



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 10:59 AM EDT

PDB ID : 5TAT
EMDB ID : EMD-8384
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.80 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.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

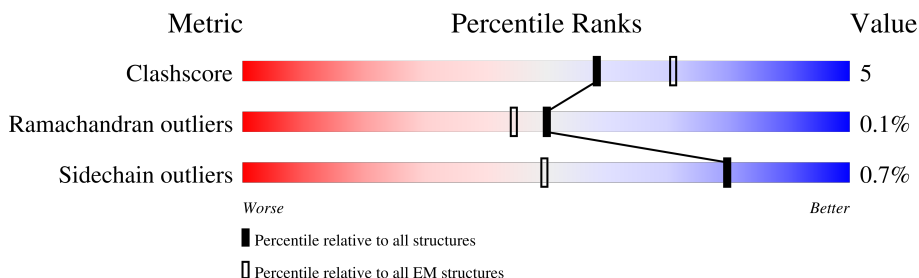
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	108	<div> <div>36%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	F	108	<div> <div>36%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	H	108	<div> <div>36%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	J	108	<div> <div>37%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	B	4416	<div> <div>39%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	E	4416	<div> <div>39%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
2	G	4416	<div> <div>39%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
2	I	4416	<div> <div>39%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

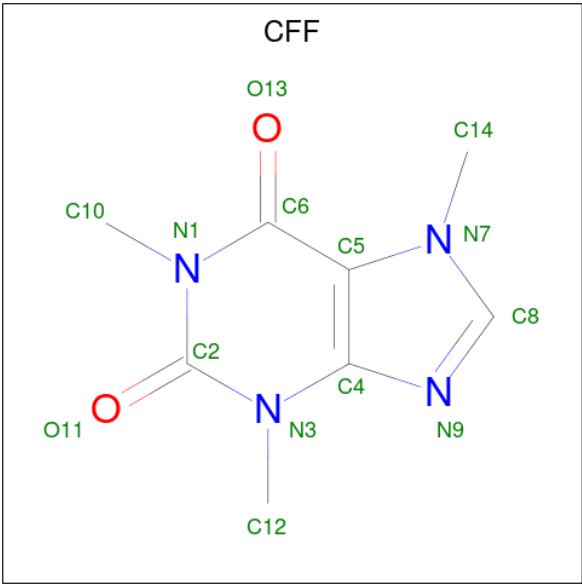
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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	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	
3	G	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	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

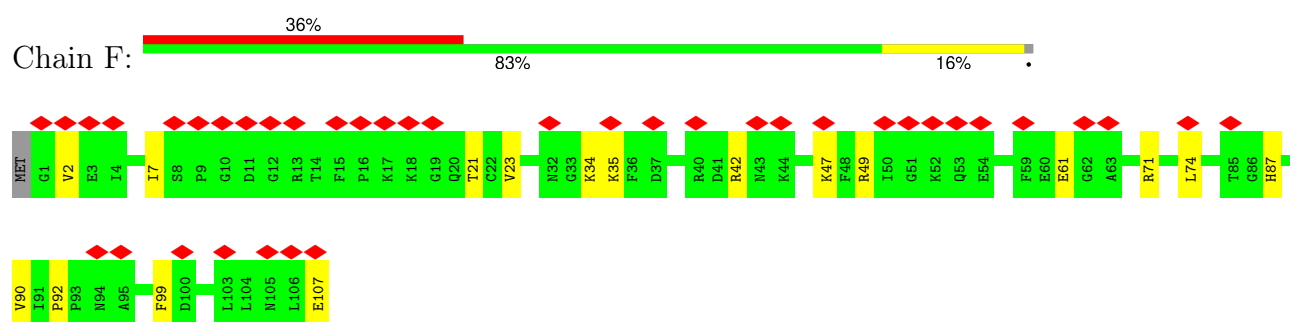
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

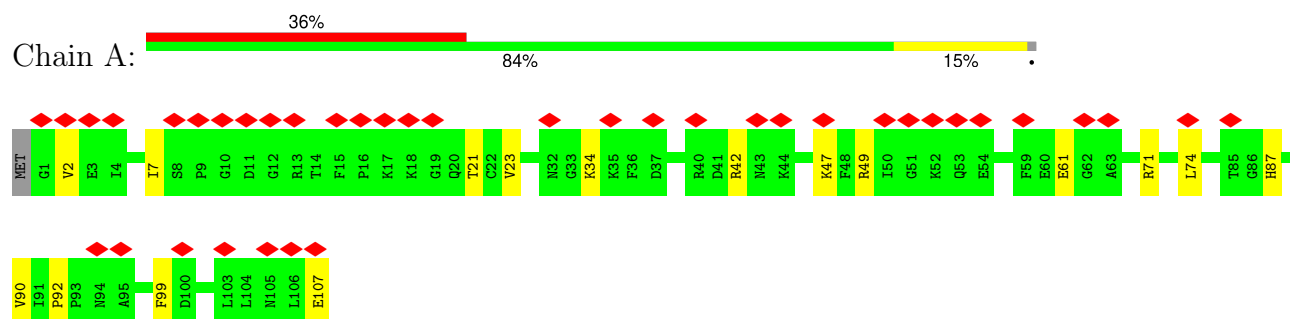
3 Residue-property plots [i](#)

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.

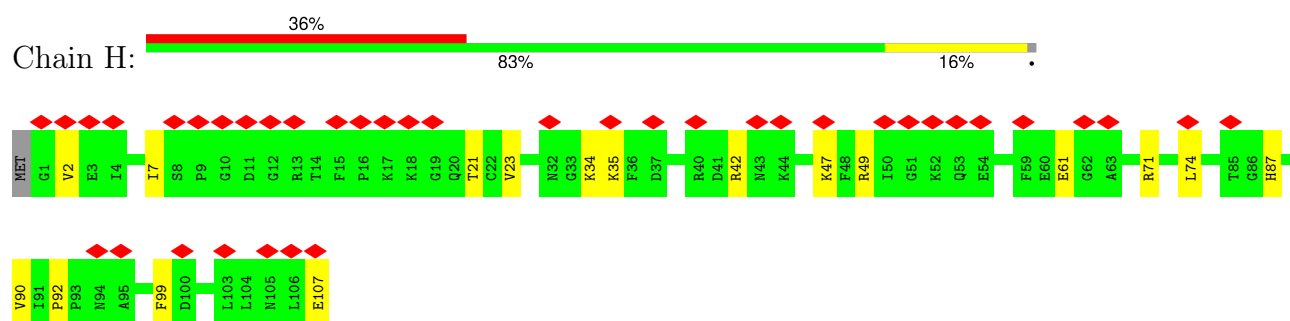
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



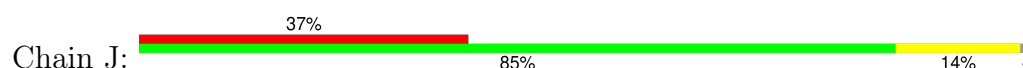
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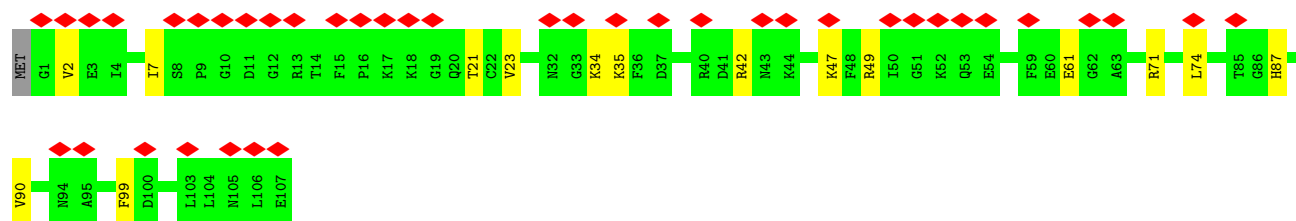


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

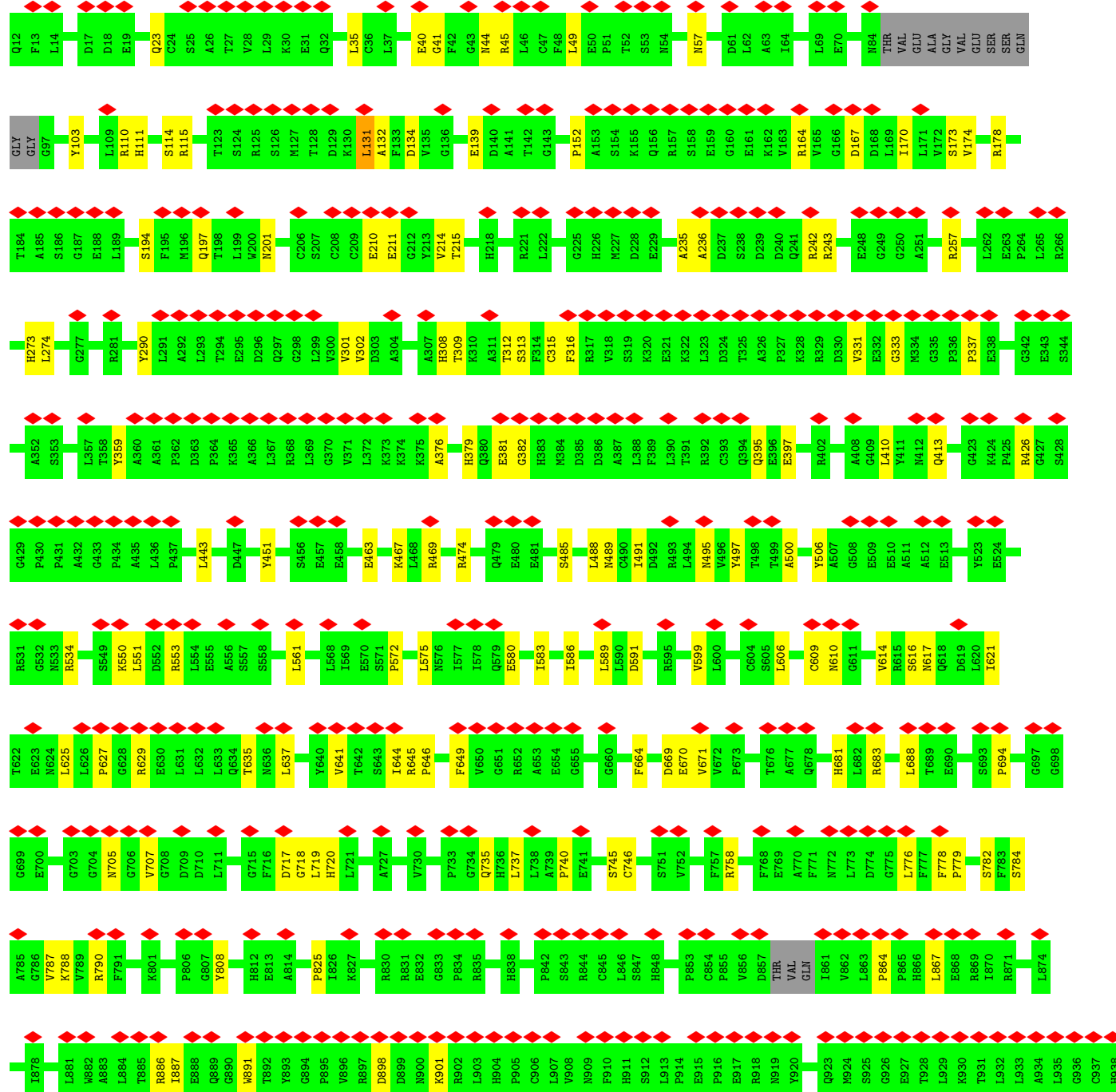
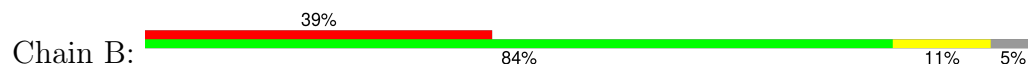


