



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:35 AM UTC

PDB ID : 6JIY / pdb_00006jiy
EMDB ID : EMD-9837
Title : Structure of RyR2 (F/A/C/H-Ca²⁺/Ca²⁺+CaM dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-24
Resolution : 3.90 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:

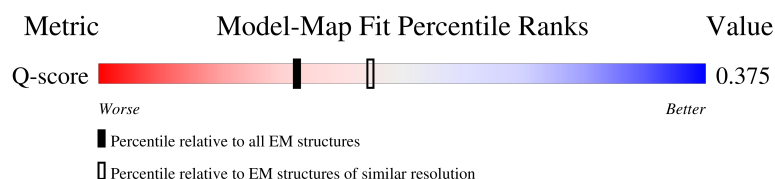
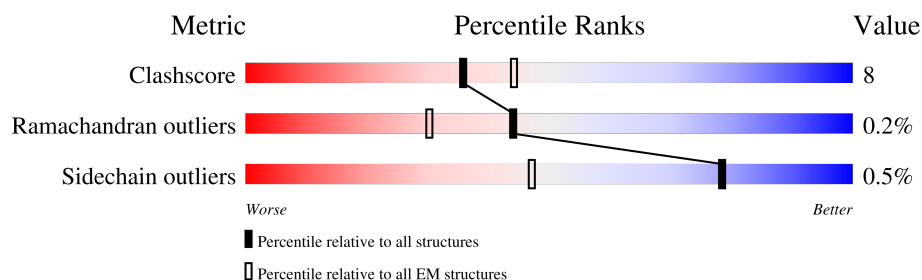
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

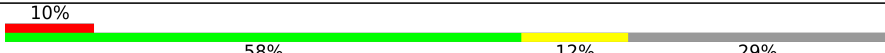
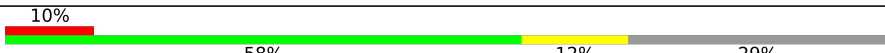
The reported resolution of this entry is 3.90 Å.

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	8855 (3.40 - 4.40)

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	4968	
1	D	4968	
1	G	4968	
1	J	4968	

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Mol	Chain	Length	Quality of chain
2	B	108	
2	E	108	
2	H	108	
2	K	108	
3	C	149	
3	F	149	
3	I	149	
3	L	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CFF	A	6003	-	X	-	-
7	CFF	D	6003	-	X	-	-
7	CFF	G	6003	-	X	-	-
7	CFF	J	6003	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 115288 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	D	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	G	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	J	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	K	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	F	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	I	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	L	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		

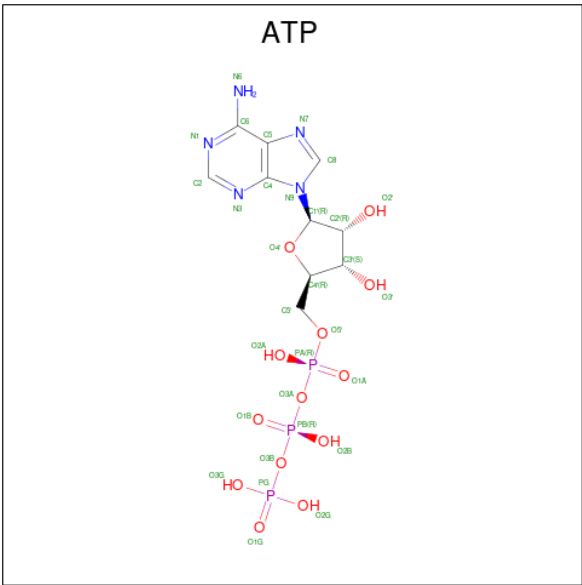
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

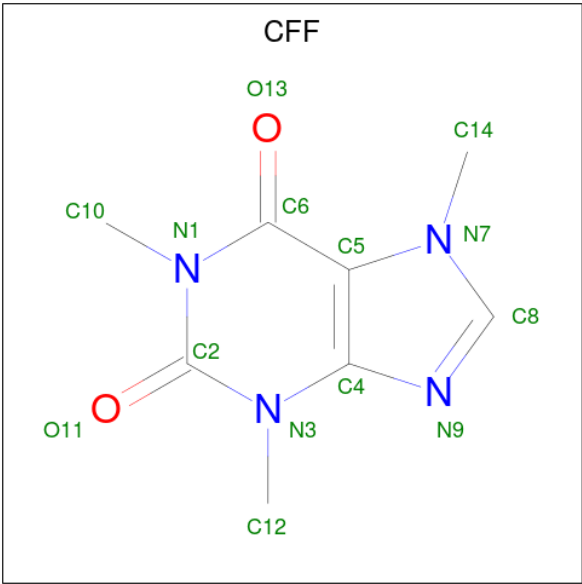
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	C	4	Total 4	Ca 4	0
5	D	1	Total 1	Ca 1	0
5	F	4	Total 4	Ca 4	0
5	G	1	Total 1	Ca 1	0
5	I	4	Total 4	Ca 4	0
5	J	1	Total 1	Ca 1	0
5	L	4	Total 4	Ca 4	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	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 CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).

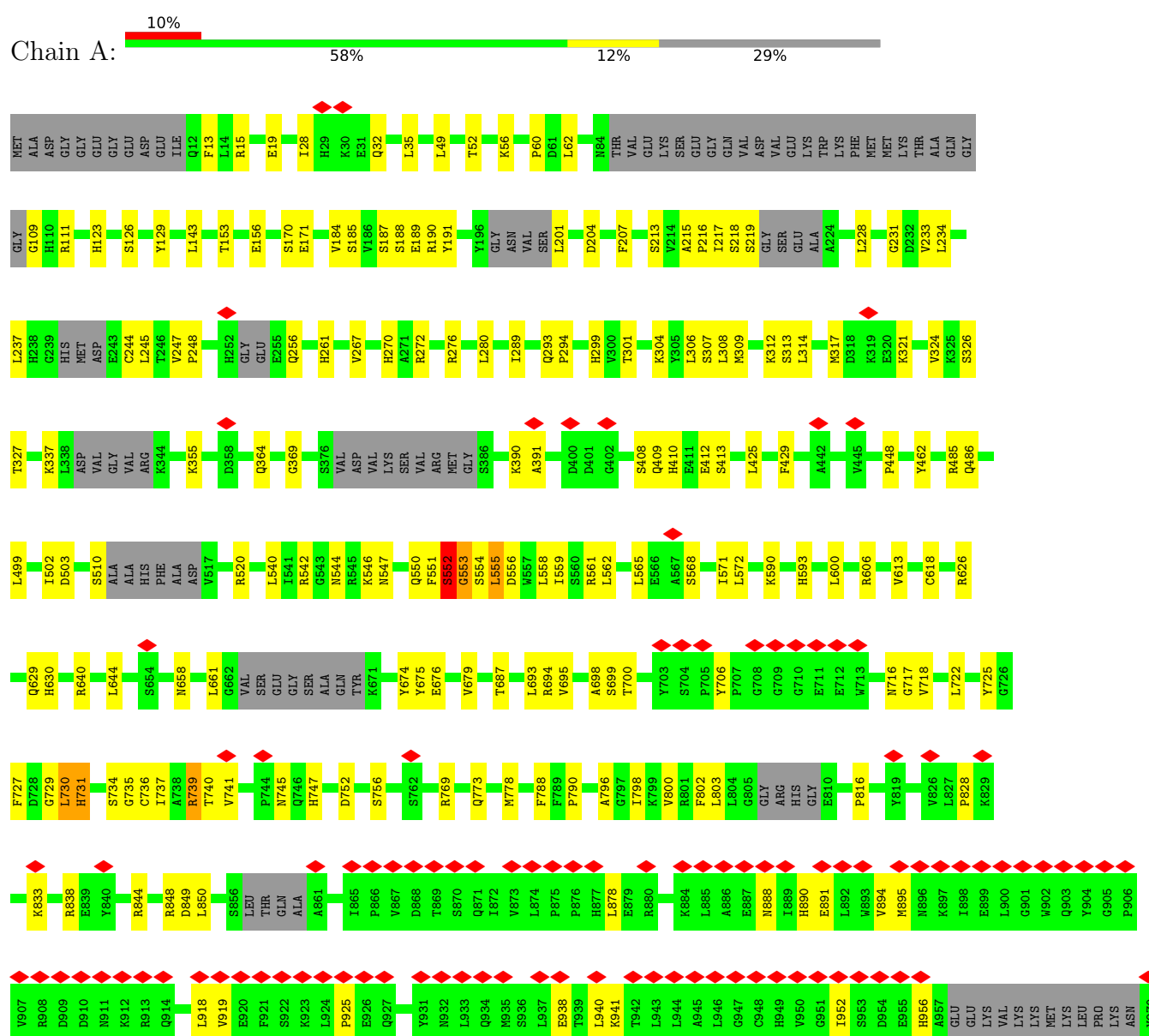


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 4	O 2	0
7	D	1	Total 14	C 8	N 4	O 2	0
7	G	1	Total 14	C 8	N 4	O 2	0
7	J	1	Total 14	C 8	N 4	O 2	0

3 Residue-property plots

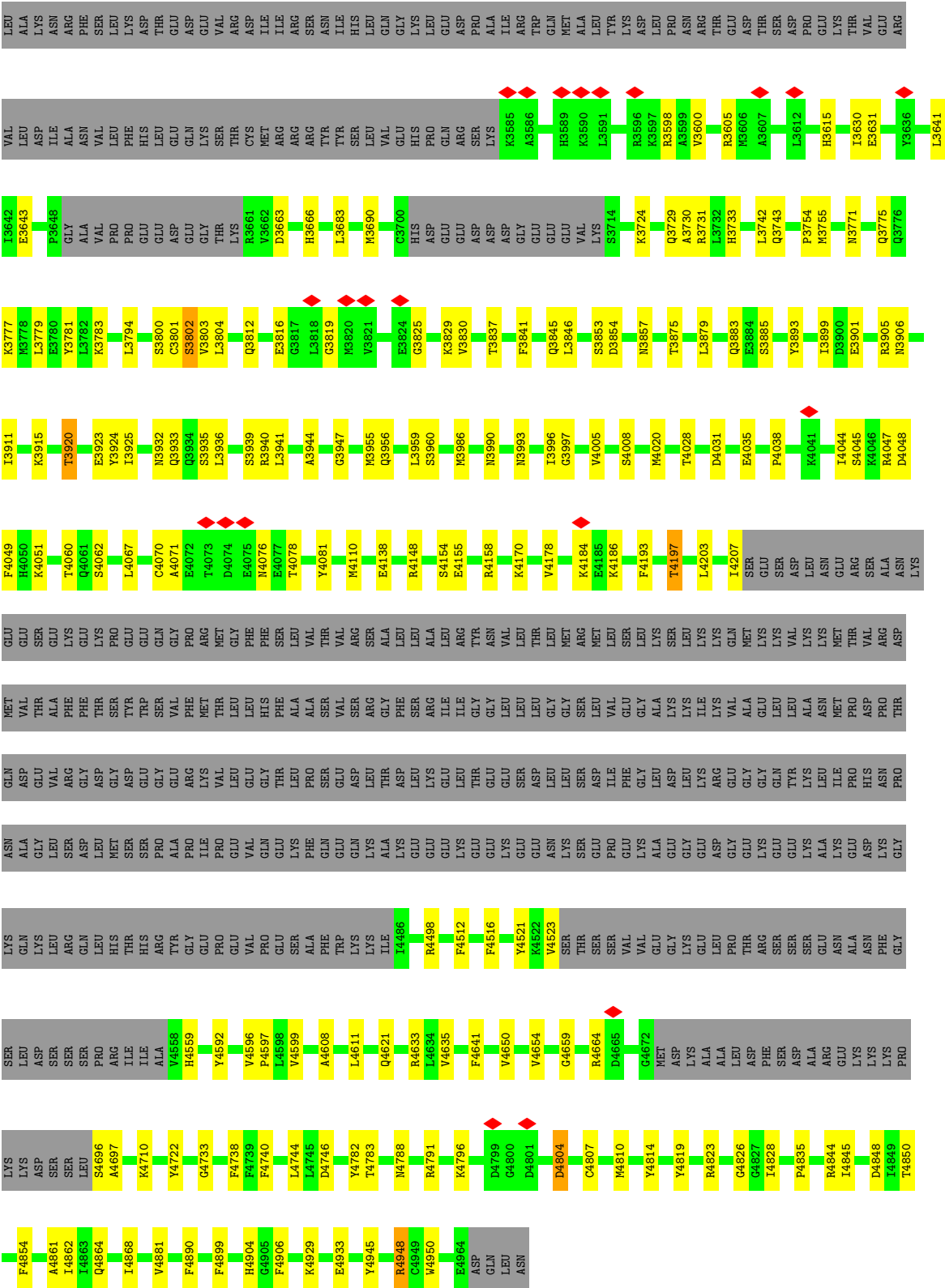
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RyR2









