



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:22 PM UTC

PDB ID : 6JH6 / pdb_00006jh6
EMDB ID : EMD-9825
Title : Structure of RyR2 (F/A/Ca2+ dataset)
Authors : Chi, X.M.; Gong, D.S.; Ren, K.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Zhou, Q.; Yan, N.
Deposited on : 2019-02-17
Resolution : 4.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

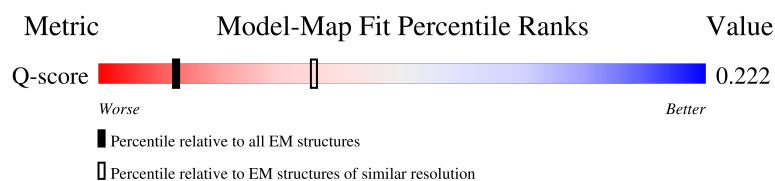
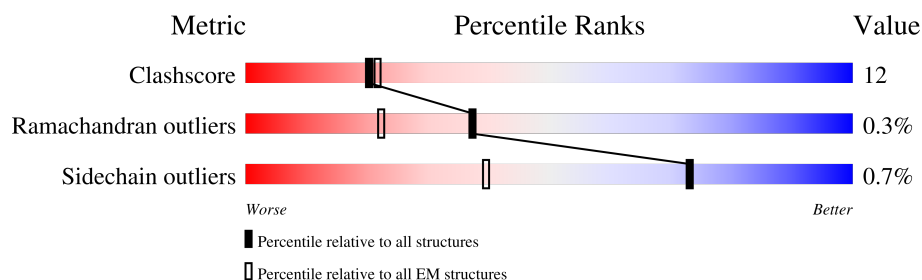
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

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



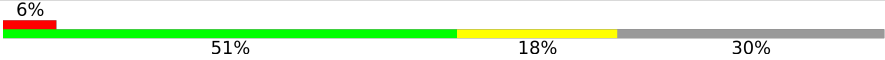
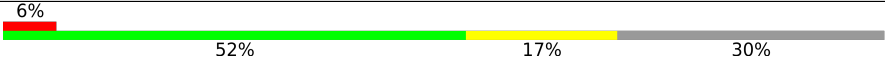
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	C	108	
1	E	108	
1	G	108	

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Mol	Chain	Length	Quality of chain
2	B	4968	
2	D	4968	
2	F	4968	
2	H	4968	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 108924 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	A	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	C	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3454	Total	C	N	O	S	0	0
			26380	16798	4512	4915	155		
2	D	3454	Total	C	N	O	S	0	0
			26380	16798	4512	4915	155		
2	F	3454	Total	C	N	O	S	0	0
			26380	16798	4512	4915	155		
2	H	3454	Total	C	N	O	S	0	0
			26380	16798	4512	4915	155		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

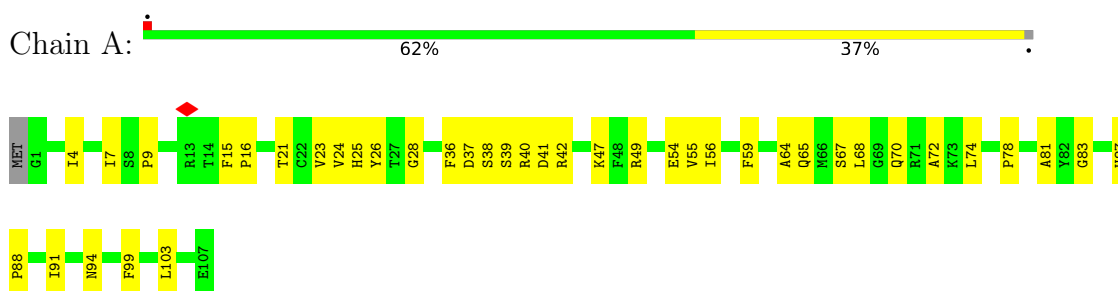
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	
4	F	1	Total	Zn	0
			1	1	
4	H	1	Total	Zn	0
			1	1	

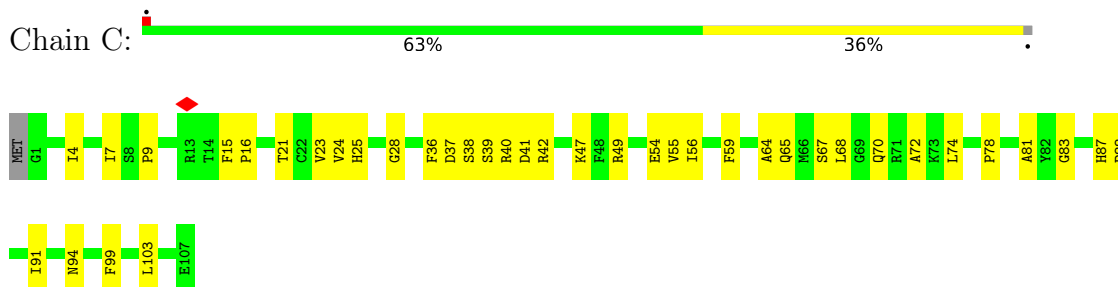
3 Residue-property plots [i](#)

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

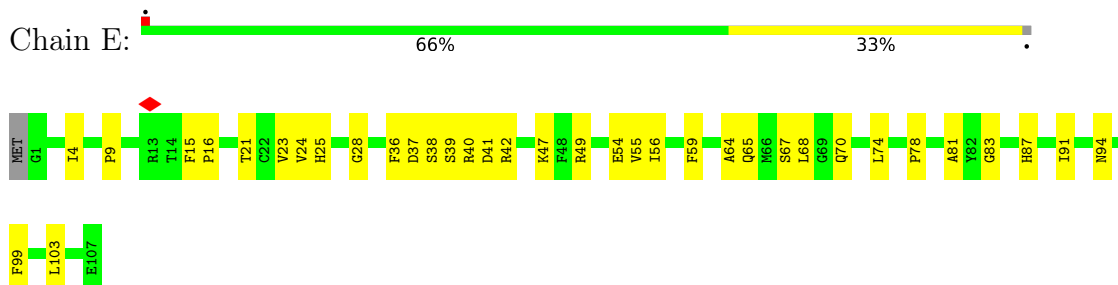
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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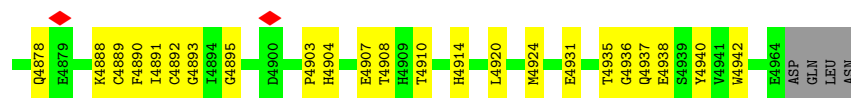




