



wwPDB EM Validation Summary Report ⓘ

Oct 26, 2024 – 08:46 AM EDT

PDB ID : 5TA3
EMDB ID : EMD-8377
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 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

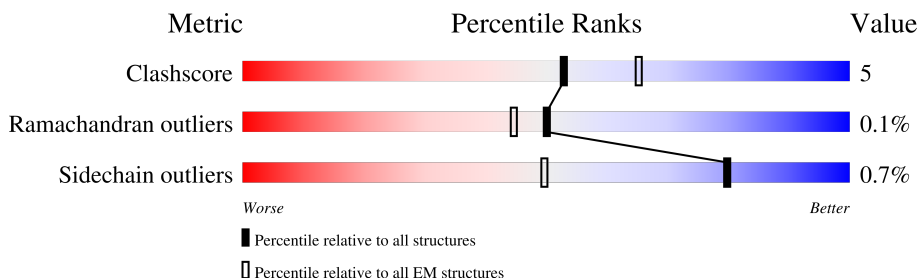
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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>69%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
1	F	108	<div> <div>69%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>
1	H	108	<div> <div>69%</div> <div>73%</div> <div>26%</div> <div>.</div> </div>
1	J	108	<div> <div>69%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>
2	B	4416	<div> <div>64%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	E	4416	<div> <div>63%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	G	4416	<div> <div>63%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	I	4416	<div> <div>63%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

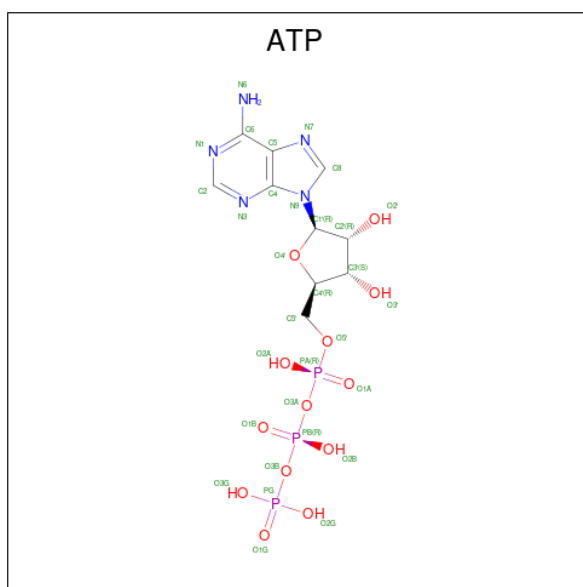
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

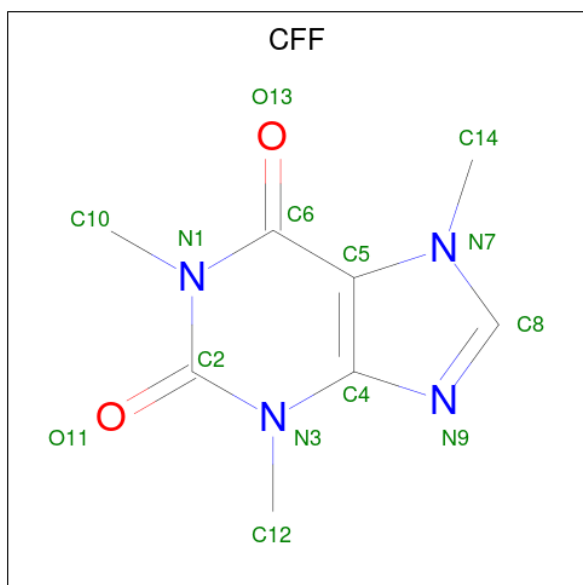
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



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

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



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

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

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

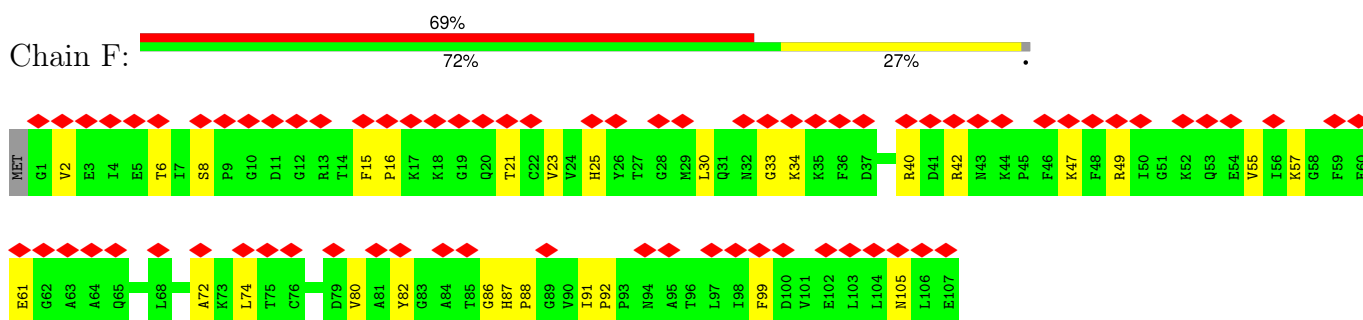
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

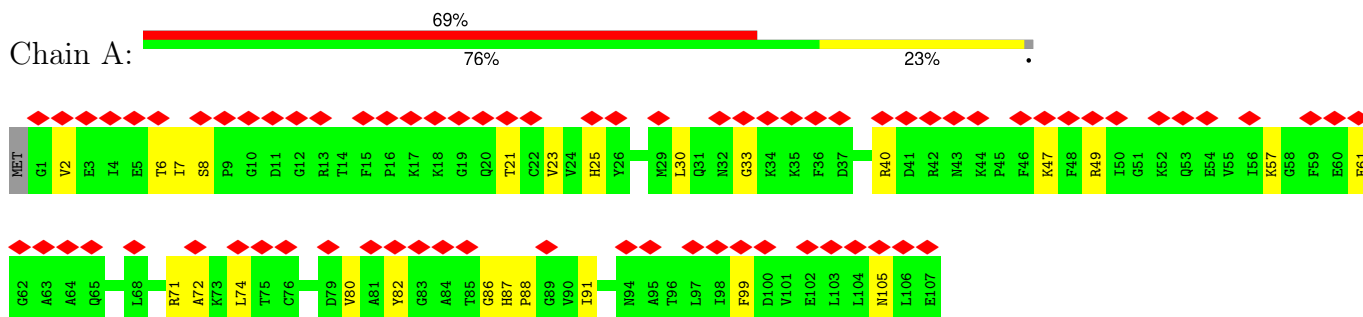
3 Residue-property plots [i](#)

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

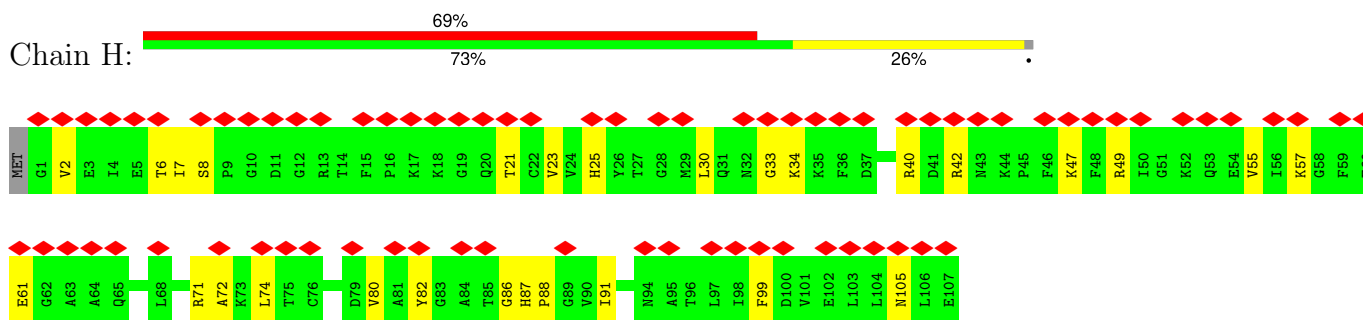
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

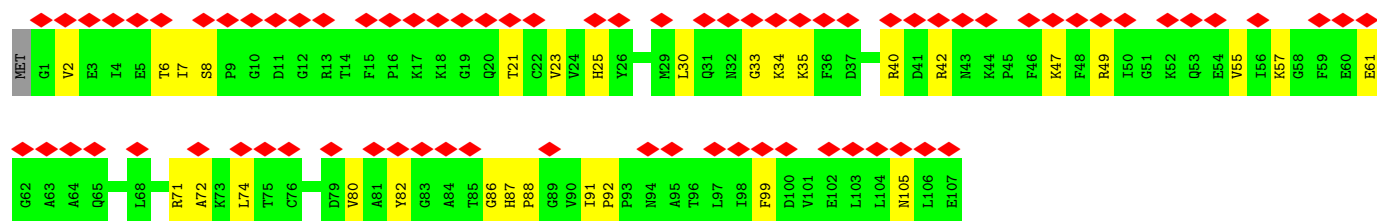


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

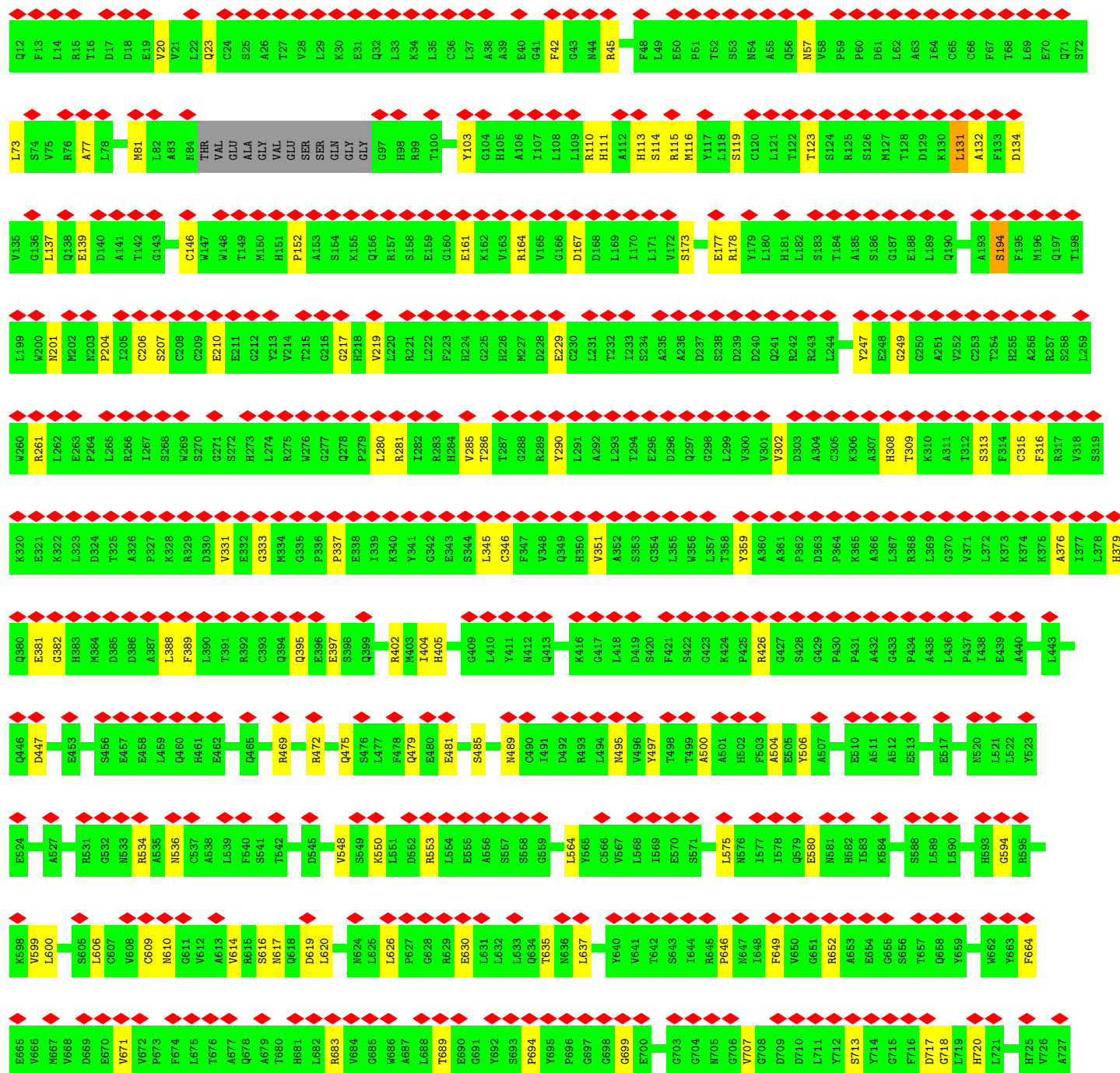
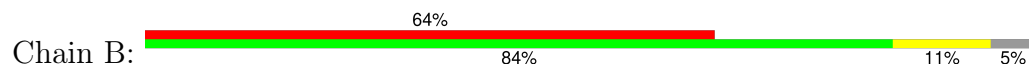