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

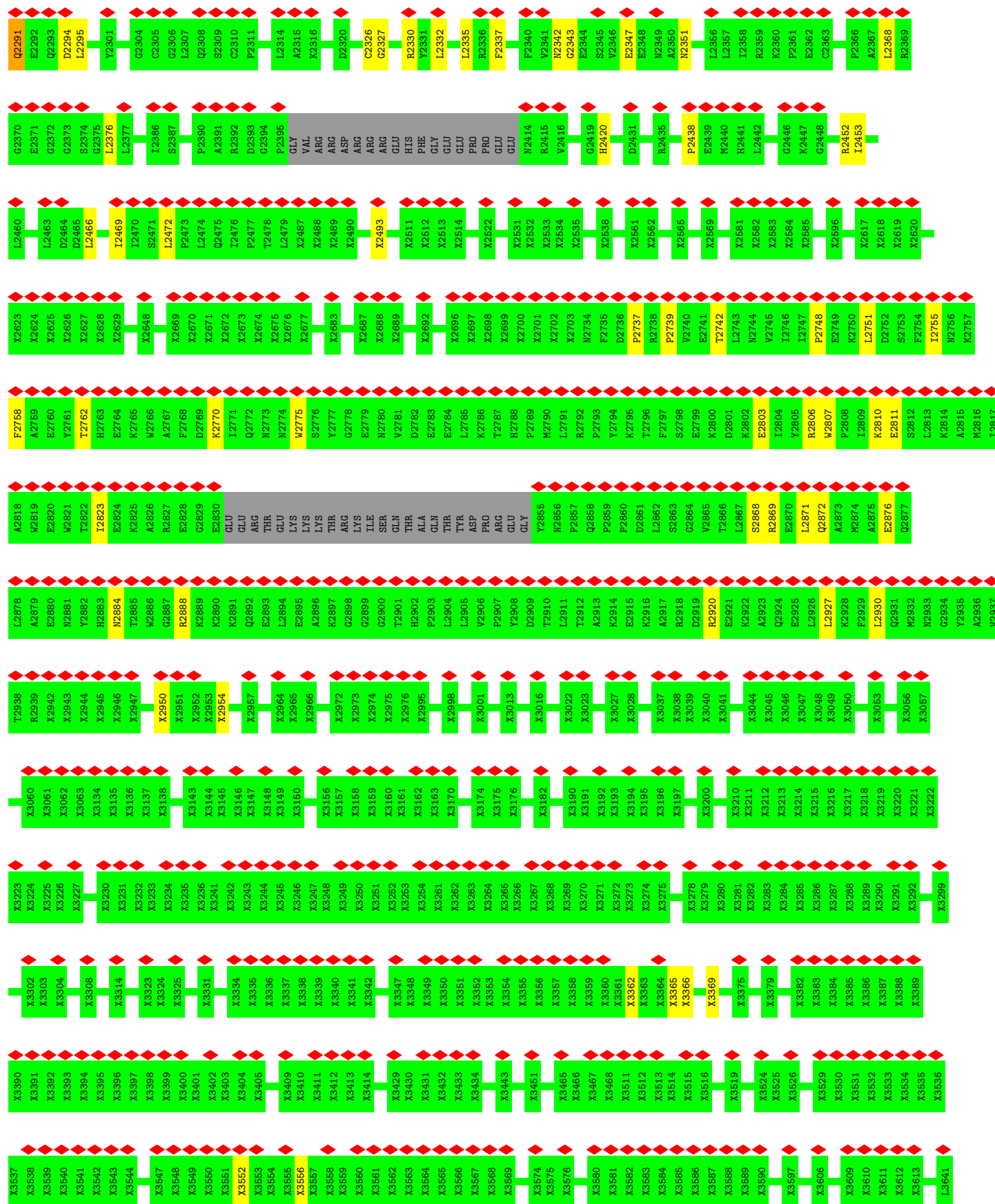




• Molecule 2: Ryanodine receptor 1



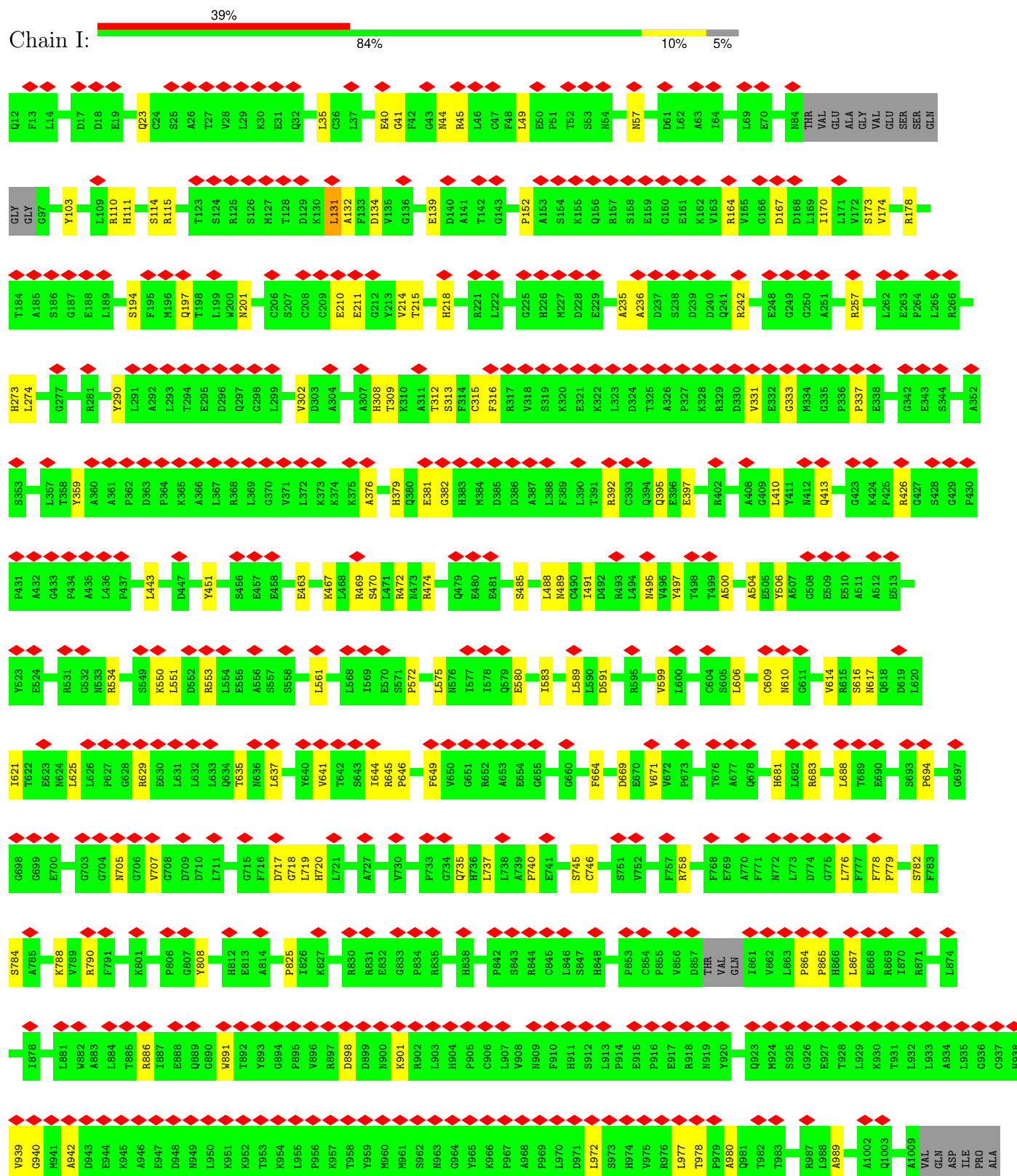
SER	R2184	S1987	GLU	A1801	S1722	A1838	X1528	G1262	L1164	Y1081	ARG	V939
	L2185	A1988	GLU	I1802	A1723	L1639	X1529	T1263	N1165	ARG	ARG	G940
	R2186	A1989	GLU	I1803	C1724	E1644	X1530	V1264	G1186	Y1089	ASN	R941
	R2187	F1990	LVS	F1903	R1725	M1645	X1531	D1265	L1169	F1092	PRO	A942
	R2188	GLU	ASP	A1806	R1727	M1648	X1532	T1266	M1170	E1093	L10120	D943
	R2189	A1992	GLU	L1807	R1728	D1649	X1543	P1267	S1171	T1096	R10125	E944
	Y2192	R1993	GLU	R1808	L1731	E1652	X1544	P1268	D1172	E1099	L10126	R945
	R2199	R1994	GLU	R1813	S1732	E1653	X1545	C1269	S1173	M1100	L10127	A946
	A2200	T1995	GLU	E1817	E1733	L1657	X1546	R1271	G1174	R1101	D10128	E947
	H2204	F1998	LVS	D1821	L1738	R1656	X1547	L1272	S1175	E1102	E10129	D948
VAL	R2212	F1999	ASP	D1821	L1738	R1657	X1548	X1276	T1177	G1103	A10130	R949
	R2213	S2000	ALA	R1827	E1741	Q1660	X1549	X1277	A1178	E1099	L10131	L950
	V2214	P2002	GLU	D1828	T1742	Q1660	X1550	X1278	A1179	E1099	L10132	R951
	L2215	Q2003	LVS	R1743	R1743	S1664	X1551	X1279	F1179	E1105	R10133	R952
	L2216	Q2005	GLU	G1832	F1748	L1667	X1555	X1281	R1180	E1106	S10134	R953
	G2217	L2006	GLU	G1832	F1748	L1667	X1556	X1281	E1181	E1108	N10135	R954
	G2217	N2007	GLU	G1832	F1748	L1667	X1557	X1281	E1181	E1109	R10136	L955
	G2218	L2010	ALA	Q1837	P1749	R1671	X1573	X1290	E1183	L1109	D10137	R956
	G2219	H2011	PRO	P1840	P1750	A1672	S1576	X1291	I1184	P1111	S10138	R957
	T2220	F2012	GLU	L1848	R1752	A1672	S1576	X1291	G1185	D1112	L10139	R958
GLU	R2221	K2013	LVS	L1848	R1752	A1675	S1576	X1291	D1186	L1115	C10140	Y959
	E2222	A2016	ASP	G1852	G1754	A1675	L1581	X1439	L1189	E1116	A10141	R960
	L2223	D2017	ASP	I1853	G1755	L1676	S1582	X1439	P1190	G1116	A10142	R961
	F2235	E2018	E1923	F1854	N1756	R1679	E1583	X1441	V1199	A1117	V10143	R962
	L2236	E2019	E1924	R1855	N1756	R1680	A1588	X1442	G1200	D1118	R10144	R963
	Q2247	E2019	G1925	R1857	A1757	A1682	P1589	X1443	H1201	E1119	T10145	G964
	D2252	D2020	L1926	E1857	R1758	H1683	Q1590	X1447	L1202	V1123	G10148	Y965
	H2253	C2021	L1927	D1858	H1760	L1685	C1591	X1447	N1203	H1127	Y10149	R966
	L2257	P2022	Q1928	V1859	G1761	C1686	Q1590	X1457	L1204	R1128	G10150	P967
	N2260	L2023	L1762	M1865	G1764	S1687	R1594	X1477	G1205	Y1051	N10152	A968
SER	R2140	E2025	GLU	E1869	V1765	Q1598	Q1598	X1476	S1209	R1131	N10153	L970
	A2141	I2027	GLU	V1870	G1766	M1599	L1600	X1477	S1210	L1134	E10154	D971
	S2147	R2028	ALA	F1871	V1767	L1694	S1605	X1479	L1211	G1140	PRO	L972
	E2150	Q2041	GLU	E1874	T1768	L1694	W1605	X1489	R1212	R1141	ASP	R973
	E2157	G2042	GLU	E1874	T1768	L1698	L1613	X1497	L1216	G1140	GLN	H974
	L2166	G2043	GLU	R1960	R1772	E1699	Q1614	X1504	C1217	R1141	GLU	Y975
	H2170	Q1973	GLU	F1961	H1775	D1700	V1615	X1505	Q1220	Q1144	PRO	R976
	Q2173	R1976	GLU	F1977	L1775	A1701	THR	X1512	Q1220	S1145	GLN	L977
	L2166	Y1977	GLU	GLU	L1783	P1704	ARG	X1513	E1221	G1146	VAL	T978
	R2166	L1980	GLU	GLU	A1784	R1708	ALA	X1514	E1224	D1147	GLU	P979
GLU	M1981	M1981	GLU	GLU	A1785	A1709	GLY	X1515	Q1231	V1148	ASN	A981
	R1982	R1982	GLU	GLU	L1786	G1710	ALA	X1516	R1232	W1153	GLN	T982
	A1983	A1983	GLU	GLU	P1787	Y1711	GLY	X1516	E1232	V1149	ARG	T983
	F1984	F1984	GLU	GLU	Y1712	Y1712	A1627	X1519	M1152	D1070	TRP	R987
	T1985	T1985	GLU	GLU	A1788	D1713	C1630	W1237	I1153	R10171	GLN	L988
	F1984	F1984	GLU	GLU	ALA	L1718	Q1631	P1247	L1155	F1076	GLU	A989
	T1985	T1985	GLU	GLU	VAL	H1719	D1632	T1156	E1157	R10176	GLU	A1002
	G2183	G2183	GLU	GLU	ALA	H1719	D1632	E1251	E1157	A10177	GLU	Q1003
	L2288	L2288	GLU	GLU	E1793	L1720	X1522	X1523	I1161	E1078	GLU	A1009
	A2289	A2289	THR	THR	A1794	E1721	M1636	X1524	F1162	K1079	ARG	VAL
SER	L2290	SER	SER	SER	A1796	E1796	M1637	X1525	T1163	T1079	GLN	GLN
					R1797	R1797		X1526			ASP	ASP
					L1798	L1798		X1527			ILE	ILE
											PRO	PRO
												A1009





