



## wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 10:55 AM EDT

PDB ID : 5TAM  
EMDB ID : EMD-8379  
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca<sup>2+</sup> dataset, class 4)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-10  
Resolution : 4.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

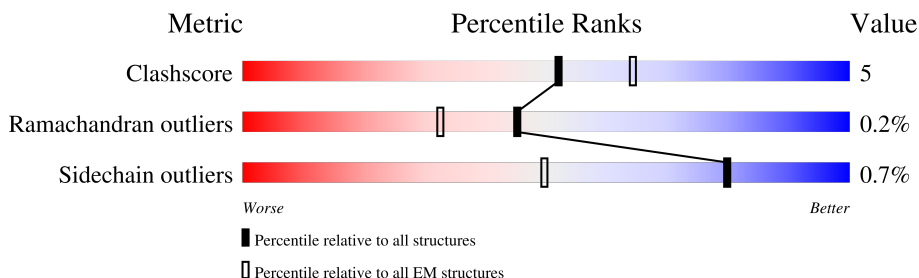
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	<div> <div>56%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	F	108	<div> <div>56%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>
1	H	108	<div> <div>57%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>
1	J	108	<div> <div>56%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>
2	B	4416	<div> <div>49%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	E	4416	<div> <div>49%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	G	4416	<div> <div>50%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	I	4416	<div> <div>50%</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.

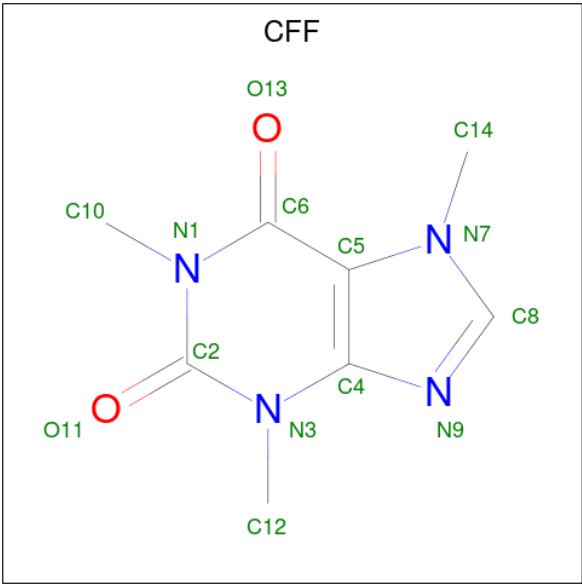
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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	E	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	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>).



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

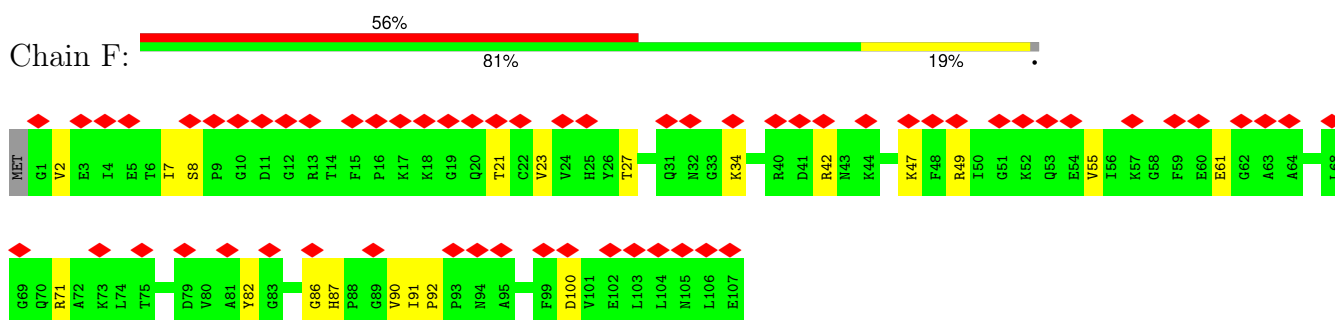
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

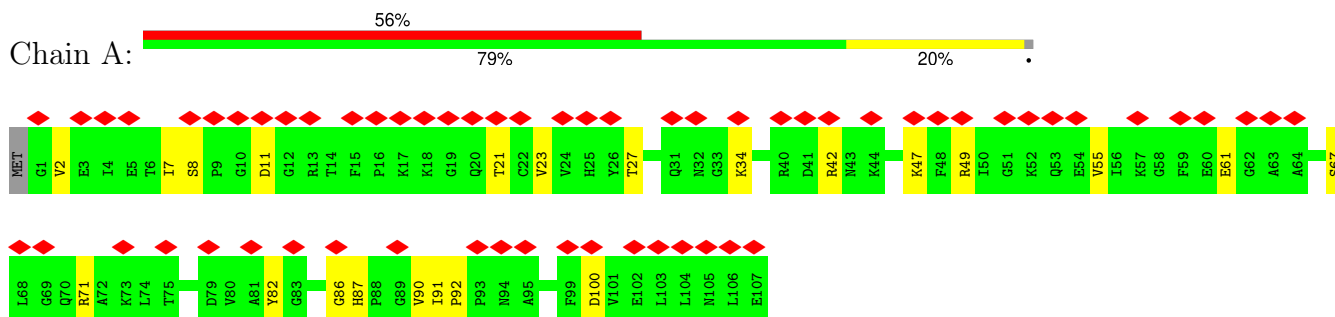
### 3 Residue-property plots [i](#)

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.

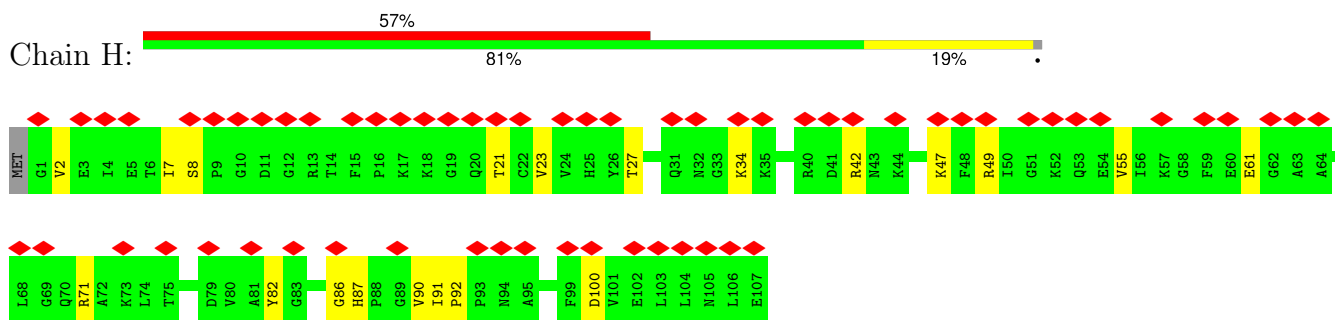
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

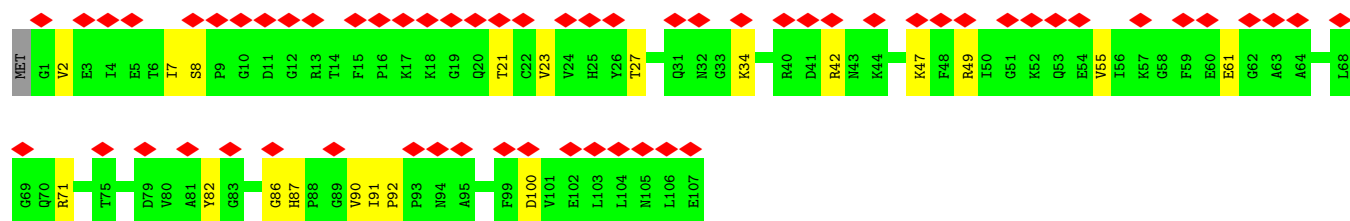


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

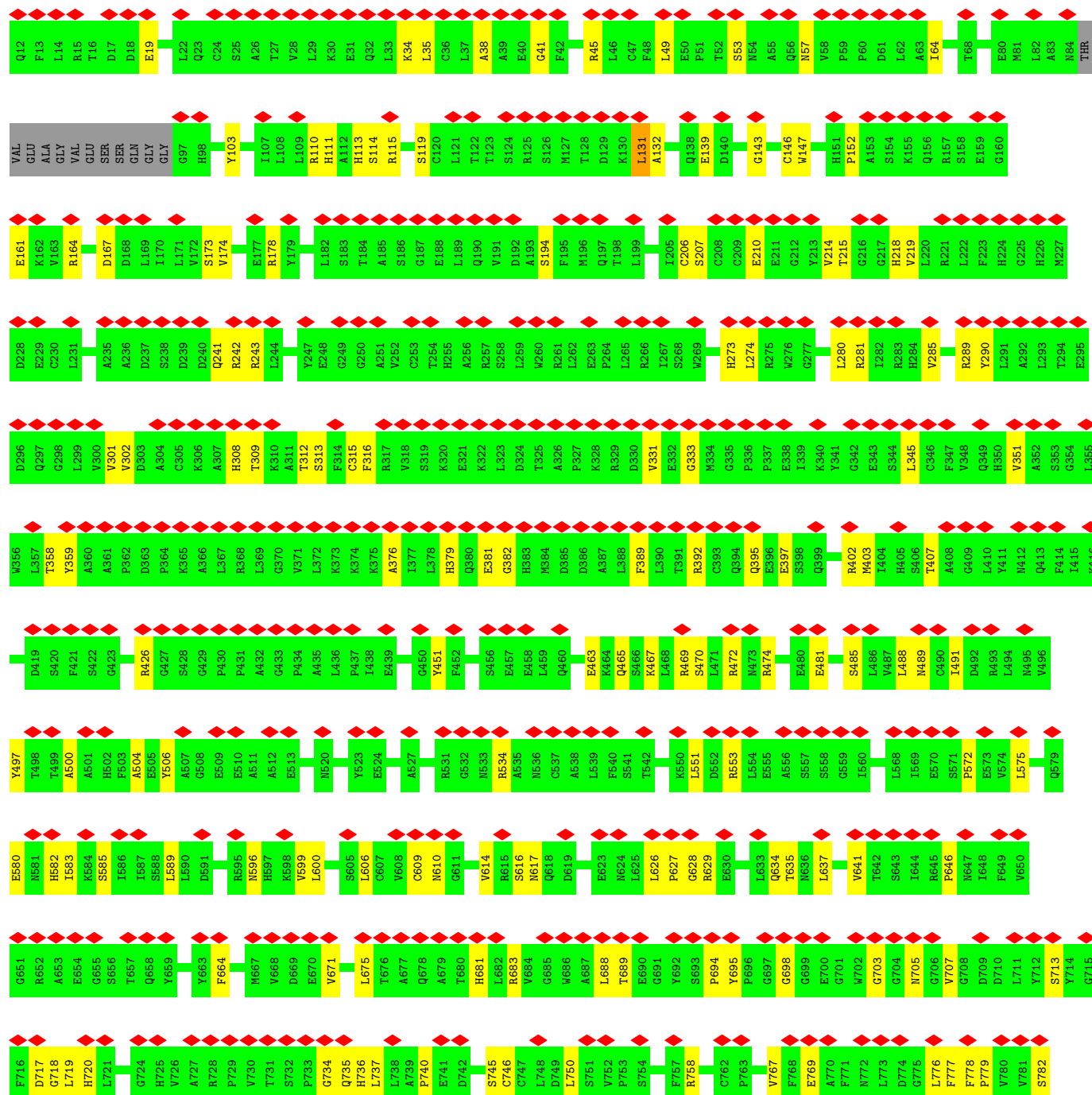
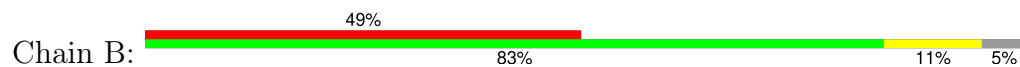