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: Ryanodine receptor 1

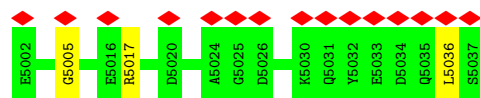


M679	R680	A684	L685	H688	L694	L695	H696	A697	L698	L699	D700	A701	H702	L703	P704	L707	R708	A709	G710	Y711	Y712	D713	I716	S717	H718	H719	L720	E721	R725	C726	R727	R728	L731	S732	E733	L738	T739	P740	E741	L742	R743	A744	L745	F748	P749	P750	G751	R752	K753	G754								
F1612	L1613	Q1614	L1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	E1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	P1633	L1634	T1635	M1636	M1637	A1638	L1639	E1643	E1644	N1645	R1646	C1647	M1648	D1649	I1650	L1651	E1652	L1653	S1654	E1655	R1656	L1657	Q1660	R1661	H1665	T1666	L1667	R1671	A1672	V1673	C1674	A1675	L1676					
X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1537	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1554	X1555	X1558	M1573	P1574	L1575	S1576	A1577	A1578	M1579	F1580	E1583	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	V1597	Q1598	M1599	L1600	V1603	S1604	W1605	M1608								
X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1457	X1458	X1459	X1460	X1464	X1473	X1474	X1475	X1476	X1479	X1480	X1486	X1487	X1488	X1489	X1492	X1495	X1496	X1497	X1502	X1503	X1504	X1505	X1506	X1507	X1510	X1511	X1512	X1513	X1514	X1515	X1516	X1519	X1520	X1521	X1522	X1523	X1524										
M1230	Q1231	R1232	T1235	T1236	K1240	S1241	L1242	P1243	Q1244	F1245	E1251	H1254	Y1255	E1256	V1257	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	P1267	C1268	L1270	R1271	L1272	L1273	H1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1297	X1430	X1434	X1435	X1436	X1437	X1438	X1439							
L1164	M1165	G1166	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	E1180	E1181	I1182	E1183	A1258	I1184	G1185	D1186	G1187	F1188	V1191	C1192	S1193	L1194	G1195	V1199	G1200	H1201	L1202	M1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	I1215	I1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1223	A1227	I1228	M1229		
W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	GLN	VAL	GLU	ASN	GLN	SER	THR	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	L1097	G1098	E1099	M1100	R1101	V1102	G1103			
V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	E990	N991	G992	A997	E998	D999	R1000	V1001	A1002	Q1003	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	M1035	R1036	D1037	S1038	L1039	C1040	Q1041	
E915	P916	E917	R918	N919	Y920	N921	L922	Q923	N924	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	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	N960	M961	S962	G964	Y965	K966	P967	A968	P969	L970	D971	S972	S973	H974
P855	V856	D857	THR	GLN	I861	V862	L863	P864	P865	H866	L867	E868	R869	I870	R871	E872	K873	L874	A875	E876	N877	I878	H879	E880	L881	W882	A883	L884	T885	R886	I887	E888	Q889	G890	W891	T892	Y893	P895	V896	D897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	
R790	F791	L792	L793	G794	G795	R796	H797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853	C854		

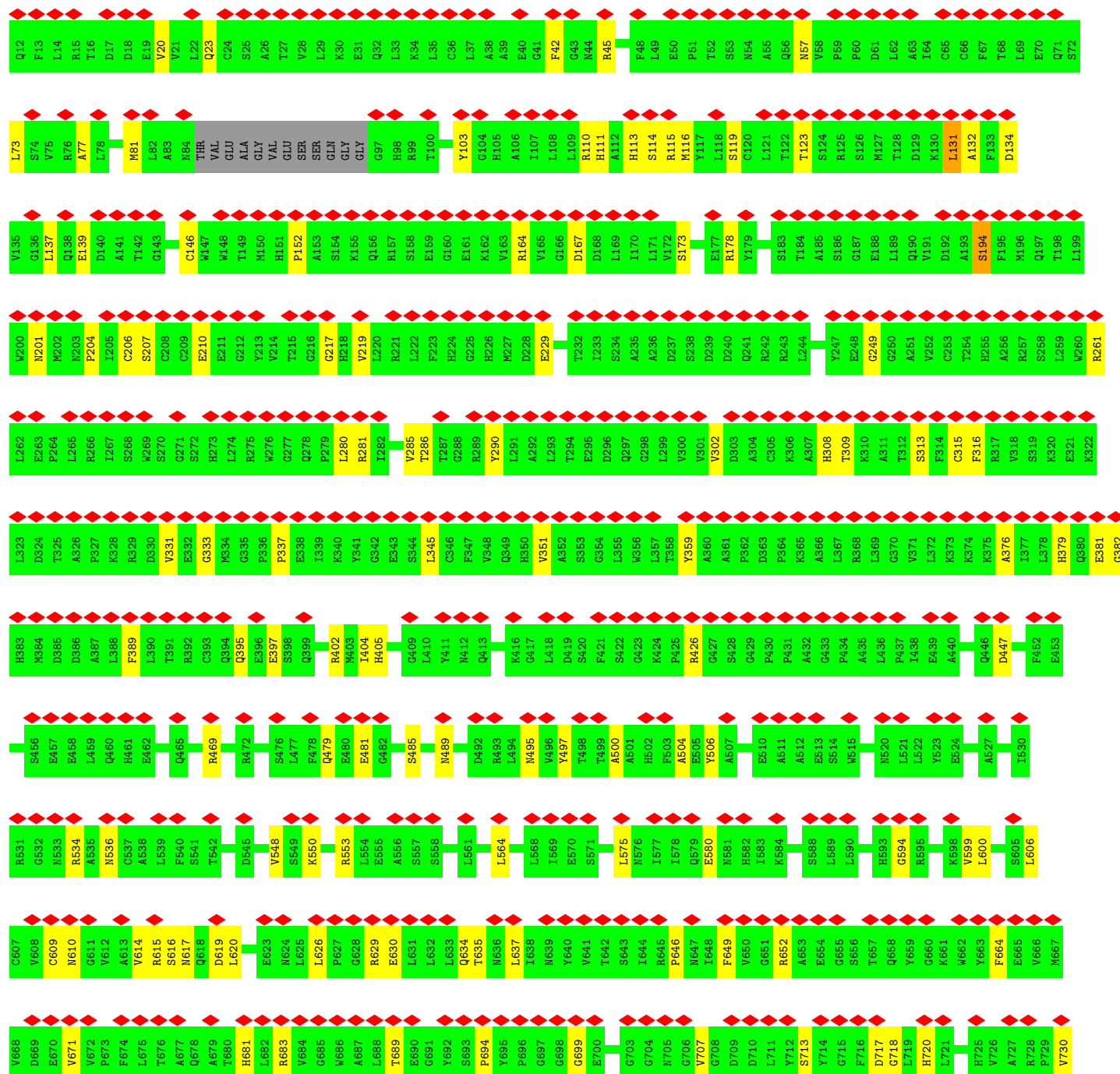
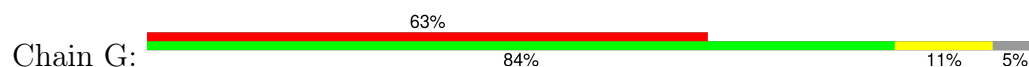


X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3603	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	L3641	X3642	N3643	L3644	H3647	R3648	M3652	E3655	S3656	Y3657	K3658	A3659	K3661	I3662	E3665	D3666	H3667	S3668	F3669	R3672	K3673	I3674	D3675	D3676																										
X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444											X3445	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525									
X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421																		
X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361																		
X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301																	
X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231																		
X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3081	X3082	X3083	X3084	X3085	X3086	X3087	X3088	X3089	X3090	X3091	X3092	X3093	X3094	X3095	X3096																	
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LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	G2863	V2864	T2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	L2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895																		
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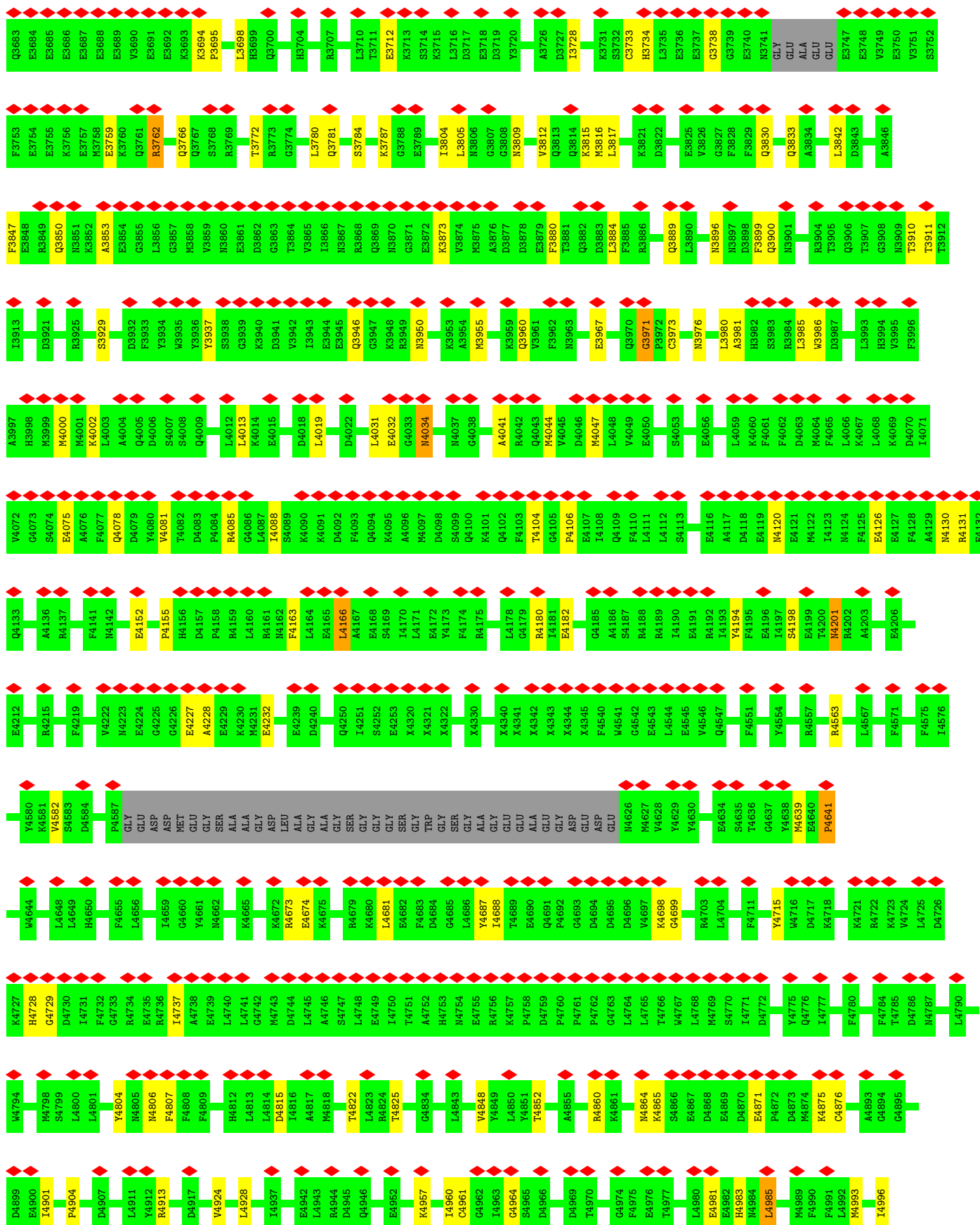
● Molecule 2: Ryanodine receptor 1