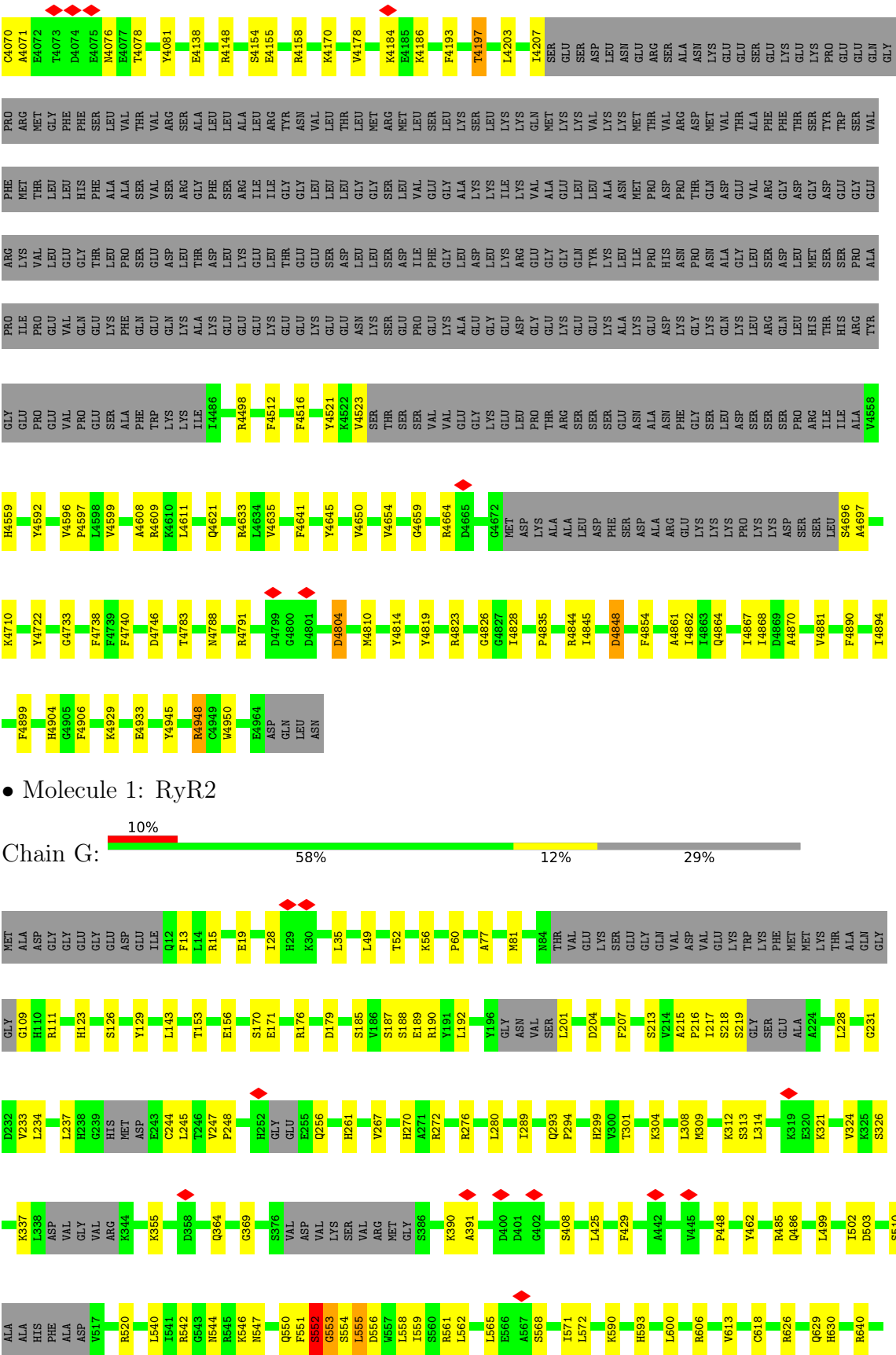
● Molecule 1: RyR2







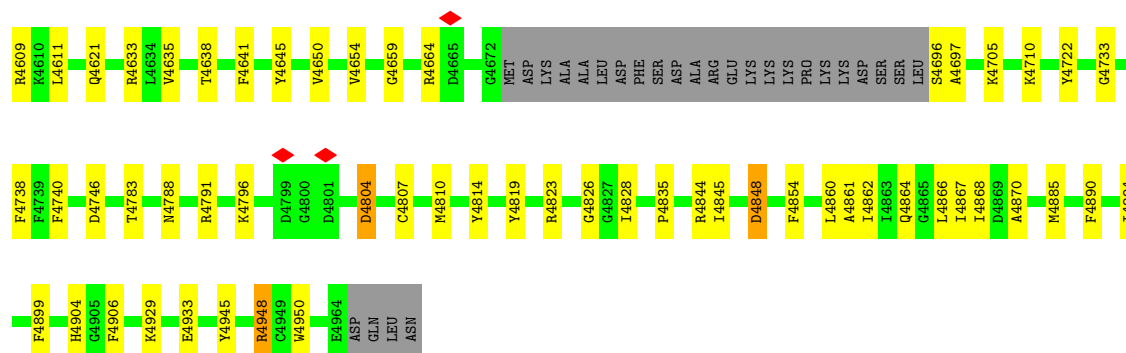




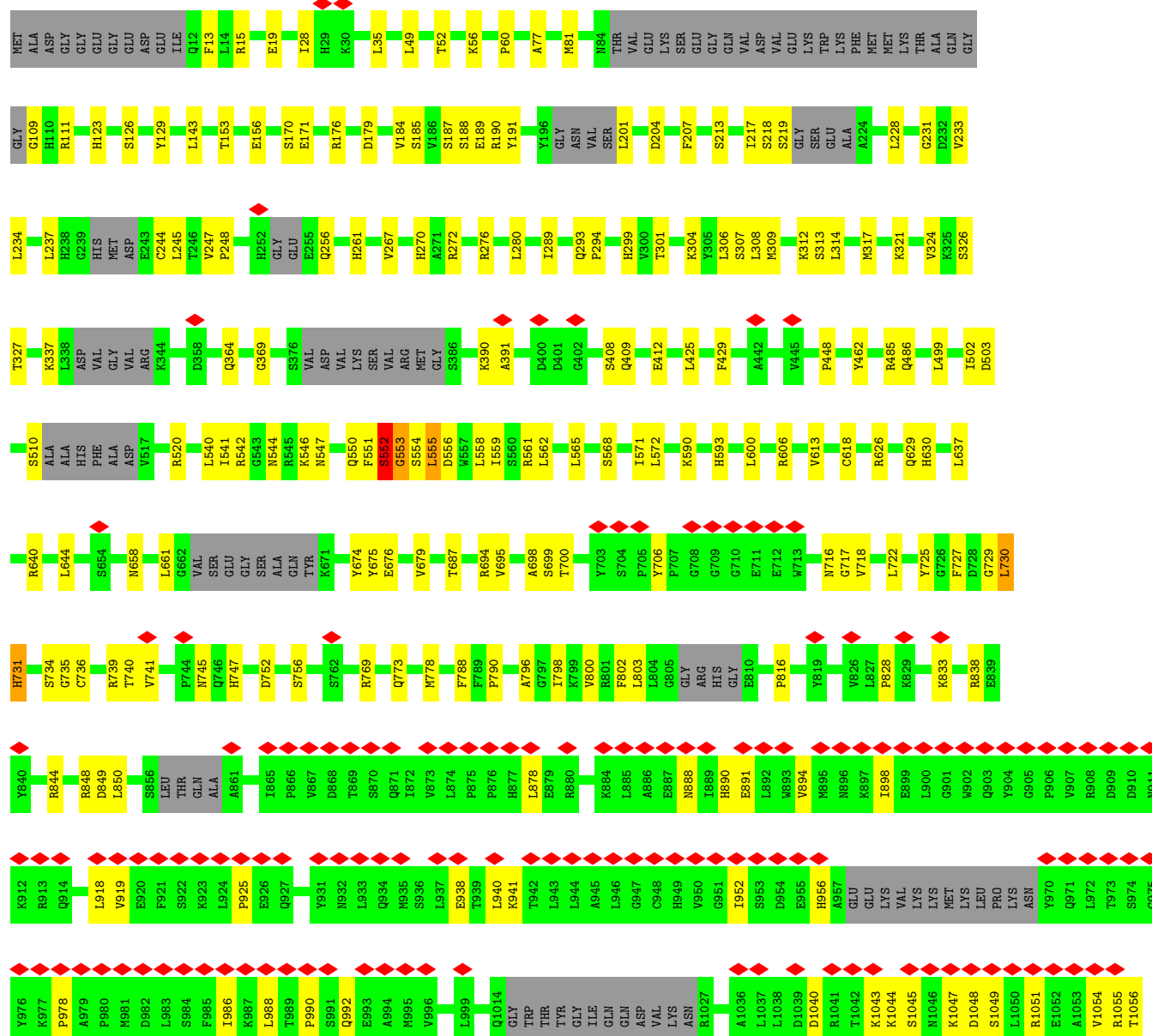






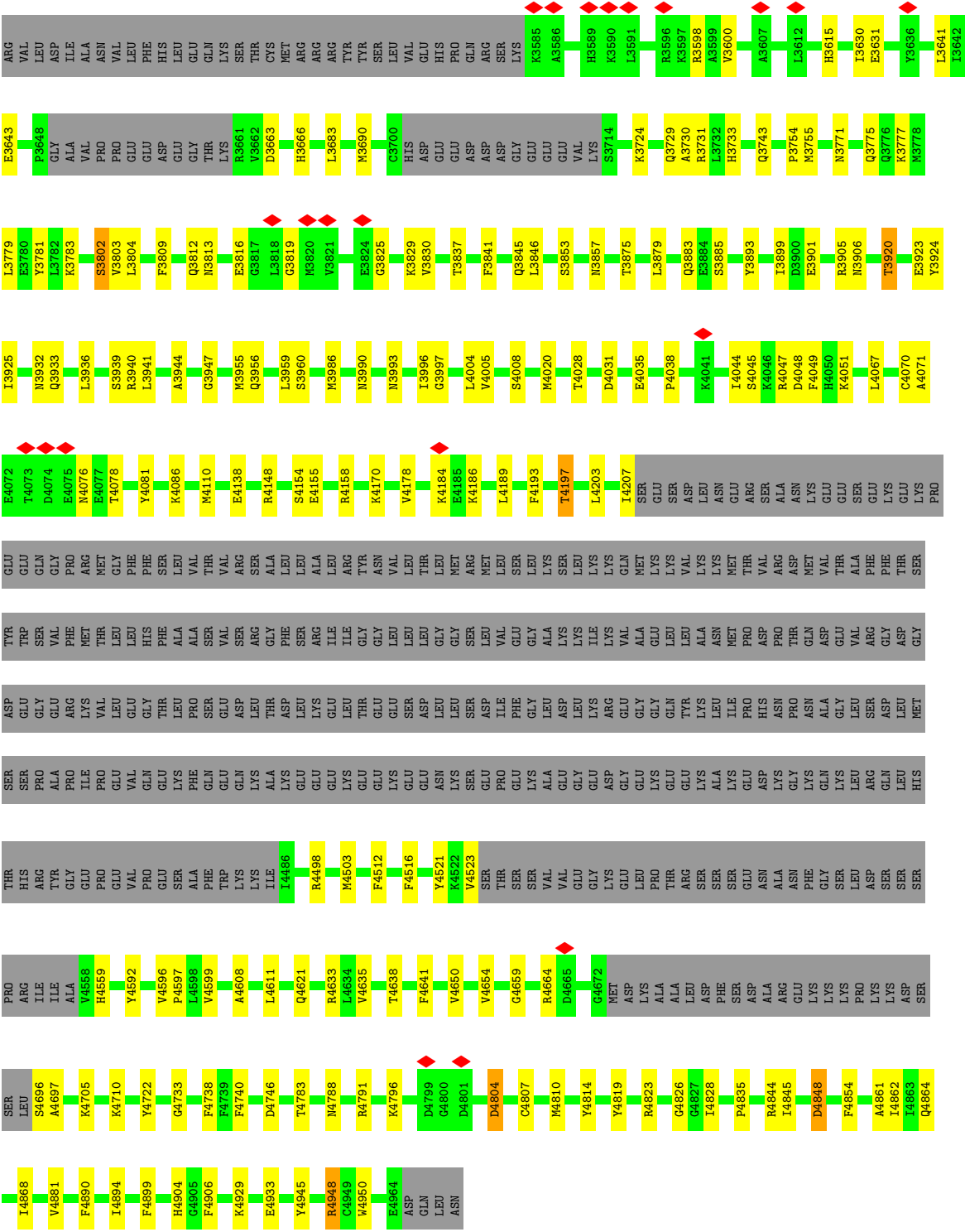


Molecule 1: RyR2

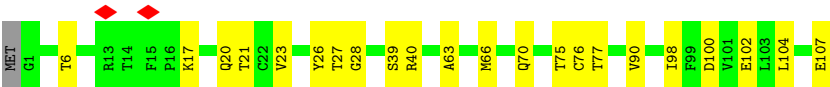
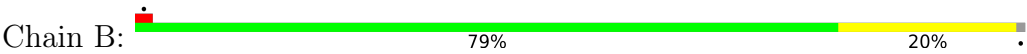


L1057	L1058	G1059	Y1060	G1061	Y1062	M1063	L1064	E1065	A1066	PRO	ASP	GLN	ASP	HIS	ALA	ALA	ARG	GLU	VAL	CYS	SER	GLY	THR	GLY	R1084	F1085	R1086	R1089	A1090	E1091	K1092	T1093	Y1094	G1099	Y1102	A1110	R1114	P1124	E1127	L1128	F1135	H1151	R1154	S1155	W1156	Q1157								
D1160	V1161	M1168	M1173	M1174	F1175	T1176	L1177	N1178	L1182	L1183	D1184	D1185	S1188	E1189	L1190	K1193	F1201	S1206	L1207	G1208	V1209	A1210	Q1211	R1214	K1219	D1220	K1225	L1229	G1230	L1232	Q1233	Y1236	E1237	A1240	V1241	W1250	L1251	S1252	K1253	R1254	L1255	P1256	Q1257	F1258										
L1259	Q1260	H1265	F1266	H1267	R1272	L1273	D1274	GLY	THR	ILE	ASP	SER	SER	PRO	CYS	LEU	V1285	T1286	S1292	Q1293	M1294	R1303	L1304	S1305	M1306	C1310	ALA	GLU	VAL	PHE	SER	THR	LYS	ALA	GLN	PRO	GLY	ILE	PRO	GLY	ALA	ASN	ASP	GLU	ASP	TYR								
ASP	ALA	ASP	ASP	PHE	GLU	VAL	LEU	MET	THR	ALA	HIS	GLY	HIS	VAL	VAL	PRO	ASP	ARG	ASP	LYS	ASP	GLU	ALA	THR	PHE	ASN	ALA	ASN	GLU	HIS	LYS	VAL	THR	ALA	GLN	LYS	PRO	ARG	GLN	ARG	THR	LYS	PRO	ASP	TYR									
SER	THR	HIS	SER	ALA	ARG	LEU	THR	ASP	VAL	LEU	ALA	ASP	ASP	ARG	ASP	TYR	TYR	LEU	MET	GLN	THR	SER	T1425	S1429	F1434	GLY	GLN	PRO	ALA	ALA	H1440	V1443	G1444	W1445	D1449	F1450	H1451	L1459	ASP	ARG	VAL	ARG	THR	E1472	K1473	G1474	K1475	V1476						
H1477	E1478	S1479	K1481	R1482	S1483	N1484	CYS	Y1486	M1487	V1488	C1489	A1490	GLY	GLU	SER	MET	PRO	GLY	GLN	GLY	ARG	ASN	N1502	V1510	Y1511	ASP	ALA	ALA	SER	G1516	S1528	P1535	V1543	E1556	LEU	GLY	ARG	ILE	LYS	ASN	VAL	MET	PRO	LEU	SER	A1568	K1572	S1573	F1574	H1575	K1576			
V1579	P1580	P1584	R1585	L1586	H1587	Y1588	Y1589	F1590	L1591	S1592	H1593	V1594	GLY	ALA	W1596	P1600	K1605	V1606	D1607	I1611	S1612	E1613	R1614	Q1615	Q1616	W1617	L1622	M1628	S1629	L1630	E1634	E1635	D1640	I1641	T1645	K1652	Y1655	R1659	L1667	G1668	N1669	H1670	R1671	E1682										