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: Ryanodine receptor 1

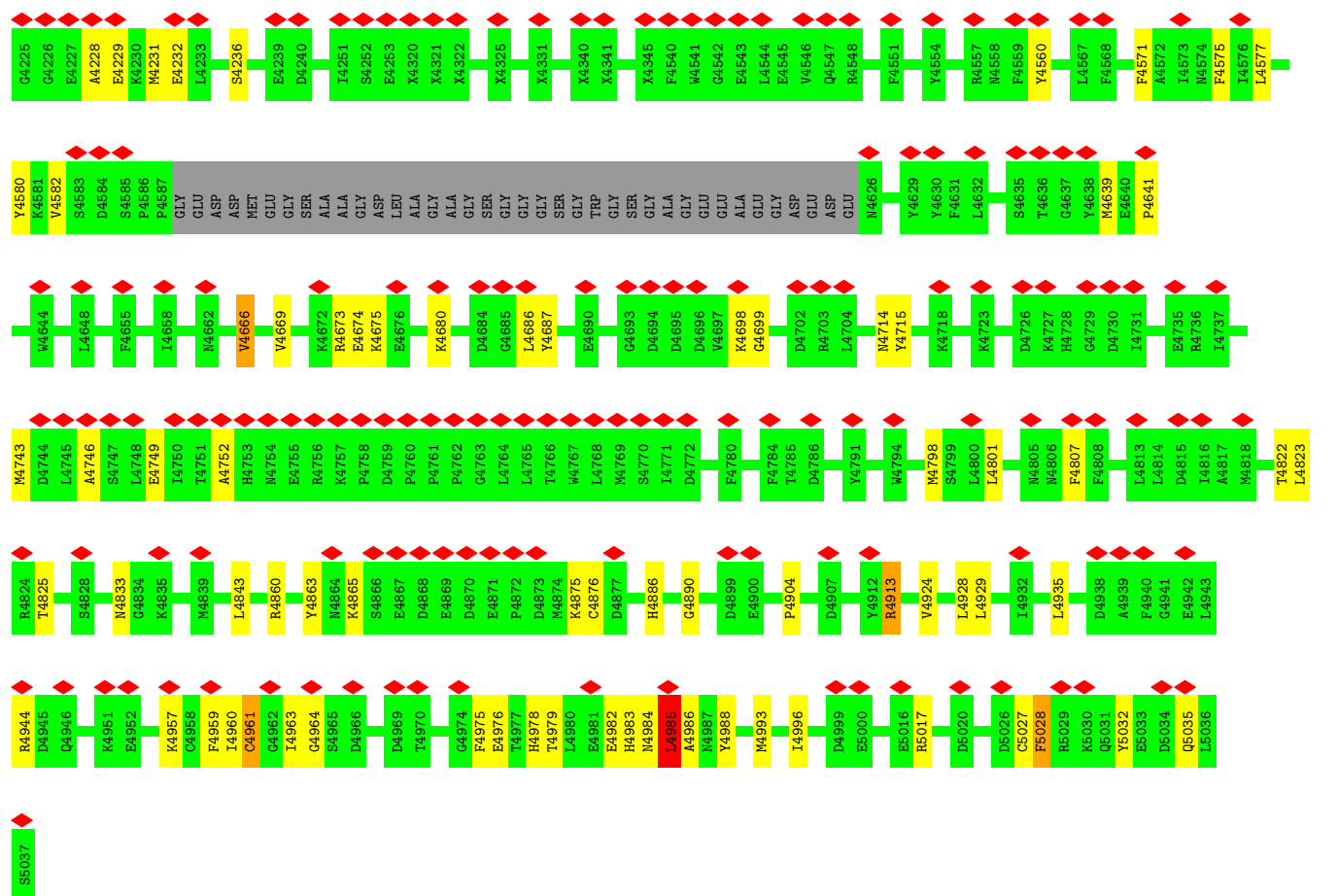


GLU	I1802	R1728	M1637	X1529	V1264	A1178	P1107	C1040	A968	V908	H848	F783
GLU	P1803		A1638	X1530	D1265	F1179	E1108	Q1041	P969	N909	T849	S784
GLU	L1804	L1731	L1639	X1531		R180	L1109	A1042	L970	F910	D850	A785
GLU	E1805	S1732	E1643	X1532	C1269	E181	R1110	V1043	D971	H911	F851	G786
GLU	A1806	E1733	E1644	X1533	L1270	I1812	R1111	L1045	L972	S912	V852	K788
GLU	L1807	E1734	E1645	X1536	R1271	E183	D1112	L1046	S973	L913	P853	
GLU	R1808	Y1734	N1645	X1537	L1272	I184	E1114	L1047	H974	P914	C854	
ASP	D1809		R1646	X1542	D1273	G185	L1115	G1048	V975	E915	P855	
GLU	A1810	L1738	E1652	X1544			G1116	G1049	A976	P916	V856	
GLU	A1811	T1739	L1653	X1545	L1189		A1117	G1050	T977	E917	D857	
GLU	L1812	P1740	S1654	X1547	L1194	L194	D1118	Y1051	T978	R918	THR	
LYS	R1813	E1741	E1655	X1548	G1195	G195	E1119	N1052	P979	N919	VAL	
GLU	T1742	R1743	R1656	X1549			L1120	I1053	A980	N921	GLN	
ASP	L1815	A1744	L1657	X1551	V1199			E1054	Q981	Y920	R918	
GLU	D1821	I1745		X1579	G1200		V1123	PRO	T982	N921	THR	
GLU	G1822		L1667	F1580	H1201		F1124	ASP	T983	L922	VAL	
GLU	Q1823	F1748	L1658	X1585		L1204		GLN	T984	Q923	GLN	
LYS	L1824	P1749	S1659	X1586	X1284	G1205	R1128	GLU	L984	M924	P864	
LYS	H1825	P1750	E1670	X1587	X1285	Q1206		PRO	V985	S925	P865	
ASP	A1826	G1751	A1672	X1588	X1430	D1207	R1131	PRO	D986	G926	H866	
ALA	R1827	R1752	A1675	X1589	X1441			GLN	R987	E927	L867	
GLU	D1828	K1753	L1676	X1591	X1442	L1211	L1134	VAL	A989	T928	E868	
LYS	G1832	G1754	L1677	L1595	X1443	L1212	G1135	GLU	D999	K930	R871	
GLU	F1838	G1755		X1457	X1445	F1213	S1136	ASN		T931	E872	
GLU	V1839	N1756	N1679	X1473	X1446	F1214		GLN	Q1003	L932	E873	
ALA	P1840	A1757	V1681	X1474	X1447	F1215	F1139	ASP	G1004	L933	K873	
GLU	V1841	P1758	A1682	X1475	X1448	I1216	G1140	GLN	W1005	A934	L874	
GLY	L1842	R1759	L1685	X1476	X1449	C1217	R1141	TRP	S1006	L935	A875	
GLU	K1843	H1760	H1688	X1497	X1450		Q1144	D1070	Y1007	G936	E876	
LYS	L1844	G1761	V1689	X1498	X1451	Q1220	S1145	R1071	S1008	C937	N877	
ASP	I1853	L1762	D1691	X1499	X1452	E1221	G1146	V1072	A1009	H938	I878	
L1922	F1854	G1763	Q1691	X1504	X1453	E1222	D1147	I1074	VAL	V939	R818	
E1923	G1855	V1765	L1694	X1513	X1474	G1223	V1148	F1075	GLN	G940	E890	
E1924	D1856	G1766		X1514	X1475		V1149	A1077	ILE	M941	L881	
G1925	E1857	V1767	L1698	X1515	X1476	A1227	C1151	E1078	PRO	A942	W882	
L1926	D1858		E1699	X1516	X1477		M1152	K1079	ALA	D943	A883	
L1927	V1859	R1772	D1700	X1519	X1480	Q1231	I1153	S1080	ARG	E944	L884	
Q1928	K1860	P1773	A1701	X1520	X1481	R1232	D1154	Y1081	ASN	T886	T885	
	Q1861	H1774		X1521	X1482		L1155	PRO	PRO	K945	K827	
	L1862		R1708	X1522	X1483	W1237	T1156	Y1089	R1020	A946	E828	
	L1863	H1775	A1709	X1523	X1484	Q1244	E1157	F1090	I887	E947	Y829	
	E1869	F1782	G1710	X1524	X1485	Q1247	N1158	F1092	E888	R830	R830	
E1944	V1870	V1783	Y1711	X1525	X1486			E1093	Q889	D948	R831	
Y1945	F1871	A1784	Y1712	X1526	X1487	E1251	L1161	A1094	N949	L950	E832	
F1946	T1872	A1785	D1713	X1527	X1488	H1252	F1162	V1095	K951	K952	G833	
	E1873	L1786		X1528	X1489	P1253	T1163		T892	Y893	P834	
	E1874	P1787	L1718	X1529	X1490		L1164	G1098	Y894	G894	R835	
	GLU	A1788	H1719	X1530	X1491	E1256		E1099	T953	P837	G836	
	GLU	ALA	L1720	X1531	X1492		L1169	M1100	K954	P837	H838	
	GLU	GLY	E1721	X1532	X1493	E1257	M1170	M1101	P895	P837	L839	
	GLU	VAL	S1722	X1533	X1494	A1258	S1171	V1102	V896	V896	L839	
	GLU	ALA		X1534	X1495	R1259	D1172	G1103	R897	R897	V840	
	GLU		R1725	X1535	X1496	M1260	S1173	W1104	D998	D998	G841	
	GLU		S1726	X1536	X1497	D1261	G1174	A1105	D899	D899	P842	
	GLU		R1727	X1537	X1498	G1262	S1175	R1036	N900	N900	S843	
				X1528	X1499	T1263	E1176	D1037	K901	K901	R844	
								S1038	R902	R902	C845	
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									H904	H904	S847	
									P905	P905		
									L907	L907		

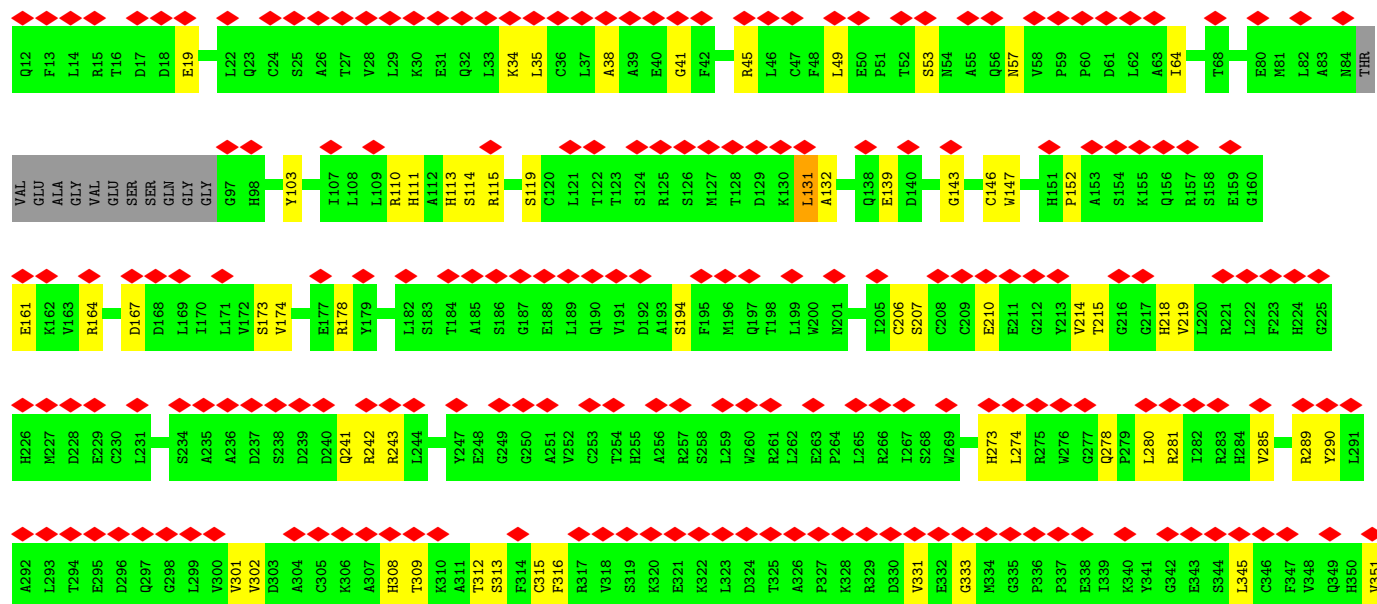
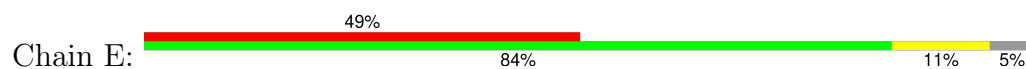


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ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	R2859	P2860	D2861	L2862	S2863	G2864	V2865	L2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	Q2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	R2899	G2900	T2901	H2902	L2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911																													
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X2702	X2703	M2734	F2735	D2736	P2737	S2738	P2739	V2740	E2741	T2742	L2743	M2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	K2756	M2757	F2758	A2759	X2760	X2761	T2762	H2763	E2764	K2765	L2766	A2767	F2768	D2769	K2770	L2771	Q2772	M2773	L2774	W2775	S2776	T2777	G2778	E2779	M2780	V2781	D2782	E2783	L2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791																													
X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2634	X2635	X2636	X2641	X2645	X2648	X2649	X2650	X2651	X2658	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2686	X2687	X2688	X2689	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701																																					
A2428	L2429	I2430	D2431	L2432	R2435	C2436	A2437	P2438	E2439	M2440	H2441	L2442	G2446	K2447	G2448	E2449	A2450	L2451	R2452	L2453	R2454	A2455	R2458	S2459	L2460	L2463	D2464	D2465	L2466	I2469	L2470	S2471	L2472	P2473	L2474	Q2475	L2476	P2477	T2478	L2479	X2487	X2488	X2489	X2490	X2493	X2494	X2499	X2502	X2511	X2512																																						
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L2295	E2296	V2299	S2300	A2303	G2304	C2305	G2306	L2307	Q2308	S2309	C2310	P2311	L2314	A2315	K2316	Q2317	Y2318	P2319	D2320	L2321	C2322	C2326	Q2327	R2330	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	A2338	V2339	F2340	V2341	N2342	G2343	V2346	E2347	E2348	N2349	R2355	L2356	L2357	I2358	R2359	K2360	C2363	F2364	G2365	P2366																																					
G2218	E2219	T2220	K2221	E2222	L2223	G2224	F2225	P2226	K2227	M2228	Y2229	S2231	C2232	C2233	R2234	F2239	I2242	N2246	Q2247	R2248	F2251	D2252	H2253	Y2256	L2257	L2258	E2259	M2260	S2261	G2262	L2263	G2264	L2265	G2266	M2267	Q2268	G2269	D2274	A2277	D2282	E2285	L2288	A2289	L2290	Q2291	E2292	Q2293	D2294																																								
K2089	K2090	P2091	Q2092	Q2095	R2104	Q2107	Y2110	L2123	Q2127	L2131	R2140	A2141	I2144	S2145	P2146	S2147	E2150	L2165	L2166	T2167	V2168	Q2169	M2170	N2176	M2184	N2187	N2188	K2189	Y2192	Q2193	N2196	R2199	A2200	L2201	H2204	N2213	V2214	L2215	G2217	G2218	E2219	T2220	K2221	E2222	L2223	R2224	F2225	P2226	K2227	L2228	T2229	S2231	C2232	C2233	R2234	F2239	I2242	N2246	Q2247	R2248	F2251	D2252	H2253	Y2256	L2257	L2258	E2259	M2260	S2261	G2262	L2263	G2264	L2265	G2266	M2267	Q2268	G2269	D2274	A2277	D2282	E2285	L2288	A2289	L2290	Q2291	E2292	Q2293	D2294
C2021	P2022	L2023	P2024	I2027	R2028	Q2029	D2030	H2035	N2041	C2042	G2043	L2044	Q2045	E2047	G2048	GLU	GLU	GLU	GLU	PRU	GLU	GLU	GLU	THR	SER	SER	LEU	SER	LEU	ARG	SER	LEU	LEU	LEU	THR	VAL	ARG	LEU	VAL	LYS	LYS	Q2003	GLU	E2004	Q2005	L2006	N2007	M2008	L2009	L2010	H2011	F2012	K2013	D2014	E2015	A2016	D2017	E2018	E2019	D2020																												

L4112	D4018	D3878	S3784	E3688	X3598	X3532	X3411	X3350	X3279	X3208	X3063	X2995
L4019	Q4020	Q3882	K3787	E3689	X3599	X3533	X3412	X3551	X3280	X3209	X3063	X2996
K4021	D4022	R3886	G3788	V3690	X3600	X3534	X3413	X3552	X3281	X3210	X3194	X2997
D4022			E3789	E3691	X3601	X3535	X3414	X3553	X3282	X3211	X3195	X2998
E4032		Q3889	K3799	K3693	X3602	X3538	X3417	X3555	X3283	X3212	X3196	X2999
G4033		N3896		K3694	X3605	X3539	X3421	X3556	X3284	X3213	X3197	X3000
N4034		N3897	L3804	R3707	X3606	X3540	X3427	X3557	X3285	X3214	X3198	X3001
V4035			L3805		X3607	X3541	X3428	X3558	X3286	X3215	X3199	X3002
V4036			N3809		X3608	X3542	X3428	X3559	X3287	X3216	X3142	X3003
M4037		G3908	V3812	L3710	X3609	X3543	X3431	X3560	X3288	X3217	X3143	X3004
G4038		N3909	V3812	T3711	X3610	X3544	X3432	X3561	X3289	X3218	X3144	X3005
M4039		T3910	K3713	E3712	X3611	X3545	X3433	X3562	X3290	X3219	X3145	X3006
E4126		T3911	K3713	K3713	X3612	X3546	X3434	X3563	X3291	X3220	X3148	X3007
E4127			S3714	K3714	X3613	X3547	X3434	X3564	X3292	X3221	X3149	X3008
N4130			K3715	S3714	X3613	X3548	X3435	X3565	X3293	X3222	X3150	X3009
R4131			K3715	X3613	X3613	X3549	X3436	X3566	X3294	X3223	X3151	X3010
R4137			X3613	T3639	X3613	X3550	X3436	X3567	X3295	X3224	X3152	X3014
			X3613		X3613	X3551	X3436	X3568	X3296	X3225	X3153	X3015
			X3613		X3613	X3552	X3436	X3569	X3297	X3226	X3154	X3016
			X3613		X3613	X3553	X3436	X3570	X3302	X3227	X3155	X3017
			X3613		X3613	X3554	X3436	X3571	X3303	X3228	X3156	X3018
			X3613		X3613	X3555	X3436	X3572	X3304	X3229	X3157	X3019
			X3613		X3613	X3556	X3436	X3573	X3305	X3230	X3158	X3020
			X3613		X3613	X3557	X3436	X3574	X3306	X3231	X3159	X3021
			X3613		X3613	X3558	X3436	X3575	X3307	X3232	X3160	X3022
			X3613		X3613	X3559	X3436	X3576	X3308	X3233	X3161	X3023
			X3613		X3613	X3560	X3436	X3577	X3309	X3234	X3162	
			X3613		X3613	X3561	X3436	X3578	X3310	X3235	X3163	X3027
			X3613		X3613	X3562	X3436	X3579	X3311	X3236	X3170	X3028
			X3613		X3613	X3563	X3436	X3580	X3312	X3237	X3171	X3029
			X3613		X3613	X3564	X3436	X3581	X3313	X3238	X3172	X3030
			X3613		X3613	X3565	X3436	X3582	X3314	X3239	X3173	X3033
			X3613		X3613	X3566	X3436	X3583	X3315	X3240	X3174	X3034
			X3613		X3613	X3567	X3436	X3584	X3316	X3241	X3175	X3035
			X3613		X3613	X3568	X3436	X3585	X3317	X3242	X3176	X3036
			X3613		X3613	X3569	X3436	X3586	X3318	X3243	X3177	X3037
			X3613		X3613	X3570	X3436	X3587	X3319	X3244	X3178	X3038
			X3613		X3613	X3571	X3436	X3588	X3320	X3245	X3179	X3039
			X3613		X3613	X3572	X3436	X3589	X3321	X3246	X3180	X3040
			X3613		X3613	X3573	X3436	X3590	X3322	X3247	X3181	X3041
			X3613		X3613	X3574	X3436	X3591	X3323	X3248	X3182	X3042
			X3613		X3613	X3575	X3436	X3592	X3324	X3249	X3183	X3043
			X3613		X3613	X3576	X3436	X3593	X3325	X3250	X3184	X3044
			X3613		X3613	X3577	X3436	X3594	X3326	X3251	X3185	X3045
			X3613		X3613	X3578	X3436	X3595	X3327	X3252	X3186	X3046
			X3613		X3613	X3579	X3436	X3596	X3328	X3253	X3187	X3047
			X3613		X3613	X3580	X3436	X3597	X3329	X3254	X3188	X3048
			X3613		X3613	X3581	X3436	X3598	X3330	X3255	X3189	X3049
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			X3613		X3613	X3583	X3436	X3600	X3332	X3257	X3191	X3051
			X3613		X3613	X3584	X3436	X3601	X3333	X3258	X3192	X3052
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			X3613		X3613	X3586	X3436	X3603	X3335	X3260	X3194	X3054
			X3613		X3613	X3587	X3436	X3604	X3336	X3261	X3195	X3055
			X3613		X3613	X3588	X3436	X3605	X3337	X3262	X3196	X3056
			X3613		X3613	X3589	X3436	X3606	X3338	X3263	X3197	X3057
			X3613		X3613	X3590	X3436	X3607	X3339	X3264	X3198	X3058
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			X3613		X3613	X3592	X3436	X3609	X3341	X3266	X3200	X3060
			X3613		X3613	X3593	X3436	X3610	X3342	X3267	X3201	X3061
			X3613		X3613	X3594	X3436	X3611	X3343	X3268	X3202	
			X3613		X3613	X3595	X3436	X3612	X3344	X3269	X3203	
			X3613		X3613	X3596	X3436	X3613	X3345	X3270	X3204	
			X3613		X3613	X3597	X3436	X3614	X3346	X3271	X3205	
			X3613		X3613	X3598	X3436	X3615	X3347	X3272	X3206	
			X3613		X3613	X3599	X3436	X3616	X3348	X3273	X3207	
			X3613		X3613	X3600	X3436	X3617	X3349	X3274		
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			X3613		X3613	X3603	X3436	X3620	X3352	X3277		
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			X3613		X3613	X3605	X3436	X3622	X3354	X3279		
			X3613		X3613	X3606	X3436	X3623	X3355	X3280		
			X3613		X3613	X3607	X3436	X3624	X3356	X3281		
			X3613		X3613	X3608	X3436	X3625	X3357	X3282		
			X3613		X3613	X3609	X3436	X3626	X3358	X3283		
			X3613		X3613	X3610	X3436	X3627	X3359	X3284		
			X3613		X3613	X3611	X3436	X3628	X3360	X3285		
			X3613		X3613	X3612	X3436	X3629	X3361	X3286		
			X3613		X3613	X3613	X3436	X3630	X3362	X3287		
			X3613		X3613	X3614	X3436	X3631	X3363	X3288		
			X3613		X3613	X3615	X3436	X3632	X3364	X3289		
			X3613		X3613	X3616	X3436	X3633	X3365	X3290		
			X3613		X3613	X3617	X3436	X3634	X3366	X3291		
			X3613		X3613	X3618	X3436	X3635	X3367	X3292		
			X3613		X3613	X3619	X3436	X3636	X3368	X3293		
			X3613		X3613	X3620	X3436	X3637	X3369	X3294		
			X3613		X3613	X3621	X3436	X3638	X3370	X3295		
			X3613		X3613	X3622	X3436	X3639	X3371	X3296		
			X3613		X3613	X3623	X3436	X3640	X3372	X3297		
			X3613		X3613	X3624	X3436	X3641	X3373	X3298		
			X3613		X3613	X3625	X3436	X3642	X3374	X3299		
			X3613		X3613	X3626	X3436	X3643	X3375	X3300		
			X3613		X3613	X3627	X3436	X3644	X3376	X3301		
			X3613		X3613	X3628	X3436	X3645	X3377	X3302		
			X3613		X3613	X3629	X3436	X3646	X3378	X3303		
			X3613		X3613	X3630	X3436	X3647	X3379	X3304		
			X3613		X3613	X3631	X3436	X3648	X3380	X3305		
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			X3613		X3613	X3633	X3436	X3650	X3382	X3307		
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			X3613		X3613	X3635	X3436	X3652	X3384	X3309		
			X3613		X3613	X3636	X3436	X3653	X3385	X3310		
			X3613		X3613	X3637	X3436	X3654	X3386	X3311		
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			X3613		X3613	X3639	X3436	X3656	X3388	X3313		
			X3613		X3613	X3640	X3436	X3657	X3389	X3314		
			X3613		X3613	X3641	X3436	X3658	X3390	X3315		
			X3613		X3613	X3642	X3436	X3659	X3391	X3316		
			X3613		X3613	X3643	X3436	X3660	X3392	X3317		
			X3613		X3613	X3644	X3436	X3661	X3393	X3318		
			X3613		X3613	X3645	X3436	X3662	X3394	X3319		
			X3613		X3613	X3646	X3436	X3663	X3395	X3320		
			X3613		X3613	X3647	X3436	X3664	X3396	X3321		
			X3613		X3613	X3648	X3436	X3665	X3397	X3322		
			X3613		X3613	X3649	X3436	X3666	X3398	X3323		
			X3613		X3613	X3650	X3436	X3667	X3399	X3324		
			X3613		X3613	X3651	X3436	X3668	X3400	X3325		
			X3613		X3613	X3652	X3436	X3669	X3401	X3326		
			X3613		X3613	X3653	X3436	X3670	X3402	X3327		
			X3613		X3613	X3654	X3436	X3671	X3403	X3328		
			X3613		X3613	X3655	X3436	X3672	X3404	X3329		
			X3613		X3613	X3656	X3436	X3673	X3405	X3330		
			X3613		X3613	X3657	X3436	X3674	X3406	X3331		
			X3613		X3613	X3658	X3436	X3675	X3407	X3332		
			X3613									