• Molecule 2: Ryanodine receptor 1

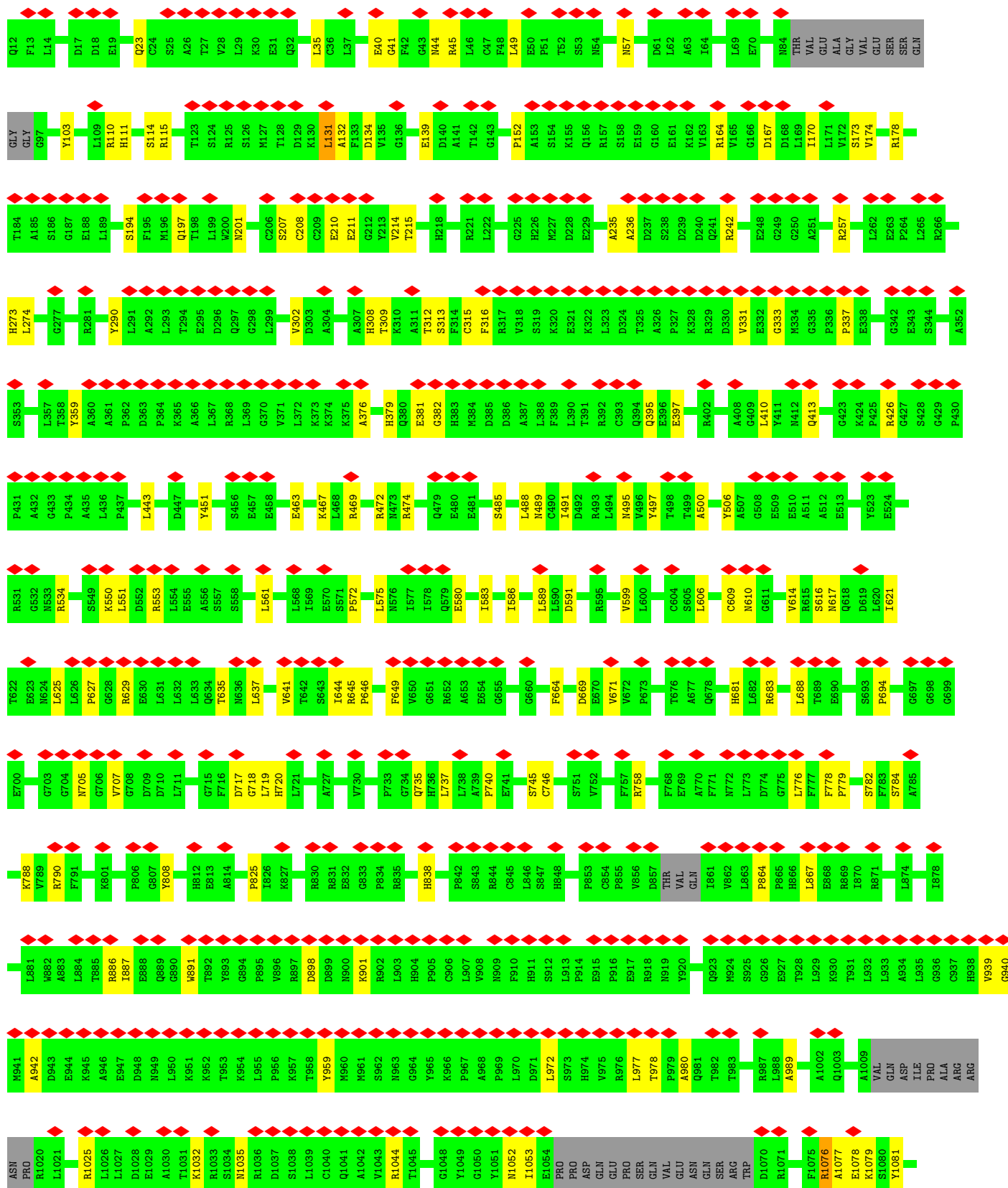
Chain I:





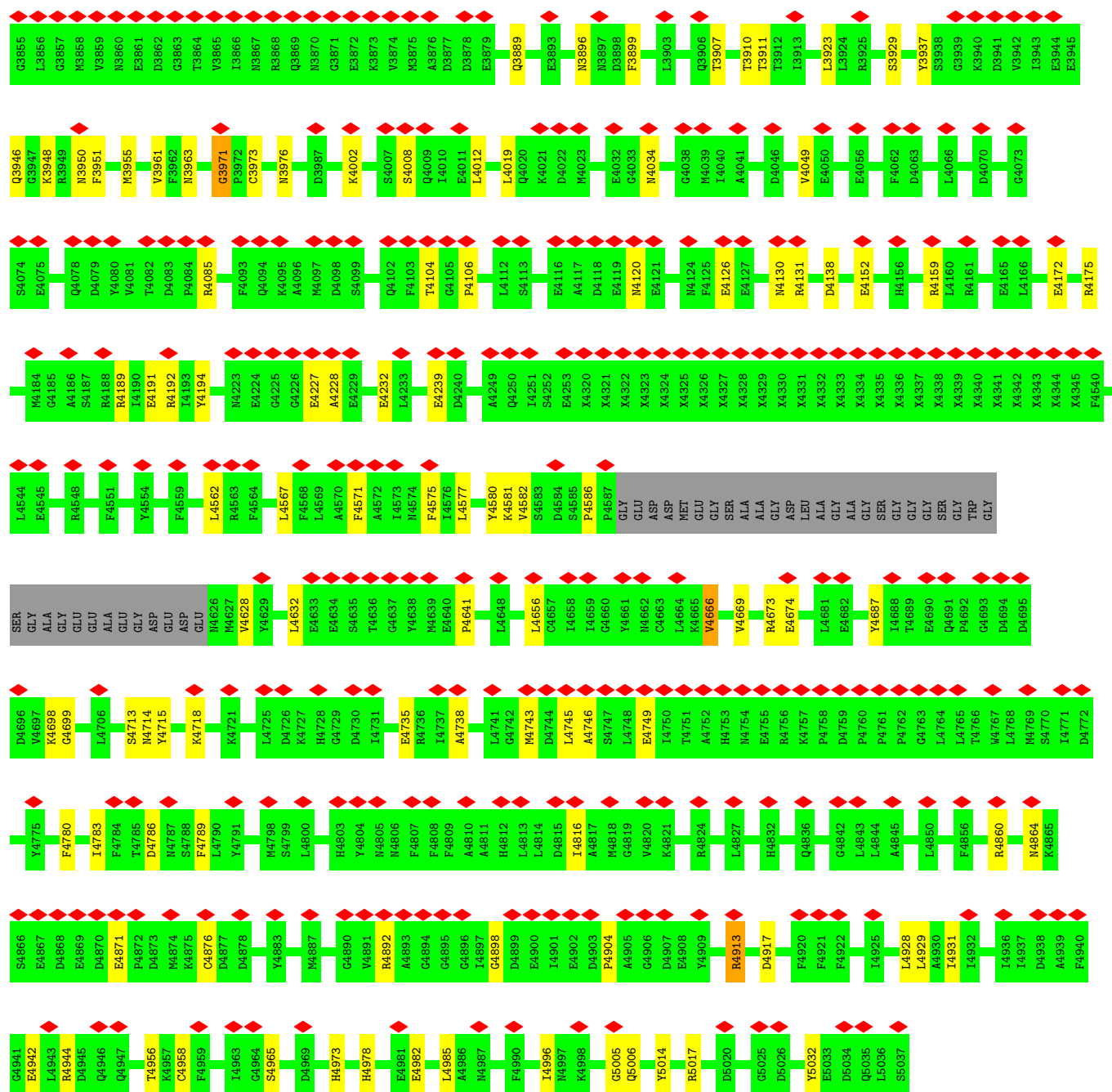




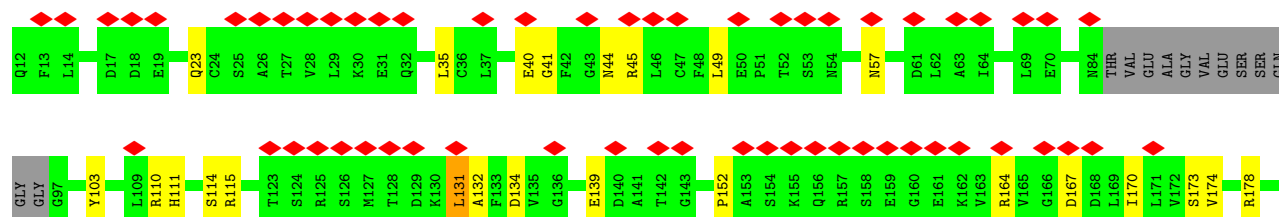
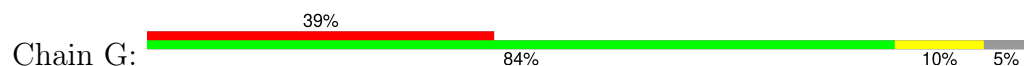


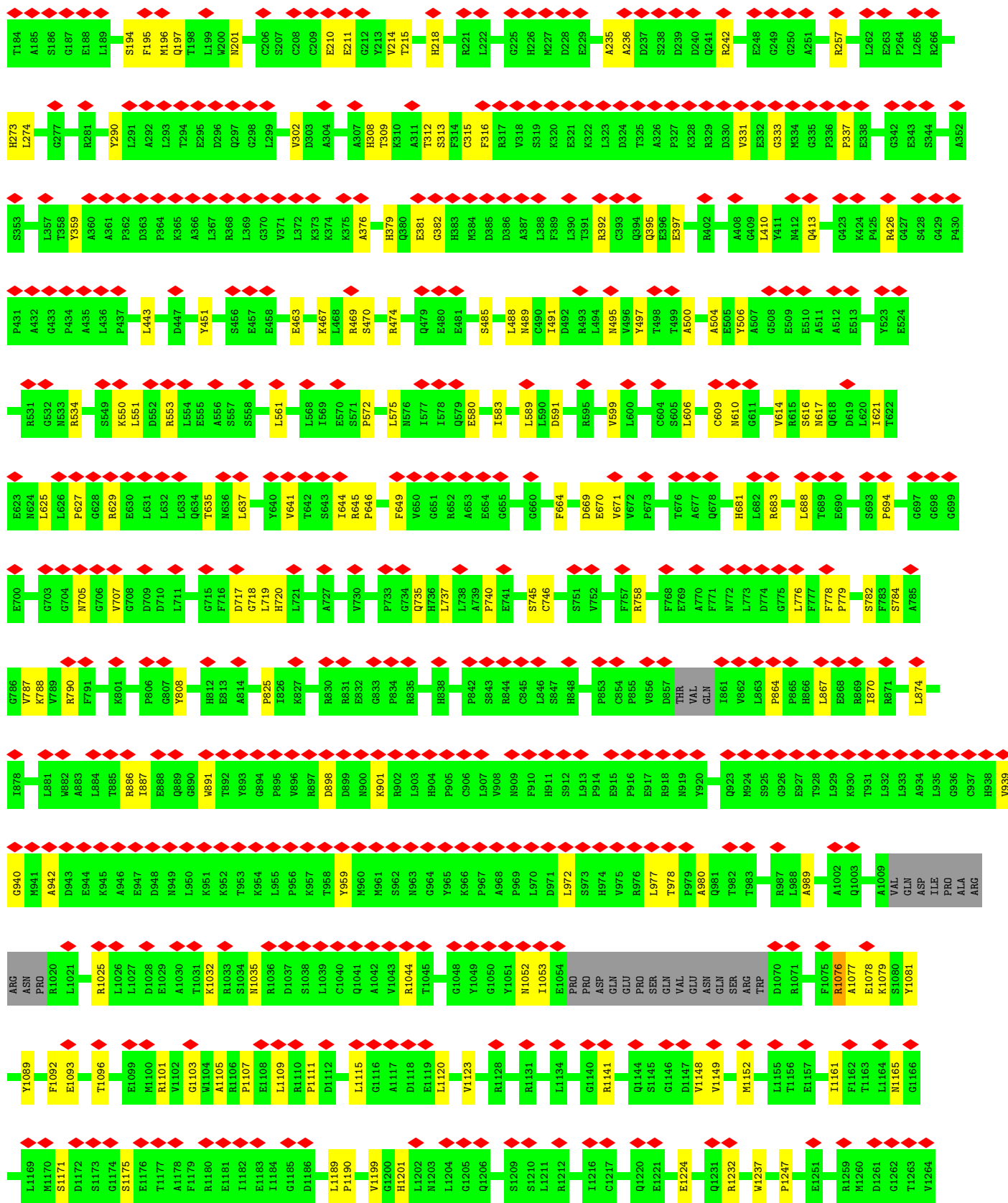


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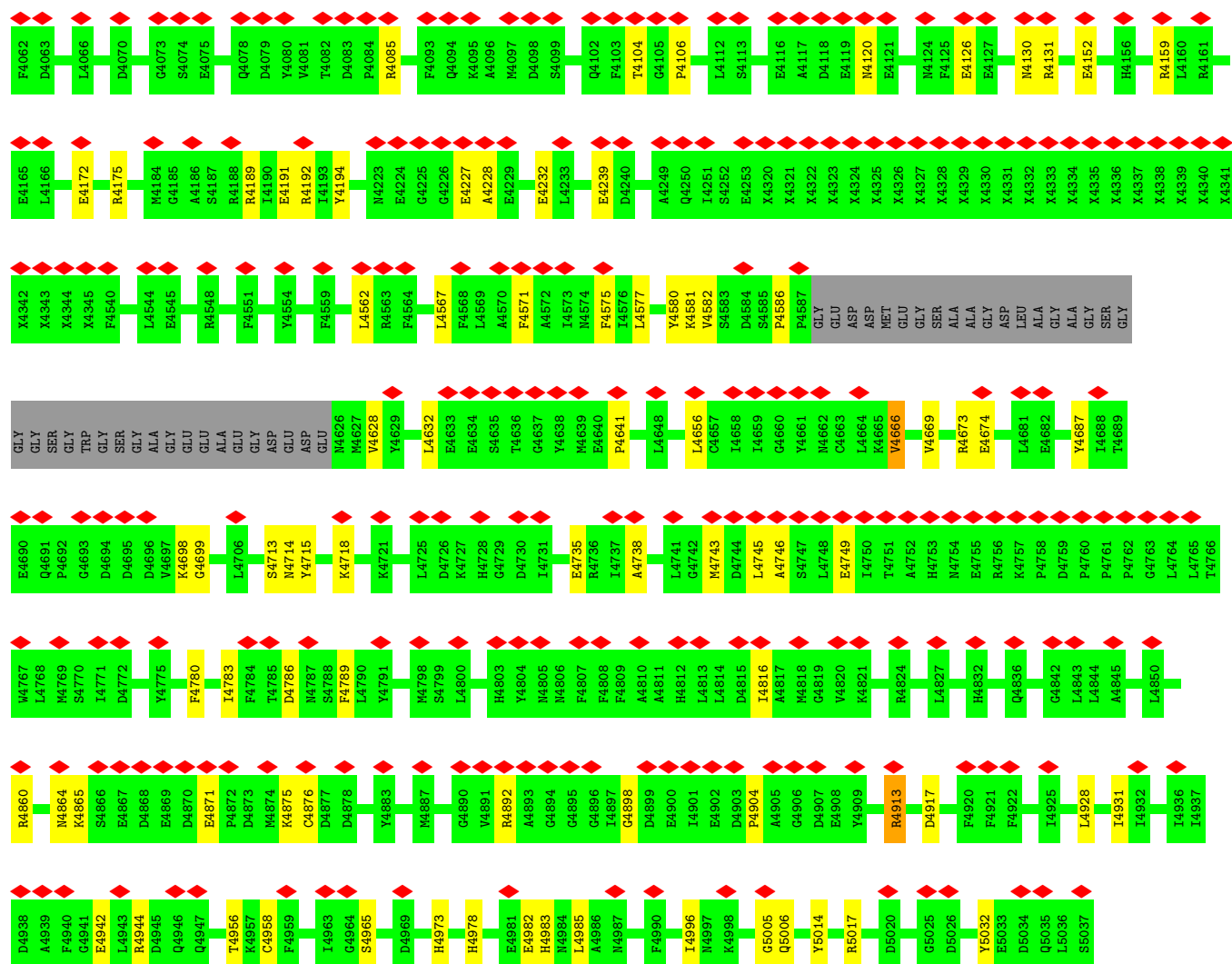
• Molecule 2: Ryanodine receptor 1