L1685	L1686	Y1687	P1695	R1699	Y1703	L1706	L1726	D1741	ASN	LYS	GLY	ASN	LYS	LYS	HIS	G1747	C1775	Y1776	Q1777	D1785	K1788	Q1800	S1803	D1808	L1824	M1831	I1842	L1843	E1847	F1848	S1849	VAL	PHE	LYS	GLU	ALA	GLY	ALA	PRO	GLU	GLU	GLU	ASP	THR										
LEU	GLU	GLU	PRO	CYS	ALA	GLU	SER	ASP	ARG	LEU	GLY	GLY	PRO	ALA	GLU	GLU	SER	LYS	GLY	GLY	LYS	ARG	PRO	LYS	GLY	G1893	M1907	V1934	L1937	N1940	Q1941	R1944	N1953	MET	SER	ALA	ALA	LEU	THR	ALA	LYS	LYS	GLU	PHE	ARG	SER	PRO							
GLN	GLU	ILE	ASN	MET	LEU	LEU	PHE	LYS	ASP	ASP	LYS	SER	G1987	P1988	C1989	P1990	I1993	R1994	L1997	D2013	GLU	ASP	GLY	SER	LEU	LEU	ASP	ALA	ASN	GLY	ASN	LYS	R2029	S2032	V2037	T2038	Y2039	LEU	LYS	LYS	LYS	ALA	GLU	GLY	VAL	GLU	SER							
ASP	SER	LYS	SER	T2058	L2059	V2075	I2076	L2088	Y2093	N2110	D2116	N2119	L2120	L2121	V2133	ARG	MET	GLY	E2138	L2147	I2150	N2153	K2154	V2155	E2174	V2177	G2181	GLY	GLU	GLY	SER	LYS	GLU	ILE	THR	PHE	P2191	Q2212	V2228	A2234														
V2235	R2236	P2240	A2246	V2267	L2270	C2273	G2274	L2275	GLN	SER	PRO	CYS	GLN	MET	LEU	VAL	SER	LYS	GLY	TYR	PRO	ASP	ILE	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435	V2436	I2437	S2438	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP
GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	GLY	F2461	D2464	H2465	K2466	V2476	Y2477	GLY	ILE	GLU	GLU	ASP	THR	THR	THR	HIS	H2487	L2503	ASP	THR	A2416	R2419	R2420	R2421	S2426	P2429	L2430	G2431	D2432	L2433	V2434	G2435</														



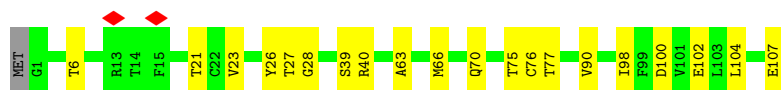


● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

Chain E: 



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

Chain H: 



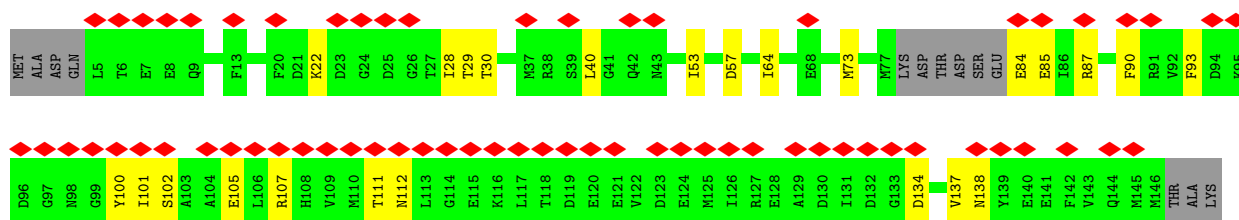
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K: 



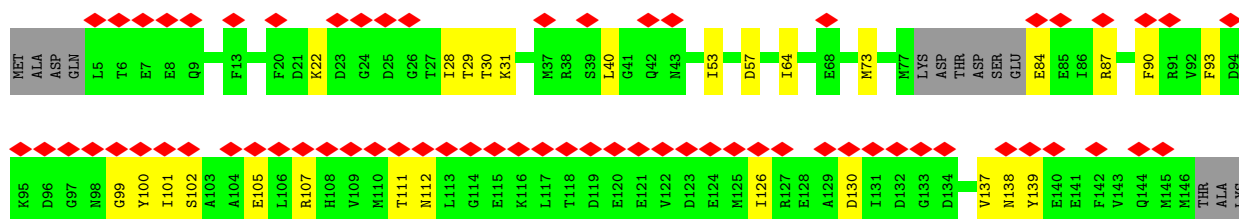
- Molecule 3: Calmodulin-1

Chain C: 



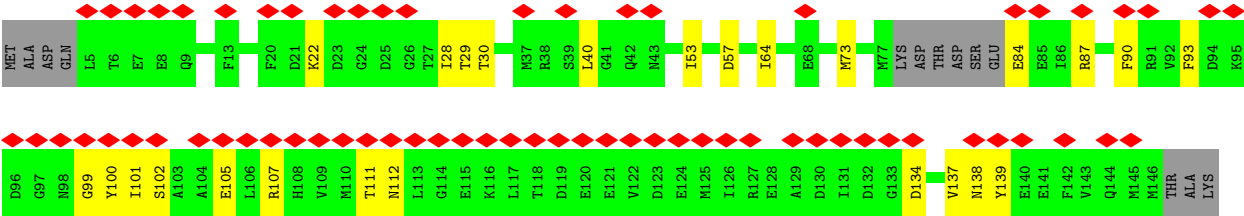
- Molecule 3: Calmodulin-1

Chain F: 