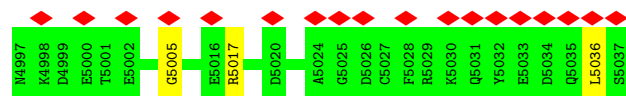


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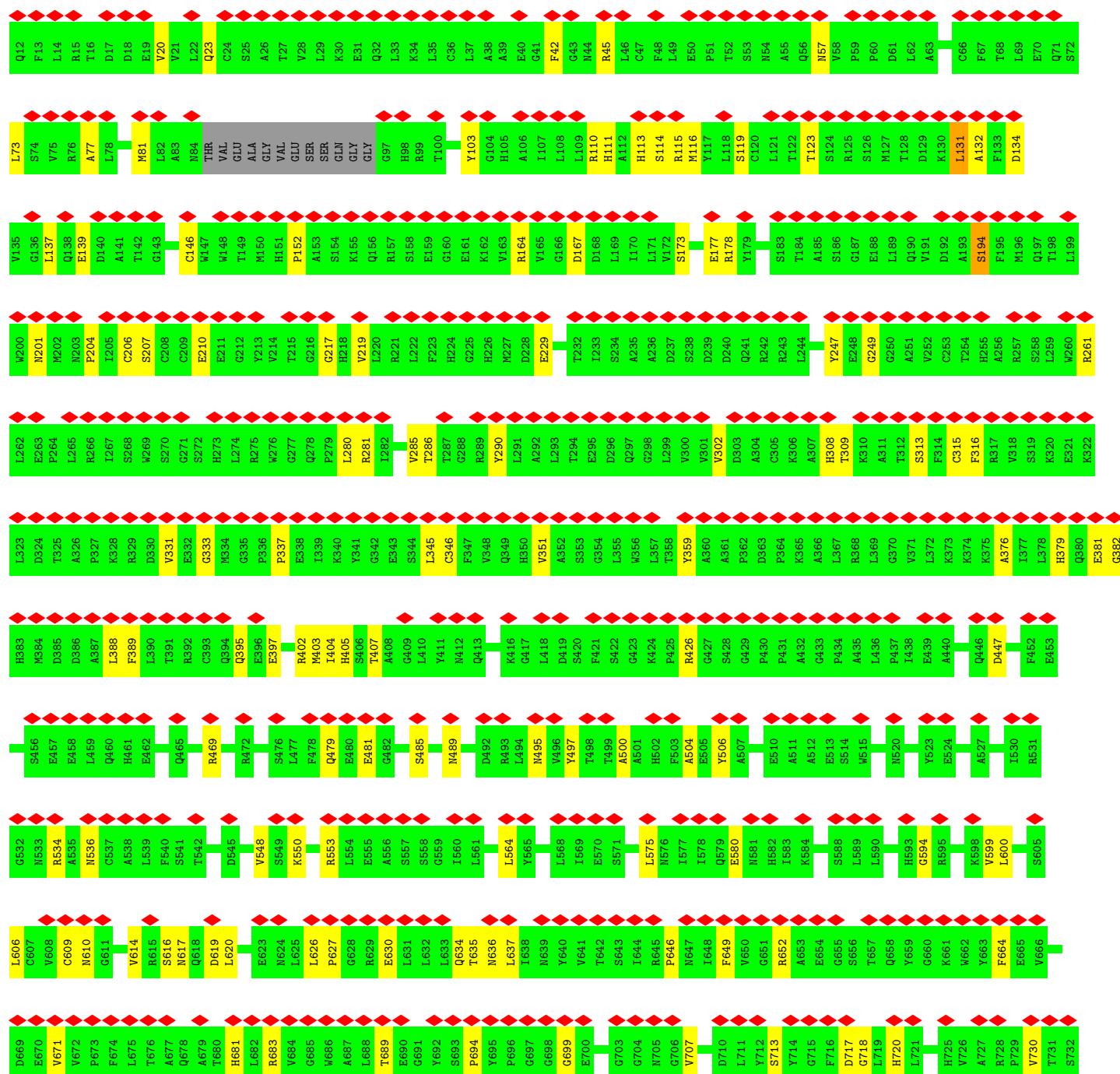






• Molecule 2: Ryanodine receptor 1

Chain I: 63% 84% 11% 5%

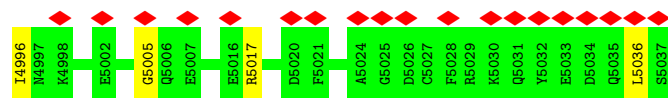


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VAL	GLN	S861	V862	L863	P864	F800	H866	L867	E868	R869	I870	R871	E872	K873	L874	A875	E876	N877	L878	H879	E880	L881	W882	A883	L884	T885	R886	I887	Q888	Q889	G890	W891	T892	T893	G894	P895	V896	R897	D898	D899	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	R917		
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P733	G734	Q735	H736	L737	L738	A739	P740	E741	D742	S745	C746	C747	L748	D749	S751	V752	P753	S754	F757	R758	N760	G761	C762	P763	V764	Q765	V767	F768	E769	A770	F771	N772	D773	L774	G775	L776	F777	F778	P779	W780	V781	S782	F783	A785	G786	V787	K788	W789	R790	F791	C854	L793	G794						

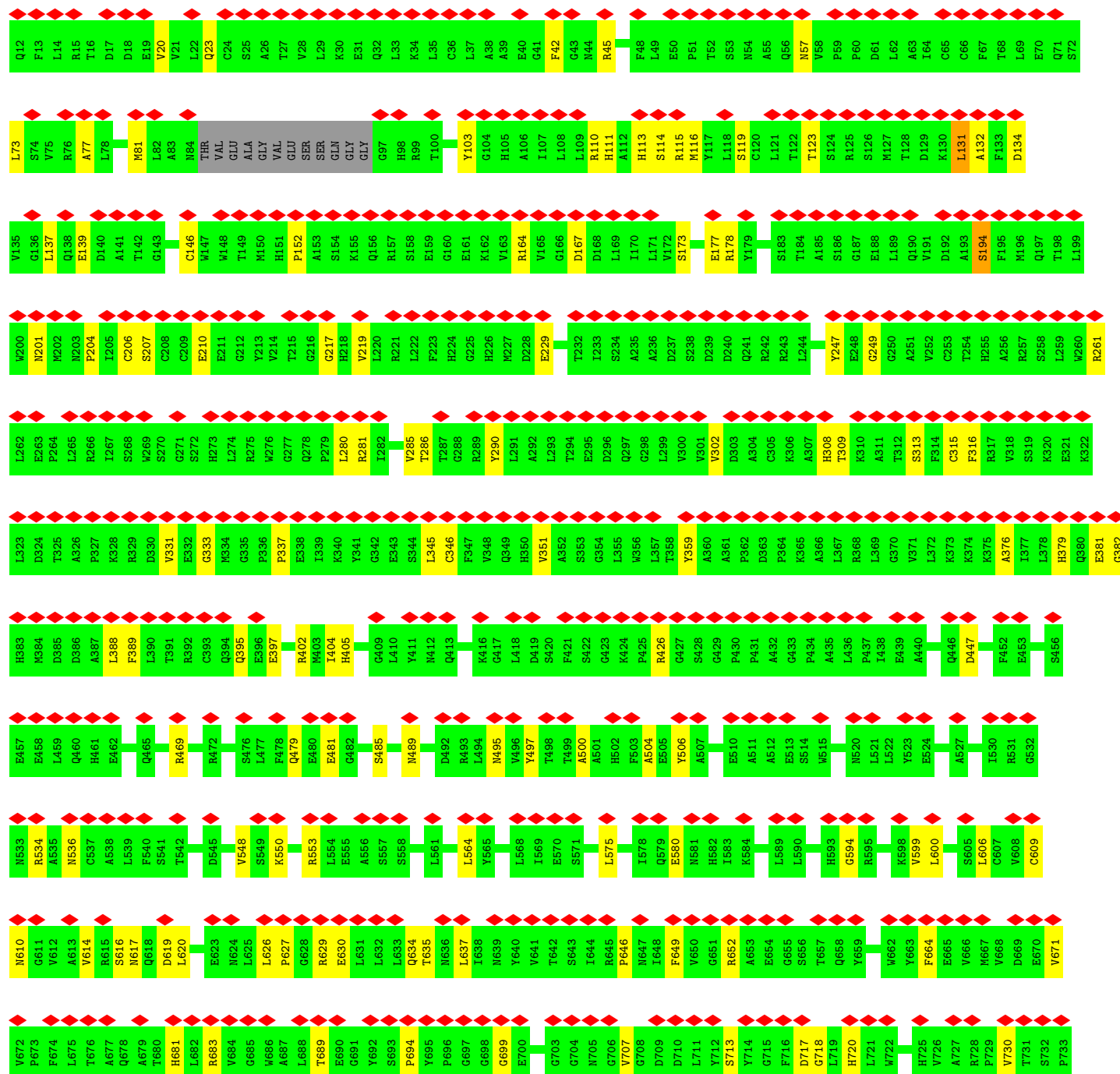
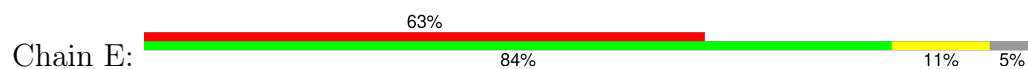


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GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	THR	LYS	LYS	SER	ILE	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	E2869	L2870	Q2871	M2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	A2891	A2892	X2893																																																																			
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• Molecule 2: Ryanodine receptor 1

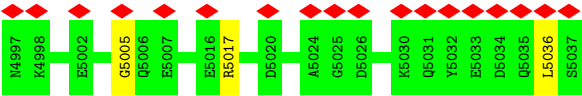


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4 Experimental information

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	0.064	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.52	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.30	0/25428	0.54	9/34534 (0.0%)
2	E	0.30	0/25428	0.54	9/34534 (0.0%)
2	G	0.30	0/25428	0.54	9/34534 (0.0%)
2	I	0.30	0/25428	0.54	9/34534 (0.0%)
All	All	0.30	0/105048	0.54	36/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	7.43	132.38	115.30
2	G	131	LEU	CA-CB-CG	7.42	132.36	115.30
2	I	131	LEU	CA-CB-CG	7.42	132.36	115.30
2	E	131	LEU	CA-CB-CG	7.41	132.34	115.30
2	G	4985	LEU	CA-CB-CG	6.93	131.25	115.30

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	18	0
1	H	818	0	824	17	0
1	J	818	0	824	19	0
2	B	29499	0	24746	271	0
2	E	29499	0	24745	276	0
2	G	29499	0	24745	266	0
2	I	29499	0	24745	278	0
3	B	31	0	12	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102365	1132	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 1132 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:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.52	0.74
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.73
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.71	0.73
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.52	0.73

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%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	44	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	44	78
2	G	3235/4416 (73%)	2881 (89%)	349 (11%)	5 (0%)	44	78
2	I	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	44	78
All	All	13360/18096 (74%)	11903 (89%)	1437 (11%)	20 (0%)	50	83

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	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	E	1676	LEU