V3942	R3849	T3664	X3548	X3234	X3143	X2950	G2987	A2767
T3943	E3854	E3665	X3549	X3235	X3144	X2951	R2888	F2768
E3944	E3855	D3666	X3550	X3236	X3145	X2952	R2889	D2769
O3946	L3856	H3667	X3551	X3241	X3146	X2957	K2890	K2770
G3947	L3857	S3668	X3552	X3242	X3147	X2964	K2891	I2771
K3948	E3857	F3669	X3553	X3243	X3148	X2965	Q2892	Q2772
K3949	E3858	R3672	X3554	X3244	X3149	X2966	E2893	N2773
N3950	V3859	M3673	X3555	X3245	X3150	X2972	L2894	N2774
F3951	V3751	I3674	X3556	X3246	X3156	X2977	E2895	N2775
M3955	F3752	D3675	X3557	X3247	X3157	X2978	A2896	S2776
M3961	F3753	D3676	X3558	X3248	X3158	X2979	A2897	I2777
F3962	E3754	A3680	X3559	X3249	X3159	X2974	Q2898	G2778
N3963	E3755	G3681	X3560	X3250	X3160	X2975	L2899	E2779
G3971	E3756	E3682	X3561	X3251	X3161	X2976	E2899	N2780
F3972	E3757	Q3683	X3562	X3252	X3162	X2995	Q2900	V2781
C3973	E3758	Q3684	X3563	X3253	X3163	X2998	T2901	D2782
N3976	R3762	Q3685	X3564	X3254	X3170	X3001	H2902	E2783
D3987	S3768	E3686	X3565	X3261	X3174	X3013	P2903	E2784
F3992	R3769	E3687	X3566	X3262	X3175	X3016	L2904	L2785
F3996	L3770	E3688	X3567	X3263	X3176	X3022	L2905	K2786
K4002	H3772	E3689	X3568	X3264	X3182	X3023	P2906	I2787
S4007	R3773	E3690	X3569	X3265	X3190	X3027	P2907	D2788
S4008	V3779	E3691	X3574	X3266	X3191	X3037	Y2855	F2789
L4010	Q3781	E3692	X3575	X3267	X3192	X3038	N2856	N2790
E4011	S3784	K3696	X3576	X3268	X3193	X3039	P2857	L2791
L4012	K3787	Q3700	X3577	X3269	X3194	X3040	Q2858	R2792
L4019	G3788	R3707	X3578	X3270	X3195	X3041	P2859	P2793
Q4020	E3789	T3711	X3579	X3271	X3196	X3044	P2860	Y2794
K4021	T3790	E3712	X3580	X3272	X3197	X3045	E2795	K2795
D4022	L3798	E3713	X3581	X3273	X3200	X3046	F2797	S2798
M4023	L3805	E3714	X3582	X3274	X3210	X3047	Q2800	K2800
E4032	N3806	K3715	X3583	X3275	X3211	X3048	D2801	D2802
G4033	G3807	L3716	X3584	X3276	X3212	X3049	L2867	E2803
M4034	E3808	D3717	X3585	X3277	X3213	X3050	Q2868	E2804
G4038	N3809	E3718	X3586	X3278	X3214	X3053	R2869	T2805
M4039	L3817	D3719	X3587	X3279	X3215	X3056	E2870	Y2806
L4041	L3821	Y3720	X3588	X3280	X3216	X3057	Q2871	R2807
D4046	K3822	X3606	X3589	X3281	X3217	X3060	L2927	K2808
V4049	D3822	X3609	X3590	X3282	X3218	X3061	K2928	P2808
E4050	A3724	X3610	X3591	X3283	X3219	X3062	F2929	M2874
E4056	K3823	X3611	X3592	X3284	X3220	X3063	L2930	E2875
	K3824	X3612	X3593	X3285	X3221	X3064	Q2876	A2873
	G3827	X3613	X3594	X3286	X3222	X3065	E2877	M2874
	Q3830	L3641	X3595	X3287	X3223	X3066	Q2877	L2878
	Q3833	N3642	X3596	X3288	X3224	X3067	N2932	L2813
	L3842	L3644	X3597	X3289	X3225	X3068	N2933	K2814
	D3843	F3653	X3598	X3290	X3226	X3069	Y2935	E2890
		K3658	X3599	X3291	X3227	X3070	N2861	N2816
		W3661	X3600	X3292	X3228	X3071	Y2937	L2817
		L3662	X3601	X3293	X3229	X3072	T2938	A2818
		L3663	X3602	X3294	X3230	X3073	N2885	W2886
			X3603	X3295	X3231	X3074		
			X3604	X3296	X3232	X3075		
			X3605	X3297	X3233	X3076		
			X3606	X3298	X3234	X3077		
			X3607	X3299	X3235	X3078		
			X3608	X3300	X3236	X3079		
			X3609	X3301	X3237	X3080		
			X3610	X3302	X3238	X3081		
			X3611	X3303	X3239	X3082		
			X3612	X3304	X3240	X3083		
			X3613	X3305	X3241	X3084		
			X3614	X3306	X3242	X3085		
			X3615	X3307	X3243	X3086		
			X3616	X3308	X3244	X3087		
			X3617	X3309	X3245	X3088		
			X3618	X3310	X3246	X3089		
			X3619	X3311	X3247	X3090		
			X3620	X3312	X3248	X3091		
			X3621	X3313	X3249	X3092		
			X3622	X3314	X3250	X3093		
			X3623	X3315	X3251	X3094		
			X3624	X3316	X3252	X3095		
			X3625	X3317	X3253	X3096		
			X3626	X3318	X3254	X3097		
			X3627	X3319	X3255	X3098		
			X3628	X3320	X3256	X3099		
			X3629	X3321	X3257	X3100		
			X3630	X3322	X3258	X3101		
			X3631	X3323	X3259	X3102		
			X3632	X3324	X3260	X3103		
			X3633	X3325	X3261	X3104		
			X3634	X3326	X3262	X3105		
			X3635	X3327	X3263	X3106		
			X3636	X3328	X3264	X3107		
			X3637	X3329	X3265	X3108		
			X3638	X3330	X3266	X3109		
			X3639	X3331	X3267	X3110		
			X3640	X3332	X3268	X3111		
			X3641	X3333	X3269	X3112		
			X3642	X3334	X3270	X3113		
			X3643	X3335	X3271	X3114		
			X3644	X3336	X3272	X3115		
			X3645	X3337	X3273	X3116		
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			X3647	X3339	X3275	X3118		
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			X3652	X3344	X3280	X3123		
			X3653	X3345	X3281	X3124		
			X3654	X3346	X3282	X3125		
			X3655	X3347	X3283	X3126		
			X3656	X3348	X3284	X3127		
			X3657	X3349	X3285	X3128		
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			X3659	X3351	X3287	X3130		
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			X3662	X3354	X3290	X3133		
			X3663	X3355	X3291	X3134		
			X3664	X3356	X3292	X3135		
			X3665	X3357	X3293	X3136		
			X3666	X3358	X3294	X3137		
			X3667	X3359	X3295	X3138		
			X3668	X3360	X3296			
			X3669	X3361	X3297			
			X3670	X3362	X3298			
			X3671	X3363	X3299			
			X3672	X3364	X3300			
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			X3675	X3367	X3303			
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			X3679	X3371	X3307			
			X3680	X3372	X3308			
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			X3683	X3375	X3311			
			X3684	X3376	X3312			
			X3685	X3377	X3313			
			X3686	X3378	X3314			
			X3687	X3379	X3315			
			X3688	X3380	X3316			
			X3689	X3381	X3317			
			X3690	X3382	X3318			
			X3691	X3383	X3319			
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			X3695	X3387	X3323			
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			X3702	X3394	X3330			
			X3703	X3395	X3331			
			X3704	X3396	X3332			
			X3705	X3397	X3333			
			X3706	X3398	X3334			
			X3707	X3399	X3335			
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			X3709	X3401	X3337			
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			X3711	X3403	X3339			
			X3712	X3404	X3340			
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			X3737	X3429	X3365			
			X3738	X3430	X3366			
			X3739	X3431	X3367			
			X3740	X3432	X3368			
			X3741	X3433	X3369	</		



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	0.095	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	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: CFF, ATP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.29	0/25428	0.53	6/34534 (0.0%)
2	E	0.29	0/25428	0.53	6/34534 (0.0%)
2	G	0.29	0/25428	0.53	6/34534 (0.0%)
2	I	0.29	0/25428	0.53	6/34534 (0.0%)
All	All	0.29	0/105048	0.53	24/142628 (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
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	8.17	134.09	115.30
2	E	131	LEU	CA-CB-CG	8.17	134.09	115.30
2	I	131	LEU	CA-CB-CG	8.17	134.08	115.30
2	G	131	LEU	CA-CB-CG	8.16	134.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1600	LEU	CA-CB-CG	7.04	131.49	115.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	312	THR	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	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	11	0
1	J	818	0	824	9	0
2	B	29499	0	24741	252	0
2	E	29499	0	24741	250	0
2	G	29499	0	24741	251	0
2	I	29499	0	24741	253	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	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102348	1016	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 1016 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:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.78	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.65
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.30	0.65
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.65

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	304 (9%)	2 (0%)	48	83
2	E	3235/4416 (73%)	2931 (91%)	302 (9%)	2 (0%)	48	83
2	G	3235/4416 (73%)	2930 (91%)	303 (9%)	2 (0%)	48	83
2	I	3235/4416 (73%)	2930 (91%)	303 (9%)	2 (0%)	48	83
All	All	13360/18096 (74%)	12093 (90%)	1259 (9%)	8 (0%)	50	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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

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%)	2476 (99%)	17 (1%)	81	87
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	80	87

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1676	LEU
2	G	3663	LEU
2	G	4120	ASN
2	I	1964	ARG
2	I	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1688	HIS

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Mol	Chain	Res	Type
2	G	2127	GLN
2	G	4553	ASN
2	I	1679	ASN
2	I	1598	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	B	5101	-	28,33,33	1.00	2 (7%)	34,52,52	1.10	2 (5%)
4	CFF	B	5102	-	8,15,15	2.05	3 (37%)	8,23,23	1.34	1 (12%)
4	CFF	E	5102	-	8,15,15	2.05	3 (37%)	8,23,23	1.32	1 (12%)
3	ATP	I	5101	-	28,33,33	1.00	2 (7%)	34,52,52	1.10	2 (5%)
4	CFF	I	5102	-	8,15,15	2.04	3 (37%)	8,23,23	1.32	1 (12%)
3	ATP	E	5101	-	28,33,33	1.01	2 (7%)	34,52,52	1.10	2 (5%)
3	ATP	G	5101	-	28,33,33	1.00	2 (7%)	34,52,52	1.10	2 (5%)
4	CFF	G	5102	-	8,15,15	2.06	3 (37%)	8,23,23	1.34	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	B	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-3.39	1.33	1.39
4	G	5102	CFF	C5-C4	-3.39	1.33	1.39
4	I	5102	CFF	C5-C4	-3.39	1.33	1.39
4	B	5102	CFF	C5-C4	-3.34	1.33	1.39
4	B	5102	CFF	C6-N1	-3.28	1.32	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-3.49	123.93	128.67
3	G	5101	ATP	N3-C2-N1	-3.49	123.94	128.67
3	I	5101	ATP	N3-C2-N1	-3.47	123.96	128.67
3	B	5101	ATP	N3-C2-N1	-3.46	123.98	128.67
4	B	5102	CFF	C14-N7-C8	-2.87	111.63	125.43