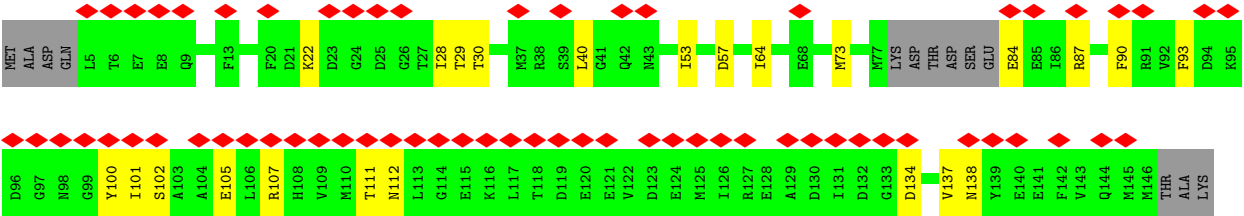
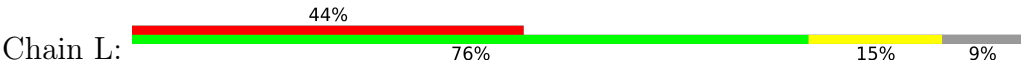


- Molecule 3: Calmodulin-1

Chain I: 



• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	96158	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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: ZN, CFF, CA, ATP

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	0.35	0/27385	0.62	7/37042 (0.0%)
1	D	0.35	0/27385	0.62	7/37042 (0.0%)
1	G	0.35	0/27385	0.62	7/37042 (0.0%)
1	J	0.35	0/27385	0.62	7/37042 (0.0%)
2	B	0.28	0/835	0.53	0/1123
2	E	0.28	0/835	0.53	0/1123
2	H	0.28	0/835	0.53	0/1123
2	K	0.28	0/835	0.53	0/1123
3	C	0.19	0/1086	0.45	0/1456
3	F	0.19	0/1086	0.46	0/1456
3	I	0.19	0/1086	0.45	0/1456
3	L	0.19	0/1086	0.46	0/1456
All	All	0.34	0/117224	0.61	28/158484 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	D	0	19
1	G	0	19
1	J	0	19
All	All	0	76

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2037	VAL	N-CA-C	-8.57	104.28	111.91
1	D	2037	VAL	N-CA-C	-8.57	104.28	111.91
1	G	2037	VAL	N-CA-C	-8.57	104.28	111.91
1	J	2037	VAL	N-CA-C	-8.54	104.31	111.91
1	A	4828	ILE	N-CA-C	-6.57	106.84	113.47

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	PHE	Peptide
1	A	552	SER	Peptide
1	A	729	GLY	Peptide
1	A	731	HIS	Peptide
1	A	739	ARG	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	26877	0	25382	467	0
1	D	26877	0	25382	477	0
1	G	26877	0	25382	468	0
1	J	26877	0	25382	460	0
2	B	819	0	824	12	0
2	E	819	0	824	12	0
2	H	819	0	824	12	0
2	K	819	0	824	13	0
3	C	1075	0	1011	16	0
3	F	1075	0	1011	17	0
3	I	1075	0	1011	17	0
3	L	1075	0	1011	15	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
5	F	4	0	0	0	0
5	G	1	0	0	0	0
5	I	4	0	0	0	0
5	J	1	0	0	0	0
5	L	4	0	0	0	0
6	A	31	0	12	1	0
6	D	31	0	12	1	0
6	G	31	0	12	1	0
6	J	31	0	12	1	0
7	A	14	0	10	1	0
7	D	14	0	10	1	0
7	G	14	0	10	1	0
7	J	14	0	10	1	0
All	All	115288	0	108956	1754	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 8.

The worst 5 of 1754 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:G:4862:ILE:HG22	1:J:4868:ILE:CD1	1.57	1.35
1:A:4868:ILE:CD1	1:J:4862:ILE:HG22	1.58	1.34
1:D:4862:ILE:HG22	1:G:4868:ILE:CD1	1.59	1.30
1:A:4862:ILE:HG22	1:D:4868:ILE:CD1	1.60	1.30
1:G:4862:ILE:CG2	1:J:4868:ILE:HD13	1.64	1.28

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	3405/4968 (68%)	2973 (87%)	423 (12%)	9 (0%)	36	69
1	D	3405/4968 (68%)	2974 (87%)	422 (12%)	9 (0%)	36	69
1	G	3405/4968 (68%)	2973 (87%)	423 (12%)	9 (0%)	36	69
1	J	3405/4968 (68%)	2974 (87%)	422 (12%)	9 (0%)	36	69
2	B	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	E	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	H	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	K	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
3	C	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	F	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	I	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	L	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
All	All	14568/20900 (70%)	12750 (88%)	1782 (12%)	36 (0%)	44	74

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	553	GLY
1	A	1776	TYR
1	D	553	GLY
1	D	1776	TYR
1	G	553	GLY

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	2701/4355 (62%)	2687 (100%)	14 (0%)	81	82
1	D	2700/4355 (62%)	2684 (99%)	16 (1%)	78	80
1	G	2700/4355 (62%)	2684 (99%)	16 (1%)	78	80
1	J	2700/4355 (62%)	2684 (99%)	16 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	88/89 (99%)	88 (100%)	0	100	100
2	E	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
2	K	88/89 (99%)	88 (100%)	0	100	100
3	C	116/127 (91%)	116 (100%)	0	100	100
3	F	116/127 (91%)	116 (100%)	0	100	100
3	I	116/127 (91%)	116 (100%)	0	100	100
3	L	116/127 (91%)	116 (100%)	0	100	100
All	All	11617/18284 (64%)	11555 (100%)	62 (0%)	78	82

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4197	THR
1	J	2419	ARG
1	G	1176	THR
1	J	2076	ILE
1	J	3920	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 233 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	112	ASN
1	J	4089	HIS
1	G	1684	GLN
1	J	3993	ASN
1	J	1587	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 24 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
6	ATP	G	6002	-	32,33,33	1.29	6 (18%)	48,52,52	1.80	9 (18%)
7	CFF	G	6003	-	15,15,15	2.15	8 (53%)	23,23,23	2.72	9 (39%)
7	CFF	A	6003	-	15,15,15	2.15	8 (53%)	23,23,23	2.72	9 (39%)
7	CFF	J	6003	-	15,15,15	2.14	8 (53%)	23,23,23	2.71	9 (39%)
6	ATP	D	6002	-	32,33,33	1.29	6 (18%)	48,52,52	1.79	9 (18%)
6	ATP	A	6002	-	32,33,33	1.29	6 (18%)	48,52,52	1.80	9 (18%)
7	CFF	D	6003	-	15,15,15	2.15	8 (53%)	23,23,23	2.72	9 (39%)
6	ATP	J	6002	-	32,33,33	1.29	6 (18%)	48,52,52	1.80	9 (18%)

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
6	ATP	G	6002	-	-	6/22/38/38	0/3/3/3
7	CFF	G	6003	-	-	-	0/2/2/2
7	CFF	A	6003	-	-	-	0/2/2/2
7	CFF	J	6003	-	-	-	0/2/2/2
6	ATP	D	6002	-	-	6/22/38/38	0/3/3/3
6	ATP	A	6002	-	-	6/22/38/38	0/3/3/3
7	CFF	D	6003	-	-	-	0/2/2/2
6	ATP	J	6002	-	-	6/22/38/38	0/3/3/3

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	6003	CFF	C6-N1	-4.34	1.31	1.40
7	A	6003	CFF	C6-N1	-4.32	1.31	1.40
7	D	6003	CFF	C6-N1	-4.32	1.31	1.40
7	J	6003	CFF	C6-N1	-4.32	1.31	1.40
6	J	6002	ATP	C5-C4	4.04	1.46	1.39

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	6003	CFF	C14-N7-C8	-7.71	111.85	126.28
7	D	6003	CFF	C14-N7-C8	-7.71	111.85	126.28
7	G	6003	CFF	C14-N7-C8	-7.71	111.85	126.28
7	J	6003	CFF	C14-N7-C8	-7.71	111.85	126.28
6	J	6002	ATP	C5-C4-N3	-5.99	118.47	126.72

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O1A
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C5'-O5'-PA-O3A
6	D	6002	ATP	C5'-O5'-PA-O1A
6	D	6002	ATP	C5'-O5'-PA-O2A

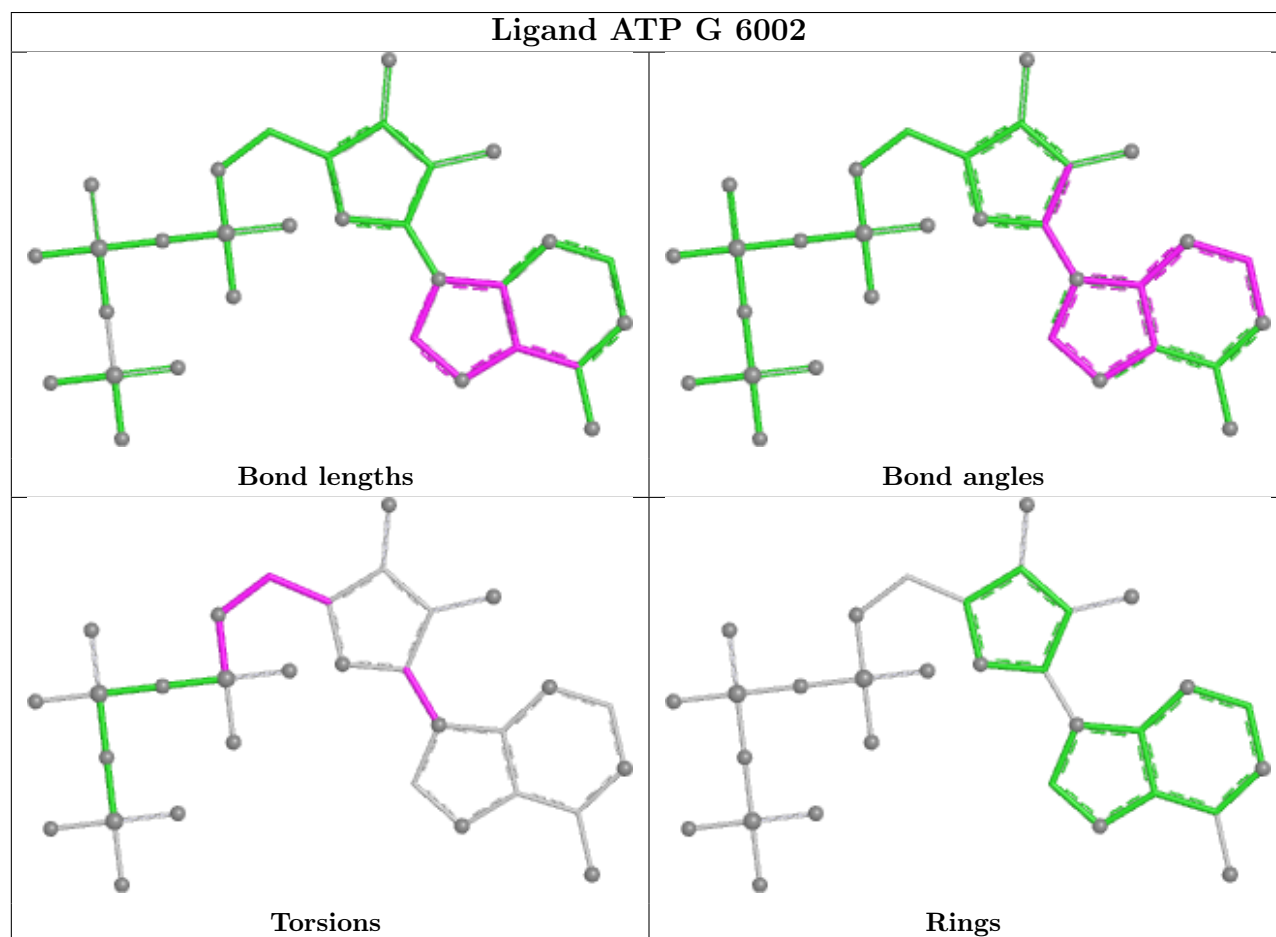
There are no ring outliers.