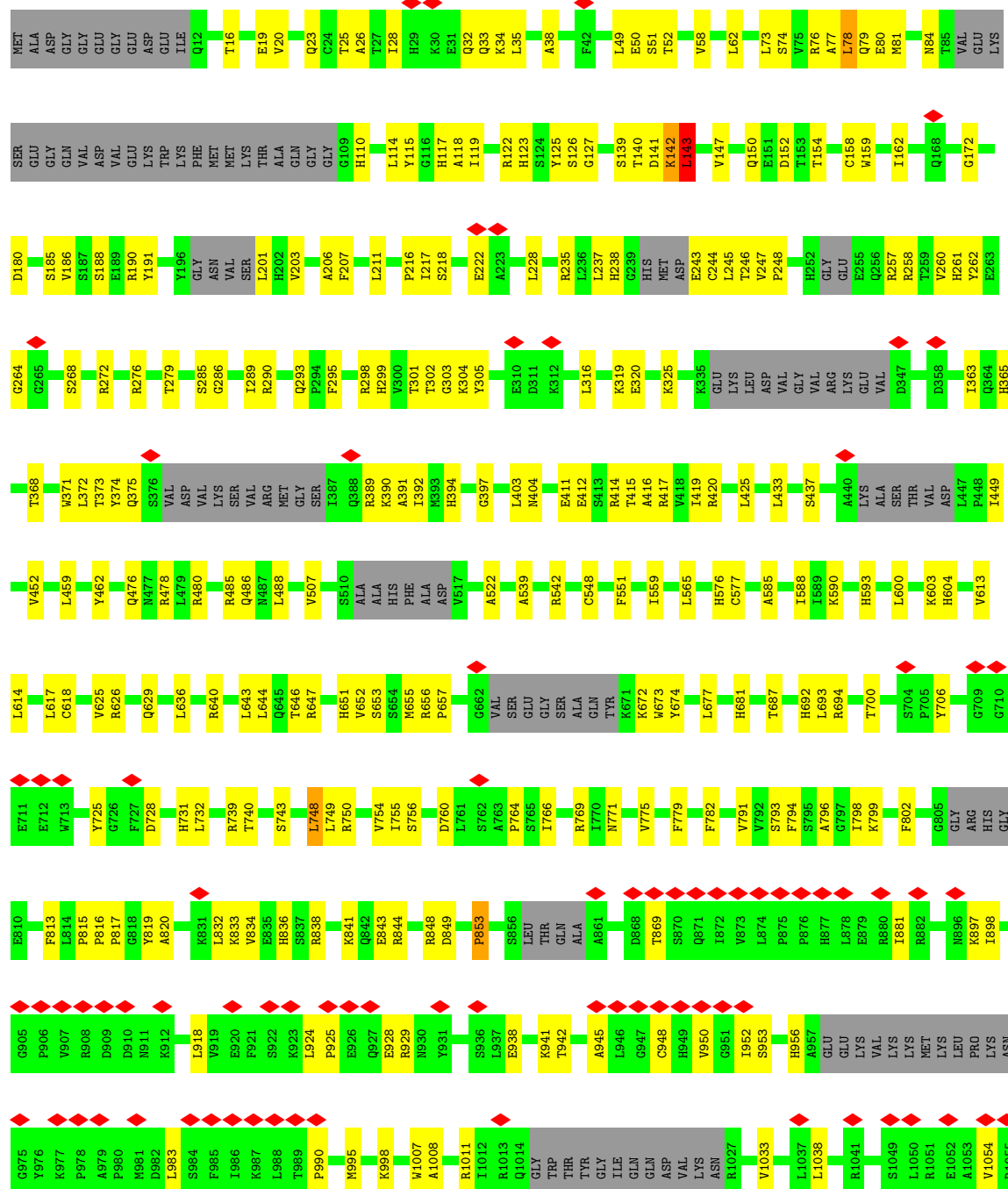








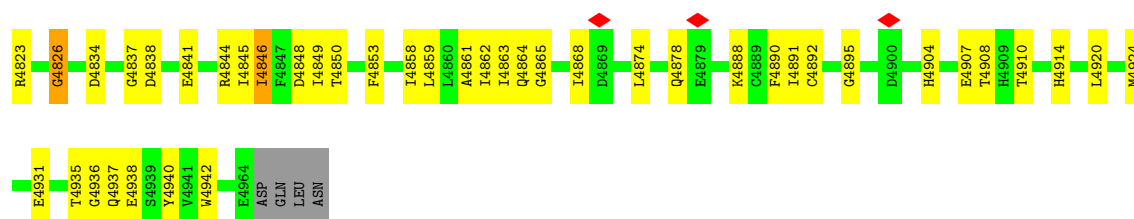
• Molecule 2: RyR2



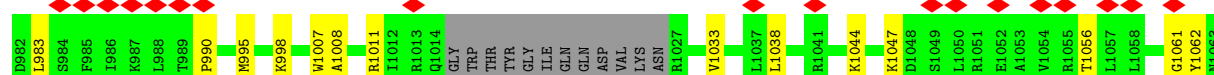
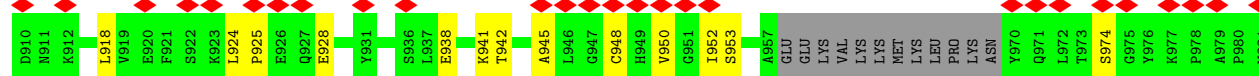
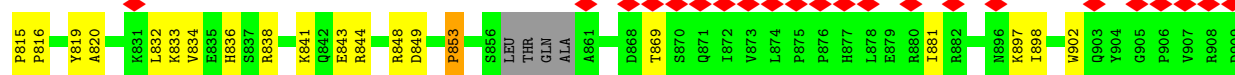
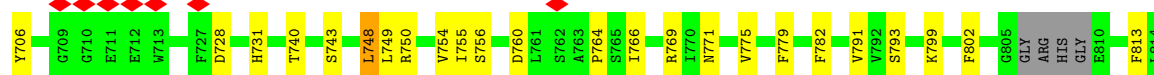
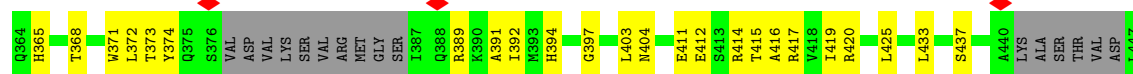
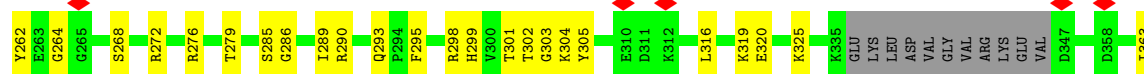
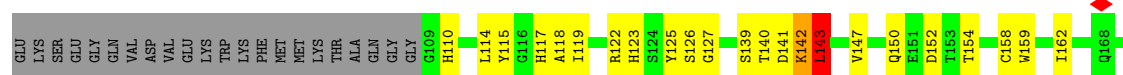
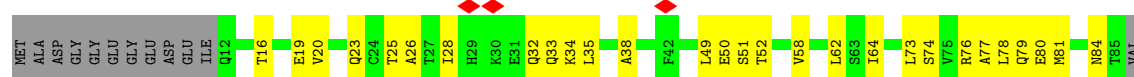
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N2211	V2082	E2011	V1934	I1830	L1719	V1619	Y1543	I1446	ARG	PRO	Y1236	R1144	G1061
Q2212	R2083	D2013	V1934	E1847	M1722	C1620	F1543	H1451	LYS	ALA	F1239	W1145	Y1062
Y2221	A2084	D2013	Q1938	P1848	M1723	L1622	A1545	T1455	GLN	GLY	N1242	Q1147	L1064
L2222	R2085	D2013	P1849	S1849	I1726	L1625	Q1546	L1459	ARG	PHE	W1250	E1150	E1065
N2225	L2089	GLU	N1940	V1849	V1727	Q1626	S1549	ASP	LEU	GLY	L1251	H1151	A1066
S2226	R2090	ASP	Q1941	PHE	L1738	S1629	P1550	ARG	LEU	PRO	S1252	Y1152	PRO
S2227	R2091	SER	F1942	GLY	L1738	L1630	N1551	VAL	ARG	ASN	G1253	R1154	ASP
V2228	Q2092	ASP	R1944	ALA	D1741	H1631	Q1554	ARG	THR	LEU	R1254	S1155	ASP
S2232	L2096	GLY	V1948	ALA	GLU	I1632	F1555	THR	LYS	LEU	L1255	W1156	HIS
P2233	V2100	ASN	Q1948	GLY	ASN	E1635	E1556	V1485	PRO	GLU	P1256	Q1157	ALA
A2102	R2101	D2023	ALA	PRO	LYS	E1635	LEU	L1489	TYR	ASP	Q1257	A1158	ALA
S2247	A2102	L2024	ALA	GLU	HIS	S1638	GLY	L1489	ASP	TYR	F1258	G1159	ARG
V2248	L2025	T2025	LEU	GLU	G1747	I1641	ARG	D1471	THR	ALA	H1267	D1160	ALA
R2249	ASN	T2026	ASN	SER	L1748	T1641	ILE	G1474	SER	ASP	M1165	VAL	GLU
T2107	R2106	R2027	MET	THR	P1749	E1643	LYS	K1475	HIS	SER	T1172	CYS	VAL
L2254	T2108	G2028	SER	THR	G1750	L1643	ASN	V1476	ALA	ASP	R1272	SER	GLY
A2255	T2109	R2029	ALA	LEU	S1756	Y1655	VAL	H1477	ARG	PHE	I1273	M1173	THR
L2256	L2109	L2030	ALA	GLU	L1757	Y1655	MET	E1478	ARG	GLU	D1274	M1174	GLY
R2259	D2116	L2031	LEU	LYS	R1758	R1659	PRO	S1479	LEU	VAL	GLY	L1177	GLY
V2267	T2117	E2036	THR	PRO	M1761	L1667	SER	R1482	GLU	THR	I1178	N1178	R1084
L2270	I2118	R2036	ARG	CYS	Q1762	G1668	A1568	R1482	ASP	ILE	G1179	G1179	R1085
G2274	L2121	V2037	LYS	ALA	S1767	G1669	G1569	S1483	VAL	LYS	E1180	F1180	R1086
LEU	V2133	T2038	LYS	GLU	S1767	H1670	L1570	N1484	LEU	ALA	I1181	L1181	R1089
GLN	R2134	Y2039	ASP	SER	S1770	R1671	S1573	CYS	ASP	GLY	L1182	L1183	R1089
CYS	R2135	L2040	PHE	THR	I1771	V1672	V1579	Y1486	ASP	HIS	G1187	D1184	Y1102
MET	R2136	LYS	ARG	ARG	N1772	A1673	P1580	M1487	ASP	LEU	G1187	G1187	E1106
GLN	G2136	ALA	SER	GLU	M1773	L1676	Q1581	V1488	ASP	VAL	V1285	S1188	E1106
LEU	L2142	GLY	PRO	PRO	E1774	H1679	C1582	C1489	TYR	ARG	T1286	E1189	T1109
SER	R2145	PRO	ALA	ALA	S1779	V1680	L1586	GLY	ASP	ASP	GLI291	L1190	A1110
VAL	R2153	GLU	GLU	GLU	P1783	D1681	H1587	SER	TYR	ARG	GLI291	A1191	G1111
LYS	N2161	ASN	ILE	GLU	I1786	Q1684	F1590	MET	LEU	VAL	M1294	F1192	G1111
GLY	N2173	GLU	LYS	LYS	L1795	Y1687	S1592	GLY	GLN	LYS	M1300	D1196	M1113
TYR	V2177	ASP	LEU	GLY	L1795	A1688	H1593	GLN	THR	ASP	Y1302	S1206	V1115
PRO	GLY	LYS	ASN	GLY	V1799	I1689	W1596	ARG	ALA	GLU	R1303	L1207	G1116
ASP	G2181	SER	PHE	LYS	E1690	E1691	P1600	ASN	THR	THR	L1304	Q1211	W1117
GLY	G2181	PRO	LYS	ARG	S1803	L1696	N1601	N1502	ALA	GLU	S1305	P1212	S1118
ASN	GLY	LYS	GLU	GLU	R1807	G1696	Q1602	GLY	PHE	GLY	M1306	G1213	P1120
P2293	GLU	LYS	SER	G1893	D1808	R1699	D1607	I1507	ASN	ALA	C1310	R1214	G121
G2296	SER	GLU	GLU	L1894	P1809	R1699	D1607	C1508	GLY	ASN	ALA	P1214	P124
E2297	LYS	PRO	CYS	L1894	V1810	Y1703	I1611	C1509	GLN	ASN	VAL	S1222	E127
R2298	GLU	PRO	PRO	P1902	G1811	I1707	S1612	V1510	LYS	HIS	T1223	L1224	L1128
L2300	THR	CYS	CYS	L1905	G1812	I1707	E1613	ASP	ASP	THR	PHE	F1227	E1132
R2304	F2190	PRO	PRO	L1905	F1816	L1711	R1614	ALA	ALA	LYS	LYS	T1228	R1133
F2305	F2191	GLU	GLU	R1920	L1817	T1716	Q1615	SER	GLN	THR	THR	G1231	A1136
	M2193	ILE	ILE	H1921	P1820	A1717	W1617	G1516	GLY	ALA	GLY	L1232	F1137
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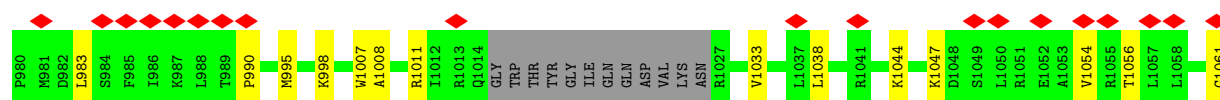
• Molecule 2: RyR2