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

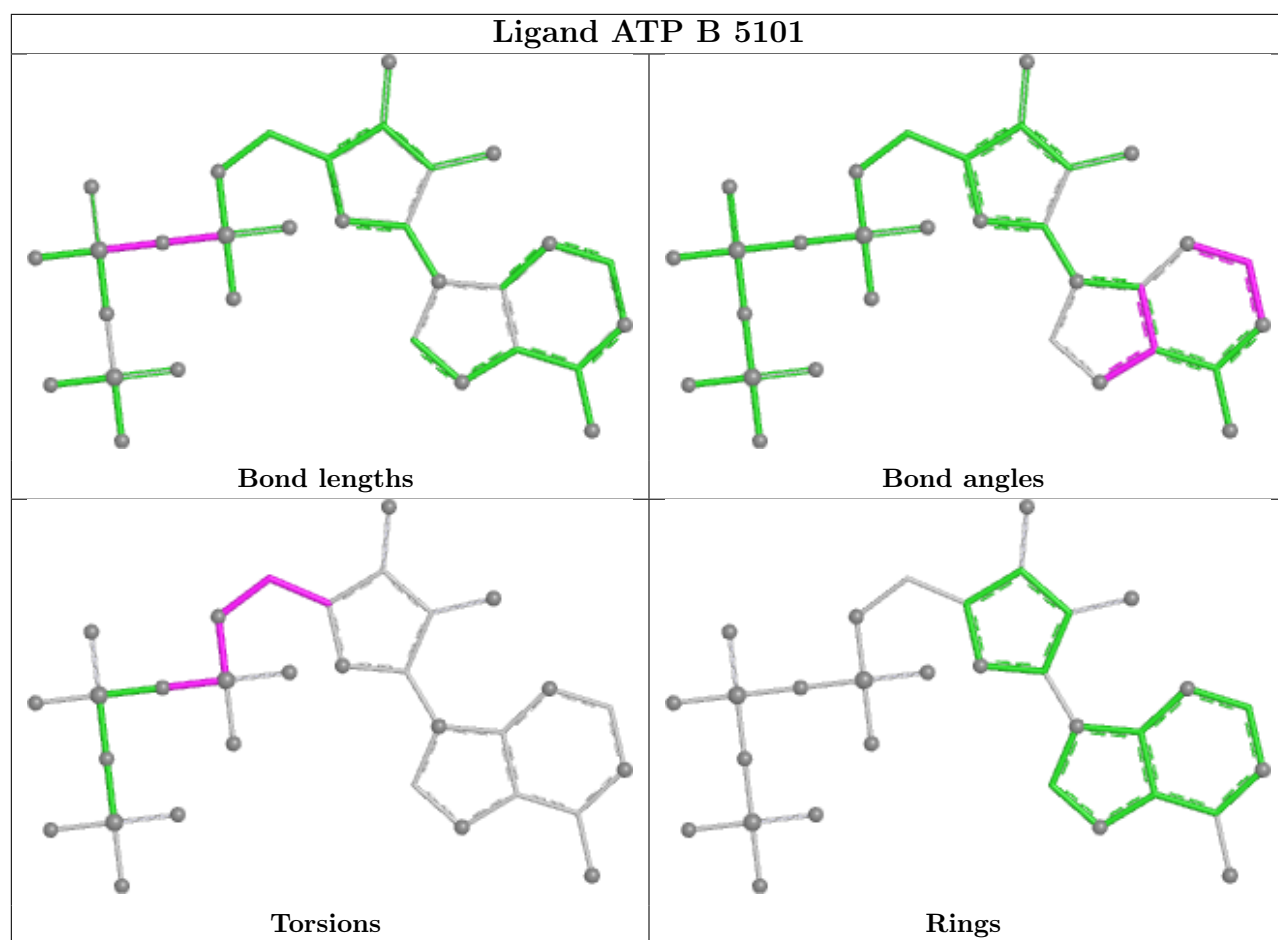
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A

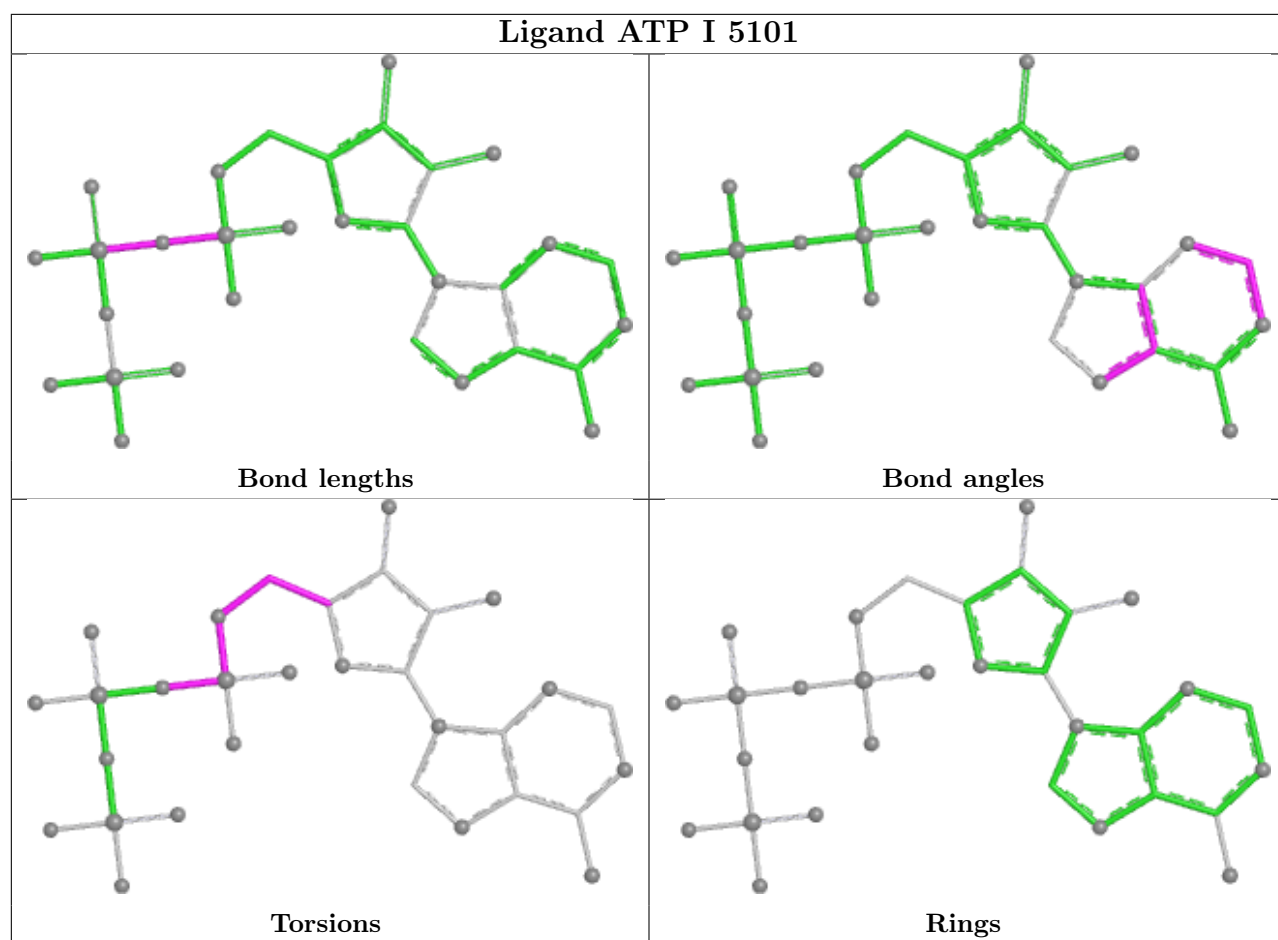
There are no ring outliers.

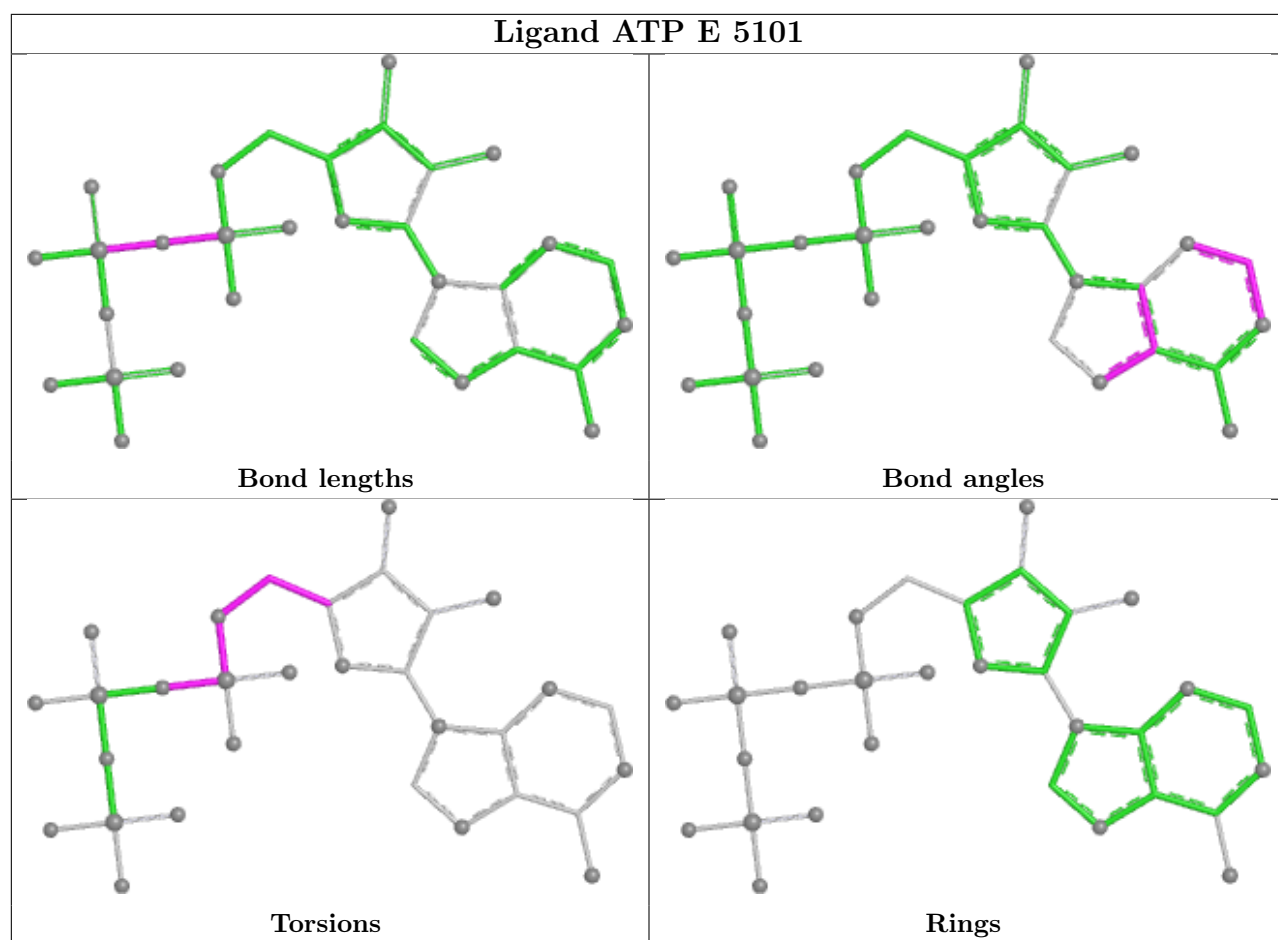
8 monomers are involved in 8 short contacts:

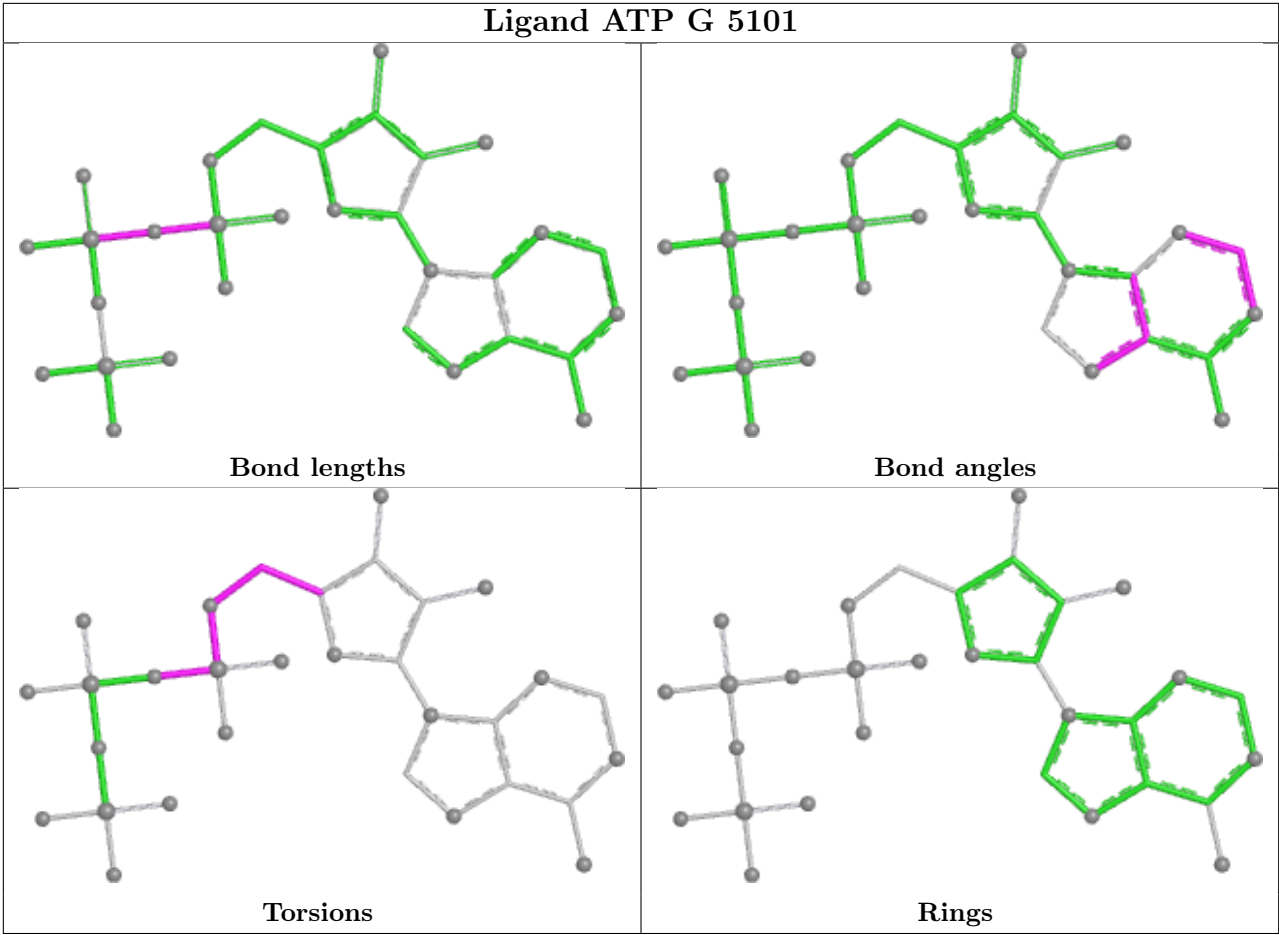
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
4	B	5102	CFF	1	0
4	E	5102	CFF	1	0
3	I	5101	ATP	1	0
4	I	5102	CFF	1	0
3	E	5101	ATP	1	0
3	G	5101	ATP	1	0
4	G	5102	CFF	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	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	74.23
1	E	4345:UNK	C	4540:PHE	N	74.23