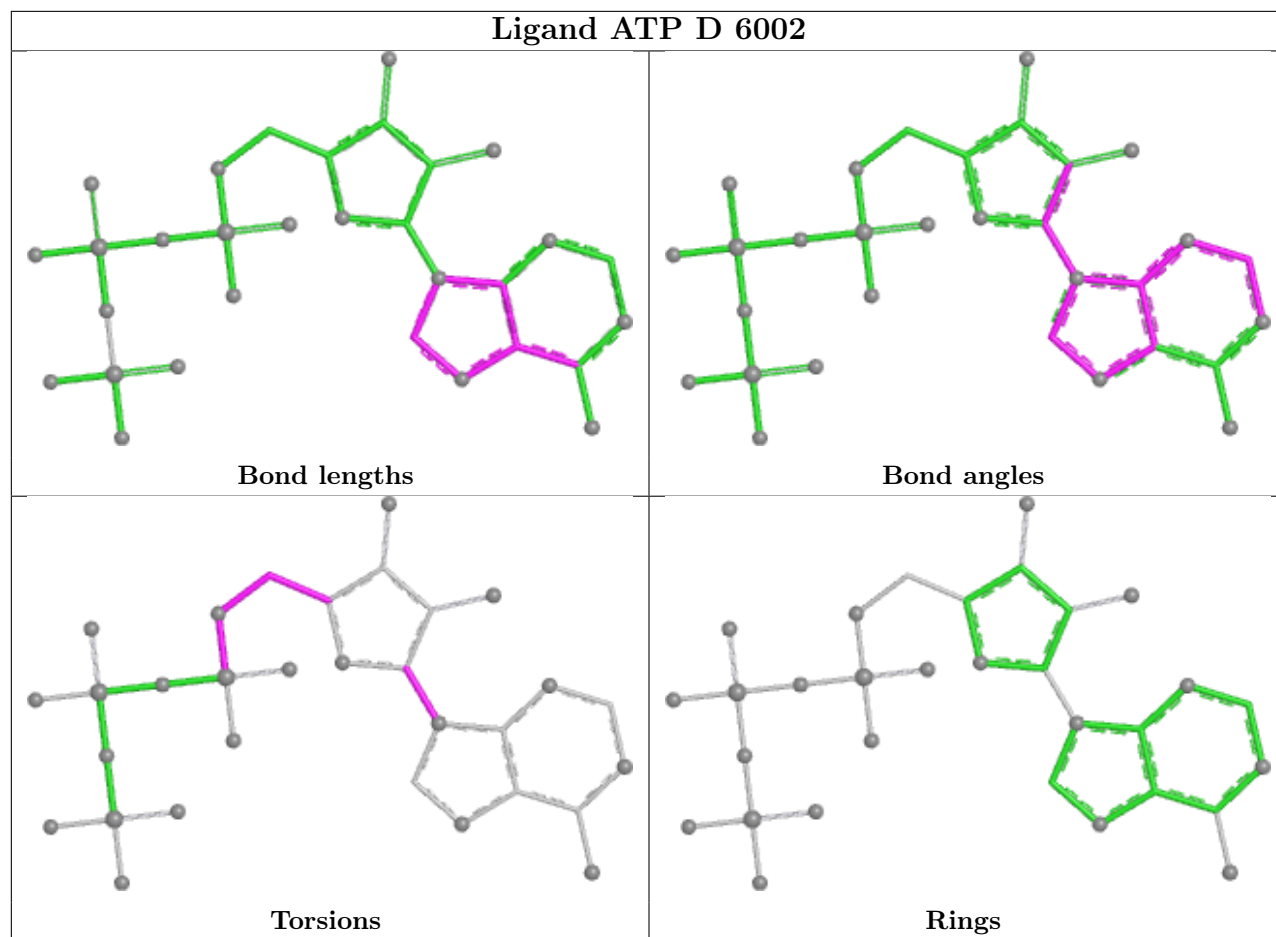
8 monomers are involved in 8 short contacts:

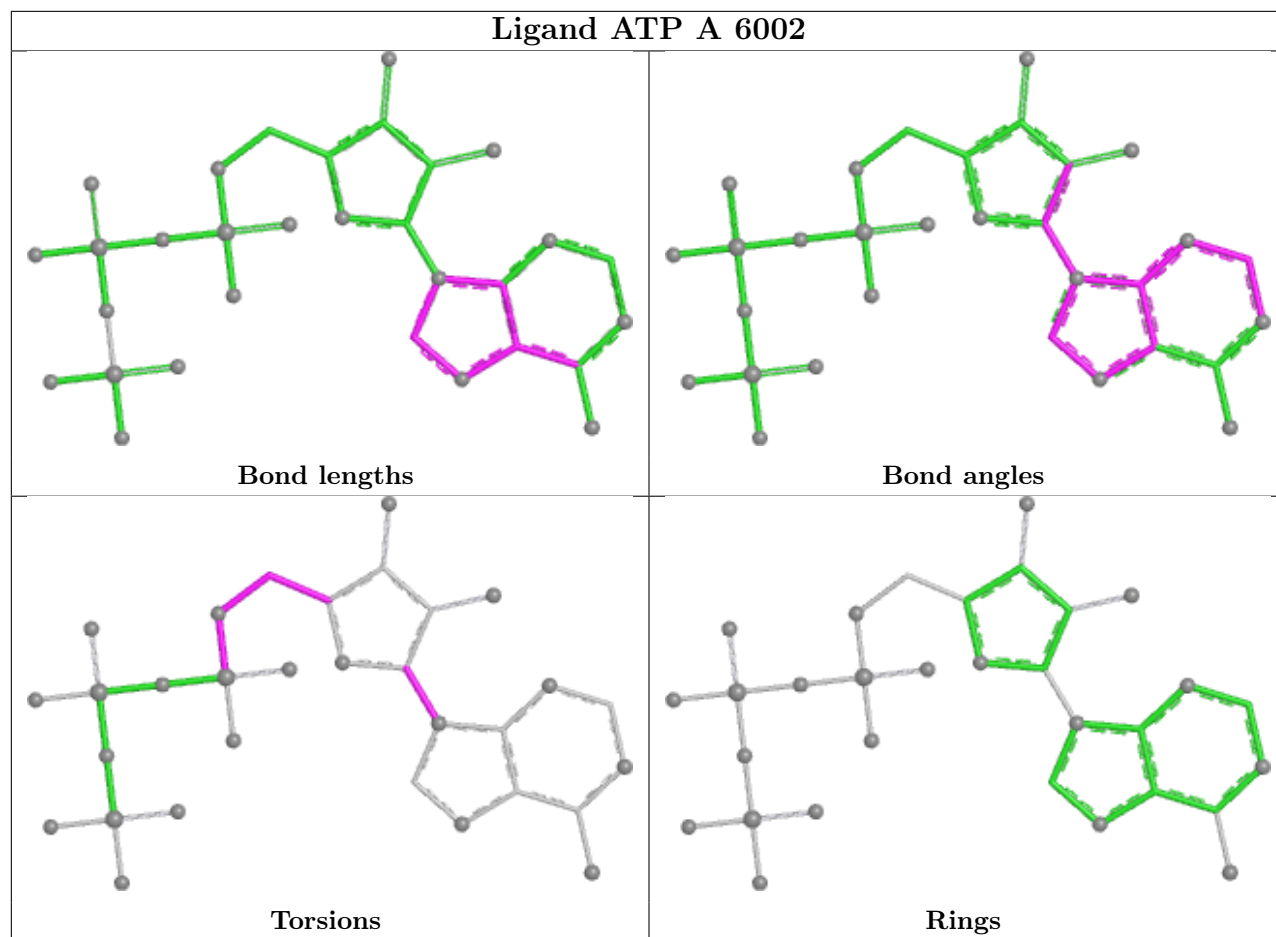
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	6002	ATP	1	0
7	G	6003	CFF	1	0
7	A	6003	CFF	1	0
7	J	6003	CFF	1	0
6	D	6002	ATP	1	0
6	A	6002	ATP	1	0
7	D	6003	CFF	1	0
6	J	6002	ATP	1	0

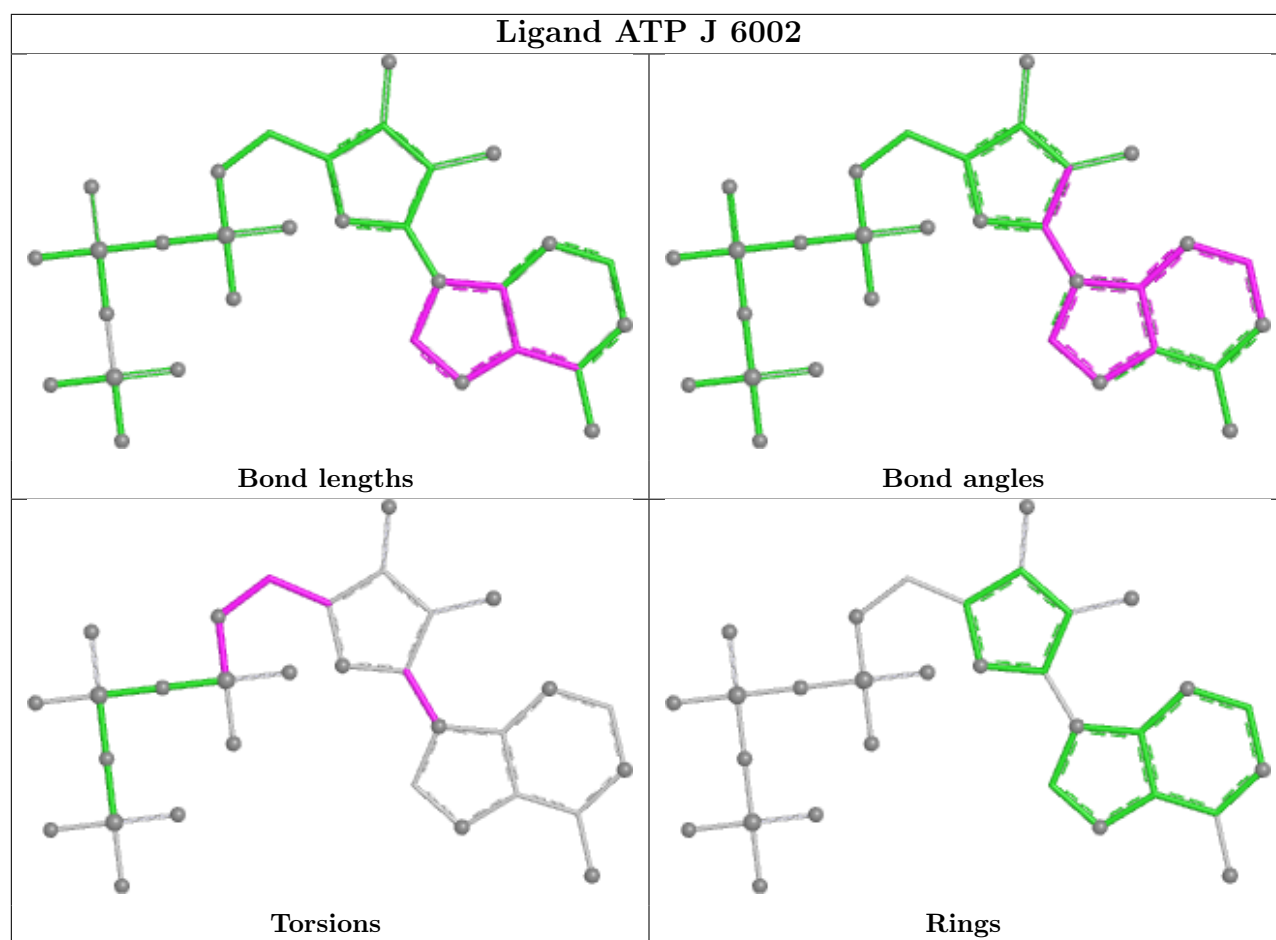
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

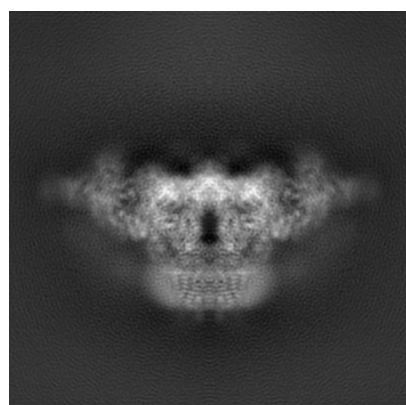
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9837. These allow visual inspection of the internal detail of the map and identification of artifacts.

