



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 10:24 PM EST

PDB ID : 9E1H
EMDB ID : EMD-47394
Title : Structure of RyR1 in the primed state in the presence of oxopyricid
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 3.26 Å (reported)
Based on initial model : 7TZC

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.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

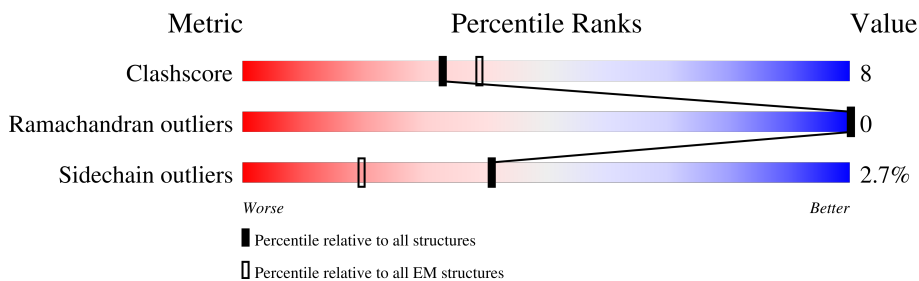
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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 ≥ 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	5037	
1	B	5037	
1	C	5037	
1	D	5037	
2	E	108	
2	F	108	
2	G	108	
2	H	108	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144120 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
1	B	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
1	D	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
1	C	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	H	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	G	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	F	107	Total 831	C 527	N 146	O 154	S 4	0	0

- 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
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

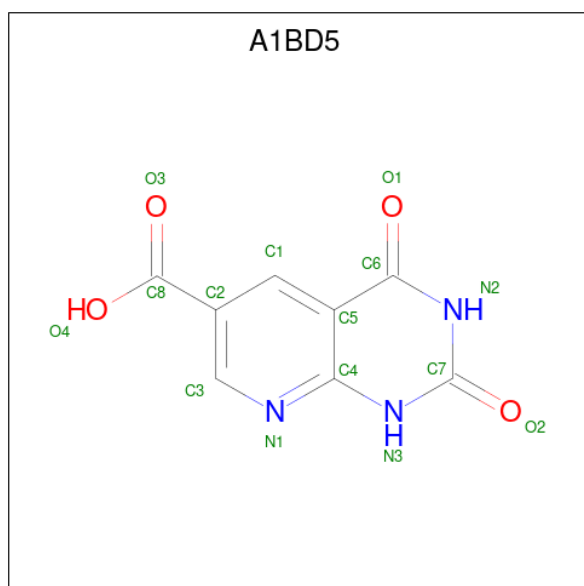
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	Total	Zn	0
			1	1	

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

- Molecule 6 is oxopyricid (three-letter code: A1BD5) (formula: $C_8H_5N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			15	8	3	4	
6	B	1	Total	C	N	O	0
			15	8	3	4	
6	D	1	Total	C	N	O	0
			15	8	3	4	
6	C	1	Total	C	N	O	0
			15	8	3	4	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	B	1	Total	O	0
			1	1	

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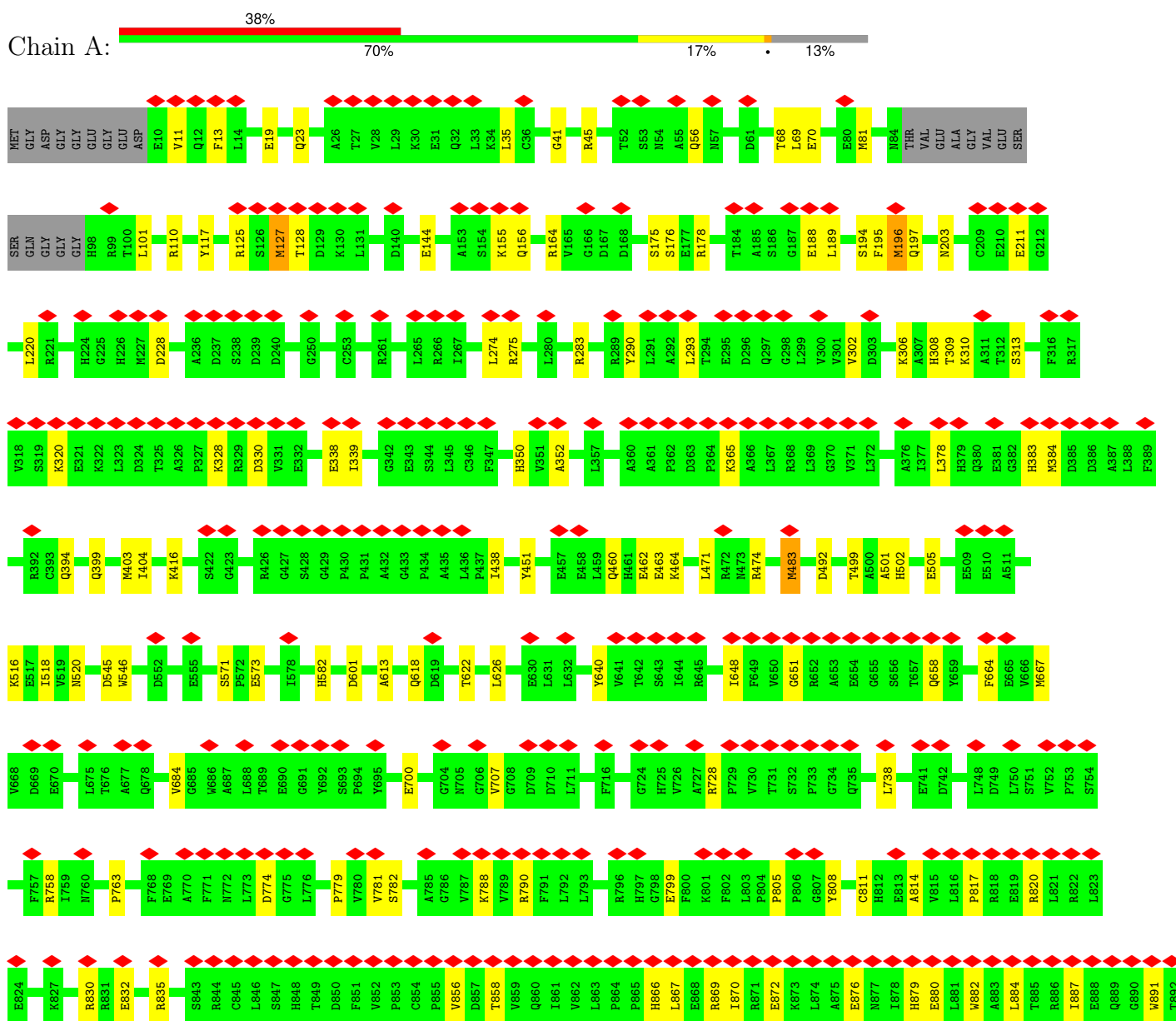
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Mol	Chain	Residues	Atoms	AltConf
7	D	1	Total O 1 1	0
7	C	1	Total O 1 1	0

3 Residue-property plots

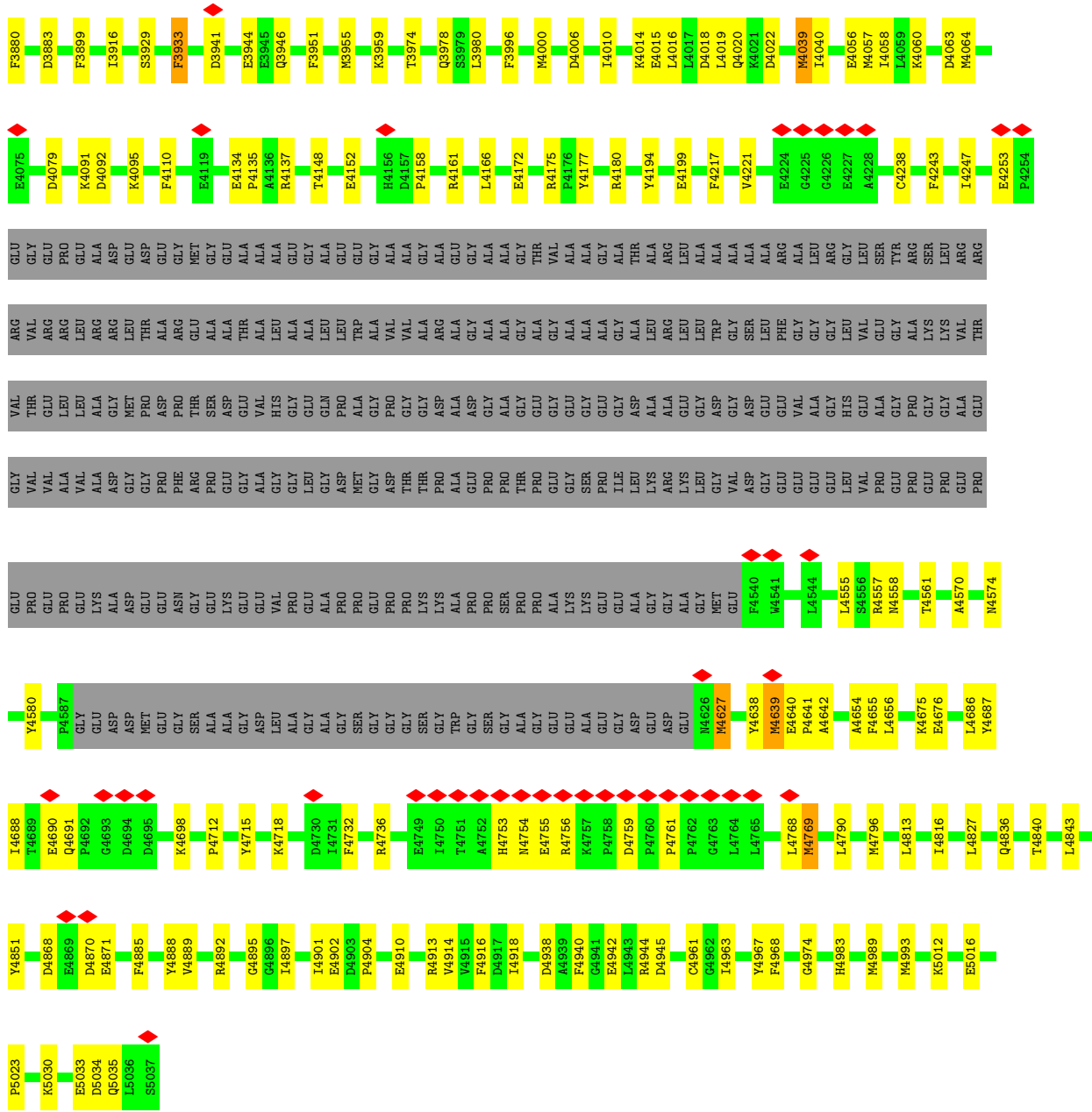
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 1