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Mol	Chain	Res	Type
2	E	3762	ARG
2	E	4131	ARG
2	G	1964	ARG
2	G	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	3950	ASN
2	E	1693	GLN
2	I	495	ASN
2	E	1679	ASN
2	E	3946	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 [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	5101	-	28,33,33	0.83	0	34,52,52	1.23	2 (5%)
4	CFF	G	5102	-	8,15,15	2.11	3 (37%)	8,23,23	1.26	1 (12%)
3	ATP	B	5101	-	28,33,33	0.83	0	34,52,52	1.24	2 (5%)
4	CFF	I	5102	-	8,15,15	2.11	3 (37%)	8,23,23	1.26	1 (12%)
3	ATP	G	5101	-	28,33,33	0.83	0	34,52,52	1.23	2 (5%)
3	ATP	I	5101	-	28,33,33	0.84	0	34,52,52	1.23	2 (5%)
4	CFF	E	5102	-	8,15,15	2.11	3 (37%)	8,23,23	1.27	1 (12%)
4	CFF	B	5102	-	8,15,15	2.10	3 (37%)	8,23,23	1.27	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C6-N1	-3.50	1.32	1.38
4	E	5102	CFF	C6-N1	-3.49	1.32	1.38
4	B	5102	CFF	C6-N1	-3.46	1.32	1.38
4	G	5102	CFF	C6-N1	-3.44	1.32	1.38
4	G	5102	CFF	C5-C4	-3.40	1.33	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	ATP	N3-C2-N1	-3.90	123.38	128.67
3	G	5101	ATP	N3-C2-N1	-3.89	123.40	128.67
3	I	5101	ATP	N3-C2-N1	-3.87	123.42	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-3.84	123.46	128.67
4	G	5102	CFF	C14-N7-C8	-2.88	111.56	125.43

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

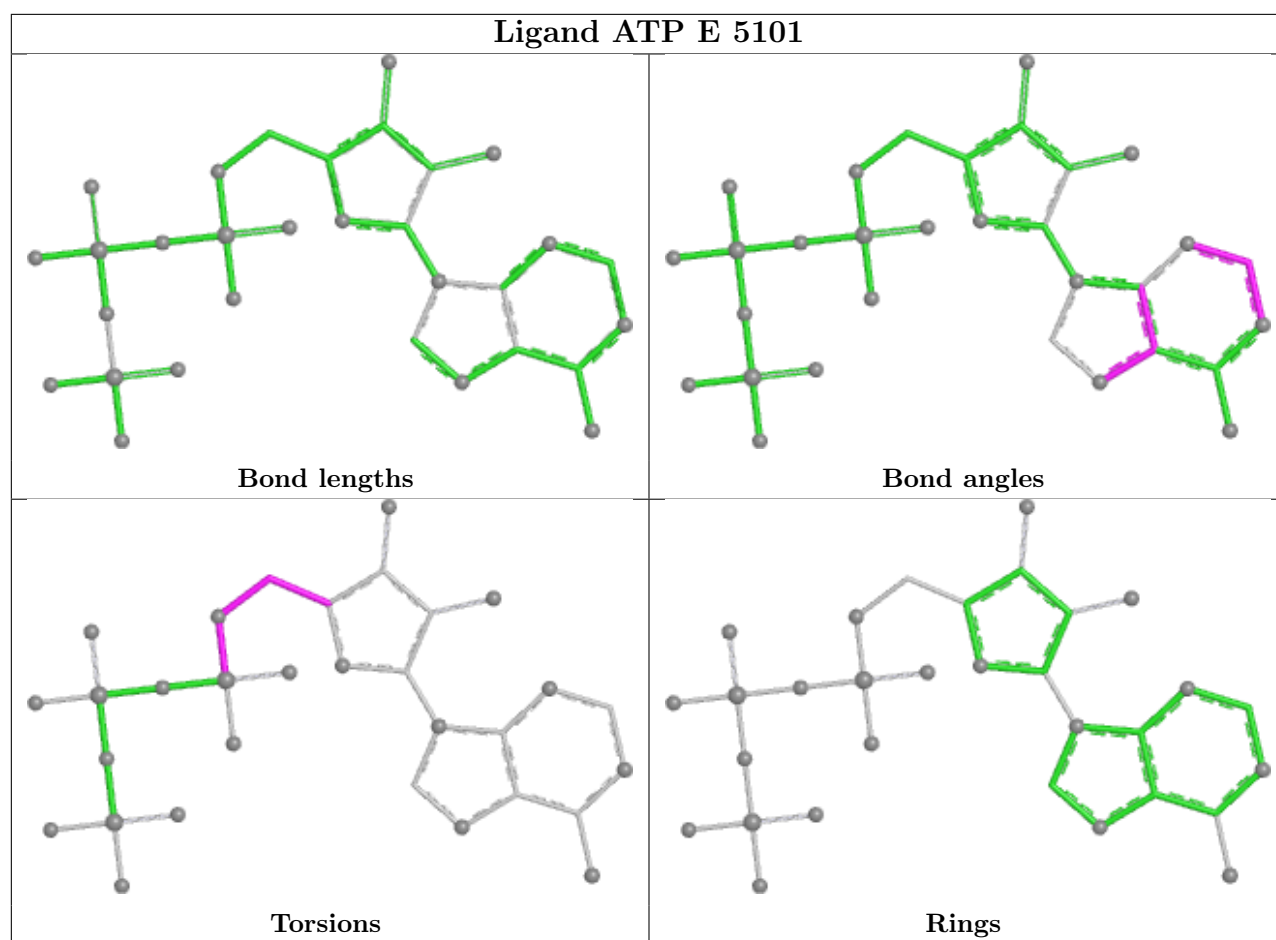
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A

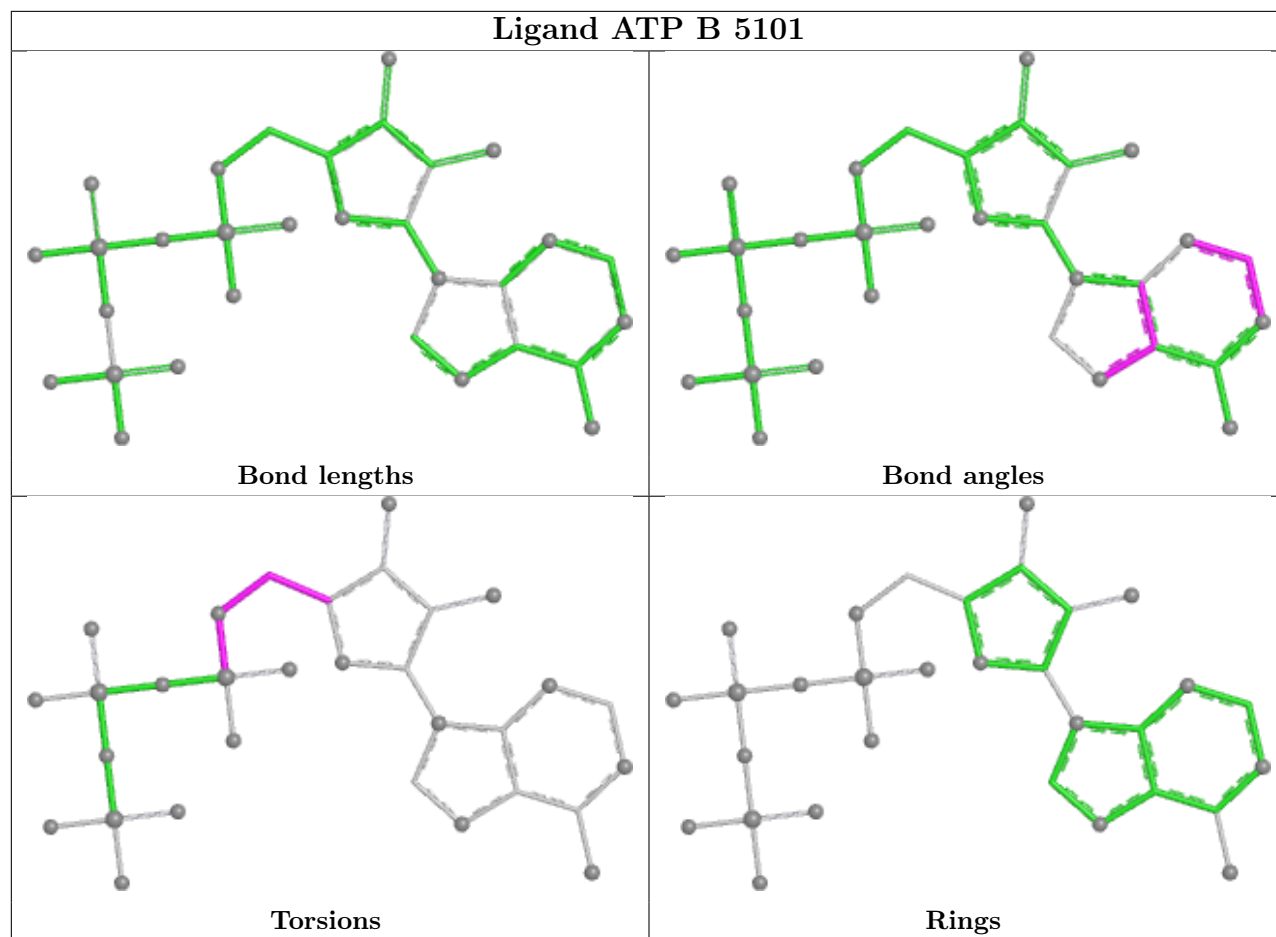
There are no ring outliers.

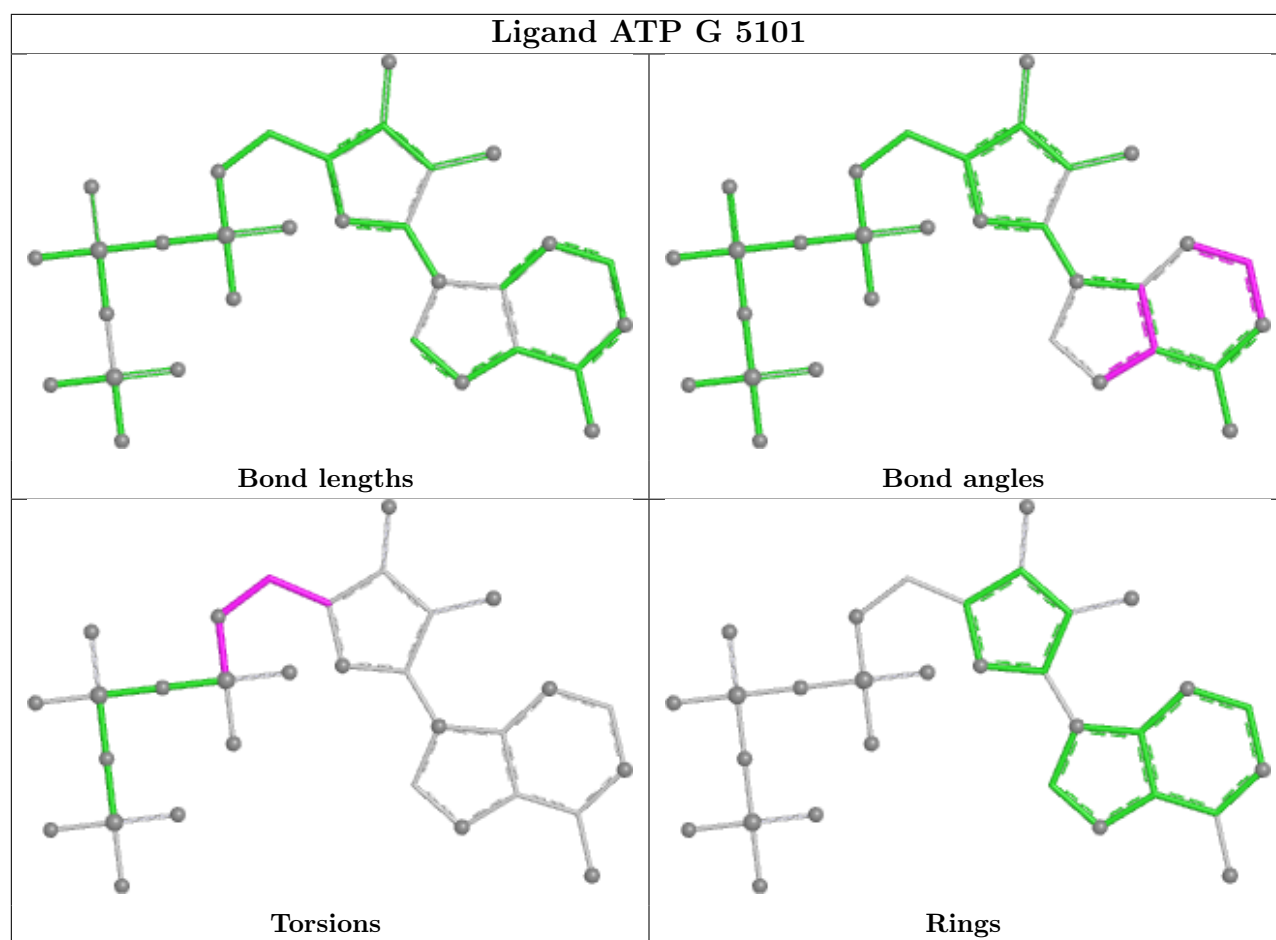
8 monomers are involved in 9 short contacts:

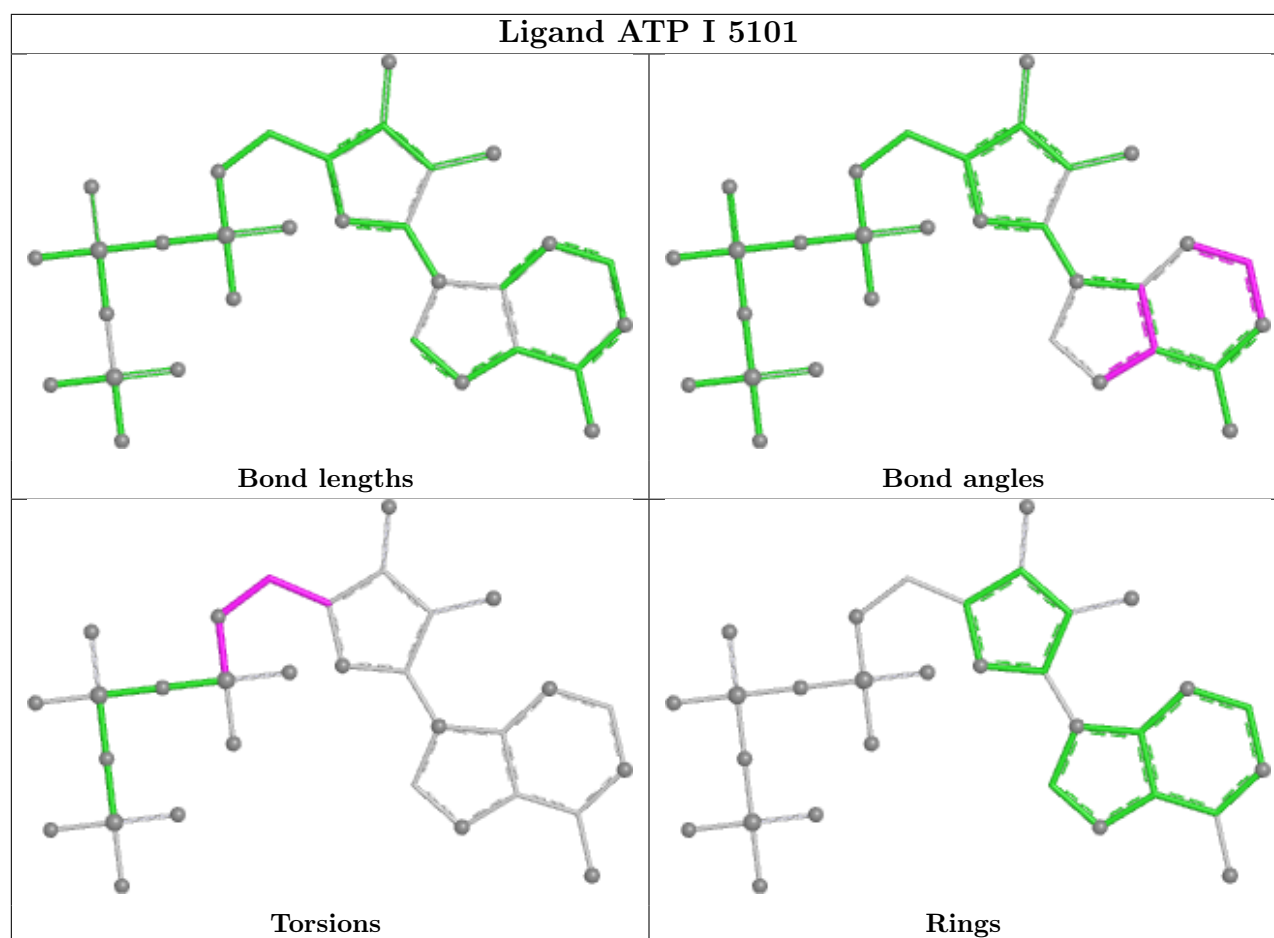
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	1	0
4	G	5102	CFF	1	0
3	B	5101	ATP	2	0
4	I	5102	CFF	1	0
3	G	5101	ATP	1	0
3	I	5101	ATP	1	0
4	E	5102	CFF	1	0
4	B	5102	CFF	1	0

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	E	14
2	B	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	E	4345:UNK	C	4540:PHE	N	73.04
1	B	4345:UNK	C	4540:PHE	N	73.02

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.01
1	G	4345:UNK	C	4540:PHE	N	73.00
1	E	3613:UNK	C	3639:THR	N	45.97

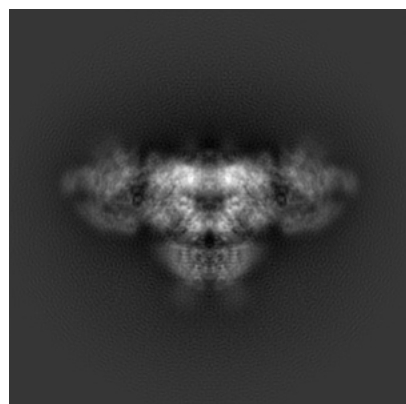
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8377. These allow visual inspection of the internal detail of the map and identification of artifacts.

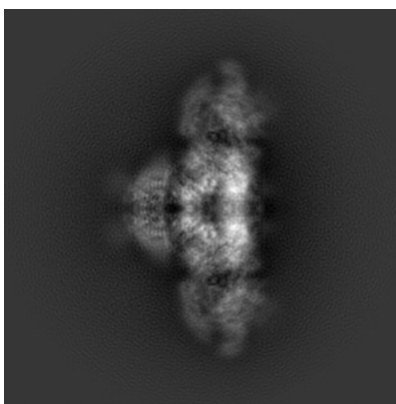
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

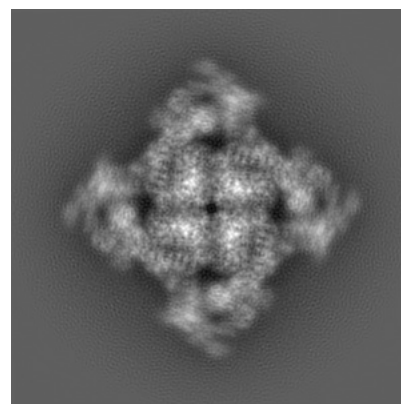
6.1.1 Primary map



X

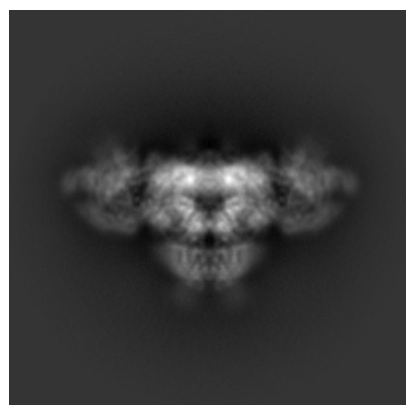


Y

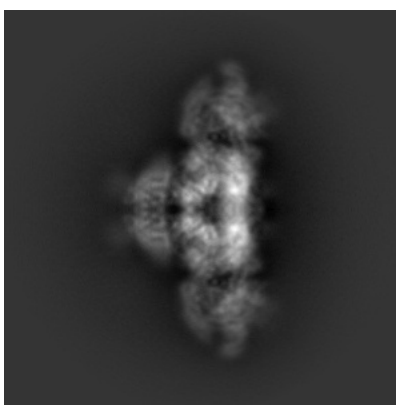


Z

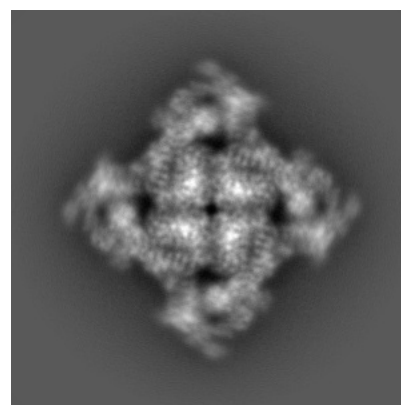
6.1.2 Raw map



X



Y

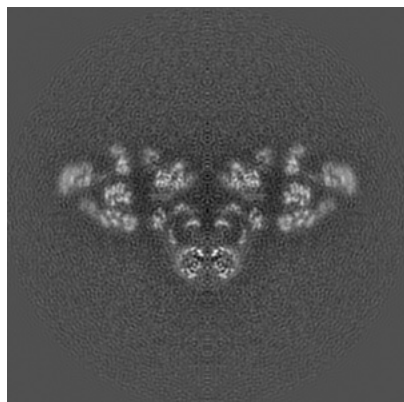


Z

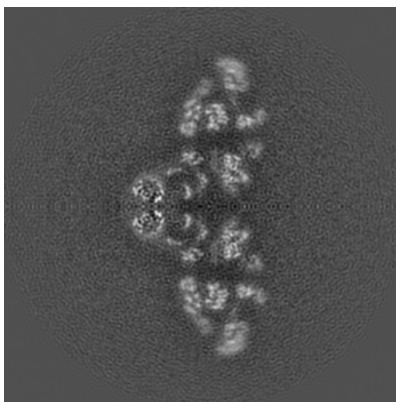
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

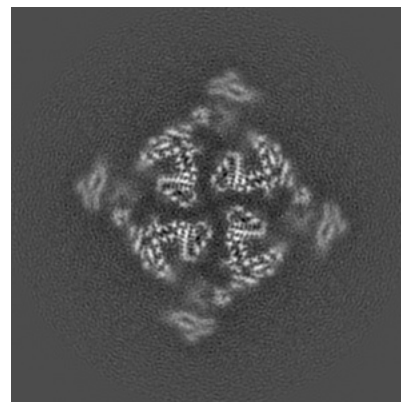
6.2.1 Primary map



X Index: 200

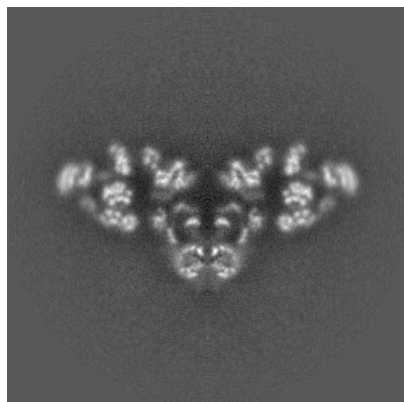


Y Index: 200

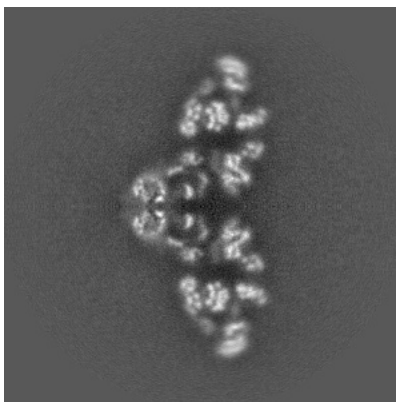


Z Index: 200

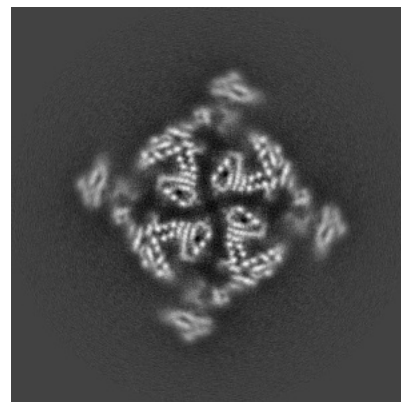
6.2.2 Raw map



X Index: 200



Y Index: 200

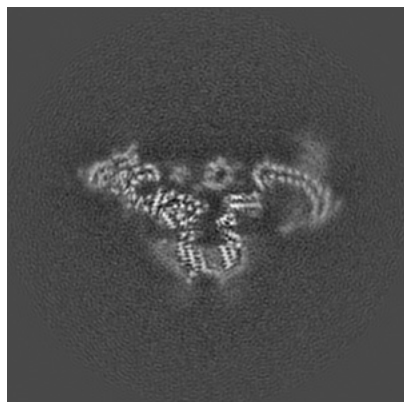


Z Index: 200

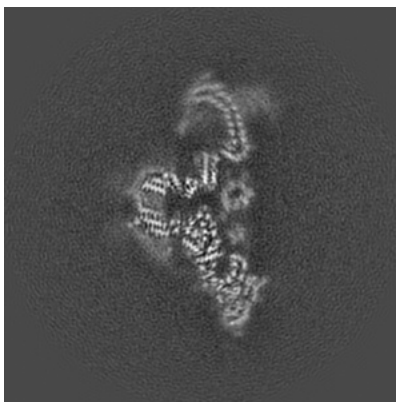
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