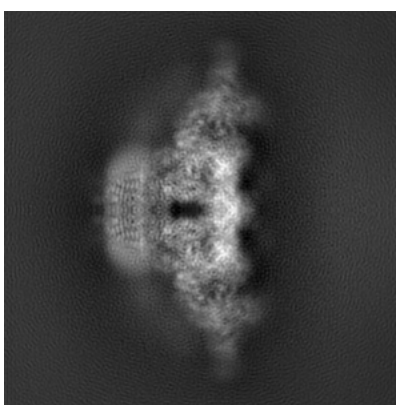
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

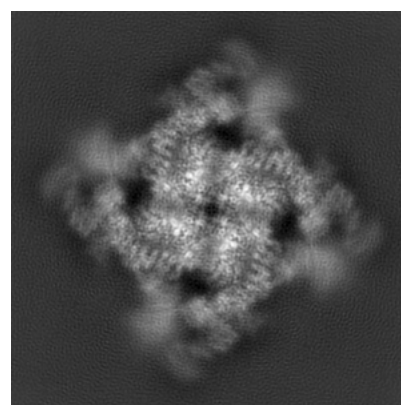
6.1.1 Primary map



X



Y

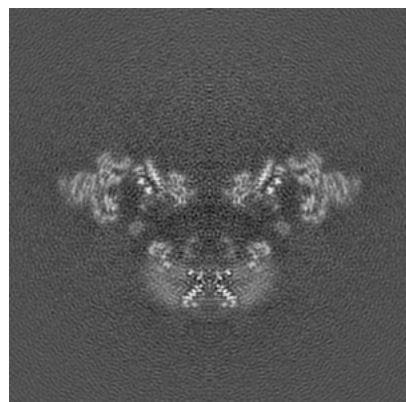


Z

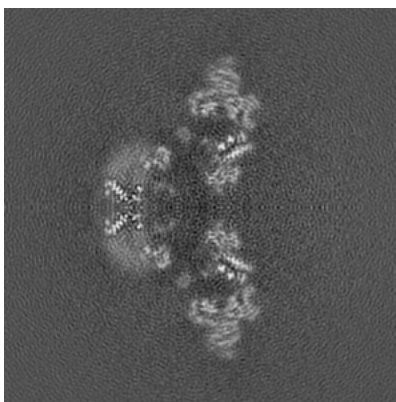
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

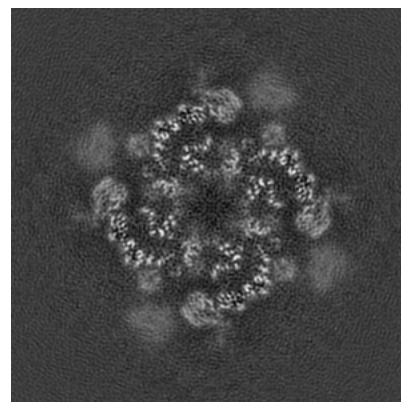
6.2.1 Primary map



X Index: 200



Y Index: 200

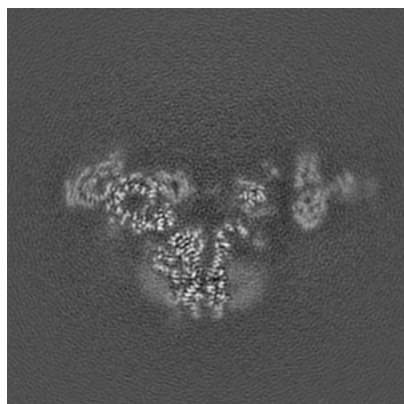


Z Index: 200

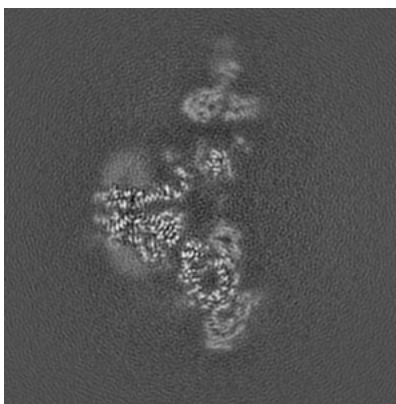
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

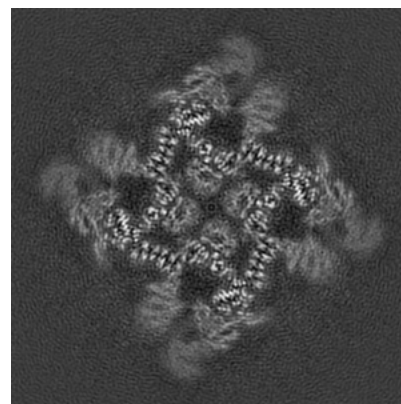
6.3.1 Primary map



X Index: 212



Y Index: 188

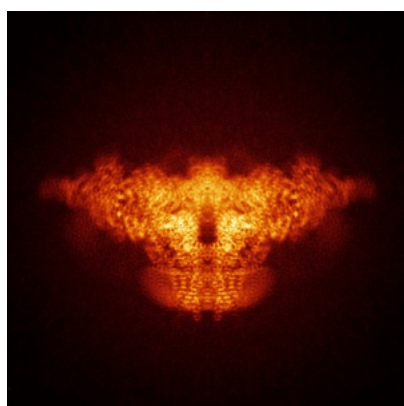


Z Index: 214

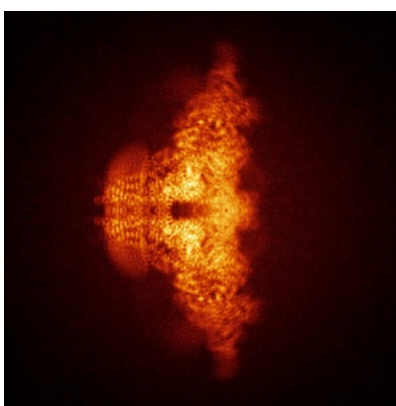
The images above show the largest variance slices of the map in three orthogonal directions.