L2081	N2196	L2081	D1999	V1934	E1847	M1723	L1626	Q1546	L1469	LEU	GLY	W1250	E1150	L1064
N2085	N2211	N2085	E2011	Q1938	S1848	I1726	Q1626	S1549	ASP	LEU	PRO	L1251	H1151	E1065
L2089	Q2212	L2089	D2013	D1939	S1849	V1727	S1629	P1550	ARG	ARG	ASN	S1252	H1151	A1066
H2090	Y2221	H2090	D2013	N1940	P1849	L1738	H1631	M1551	VAL	THR	ASP	R1254	R1153	PRO
Q2092	L2222	Q2092	ASP	R1942	GLY	D1741	I1632	Q1554	THR	PRO	LEU	L1255	R1154	ASP
L2096	N2225	L2096	GLY	F1943	ALA	GLU	P1633	F1555	V1465	ASP	ASP	P1256	W1155	GLN
V2100	S2226	V2100	ASP	R1944	GLY	LYS	E1635	E1556	L1469	THR	TYR	Q1257	W1156	ASP
R2101	S2227	R2101	GLY	V1948	ALA	LYS	S1638	GLY	G1470	THR	ALA	Q1257	W1157	HIS
A2102	V2228	A2102	ASN	GLN	PRO	HIS	S1638	ILE	D1471	SER	ALA	H1267	G1159	ALA
R2105	S2232	R2105	S2022	ALA	GLU	G1747	T1641	LYS	G1474	SER	SER	I1268	D1160	ALA
T2106	P2233	T2106	D2023	LEU	GLU	P1748	E1642	ASN	K1475	VAL	ASP	R1272	M1165	GLU
T2108	S2247	T2108	L2024	ASN	SER	P1749	E1643	VAL	V1476	ARG	GLU	I1273	T1172	VAL
T2109	V2248	T2109	T2025	MET	ASP	G1750	E1643	MET	H1477	LEU	VAL	D1274	M1173	CYS
D2116	N2249	D2116	I2026	SER	THR	S1756	Y1655	PRO	E1478	THR	LEU	GLY	M1174	GLY
A2255	L2256	A2255	R2027	ALA	LEU	I1757	R1659	LEU	S1479	ASP	MET	THR	L1177	THR
L2118	R2259	L2118	G2028	ALA	GLU	R1758	R1659	SER	R1482	VAL	LYS	ASP	N1178	GLU
L2121	V2267	L2121	R2029	LEU	GLU	S1758	L1687	A1568	S1483	LEU	THR	SER	G1179	R1084
L2124	L2270	L2124	L2030	THR	GLU	M1761	L1687	G1569	S1483	LEU	ALA	SER	G1179	F1085
L2127	G2274	L2127	L2031	ALA	PRO	Q1762	N1669	L1570	N1484	ASP	HIS	PRO	I1181	R1086
V2133	LEU	V2133	E2035	LYS	ALA	P1766	V1672	S1573	CYS	ASP	HIS	CYS	L1182	R1089
R2134	GLN	R2134	R2036	PRO	SER	S1767	V1673	V1579	M1486	ARG	LEU	LEU	L1183	B1089
G2135	SER	G2135	V2037	GLN	GLU	S1767	A1673	P1580	M1487	ASP	VAL	V1286	D1184	A1098
L2142	GLN	L2142	T2038	GLU	ASP	S1770	L1676	Q1581	V1488	TYR	ASP	G1291	G1187	W1101
N2143	VAL	N2143	Y2039	ARG	SER	S1770	L1676	Q1581	C1489	ASP	ARG	M1294	S1188	Y1102
R2144	SER	R2144	L2040	ARG	LEU	N1772	H1679	C1582	A1490	TYR	VAL	F1301	E1189	E1106
R2145	LEU	R2145	LYS	SER	GLU	E1774	V1680	L1586	GLY	LEU	ASP	M1300	L1190	T1109
N2153	GLY	N2153	GLY	LEU	GLY	E1774	D1681	H1587	SER	MET	LYS	F1301	L1191	G1111
N2161	ASP	N2161	ASP	ASN	GLY	L1795	G1684	F1590	SER	GLN	LYS	M1300	F1192	G1111
N2177	LYS	N2177	SER	PHE	GLY	V1799	G1696	P1600	N1502	SER	PHE	G1310	S1206	E1106
G2181	LYS	G2181	LYS	LYS	ARG	S1803	R1699	Q1602	I1507	GLY	ASN	ALA	L1207	T1109
GLY	ASP	GLY	SER	ASP	PRO	S1803	R1699	Q1602	G1508	GLN	ASN	ALA	G1111	A1110
GLY	ASP	GLY	SER	ASP	PRO	R1807	Y1703	D1607	C1509	GLU	HIS	VAL	G1111	G1111
TRP	ASP	TRP	T2058	SER	GLY	P1808	L1704	I1611	V1511	PRO	LYS	PHE	F1227	G1222
ASN	ASN	ASN	L2059	GLY	L1894	V1810	L1705	S1612	ASP	ALA	ALA	LYS	T1228	T1222
P2293	GLY	P2293	Q2060	CYS	P1902	G1811	L1706	E1613	ALA	R1440	ALA	THR	F1227	L1224
G2296	SER	G2296	M2067	PRO	P1902	G1812	I1707	R1614	ALA	V1441	GLN	SER	T1228	P1224
Y2299	LYS	Y2299	M2067	CYS	L1905	G1812	L1711	Q1615	SER	V1443	LYS	THR	G1231	E1227
R2304	GLU	R2304	W2070	PRO	L1905	F1816	T1716	G1616	G1516	G1444	GLY	GLY	L1232	R1133
F2305	THR	F2305	A2071	ILE	H1921	L1817	A1717	W1617	T1521	W1445	ILE	PRO	G1236	A1136
F2308	THR	F2308	S2074	R1994	R1922	P1820	A1717	V1619	Y1531	I1446	ARG	GLY	Y1236	F1137
			S2075	R1997	R1922	L1821	R1718	Q1620	Y1531	H1451	LYS	ALA	F1239	Q1143
			I2076	L1997	V1927	L1821	L1719	C1621	V1543	Q1452	GLN	SER	N1242	R1144
				L1998		I1830	N1722	L1622	A1545	T1455	ARG	LEU	W1145	W1146



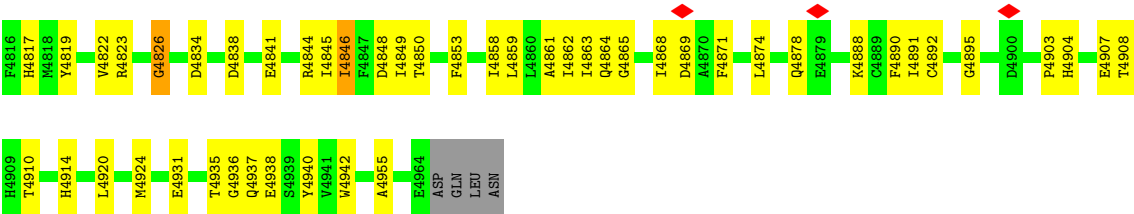






ASN	PHE	GLY	ALA	ASP	MET	PHE	P3082	PRO	F2896	L2834	V2774	LEU	C2462	ASP	THR	P2293
ARG	LYS	LEU	GLU	GLY	PRO	VAL	THR	TYR	L2897	S2835	P2775	R2682	Y2476	THR	ILE	G2296
GLY	ASN	LEU	ILE	GLN	GLU	GLN	ARG	GLN	Q2898	R2836	I2776	N2601	Y2477	HIS	ILE	Y2299
ASN	GLN	LEU	ASN	LYS	ILE	LYS	ASN	ILE	I2899	D2837	K2717	HIS	ILE	MET	ILE	Y2304
ASN	GLN	LEU	PRO	PRO	PRO	PRO	GLN	PRO	N2900	H2838	E2778	ALA	GLU	GLY	GLU	F2305
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	Y2902	A2840	S2779	R2605	Y2481	PRO	GLU	F2308
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	A2903	M2841	T2782	G2627	VAL	MET	VAL	S2313
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	V2904	A2842	L2784	ASP	G2492	HIS	GLY	I2326
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	S2905	E2843	M2783	ALA	THR	ILE	ILE	R2327
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	R2906	M2844	L2784	A2634	L2503	HIS	THR	E2330
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	G2907	M2845	A2785	LYS	ASP	ALA	ALA	CYS
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	PHE	A2846	V2786	LYS	ASP	ALA	PHE	GLY
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	LYS	E2847	G2787	LYS	ASP	ALA	ALA	PRO
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ASP	M2848	V2788	GLN	ASP	ALA	LYS	GLY
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	LEU	Y2849	R2789	LYS	ASP	ALA	ALA	PRO
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLU	H2850	I2790	LYS	ASP	ALA	ALA	LEU
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	THR	M2851	E2791	LYS	ASP	ALA	ALA	ARG
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	PRO	I2852	R2792	LYS	ASP	ALA	ALA	GLY
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	SER	L2852	T2793	LYS	ASP	ALA	ALA	GLU
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ILE	K2855	E2794	ASP	ASP	ALA	ALA	GLY
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	LYS	K2856	R2794	TYR	ASP	ALA	ALA	GLY
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ARG	K2857	E2795	MET	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	PHE	K2858	G2796	GLU	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ALA	L2859	D2797	GLU	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ALA	E2860	I2798	ASN	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	SER	L2861	A2799	TYR	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	PHE	E2862	I2740	VAL	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	LEU	L2863	G2741	SER	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLN	K2864	E2742	MET	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ILE	G2865	I2743	MET	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ARG	G2866	E2744	SER	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	TYR	G2867	G2745	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	H2868	I2747	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ASP	H2869	G2748	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLU	L2870	S2749	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	HIS	L2871	D2750	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLN	L2872	S2751	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	TYR	G2873	S2752	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ILE	P2874	K2753	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	LEU	Y2875	E2754	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	PHE	D2876	G2755	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ASP	T2877	P2756	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	T2878	G2757	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	ARG	T2879	I2757	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	SER	A2880	K2758	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	LYS	E2881	S2823	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	K2882	P2824	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	HIS	A2883	R2825	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	E2884	A2826	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	K2885	I2827	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	D2886	L2764	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	E2887	S2765	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	E2888	K2767	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	Q2891	E2768	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	D2892	K2769	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	L2893	E2770	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	K2895	I2771	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	K2895	E2772	GLY	ASP	ALA	ALA	ASN
ASN	GLN	LEU	VAL	VAL	VAL	VAL	VAL	VAL	GLY	K2895	R2773	GLY	ASP	ALA	ALA	ASN





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	44288	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 ($e^-/\text{\AA}^2$)	48.6	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	0.071	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	522.616, 522.616, 522.616	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/835	0.49	0/1123
1	C	0.24	0/835	0.49	0/1123
1	E	0.24	0/835	0.49	0/1123
1	G	0.24	0/835	0.49	0/1123
2	B	0.27	0/26871	0.62	26/36338 (0.1%)
2	D	0.27	0/26871	0.62	26/36338 (0.1%)
2	F	0.27	0/26871	0.62	26/36338 (0.1%)
2	H	0.27	0/26871	0.62	26/36338 (0.1%)
All	All	0.27	0/110824	0.62	104/149844 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	21
2	D	0	21
2	F	0	21
2	H	0	21
All	All	0	84

There are no bond length outliers.

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2327	ARG	N-CA-C	-8.65	101.17	112.68
2	B	2039	TYR	N-CA-C	8.12	126.03	113.28
2	F	2039	TYR	N-CA-C	8.12	126.03	113.28
2	D	2039	TYR	N-CA-C	8.12	126.03	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2039	TYR	N-CA-C	8.12	126.02	113.28

There are no chirality outliers.

