



## wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 07:04 AM EST

PDB ID : 8DVE  
EMDB ID : EMD-27736  
Title : RyR1 in presence of IpCa-T26E phosphomimetic and activating ligands  
Authors : Haji-Ghassemi, O.; Van Petegm, F.  
Deposited on : 2022-07-28  
Resolution : 3.84 Å(reported)  
Based on initial model : 6M2W

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>.

---

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

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



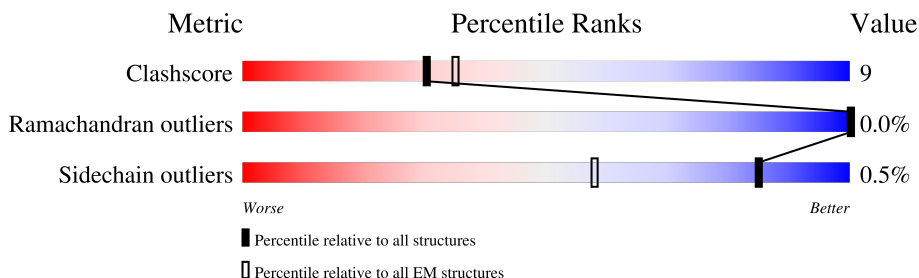
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.84 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	5037	<div> <div>6%</div> <div>66%</div> <div>12%</div> <div>22%</div> </div>
1	D	5037	<div> <div>10%</div> <div>64%</div> <div>14%</div> <div>22%</div> </div>
1	G	5037	<div> <div>7%</div> <div>65%</div> <div>13%</div> <div>22%</div> </div>
1	J	5037	<div> <div>11%</div> <div>64%</div> <div>15%</div> <div>22%</div> </div>
2	B	107	<div> <div>81%</div> <div>19%</div> </div>
2	E	107	<div> <div>79%</div> <div>21%</div> </div>
2	H	107	<div> <div>79%</div> <div>21%</div> </div>
2	K	107	<div> <div>71%</div> <div>29%</div> </div>

Continued on next page...



*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	C	149	<p>27% 91% 7%</p>
3	F	149	<p>58% 89% 7%</p>
3	I	149	<p>30% 84% 9% 7%</p>
3	L	149	<p>44% 88% 8%</p>



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 114229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	3942	Total	C	N	O	S	0	0
			26818	17244	4812	4614	148		
1	A	3943	Total	C	N	O	S	0	0
			27274	17556	4883	4676	159		
1	G	3944	Total	C	N	O	S	0	0
			27137	17456	4860	4662	159		
1	J	3943	Total	C	N	O	S	0	0
			26962	17331	4814	4668	149		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			743	475	132	133	3		
2	B	107	Total	C	N	O	S	0	0
			743	473	134	132	4		
2	H	107	Total	C	N	O	S	0	0
			745	474	134	134	3		
2	K	107	Total	C	N	O	S	0	0
			728	466	128	131	3		

- Molecule 3 is a protein called Calmodulin-1.

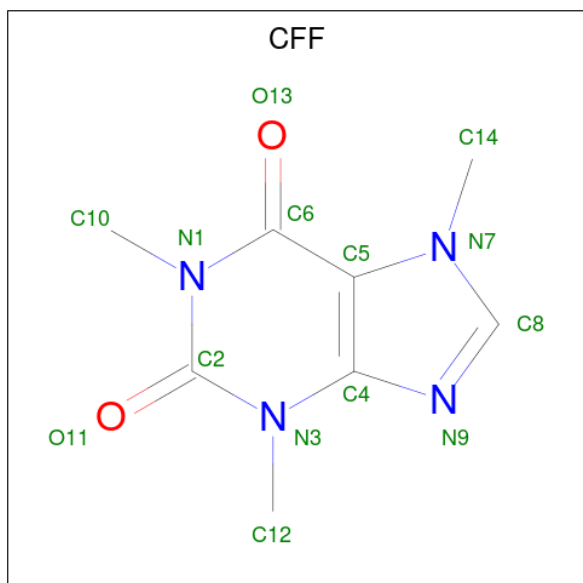
Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	138	Total	C	N	O	S	0	0
			715	437	138	139	1		
3	C	138	Total	C	N	O	S	0	0
			720	437	139	142	2		
3	I	138	Total	C	N	O	S	0	0
			730	447	140	142	1		
3	L	137	Total	C	N	O	S	0	0
			726	443	138	141	4		

There are 16 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

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



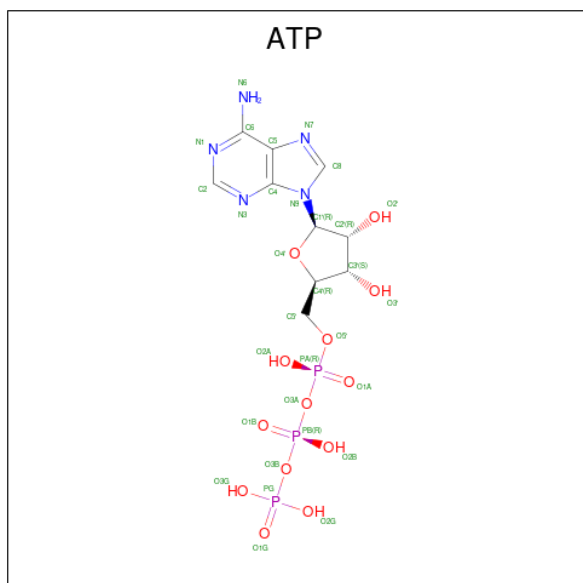
Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	4	2	
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	
4	J	1	Total	C	N	O	0
			14	8	4	2	



- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Ca	0
			1	1	
5	A	1	Total	Ca	0
			1	1	
5	G	1	Total	Ca	0
			1	1	
5	J	1	Total	Ca	0
			1	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	Zn 1	0
7	A	1	Total 1	Zn 1	0
7	G	1	Total 1	Zn 1	0
7	J	1	Total 1	Zn 1	0







L1115	L1120	L1122	L1123	F1124	N1125	G1126	Q1130	R1131	W1132	F1139	W1143	W1152	T1153	D1154	I1161	S1171	G1174	S1193	L1194	G1205	L1211	E1221	G1222	F1223	E1224	P1225	I1228	T1235	T1236	W1237	F1238	S1239	K1240	P1243	R1259	C1269	L1272	L1289	R1290								
L1291	P1294	A1121	F1297	R1302	CYS	THR	GLY	ALA	THR	ALA	PRO	GLY	ASN	LEU	GLN	PRO	GLU	ASP	GLU	ALA	ALA	PRO	ASP	TYR	GLU	ASN	LEU	ALA	ARG	SER	ALA	THR	GLN	GLY	TRP	PRO	GLY	ALA	GLU	ALA	GLY	GLY	THR	ALA	LYS	ASP	VAL
VAL	PRO	ALA	ASN	ARG	D1422	D1423	P1424	E1425	I1426	I1427	L1428	T1431	T1432	Y1433	Y1434	Y1435	S1446	C1447	V1448	G1451	W1452	F1464	D1465	L1466	D1478	E1479	Q1480	N1491	M1494	W1495	W1496	F1500	V1501	SER	PRO	GLY	GLN	GLN	GLY	ARG	SER	H1511	V1520	D1521	L1522	A1523	A1531
L1548	P1549	P1550	F1553	V1554	Q1563	F1564	E1565	L1566	Q1569	K1570	N1571	I1572	M1573	P1574	A1578	F1580	P1592	F1593	L1594	L1595	L1600	R1607	M1608	P1609	F1612	G1621	L1624	G1625	W1626	A1627	M1637	L1638	L1639	C1647	L1651	E1652	D1658	L1659	H1665	T1666	L1667						
V1673	L1676	V1681	S1687	H1688	V1689	Q1693	L1694	L1695	L1698	E1699	H1702	D1713	L1714	L1715	I1716	S1717	I1718	H1719	L1720	E1721	R1725	L1731	S1732	E1733	Y1734	I1735	L1738	T1742	I1745	T1746	L1747	P1750	GLY	ARG	LYS	GLY	ASN	ALA	ARG	R1759	H1760	G1761	L1762	L1771			
R1772	P1773	F1782	P1787	ALA	ALA	VAL	ALA	GLU	A1794	P1795	I1802	P1803	L1804	K1810	M1814	T1847	L1848	Y1850	M1851	G1852	I1853	F1854	L1863	I1866	F1871	T1872	E1873	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU		
LYS	GLU	ASP	GLU	GLU	GLU	GLU	GLU	GLU	ASP	ALA	GLU	LYS	GLU	PRO	GLY	LYS	GLU	ASP	E1923	Q1928	L1931	P1932	V1935	K1936	C1947	D1948	Q1949	Q1952	E1963	R1964	Y1965	V1966	R1982	A1988	A1989	E1990	T1995	S2000	Q2003								
E2004	Q2005	I2006	N2007	L2010	D2014	GLU	ALA	ASP	GLU	GLU	D2020	E2025	D2026	I2027	R2028	L2031	L2038	H2041	Q2045	LEU	GLY	GLU	GLU	GLU	GLU	THR	SER	LEU	SER	ARG	LEU	ARG	SER	LEU	GLU	THR	VAL	ARG	LEU	VAL	LYS	LYS	LYS	GLU	GLU		
LYS	PRO	GLU	GLU	LEU	PRO	ALA	GLU	GLU	LYS	P2091	L2094	V2103	R2104	Q2107	F2121	S2122	L2123	H2125	R2126	Q2127	Y2128	L2134	L2138	P2139	R2140	P2146	M2153	L2156	Q2161	L2165	M2178	S2181	Y2185	N2188	K2189	V2190	Q2193	M2203									
V2207	V2210	M2211	V2212	L2215	G2216	GLY	GLU	THR	LYS	E2222	F2225	V2229	T2230	F2235	F2251	Y2256	G2262	T2263	G2264	W2267	S2270	T2271	P2272	L2273	L2286	V2299	G2304	L2307	Q2308	S2309	C2310	P2311	M2312	D2320	N2324	M2324	G2327	L2332	R2336								
V2339	V2346	N2349	R2355	L2356	L2357	L2358	R2359	G2370	E2371	L2376	L2386	R2392	D2393	GLY	PRO	GLY	VAL	ARG	ASP	ARG	ARG	ARG	GLU	GLU	PRO	PRO	GLU	L2414	L2418	G2419	H2420	A2421	L2422	L2430	A2437	M2440	L2443	A2455	L2460								
L2463	I2476	P2477	THR	LEU	GLY	LYS	ASP	GLY	ALA	LEU	V2486	Q2487	P2488	K2489	M2490	S2491	V2495	P2496	D2497	A2500	V2503	L2504	F2505	D2507	R2508	V2509	Y2510	G2511	I2512	E2513	N2514	Q2515	F2517	L2518	L2519	H2520	V2521	L2522	D2523	F2526	M2546	N2551	R2552	Y2553	A2557	T2563	
P2567	L2568	F2569	A2570	Q2571	T2572	E2573	V2579	D2580	S2581	H2584	S2594	L2595	L2603	C2606	Y2613	M2618	H2621	R2624	R2625	F2628	D2629	V2630	P2631	N2634	K2638	N2646	Y2654	T2659	G2660	N2663	F2664	G2665	V2666	T2667	E2669	E2670	E2671	L2672	V2680	Q2681	T2682						