• Molecule 2: Ryanodine receptor 1



T1177	E1108	L1109	P1111	E1181	E1182	E1183	I1184	G1185	D1186	L1189	L1194	G1195	V1199	G1200	H1201	L1204	G1205	Q1206	D1207	L1211	R1212	F1213	F1214	A1215	I1216	C1217	Q1220	E1221	G1222	F1223	A1227	Q1231	R1232	W1237	Q1244	P1247	E1251	H1252	P1253	E1256	V1257	R1258	R1259	M1260	D1261	G1262												
P1107	E1108	L1109	P1111	E1181	E1182	E1183	I1184	G1185	D1186	L1189	L1194	G1195	V1199	G1200	H1201	L1204	G1205	Q1206	D1207	L1211	R1212	F1213	F1214	A1215	I1216	C1217	Q1220	E1221	G1222	F1223	A1227	Q1231	R1232	W1237	Q1244	P1247	E1251	H1252	P1253	E1256	V1257	R1258	R1259	M1260	D1261	G1262												
D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	I1074	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	R1025	L1026	L1027	D1028	E1029	A1030	Y1102	G1103	L1032	W1173	A1105	R1106
Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	D999	Q1003	G1004	W1005	S1006	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	R1025	L1026	L1027	D1028	E1029	A1030	Y1102	G1103	L1032	W1173	A1105	R1106		
P905	C906	L907	V908	R909	F910	H911	S912	L913	P914	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	N941	A942	D943	L944	ARG	ARG	ASN	PRO	R1020	L1021	R1025	L1026	L1027	D1028	E1029	A1030	Y1102	G1103	L1032	W1173	A1105	R1106	
C945	L946	S947	H948	T949	D950	F951	H952	P953	C954	P955	H956	D957	THR	VAL	GLN	T961	V962	L963	P964	P965	H966	L967	E968	R969	T970	R971	E972	K973	L974	A975	E976	H977	L978	H979	E980	L981	H982	A983	T985	R986	L987	E988	Q989	G990	W991	T992	Y993	G994	P995	V996	R997	D998	D999	N900	K901	R902	L903	H904
V780	V781	S782	F783	A784	G785	V786	V787	K788	V789	R790	F791	L792	L793	G794	G795	R796	F799	K801	F802	L803	P804	P805	P806	G807	Y808	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	V840	G841	P842	S843	R844			
S713	Y714	G715	F716	D717	G718	L719	H720	L721	G724	H725	V726	A727	R728	F729	V730	T731	S732	F733	G734	Q735	H736	L737	L738	A739	P740	E741	D742	S745	C746	C747	L748	D749	L750	S751	V752	P753	S754	F757	R758	C762	F763	Y767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779				
I648	F649	V650	G651	R652	A653	E654	G655	S656	T657	Q658	Y659	Y663	F664	H667	V668	D669	E670	V671	L675	T676	A677	Q678	E679	T680	H681	L682	A683	N617	Q618	D619	E623	N624	L625	L626	P627	G628	R629	E630	L631	L632	L633	Q634	T635	R636	G699	E700	G701	W702	G703	G704	N705	G706	V707	G708	D709	L711	Y712	
L494	N495	V496	Y497	T498	T499	A500	A501	H502	F503	A504	Y506	A507	G508	E509	E510	A511	A512	E513	N520	Y523	E524	A527	R531	G532	N533	R534	A535	N536	C537	A538	L539	F540	S541	T542	K550	L551	D552	R553	L554	E555	A556	S557	S558	G559	I560	L568	I569	E570	S571	P572	E573	V574						
Q413	F414	I415	K416	D419	S420	F421	S422	G423	R426	G427	S428	G429	P430	P431	A432	G433	P434	A435	L436	P437	I438	E439	Y451	F452	S456	E457	E458	L459	Q460	E463	K464	Q465	S466	K467	L468	R469	S470	L471	R472	N473	R474	E480	E481	S485	L486	V487	L488	M489	C490	I491	D492	R493						
A352	S353	G354	L355	W356	L357	L358	Y359	A360	A361	P362	P363	P364	K365	A366	L367	R368	L369	G370	V371	L372	K373	K374	K375	A376	I377	L378	H379	Q380	E381	G382	H383	M384	D385	D386	A387	L388	F389	L390	T391	R392	C393	Q394	Q395	E396	E397	S398	Q399	R402	M403	I404	H405	S406	T407	A408	G409	L410	Y411	N412



X3532	X3410	X3349	X3278	X3207	X2976	L2911	PRO	L2791	X2701	X2620	X2502
X3533	X3411	X3350	X3279	X3208	X2995	T2912	ARG	R2792	X2702	X2621	
X3534	X3412	X3351	X3280	X3209	X2996	A2913	GLU	P2793	X2703	X2622	
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			X3335	X3254		X2957		ARG			
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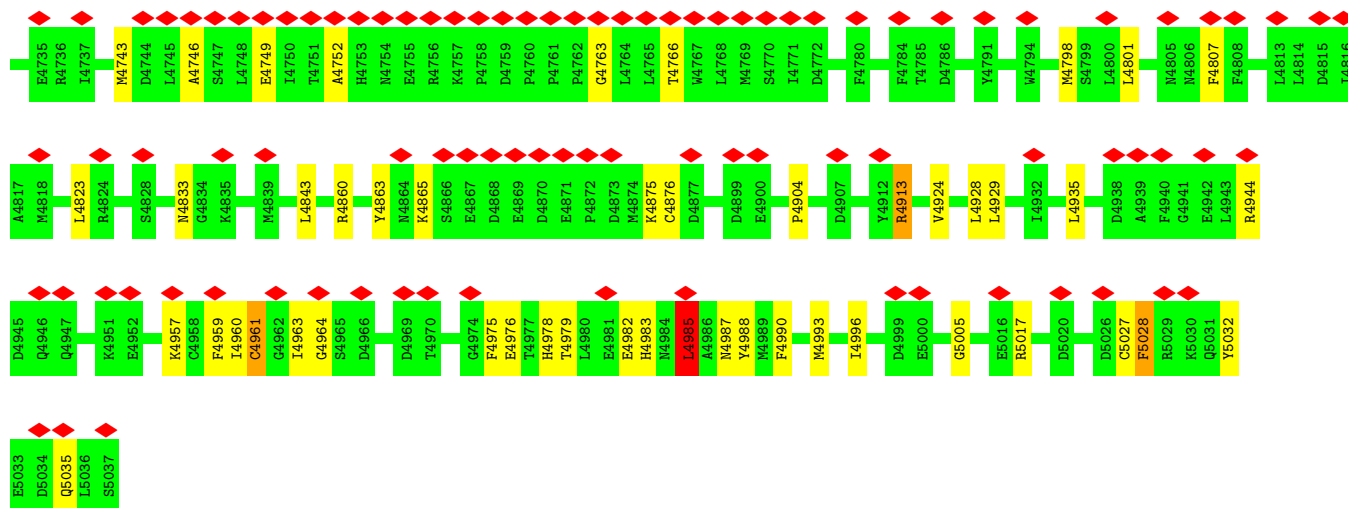
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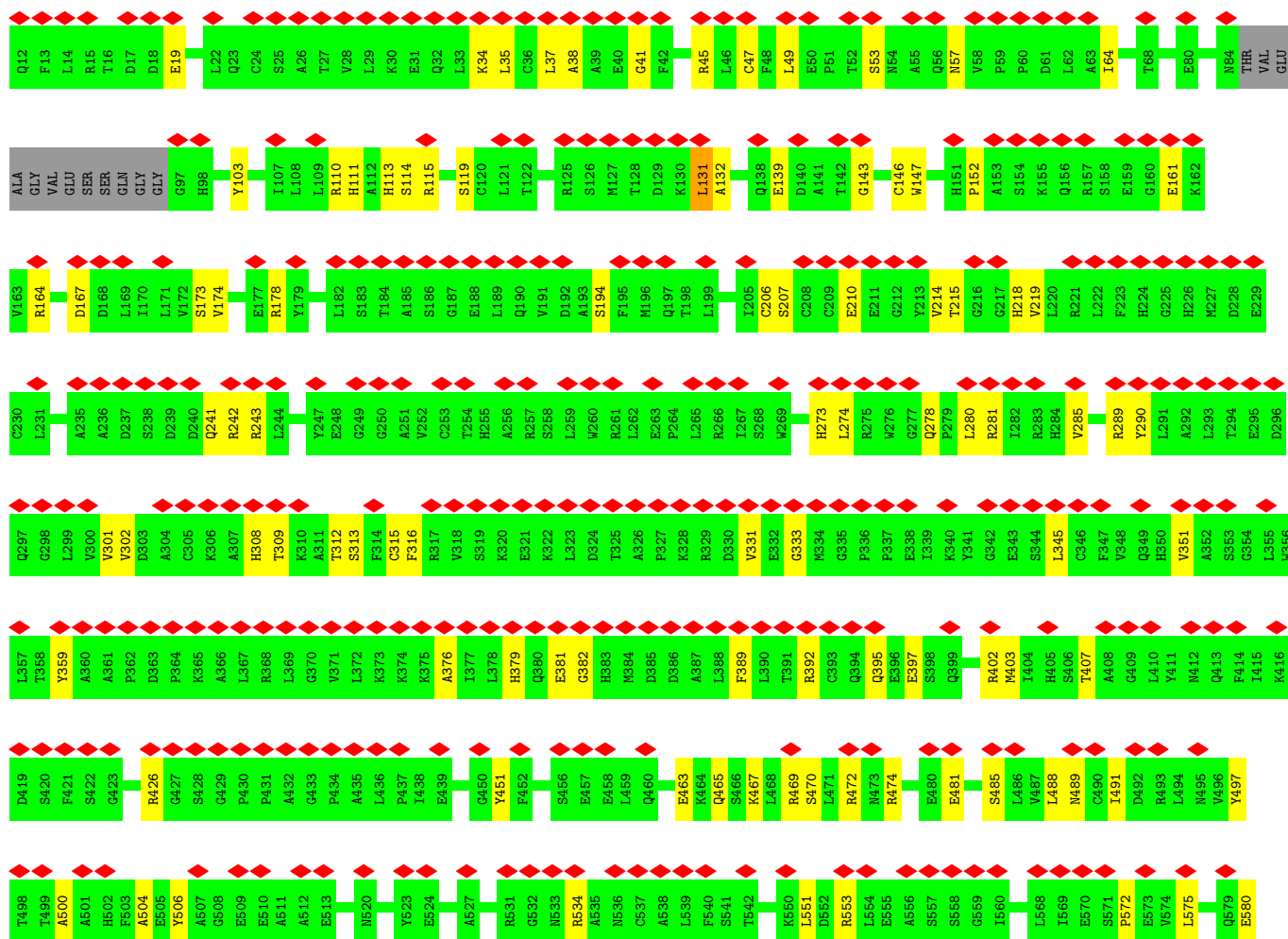
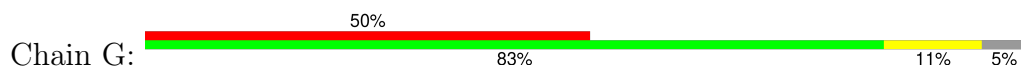