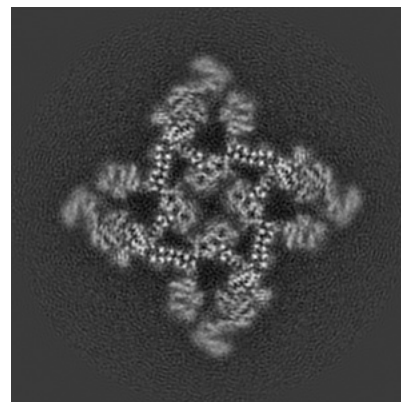
6.3.1 Primary map



X Index: 225

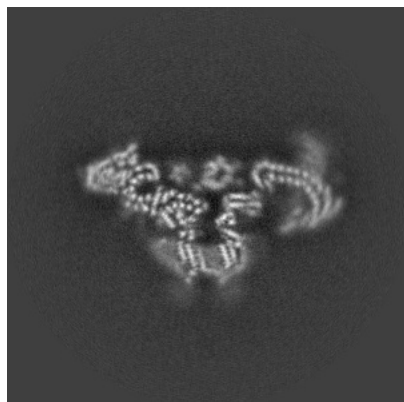


Y Index: 175

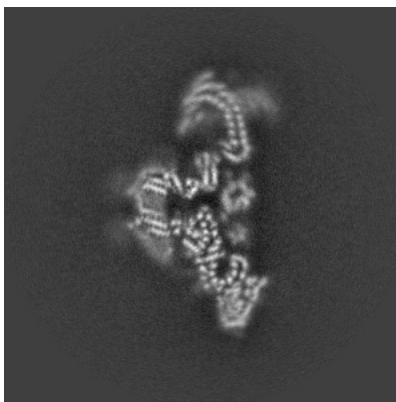


Z Index: 226

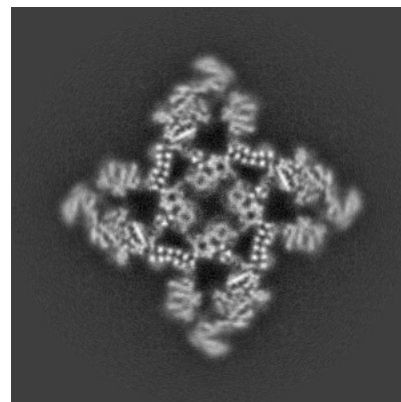
6.3.2 Raw map



X Index: 225



Y Index: 175

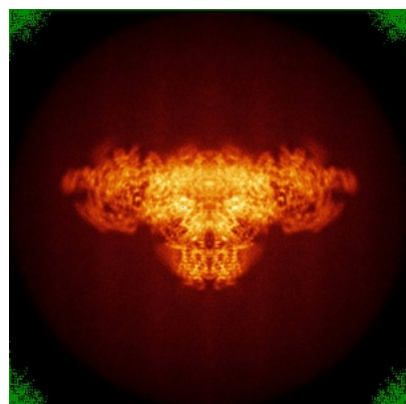


Z Index: 226

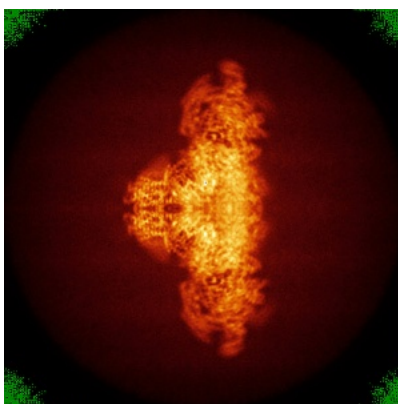
The images above show the largest variance slices of the map in three orthogonal directions.

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

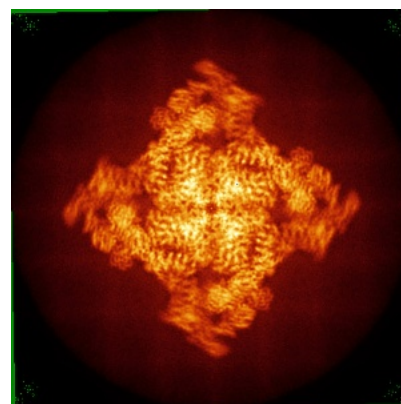
6.4.1 Primary map



X

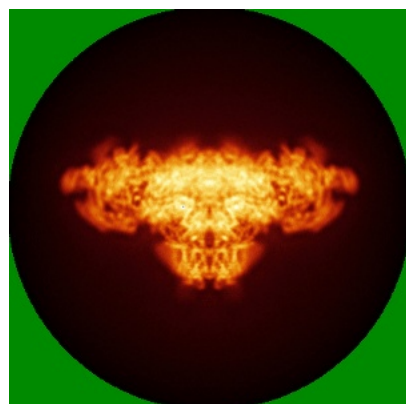


Y

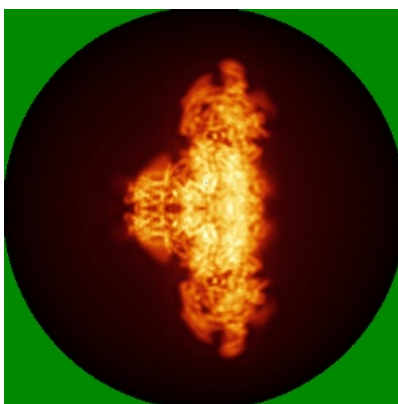


Z

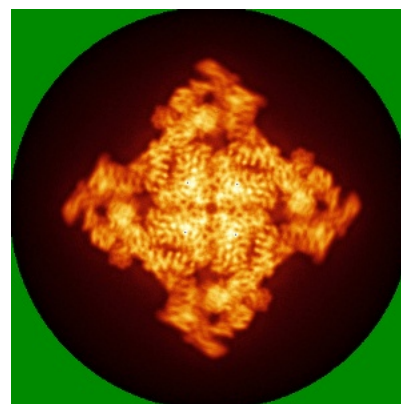
6.4.2 Raw map



X



Y

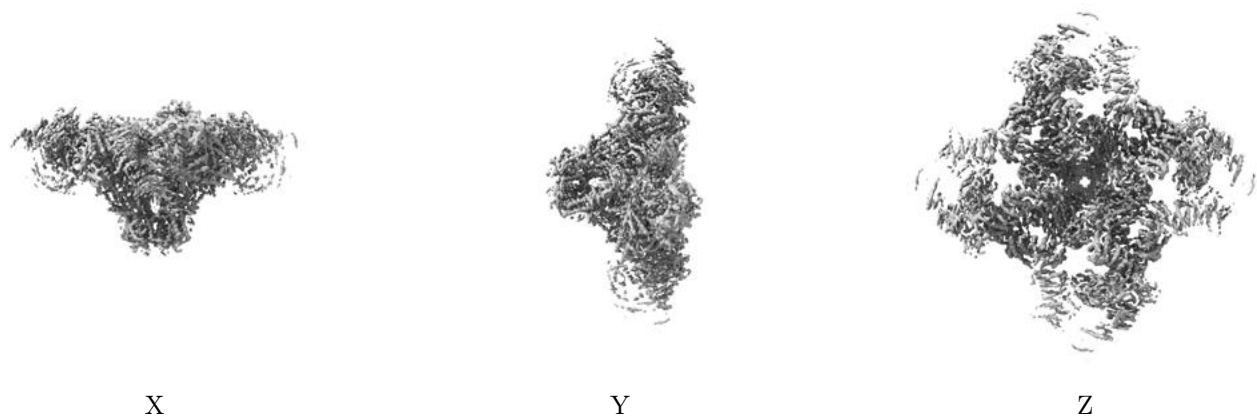


Z

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.

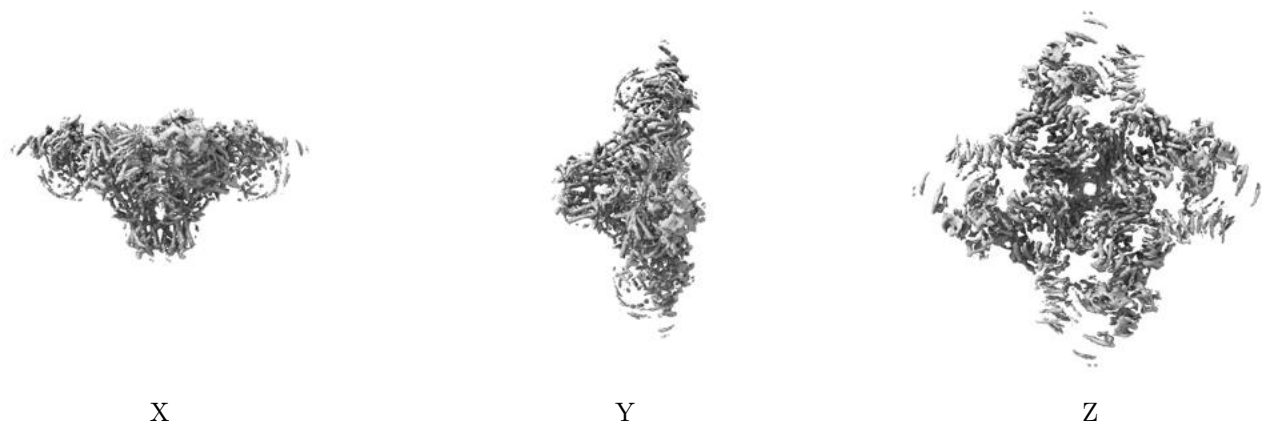
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