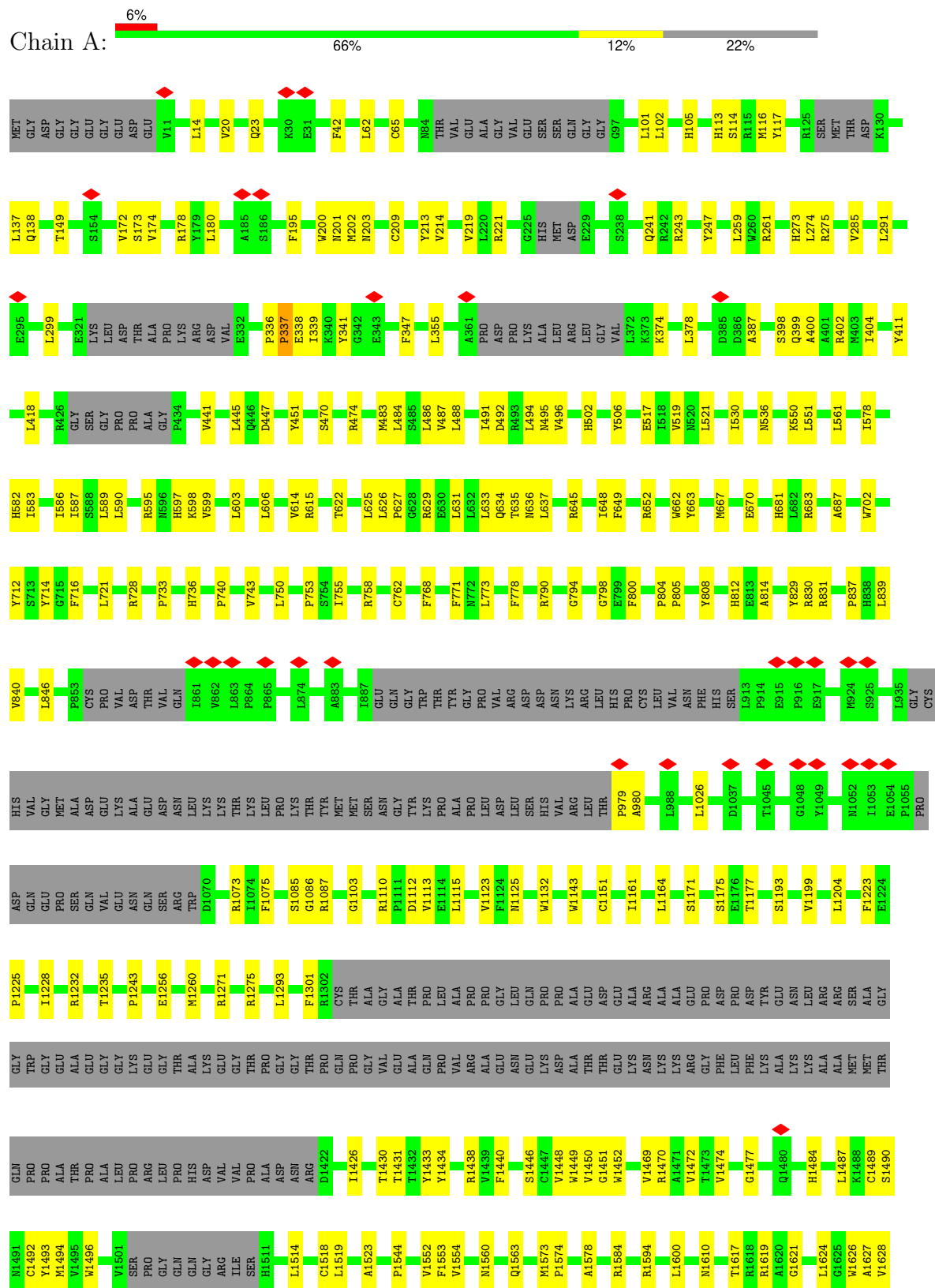
SER	PRO	SER	LEU	ARG	LYS	LYS	TRP	GLN	ARG	ALA	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
E3397	F3398	S3399	V3400	R3403	D3404	L3408	L3411	L3412	L3424	T3425	E3426	P3427	N3428	A3429	N3430	V3438	W3445	S3448	H3449	N3450	E3454	E3463	ILE	ASN	ASN	MET	SER	PHE	LEU	TRP	THR	ALA	ASP	SER	LYS	SER	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754	
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL	ASP	GLY	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	GLU	THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754
GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	TYR	ARG	GLY	LEU	VAL	GLN	THR	GLY	SER	TYR	GLY	GLU	GLU	GLU	ASP	ASP	PRO	PRO	ASP</																																							







• Molecule 1: Ryanodine receptor 1



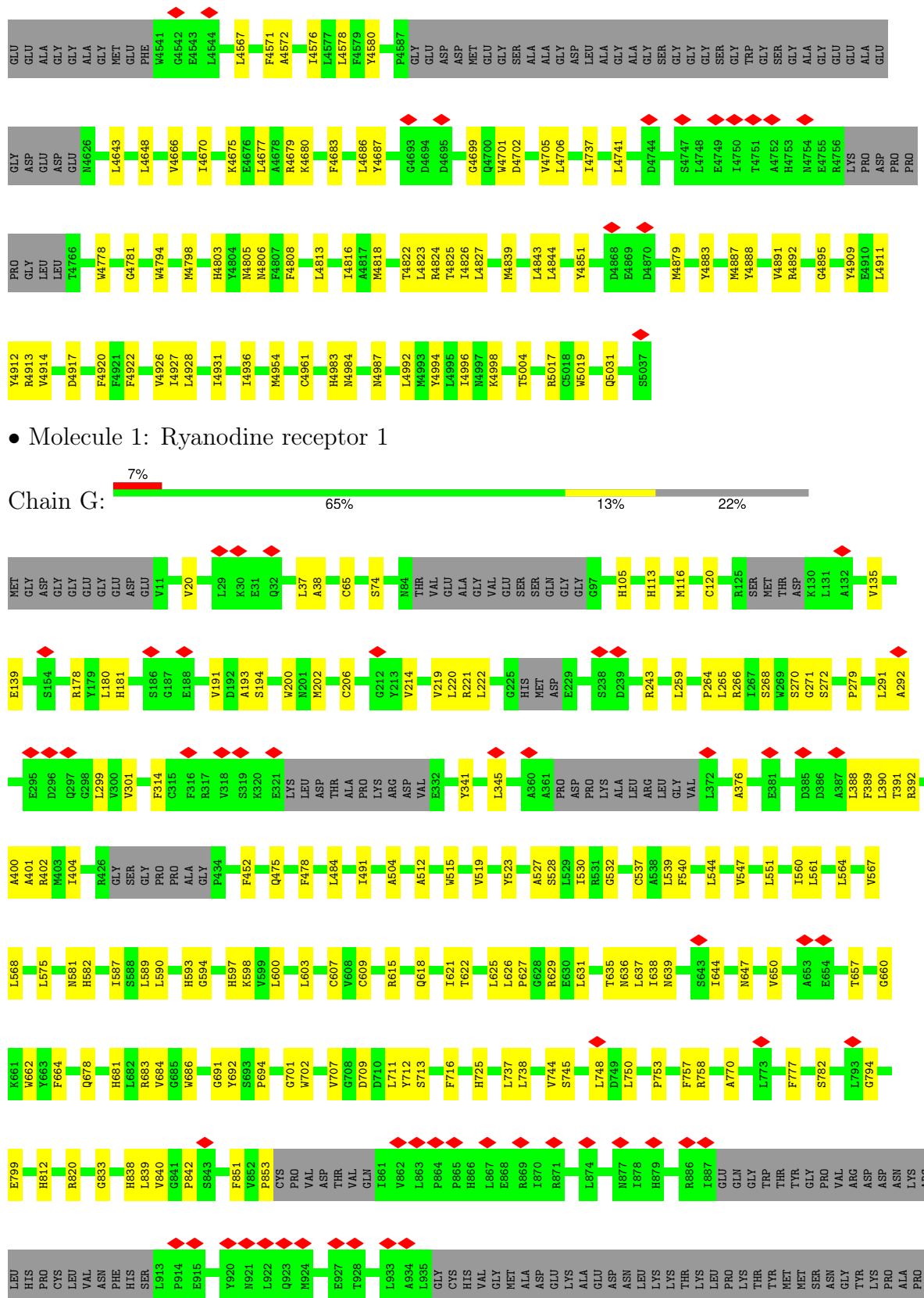


--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--









• Molecule 1: Ryanodine receptor 1
























H3771	I3662	GLY	R3337	ASP	S3174	MET	SER	T2912	R2852	R2792	GLU
I3772	H3667	LYS	Q3343	ILE	L3175	LYS	PRO	A2913	E2853	P2793	GLY
G3773	R3773	VAL	P3344	PRO	GLY	SER	H2991	K2914	G2854	Y2794	ASN
A3774	E3670	GLU	P3344	VAL	THR	THR	E2992	E2915	G2854	K2795	PHE
A3775	R3349	LYS	ASP	LEU	THR	PRO	Q2993	E2916	G2855	K2796	ASP
E3777	R3349	ASN	R3248	ASP	ASN	GLU	E2994	A2917	G2856	F2797	PRO
R3778	R3350	THR	A3257	THR	THR	ILE	I3001	R2918	P2857	F2797	ARG
V3779	P3351	TYR	GLU	GLY	TYR	VAL	L3002	R2919	Q2858	S2798	PRO
Q3780	E3376	VAL	GLY	SER	VAL	GLU	L3002	D2919	P2859	S2799	GLU
L3780	E3376	LYS	GLY	GLY	LYS	LYS	P3004	E2920	R2860	K2800	LEU
K3821	E3377	LEU	ALA	ALA	R3187	LEU	N3007	E2921	D2861	D2801	ASN
F3829	Q3378	ARG	TYR	ARG	L3190	GLY	F3010	K2922	L2862	K2802	VAL
L3842	Q3379	THR	GLU	THR	A3199	THR	F3010	Q2924	S2863	E2803	ILE
K3851	Q3379	GLU	MET	MET	ALA	THR	S3019	L2926	G2864	I2804	ILE
A3852	LEU	GLU	P3267	P3267	ALA	THR	S3019	L2927	T2866	Y2805	
A3853	ALA	GLU	M3276	M3276	ALA	PRO	ALA	K2928	L2867	R2806	
L3856	ALA	GLU	V3284	V3284	VAL	LYS	VAL	F2929	R2868	P2808	
I3862	ALA	GLU	TRP	TRP	PHE	VAL	VAL	K2930	R2869	L2809	
I3867	ALA	GLU	GLU	GLU	LEU	LEU	LEU	L2930	E2870	K2810	
I3868	ALA	GLU	GLU	GLU	GLU	GLY	GLY	Q2931	L2871	E2811	
I3869	ALA	GLU	GLU	GLU	GLU	GLY	GLY	K2932	L2872	S2812	
I3870	ALA	GLU	GLU	GLU	GLU	GLY	GLY	M2874	Q2873	L2813	
M3875	ALA	GLU	GLU	GLU	GLU	GLY	GLY	E2935	A2875	K2814	
Q3882	ALA	GLU	GLU	GLU	GLU	GLY	GLY	A2936	E2876	A2815	
Q3889	ALA	GLU	GLU	GLU	GLU	GLY	GLY	V2937	E2877	M2816	
L3890	ALA	GLU	GLU	GLU	GLU	GLY	GLY	T2938	Q2877	L2817	
E3893	ALA	GLU	GLU	GLU	GLU	GLY	GLY	R2939	L2878	A2818	
F3899	ALA	GLU	GLU	GLU	GLU	GLY	GLY	E2880	A2879	W2819	
Y3902	ALA	GLU	GLU	GLU	GLU	GLY	GLY	E2881	E2880	E2820	
L3903	ALA	GLU	GLU	GLU	GLU	GLY	GLY	L2881	E2881	E2821	
R3904	ALA	GLU	GLU	GLU	GLU	GLY	GLY	Y2882	Y2882	T2822	
Q3906	ALA	GLU	GLU	GLU	GLU	GLY	GLY	M2883	M2883	I2823	
T3907	ALA	GLU	GLU	GLU	GLU	GLY	GLY	L2884	E2824	K2825	
T3910	ALA	GLU	GLU	GLU	GLU	GLY	GLY	T2885	E2825	A2826	
L3923	ALA	GLU	GLU	GLU	GLU	GLY	GLY	W2886	W2886	R2827	
Q3927	ALA	GLU	GLU	GLU	GLU	GLY	GLY	G2887	G2887	R2827	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	R2888	R2888	I2771	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	K2889	K2889	Q2772	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	E2890	E2890	R2773	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	K2891	K2891	W2774	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	Q2892	Q2892	W2775	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	E2893	E2893	S2776	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	L2894	L2894	Y2777	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	E2895	E2895	Q2778	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	A2896	A2896	E2779	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	K2897	K2897	W2780	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	G2898	G2898	V2781	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	E2899	E2899	K2782	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	G2900	G2900	E2783	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	T2901	T2901	E2784	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	H2902	H2902	L2785	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	P2903	P2903	K2786	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	L2904	L2904	T2787	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	V2906	V2906	H2788	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	P2907	P2907	P2789	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	Y2908	Y2908	W2790	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	T2910	T2910	L2791	
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	D2909	D2909		
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	T2848	T2848		
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	D2850	D2850		
	ALA	GLU	GLU	GLU	GLU	GLY	GLY	P2851	P2851		








- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B:  81% 19%



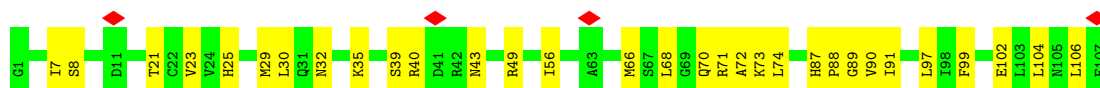
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:  79% 21%



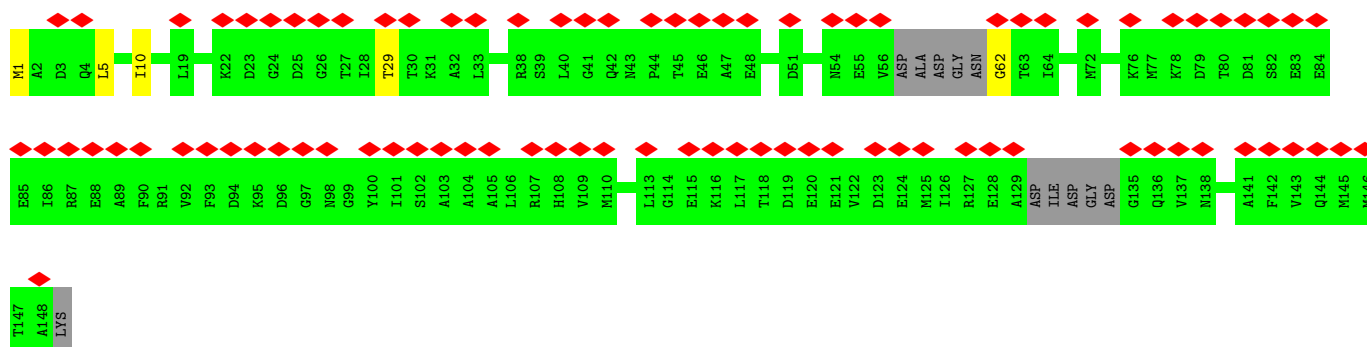
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:  71% 29%




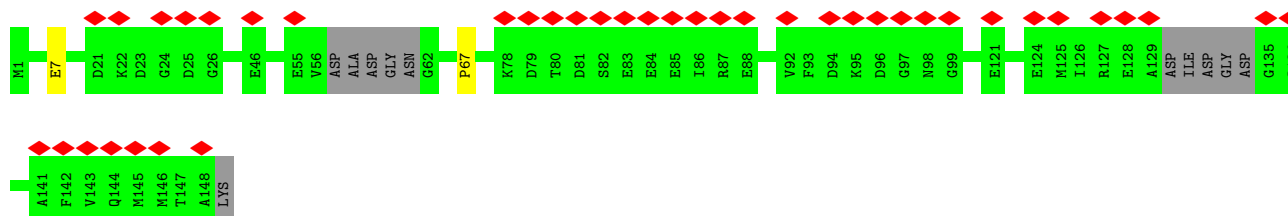
- Molecule 3: Calmodulin-1

Chain F:  58% 89% 7%




- Molecule 3: Calmodulin-1

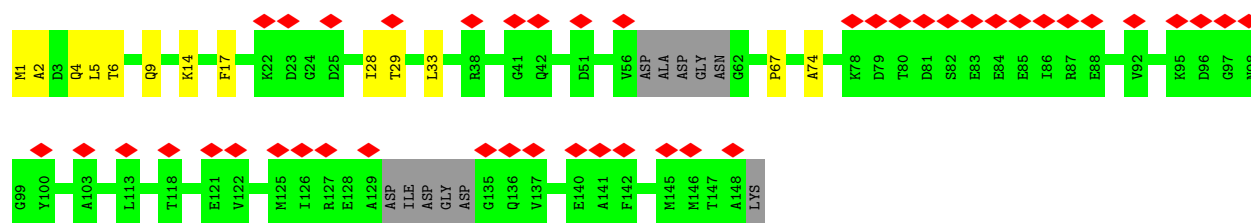
Chain C:  27% 91% 7%




- Molecule 3: Calmodulin-1

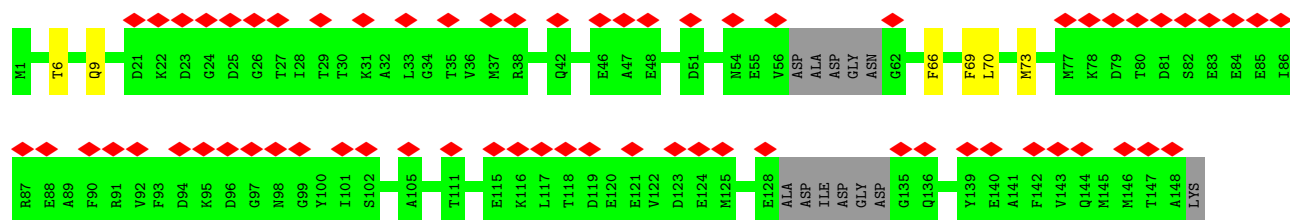


Chain I: 



• Molecule 3: Calmodulin-1

Chain L: 





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	481.28, 481.28, 481.28	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/27849	0.47	0/38070
1	D	0.27	0/27383	0.47	0/37497
1	G	0.26	0/27706	0.47	0/37888
1	J	0.26	0/27526	0.47	0/37679
2	B	0.26	0/758	0.51	0/1032
2	E	0.30	0/758	0.50	0/1033
2	H	0.32	0/761	0.54	0/1036
2	K	0.25	0/744	0.51	0/1018
3	C	0.24	0/720	0.37	0/993
3	F	0.24	0/716	0.37	0/989
3	I	0.24	0/731	0.36	0/1007
3	L	0.24	0/727	0.38	0/1001
All	All	0.26	0/116379	0.47	0/159243

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	27274	0	23938	406	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	26818	0	23065	467	0
1	G	27137	0	23674	449	0
1	J	26962	0	23301	513	0
2	B	743	0	703	12	0
2	E	743	0	703	17	0
2	H	745	0	694	17	0
2	K	728	0	670	21	0
3	C	720	0	401	2	0
3	F	715	0	391	3	0
3	I	730	0	421	8	0
3	L	726	0	425	3	0
4	A	14	0	10	0	0
4	D	14	0	10	0	0
4	G	14	0	10	1	0
4	J	14	0	10	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
6	A	31	0	12	0	0
6	D	31	0	12	2	0
6	G	31	0	12	4	0
6	J	31	0	12	2	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	114229	0	98474	1865	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 9.

The worst 5 of 1865 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4577:LEU:HD12	1:D:4580:TYR:HE2	1.12	1.10
1:D:4577:LEU:HD12	1:D:4580:TYR:CE2	1.96	1.00
1:J:4017:LEU:HD12	1:J:4139:ILE:HG21	1.50	0.92
2:H:10:GLY:HA3	2:H:70:GLN:HB2	1.53	0.91
1:D:4577:LEU:CD1	1:D:4580:TYR:HE2	1.85	0.90



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	3853/5037 (76%)	3782 (98%)	68 (2%)	3 (0%)	48	80
1	D	3852/5037 (76%)	3792 (98%)	60 (2%)	0	100	100
1	G	3854/5037 (76%)	3797 (98%)	57 (2%)	0	100	100
1	J	3853/5037 (76%)	3778 (98%)	75 (2%)	0	100	100
2	B	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	E	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	H	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	K	105/107 (98%)	104 (99%)	1 (1%)	0	100	100
3	C	132/149 (89%)	131 (99%)	1 (1%)	0	100	100
3	F	132/149 (89%)	131 (99%)	1 (1%)	0	100	100
3	I	132/149 (89%)	131 (99%)	1 (1%)	0	100	100
3	L	131/149 (88%)	128 (98%)	3 (2%)	0	100	100
All	All	16359/21172 (77%)	16079 (98%)	277 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	PRO
1	A	2859	PRO
1	A	2857	PRO

### 5.3.2 Protein sidechains [i](#)

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



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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2211/4276 (52%)	2202 (100%)	9 (0%)	89	91
1	D	2095/4276 (49%)	2077 (99%)	18 (1%)	75	83
1	G	2176/4276 (51%)	2165 (100%)	11 (0%)	86	90
1	J	2139/4276 (50%)	2130 (100%)	9 (0%)	89	91
2	B	68/88 (77%)	68 (100%)	0	100	100
2	E	68/88 (77%)	68 (100%)	0	100	100
2	H	68/88 (77%)	68 (100%)	0	100	100
2	K	65/88 (74%)	65 (100%)	0	100	100
3	C	11/123 (9%)	11 (100%)	0	100	100
3	F	9/123 (7%)	9 (100%)	0	100	100
3	I	13/123 (11%)	13 (100%)	0	100	100
3	L	15/123 (12%)	15 (100%)	0	100	100
All	All	8938/17948 (50%)	8891 (100%)	47 (0%)	85	90

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3679	LYS
1	G	4792	LEU
1	G	3721	LEU
1	G	3763	LEU
1	G	4865	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	3889	GLN
1	J	705	ASN
1	G	4009	GLN
1	J	138	GLN
1	J	1678	ASN

### 5.3.3 RNA ⓘ

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$
4	CFF	J	5101	-	8,15,15	1.18	1 (12%)	8,23,23	2.66	3 (37%)
6	ATP	J	5103	-	28,33,33	0.62	0	34,52,52	0.81	2 (5%)
4	CFF	G	5101	-	8,15,15	1.17	1 (12%)	8,23,23	2.66	3 (37%)
6	ATP	D	5103	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
6	ATP	A	5103	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
6	ATP	G	5103	-	28,33,33	0.63	0	34,52,52	0.62	1 (2%)
4	CFF	A	5101	-	8,15,15	1.17	1 (12%)	8,23,23	2.64	3 (37%)
4	CFF	D	5101	-	8,15,15	1.17	1 (12%)	8,23,23	2.64	3 (37%)

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
4	CFF	J	5101	-	-	-	0/2/2/2
6	ATP	J	5103	-	-	9/18/38/38	0/3/3/3
4	CFF	D	5101	-	-	-	0/2/2/2
4	CFF	G	5101	-	-	-	0/2/2/2
6	ATP	D	5103	-	-	7/18/38/38	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	G	5103	-	-	5/18/38/38	0/3/3/3
4	CFF	A	5101	-	-	-	0/2/2/2
6	ATP	A	5103	-	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5101	CFF	C6-N1	2.88	1.42	1.38
4	D	5101	CFF	C6-N1	2.86	1.42	1.38
4	G	5101	CFF	C6-N1	2.85	1.42	1.38
4	A	5101	CFF	C6-N1	2.83	1.42	1.38

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	5101	CFF	C5-C6-N1	-5.60	112.51	118.20
4	D	5101	CFF	C5-C6-N1	-5.51	112.60	118.20
4	A	5101	CFF	C5-C6-N1	-5.51	112.60	118.20
4	G	5101	CFF	C5-C6-N1	-5.47	112.65	118.20
4	D	5101	CFF	C4-C5-C6	3.88	122.91	119.96

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	5103	ATP	PB-O3B-PG-O3G
6	D	5103	ATP	C5'-O5'-PA-O1A
6	D	5103	ATP	C5'-O5'-PA-O3A
6	G	5103	ATP	O4'-C4'-C5'-O5'
6	J	5103	ATP	PB-O3B-PG-O2G

There are no ring outliers.