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L4577	L4577	D4220	F4103	A3997	Q3869	E3777	E3682	X3591	X3404	X3343	X3272
Y4580	Y4580	D4220	T4104	L3778	N3870	G3778	Q3683	X3592	X3405	X3344	X3273
K4581	K4581	G4106	G4106	M4000	G3871	V3779	E3684	X3595	X3406	X3345	X3274
V4582	V4582	P4109	P4109	M4001	E3872	Q3781	E3685	X3596	X3407	X3346	X3275
S4583	S4583	Q4109	Q4109	K4002	K3873	S3784	E3686	X3597	X3408	X3347	X3276
D4584	D4584	L4112	L4112	L4017	D3878	K3787	E3687	X3598	X3409	X3348	X3277
S4585	S4585	S4113	S4113	D4018	Q3882	K3788	E3688	X3599	X3410	X3349	X3278
P4586	P4586	E4119	E4119	L4019	Q3882	G3788	E3689	X3600	X3411	X3350	X3279
P4587	P4587	Q4020	Q4020	L4020	R3886	E3789	V3690	X3601	X3412	X3351	X3280
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ASP	ASP	E4232	E4232	D4022	Q3889	K3799	E3693	X3604	X3417	X3354	X3283
MET	MET	L4233	L4233	D4022	N3896	I3804	K3694	X3605	X3421	X3355	X3284
GLU	GLU	S4236	S4236	D4022	N3897	L3805	K3694	X3606	X3421	X3356	X3285
SER	SER	D4240	D4240	D4022	N3897	N3809	R3707	X3607	X3421	X3357	X3286
ALA	ALA	D4240	D4240	D4022	N3897	N3809	R3707	X3607	X3421	X3357	X3286
ALA	ALA	D4240	D4240	D4022	N3897	N3809	R3707	X3607	X3421	X3357	X3286
GLY	GLY	D4240	D4240	D4022	N3897	N3809	R3707	X3607	X3421	X3357	X3286
ASP	ASP	D4240	D4240	D4022	N3897	N3809	R3707	X3607	X3421	X3357	X3286
LEU	LEU	D4240	D4240	D4022	N3897	N3809	R3707	X3607	X3421	X3357	X3286
ALA	ALA	D4240	D4240	D4022	N3897	N3809	R3707	X3607	X3421	X3357	X3286
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SER	SER	D4240	D4240	D4022	N3897	N3809	R3707	X3607	X3421	X3357	X3286
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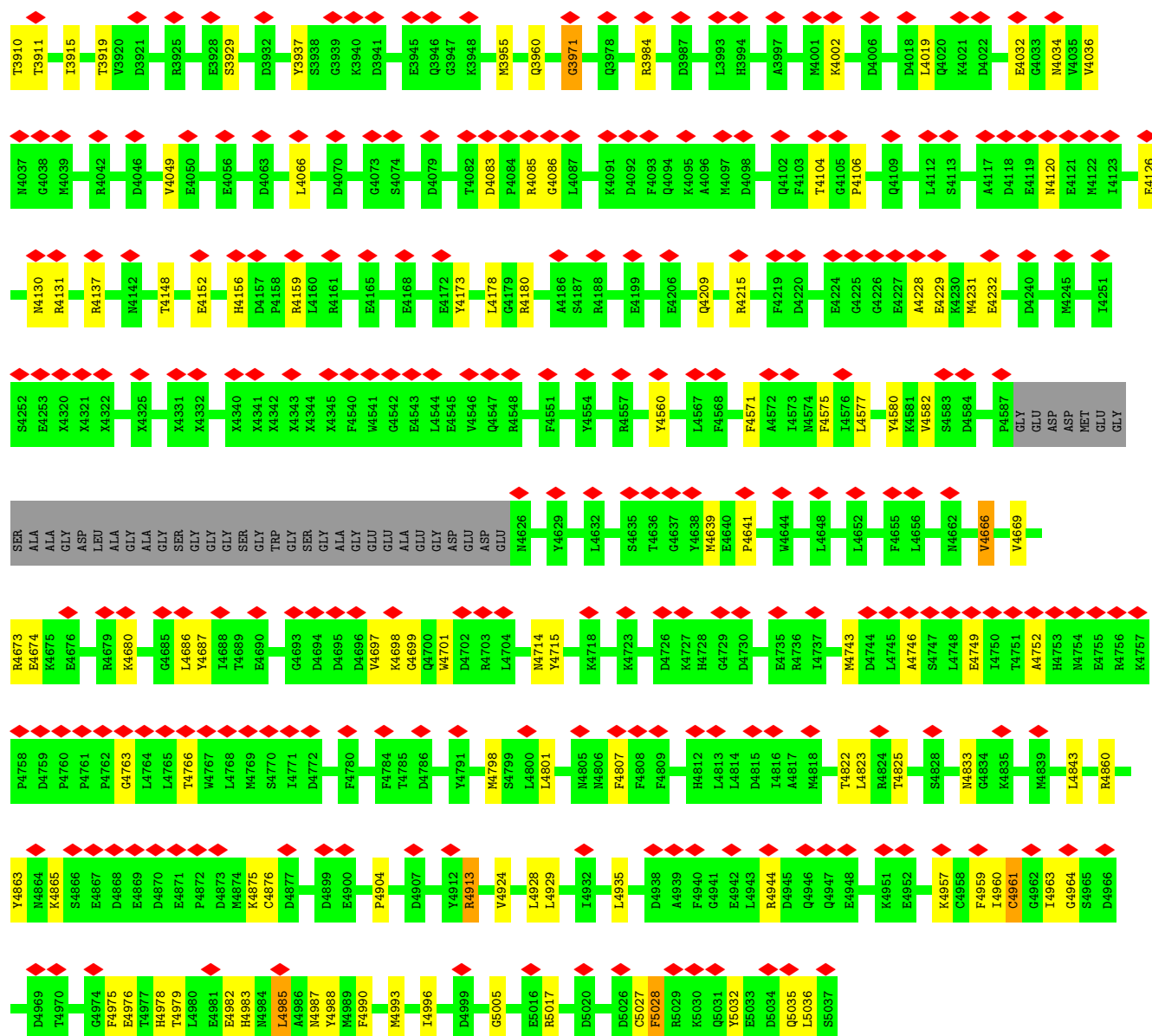
• Molecule 2: Ryanodine receptor 1





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L1732	L1804	L1804	H2041	P2226	L2307	L2377	M2440	X2531	X2646	L2747
E1733	E1805	E1805	C2042	K2227	Q2308	A2378	H2441	X2532	X2649	P2748
Y1734	E1806	A1806	G2043	M2228	S2309	A2379	L2442	X2533	X2650	E2749
L1738	L1807	L1807	T2044	T2229	C2310	I2380	G2446	X2534	X2651	K2750
T1739	R1808	R1808	L2044	S2231	P2311	E2382	K2447	X2535	X2658	L2751
P1740	L1812	L1812	Q2045	R2234	L2314	R2385	G2448	X2536	X2659	D2752
E1741	R1813	R1813	L2046	R2239	A2315	I2386	A2449	X2537	X2660	S2753
T1742	R1814	R1814	E2047	F2239	K2316	I2387	A2450	X2538	X2661	T2754
A1743	L1815	L1815	G2048	I2242	G2317	E2388	L2451	X2550	X2662	L2755
L1744	G1816	G1816	GLU	S2243	Y2318	D2389	R2452	X2551	X2663	K2756
L1745	D1821	D1821	GLU	R2244	D2320	A2391	R2453	X2561	X2664	K2757
F1748	G1822	G1822	PRO	Q2245	I2321	D2392	A2455	X2562	X2665	F2758
P1749	G1823	G1823	GLU	N2246	G2322	D2393	R2458	X2563	X2666	A2759
P1750	ASP	ASP	GLU	Q2247	C2326	G2394	S2459	X2567	X2667	E2760
P1751	ALA	ALA	THR	R2248	C2327	P2395	L2460	X2568	X2668	T2761
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R1753	E1990	E1990	SER	D2252	R2330	ARG	D2464	X2578	X2670	H2763
K1753	GLU	GLU	SER	Y2256	Y2331	ARG	D2465	X2579	X2671	E2764
G1754	GLU	GLU	ARG	L2257	L2332	ASP	L2466	X2580	X2672	K2765
G1755	ALA	ALA	LEU	L2258	D2333	ASP	D2467	X2581	X2673	A2766
G1756	PRO	PRO	ARG	L2259	F2334	ARG	L2468	X2582	X2674	X2675
N1756	GLY	GLY	SER	E2259	G2335	ARG	I2469	X2583	X2675	X2676
A1757	GLY	GLY	LEU	N2260	R2336	GLU	T2470	X2584	X2676	X2677
R1758	L1842	L1842	LEU	S2261	R2337	HIS	S2471	X2585	X2677	X2678
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L1762	F1854	F1854	LEU	G2268	F2340	GLU	Q2475	X2589	X2686	X2686
P1763	G1855	G1855	VAL	Q2269	G2341	GLU	T2476	X2590	X2687	X2687
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V1765	E1857	E1857	LYS	K2090	G2343	GLU	T2478	X2600	X2689	X2689
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V1767	V1859	V1859	LYS	Q2092	E2347	R2415	L2480	X2613	X2691	X2691
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P1773	F1870	F1870	ALA	Q2098	E2285	L2419	X2490	X2617	X2695	X2695
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H1775	E1872	E1872	LEU	Q2099	L2288	L2421	L2422	X2619	X2697	X2697
L1782	F1873	F1873	PRO	Q2099	A2289	L2422	L2423	X2620	X2698	X2698
V1783	E1874	E1874	ALA	Q2099	L2290	S2424	S2424	X2621	X2699	X2699
A1784	A1785	A1785	K2089	Q2092	E2292	Y2426	Y2426	X2622	X2700	X2700
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P1787	GLU	GLU	Q2091	Q2092	L2295	L2432	L2432	X2625	X2703	X2703
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ALA	GLU	GLU	Q2091	Q2092	E2296	A2437	A2437	X2630	X2708	X2708
E1793	GLU	GLU	Q2091	Q2092	E2296	P2438	P2438	X2631	X2709	X2709
A1794	GLU	GLU	Q2091	Q2092	E2296	L2439	L2439	X2632	X2710	X2710
P1795	GLU	GLU	Q2091	Q2092	E2296	L2440	L2440	X2633	X2711	X2711
A1796	GLU	GLU	Q2091	Q2092	E2296	L2441	L2441	X2634	X2712	X2712
R1797	GLU	GLU	Q2091	Q2092	E2296	L2442	L2442	X2635	X2713	X2713
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						L2512	L2512	X2705	X2783	X2783
						L2513	L2513	X2706	X2784	X2784
						L2514	L2514	X2707	X2785	X2785
						L2515	L2515	X2708	X2786	X2786
						L2516	L2516	X2709	X2787	X2787
						L2517	L2517	X2710	X2788	X2788
						L2518	L2518	X2711	X2789	X2789
						L2519	L2519	X2712	X2790	X2790
						L2520	L2520	X2713	X2791	X2791
						L2521	L2521	X2714	X2792	X2792
						L2522	L2522	X2715	X2793	X2793
						L2523	L2523	X2716	X2794	X2794
						L2524	L2524	X2717	X2795	X2795
						L2525	L2525	X2718	X2796	X2796
						L2526	L2526	X2719	X2797	X2797
						L2527	L2527	X2720	X2798	X2798
						L2528	L2528	X2721	X2799	X2799
						L2529	L2529	X2722	X2800	X2800
						L2530	L2530	X2723	X2801	X2801
						L2531	L2531	X2724	X2802	X2802
						L2532	L2532	X2725	X2803	X2803
						L253				