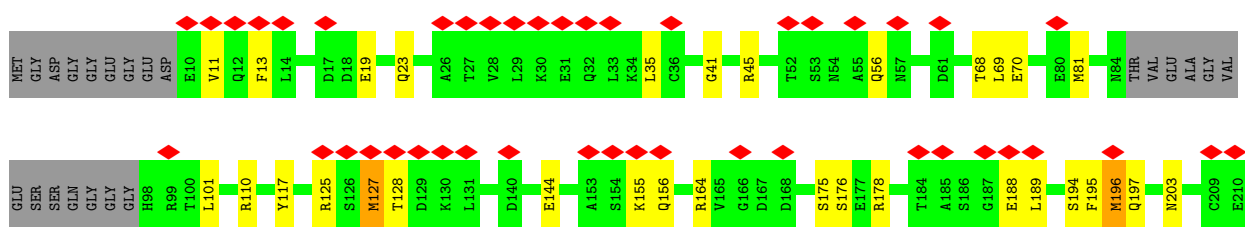


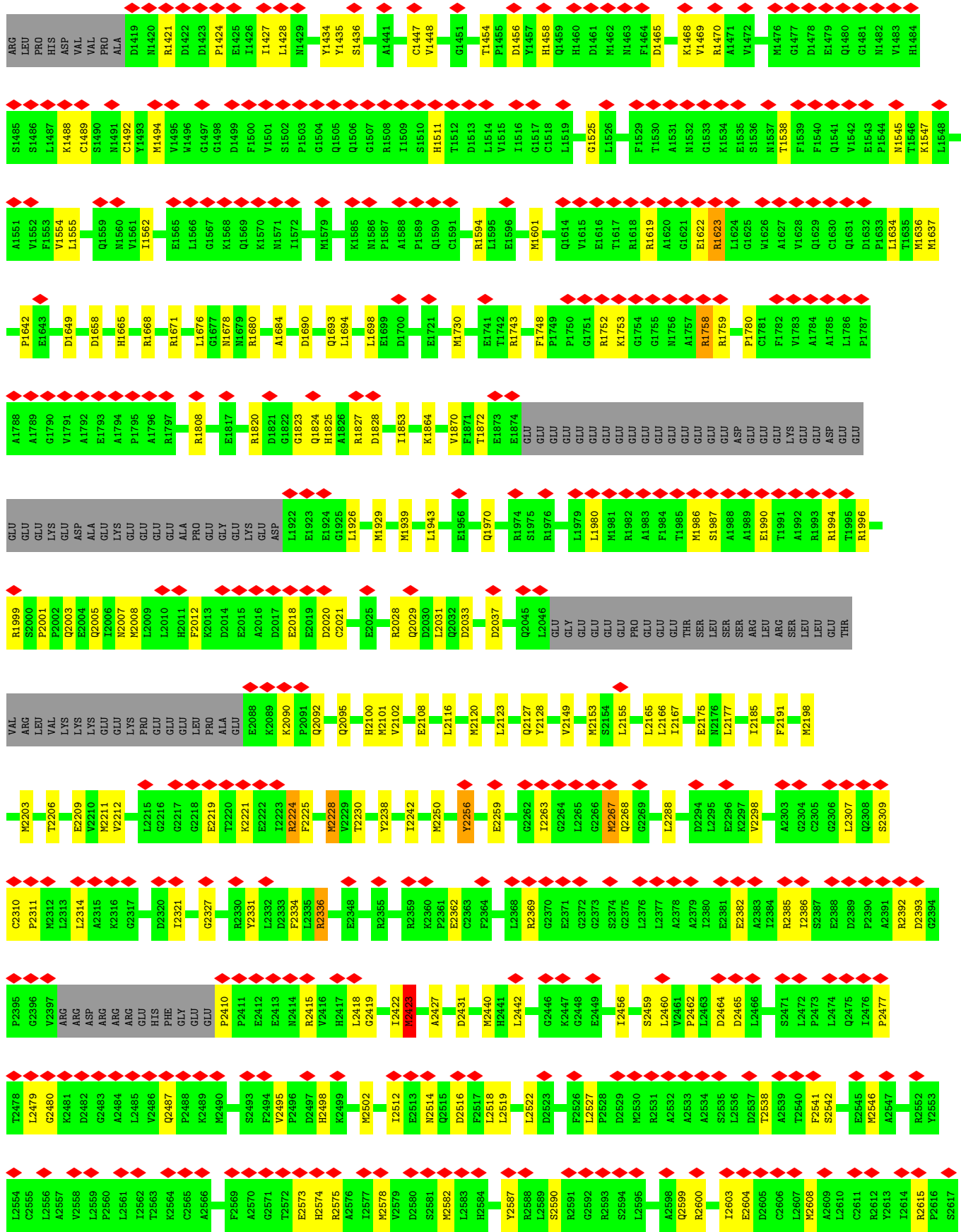
Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949	K951	K952
T953	K954	L955	P956	K957	T958	Y959	N960	N961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	Y975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	E989	E990	N991	A997	P998	R999	L1000	A1001	Q1002	G1004	W1005	S1006	Y1007	S1008	A1009	V1010	Q1011	D1012	I1013	P1014	A1015	R1016	
R1017	N1018	P1019	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	D1027	D1028	E1029	A1030	T1031	K1032	A1033	S1034	N1035	D1037	S1038	L1039	C1040	Q1041	A1042	N1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	L1053	E1054	P1055	P1056	D1057	Q1058	E1059	P1060	S1061	Q1062	V1063	E1064	N1065	Q1066	S1067	R1068	W1069	Q1070	R1071	V1072	E1078	K1079		
G1086	E1093	A1094	V1095	T1096	E1099	M1100	R1101	D1112	M1113	E1114	L1115	G1116	D1118	E1119	F1124	M1125	H1127	R1128	W1132	F1139	W1143	Q1144	S1145	G1146	D1147	G1150	D1154	L1155	T1156	E1157	T1163	L1164	N1165	G1166	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179											
R1180	E1181	I1182	E1183	I1184	G1185	D1186	L1189	L1202	G1205	Q1206	D1207	S1210	L1211	R1212	F1213	I1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1226	A1227	I1228	R1232	E1251	H1252	E1256	R1259	M1260	D1261	G1262	V1264	D1265	L1272	A1273	H1274	R1275	T1276	W1277	G1278	S1279	Q1280	M1281	S1282	L1283											
V1284	E1285	M1286	L1287	L1288	L1289	L1293	F1297	H1298	Q1299	H1300	F1301	R1302	C1303	T1304	ALA	GLY	ALA	ALA	THR	PRO	ARG	LEU	ALA	ALA	PRO	GLU	ASP	GLU	ALA	ARG	ALA	ALA	LEU	PRO	ASP	ASP	TYR	ASN	LEU	ARG	SER	ALA	GLY	GLY	TRP	GLY	GLY	ALA	GLU	GLY								
GLY	LYS	GLU	GLY	THR	ALA	LYS	GLY	PRO	THR	GLY	THR	PRO	GLN	VAL	GLU	ALA	GLN	PRO	VAL	ARG	ALA	ALA	GLU	ASN	GLY	LYS	ARG	ALA	ALA	LEU	PRO	ASP	ALA	LYS	LYS	ALA	ALA	LYS	THR	GLN	ALA	PRO	ALA	ALA	GLU	ALA												
LEU	PRO	ARG	LEU	PRO	HIS	ASP	VAL	VAL	PRO	ALA	D1419	N1420	R1421	D1422	D1423	P1424	E1425	I1426	I1427	L1428	N1429	Y1434	Y1435	S1436	A1441	C1447	V1448	G1451	T1454	P1455	D1456	Y1457	H1458	Q1459	H1460	D1461	M1462	N1463	F1464	D1465	K1466	V1469	R1470	A1471	V1472	M1476	G1477	D1478	Q1480	G1481	N1482							
V1483	H1484	S1485	S1486	L1487	K1488	C1489	S1490	N1491	C1492	Y1493	M1494	V1495	W1496	G1497	G1498	D1499	F1500	V1501	W1501	S1502	P1503	G1504	Q1505	Q1506	G1507	N1508	I1509	S1510	H1511	L1512	D1513	L1514	V1515	I1516	G1517	C1518	L1519	G1525	L1526	M1527	T1528	F1529	T1530	A1531	M1532	G1533	K1534	L1535	S1536	N1537	F1539	F1540	Q1541	V1542	P1544	M1545	T1546	
K1547	L1548	A1551	V1552	F1553	V1554	L1555	Q1559	N1560	V1561	I1562	E1565	L1566	G1567	K1568	Q1569	K1570	L1571	I1572	L1575	M1579	K1585	N1586	P1587	A1588	Q1590	C1591	R1594	L1595	E1596	M1601	Q1614	V1615	E1616	T1617	R1618	R1619	A1620	G1621	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	E1631	D1632									
M1636	M1637	P1642	E1643	D1649	S1654	D1658	H1665	R1668	R1671	L1676	G1677	M1678	N1679	R1680	A1684	D1690	Q1693	H1694	L1698	E1699	D1700	E1721	M1730	E1741	T1742	R1743	F1748	P1749	P1750	G1751	R1752	K1753	G1754	G1755	M1756	A1757	R1758	R1759	P1780	C1781	F1782																	
V1783	A1784	A1785	L1786	P1787	A1788	G1789	V1791	A1792	E1793	A1794	P1795	A1796	R1797	R1808	E1817	R1820	D1821	G1822	G1823	H1824	H1825	A1826	R1827	D1828	I1853	F1884	K1884	V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU							
LYS	GLU	ASP	GLU	GLU	GLU	LYS	ASP	ALA	GLU	LYS	GLU	GLU	GLU	ALA	PRO	GLU	GLY	LYS	GLU	ASP	L1922	E1923	E1924	G1925	L1926	M1929	M1939	L1943	E1956	Q1970	R1974	S1975	R1976	L1979	M1980	M1981	A1982	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991												

GLU	M9638	R3577	Q3456	D3396	K3336	M3276	C3216	V3156	F3096	K3036	H2976
GLU	Y3642	G3578	N3457	F3397	R3337	L3277	S3217	I3157	E3097	E3037	L2977
	D3666	L3579	F3458	F3398	L3338	C3278	V3218	L3158	E2978	M3038	E2978
		P3680	V3459	S3399	A3339	S3279	Y3219	D3159	A3099	I3039	A2979
		G3581	V3460	V3400	F3340	Y3280	Y3220	S3160	V2980	T3040	V2980
		R3582	Q3461	L3401	F3341	L3281	T3221	V3161	V2981	S3041	V2981
		E3683	N3462	C3402	A3342	Q3162	K3222	Q3162	S2982	L3042	S2982
		E3684	E3463	R3403	Q3343	V3163	S3223	V3163	S2983	F3043	S2983
		D3685	I3464	D3404	Q3344	S3164	P3224	S3164	G2984	C3044	G2984
		A3686	N3465	L3405	I3345	C3165	R3225	C3165	R2985	K3045	R2985
		A3687	N3466	Y3406	V3346	Y3166	E3226	Y3166	V2986	L3046	V2986
		P3688	M3467	A3407	S3347	R3287	R3227	V3107	E2987	A3047	E2987
		P3689	S3468	L3408	R3348	G3288	A3228	E3108	R2988	A3048	R2988
		E3690	F3469	P3410	R3350	P3289	I3229	N3109	S2989	L3049	S2989
		K3691	L3470	P3411	R3351	E3290	L3230	L3110	P2990	V3050	P2990
		L3692	T3471	L3411	P3351	A3291	G3231	R3111	H2991	R3051	H2991
		V3693	A3472	L3412	E3352	P3292	L3232	L3112	E2992	H3052	E2992
		R3694	D3473	I3413	L3353	P3293	P3233	G3113	Q2993	R3053	Q2993
		S3695	S3474	R3414	L3354	P3294	N3234	K3114	E2994	V3054	E2994
		V3696	K3475	Y3415	H3355	A3295	S3235	L3175	I2995	S3055	I2995
		Q3697	S3476	V3416	S3356	L3296	V3236	G3176	K2996	F3056	K2996
		E3698	K3477	D3417	H3357	P3297	E3237	T3177	F2997	F3057	F2997
		V3699	M3478	N3418	F3358	A3298	E3238	ALA	F2998	G3058	F2998
		V3700	A3479	N3419	I3359	G3299	M3239	ARG	A2999	T3059	A2999
		L3603	LYS	R3420	P3360	A3300	C3240	THR	K3000	D3060	K3000
		L3604	ALA	R3421	T3361	P3301	P3241	GLN	K3001	A3061	I3001
		Y3604	GLY	H3422	I3362	R3302	D3242	VAL	L3002	P3062	L3002
		H3605	ASP	W3423	G3363	P3303	I3243	G3124	L3003	A3063	L3003
		L3606	ALA	L3424	R3364	R3304	I3244	V3125	P3004	V3064	P3004
		E3607	SER	T3425	L3365	T3305	P3245	G3126	L3005	V3065	L3005
		Q3608	GLY	E3426	R3366	A3306	L3246	Q3127	I3006	N3066	I3006
		T3609	GLY	P3427	K3367	V3307	L3247	R3128	N3007	C3067	N3007
		E3610	ASP	N3428	R3368	R3308	R3248	P3188	Q3008	L3068	Q3008
		H3611	GLN	A3429	A3369	S3309	R3249	A3189	Q3009	H3069	Q3009
		P3612	GLU	N3430	G3370	S3309	L3249	Y3131	F3010	I3070	F3010
		V3613	ARG	A3431	R3371	D3310	M3250	L3130	S3011	I3071	S3011
		K3614	THR	A3432	H3372	H3311	A3251	G3191	N3012	L3071	N3012
		S3615	LYS	E3433	V3373	N3312	D3252	E3192	H3013	A3072	H3013
		K3616	LYS	F3434	V3374	L3312	I3253	C3193	C3014	R3073	C3014
		L3617	LYS	R3435	A3375	N3313	I3254	L3194	L3015	S3074	L3015
		A3618	ASP	F3436	E3376	L3314	G3254	A3195	L3016	L3075	L3016
		V3619	GLN	R3437	E3377	L3315	G3255	R3196	F3017	D3076	F3017
		W3620	ARG	M3437	Q3378	L3316	L3256	L3197	L3018	A3077	L3018
		H3621	THR	Y3438	Q3379	N3318	A3257	A3199	S3019	R3078	S3019
		K3622	LYS	F3439	R3380	L3319	E3259	A3198	T3020	T3079	T3020
		L3623	LYS	I3441	K3381	L3320	G3260	A3200	P3021	V3080	P3021
		L3624	LYS	L3442	L3381	R3321	A3261	M3201	A3022	M3081	A3022
		S3625	GLU	L3443	E3382	I3322	R3262	P3202	K3023	K3082	K3023
		K3626	ALA	Y3444	K3384	V3324	Y3263	V3203	V3024	S3083	V3024
		Q3627	ALA	W3446	A3385	N3325	T3264	A3204	L3025	G3084	L3025
		R3628	ALA	S3447	E3386	E3265	E3265	F3205	G3026	P3085	G3026
		R3629	LYS	S3448	E3387	N3326	M3266	L3206	S3027	E3086	S3027
		A3631	LYS	H3449	A3388	L3327	P3267	A3148	G3028	I3087	G3028
		V3632	LYS	N3450	E3389	I3329	H3268	Q3209	H3029	V3088	H3029
		V3633	LYS	F3451	G3390	D3330	I3270	L3210	H3030	K3089	H3030
		A3634	LYS	K3452	E3391	E3331	I3271	N3211	A3031	A3090	A3031
		C3635	LYS	R3453	L3392	A3332	I3272	E3212	S3032	G3091	S3032
		F3636	LYS	E3454	L3393	T3333	T3273	Y3213	H3033	R3093	H3033
		R3637	LYS	E3455	V3394	A3334	L3274	A3214	K3034	S3094	K3034
					R3395	M3335	P3275	A3215	E3035	F3095	E3035