5 of 84 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	141	ASP	Peptide
2	B	142	LYS	Peptide
2	B	143	LEU	Peptide
2	B	748	LEU	Peptide
2	B	816	PRO	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	819	0	824	30	0
1	C	819	0	824	29	0
1	E	819	0	824	26	0
1	G	819	0	824	28	0
2	B	26380	0	24897	714	0
2	D	26380	0	24897	704	0
2	F	26380	0	24897	701	0
2	H	26380	0	24897	706	0
3	B	31	0	12	2	0
3	D	31	0	12	2	0
3	F	31	0	12	2	0
3	H	31	0	12	2	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	108924	0	102932	2582	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 12.

The worst 5 of 2582 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:4861:ALA:CB	2:D:4864:GLN:HG2	1.60	1.32
2:D:4861:ALA:CB	2:F:4864:GLN:HG2	1.61	1.30
2:F:4861:ALA:CB	2:H:4864:GLN:HG2	1.65	1.27
2:F:4814:TYR:CE2	2:H:4518:LEU:HD13	1.71	1.24
2:D:4780:TYR:CE1	2:F:4518:LEU:HD22	1.73	1.23

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%)	101 (96%)	4 (4%)	0	100	100
1	C	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	B	3332/4968 (67%)	2955 (89%)	368 (11%)	9 (0%)	36	71
2	D	3332/4968 (67%)	2955 (89%)	368 (11%)	9 (0%)	36	71
2	F	3332/4968 (67%)	2955 (89%)	368 (11%)	9 (0%)	36	71
2	H	3332/4968 (67%)	2958 (89%)	365 (11%)	9 (0%)	36	71
All	All	13748/20304 (68%)	12227 (89%)	1485 (11%)	36 (0%)	37	71

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4595	LYS
2	D	4595	LYS
2	F	4595	LYS
2	H	4595	LYS

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Mol	Chain	Res	Type
2	B	143	LEU

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	C	88/89 (99%)	88 (100%)	0	100	100
1	E	88/89 (99%)	88 (100%)	0	100	100
1	G	88/89 (99%)	88 (100%)	0	100	100
2	B	2657/4355 (61%)	2641 (99%)	16 (1%)	78	81
2	D	2658/4355 (61%)	2639 (99%)	19 (1%)	76	79
2	F	2657/4355 (61%)	2640 (99%)	17 (1%)	78	81
2	H	2658/4355 (61%)	2638 (99%)	20 (1%)	73	78
All	All	10982/17776 (62%)	10910 (99%)	72 (1%)	73	79

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	625	VAL
2	H	4863	ILE
2	H	881	ILE
2	H	1738	LEU
2	D	925	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 243 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	4128	ASN
2	H	3635	HIS
2	F	1452	GLN
2	H	2831	ASN

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Mol	Chain	Res	Type
2	H	4160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	F	5101	-	32,33,33	1.33	4 (12%)	48,52,52	1.92	12 (25%)
3	ATP	B	5101	-	32,33,33	1.34	4 (12%)	48,52,52	1.92	12 (25%)
3	ATP	D	5101	-	32,33,33	1.34	4 (12%)	48,52,52	1.92	12 (25%)
3	ATP	H	5101	-	32,33,33	1.34	4 (12%)	48,52,52	1.92	12 (25%)

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	F	5101	-	-	7/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	7/22/38/38	0/3/3/3
3	ATP	D	5101	-	-	7/22/38/38	0/3/3/3
3	ATP	H	5101	-	-	7/22/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5101	ATP	C5-C4	4.27	1.46	1.39
3	H	5101	ATP	C5-C4	4.27	1.46	1.39
3	B	5101	ATP	C5-C4	4.25	1.46	1.39
3	F	5101	ATP	C5-C4	4.24	1.46	1.39
3	B	5101	ATP	C5-C6	2.58	1.48	1.41

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5101	ATP	C5-C4-N3	-6.31	118.03	126.72
3	B	5101	ATP	C5-C4-N3	-6.30	118.04	126.72
3	D	5101	ATP	C5-C4-N3	-6.30	118.04	126.72
3	H	5101	ATP	C5-C4-N3	-6.30	118.04	126.72
3	D	5101	ATP	N3-C4-N9	5.08	135.80	127.17

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

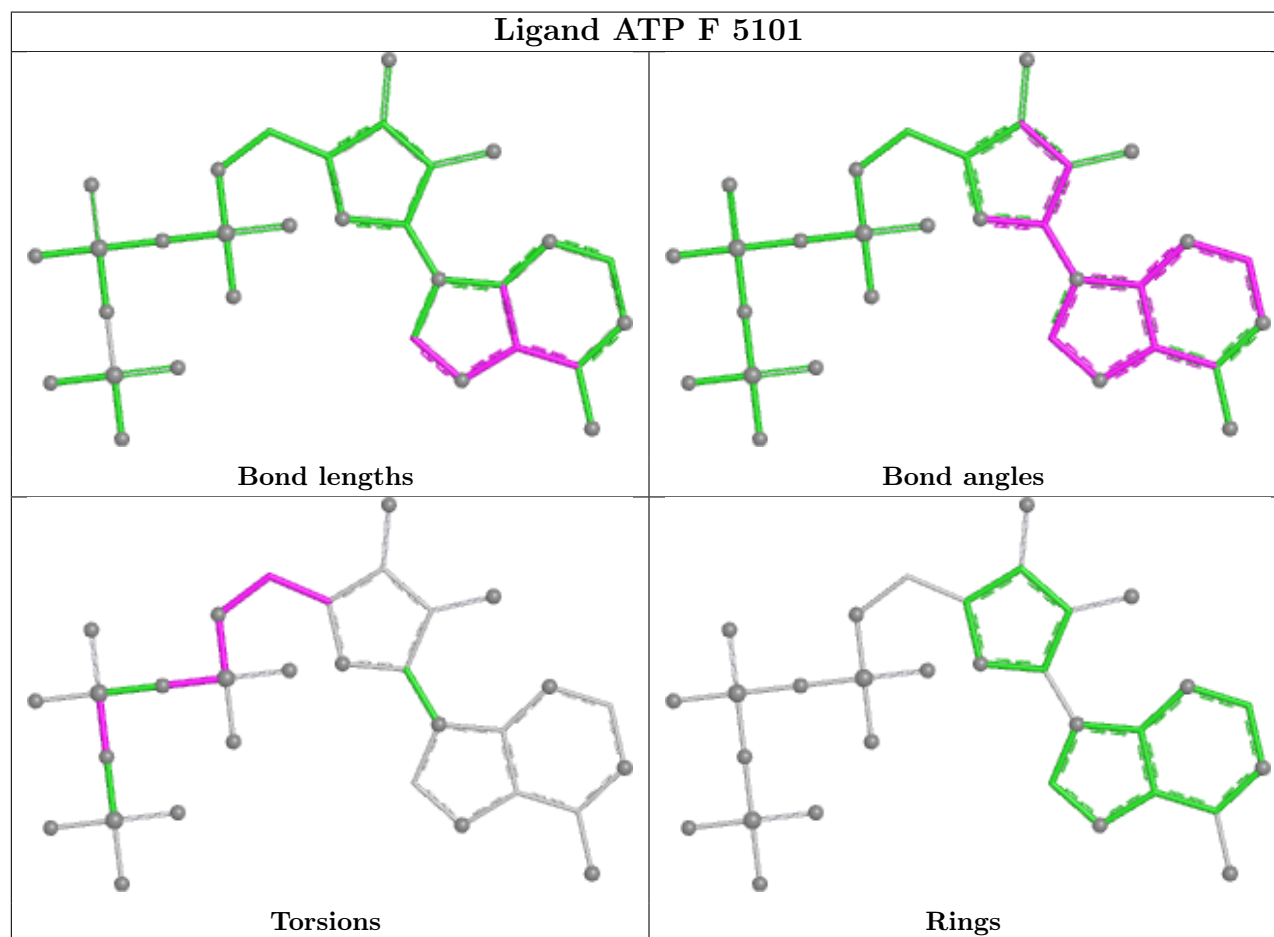
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	D	5101	ATP	C5'-O5'-PA-O2A
3	D	5101	ATP	C5'-O5'-PA-O3A
3	F	5101	ATP	C5'-O5'-PA-O2A

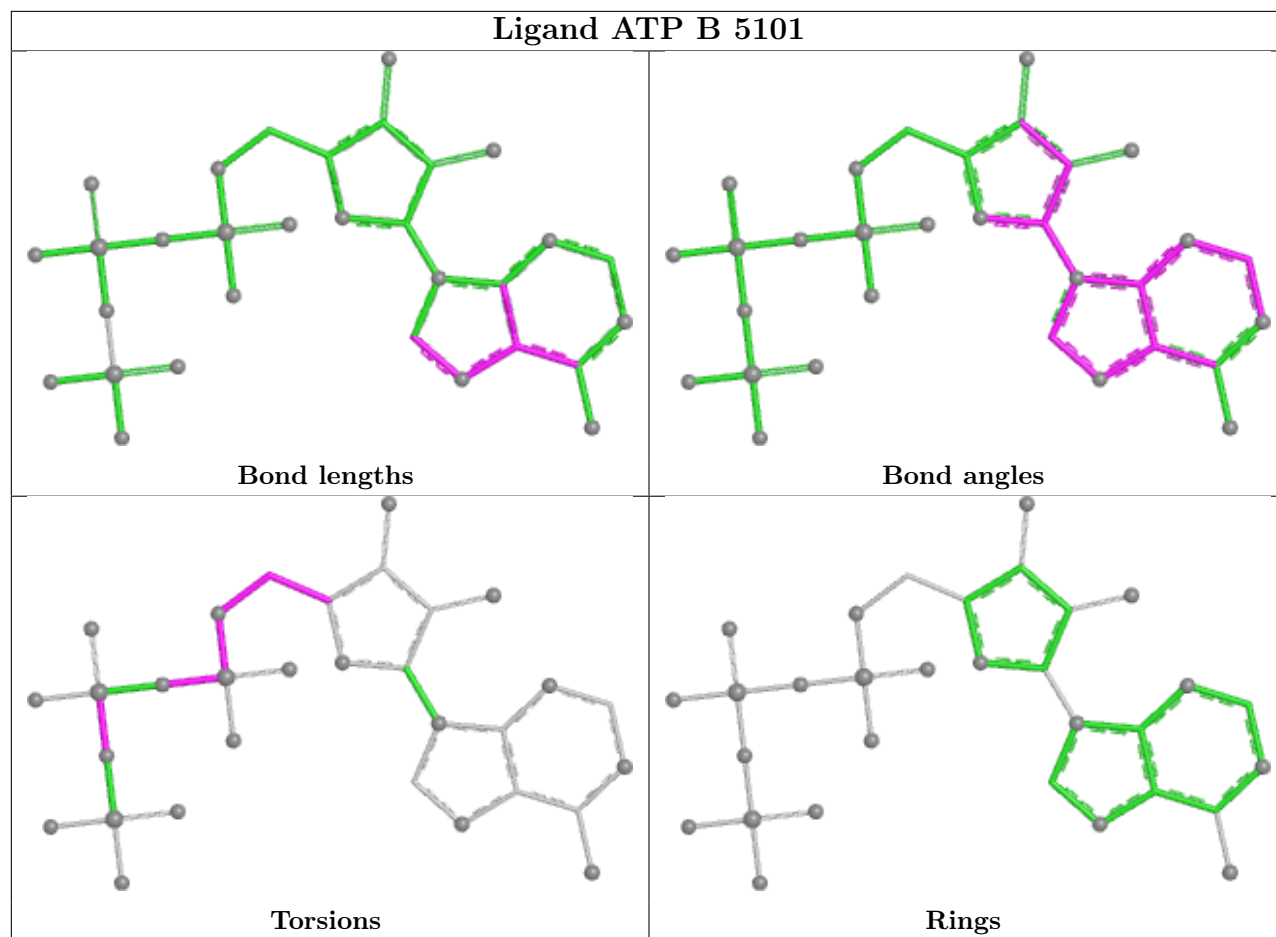
There are no ring outliers.