V3812	L3716	T3639	X3549	X3433	X3364	X3292	X3221	X3148	X3009	L2926	R2806
L3817	D3717	Y3642	X3548	X3434	X3365	X3293	X3222	X3149	X3010	L2927	W2807
D3818	E3718	N3643	X3550	X3435	X3366	X3294	X3223	X3150	X3014	L2928	F2808
K3821	D3719	L3644	X3551	X3436	X3367	X3295	X3224	X3151	X3015	F2929	T2809
D3822	X3720	P3645	X3552	X3436	X3368	X3296	X3225	X3152	X3016	L2930	K2810
E3825	D3727	H3647	X3553	X3437	X3369	X3297	X3226	X3153	X3017	Q2831	E2811
F3829	H3734	R3648	X3554	X3441	X3370	X3302	X3229	X3154	X3018	Q2872	S2812
Q3830	L3735	X3649	X3555	X3442	X3371	X3303	X3230	X3155	X3019	A2873	L2813
Q3833	L3736	N3651	X3556	X3450	X3372	X3308	X3231	X3156	X3020	M2874	K2814
M3836	E3737	H3652	X3557	X3451	X3373	X3309	X3232	X3157	X3021	A2875	A2815
L3842	E3738	F3653	X3558	X3452	X3374	X3310	X3233	X3158	X3022	E2876	M2816
D3843	G3739	S3656	X3559	X3453	X3375	X3311	X3234	X3159	X3023	T2937	T2817
L3844	G3740	Y3657	X3560	X3454	X3376	X3312	X3235	X3160	X3027	T2938	A2818
N3845	N3741	X3658	X3561	X3455	X3377	X3313	X3236	X3161	X3028	R2939	W2819
E3849	GLU	A3659	X3562	X3456	X3378	X3314	X3237	X3162	X3029	R2942	E2820
Q3850	ALA	A3660	X3563	X3457	X3379	X3315	X3238	X3163	X3030	G2943	W2821
N3851	GLU	V3661	X3564	X3458	X3380	X3316	X3239	X3164	X3033	X2944	T2822
E3854	GLU	T3662	X3565	X3459	X3381	X3317	X3240	X3165	X3034	X2945	T2823
G3855	E3747	L3663	X3566	X3462	X3382	X3318	X3241	X3166	X3035	X2946	E2824
L3856	E3748	L3664	X3567	X3463	X3383	X3319	X3242	X3167	X3036	X2947	K2825
G3857	V3749	E3665	X3568	X3464	X3384	X3320	X3243	X3168	X3037	X2948	A2826
N3858	E3750	D3666	X3569	X3465	X3385	X3321	X3244	X3169	X3038	X2949	R2827
E3861	V3751	H3667	X3570	X3466	X3386	X3322	X3245	X3170	X3039	X2950	E2828
G3862	S3752	S3668	X3571	X3467	X3387	X3323	X3246	X3171	X3040	X2951	G2829
L3863	F3753	F3669	X3572	X3468	X3388	X3324	X3247	X3172	X3041	X2952	E2830
E3864	E3754	E3670	X3573	X3469	X3389	X3325	X3248	X3173	X3042	X2953	GLU
V3865	E3755	D3671	X3574	X3470	X3390	X3326	X3249	X3174	X3043	X2954	GLU
L3866	X3759	R3672	X3575	X3471	X3391	X3327	X3250	X3175	X3044	X2955	ARG
N3867	D3760	N3673	X3576	X3472	X3392	X3328	X3251	X3176	X3045	X2956	THR
G3868	E3761	E3674	X3577	X3473	X3393	X3329	X3252	X3177	X3046	X2957	GLU
L3869	S3762	L3675	X3578	X3474	X3394	X3330	X3253	X3178	X3047	X2958	LYS
E3870	F3763	D3676	X3579	X3475	X3395	X3331	X3254	X3179	X3048	X2959	LYS
G3871	E3764	N3677	X3580	X3476	X3396	X3332	X3255	X3180	X3049	X2960	THR
E3872	E3765	E3678	X3581	X3477	X3397	X3333	X3256	X3181	X3050	X2961	ARG
K3873	E3766	E3679	X3582	X3478	X3398	X3334	X3257	X3182	X3051	X2962	LYS
D3878	G3767	A3680	X3583	X3479	X3399	X3335	X3258	X3183	X3052	X2963	ILE
L3880	L3770	G3681	X3584	X3480	X3400	X3336	X3259	X3184	X3053	X2964	GLN
N3881	R3773	E3682	X3585	X3481	X3401	X3337	X3260	X3185	X3054	X2965	ALA
G3882	G3774	E3683	X3586	X3482	X3402	X3338	X3261	X3186	X3055	X2966	THR
E3883	A3775	Q3684	X3587	X3483	X3403	X3339	X3262	X3187	X3056	X2967	ARG
L3884	E3776	E3685	X3588	X3484	X3404	X3340	X3263	X3188	X3057	X2968	LYS
V3885	E3777	E3686	X3589	X3485	X3405	X3341	X3264	X3189	X3058	X2969	LYS
N3886	M3778	E3687	X3590	X3486	X3406	X3342	X3265	X3190	X3059	X2970	THR
G3887	V3779	E3688	X3591	X3487	X3407	X3343	X3266	X3191	X3060	X2971	ALA
L3888	L3780	E3689	X3592	X3488	X3408	X3344	X3267	X3192	X3061	X2972	GLN
E3889	Q3781	X3593	X3593	X3489	X3409	X3345	X3268	X3193	X3062	X2973	THR
D3890	E3784	X3594	X3594	X3490	X3410	X3346	X3269	X3194	X3063	X2974	ASP
L3891	K3787	E3690	X3595	X3491	X3411	X3347	X3270	X3195	X3064	X2975	PRO
G3892	G3788	E3691	X3596	X3492	X3412	X3348	X3271	X3196	X3065	X2976	GLU
E3893	E3789	E3692	X3597	X3493	X3413	X3349	X3272	X3197	X3066	X2977	GLY
K3894	K3799	X3693	X3598	X3494	X3414	X3350	X3273	X3198	X3067	X2978	Y2855
L3895	L3804	R3707	X3599	X3495	X3415	X3351	X3274	X3199	X3068	X2979	H2856
N3896	L3805	L3710	X3600	X3496	X3416	X3352	X3275	X3200	X3069	X2980	P2857
E3897	N3809	L3711	X3601	X3497	X3417	X3353	X3276	X3201	X3070	X2981	Q2858
G3908	E3712	E3713	X3602	X3498	X3418	X3354	X3277	X3202	X3071	X2982	P2859
N3909	E3714	S3715	X3603	X3499	X3419	X3355	X3278	X3203	X3072	X2983	E2860
E3910	E3715	E3716	X3604	X3500	X3420	X3356	X3279	X3204	X3073	X2984	D2861
L3911	E3716	E3717	X3605	X3501	X3421	X3357	X3280	X3205	X3074	X2985	L2862
E3912	E3717	E3718	X3606	X3502	X3422	X3358	X3281	X3206	X3075	X2986	S2863
G3913	E3718	E3719	X3607	X3503	X3423	X3359	X3282	X3207	X3076	X2987	G2864
L3914	E3719	E3720	X3608	X3504	X3424	X3360	X3283	X3208	X3077	X2988	Y2865
E3915	E3720	E3721	X3609	X3505	X3425	X3361	X3284	X3209	X3078	X2989	
G3916	E3721	E3722	X3610	X3506	X3426	X3362	X3285	X3210	X3079	X2990	
L3917	E3722	E3723	X3611	X3507	X3427	X3363	X3286	X3211	X3080	X2991	
E3918	E3723	E3724	X3612	X3508	X3428	X3364	X3287	X3212	X3081	X2992	
G3919	E3724	E3725	X3613	X3509	X3429	X3365	X3288	X3213	X3082	X2993	
L3920	E3725	E3726	X3614	X3510	X3430	X3366	X3289	X3214	X3083	X2994	
E3921	E3726	E3727	X3615	X3511	X3431	X3367	X3290	X3215	X3084	X2995	
G3922	E3727	E3728	X3616	X3512	X3432	X3368	X3291	X3216	X3085	X2996	
L3923	E3728	E3729	X3617	X3513	X3433	X3369	X3292	X3217	X3086	X2997	
E3924	E3729	E3730	X3618	X3514	X3434	X3370	X3293	X3218	X3087	X2998	
G3925	E3730	E3731	X3619	X3515	X3435	X3371	X3294	X3219	X3088	X2999	
L3926	E3731	E3732	X3620	X3516	X3436	X3372	X3295	X3220	X3089	X3000	
E3927	E3732	E3733	X3621	X3517	X3437	X3373	X3296	X3221	X3090	X3001	
G3928	E3733	E3734	X3622	X3518	X3438	X3374	X3297	X3222	X3091	X3002	
L3929	E3734	E3735	X3623	X3519	X3439	X3375	X3298	X3223	X3092	X3003	
E3929	E3735	E3736	X3624	X3520	X3440	X3376	X3299	X3224	X3093	X3004	
G3930	E3736	E3737	X3625	X3521	X3441	X3377	X3300	X3225	X3094	X3005	
L3931	E3737	E3738	X3626	X3522	X3442	X3378	X3301	X3226	X3095	X3006	
E3931	E3738	E3739	X3627	X3523	X3443	X3379	X3302	X3227	X3096	X3007	
G3932	E3739	E3740	X3628	X3524	X3444	X3380	X3303	X3228	X3097	X3008	
L3933	E3740	E3741	X3629	X3525	X3445	X3381	X3304	X3229	X3098	X3009	
E3933	E3741	E3742	X3630	X3526	X3446	X3382	X3305	X3230	X3099	X3010	
G3934	E3742	E3743	X3631	X3527	X3447	X3383	X3306	X3231	X3100	X3011	
L3935	E3743	E3744	X3632	X3528	X3448	X3384	X3307	X3232	X3101	X3012	
E3935	E3744	E3745	X3633	X3529	X3449	X3385	X3308	X3233	X3102	X3013	
G3936	E3745	E3746	X3634	X3530	X3450	X3386	X3309	X3234	X3103	X3014	
L3937	E3746	E3747	X3635	X3531	X3451	X3387	X3310	X3235	X3104	X3015	
E3937	E3747	E3748	X3636	X3532	X3452	X3388	X3311	X3236	X3105	X3016	
G3938	E3748	E3749	X3637	X3533	X3453	X3389	X3312	X3237	X3106	X3017	
L3939	E3749	E3750	X3638	X3534	X3454	X3390	X3313	X3238	X3107	X3018	
E3939	E3750	E3751	X3639	X3535	X3455	X3391	X3314	X3239	X3108	X3019	
G3940	E3751	E3752	X3640	X3536	X3456	X3392	X3315	X3240	X3109	X3020	
L3941	E3752	E3753	X3641	X3537	X3457	X3393	X3316	X3241	X3110	X3021	
E3941	E3753	E3754	X3642	X3538	X3458	X3394	X3317	X3242	X3111	X3022	
G3942	E3754	E3755	X3643	X3539	X3459	X3395	X3318	X3243	X3112	X3023	
L3943	E3755	E3756	X3644	X3540	X3460	X3396	X3319	X3244	X3113	X3024	
E3943	E3756	E3757	X3645	X3541	X3461	X3397	X3320	X3245	X3114	X3025	
G3944	E3757	E3758	X3646	X3542	X3462	X3398	X3321	X3246	X3115	X3026	
L3945	E3758	E3759	X3647	X3543	X3463	X3399	X3322	X3247	X3116	X3027	
E3945	E3759	E3760	X3648	X3544	X3464	X3400	X3323	X3248	X3117	X3028	
G3946	E3760	E3761	X3649	X3545	X3465	X3401	X3324	X3249	X3118	X3029	
L3947	E3761	E3762	X3650	X3546	X3466	X3402	X3325	X3250	X3119	X3030	
E3947	E3762	E3763	X3651	X3547	X3467	X3403	X3326	X3251	X3120	X3031	
G3948	E3763	E3764	X3652	X3548	X3468	X3404	X3327	X3252	X3121	X3032	
L3949	E3764	E3765	X3653	X3549	X3469	X3405	X3328	X3253	X3122	X3033	
E3949	E3765	E3766	X3654	X3550	X3470	X3406	X3329	X3254	X3123	X3034	
G3950	E3766	E3767	X3655	X3551	X3471	X3407	X3330	X3255	X3124	X3035	
L3951	E3767	E3768	X3656	X3552	X3472	X3408	X3331	X3256	X3125	X3036	
E3951	E3768	E3769	X3657	X3553	X3473	X3409	X3332	X3257	X3126	X3037	
G3952	E3769	E3770	X3658	X3554	X3474	X3410	X3333	X3258	X3127	X3038	
L3953	E3770	E3771	X3659	X3555	X3475	X3411	X3334	X3259	X3128	X3039	
E3953	E3771										





## 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	0.065	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size ( $\text{\AA}$ )	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.255, 1.255, 1.255	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CFF, ATP, 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	0.31	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	0.31	0/25428	0.55	9/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	9/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	34/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	8.16	134.07	115.30
2	G	131	LEU	CA-CB-CG	8.16	134.07	115.30
2	B	131	LEU	CA-CB-CG	8.15	134.04	115.30
2	I	131	LEU	CA-CB-CG	8.13	133.99	115.30
2	E	4985	LEU	CA-CB-CG	7.48	132.50	115.30

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	15	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	14	0
2	B	29499	0	24747	289	0
2	E	29499	0	24747	286	0
2	G	29499	0	24747	288	0
2	I	29499	0	24748	285	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	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	102373	1167	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 1167 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:B:4975:PHE:O	2:B:4979:THR:HG23	1.85	0.77
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.85	0.76
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.86	0.76
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.86	0.76
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.78	0.71

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%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	J	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	44	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2892 (89%)	338 (10%)	5 (0%)	44	78
2	G	3235/4416 (73%)	2890 (89%)	340 (10%)	5 (0%)	44	78
2	I	3235/4416 (73%)	2889 (89%)	340 (10%)	6 (0%)	44	78
All	All	13360/18096 (74%)	11954 (90%)	1384 (10%)	22 (0%)	45	78

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1932	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%)	2475 (99%)	18 (1%)	81	87
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	79	85
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
All	All	10324/12444 (83%)	10251 (99%)	73 (1%)	80	87

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	553	ARG

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Mol	Chain	Res	Type
2	G	4944	ARG
2	G	1141	ARG
2	G	4034	ASN
2	E	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	4209	GLN
2	G	3889	GLN
2	G	57	ASN
2	G	725	HIS
2	G	4054	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	0.87	0	34,52,52	1.11	2 (5%)
4	CFF	G	5102	-	8,15,15	2.18	3 (37%)	8,23,23	1.25	1 (12%)
3	ATP	G	5101	-	28,33,33	0.87	0	34,52,52	1.11	2 (5%)
4	CFF	E	5102	-	8,15,15	2.18	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	B	5102	-	8,15,15	2.18	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	I	5102	-	8,15,15	2.18	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	B	5101	-	28,33,33	0.88	0	34,52,52	1.11	2 (5%)
3	ATP	I	5101	-	28,33,33	0.87	0	34,52,52	1.11	2 (5%)

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	-	-	6/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	I	5101	-	-	6/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	CFF	C5-C4	-3.53	1.33	1.39
4	E	5102	CFF	C5-C4	-3.53	1.33	1.39
4	I	5102	CFF	C5-C4	-3.53	1.33	1.39
4	G	5102	CFF	C5-C4	-3.53	1.33	1.39
4	G	5102	CFF	C6-N1	-3.41	1.32	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-3.53	123.88	128.67
3	B	5101	ATP	N3-C2-N1	-3.52	123.90	128.67
3	I	5101	ATP	N3-C2-N1	-3.50	123.92	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-3.50	123.93	128.67
4	I	5102	CFF	C14-N7-C8	-2.85	111.73	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	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A

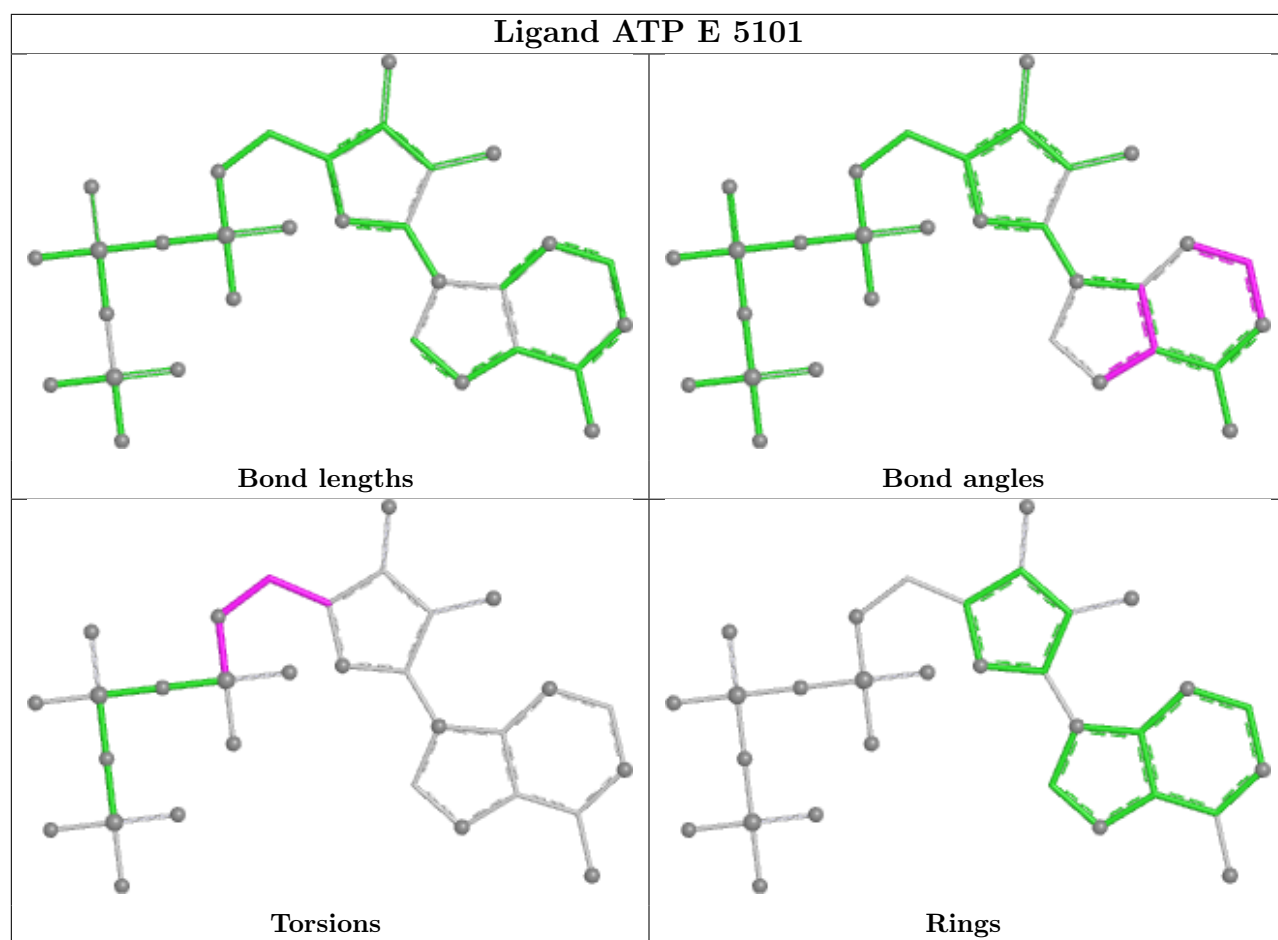
There are no ring outliers.

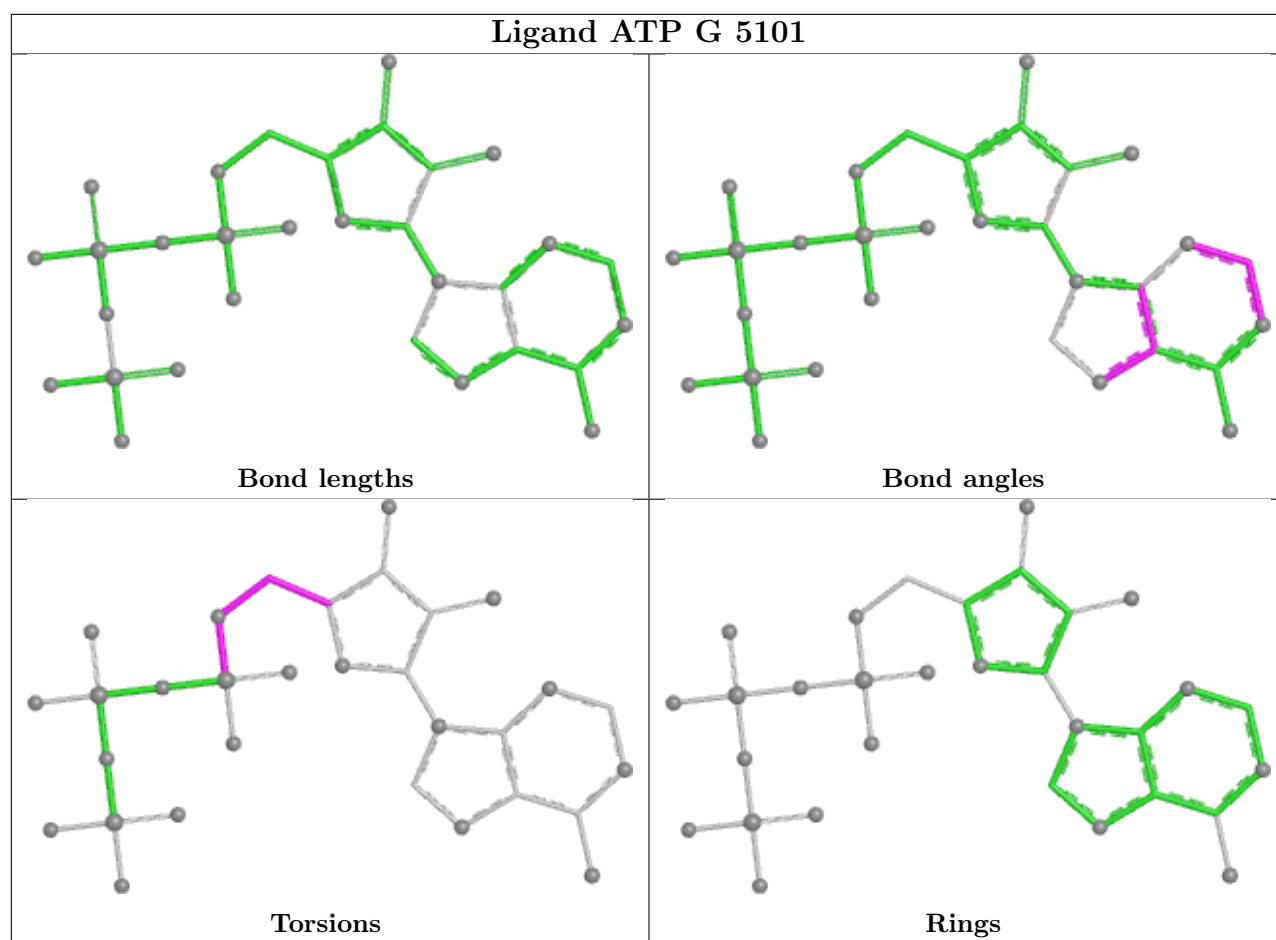
8 monomers are involved in 12 short contacts:

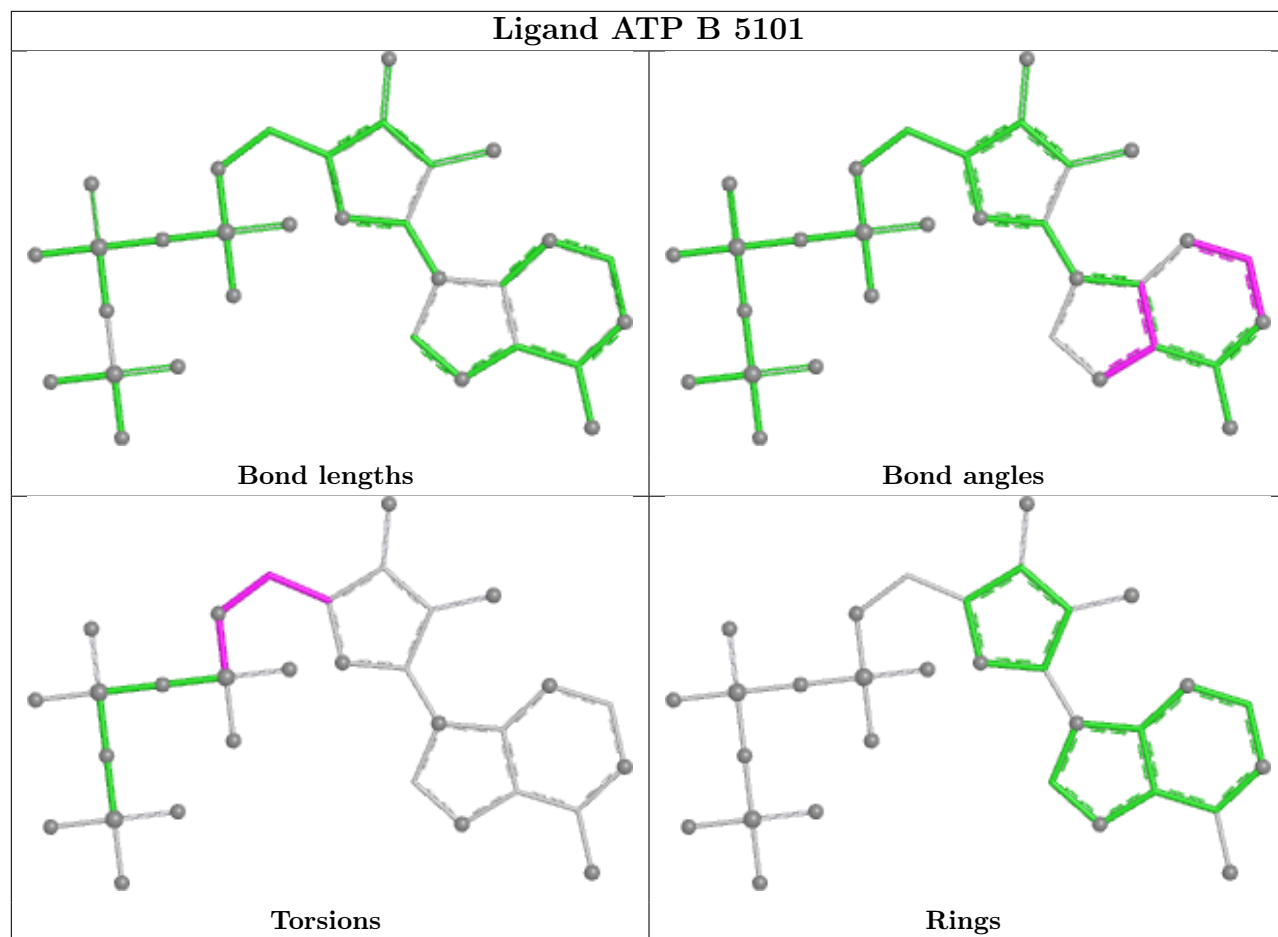
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	2	0
4	G	5102	CFF	1	0
3	G	5101	ATP	2	0
4	E	5102	CFF	1	0
4	B	5102	CFF	1	0
4	I	5102	CFF	1	0
3	B	5101	ATP	2	0
3	I	5101	ATP	2	0

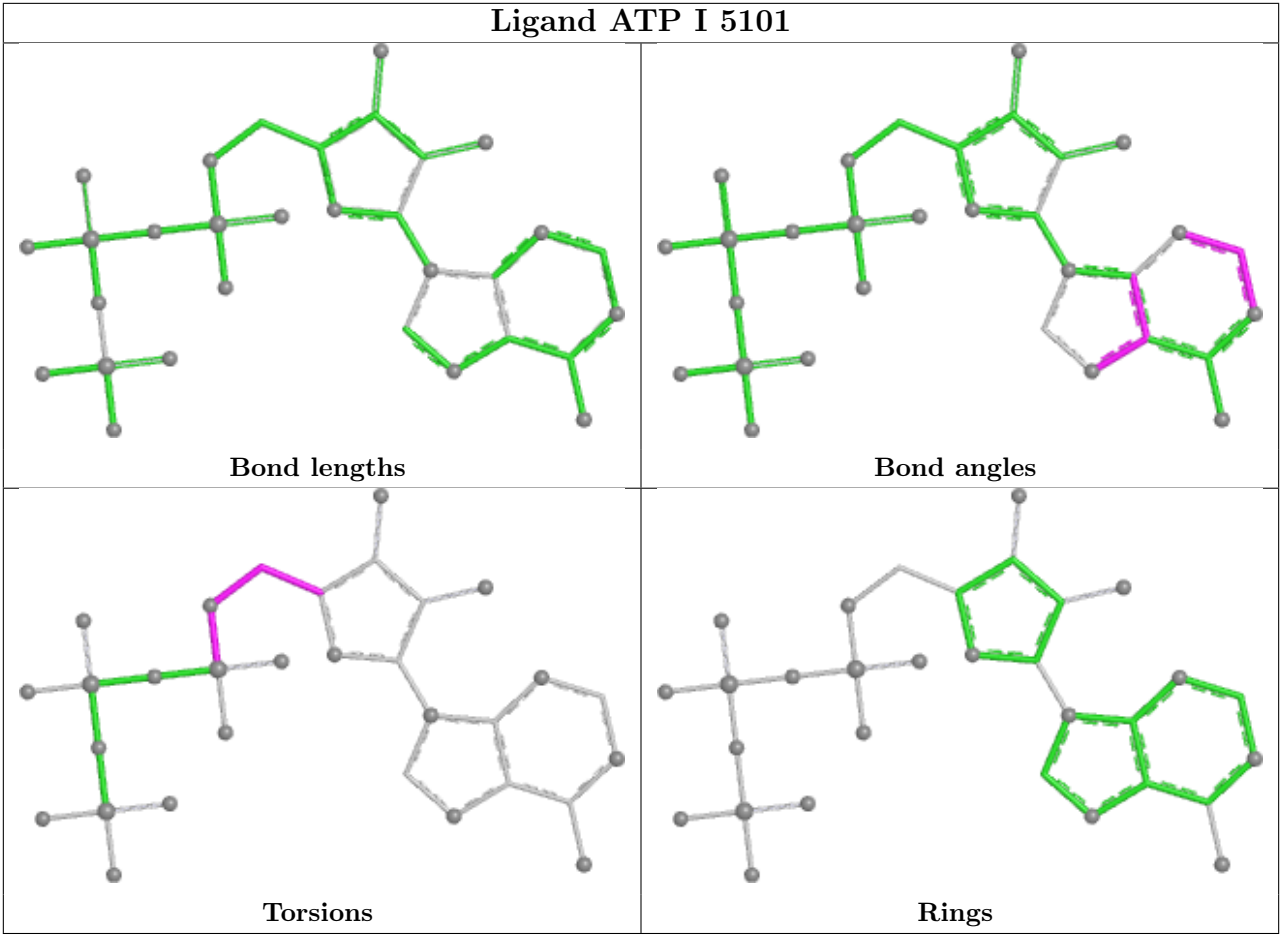
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	72.88
1	E	4345:UNK	C	4540:PHE	N	72.88

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.88
1	G	4345:UNK	C	4540:PHE	N	72.88
1	B	3613:UNK	C	3639:THR	N	43.44

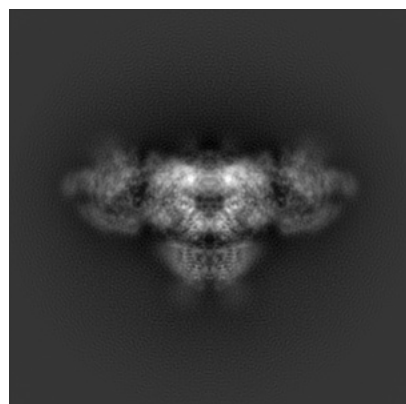
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8379. These allow visual inspection of the internal detail of the map and identification of artifacts.

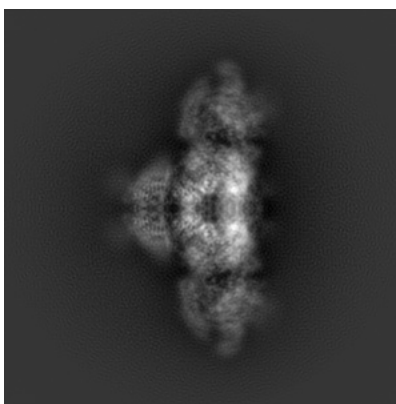
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

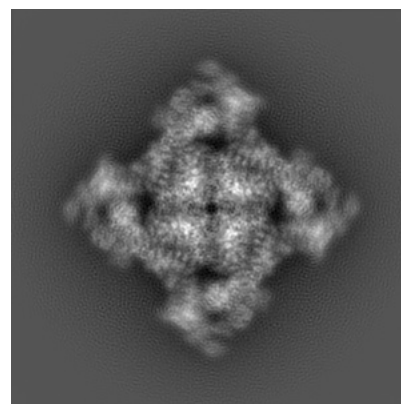
#### 6.1.1 Primary map



X

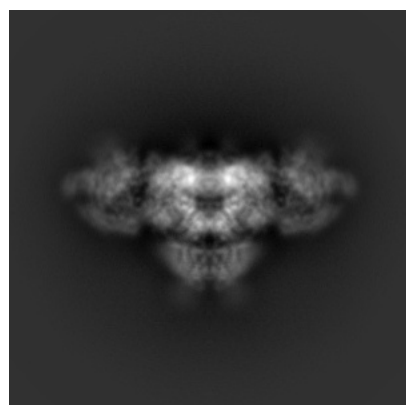


Y

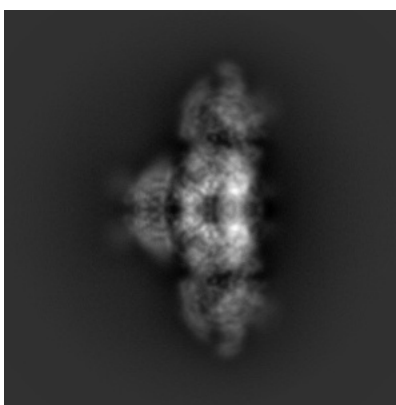


Z

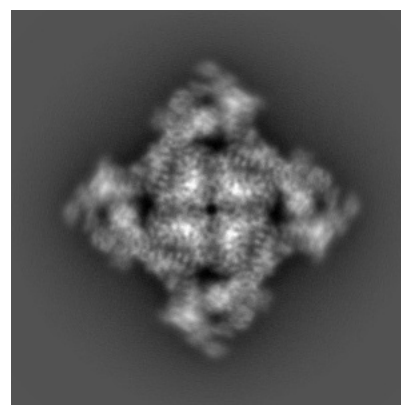
#### 6.1.2 Raw map



X



Y

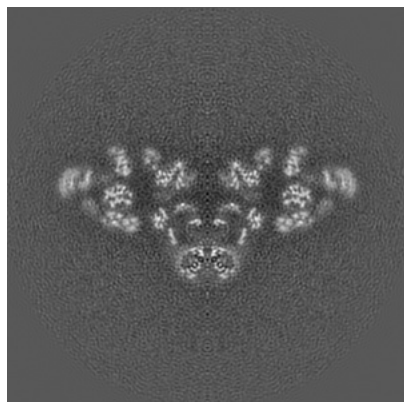


Z

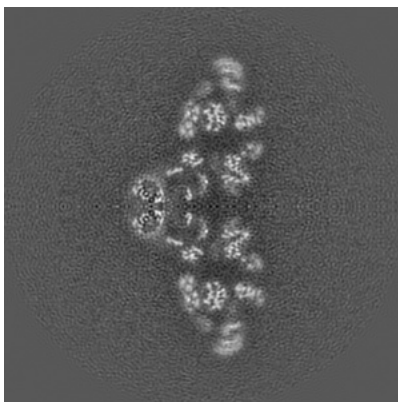
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

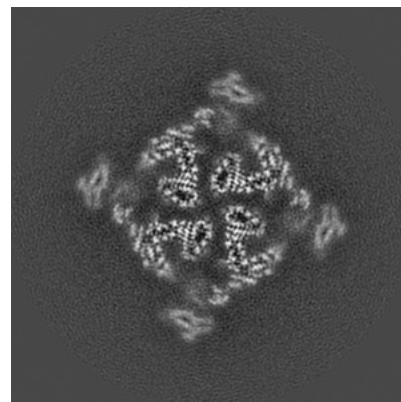
### 6.2.1 Primary map



X Index: 200

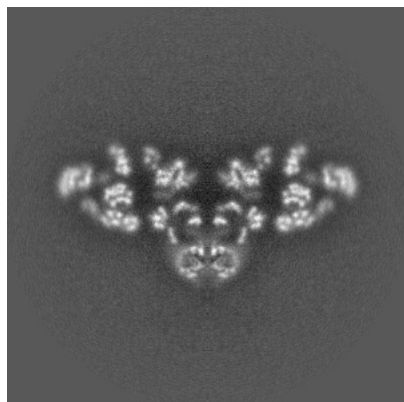


Y Index: 200

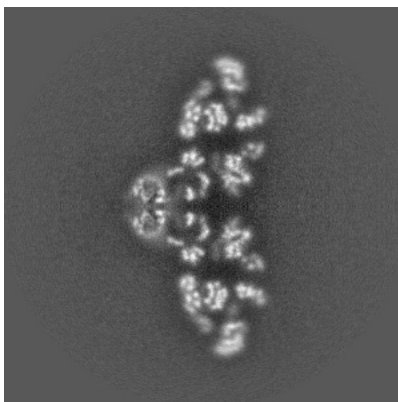


Z Index: 200

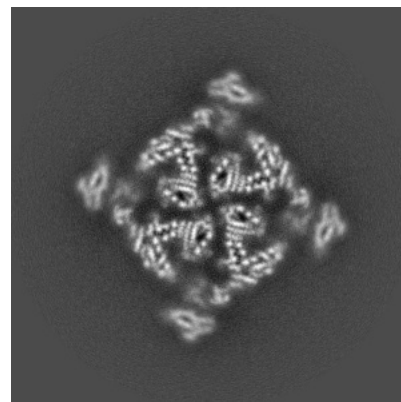
### 6.2.2 Raw map



X Index: 200



Y Index: 200

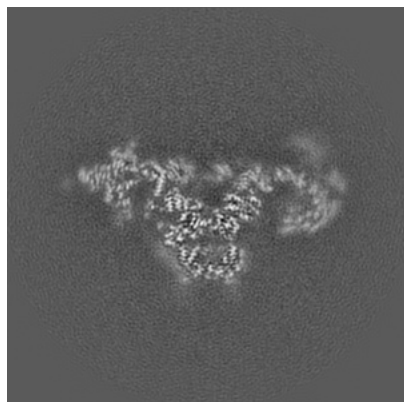


Z Index: 200

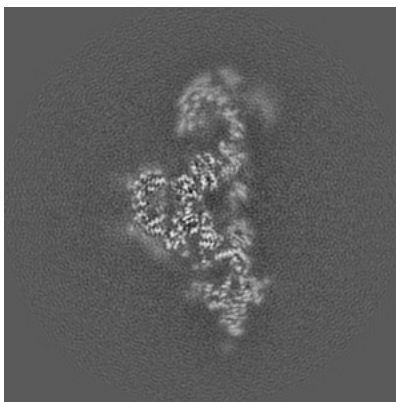
The images above show central slices of the map in three orthogonal directions.