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

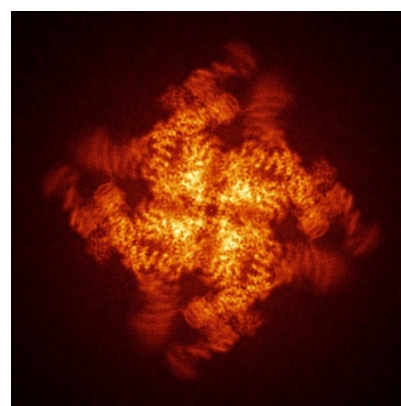
6.4.1 Primary map



X



Y

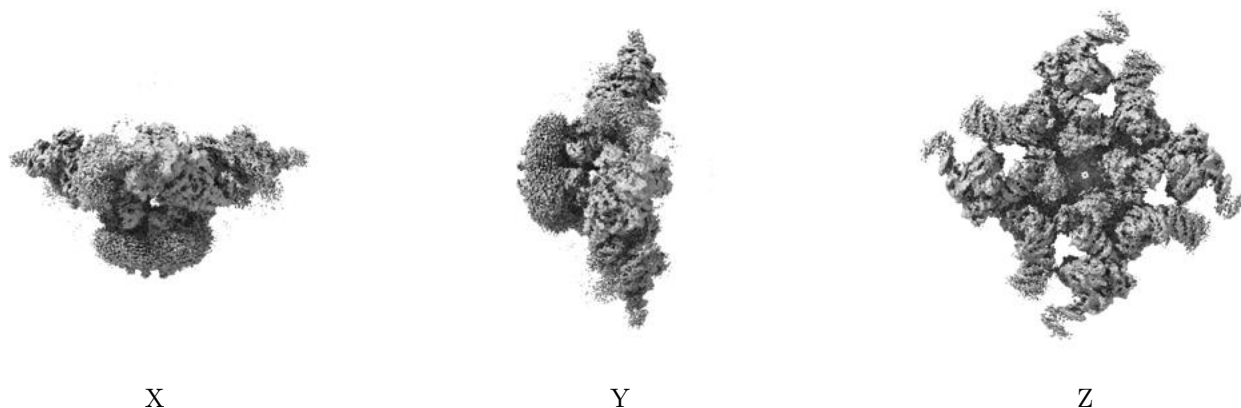


Z

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

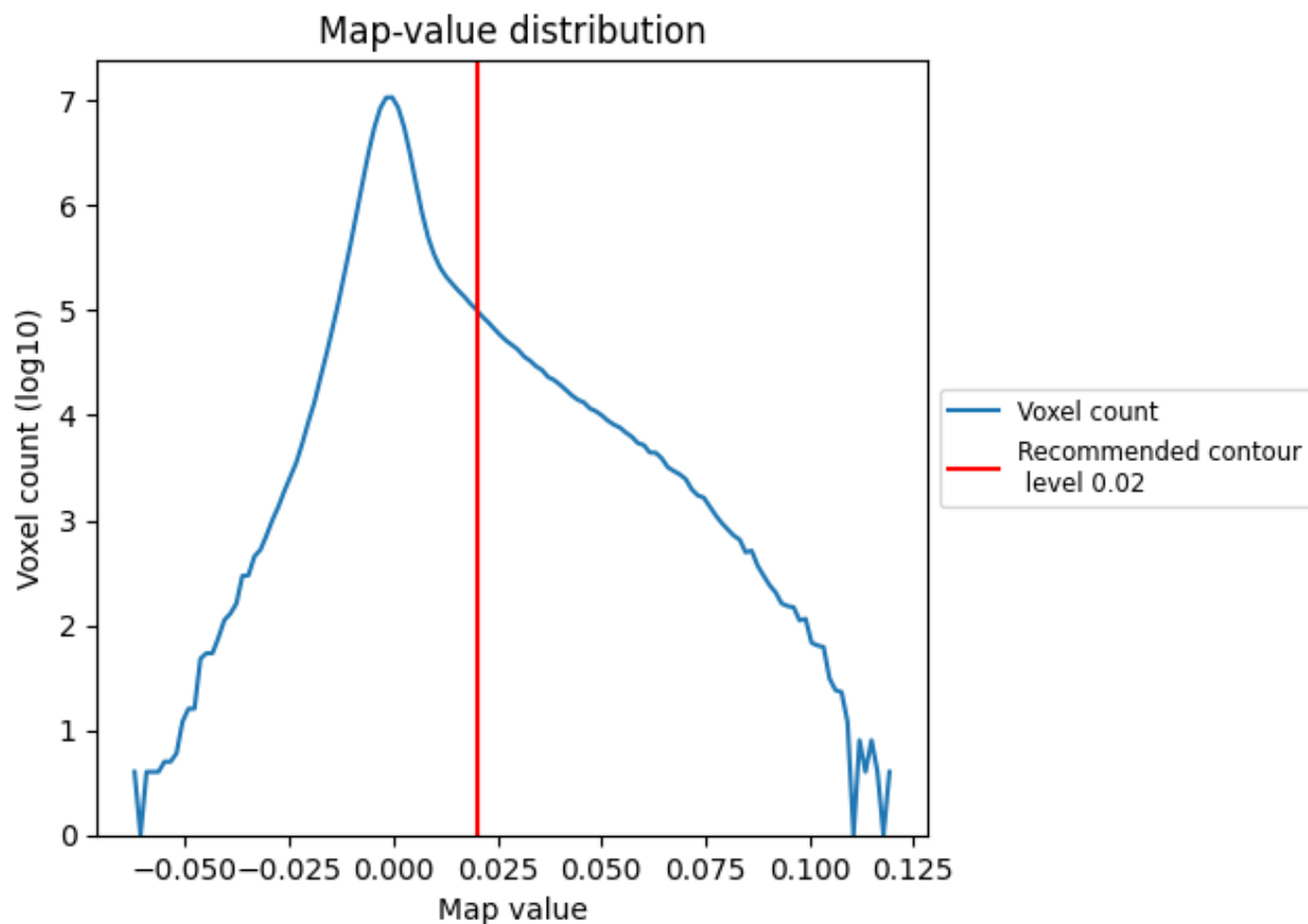
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

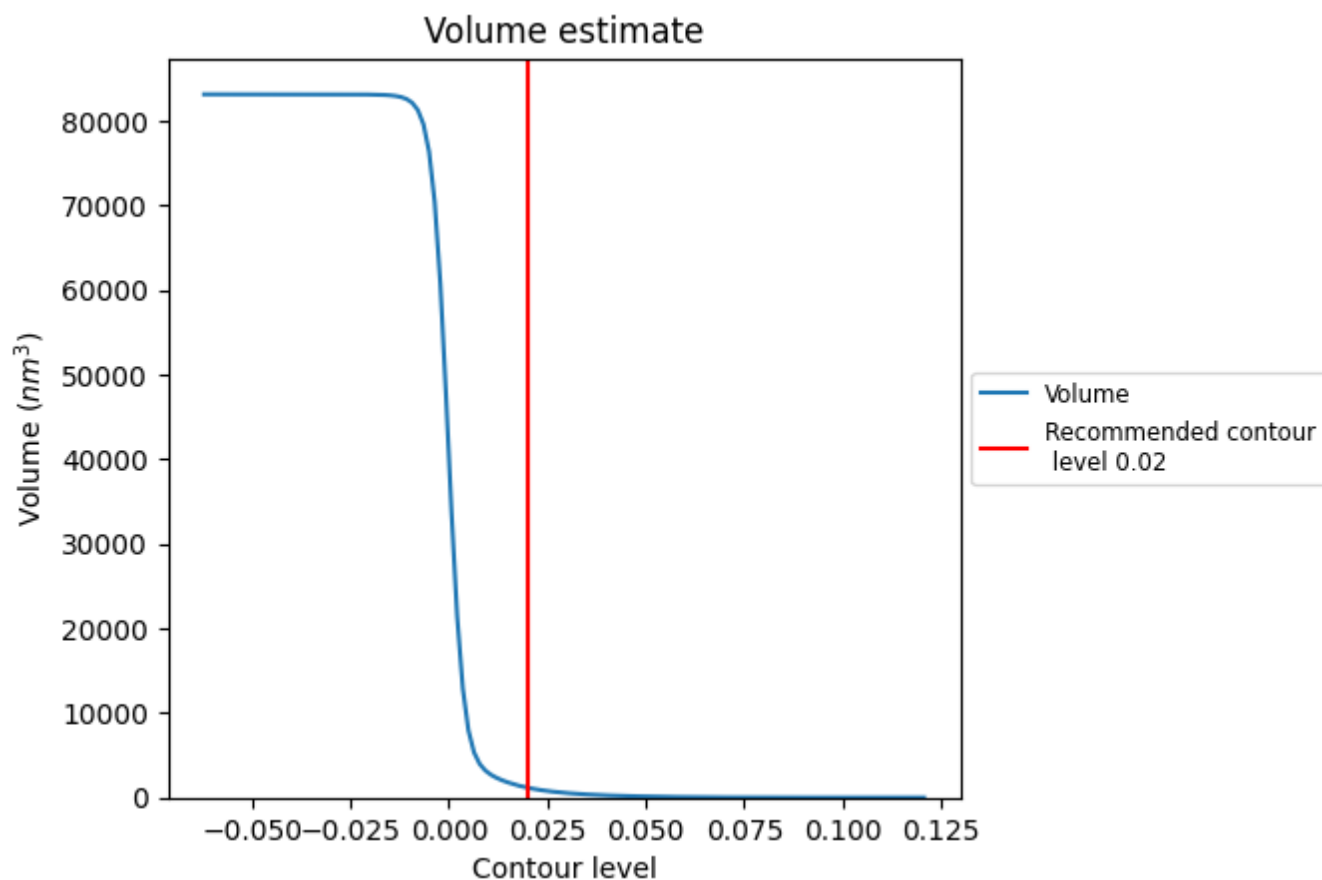
This section contains the results of statistical analysis of the map.

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.

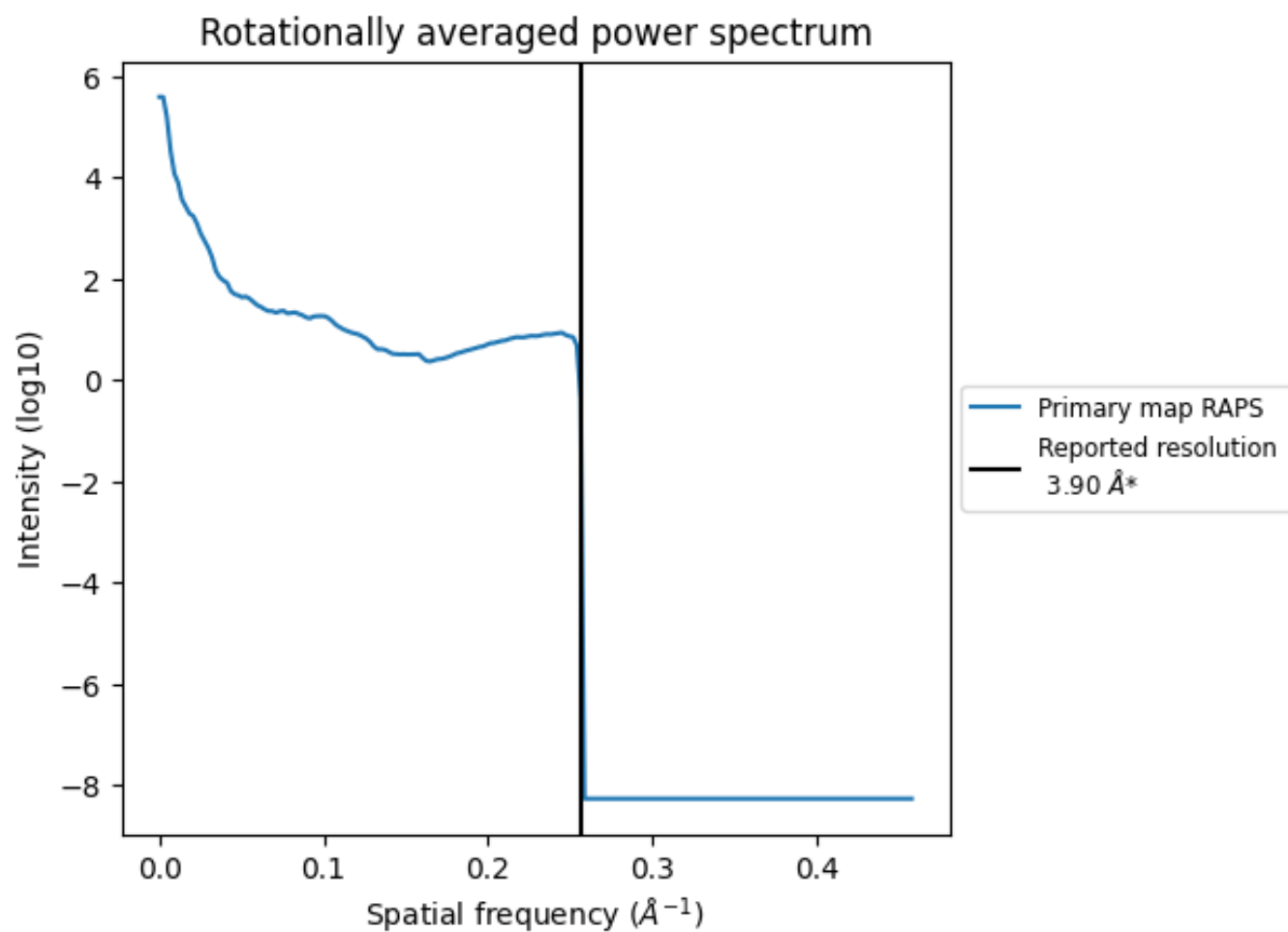
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1164 nm³; this corresponds to an approximate mass of 1051 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 ⓘ