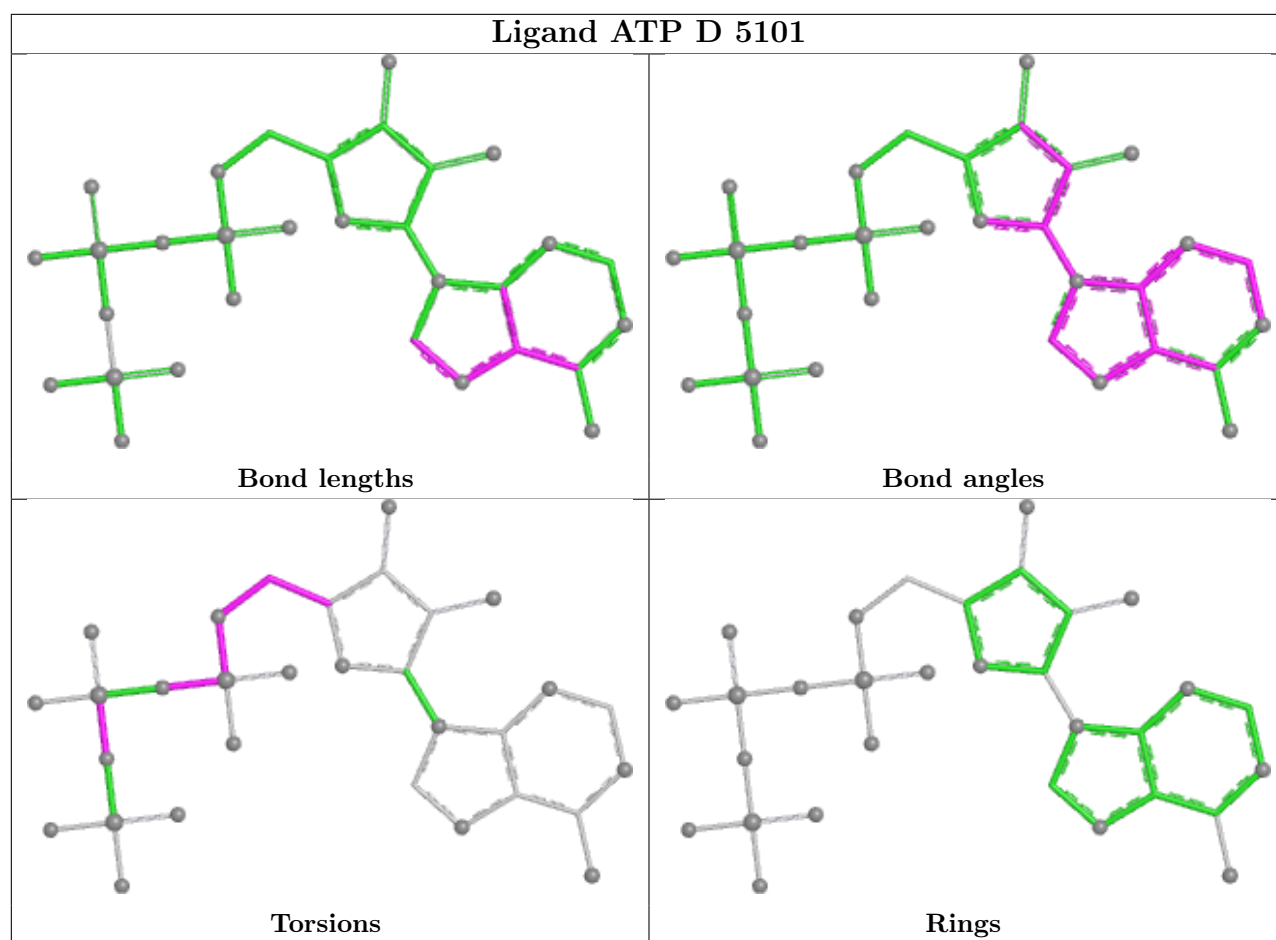
4 monomers are involved in 8 short contacts:

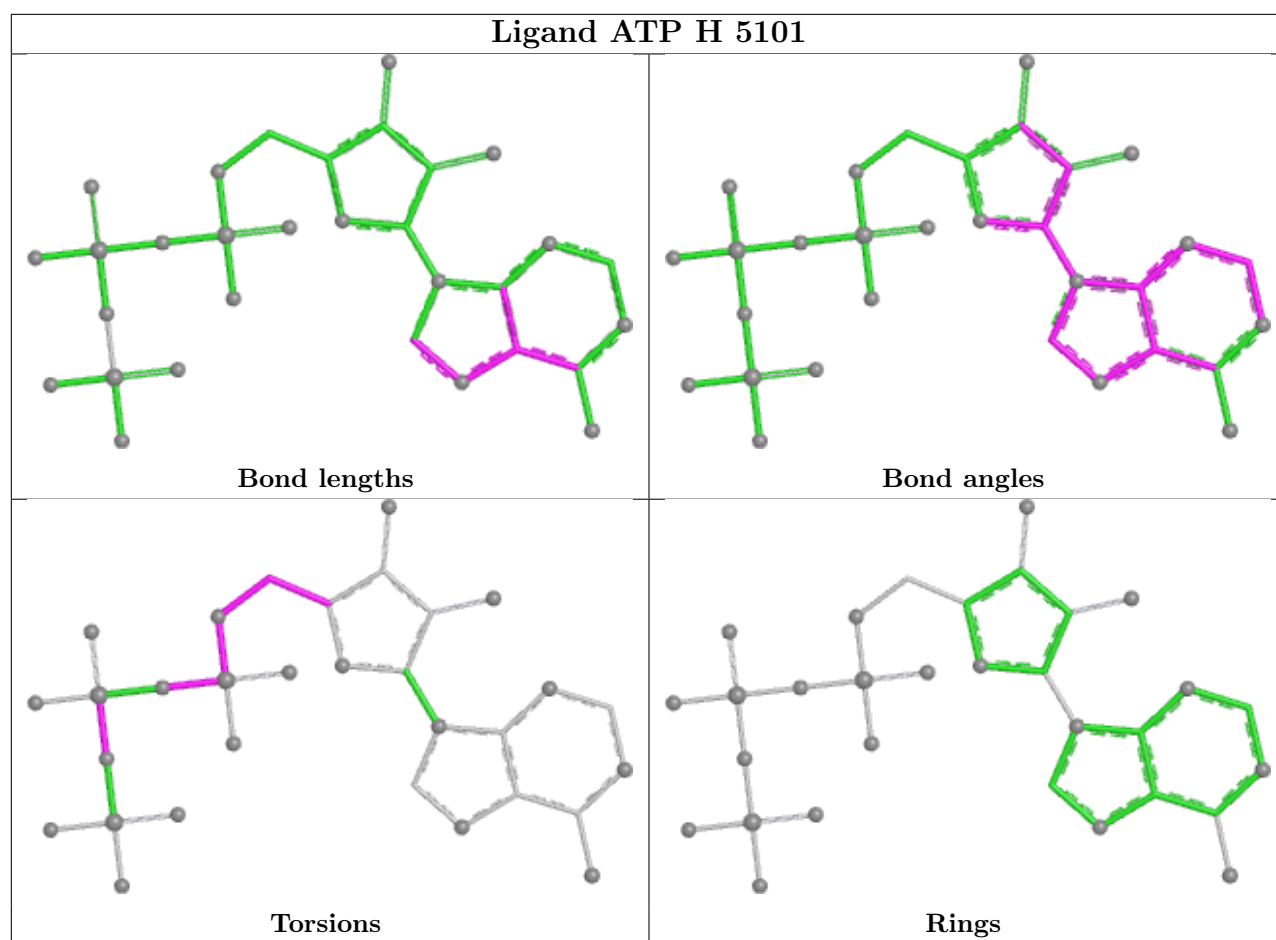
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5101	ATP	2	0
3	B	5101	ATP	2	0
3	D	5101	ATP	2	0
3	H	5101	ATP	2	0

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](#)

There are no chain breaks in this entry.

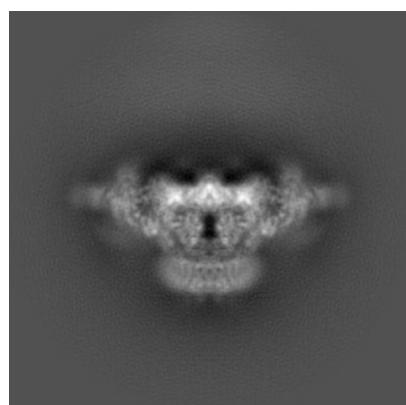
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9825. These allow visual inspection of the internal detail of the map and identification of artifacts.