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

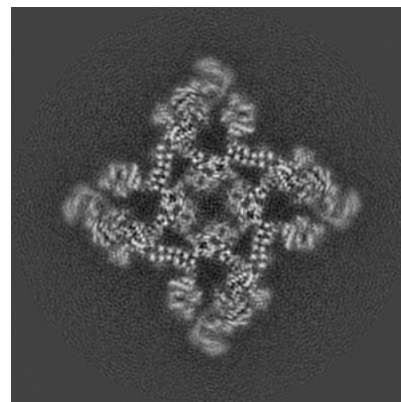
### 6.3.1 Primary map



X Index: 217

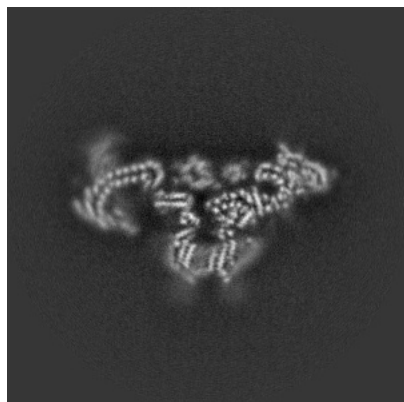


Y Index: 183

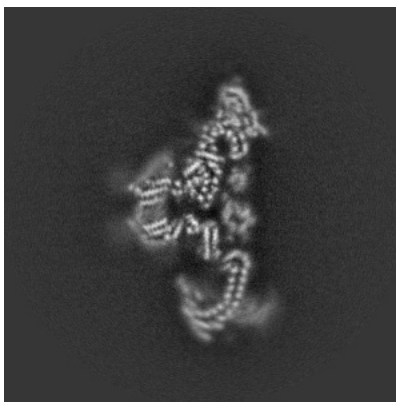


Z Index: 226

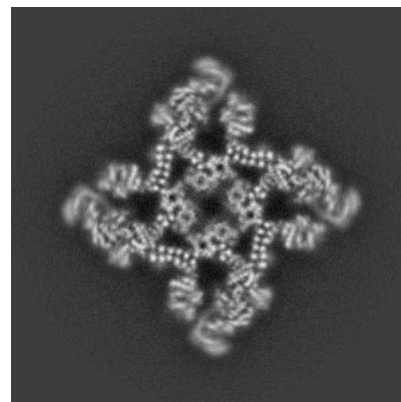
### 6.3.2 Raw map



X Index: 176



Y Index: 224



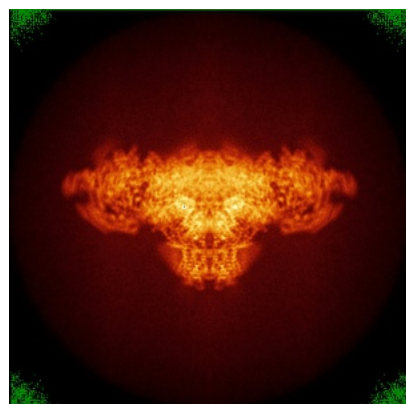
Z Index: 227

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

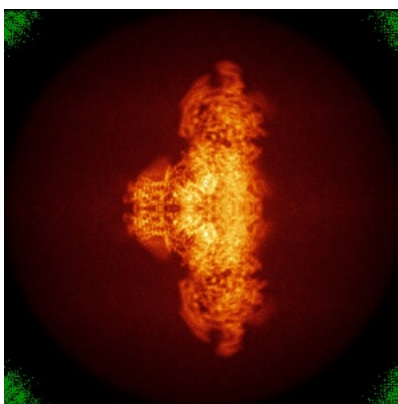


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

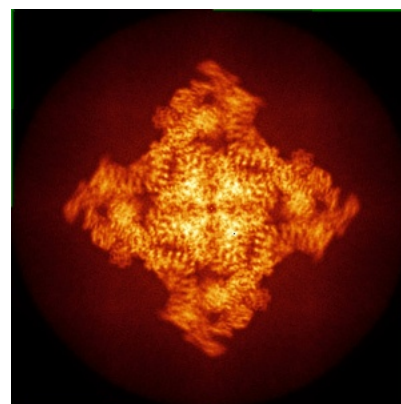
### 6.4.1 Primary map



X



Y

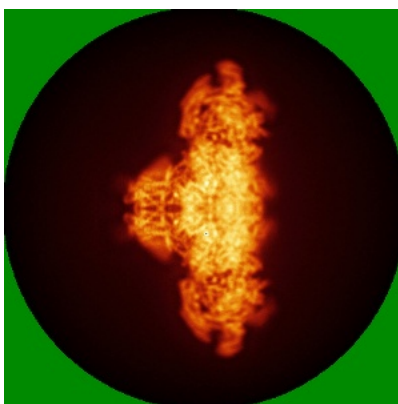


Z

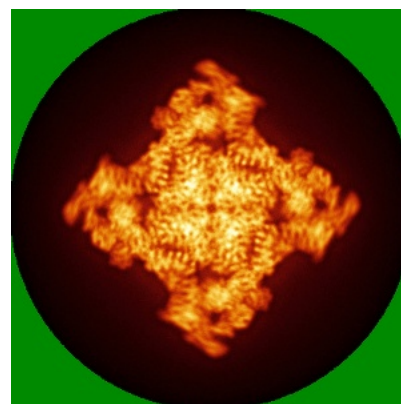
### 6.4.2 Raw map



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.

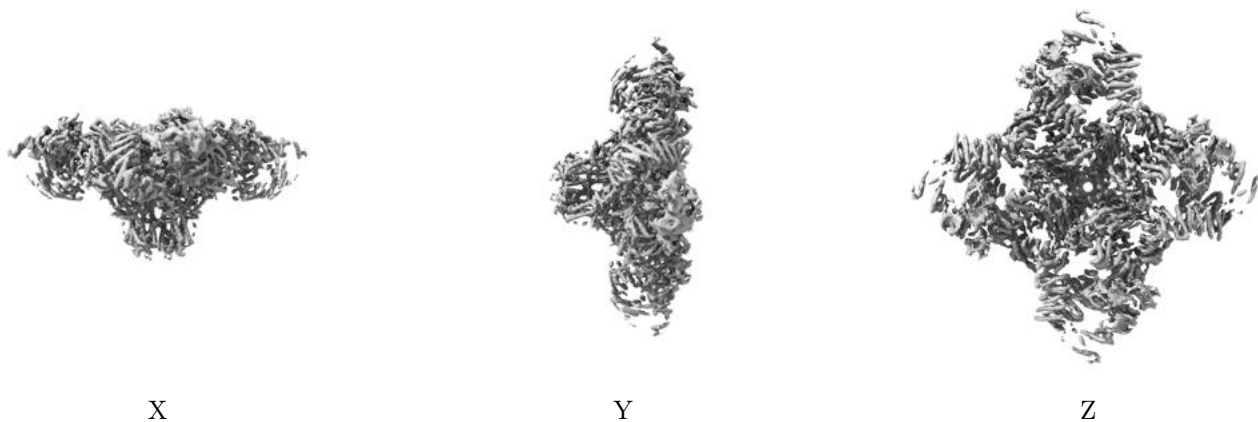
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

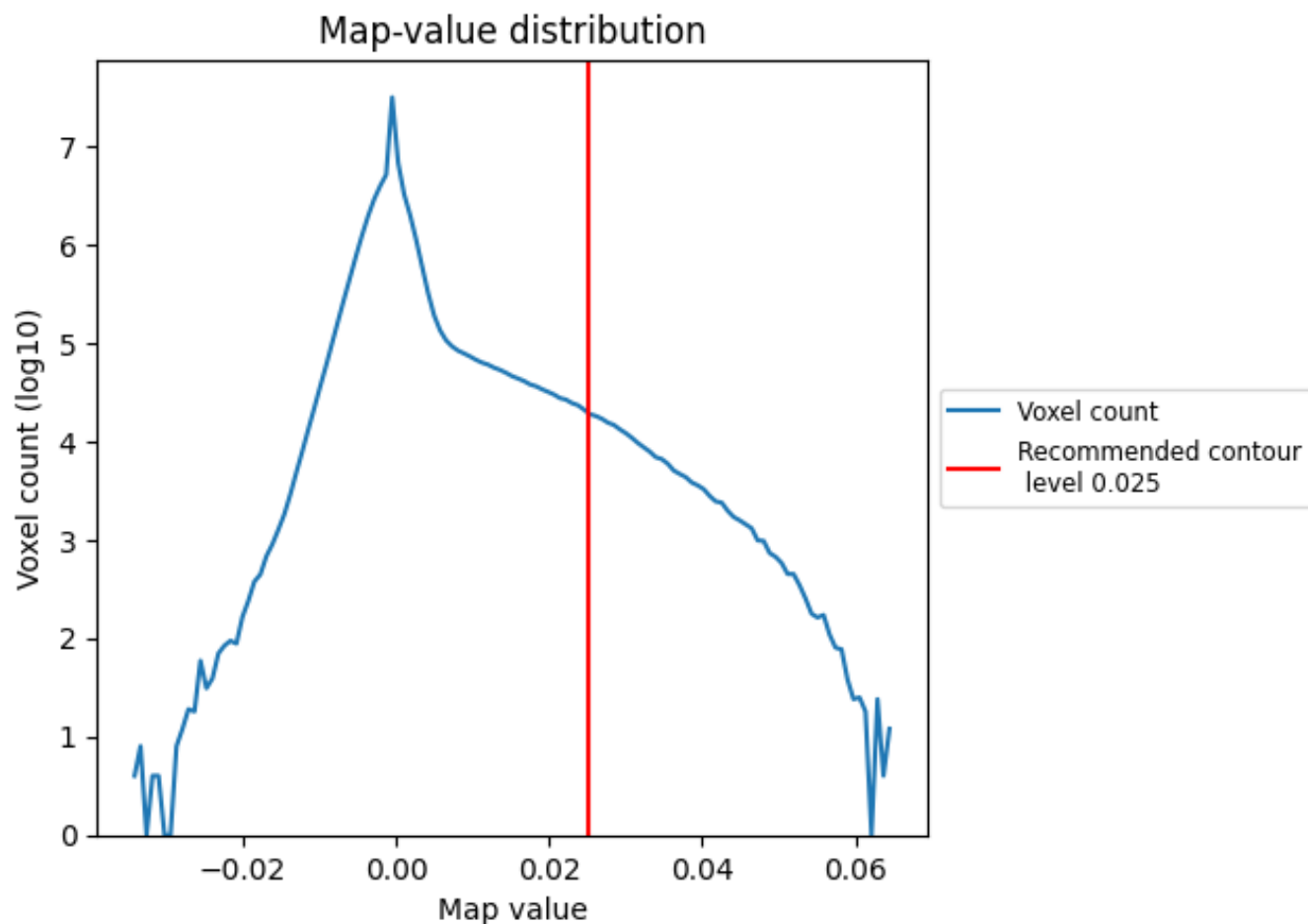
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

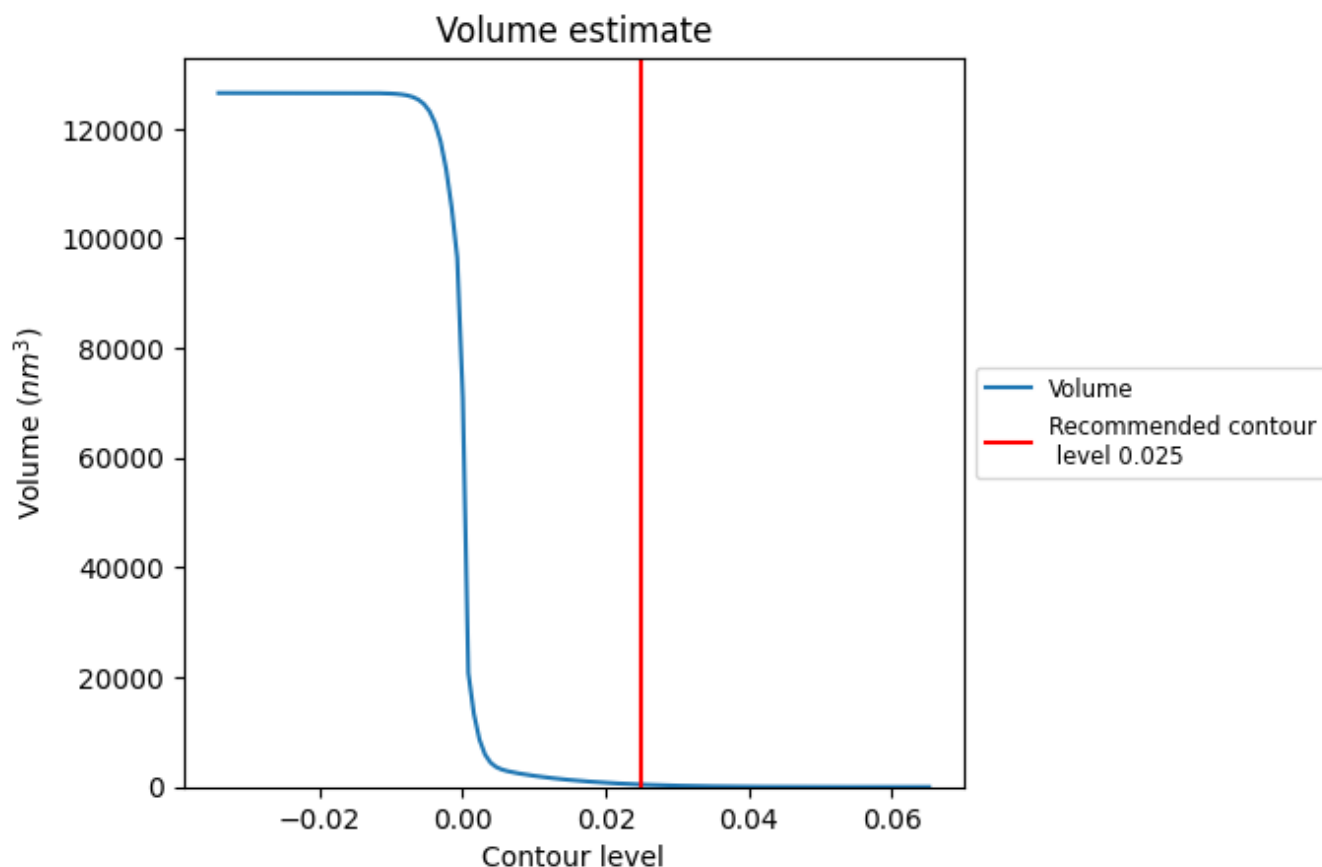
This section contains the results of statistical analysis of the map.