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	74.22
1	G	4345:UNK	C	4540:PHE	N	74.22
1	I	3613:UNK	C	3639:THR	N	43.91

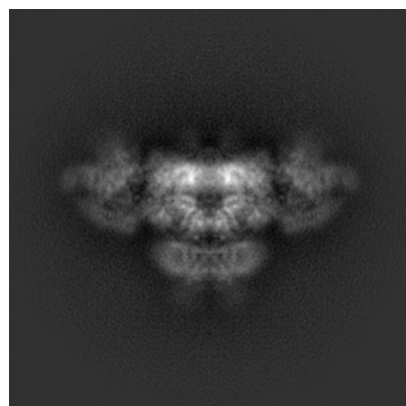
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8384. These allow visual inspection of the internal detail of the map and identification of artifacts.

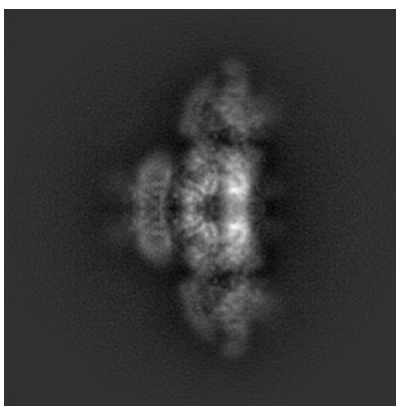
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

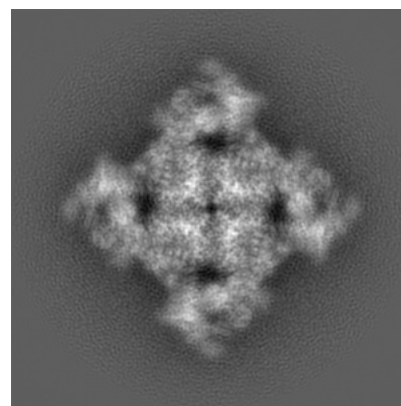
6.1.1 Primary map



X

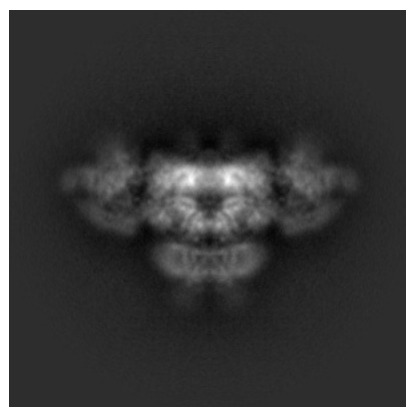


Y

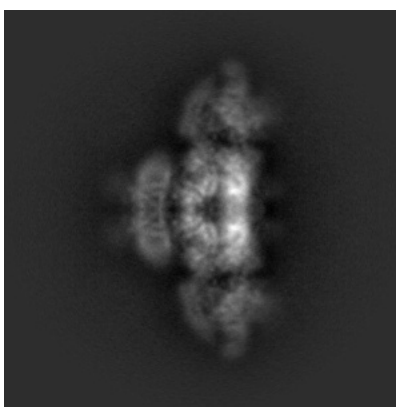


Z

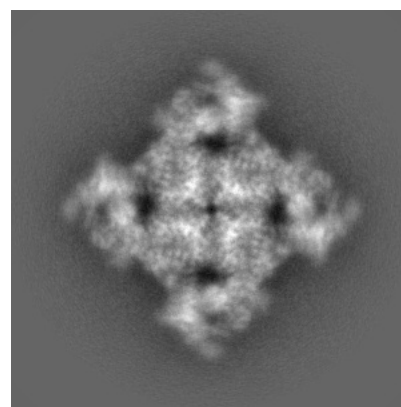
6.1.2 Raw map



X



Y

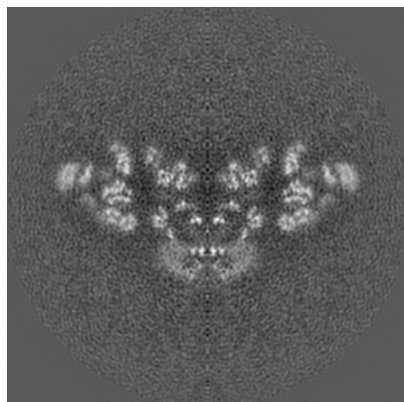


Z

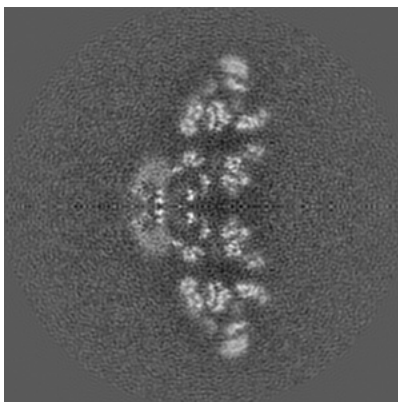
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

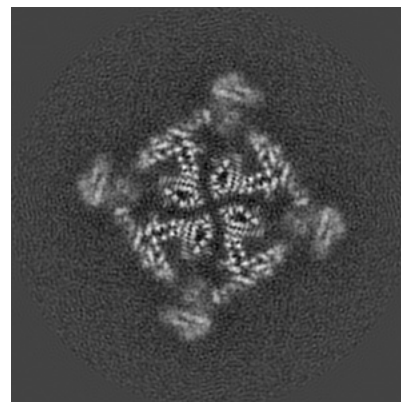
6.2.1 Primary map



X Index: 200

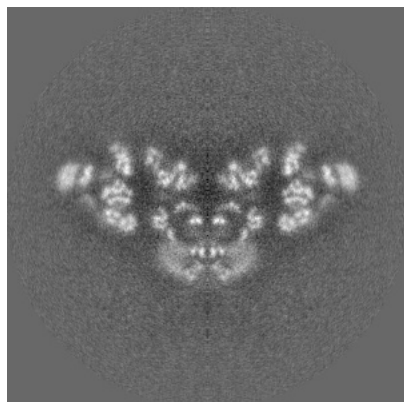


Y Index: 200

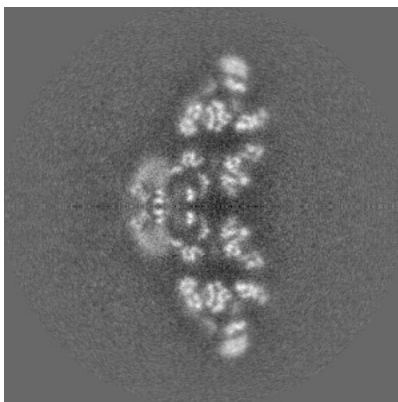


Z Index: 200

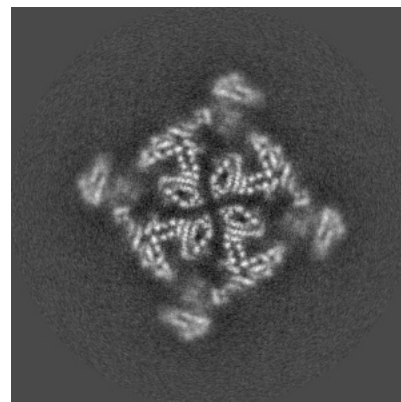
6.2.2 Raw map



X Index: 200



Y Index: 200

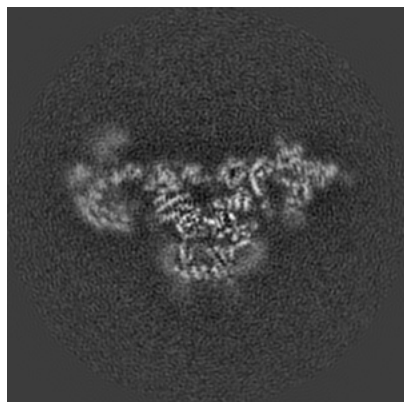


Z Index: 200

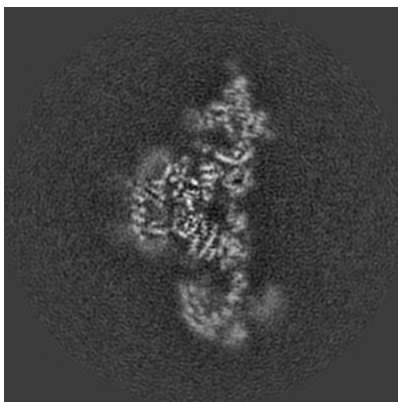
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

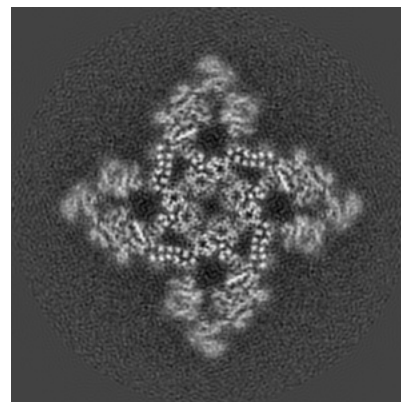
6.3.1 Primary map



X Index: 184

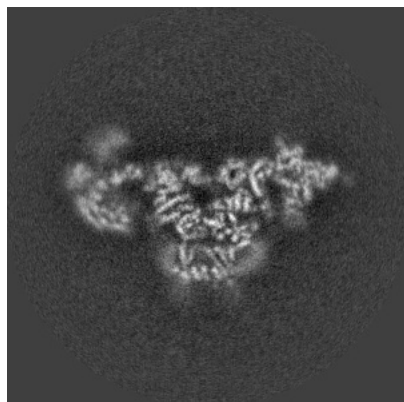


Y Index: 216

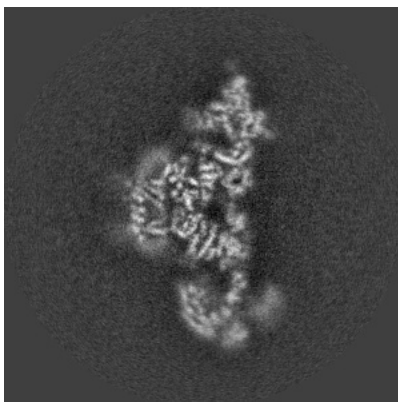


Z Index: 227

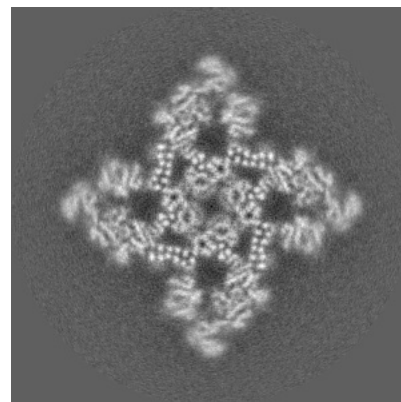
6.3.2 Raw map



X Index: 184



Y Index: 216

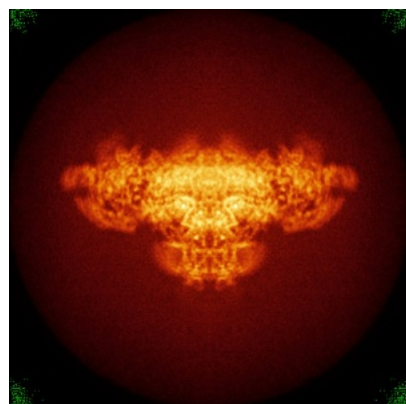


Z Index: 227

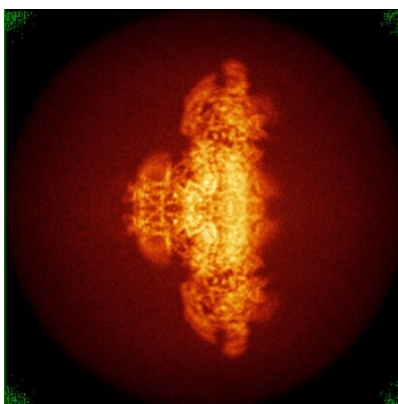
The images above show the largest variance slices of the map in three orthogonal directions.