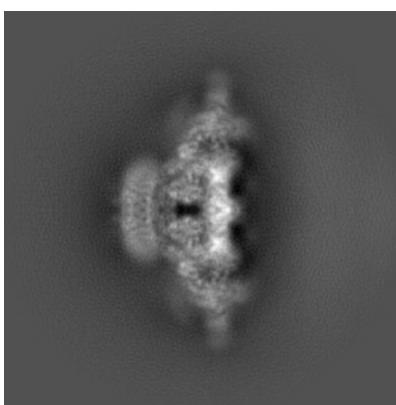
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

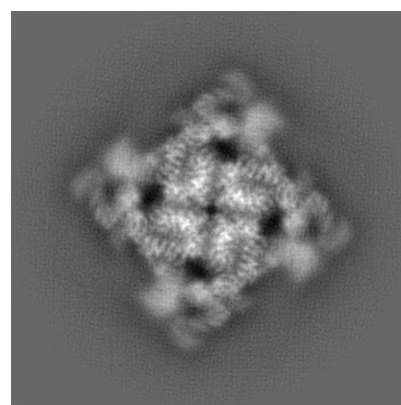
6.1.1 Primary map



X



Y

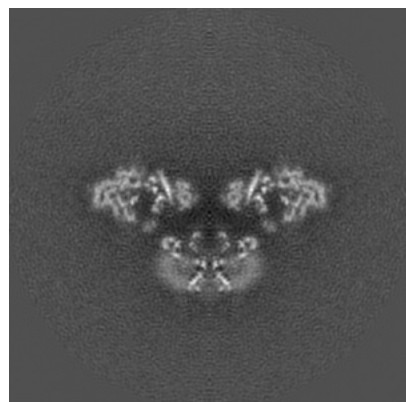


Z

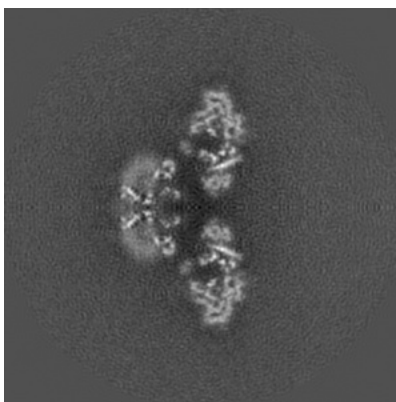
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

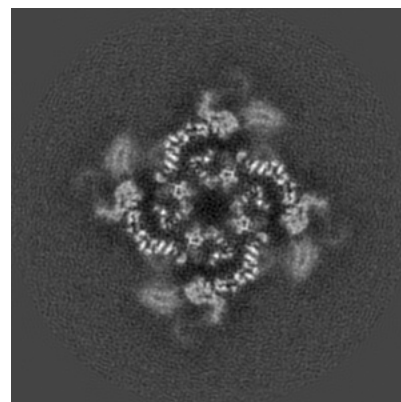
6.2.1 Primary map



X Index: 200



Y Index: 200

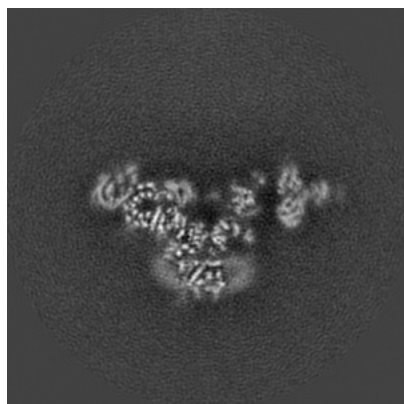


Z Index: 200

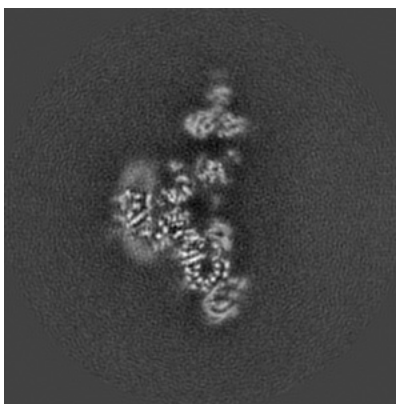
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

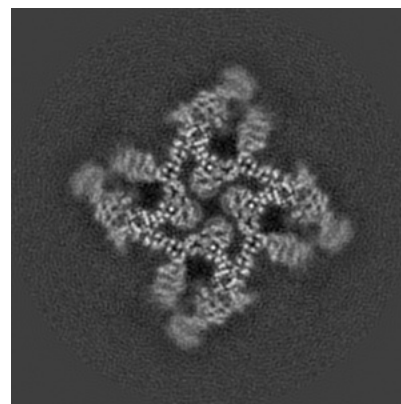
6.3.1 Primary map



X Index: 211



Y Index: 189

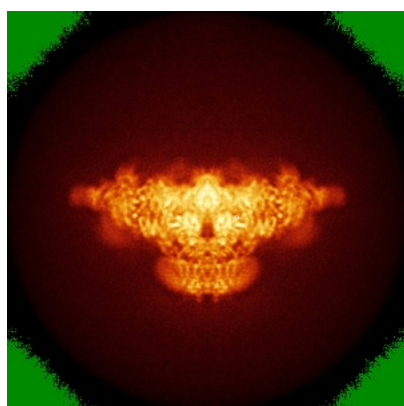


Z Index: 212

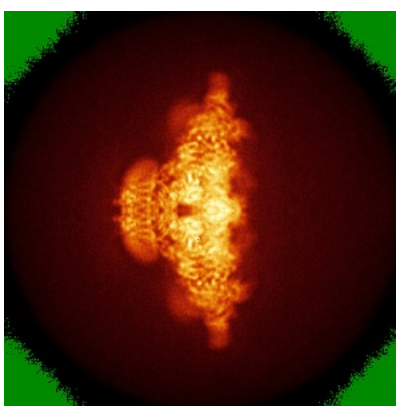
The images above show the largest variance slices of the map in three orthogonal directions.

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

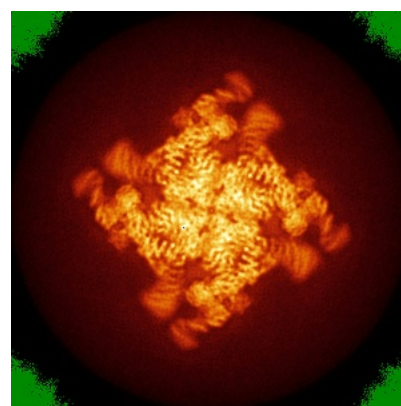
6.4.1 Primary map



X



Y

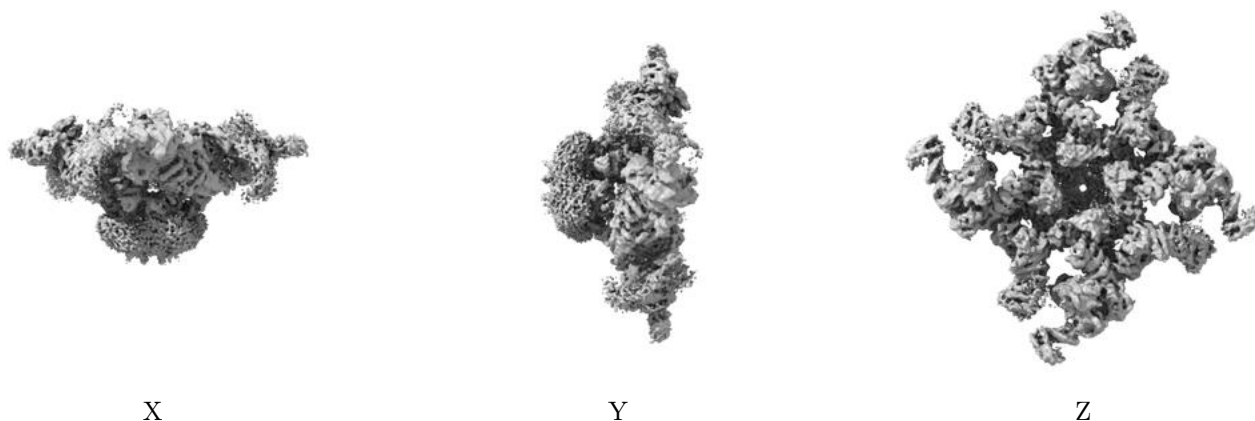


Z

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 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

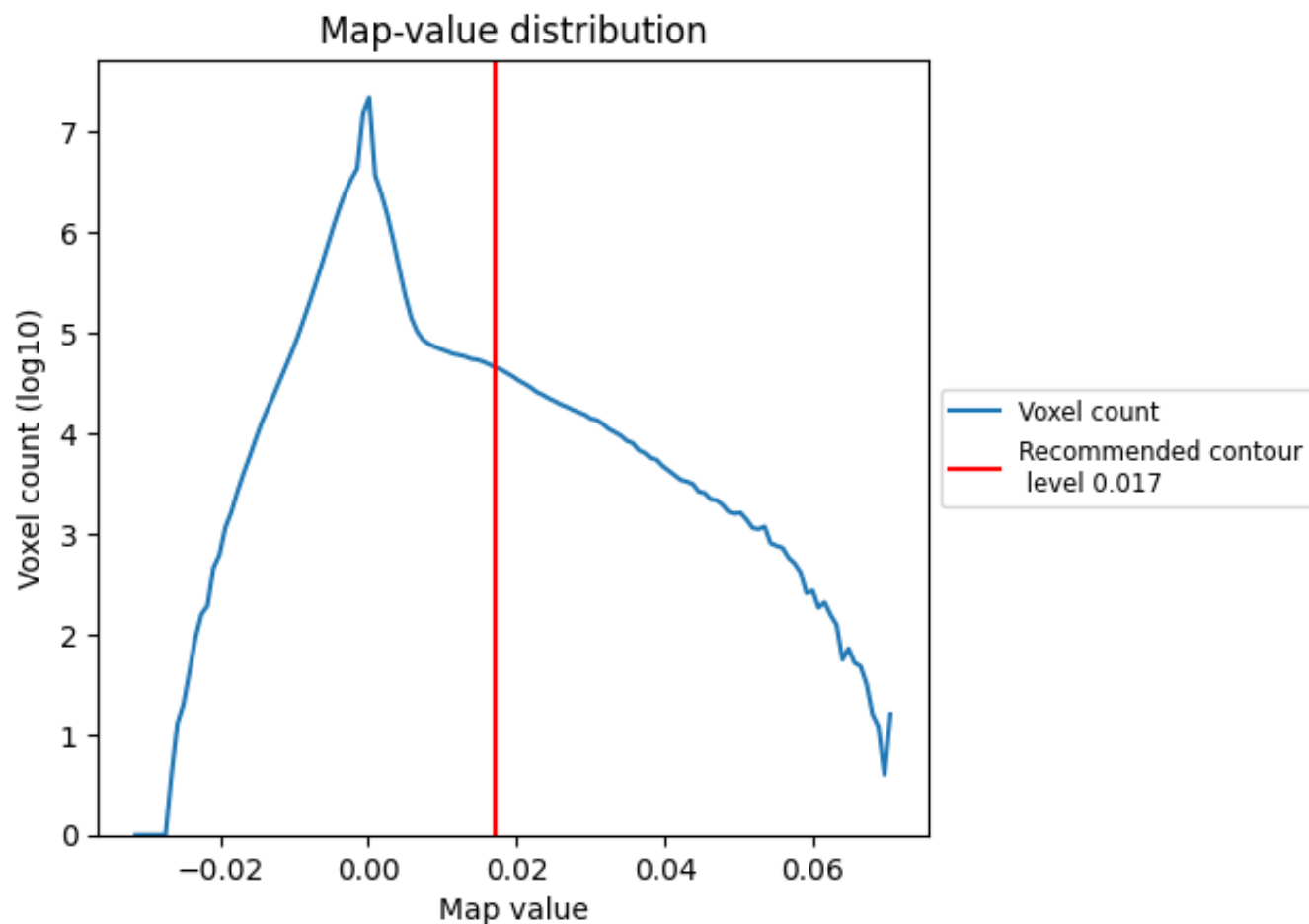
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