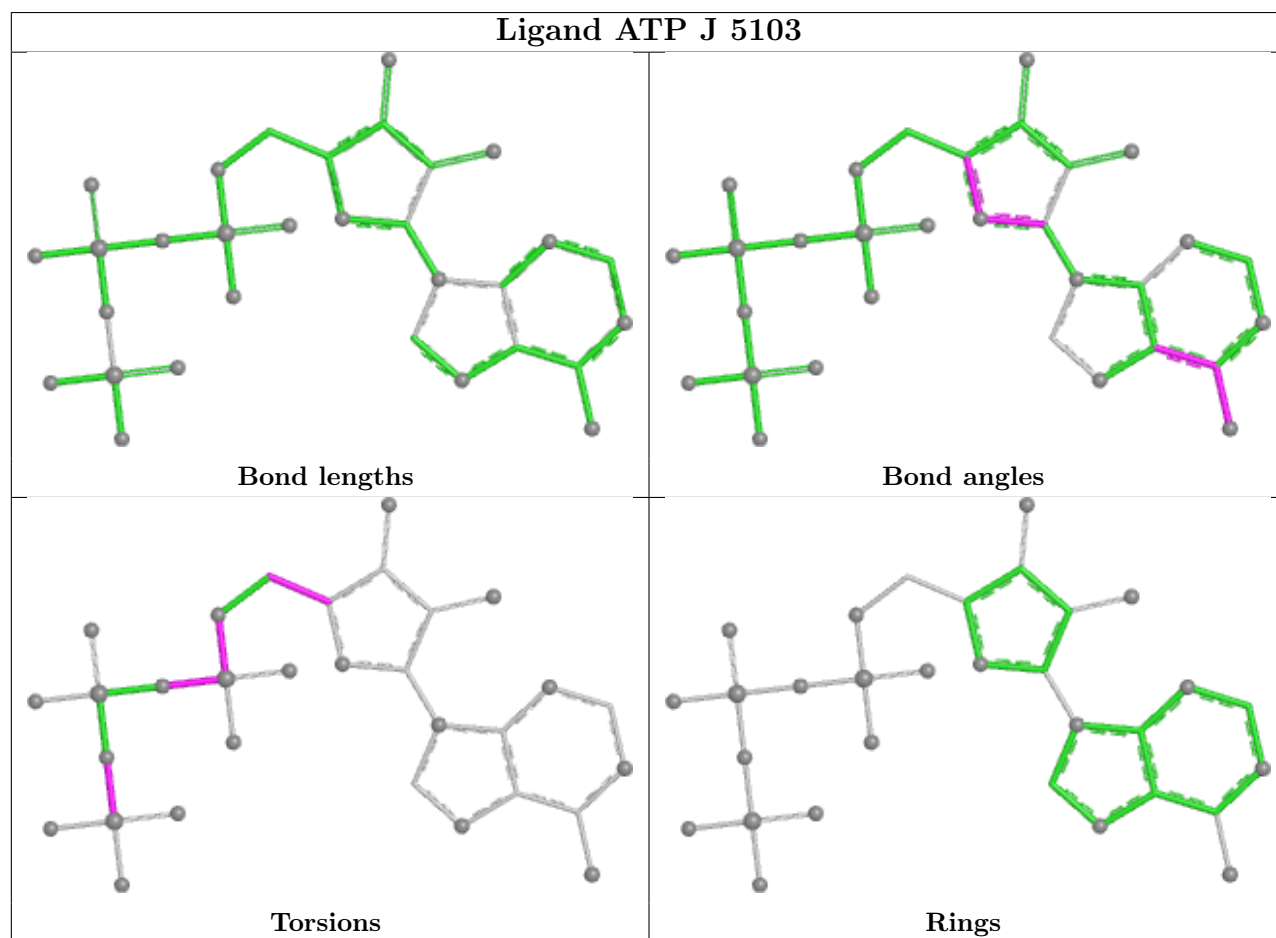
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	5103	ATP	2	0
4	G	5101	CFF	1	0
6	D	5103	ATP	2	0
6	G	5103	ATP	4	0

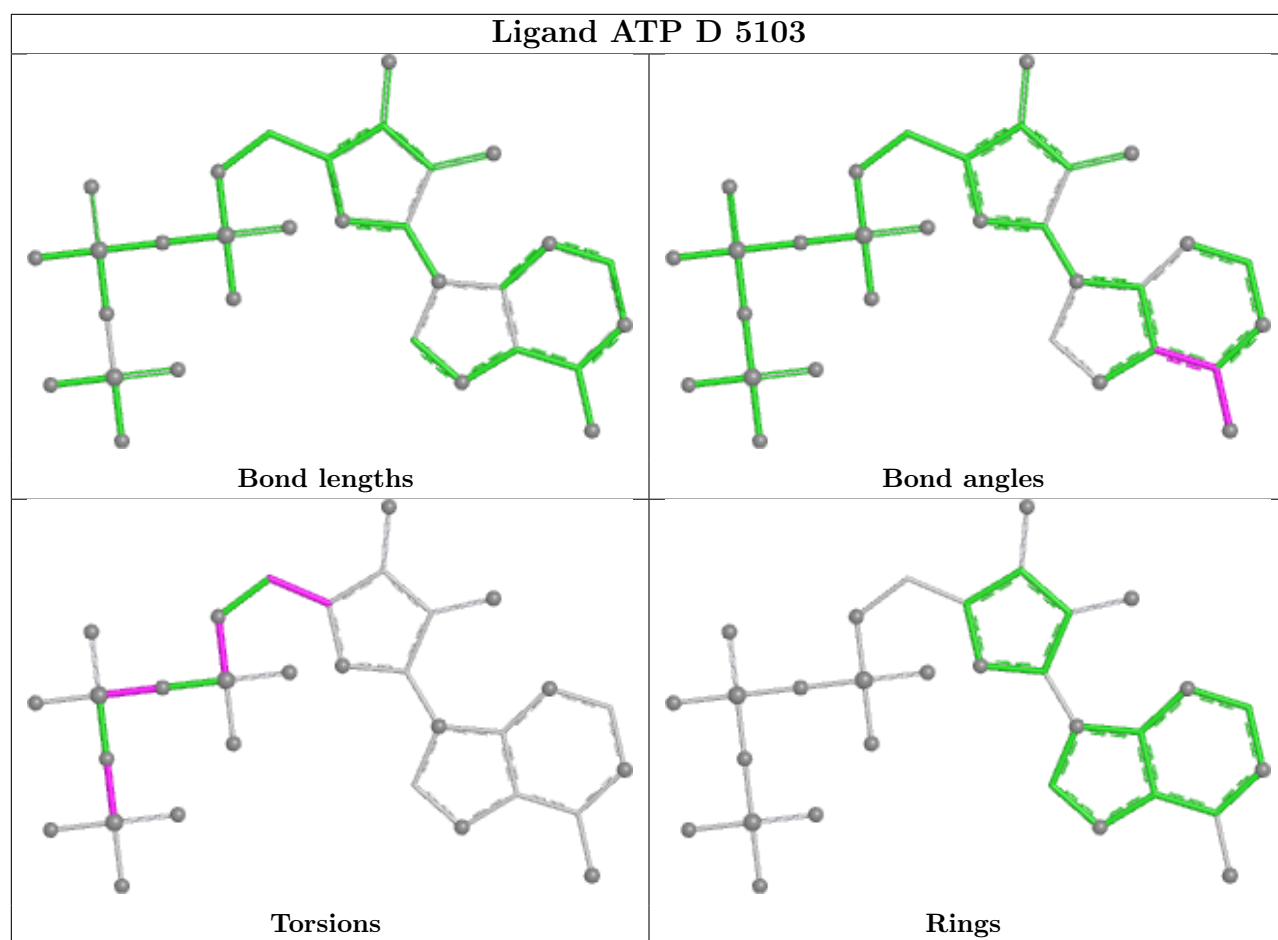
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



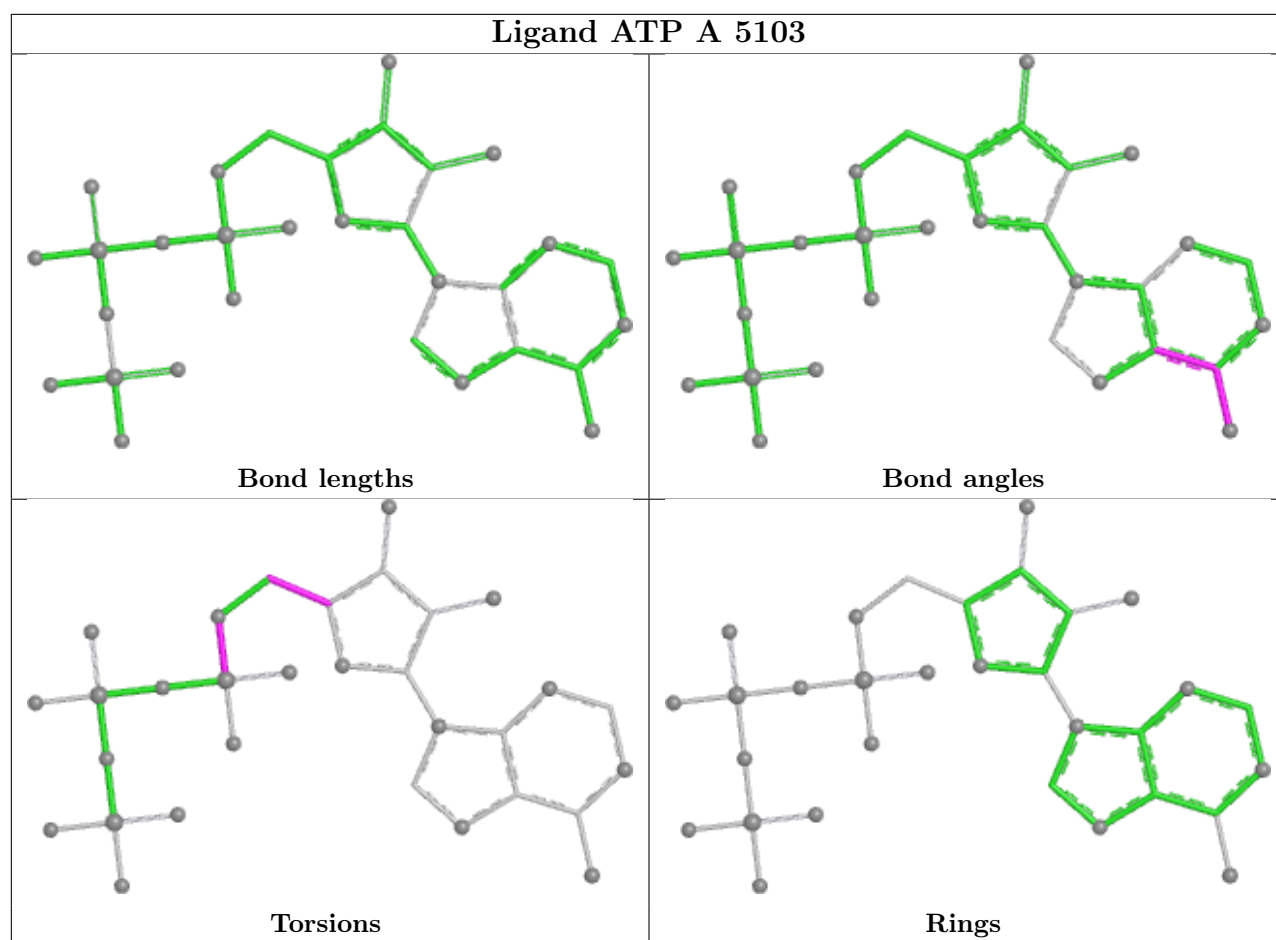
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