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

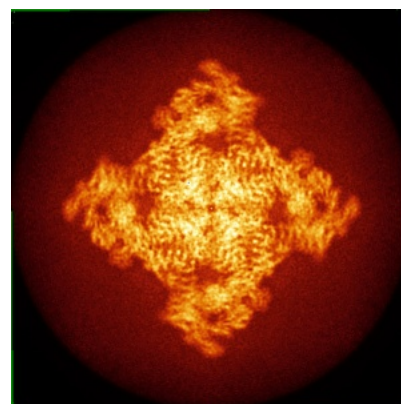
6.4.1 Primary map



X

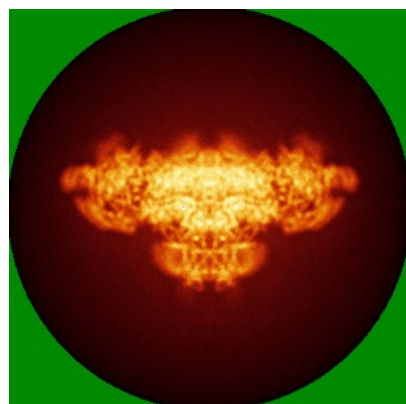


Y

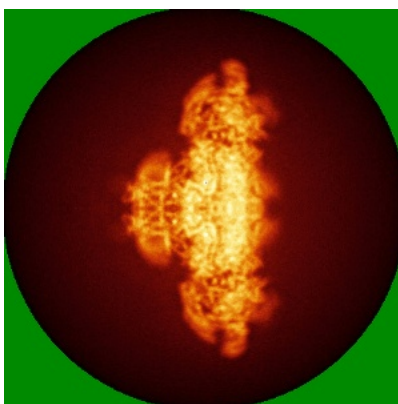


Z

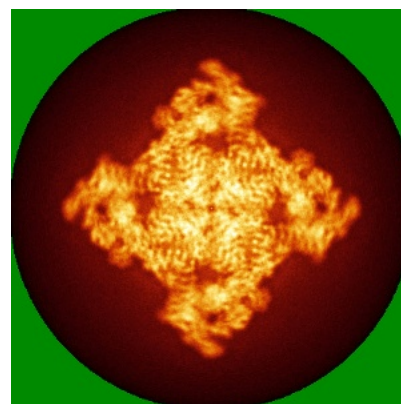
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

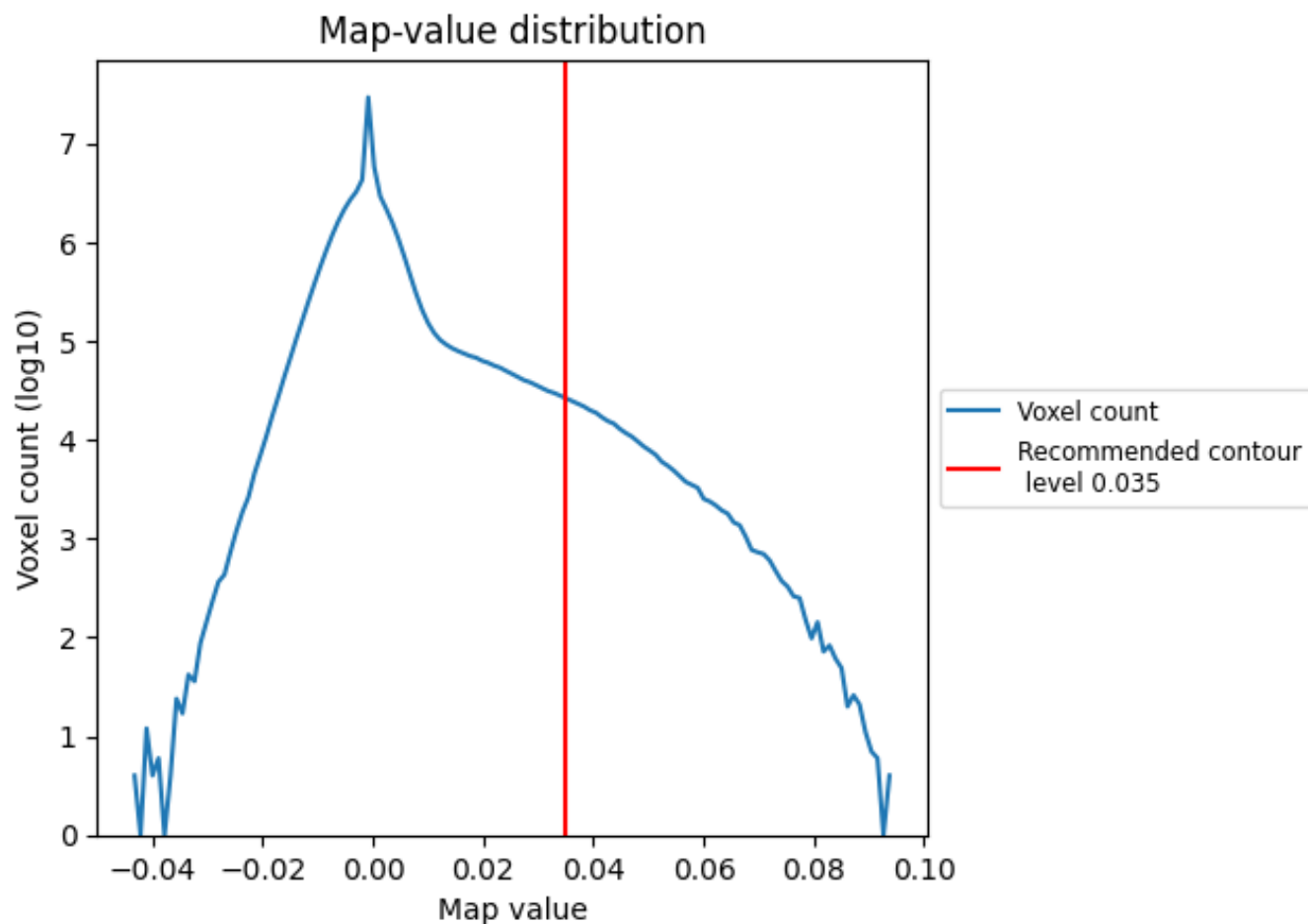
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

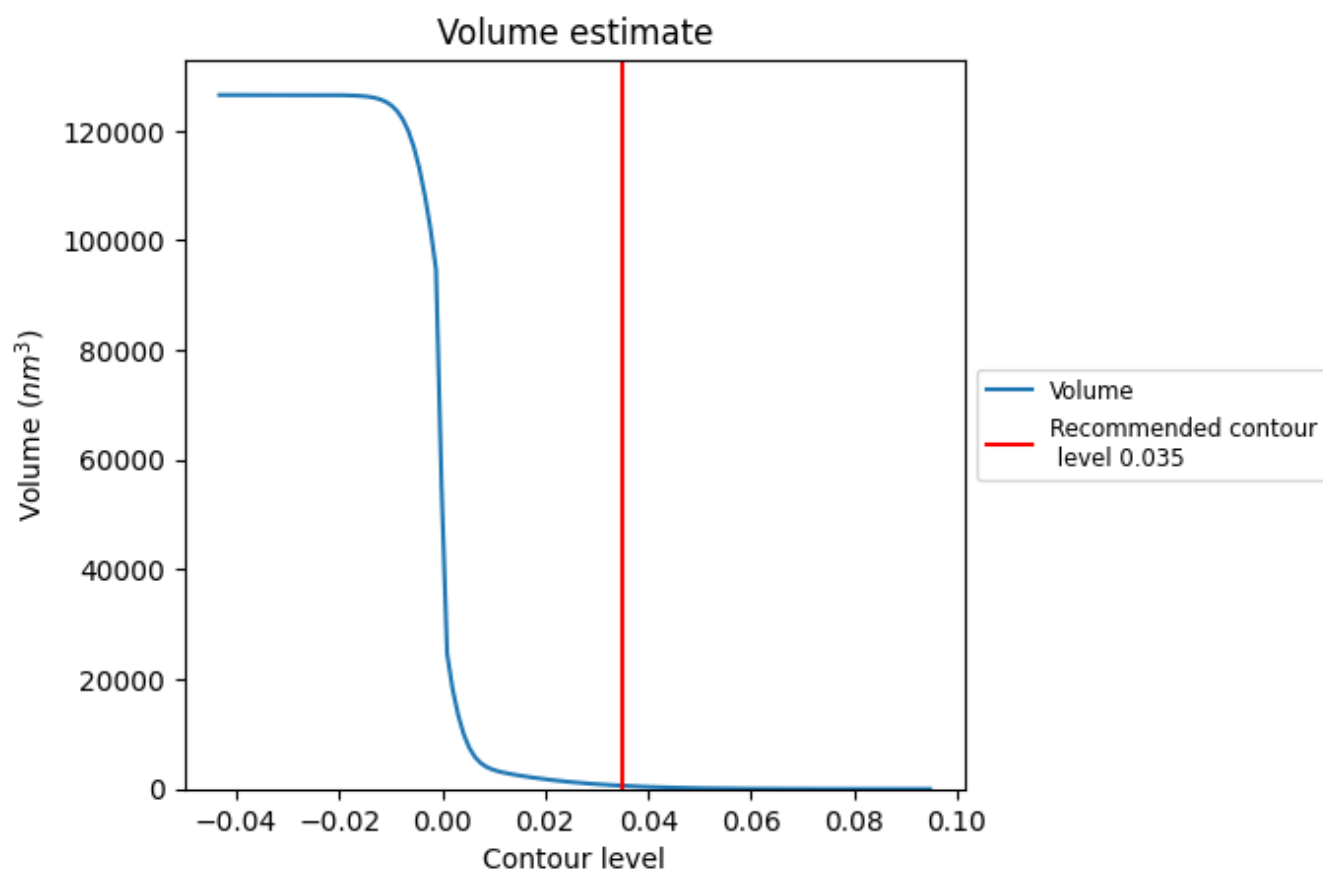
This section contains the results of statistical analysis of the map.

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.

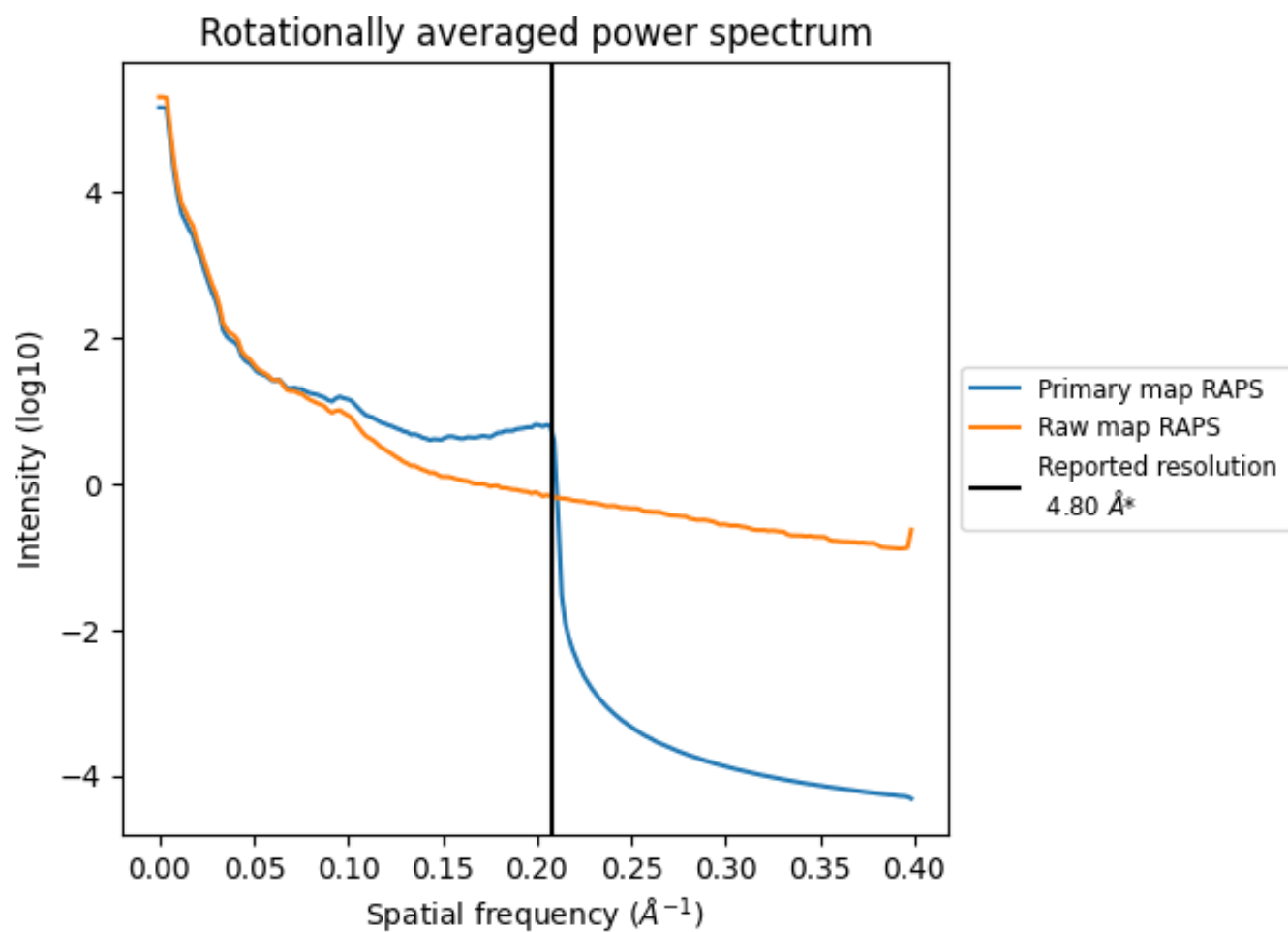
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 596 nm³; this corresponds to an approximate mass of 539 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 ⓘ