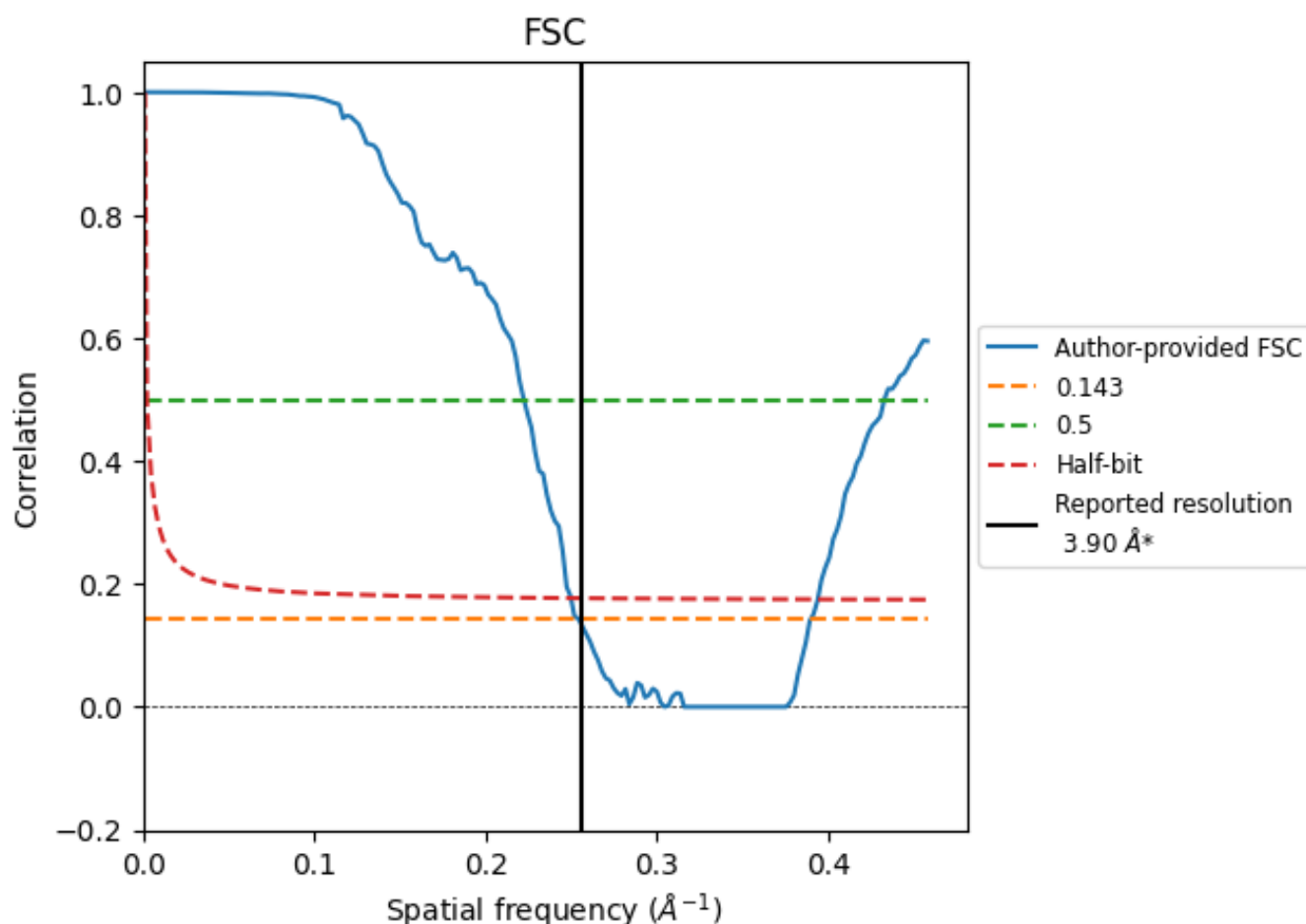


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

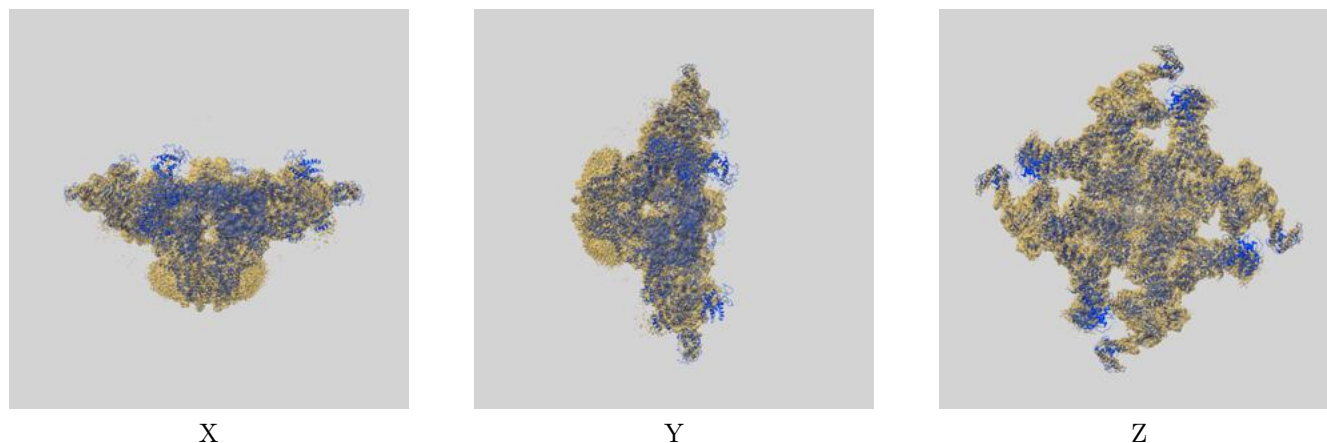
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.49	4.00
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

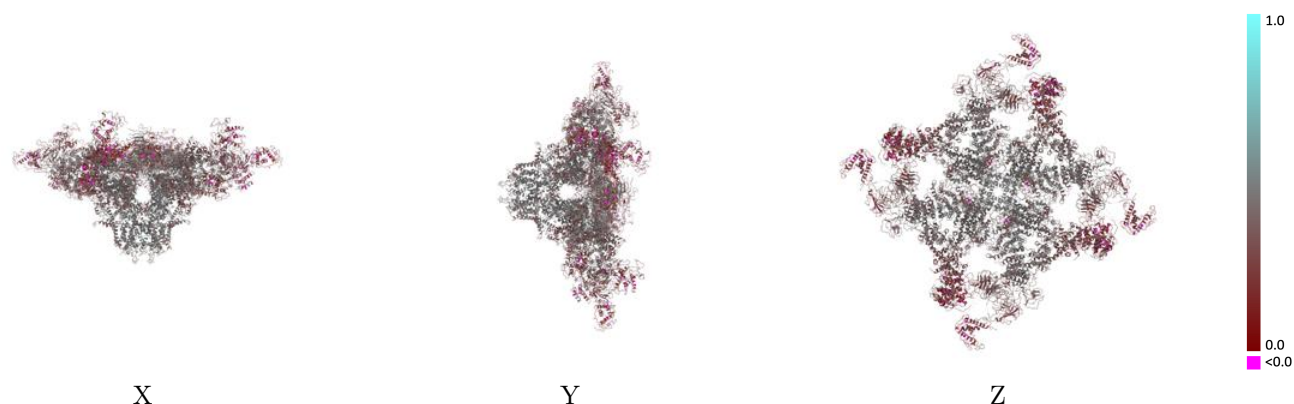
This section contains information regarding the fit between EMDB map EMD-9837 and PDB model 6JIY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



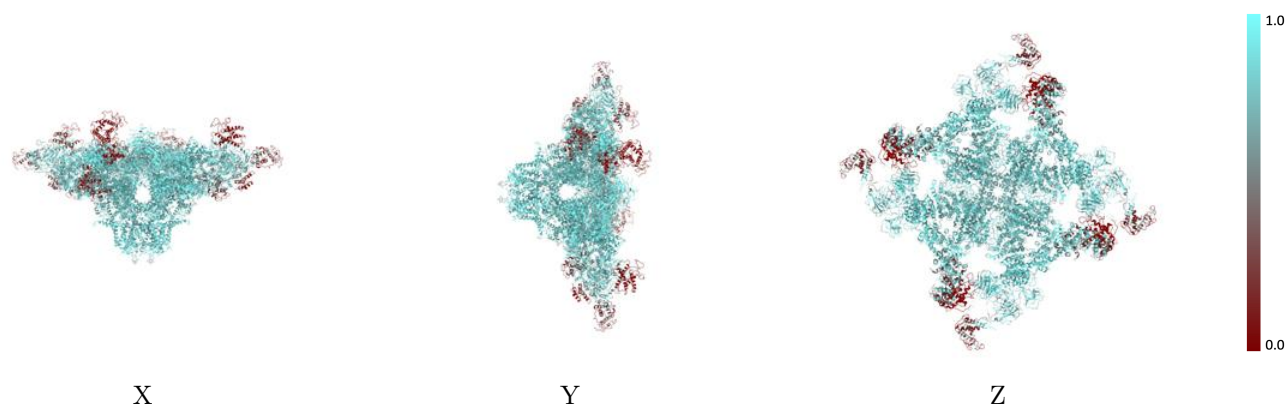
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



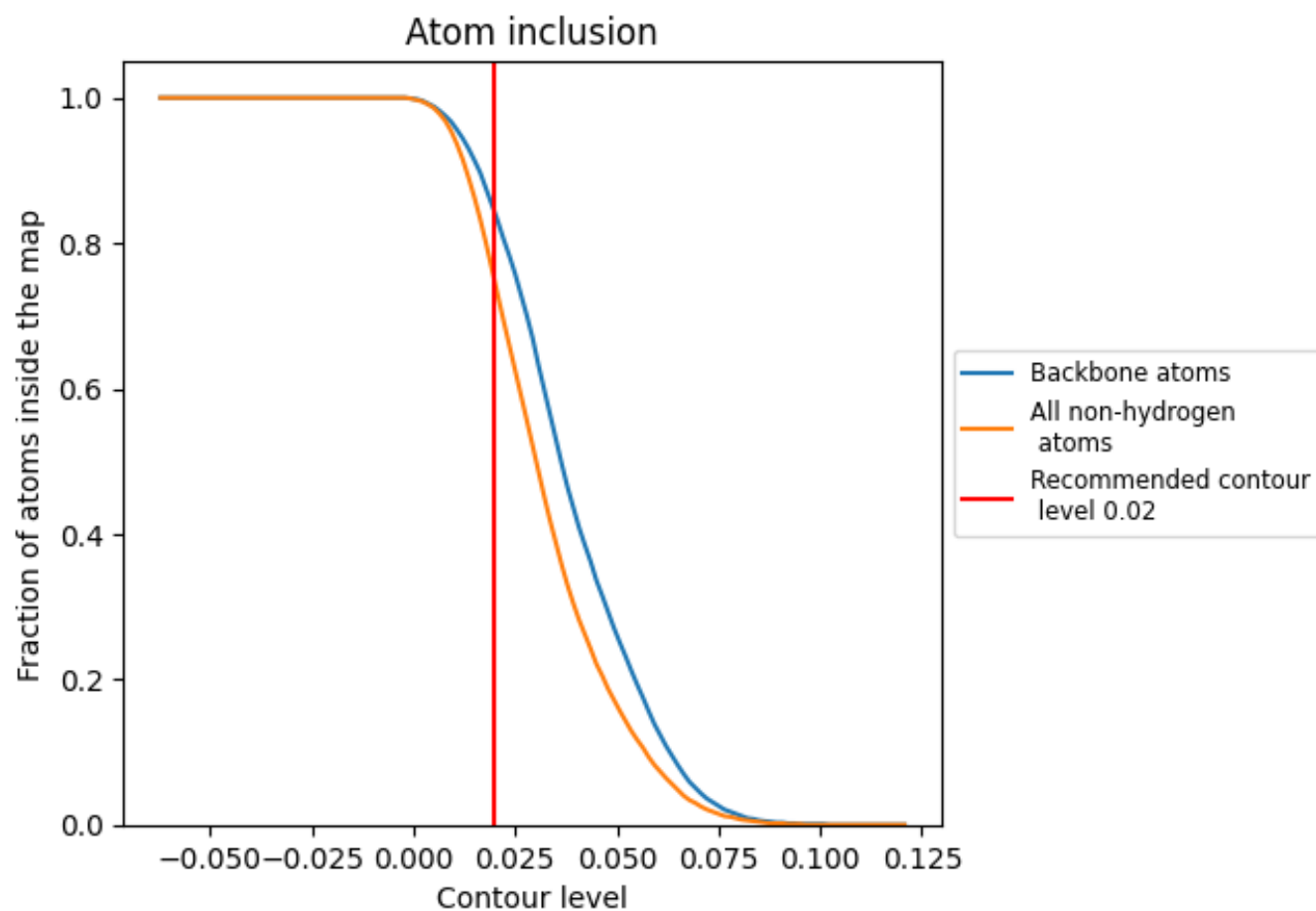
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.3750
A	0.7590	0.3790
B	0.7990	0.3990
C	0.3940	0.2820
D	0.7590	0.3790
E	0.7990	0.3990
F	0.3960	0.2820
G	0.7590	0.3780
H	0.7990	0.3970
I	0.3930	0.2810
J	0.7580	0.3780
K	0.7970	0.3980
L	0.3970	0.2820