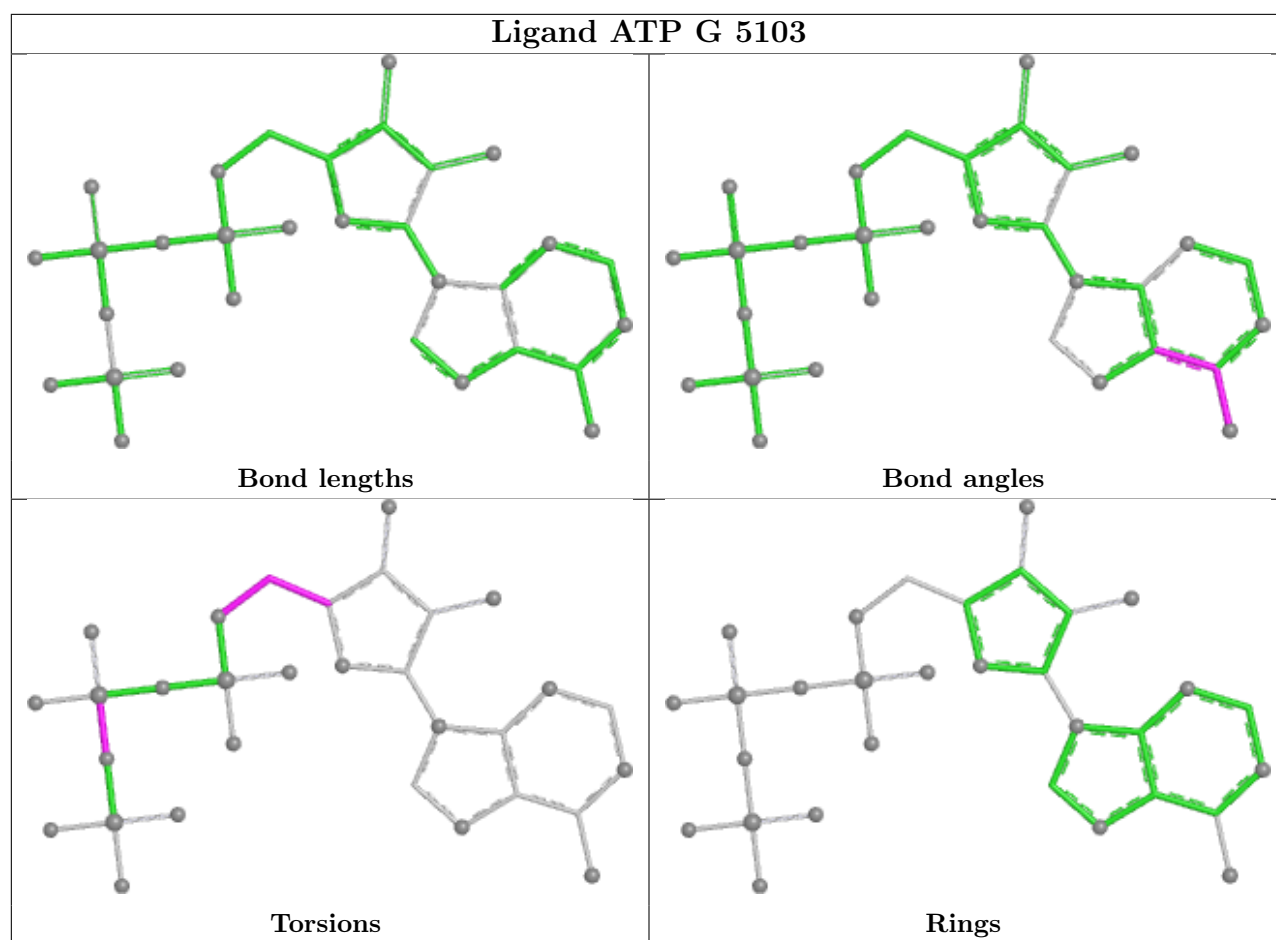












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



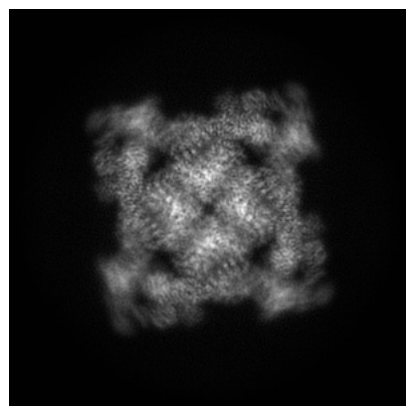
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27736. These allow visual inspection of the internal detail of the map and identification of artifacts.

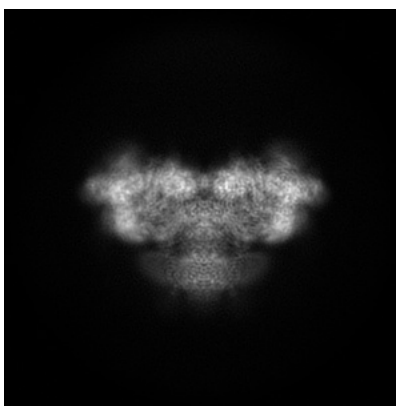
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