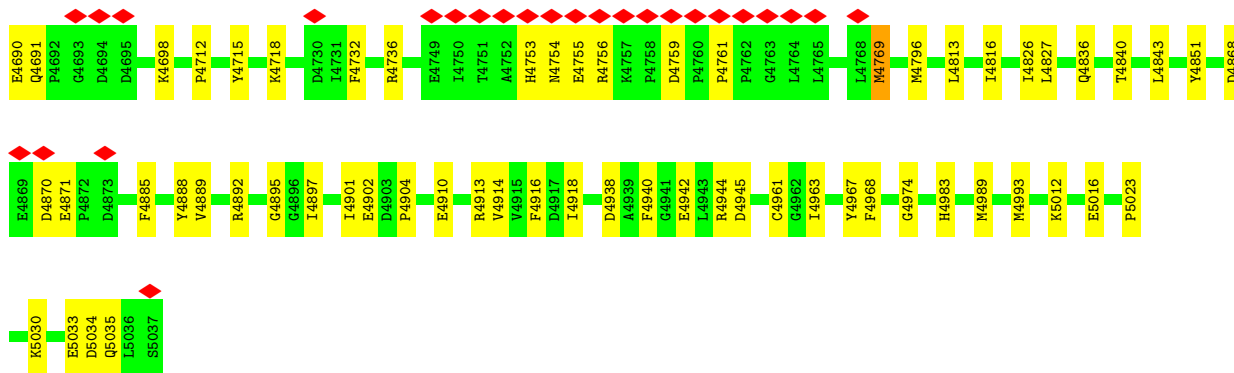


● Molecule 1: Ryanodine receptor 1

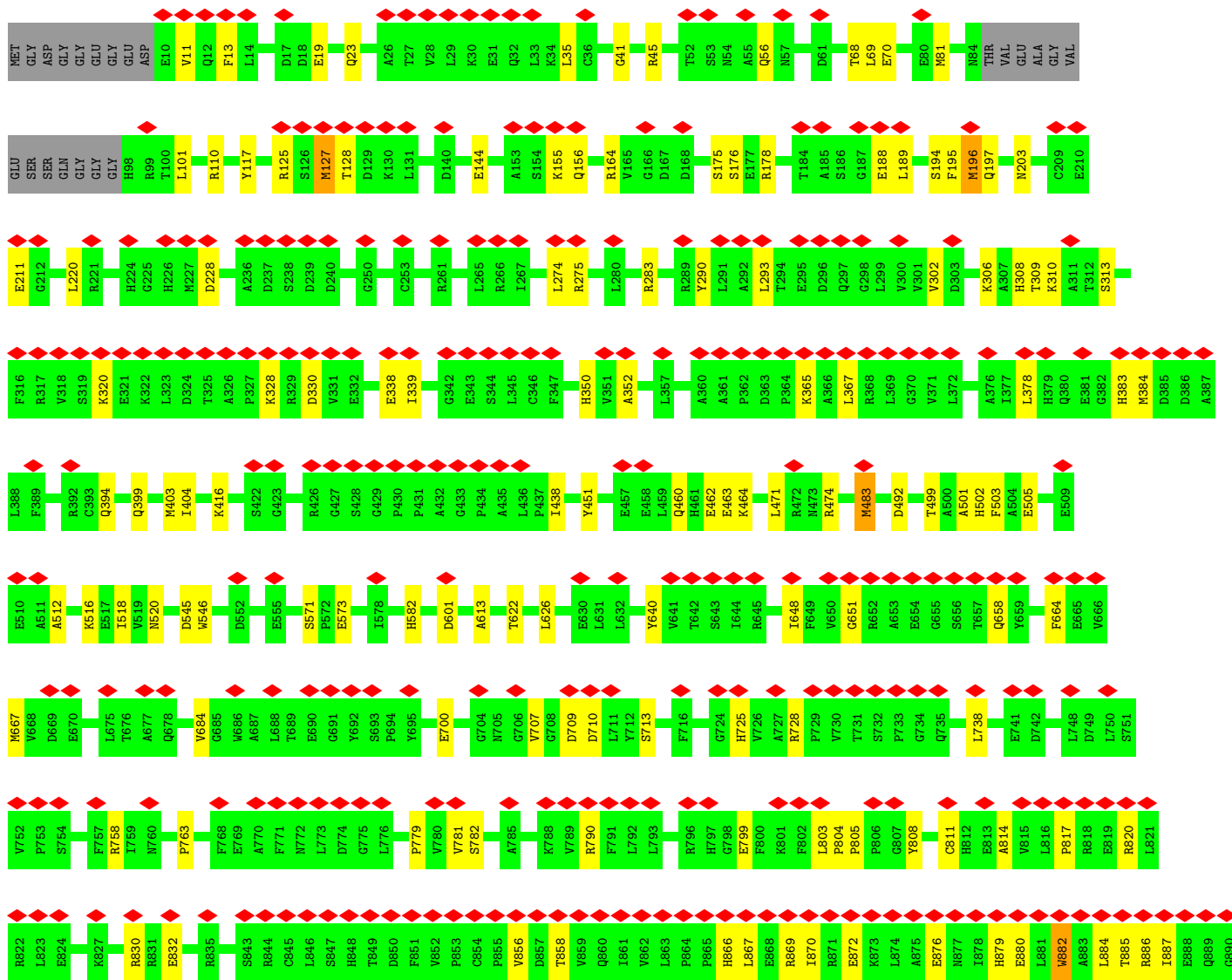




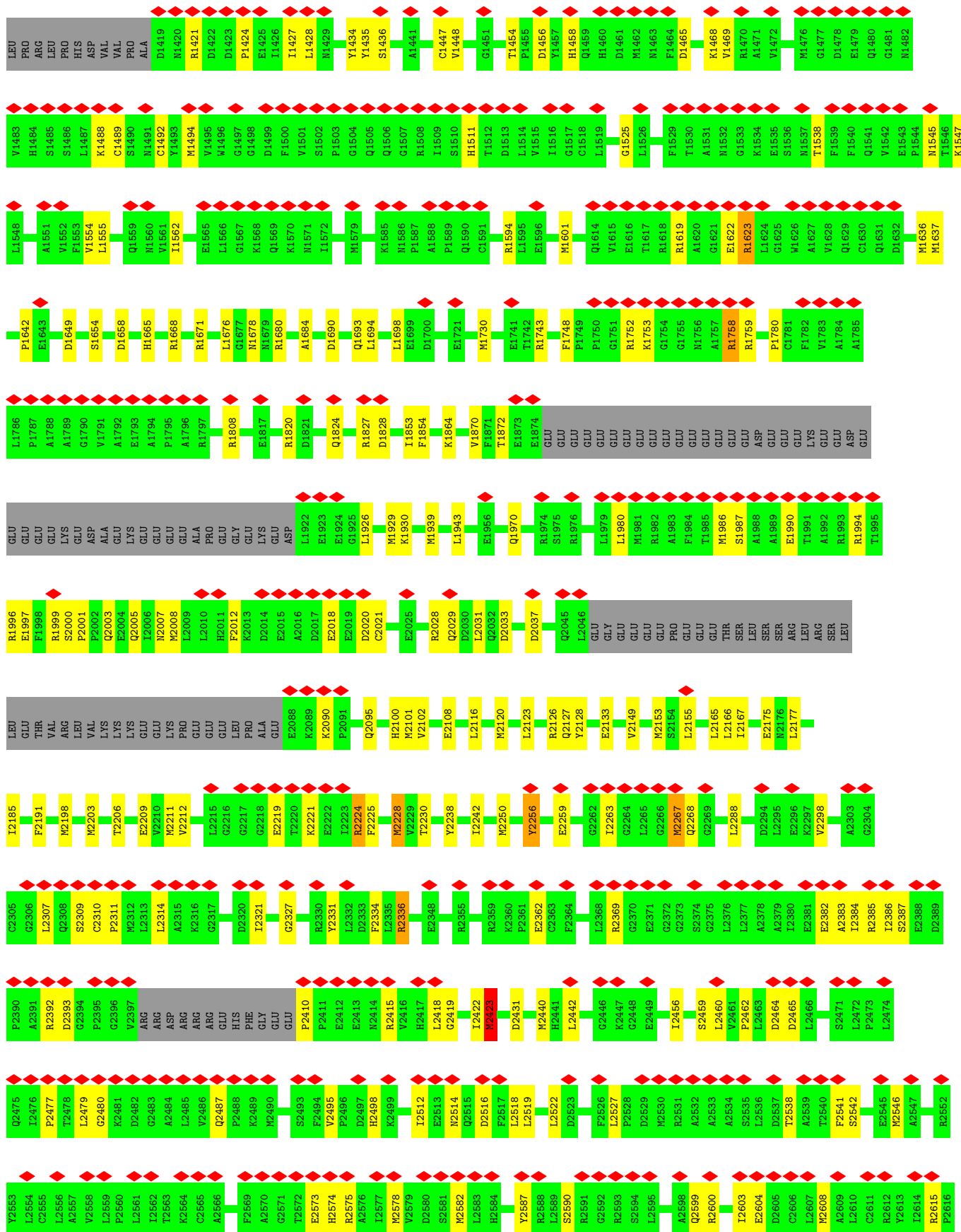
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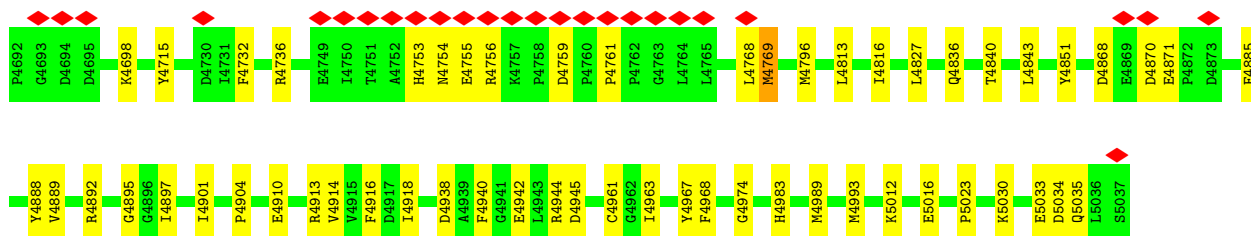
● Molecule 1: Ryanodine receptor 1



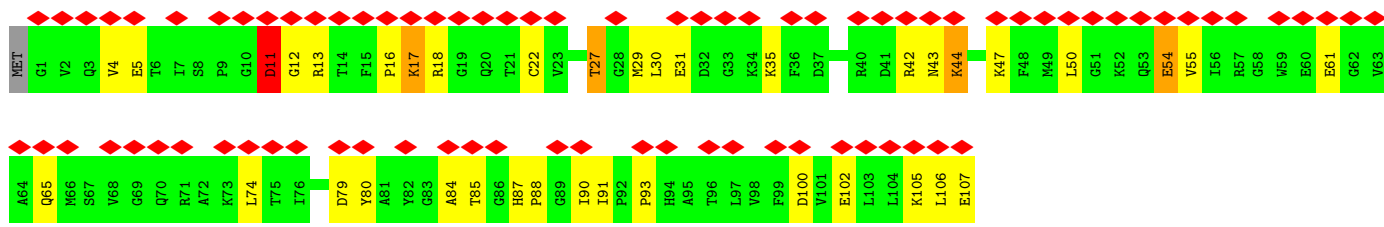
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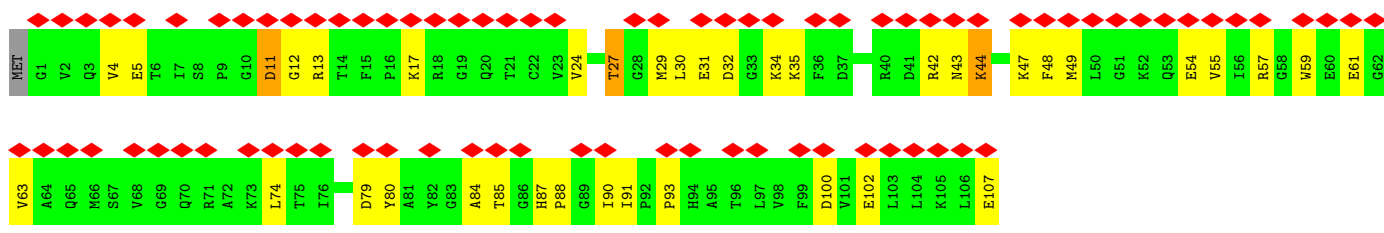
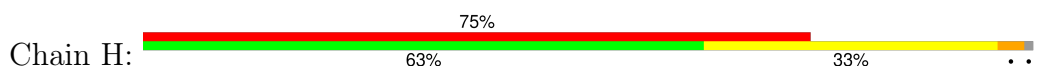
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F2679	W2680	G2681	I2682	F2683	D2684	S2685	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	Y2696	R2697	M2698	A2699	M2700	P2701	C2702	L2703	C2704	A2705	I2706	A2707	G2708	A2709	L2710	P2711	P2712	D2713	Y2714	W2715	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2794	P2795	D2796	P2797	R2798		
P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	G2767	F2768	D2769	K2770	I2771	D2772	K2773	N2774	W2775	A2776	Y2777	G2778	L2779	S2780	I2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	L2796	F2797	S2798		
E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	G2828	E2829	E2830	GLU	GLU	ARG	THR	GLU	L2894	L2895	L2896	L2897	L2898	L2899	L2900	L2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	A2913	K2914	E2915	K2916	A2917	R2918	
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	W2886	R2887	G2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	E2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	A2913	K2914	E2915	K2916	A2917	R2918			
D2919	R2920	E2921	K2922	S2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	W2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	L2940	L2941	D2942	T2943	S2944	S2945	L2946	E2947	E2948	E2949	E2950	E2951	K2952	R2953	R2954	F2955	E2956	F2957	G2958	F2959	L2960	Q2961	Q2962	L2963	L2964	R2965	W2966	W2967	D2968	T2969	S2970	Q2971	E2972	F2973	T2974	A2975	H2976	L2977	E2978
A2979	V2980	V2981	S2982	S2983	Q2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	I2995	K2996	F2997	P2998	A2999	K3000	I3001	L3002	L3003	P3004	L3005	I3006	N3007	Q3008	S3009	F3010	S3011	N3012	H3013	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	P3021	Q3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	N3033	K3034	E3035	K3036	E3037	H3038		
I3039	T3040	S3041	L3042	F3043	C3044	K3045	L3046	A3047	L3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3061	P3062	A3063	V3064	V3065	N3066	C3067	L3068	H3069	I3070	L3071	A3072	R3073	S3074	L3075	D3076	A3077	R3078	F3079	V3080	M3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	K3089	A3090	G3091	L3092	R3093	S3094	F3095	F3096	E3097	S3098		
A3099	S3100	E3101	D3102	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	K3114	Y3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	K3126	Q3127	N3128	L3129	T3130	Y3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	T3141	L3142	L3143	F3144	Q3145	H3146	I3147	A3148	Q3149	H3150	Q3151	F3152	G3153	N3154	D3155	V3156	I3157	L3158		
D3159	D3160	V3161	Q3162	S3163	S3164	C3165	V3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181	Y3182	V3183	E3184	K3185	L3186	R3187	F3188	A3189	L3190	G3191	E3192	C3193	L3194	A3195	R3196	A3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	N3213	Y3214	L3215	A3216	C3216	S3217	V3218	
Y3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	C3240	P3241	D3242	I3243	P3244	V3245	L3246	D3247	R3248	L3249	M3250	A3251	L3252	I3253	G3254	G3255	L3256	L3257	E3258	S3259	G3260	A3261	R3262	Y3263	T3264	E3265	N3266	P3267	H3268	V3269	I3270	E3271	L3272	T3273	L3274	P3275	N3276	L3277	C3278		
S3279	Y3280	L3281	P3282	R3283	V3284	W3285	E3286	R3287	G3288	P3289	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	V3307	T3308	S3309	D3310	H3311	L3312	N3313	S3314	L3315	L3316	G3317	N3318	I3319	L3320	L3321	I3322	I3323	V3324	N3325	N3326	G3328	I3329	D3330	E3331	A3332	L3333	W3334	M3335	K3336	R3337	F3338			
A3339	V3340	F3341	A3342	Q3343	P3344	I3345	V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	L3354	H3355	S3356	H3357	F3358	I3359	P3360	T3361	L3362	K3363	L3364	L3365	R3366	K3367	R3368	A3369	G3370	H3371	V3372	V3373	A3374	E3375	E3376	E3377	G3378	L3379	R3380	L3381	E3382	E3383	V3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	F3398		



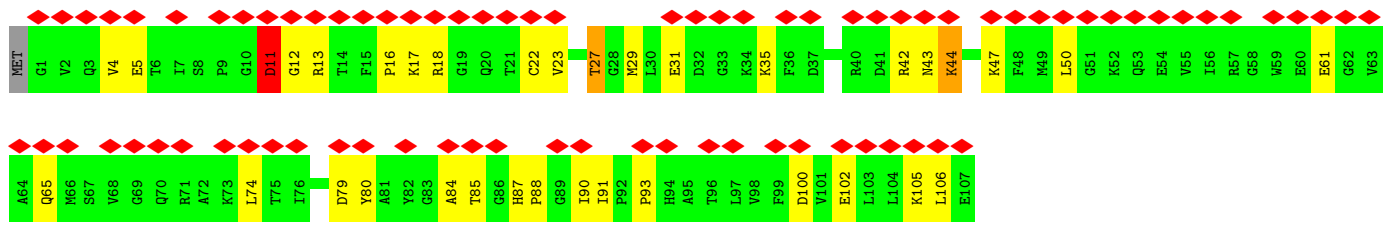
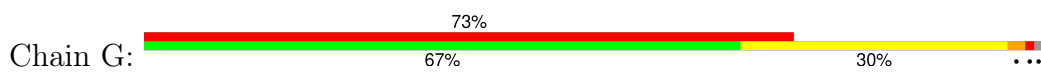
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



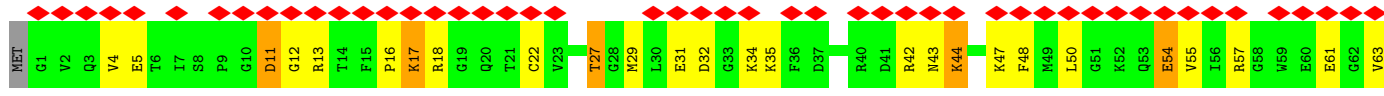
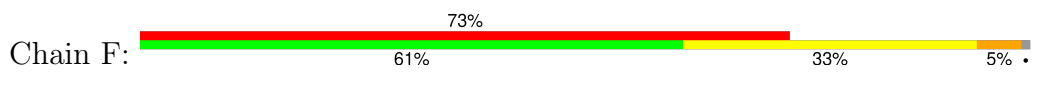
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

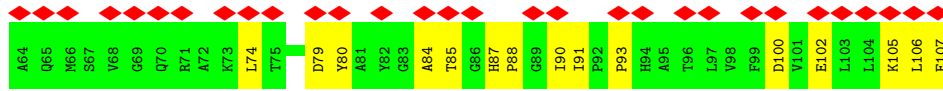


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.395	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	423.424, 423.424, 423.424	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1BD5, ATP, ZN, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/35977	0.51	7/48726 (0.0%)
1	B	0.34	0/35977	0.51	7/48726 (0.0%)
1	C	0.34	0/35977	0.51	7/48726 (0.0%)
1	D	0.34	0/35977	0.51	7/48726 (0.0%)
2	E	0.34	0/850	0.60	1/1146 (0.1%)
2	F	0.34	0/850	0.60	0/1146
2	G	0.34	0/850	0.60	1/1146 (0.1%)
2	H	0.34	0/850	0.59	0/1146
All	All	0.34	0/147308	0.51	30/199488 (0.0%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3603	LEU	CA-CB-CG	8.06	133.84	115.30
1	B	3603	LEU	CA-CB-CG	8.05	133.82	115.30
1	D	3603	LEU	CA-CB-CG	8.05	133.82	115.30
1	C	3603	LEU	CA-CB-CG	8.05	133.81	115.30
1	D	3623	LEU	CA-CB-CG	6.22	129.61	115.30

There are no chirality outliers.