### 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.

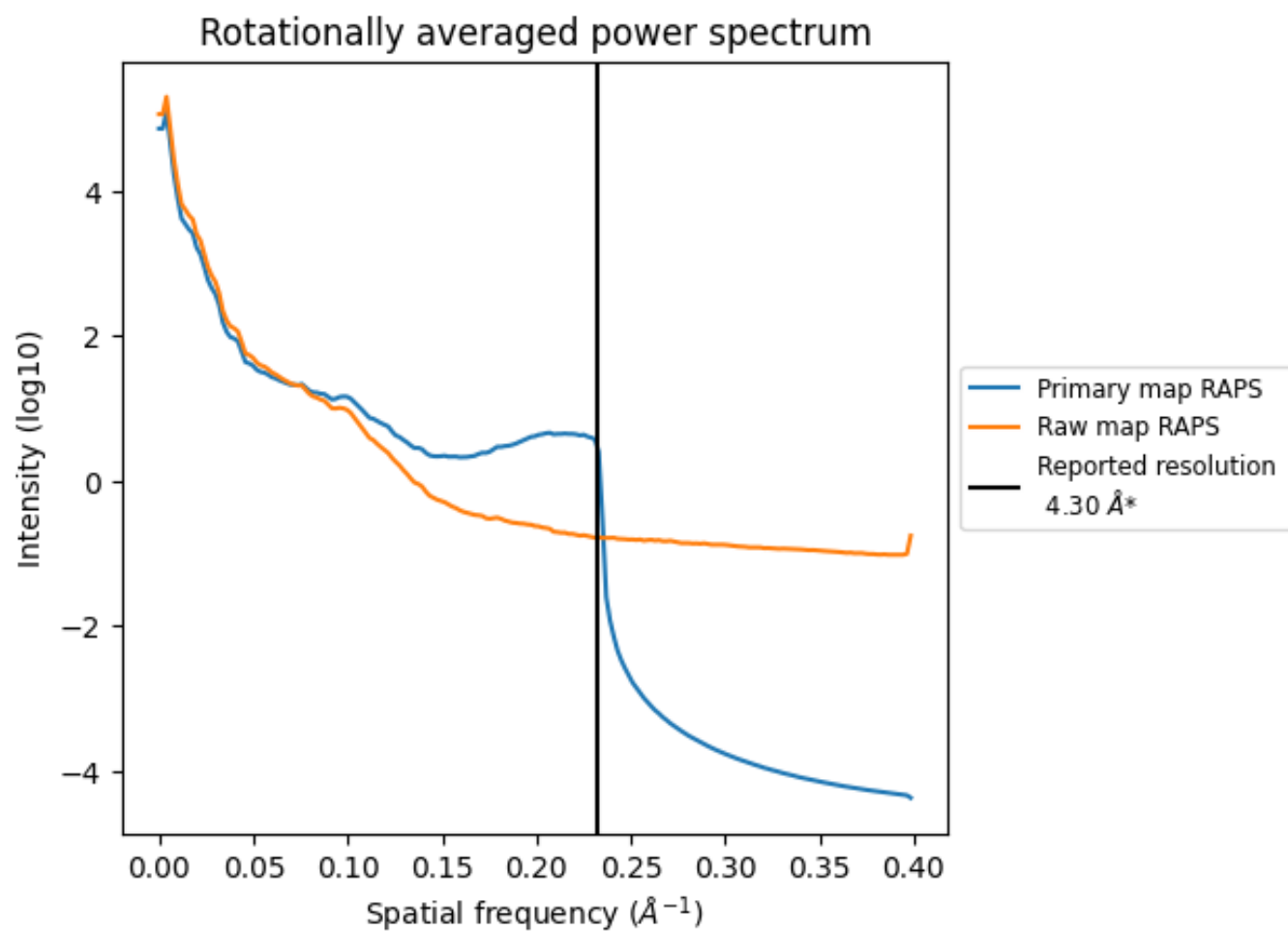
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 437 nm<sup>3</sup>; this corresponds to an approximate mass of 395 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

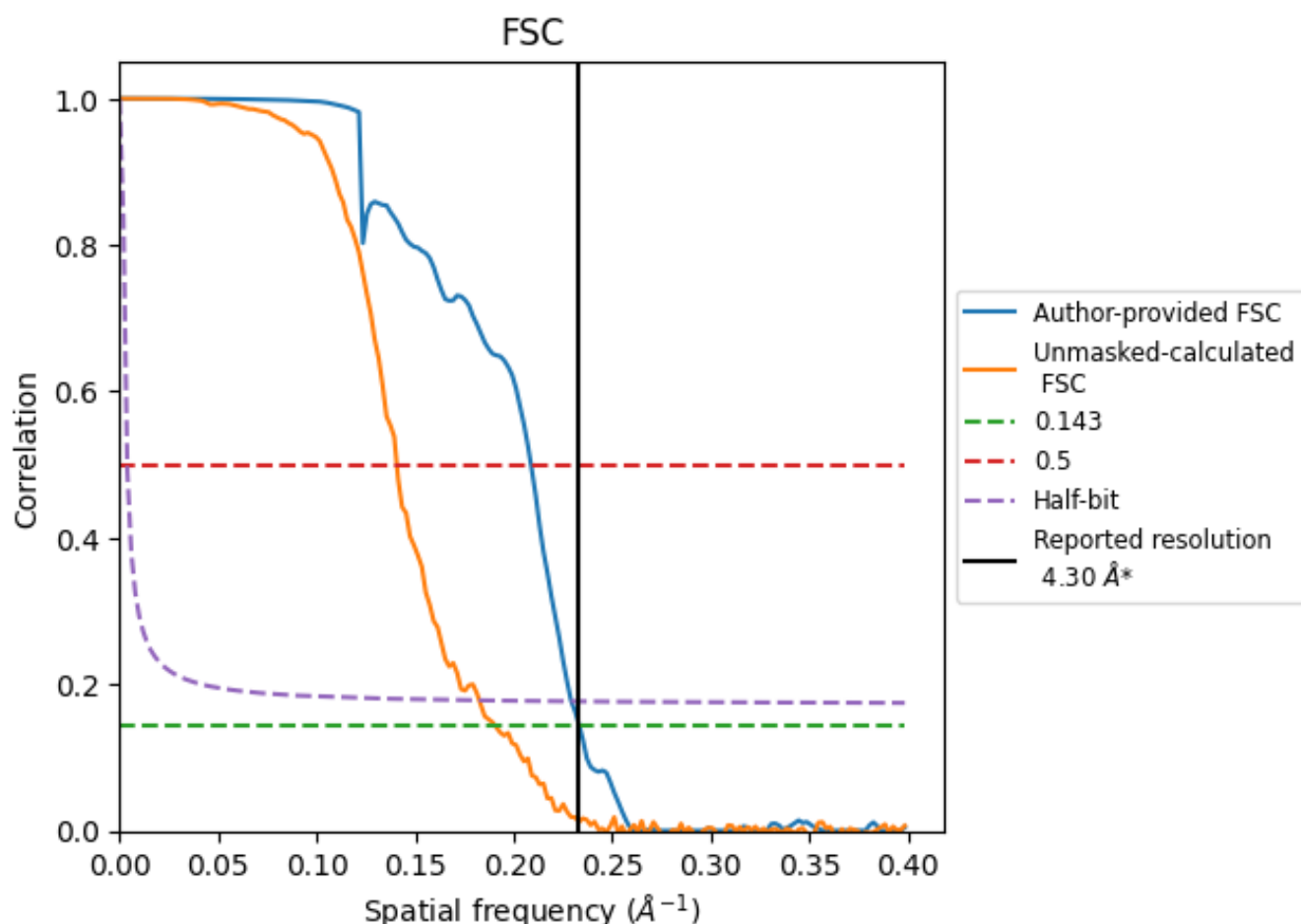


\*Reported resolution corresponds to spatial frequency of  $0.233 \text{ \AA}^{-1}$

## 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 0.233  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

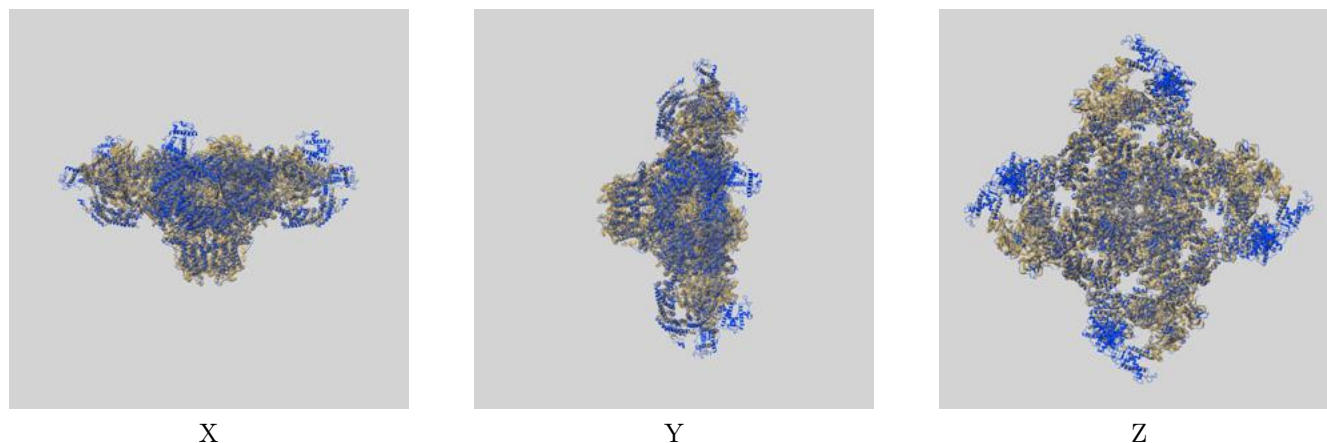
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.29	4.79	4.36
Unmasked-calculated*	5.25	7.11	5.48

\*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 5.25 differs from the reported value 4.3 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-8379 and PDB model 5TAM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

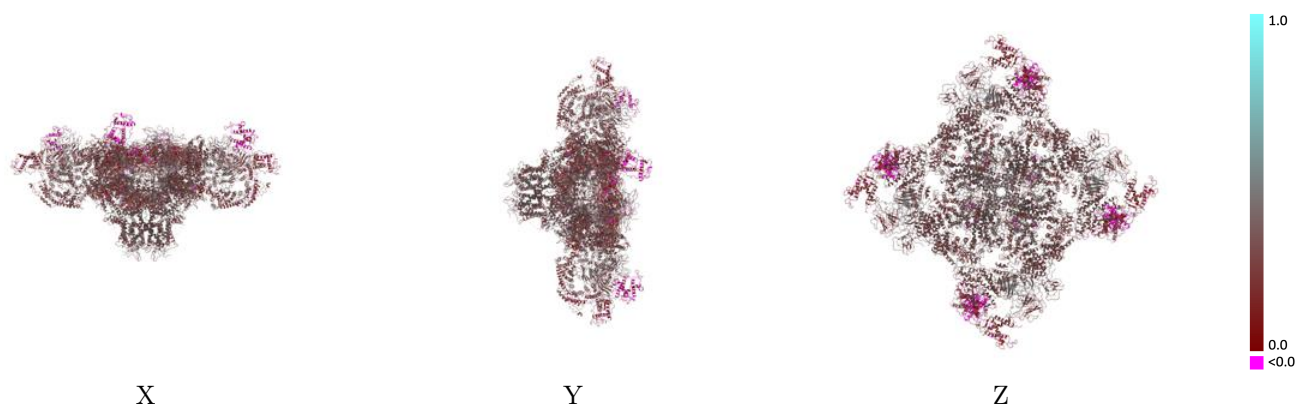
### 9.1 Map-model overlay [i](#)



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.

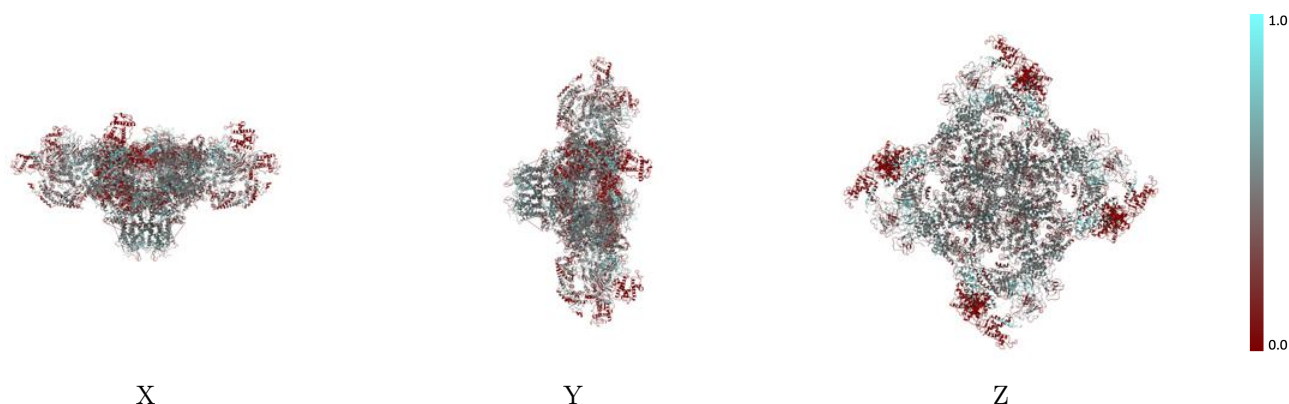


## 9.2 Q-score mapped to coordinate model [i](#)



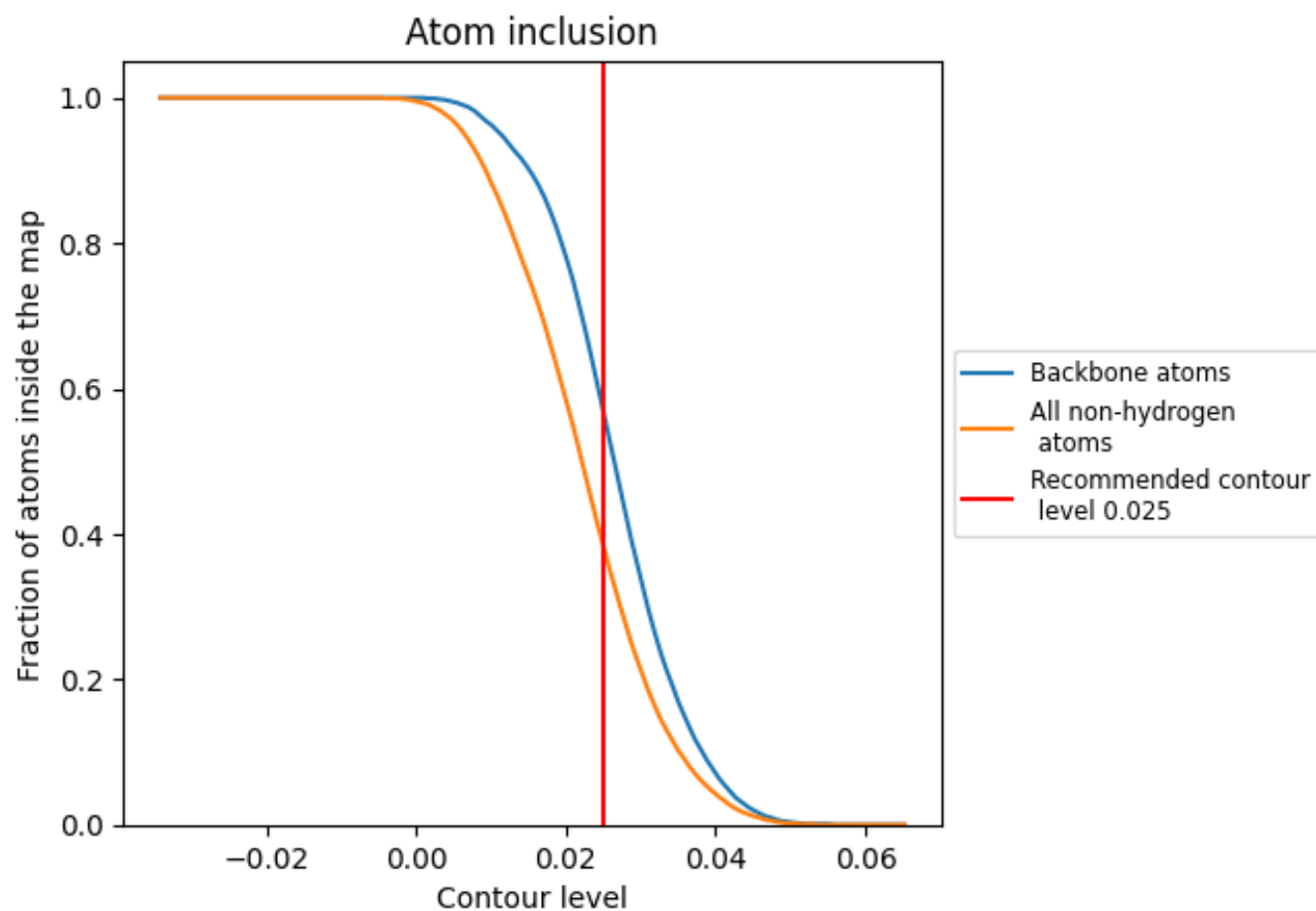
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 57% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	<div></div> 0.3840	<div></div> 0.3030
A	<div></div> 0.3520	<div></div> 0.3310
B	<div></div> 0.3850	<div></div> 0.3020
E	<div></div> 0.3850	<div></div> 0.3020
F	<div></div> 0.3570	<div></div> 0.3360
G	<div></div> 0.3850	<div></div> 0.3020
H	<div></div> 0.3540	<div></div> 0.3360
I	<div></div> 0.3840	<div></div> 0.3020
J	<div></div> 0.3560	<div></div> 0.3340

1.0

0.0

<0.0