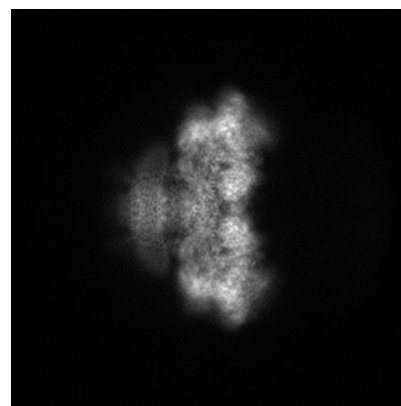
#### 6.1.1 Primary map



X

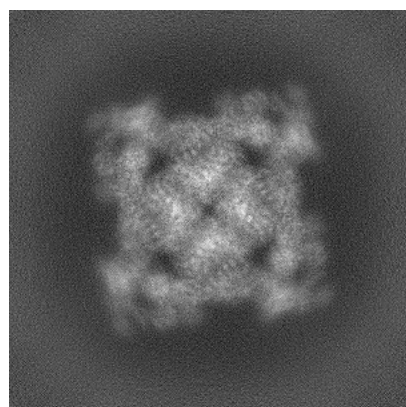


Y

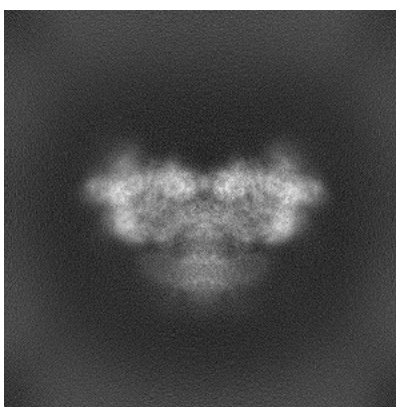


Z

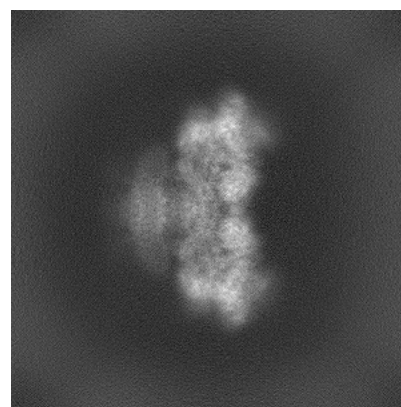
#### 6.1.2 Raw map



X



Y



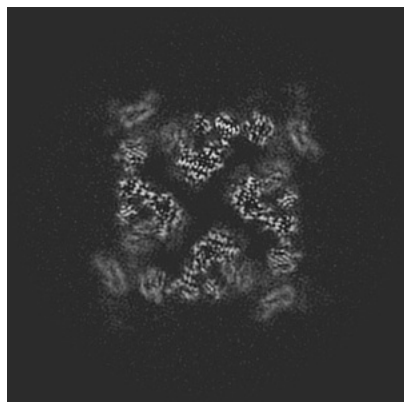
Z

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

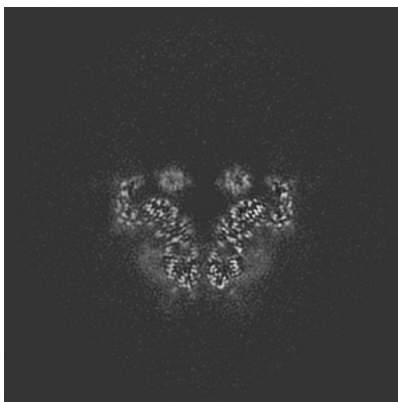


## 6.2 Central slices [i](#)

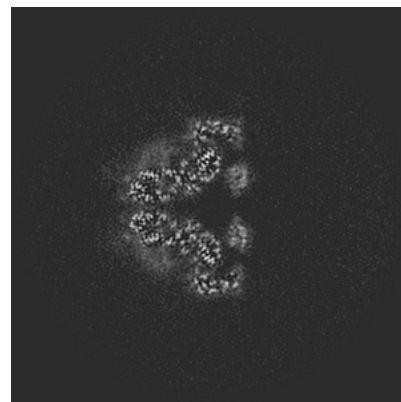
### 6.2.1 Primary map



X Index: 256

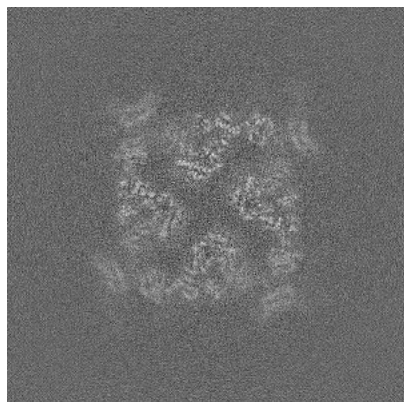


Y Index: 256

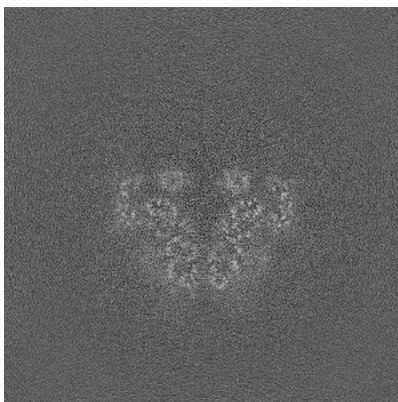


Z Index: 256

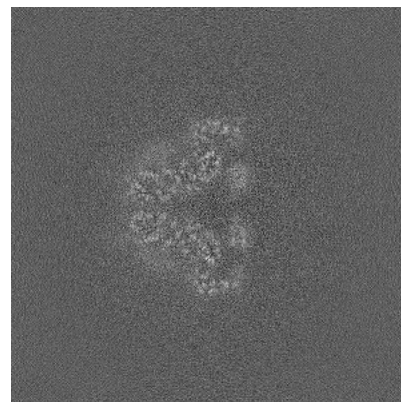
### 6.2.2 Raw map



X Index: 256



Y Index: 256



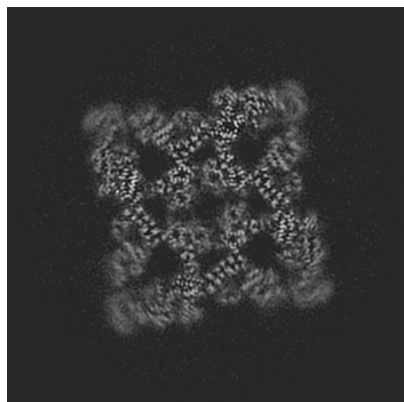
Z Index: 256

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

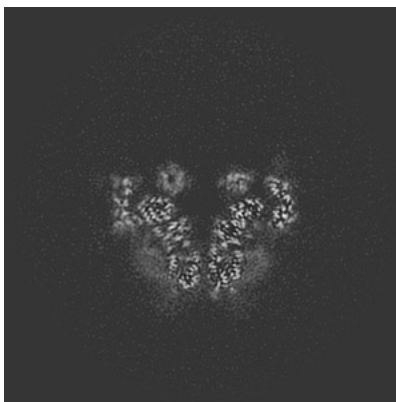


## 6.3 Largest variance slices [i](#)

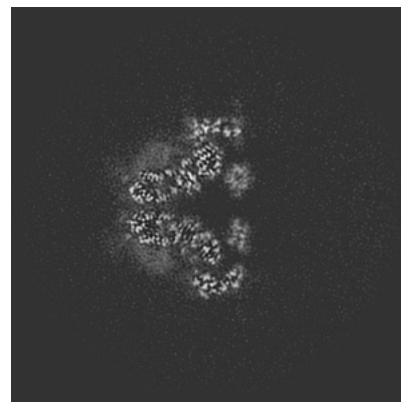
### 6.3.1 Primary map



X Index: 281

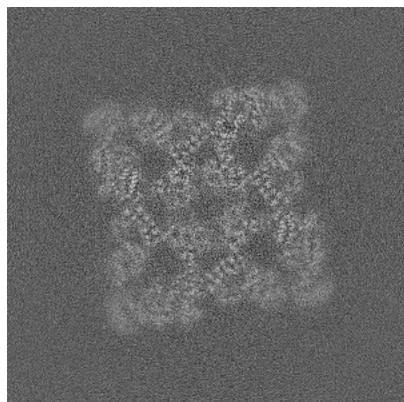


Y Index: 253

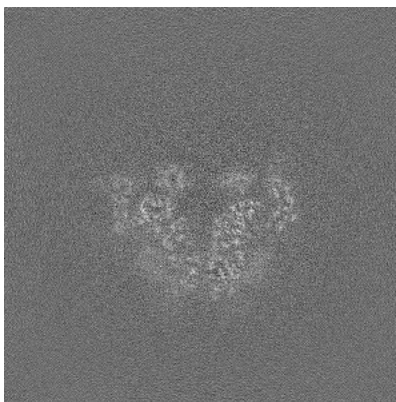


Z Index: 254

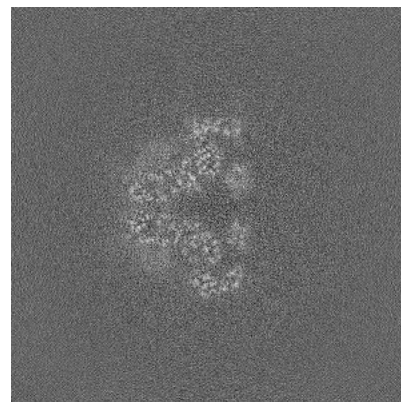
### 6.3.2 Raw map



X Index: 281



Y Index: 251



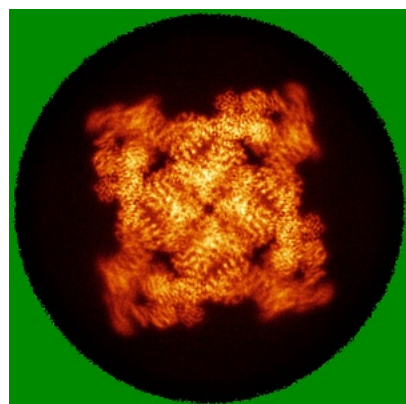
Z Index: 254

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

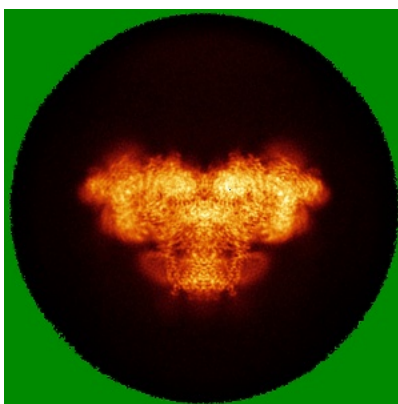


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

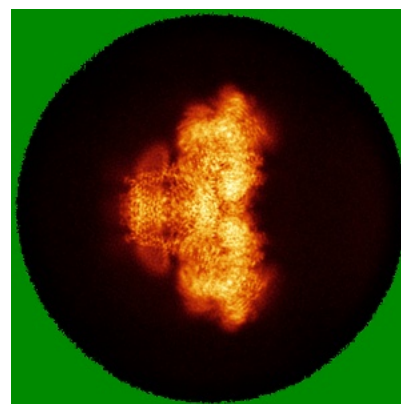
### 6.4.1 Primary map



X

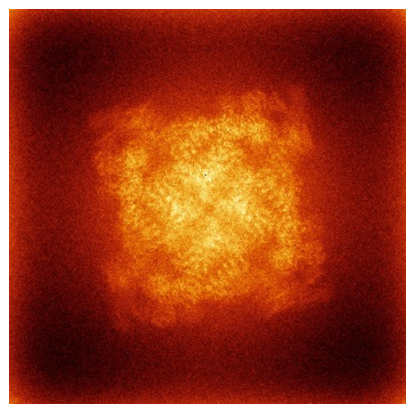


Y

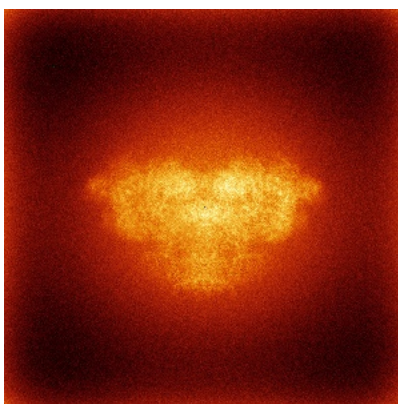


Z

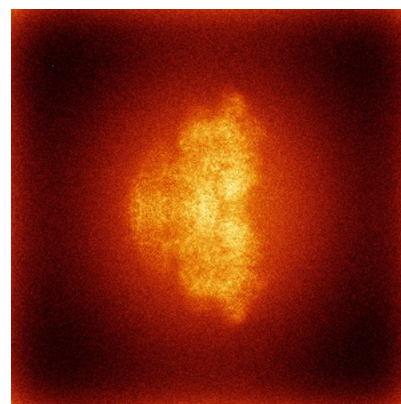
### 6.4.2 Raw map



X



Y



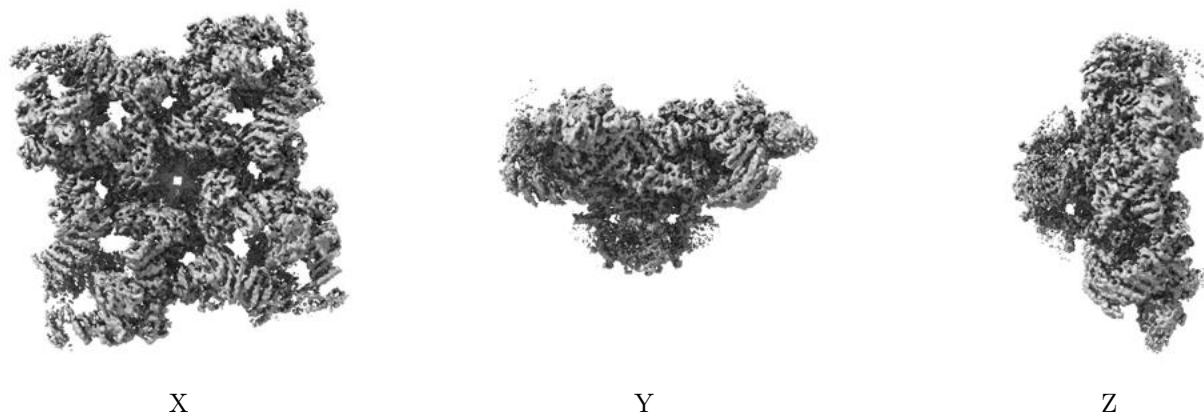
Z

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.



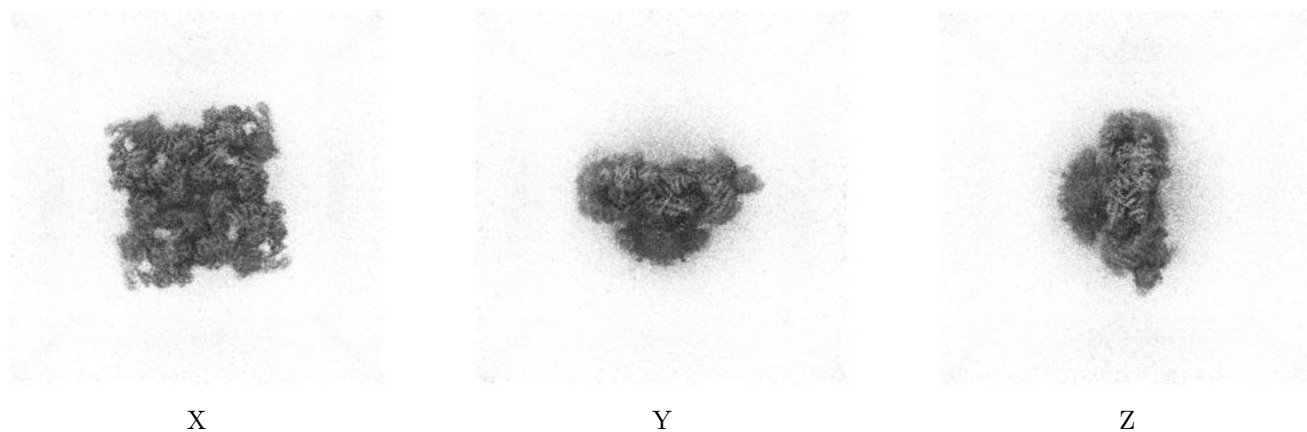
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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](#)