There are no planarity outliers.

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	35150	0	34797	577	0
1	B	35150	0	34797	567	0
1	C	35150	0	34797	570	0
1	D	35150	0	34797	579	0
2	E	831	0	831	28	0
2	F	831	0	831	30	0
2	G	831	0	831	25	0
2	H	831	0	831	21	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0
6	C	15	0	0	0	0
6	D	15	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	144120	0	142560	2359	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 8.

The worst 5 of 2359 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:2765:LYS:HZ3	1:C:2857:PRO:HB2	1.39	0.88
2:F:18:ARG:HH21	2:F:50:LEU:HD22	1.43	0.83
1:D:3539:ARG:HH12	1:D:3542:LEU:HD22	1.43	0.83
2:E:61:GLU:OE2	2:E:61:GLU:N	2.12	0.82
1:A:3539:ARG:HH12	1:A:3542:LEU:HD22	1.43	0.82

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	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	B	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	C	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	D	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
2	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17960/20580 (87%)	17398 (97%)	562 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	3836/4276 (90%)	3738 (97%)	98 (3%)	41	64
1	B	3836/4276 (90%)	3738 (97%)	98 (3%)	41	64
1	C	3836/4276 (90%)	3738 (97%)	98 (3%)	41	64
1	D	3836/4276 (90%)	3738 (97%)	98 (3%)	41	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	89/90 (99%)	78 (88%)	11 (12%)	4	16
2	F	89/90 (99%)	77 (86%)	12 (14%)	3	13
2	G	89/90 (99%)	78 (88%)	11 (12%)	4	16
2	H	89/90 (99%)	78 (88%)	11 (12%)	4	16
All	All	15700/17464 (90%)	15263 (97%)	437 (3%)	41	62

5 of 437 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3899	PHE
1	D	2267	MET
1	C	2738	ARG
1	B	4769	MET
1	D	1044	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2092	GLN
1	C	4009	GLN
1	B	4009	GLN
1	D	991	ASN
1	D	4009	GLN

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

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	D	5301	-	28,33,33	0.66	0	34,52,52	0.99	2 (5%)
6	A1BD5	B	5304	-	16,16,16	0.96	0	21,23,23	0.73	0
6	A1BD5	A	5304	-	16,16,16	0.97	0	21,23,23	0.73	0
3	ATP	B	5301	-	28,33,33	0.65	0	34,52,52	0.99	2 (5%)
3	ATP	C	5301	-	28,33,33	0.67	0	34,52,52	1.00	2 (5%)
6	A1BD5	C	5304	-	16,16,16	0.96	0	21,23,23	0.73	0
3	ATP	A	5301	-	28,33,33	0.66	0	34,52,52	0.99	2 (5%)
6	A1BD5	D	5304	-	16,16,16	0.96	0	21,23,23	0.73	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
3	ATP	D	5301	-	-	9/18/38/38	0/3/3/3
6	A1BD5	B	5304	-	-	0/4/4/4	0/2/2/2
6	A1BD5	A	5304	-	-	0/4/4/4	0/2/2/2
3	ATP	B	5301	-	-	9/18/38/38	0/3/3/3
3	ATP	C	5301	-	-	9/18/38/38	0/3/3/3
6	A1BD5	C	5304	-	-	0/4/4/4	0/2/2/2
3	ATP	A	5301	-	-	9/18/38/38	0/3/3/3
6	A1BD5	D	5304	-	-	0/4/4/4	0/2/2/2

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(°)
3	C	5301	ATP	C4'-O4'-C1'	-4.65	105.67	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5301	ATP	C4'-O4'-C1'	-4.59	105.72	109.92
3	A	5301	ATP	C4'-O4'-C1'	-4.59	105.72	109.92
3	D	5301	ATP	C4'-O4'-C1'	-4.58	105.73	109.92
3	C	5301	ATP	C5-C6-N6	2.36	123.90	120.31

There are no chirality outliers.

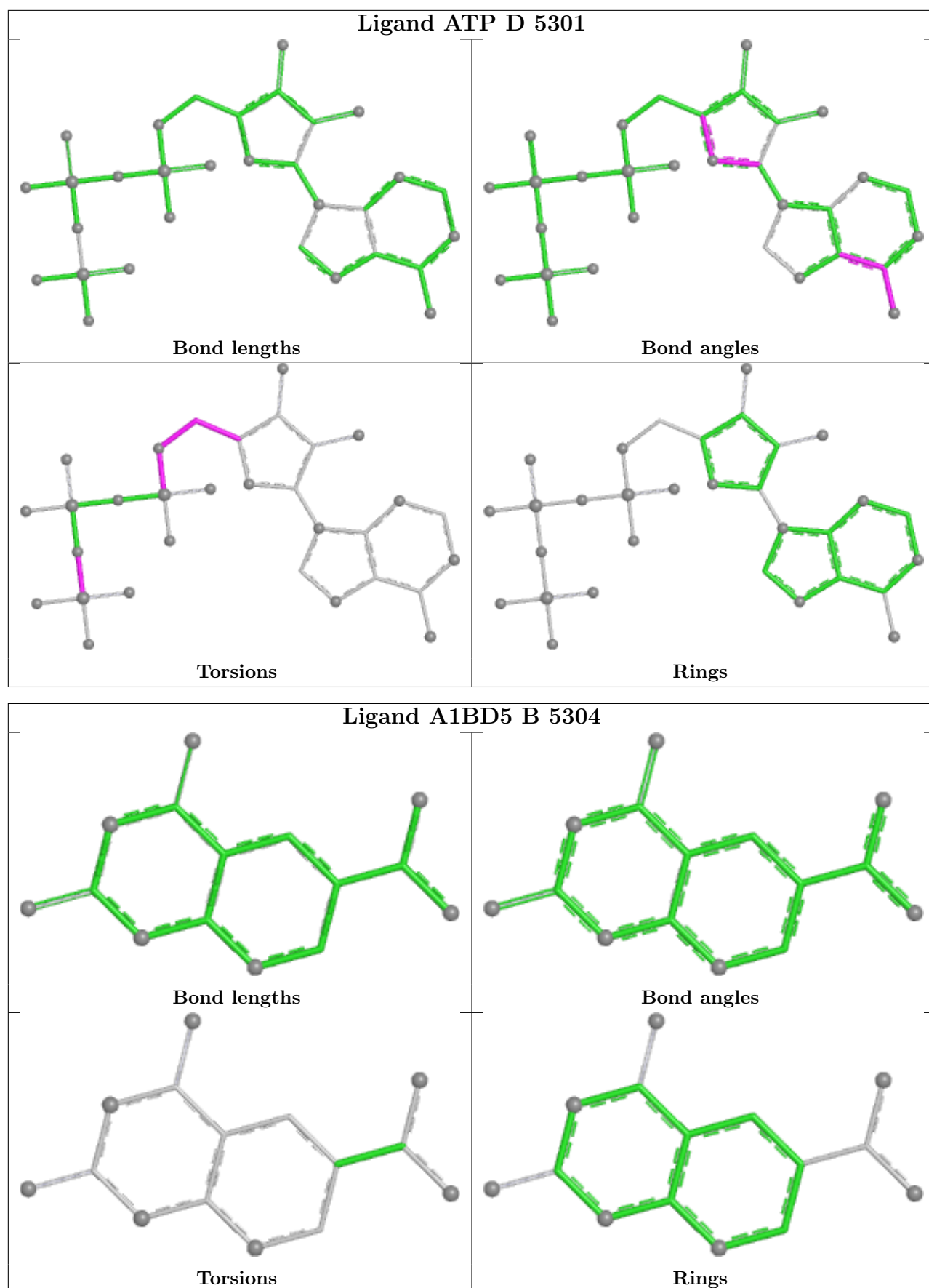
5 of 36 torsion outliers are listed below:

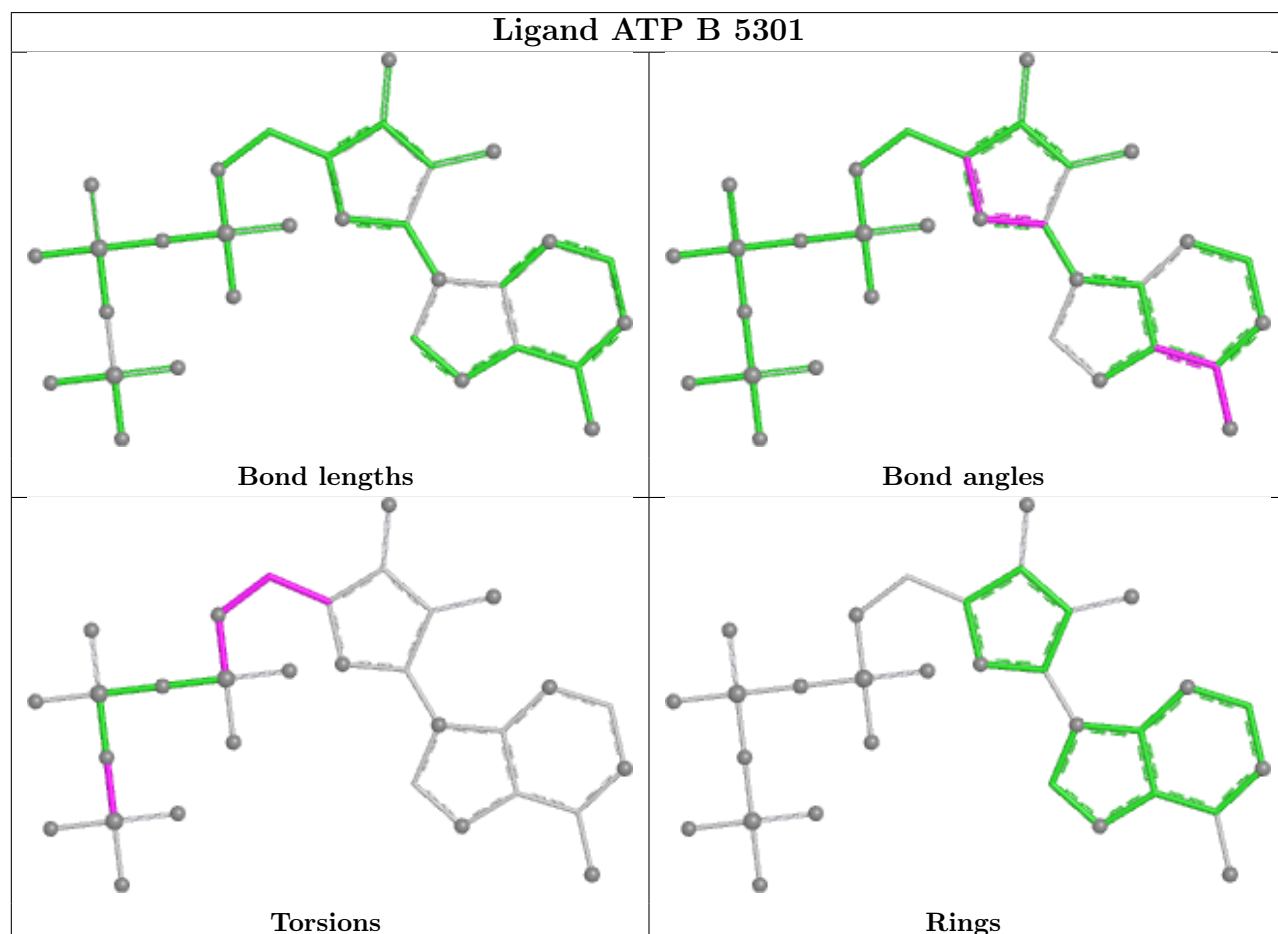
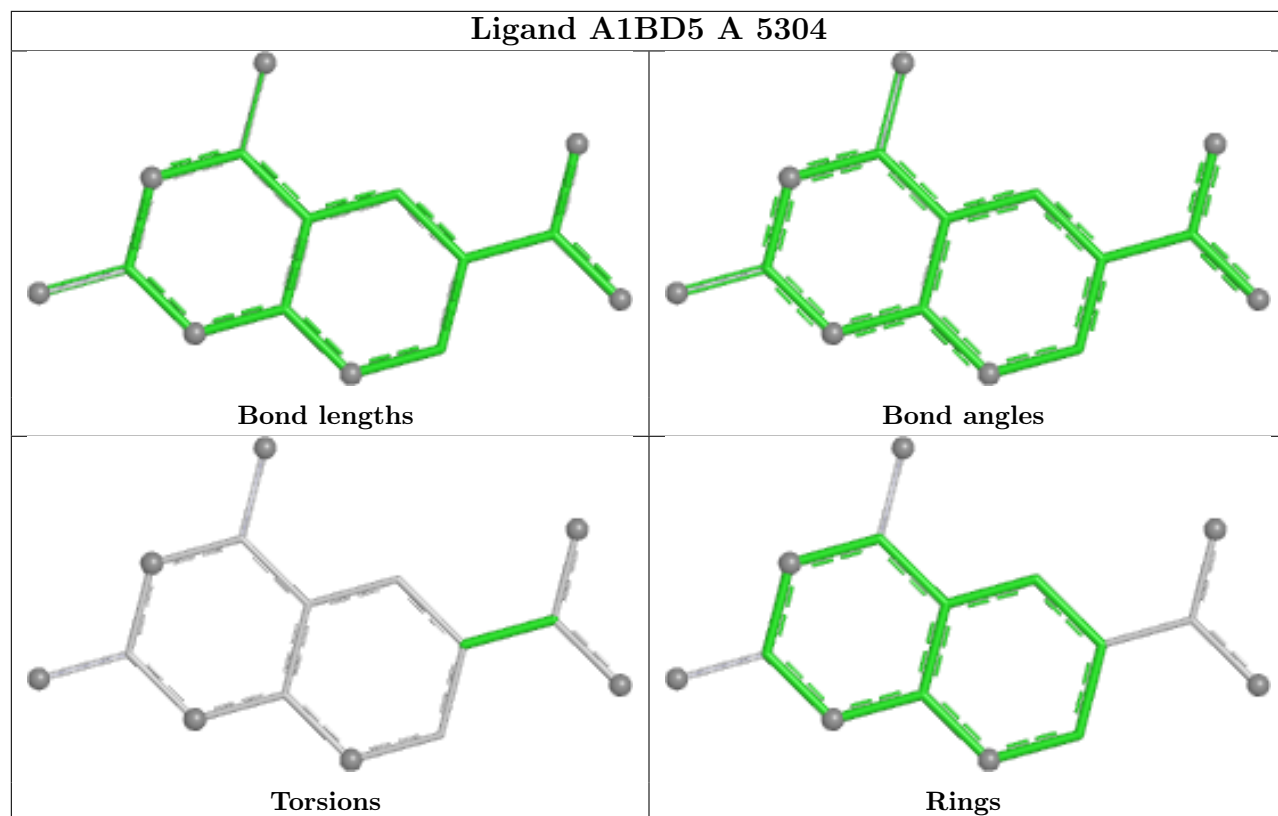
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	PB-O3B-PG-O2G
3	A	5301	ATP	C5'-O5'-PA-O1A
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	PB-O3B-PG-O2G