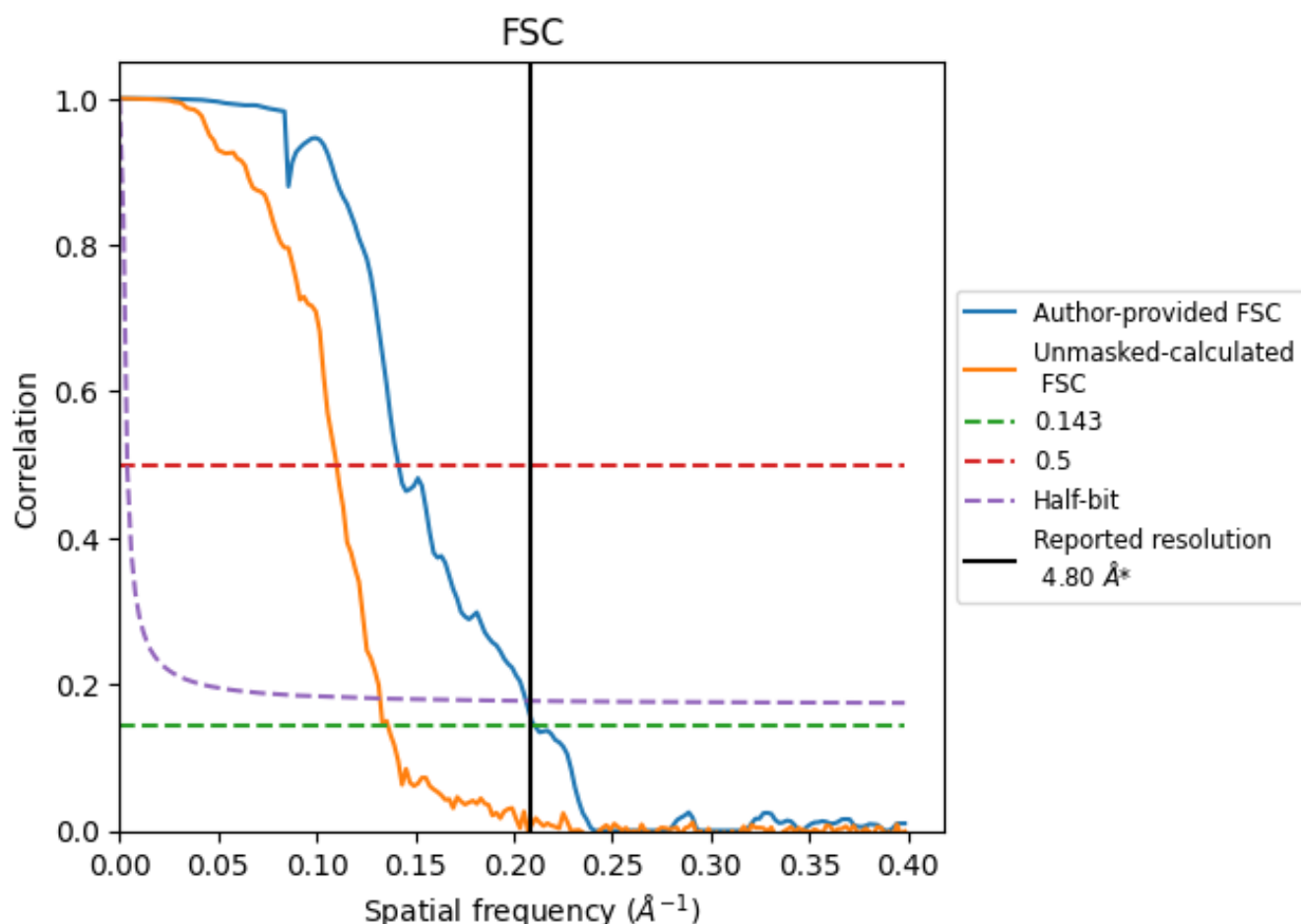


*Reported resolution corresponds to spatial frequency of 0.208 \AA^{-1}

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 0.208 \AA^{-1}

8.2 Resolution estimates [i](#)

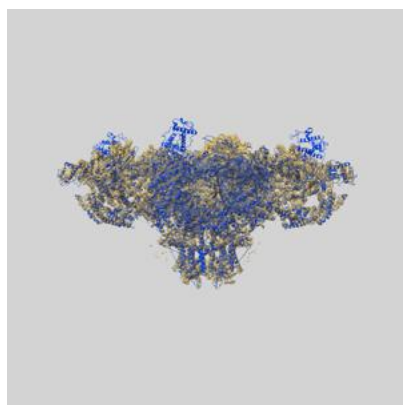
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.75	7.07	4.85
Unmasked-calculated*	7.34	9.09	7.57

*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 7.34 differs from the reported value 4.8 by more than 10 %

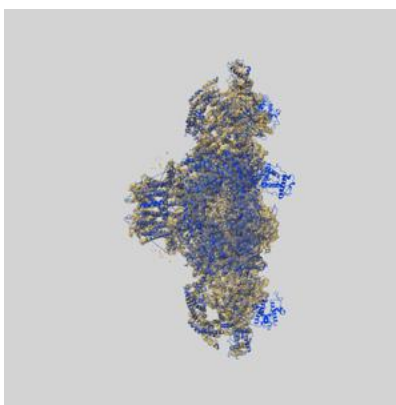
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8384 and PDB model 5TAT. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

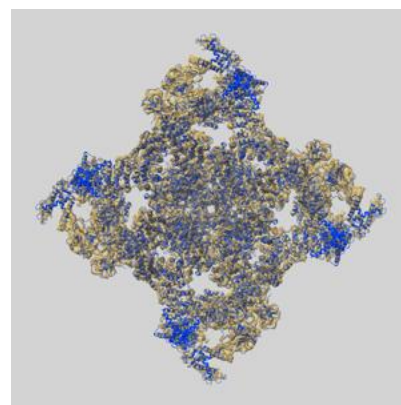
9.1 Map-model overlay [i](#)



X



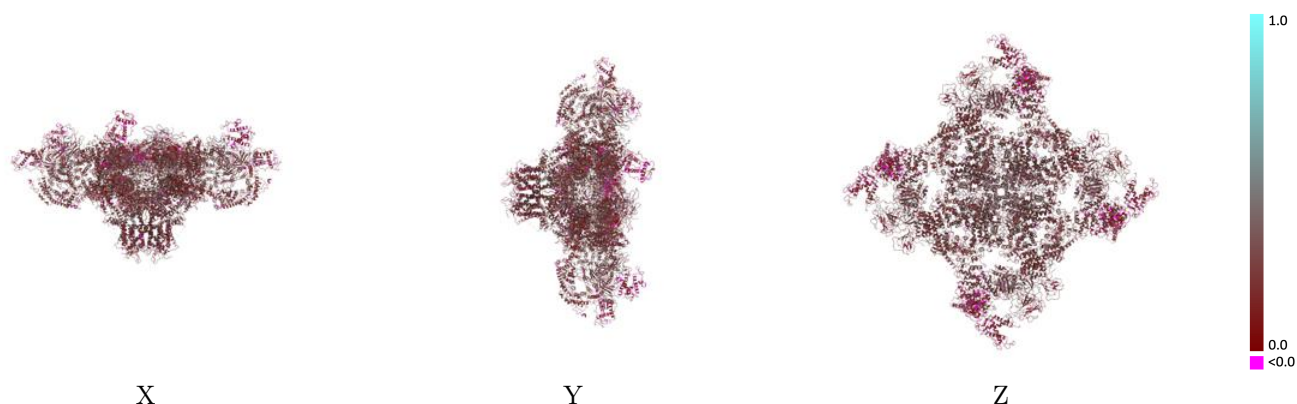
Y



Z

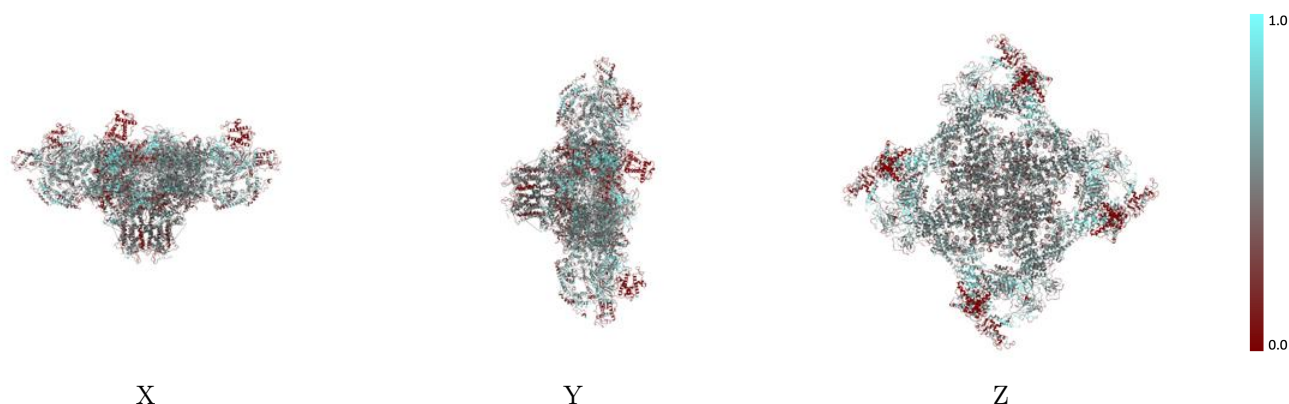
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



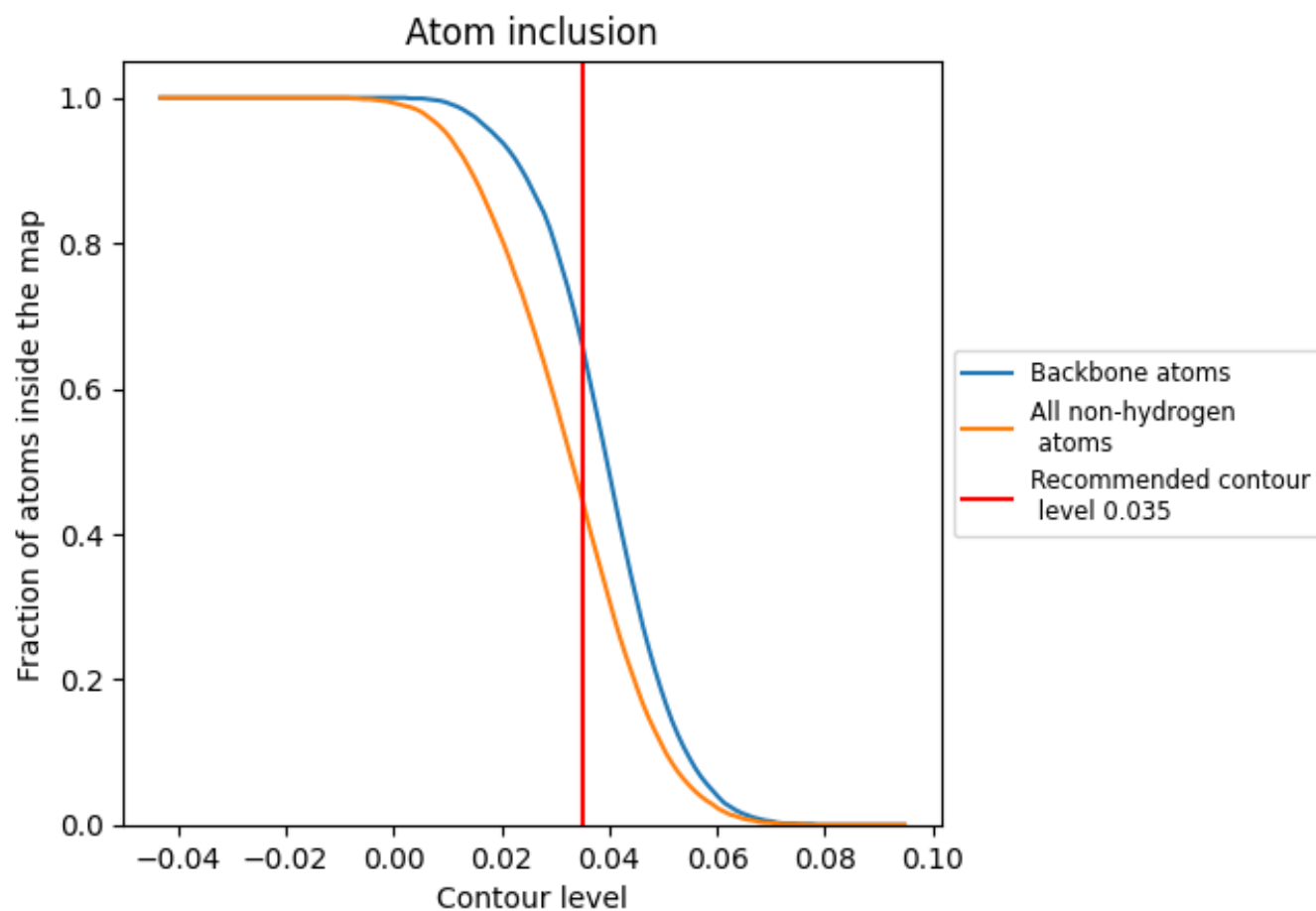
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 45% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4470	<div></div> 0.2510
A	<div></div> 0.4490	<div></div> 0.2490
B	<div></div> 0.4470	<div></div> 0.2510
E	<div></div> 0.4470	<div></div> 0.2510
F	<div></div> 0.4490	<div></div> 0.2530
G	<div></div> 0.4470	<div></div> 0.2510
H	<div></div> 0.4450	<div></div> 0.2510
I	<div></div> 0.4480	<div></div> 0.2520
J	<div></div> 0.4440	<div></div> 0.2510

1.0

0.0

<0.0