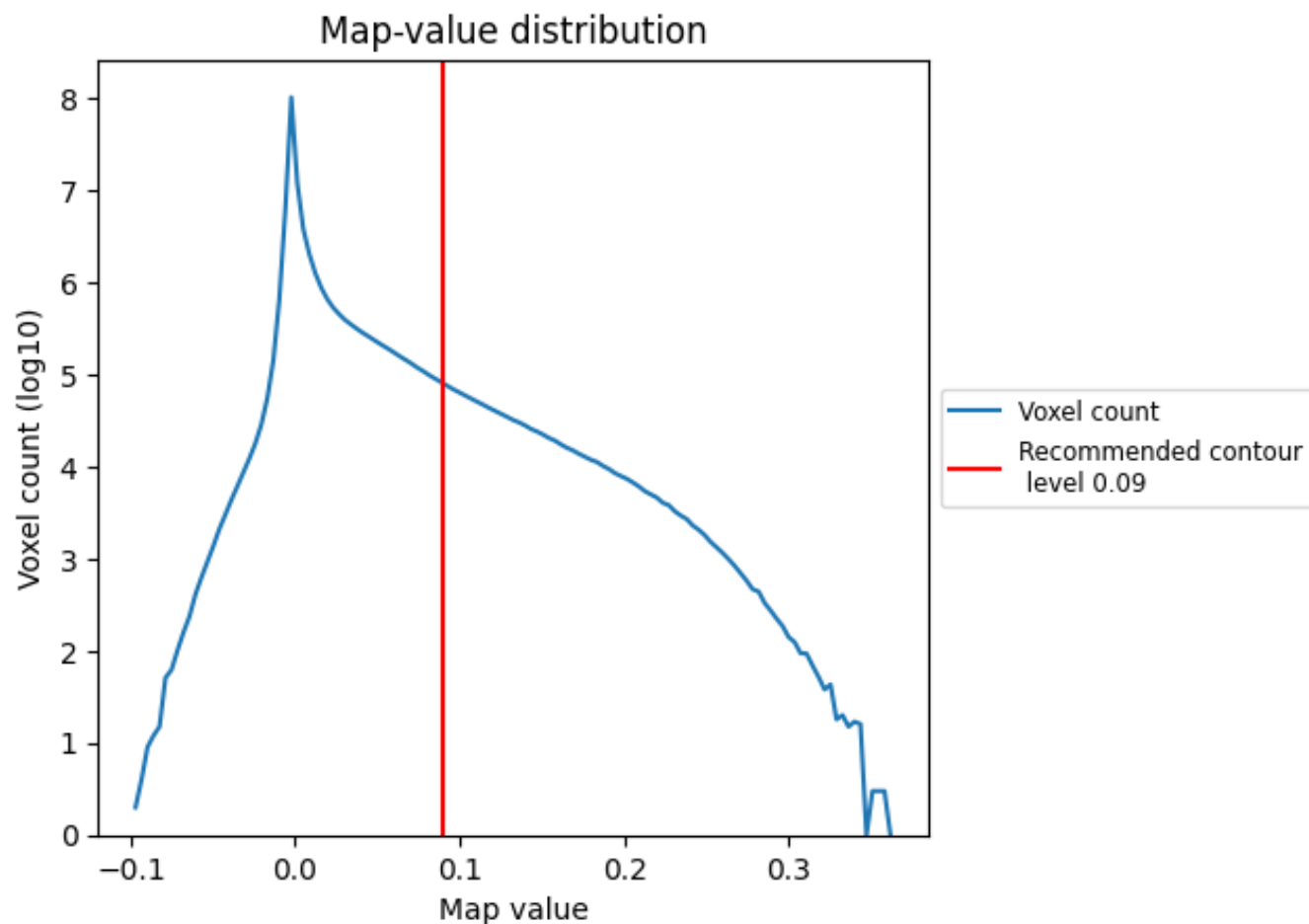
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

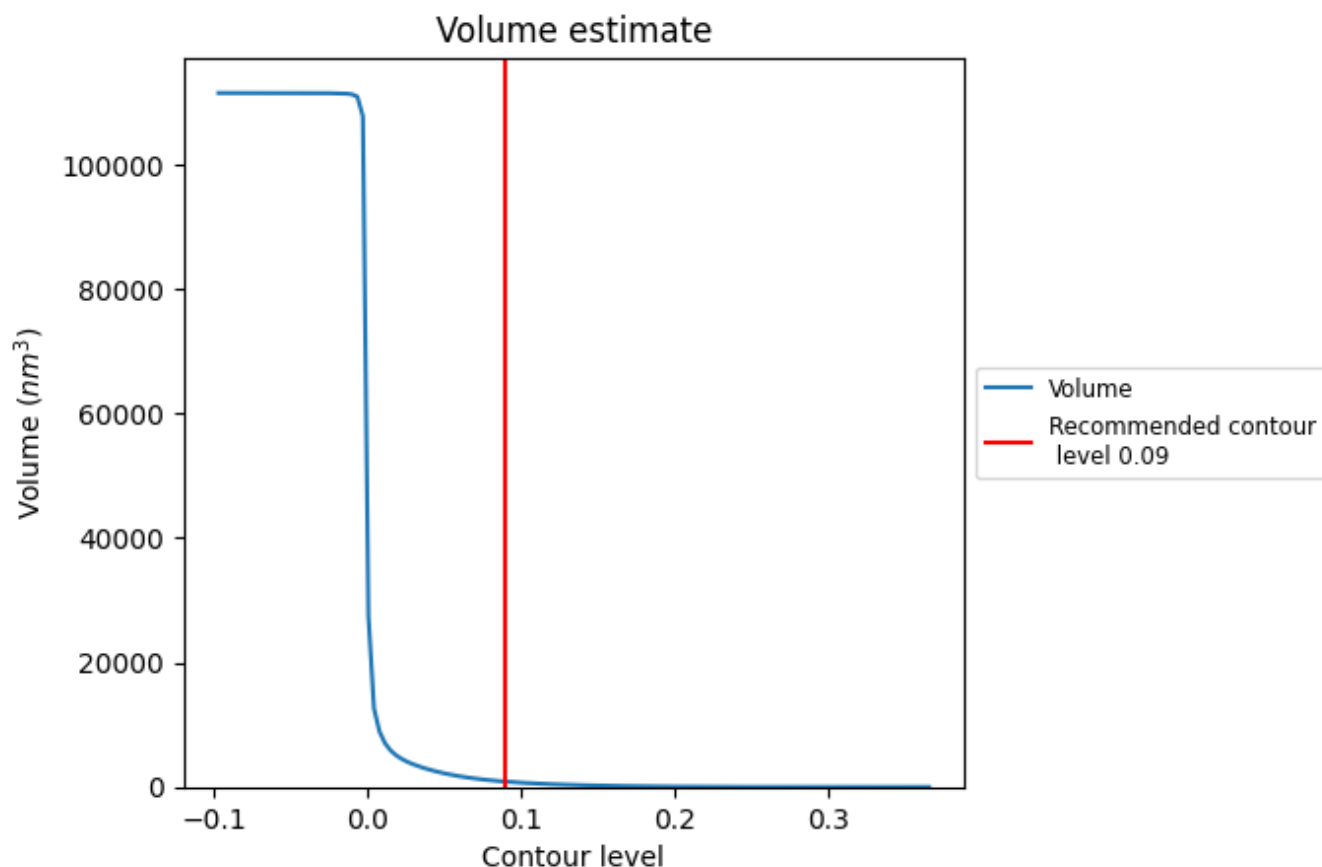
### 7.1 Map-value distribution [i](#)



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](#)

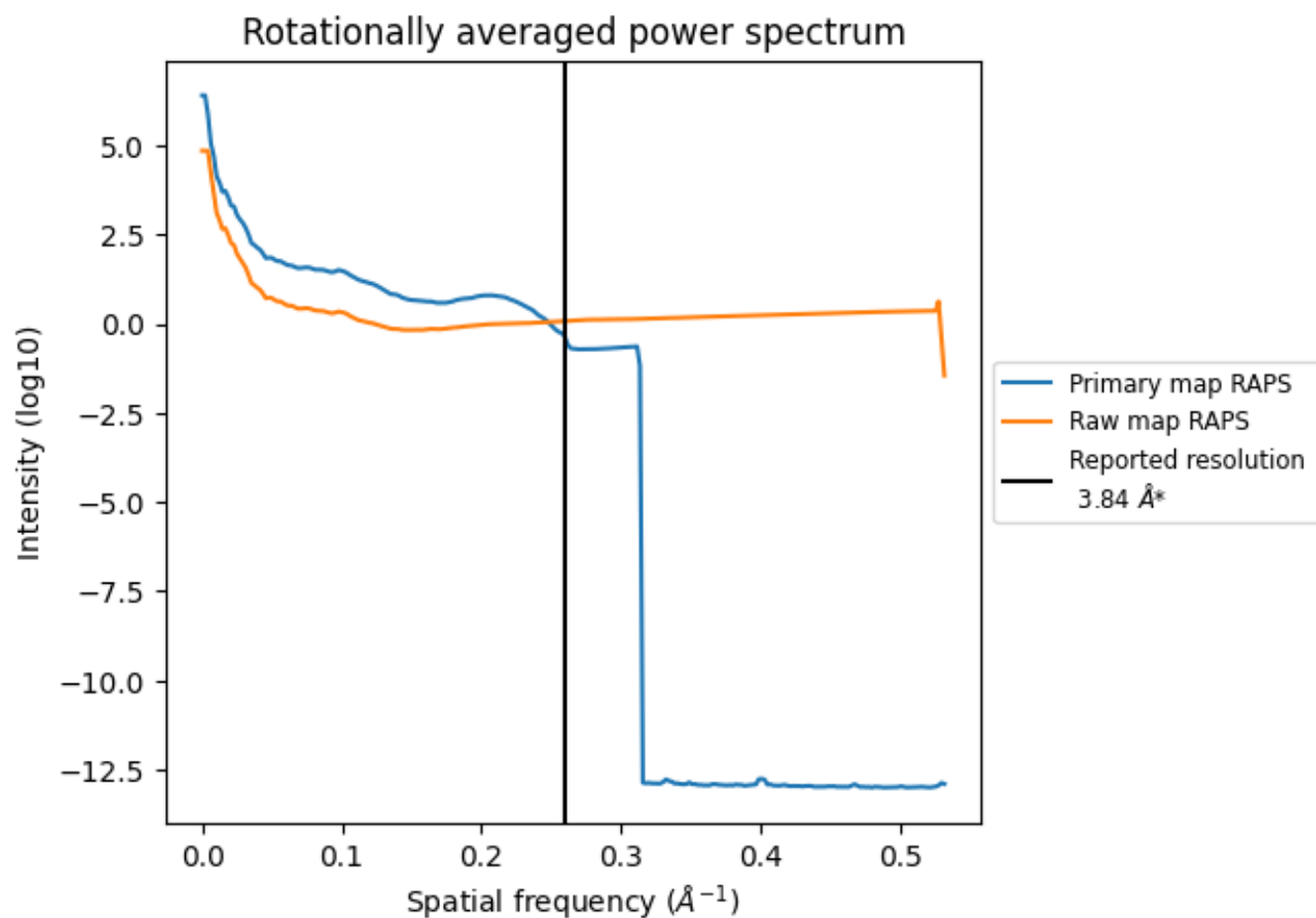


The volume at the recommended contour level is 854 nm<sup>3</sup>; this corresponds to an approximate mass of 772 kDa.

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 ⓘ



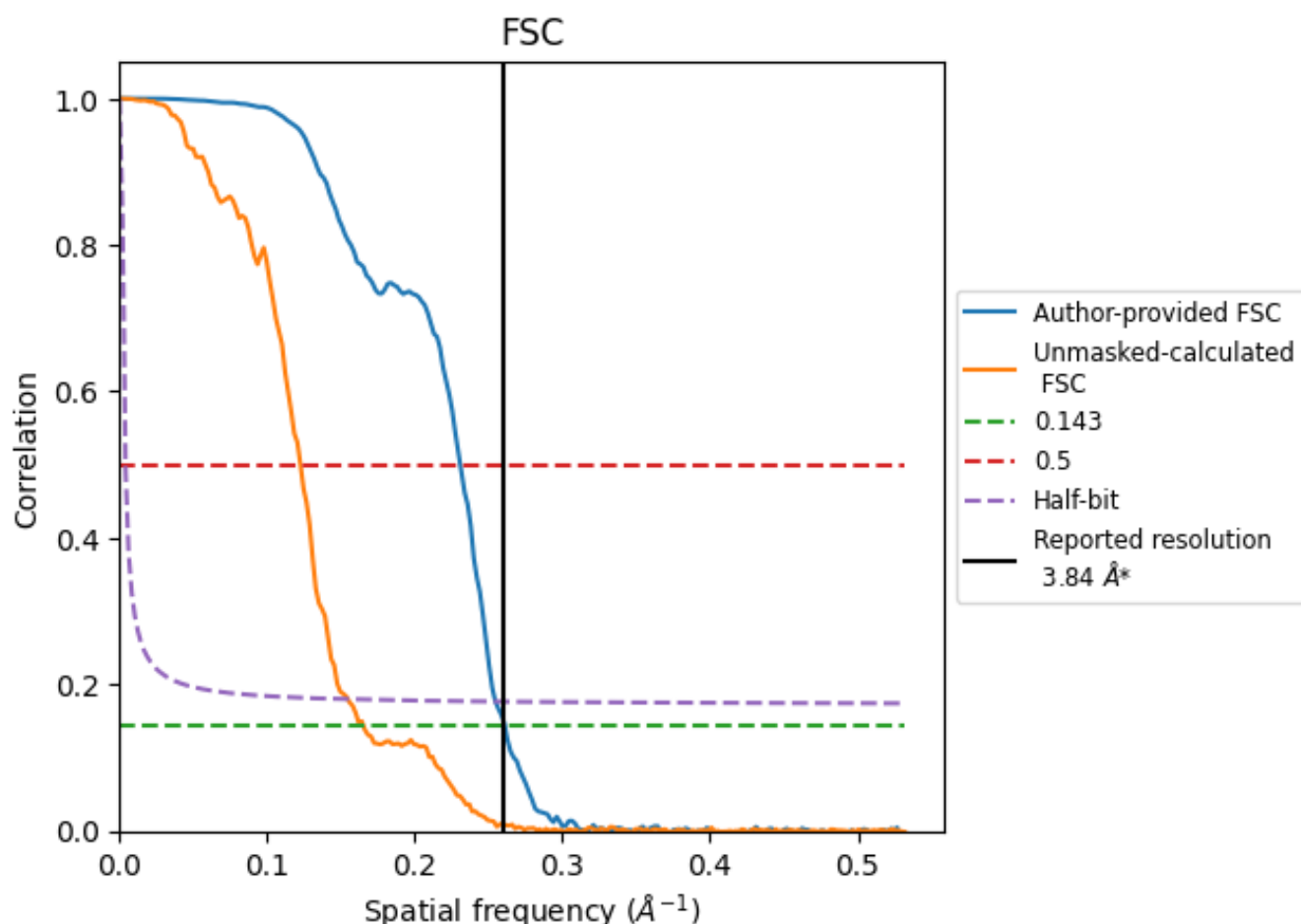
\*Reported resolution corresponds to spatial frequency of 0.260  $\text{\AA}^{-1}$