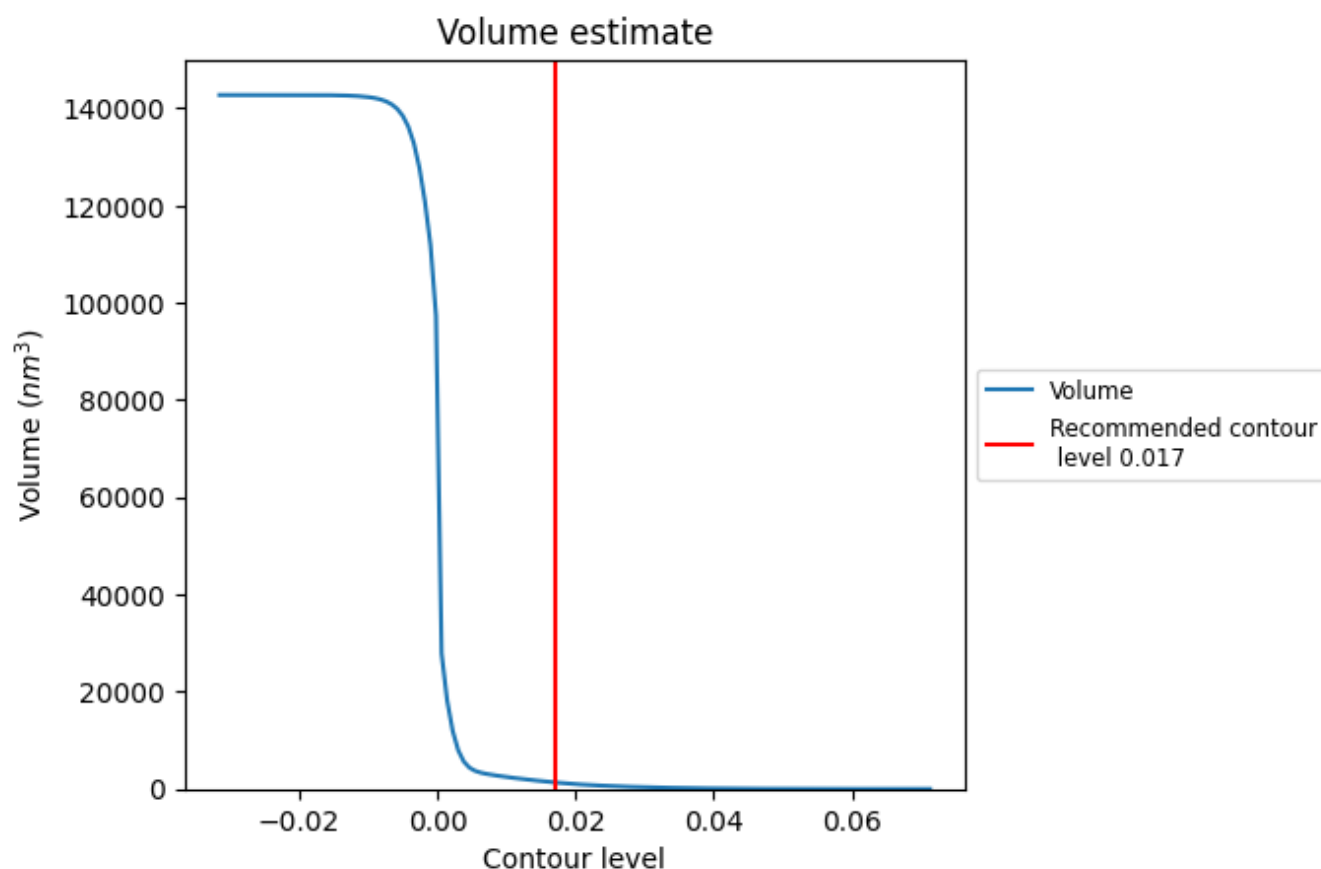
This section contains the results of statistical analysis of the map.

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.

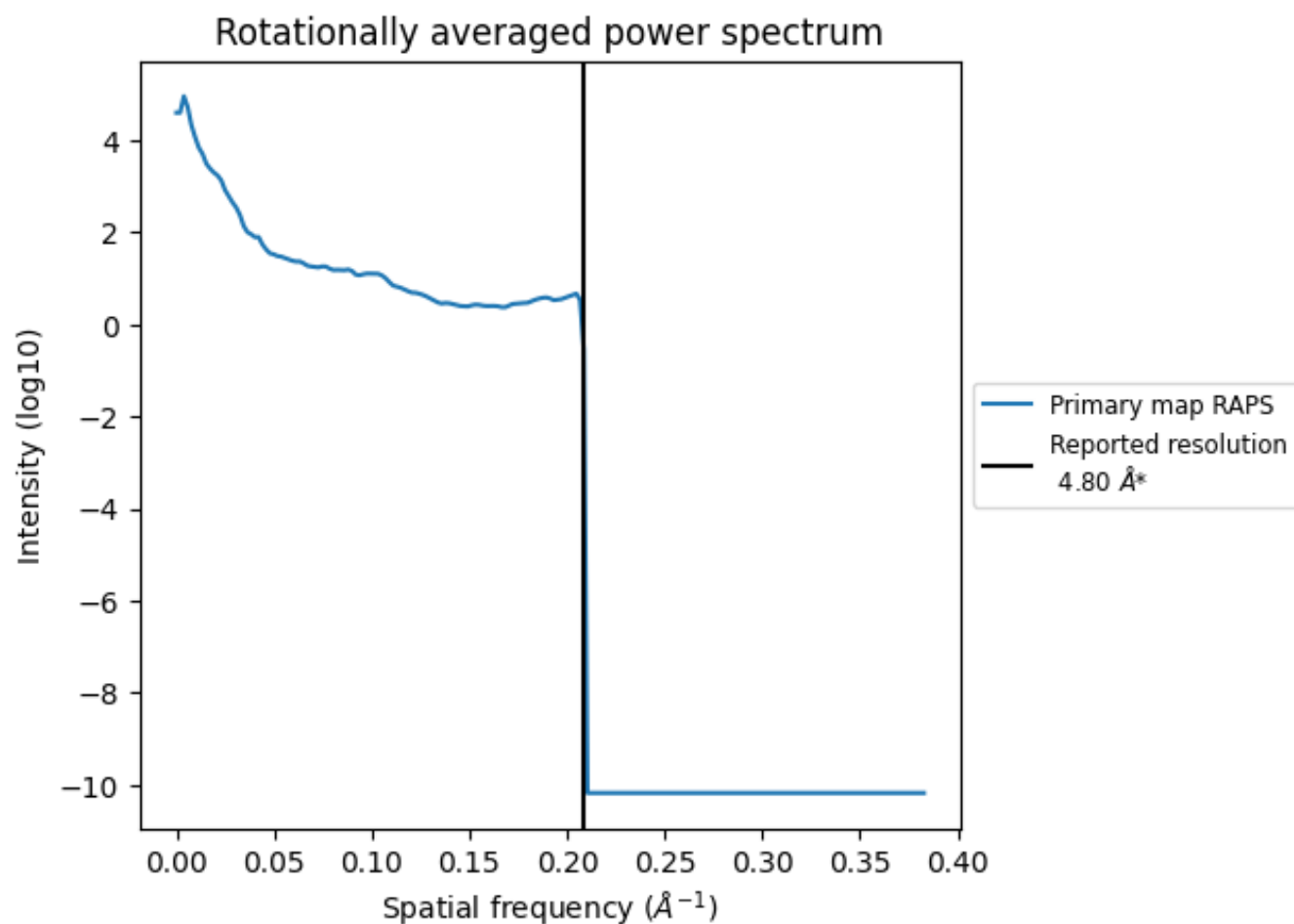
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1350 nm³; this corresponds to an approximate mass of 1219 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