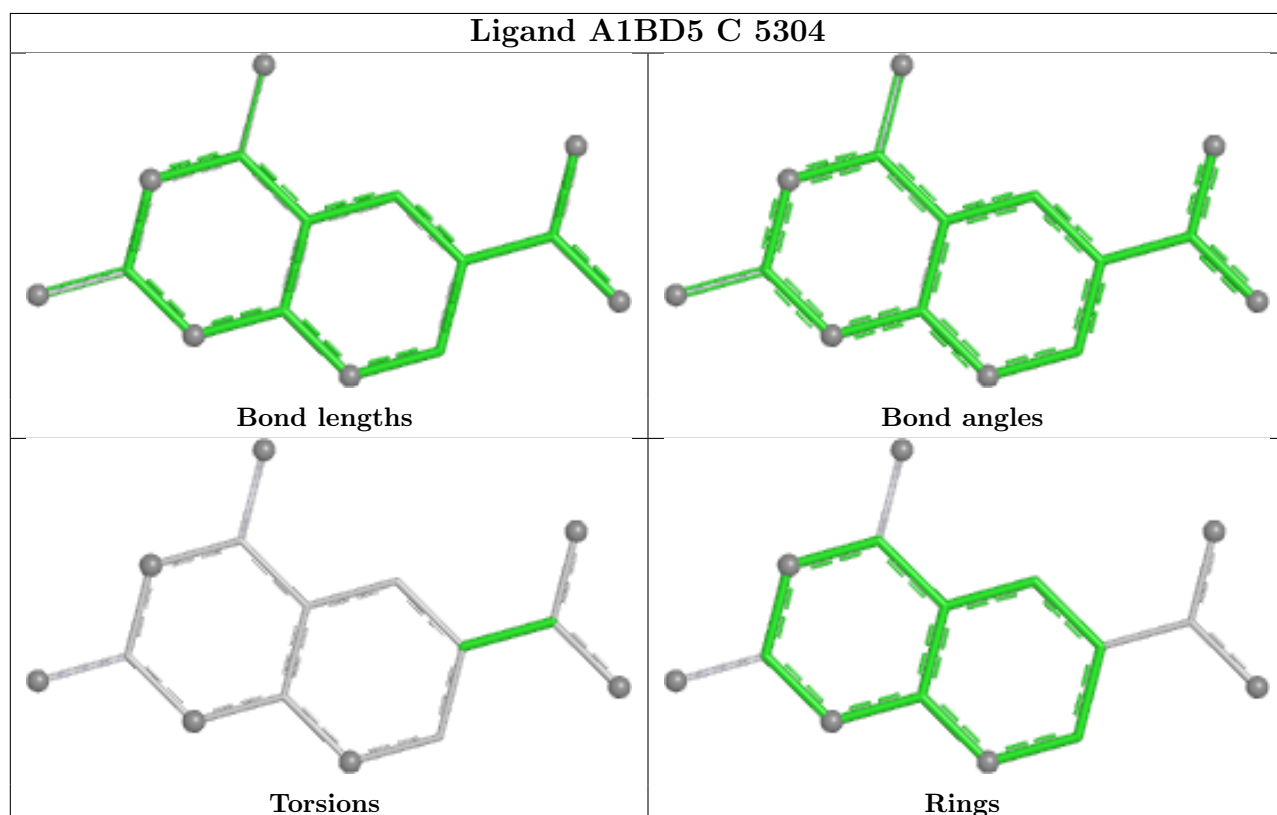
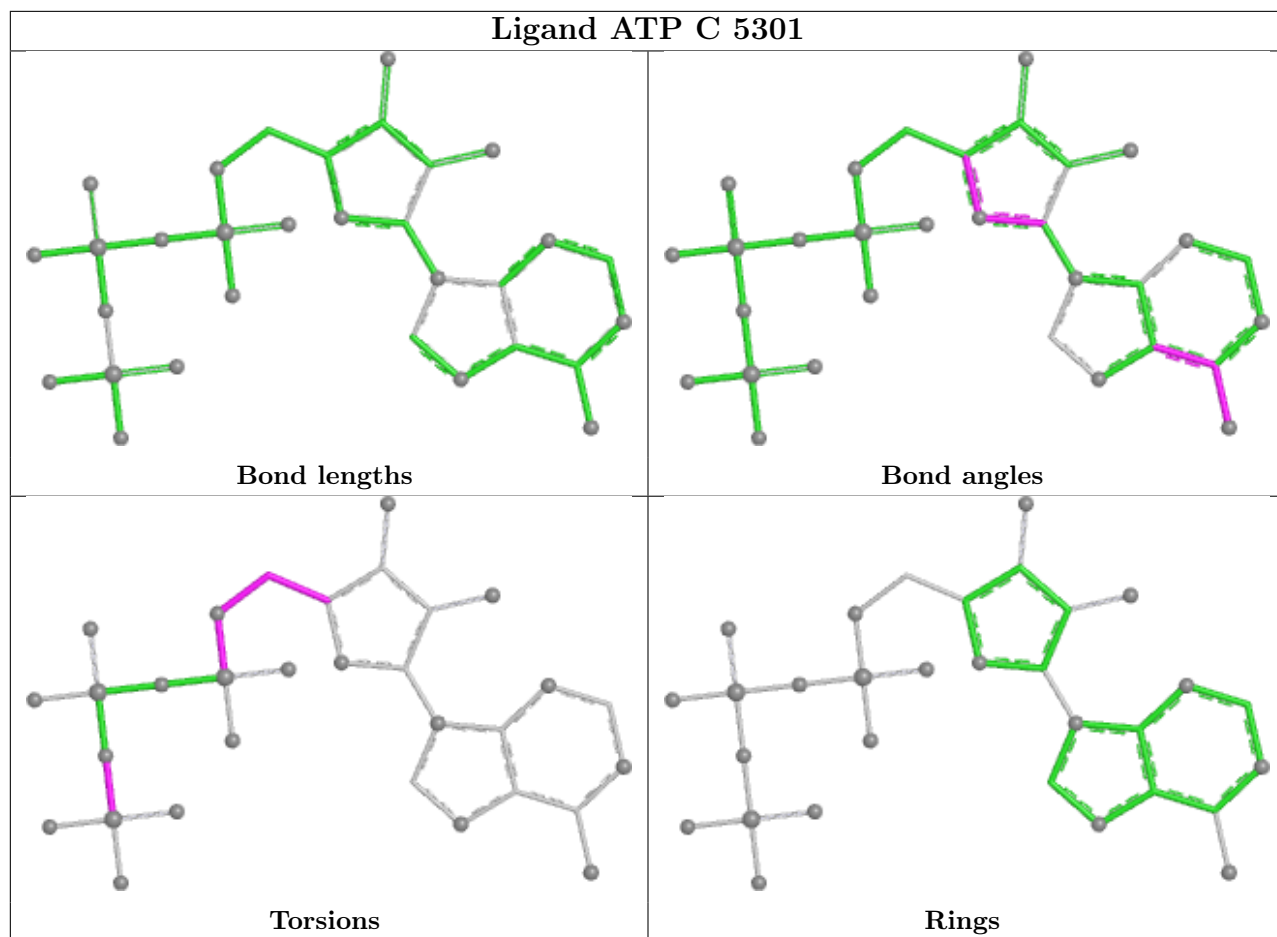
There are no ring outliers.

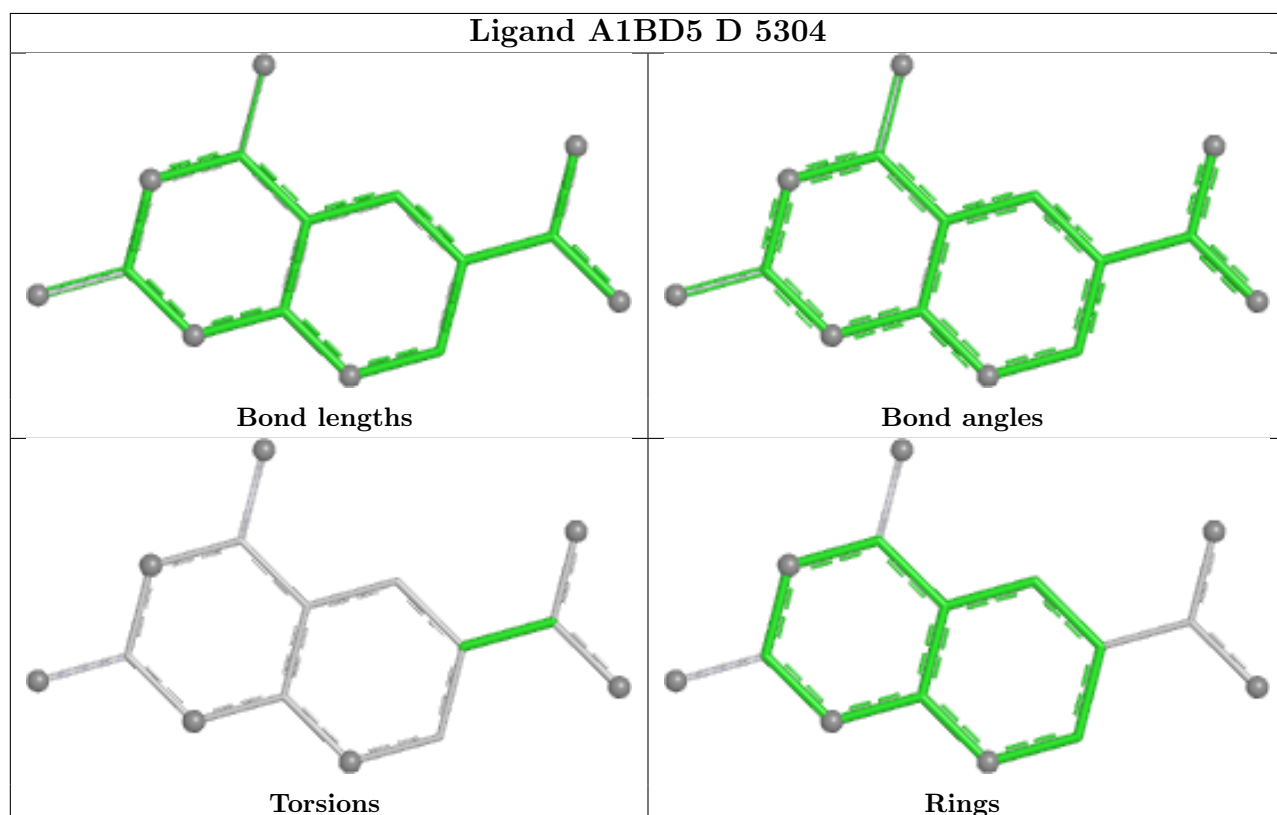
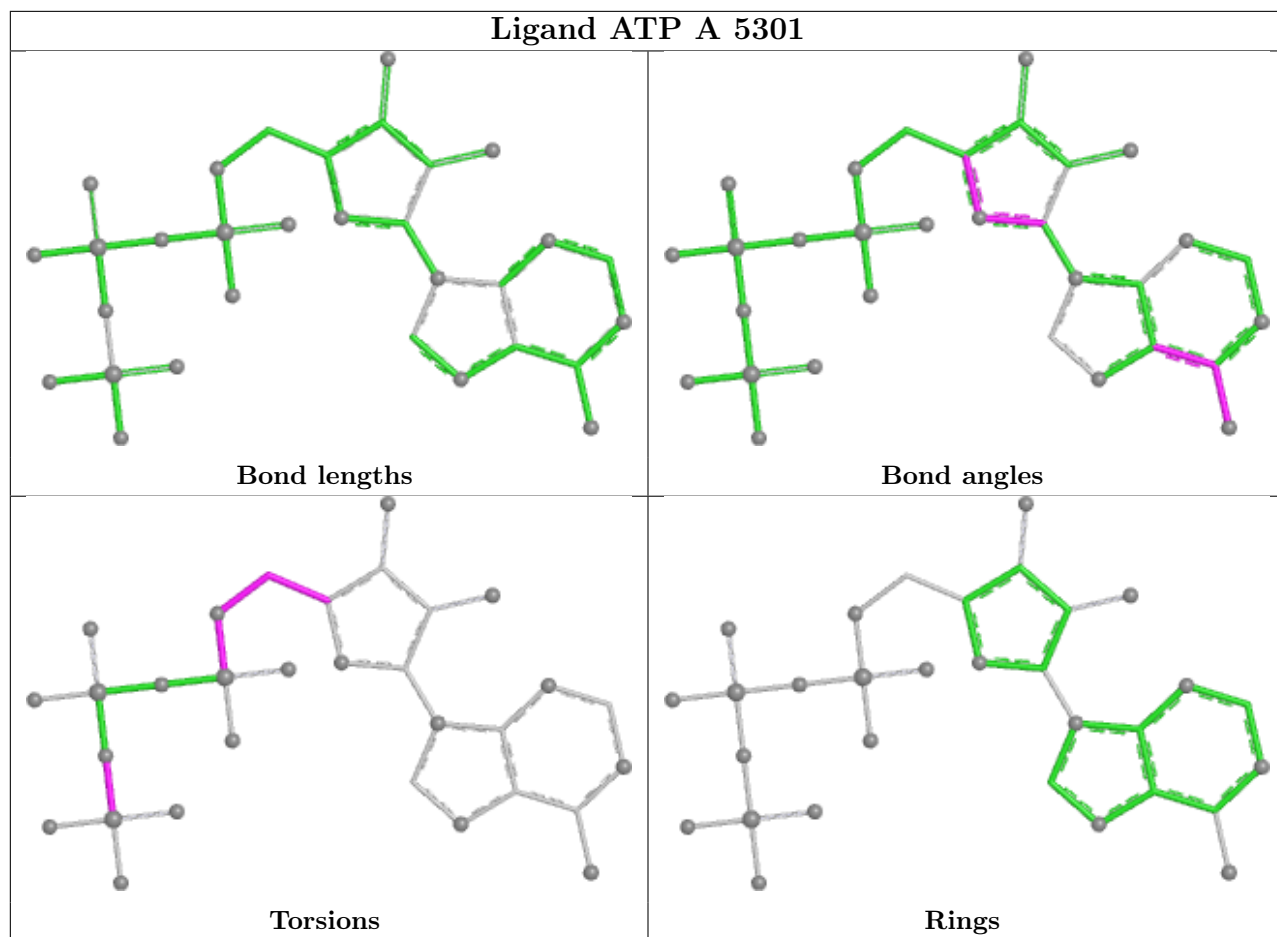
No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