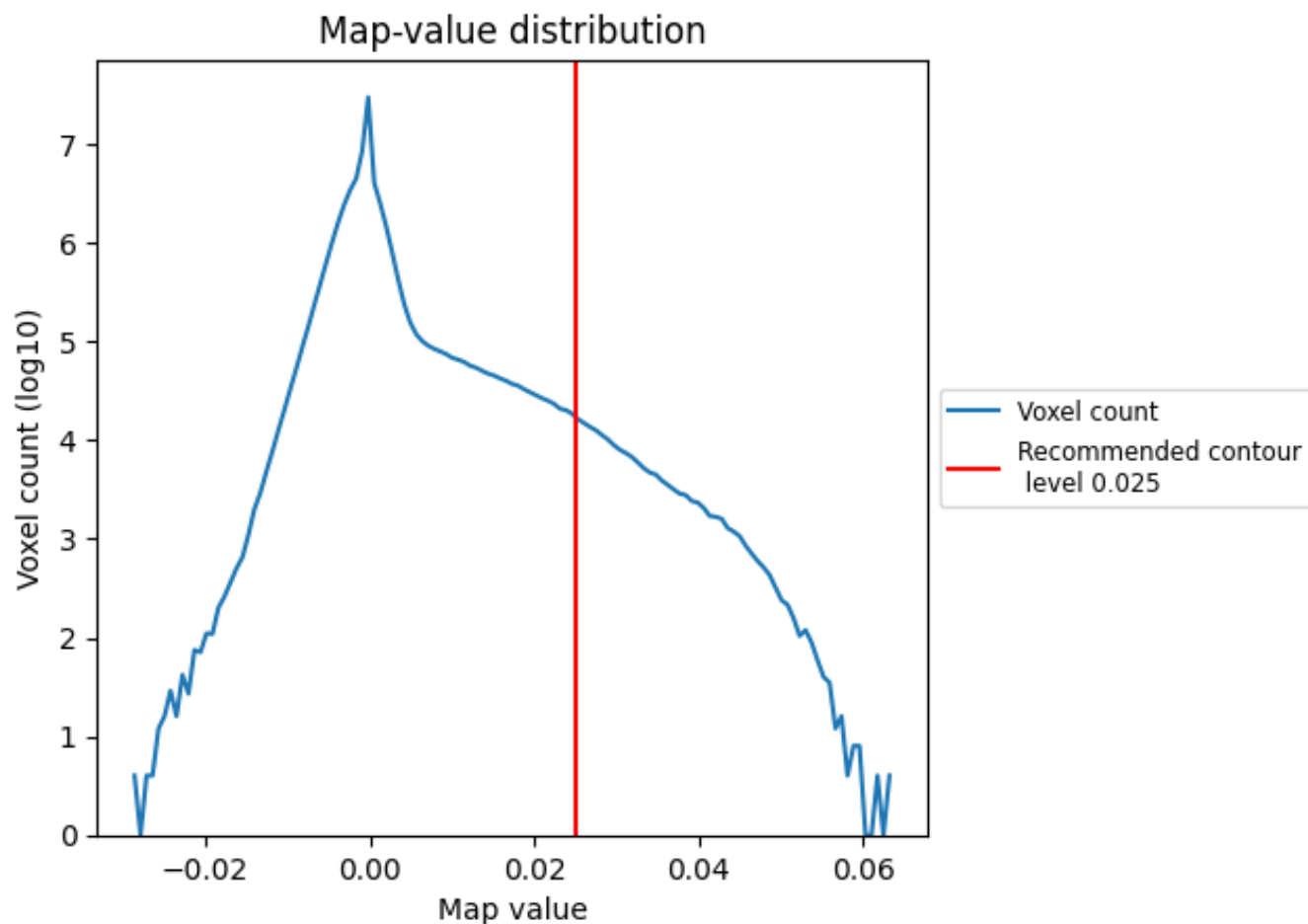
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

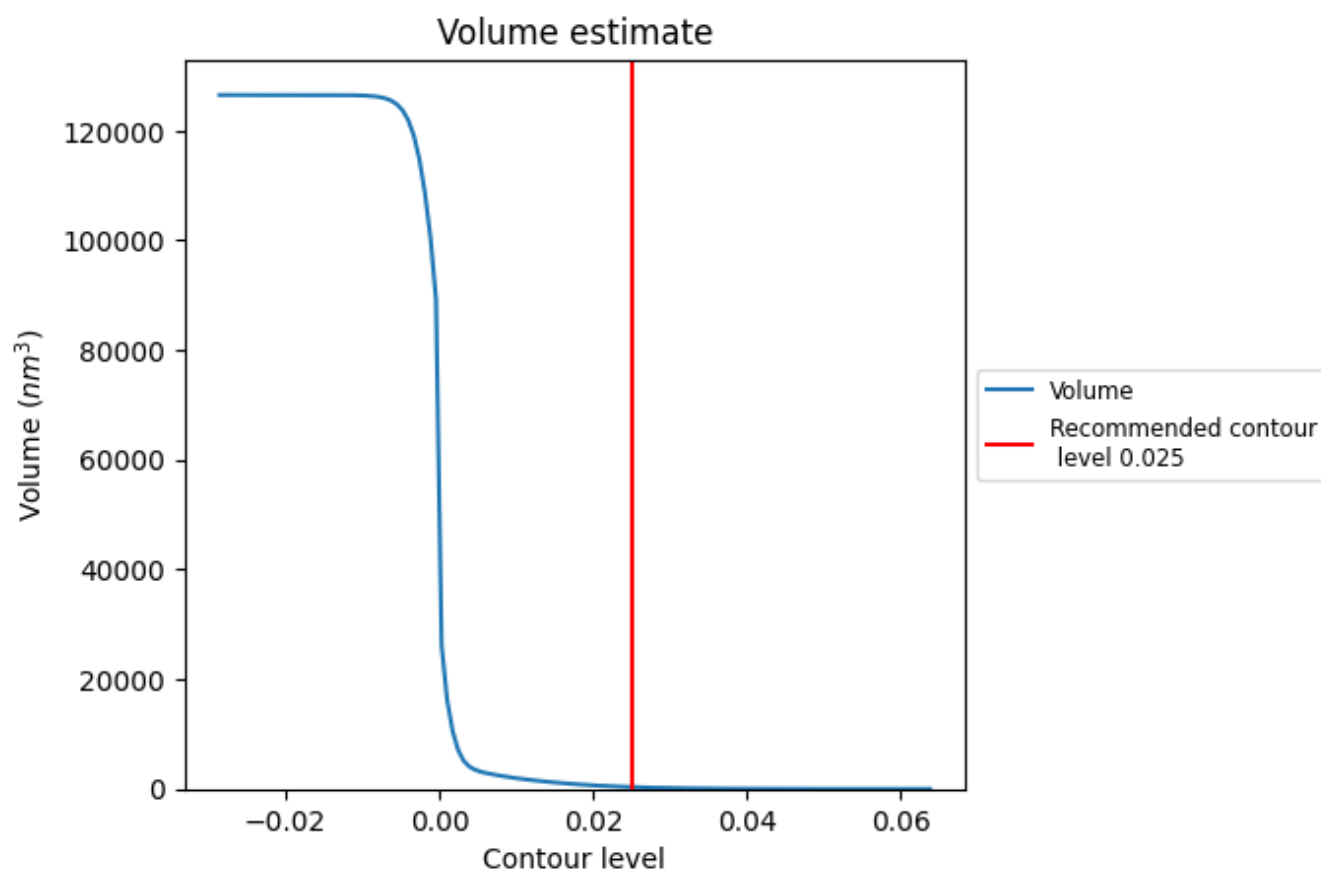
This section contains the results of statistical analysis of the map.

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.

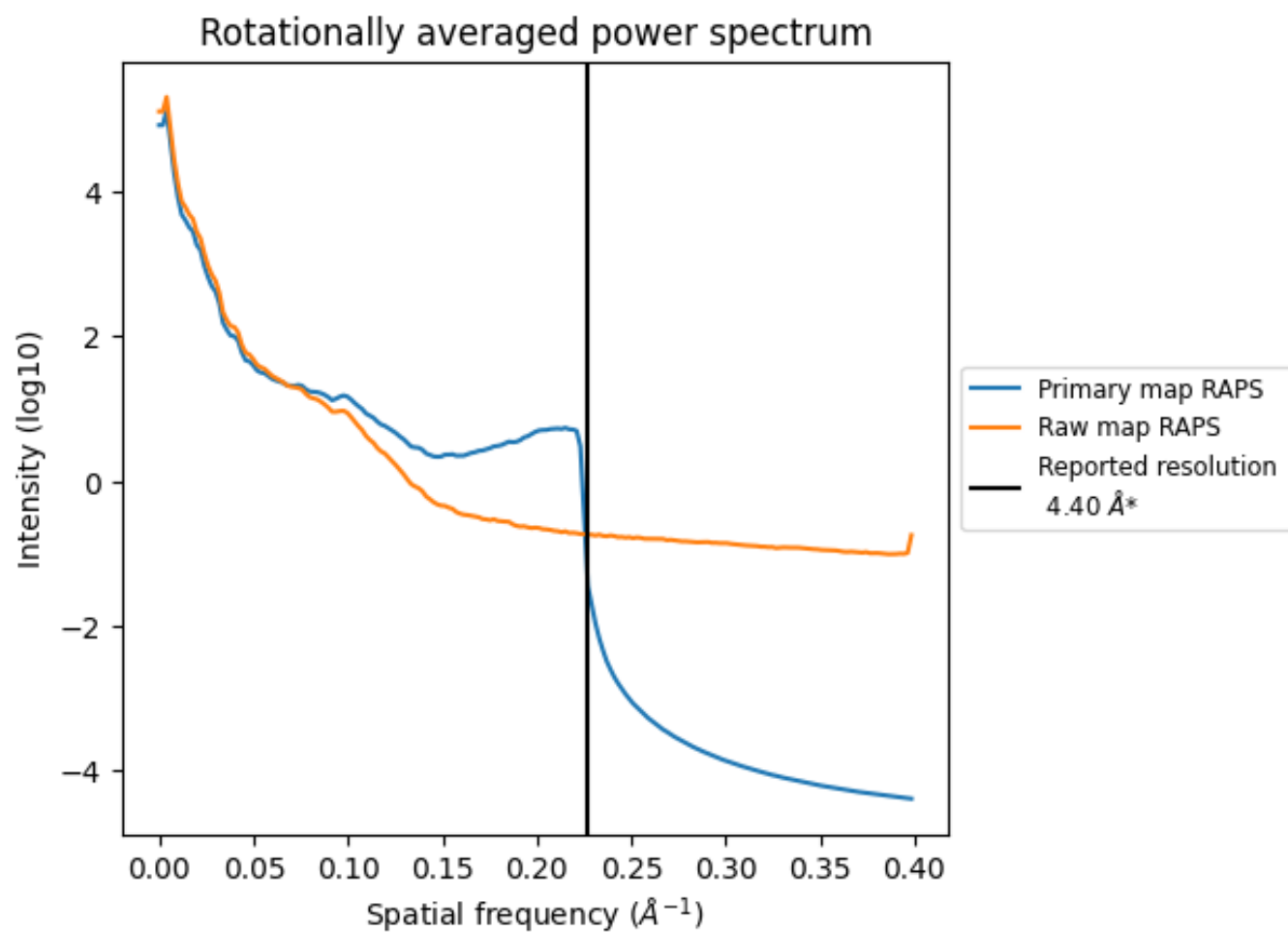
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 311 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 ⓘ