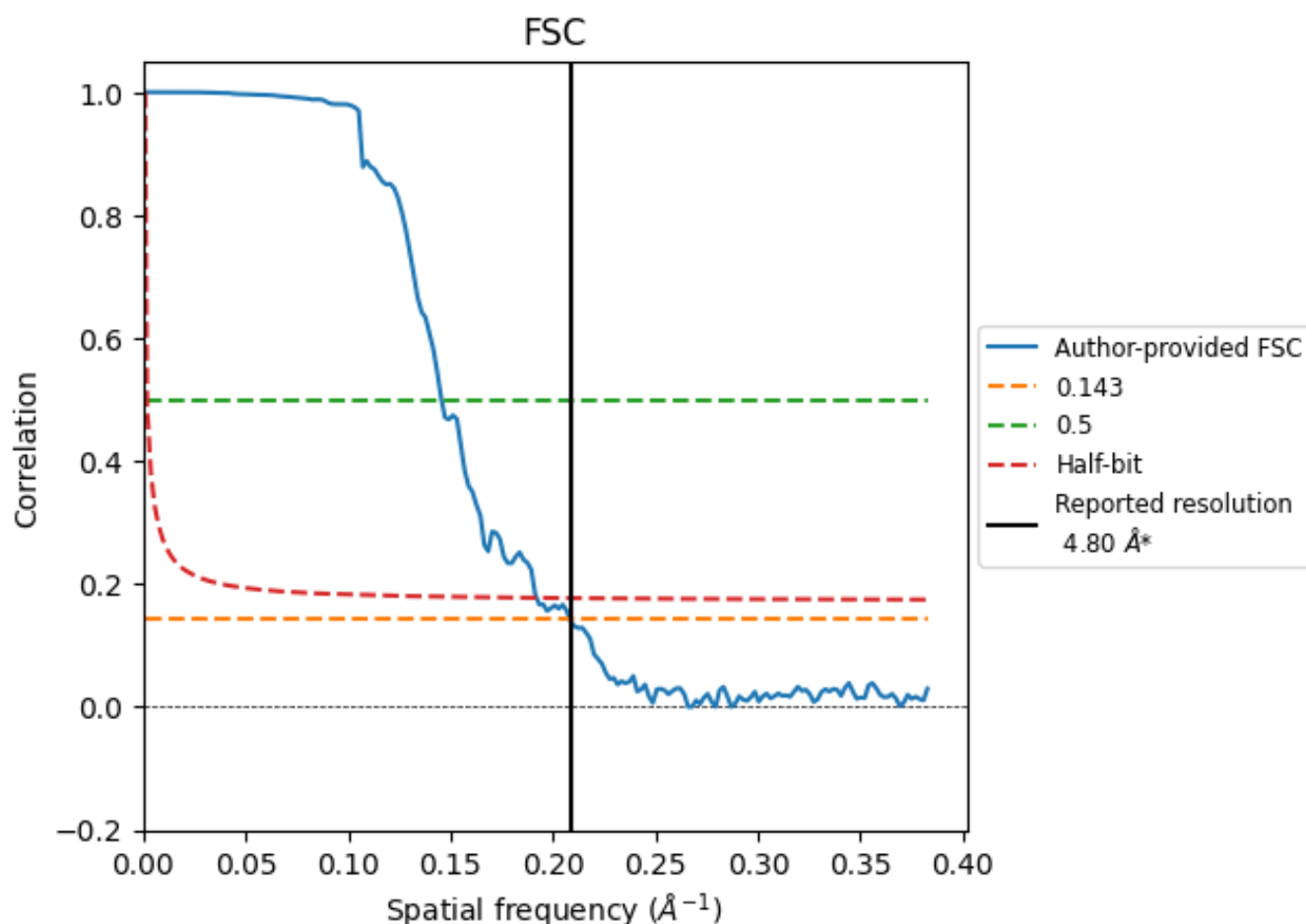


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

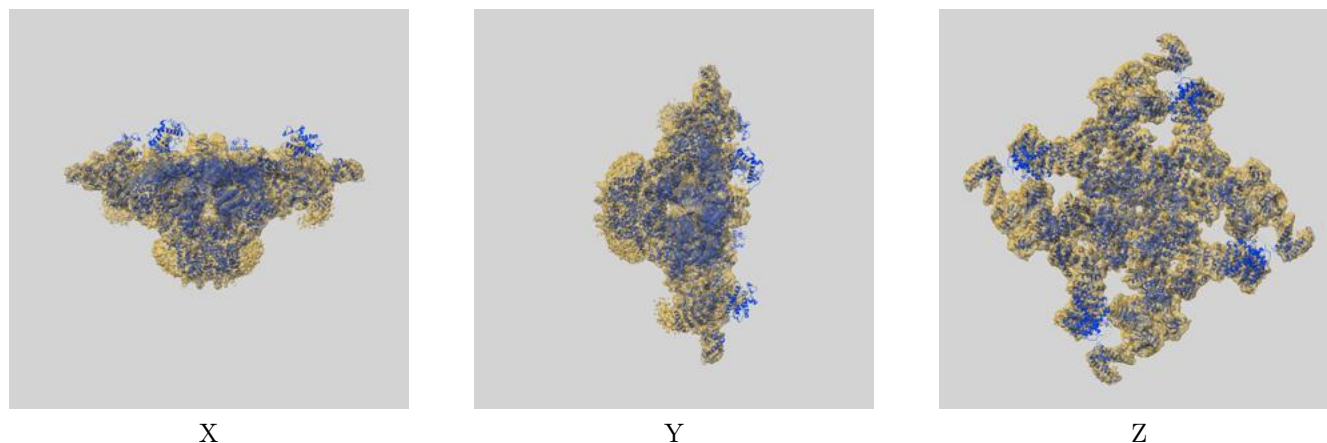
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.81	6.87	5.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

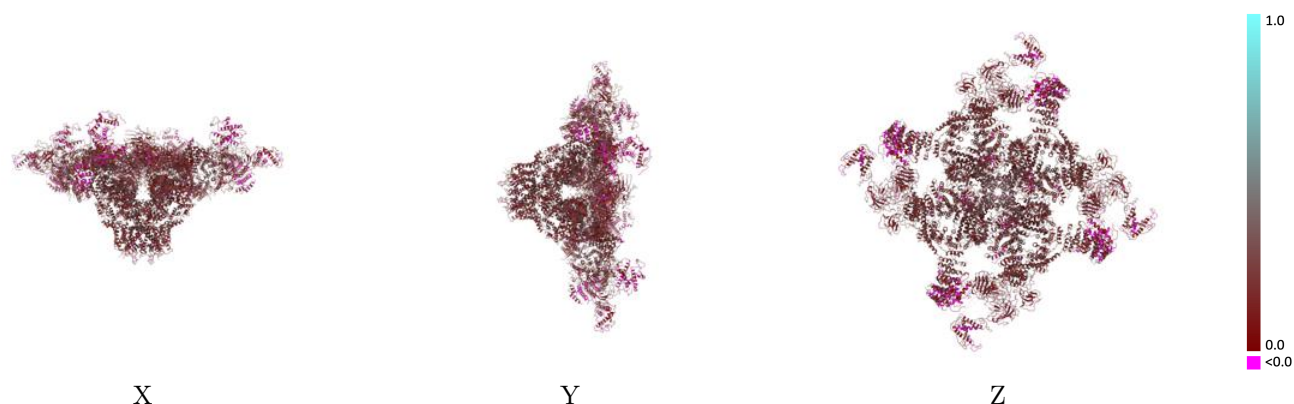
This section contains information regarding the fit between EMDB map EMD-9825 and PDB model 6JH6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



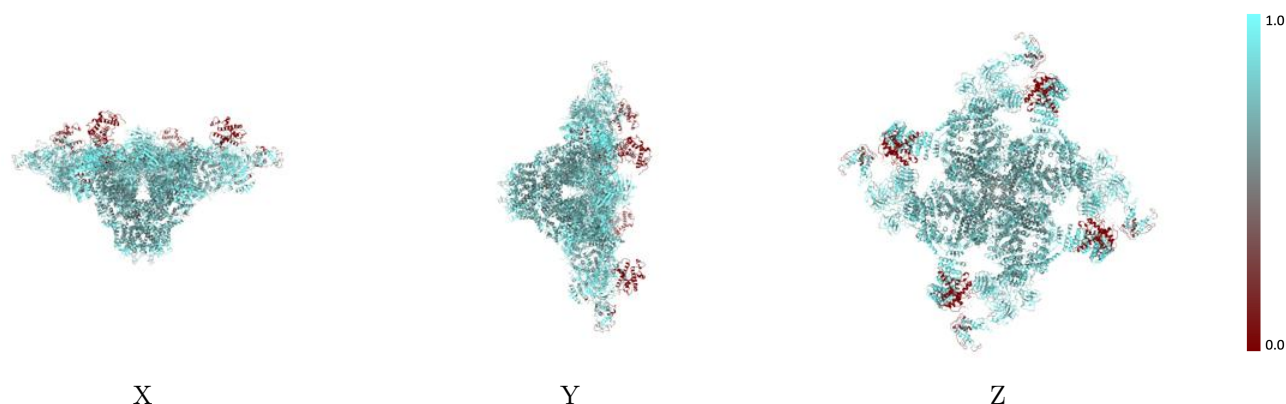
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



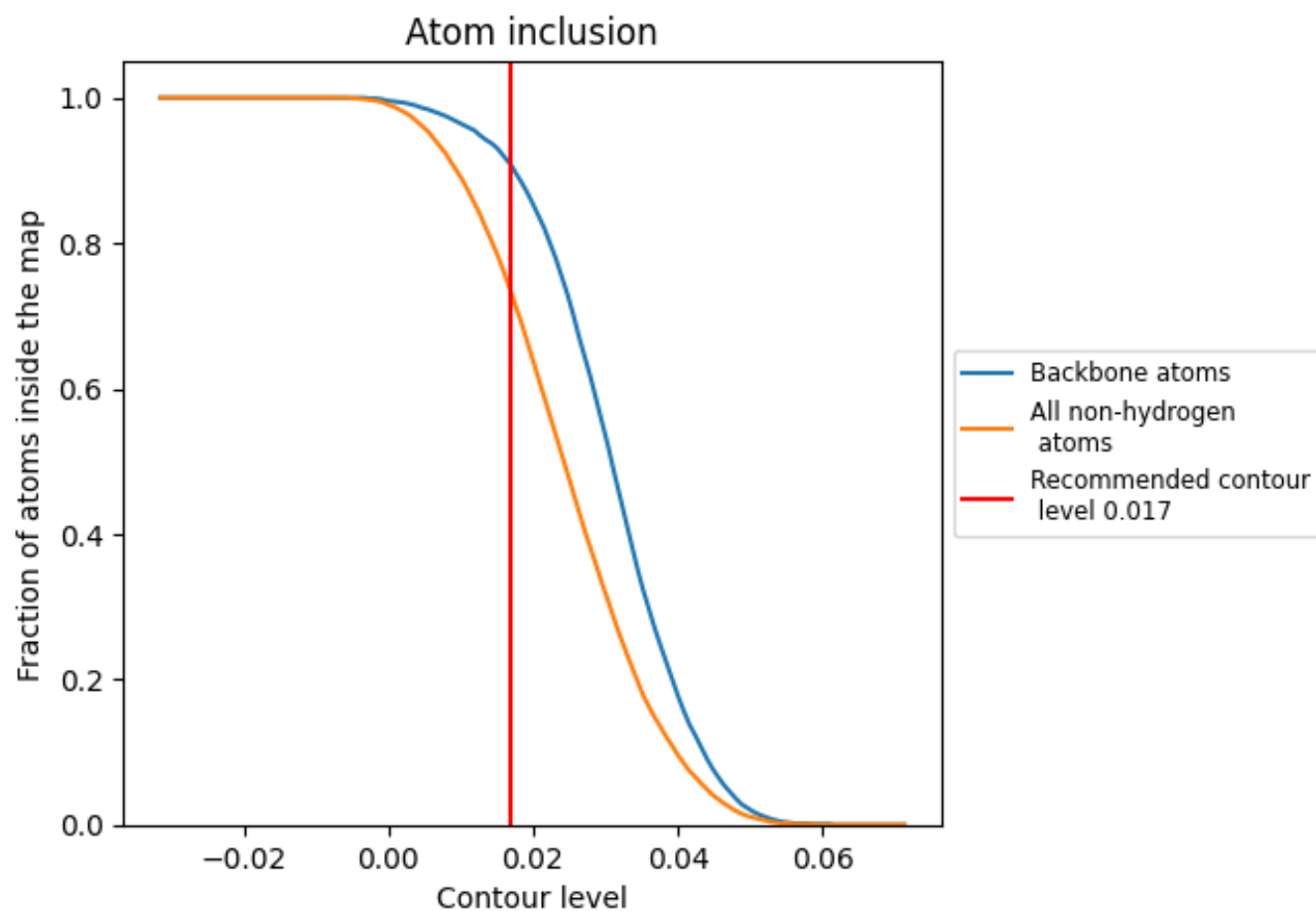
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 73% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.2220
A	0.7920	0.2290
B	0.7300	0.2220
C	0.7920	0.2300
D	0.7290	0.2220
E	0.7880	0.2300
F	0.7290	0.2220
G	0.7890	0.2260
H	0.7290	0.2210