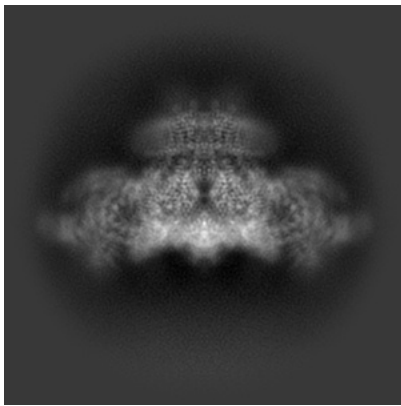
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47394. These allow visual inspection of the internal detail of the map and identification of artifacts.

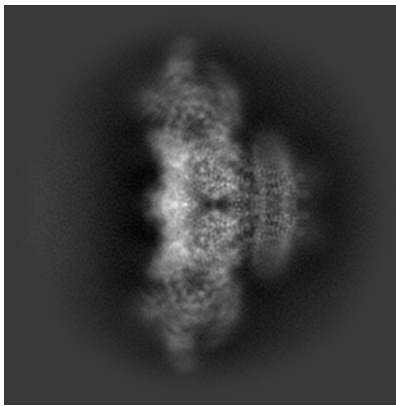
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

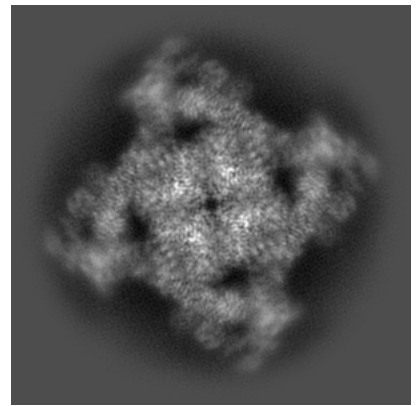
6.1.1 Primary map



X

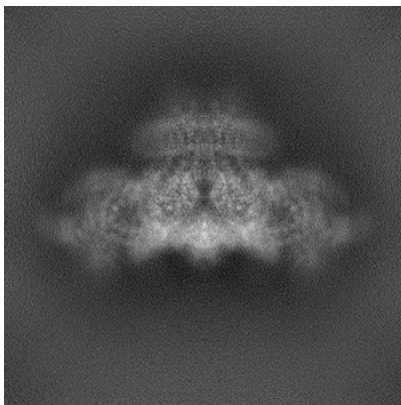


Y

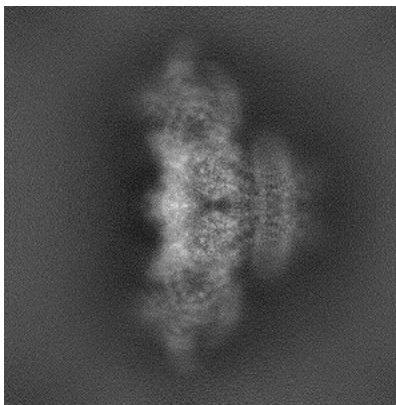


Z

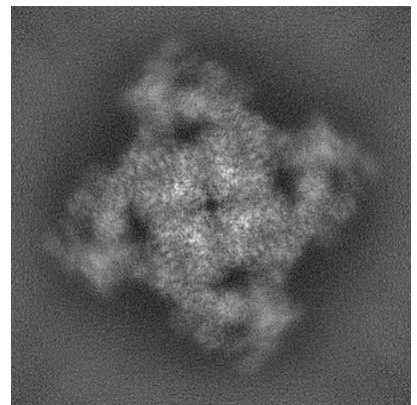
6.1.2 Raw map



X



Y

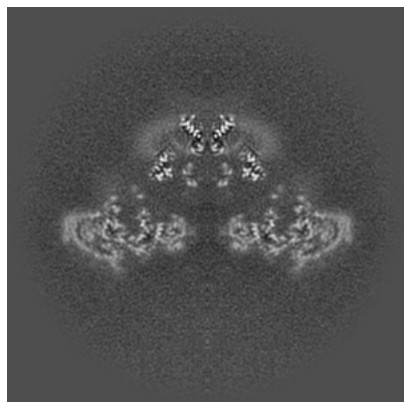


Z

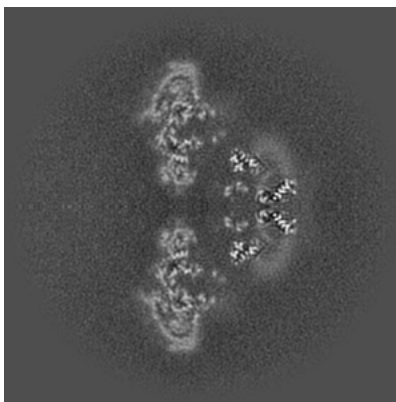
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

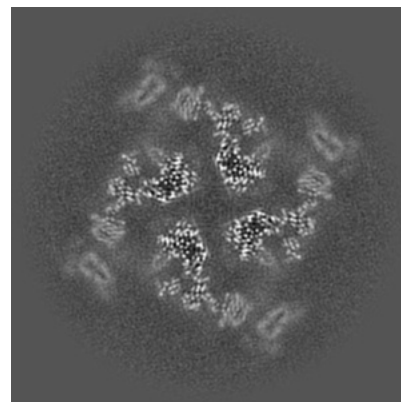
6.2.1 Primary map



X Index: 256

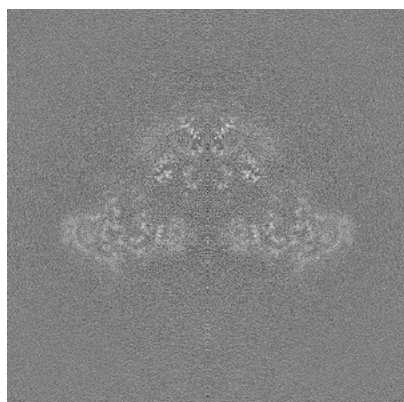


Y Index: 256

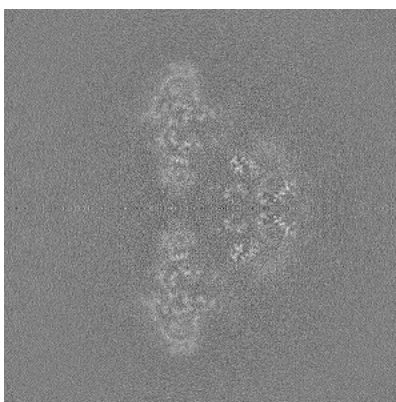


Z Index: 256

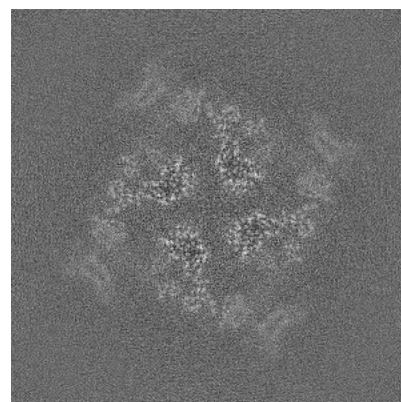
6.2.2 Raw map



X Index: 256



Y Index: 256

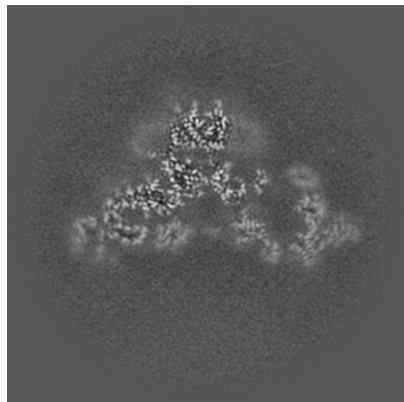


Z Index: 256

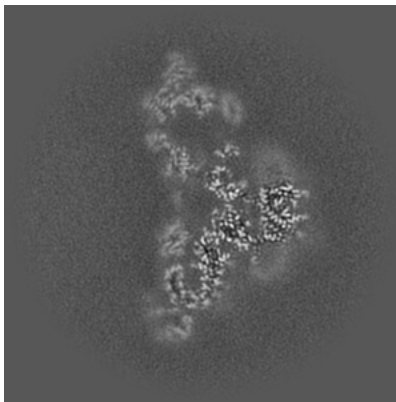
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

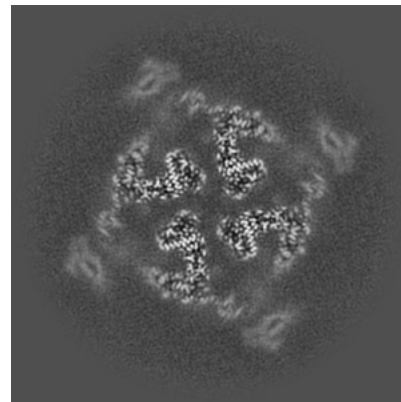
6.3.1 Primary map



X Index: 239

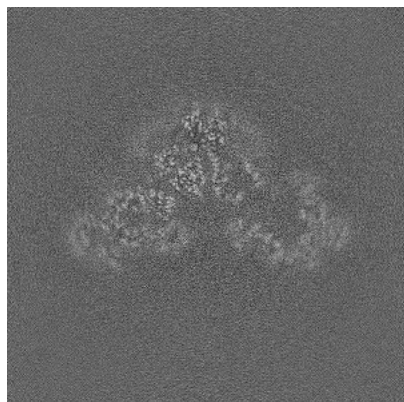


Y Index: 273

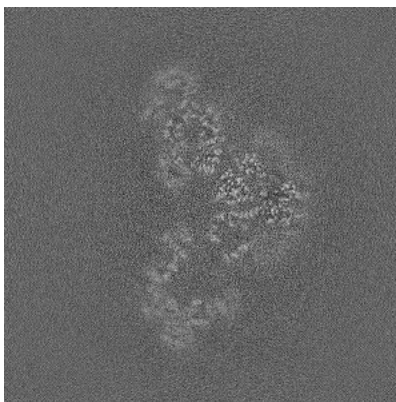


Z Index: 265

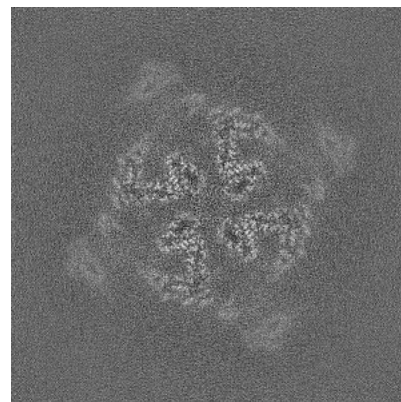
6.3.2 Raw map



X Index: 244



Y Index: 244

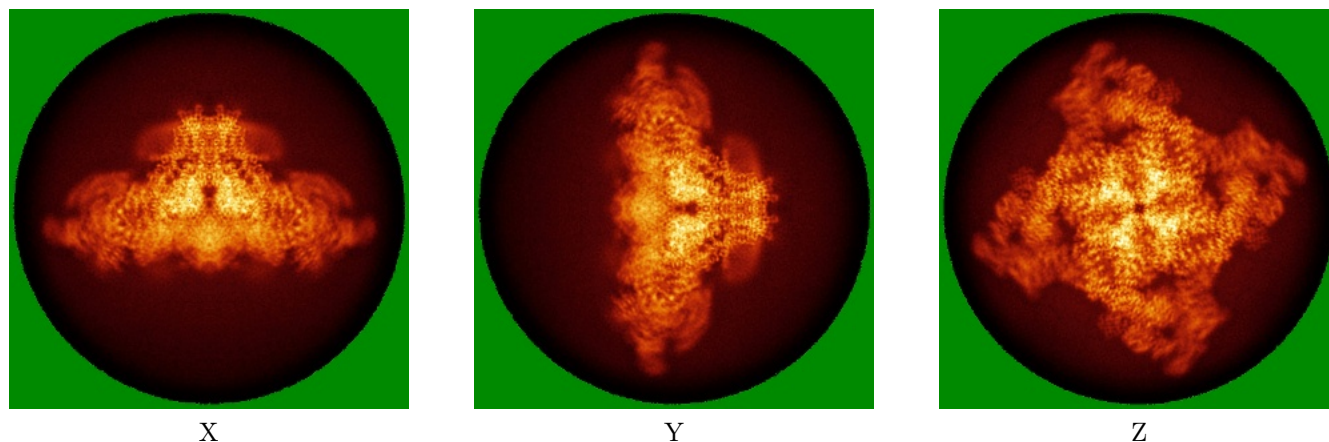


Z Index: 266

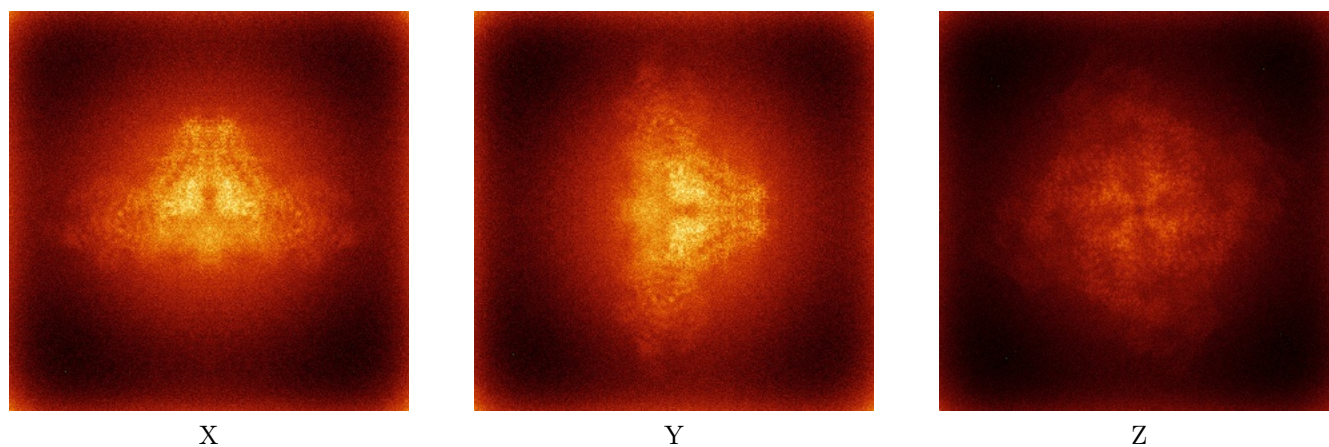
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