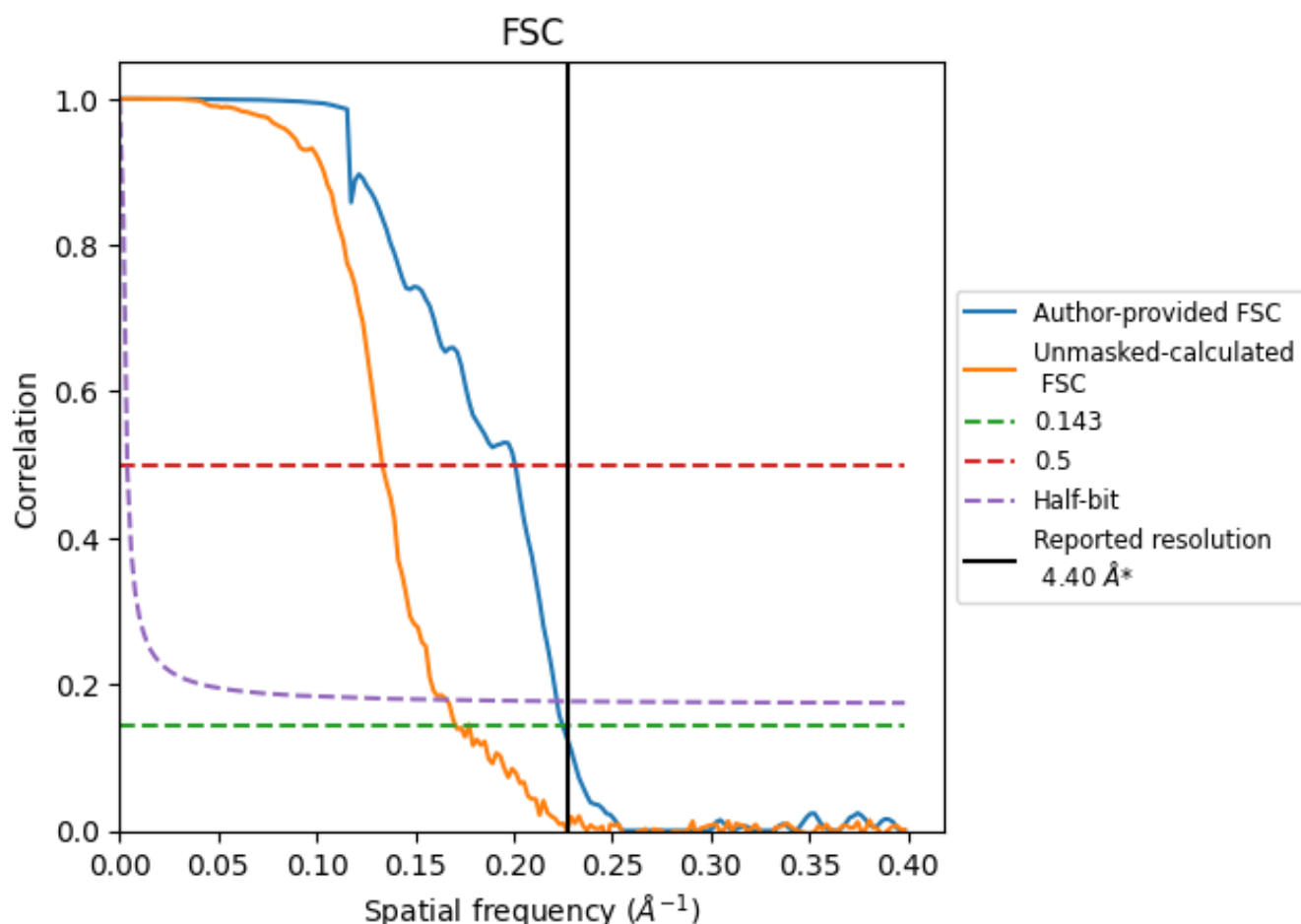


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

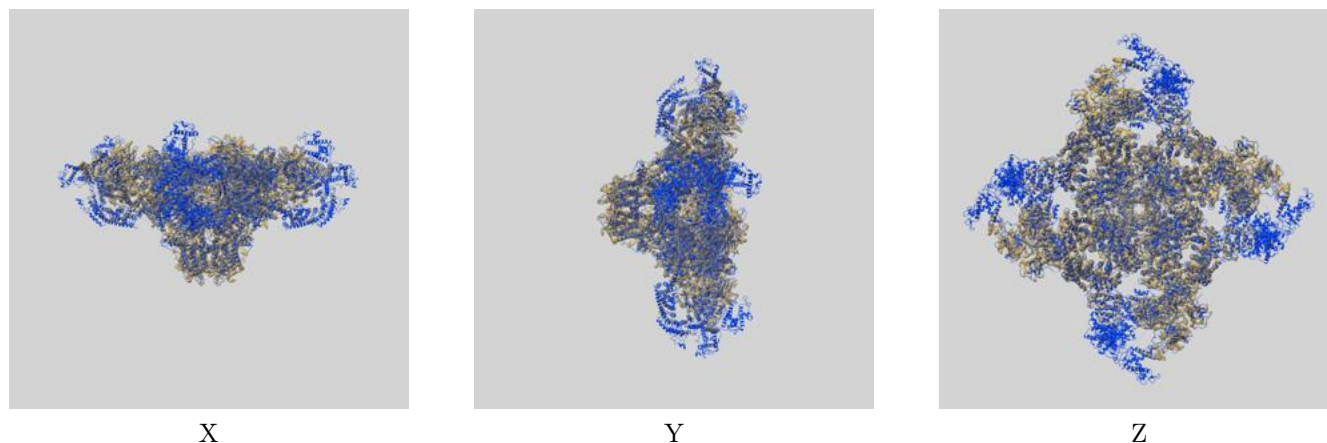
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.45	4.99	4.50
Unmasked-calculated*	5.86	7.50	6.03

*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 5.86 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

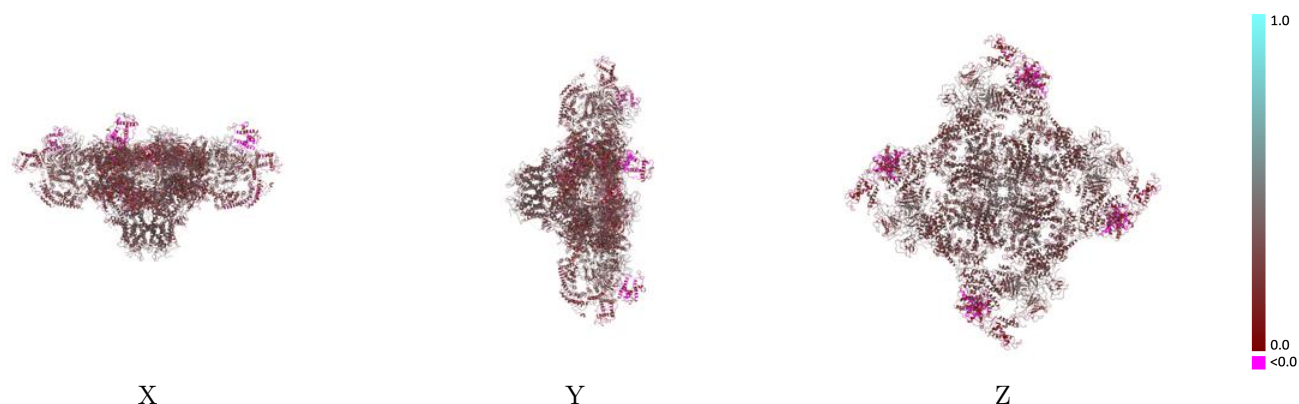
This section contains information regarding the fit between EMDB map EMD-8377 and PDB model 5TA3. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



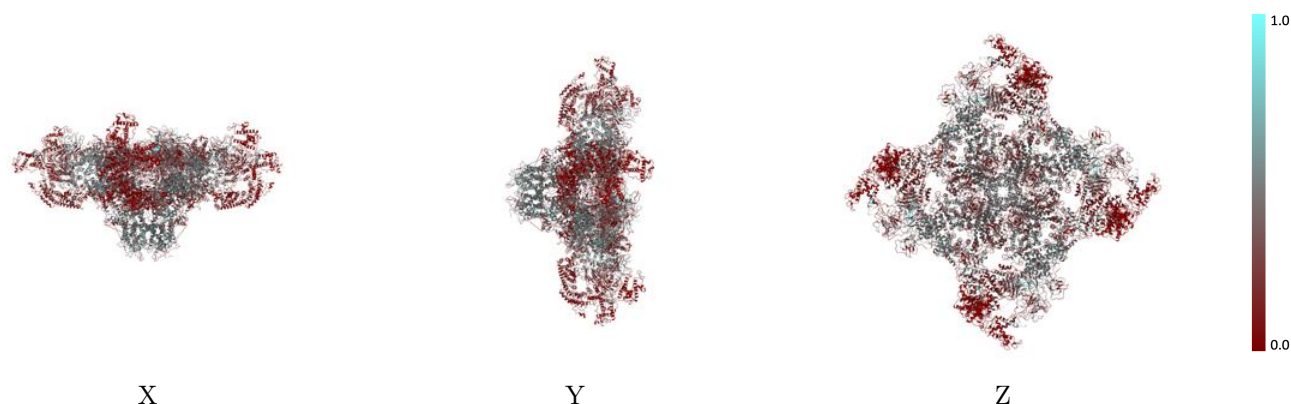
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



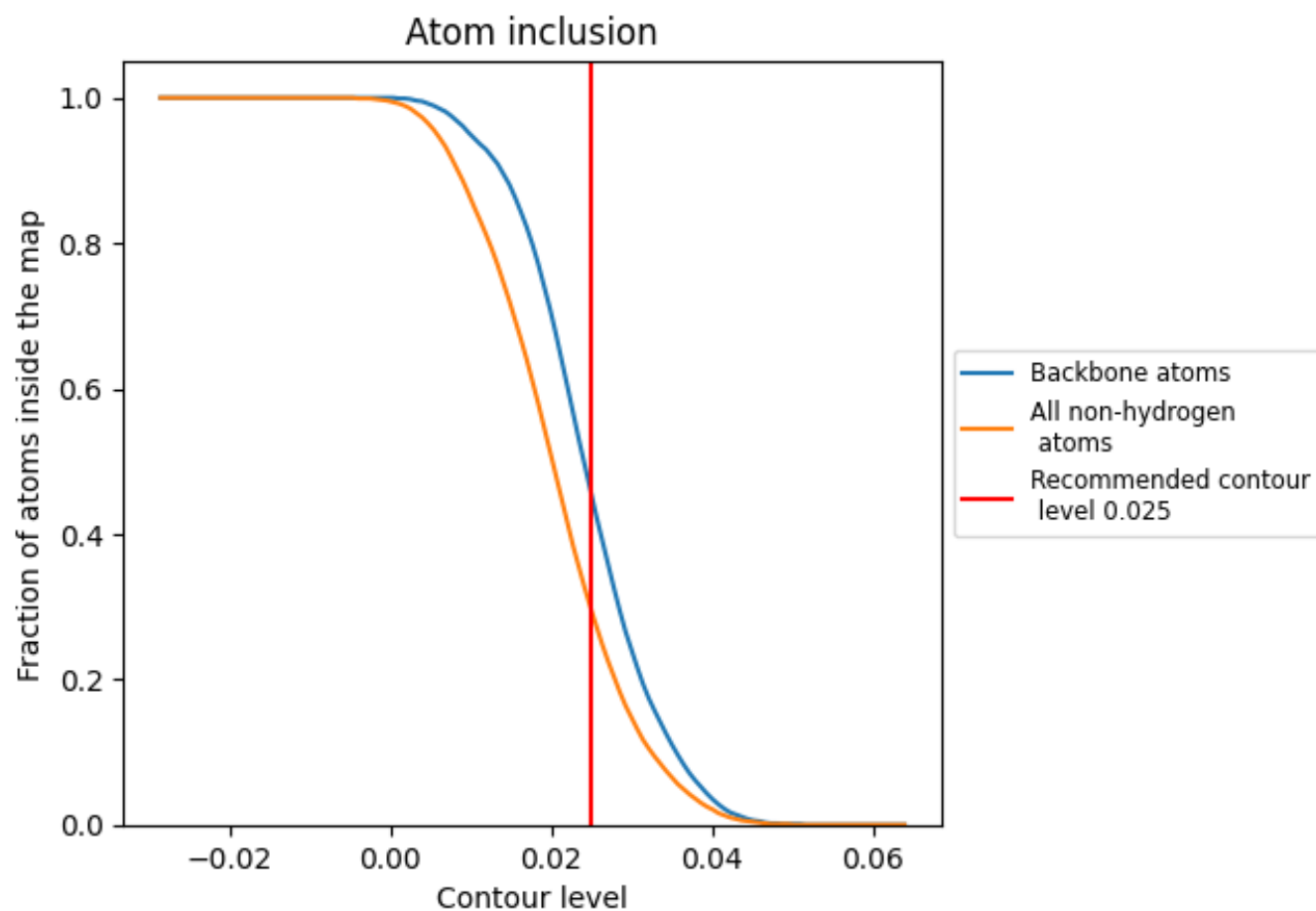
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.2940</div>	<div><div></div>0.2750</div>
A	<div><div></div>0.3000</div>	<div><div></div>0.3110</div>
B	<div><div></div>0.2950</div>	<div><div></div>0.2780</div>
E	<div><div></div>0.2940</div>	<div><div></div>0.2720</div>
F	<div><div></div>0.2960</div>	<div><div></div>0.3140</div>
G	<div><div></div>0.2940</div>	<div><div></div>0.2750</div>
H	<div><div></div>0.3010</div>	<div><div></div>0.3150</div>
I	<div><div></div>0.2930</div>	<div><div></div>0.2730</div>
J	<div><div></div>0.3030</div>	<div><div></div>0.3120</div>

1.0

0.0

<0.0