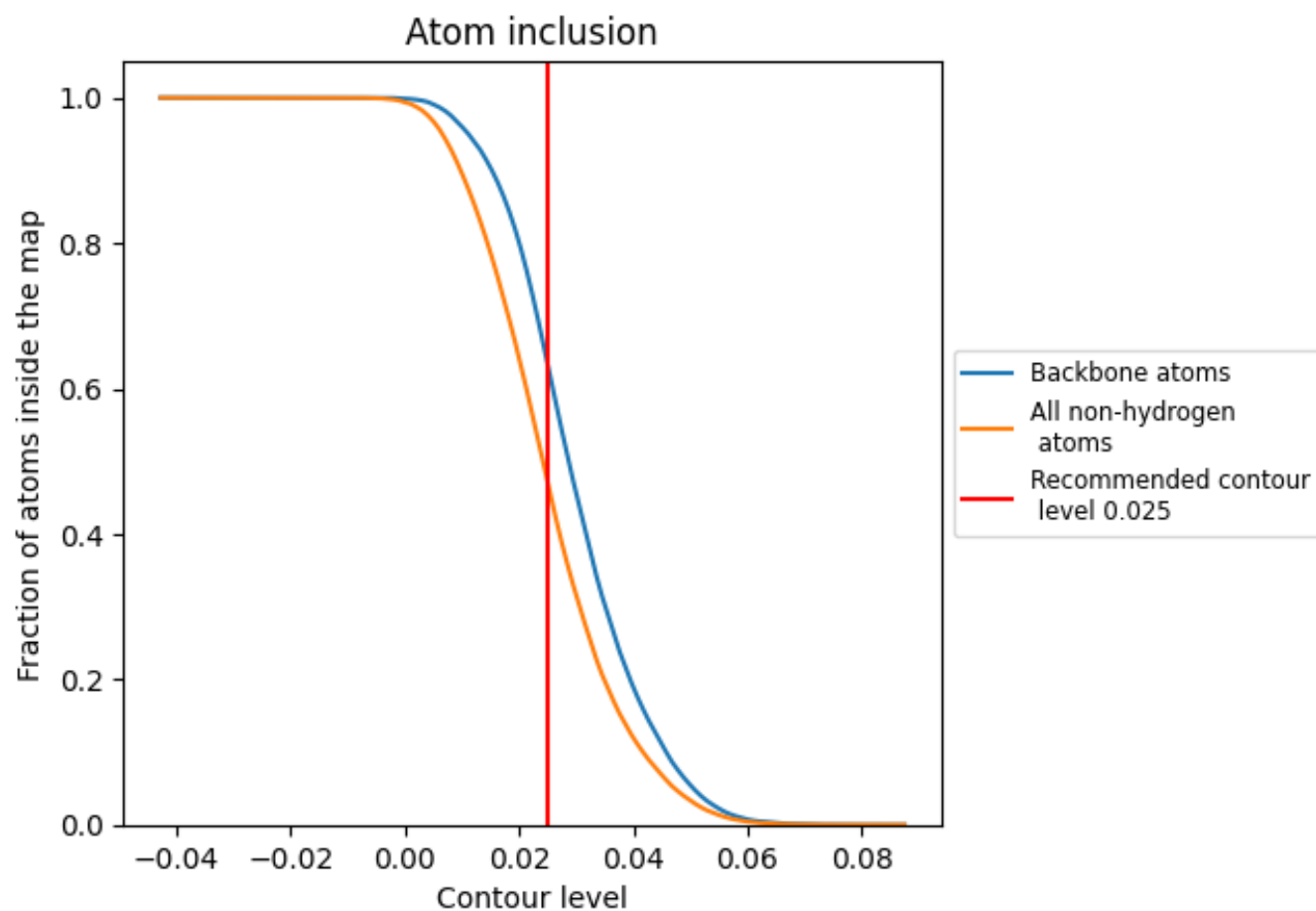
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 47% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4705	<div></div> 0.3030
A	<div></div> 0.5385	<div></div> 0.3550
B	<div></div> 0.4725	<div></div> 0.3050
E	<div></div> 0.4660	<div></div> 0.2980
F	<div></div> 0.5434	<div></div> 0.3580
G	<div></div> 0.4697	<div></div> 0.3030
H	<div></div> 0.5360	<div></div> 0.3570
I	<div></div> 0.4663	<div></div> 0.2990
J	<div></div> 0.5360	<div></div> 0.3550

1.0

0.0

<0.0