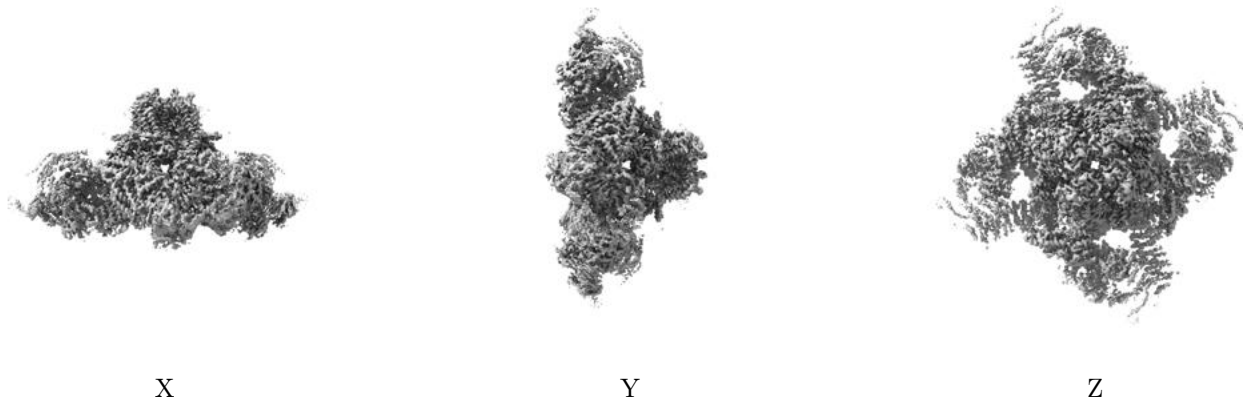
6.4.2 Raw map



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

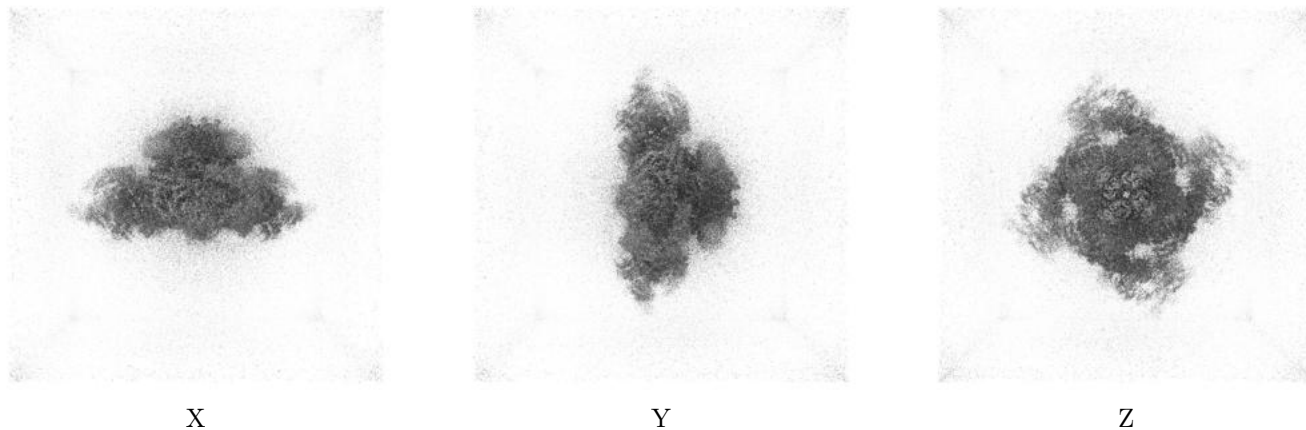
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 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.

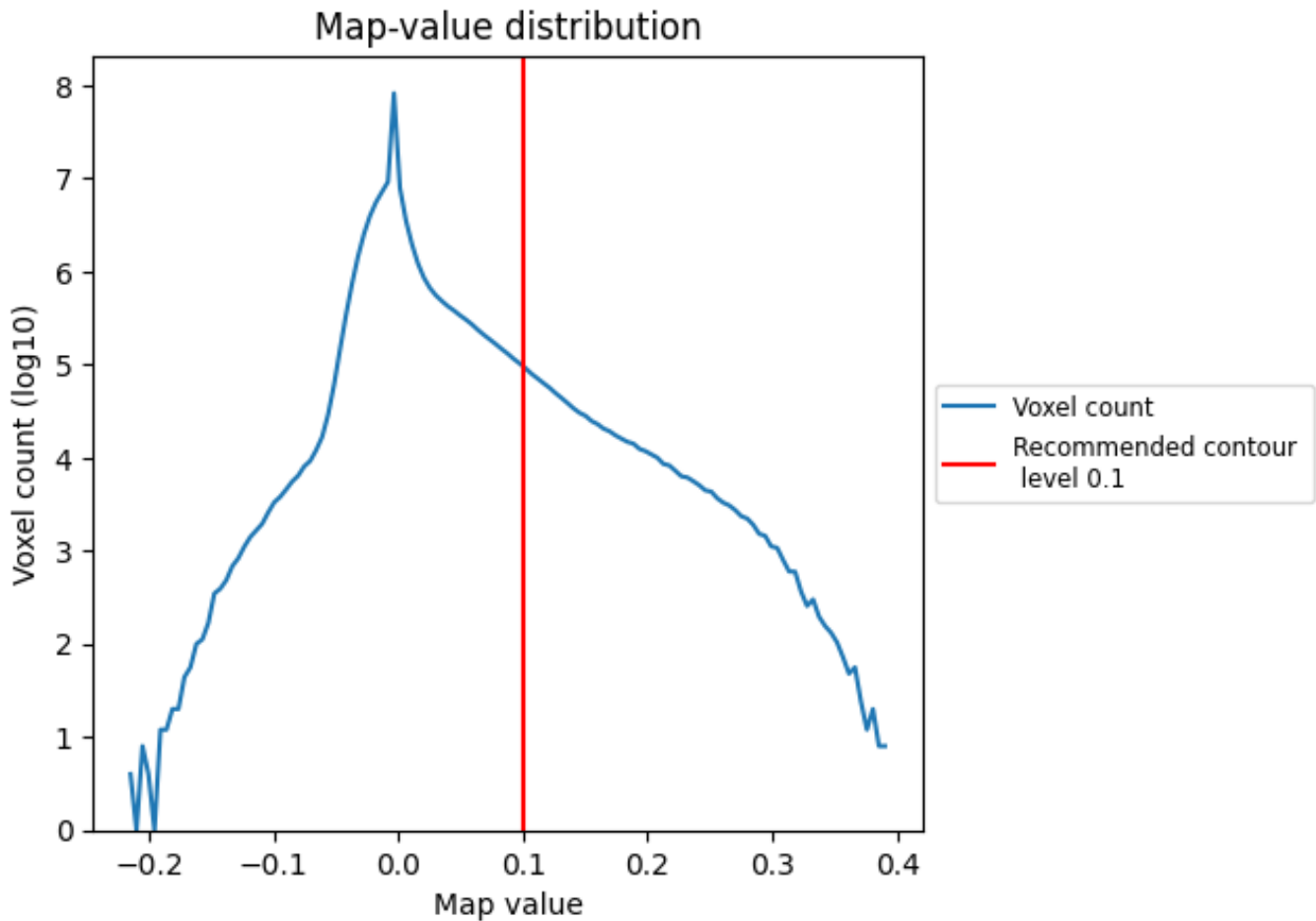
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

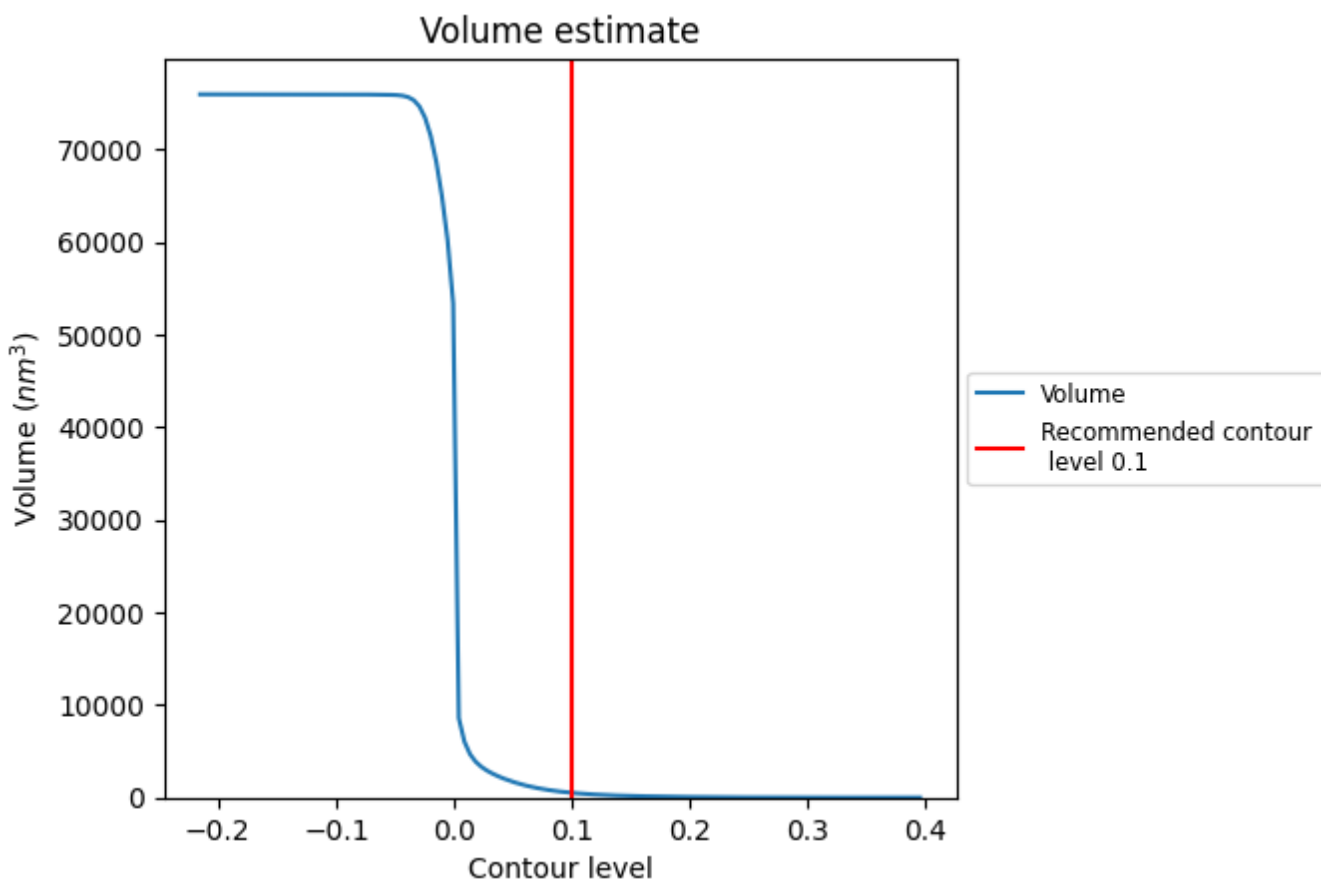
This section contains the results of statistical analysis of the map.

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.

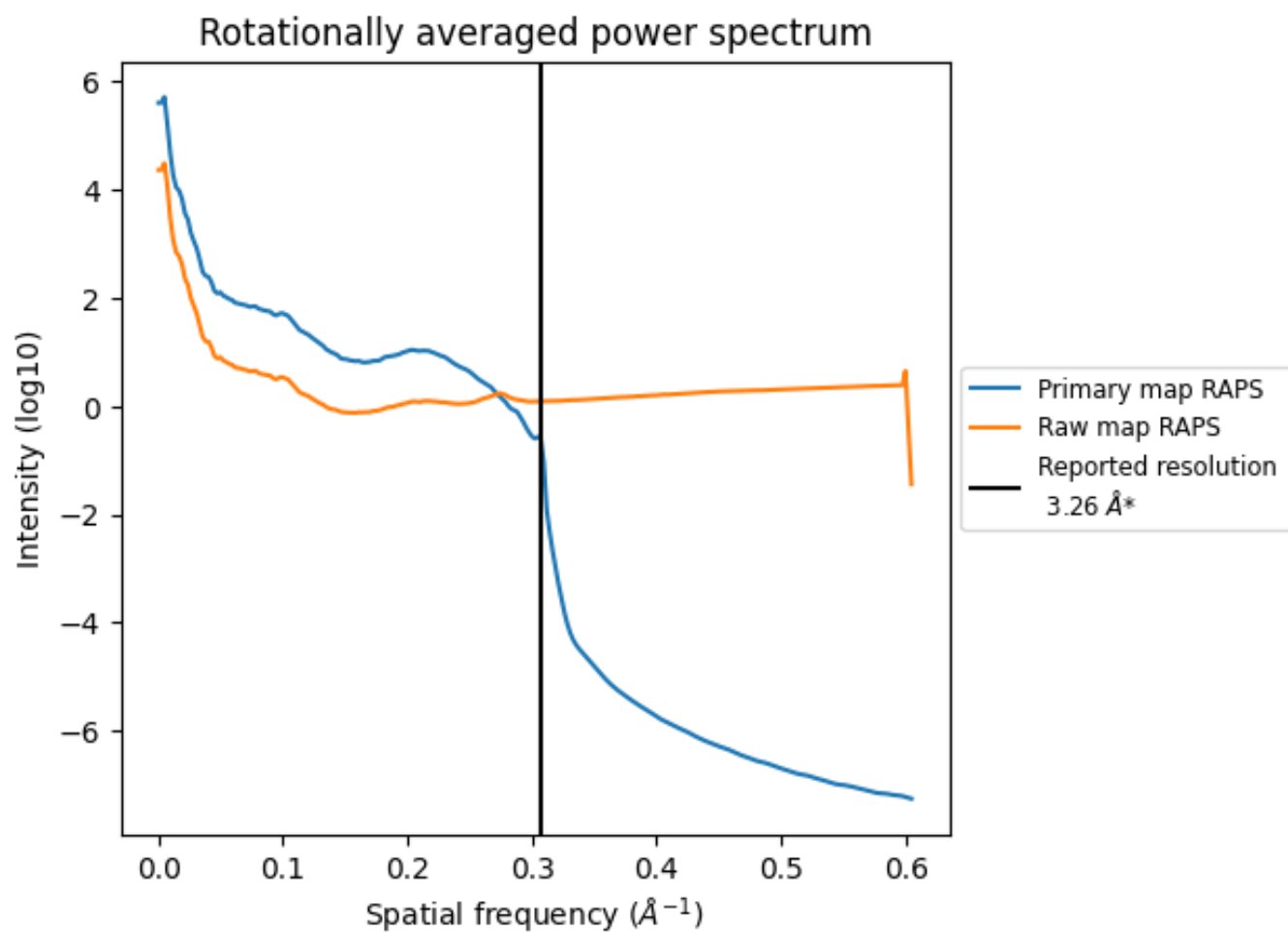
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm^3 ; this corresponds to an approximate mass of 463 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 i