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



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.83	4.33	3.93
Unmasked-calculated*	6.05	8.16	6.46

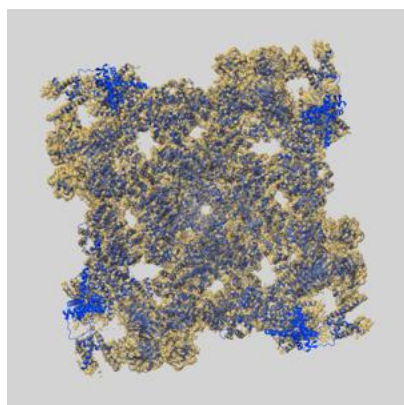
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.05 differs from the reported value 3.84 by more than 10 %



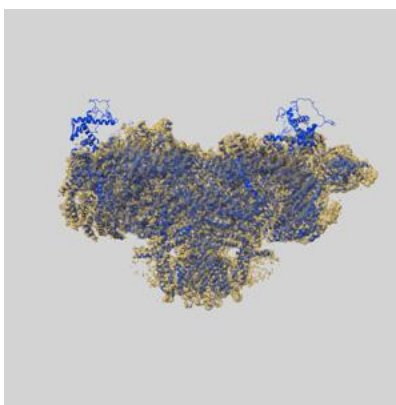
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27736 and PDB model 8DVE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

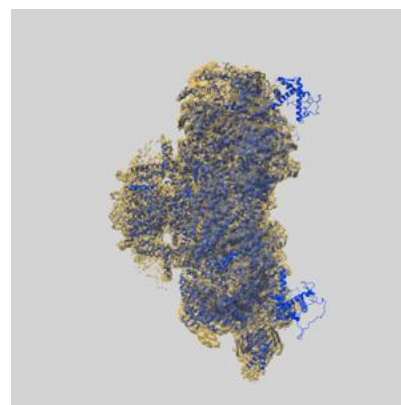
### 9.1 Map-model overlay [i](#)



X



Y

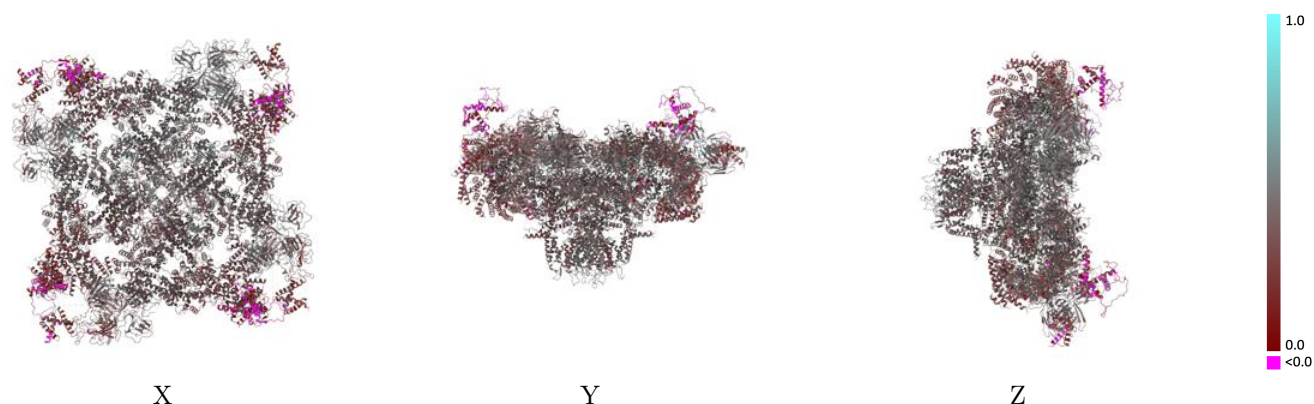


Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

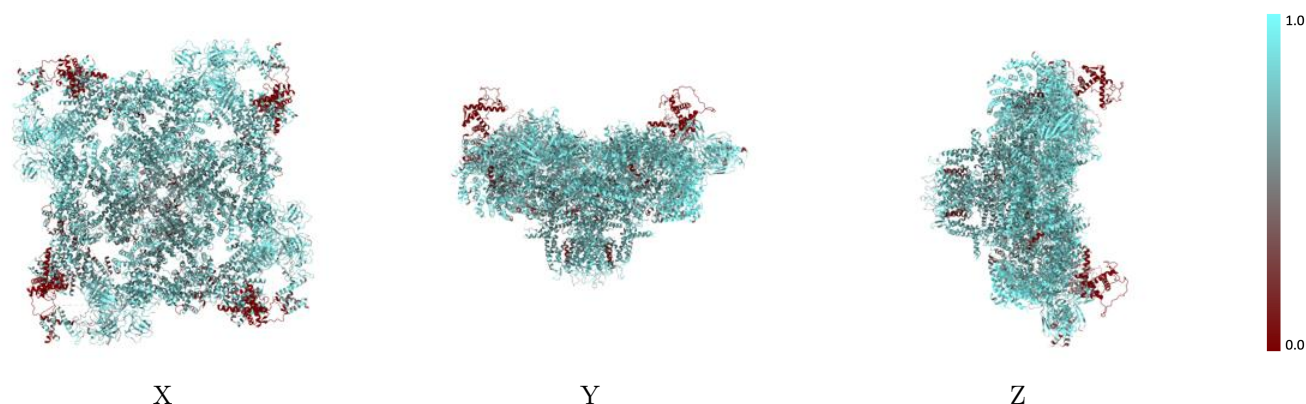


## 9.2 Q-score mapped to coordinate model [i](#)



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

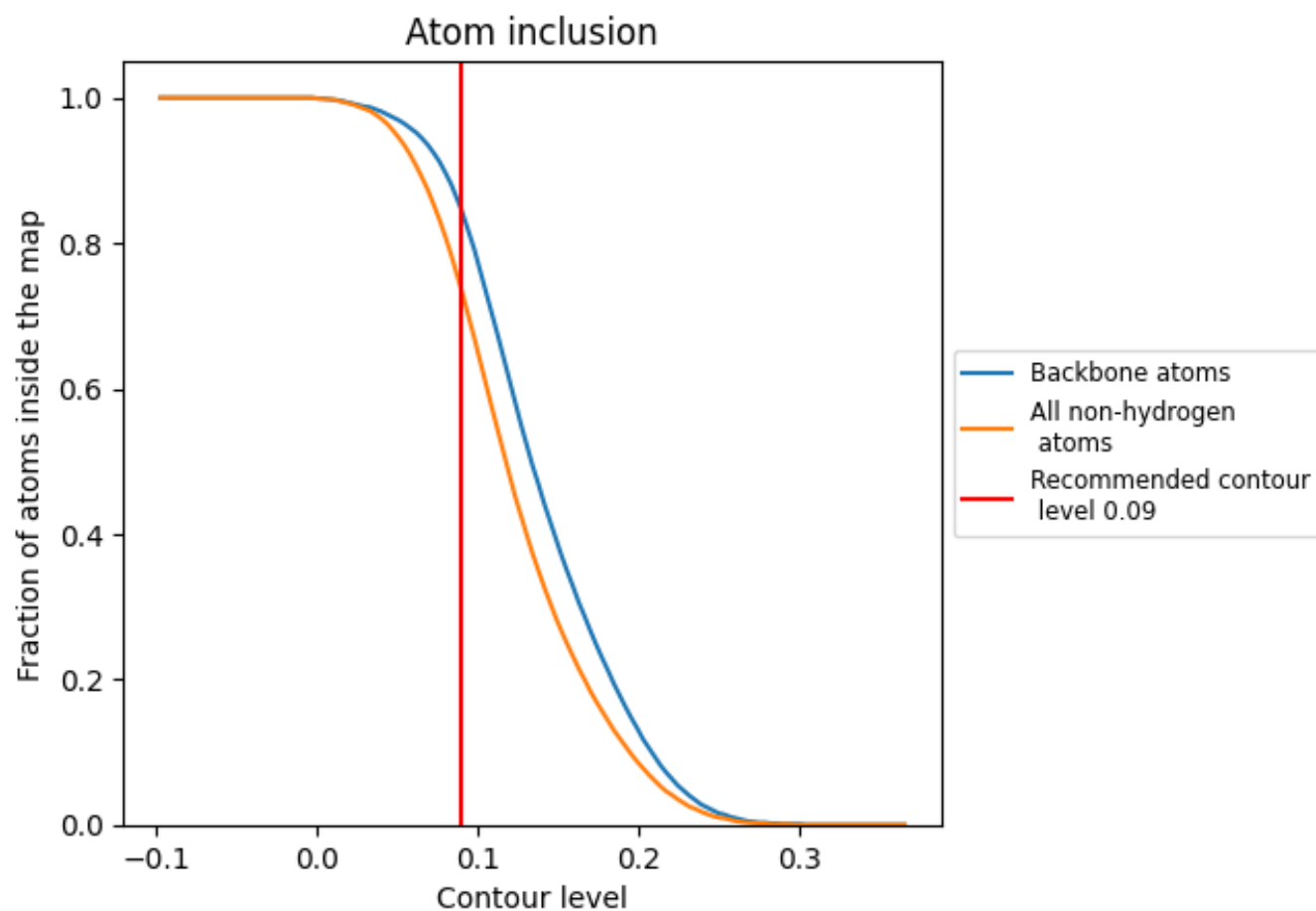
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7350	<div></div> 0.3920
A	<div></div> 0.7850	<div></div> 0.4170
B	<div></div> 0.8400	<div></div> 0.4640
C	<div></div> 0.6260	<div></div> 0.3710
D	<div></div> 0.7290	<div></div> 0.3920
E	<div></div> 0.8030	<div></div> 0.4430
F	<div></div> 0.3730	<div></div> 0.3380
G	<div></div> 0.7510	<div></div> 0.3940
H	<div></div> 0.7880	<div></div> 0.4340
I	<div></div> 0.5750	<div></div> 0.3400
J	<div></div> 0.6930	<div></div> 0.3630
K	<div></div> 0.7510	<div></div> 0.4140
L	<div></div> 0.4590	<div></div> 0.3390