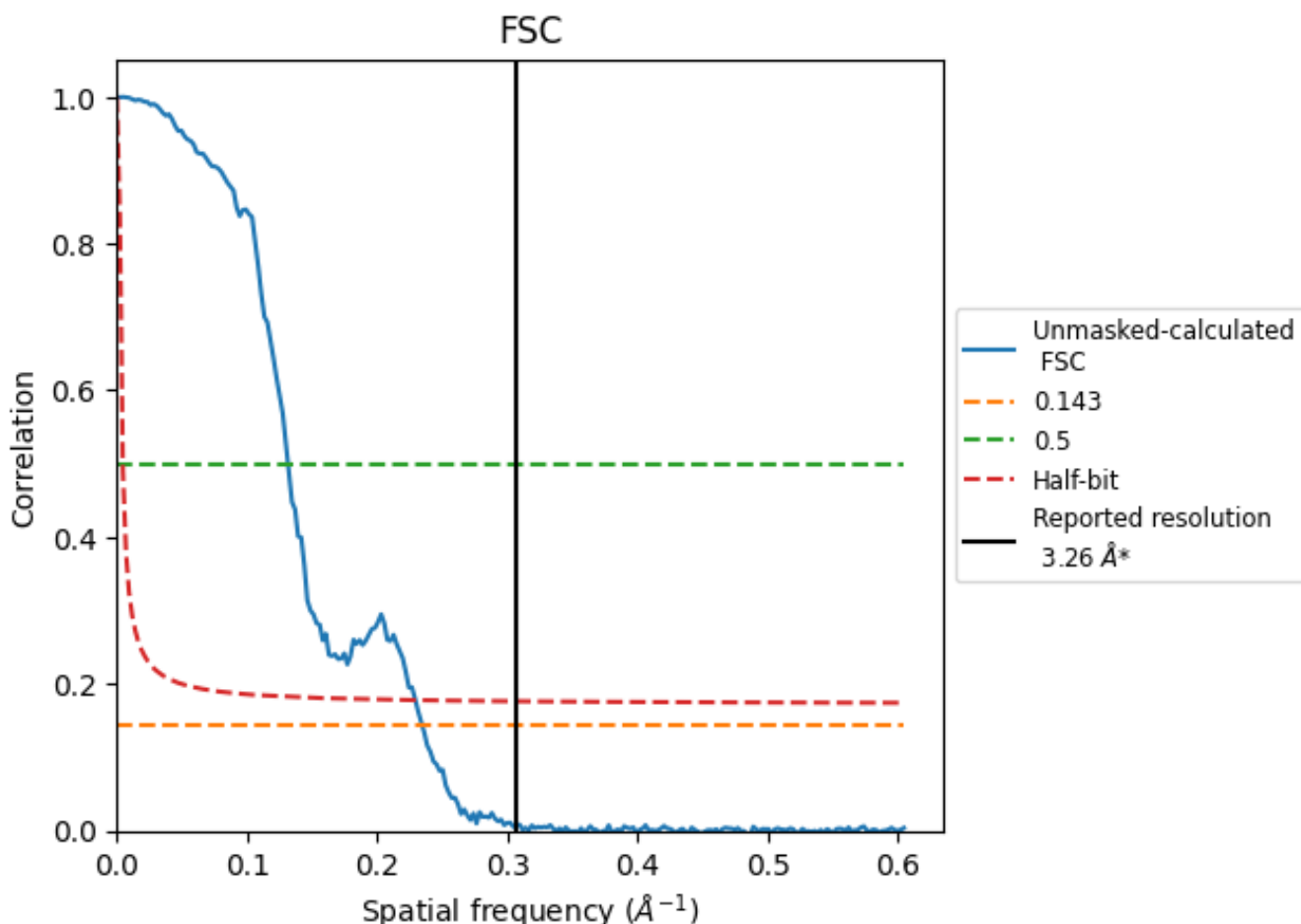


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

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 0.307 Å⁻¹

8.2 Resolution estimates [i](#)

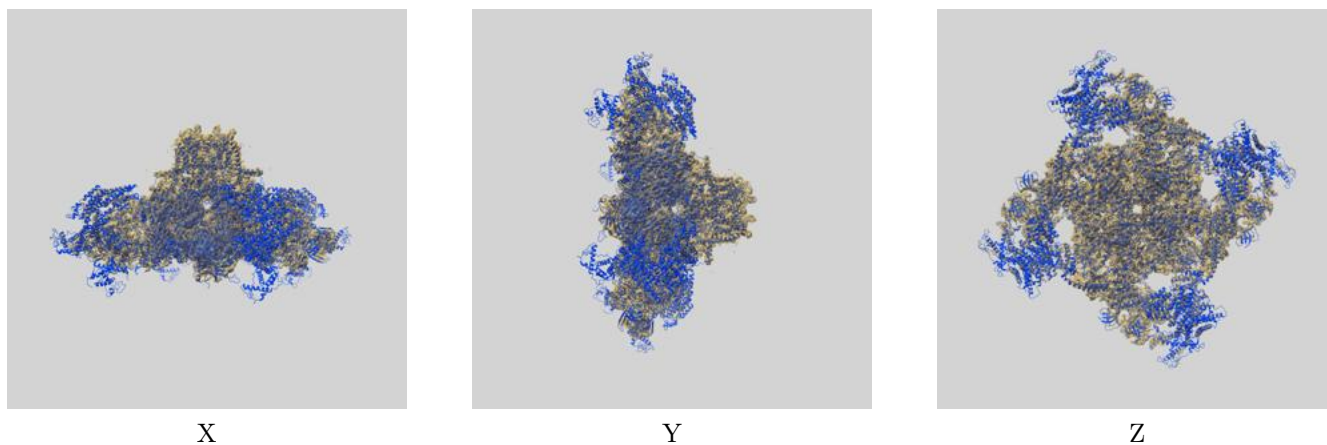
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	7.60	4.36

*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 4.26 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

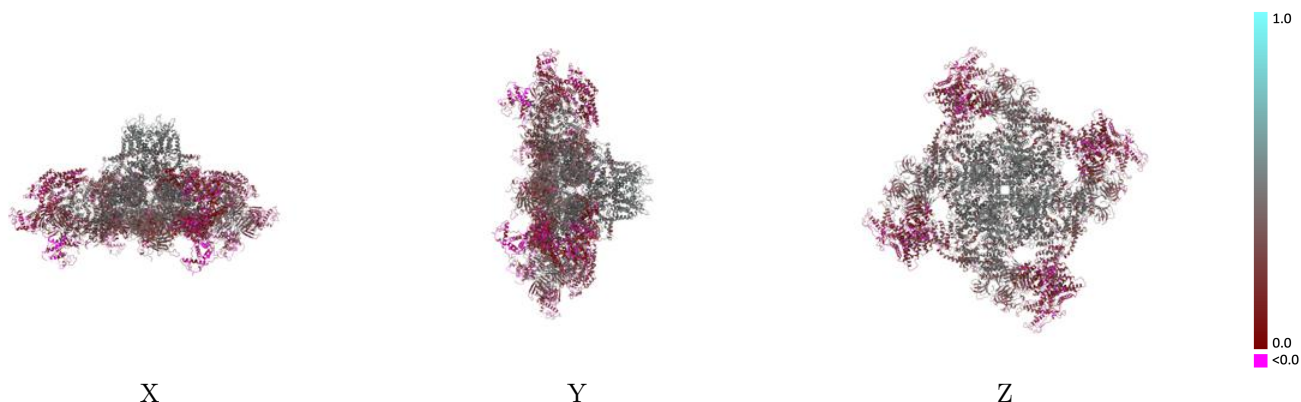
This section contains information regarding the fit between EMDB map EMD-47394 and PDB model 9E1H. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



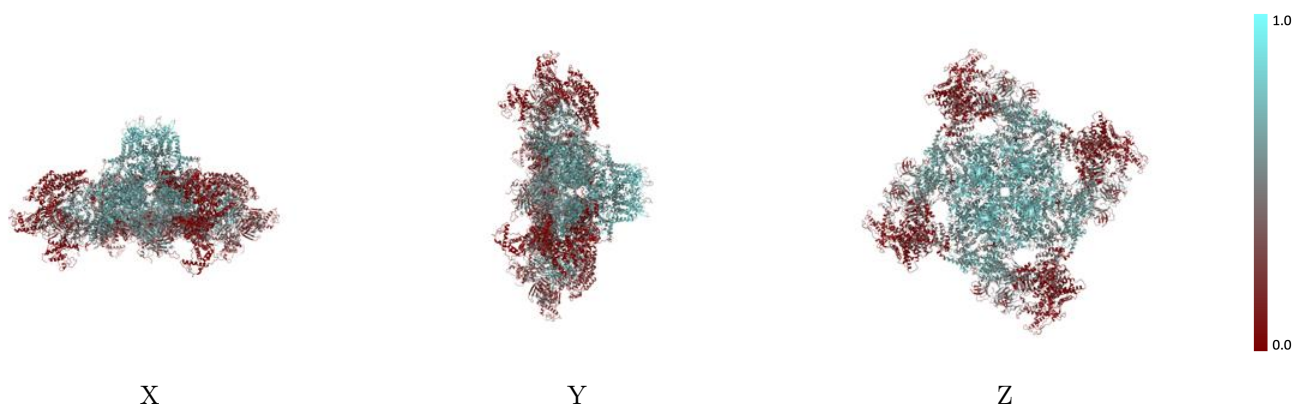
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



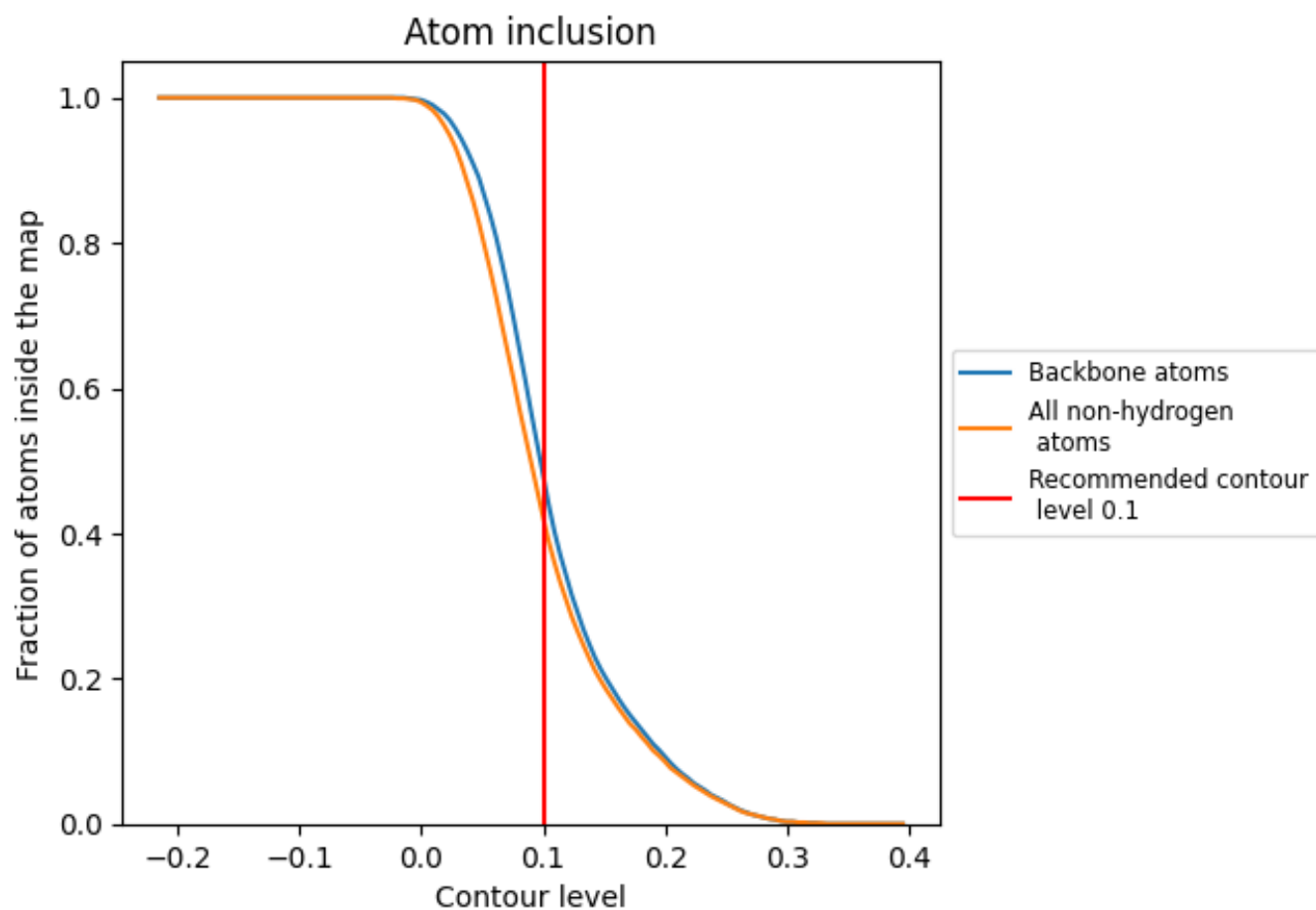
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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



















9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4210	 0.3140
A	 0.4340	 0.3130
B	 0.4350	 0.3130
C	 0.4340	 0.3130
D	 0.4340	 0.3130
E	 0.2440	 0.3570
F	 0.2440	 0.3560
G	 0.2470	 0.3530
H	 0.2420	 0.3560

