



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 08:08 pm GMT

PDB ID : 6EMK  
EMDB ID : EMD-3896  
Title : Cryo-EM Structure of *Saccharomyces cerevisiae* Target of Rapamycin Complex 2  
Authors : Karuppasamy, M.; Kusmider, B.; Oliveira, T.M.; Gaubitz, C.; Prouteau, M.; Loewith, R.; Schaffitzel, C.  
Deposited on : 2017-10-02  
Resolution : 8.00 Å (reported)  
Based on initial model : 5FVM

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

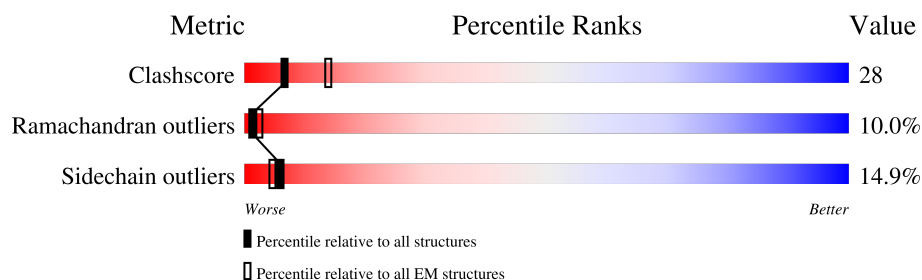
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2474	
1	C	2474	
2	B	303	
2	D	303	
3	E	303	
3	F	303	
4	G	426	
4	H	426	

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Mol	Chain	Length	Quality of chain
5	I	1176	 6% 5% 88%
5	J	1176	 6% 5% 88%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48012 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 Serine/threonine-protein kinase TOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2262	Total	C	N	O	S	0	0
			18186	11650	3110	3345	81		
1	C	2262	Total	C	N	O	S	0	0
			18186	11650	3110	3345	81		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	300	Total	C	N	O	S	0	0
			2372	1468	433	460	11		
2	D	300	Total	C	N	O	S	0	0
			2372	1468	433	460	11		

- Molecule 3 is a protein called Target of rapamycin complex 2 subunit TSC11.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	303	Total	C	N	O	0	0
			1515	909	303	303		
3	F	303	Total	C	N	O	0	0
			1515	909	303	303		

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit AVO2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	155	Total	C	N	O	0	0
			762	452	155	155		
4	H	155	Total	C	N	O	0	0
			762	452	155	155		

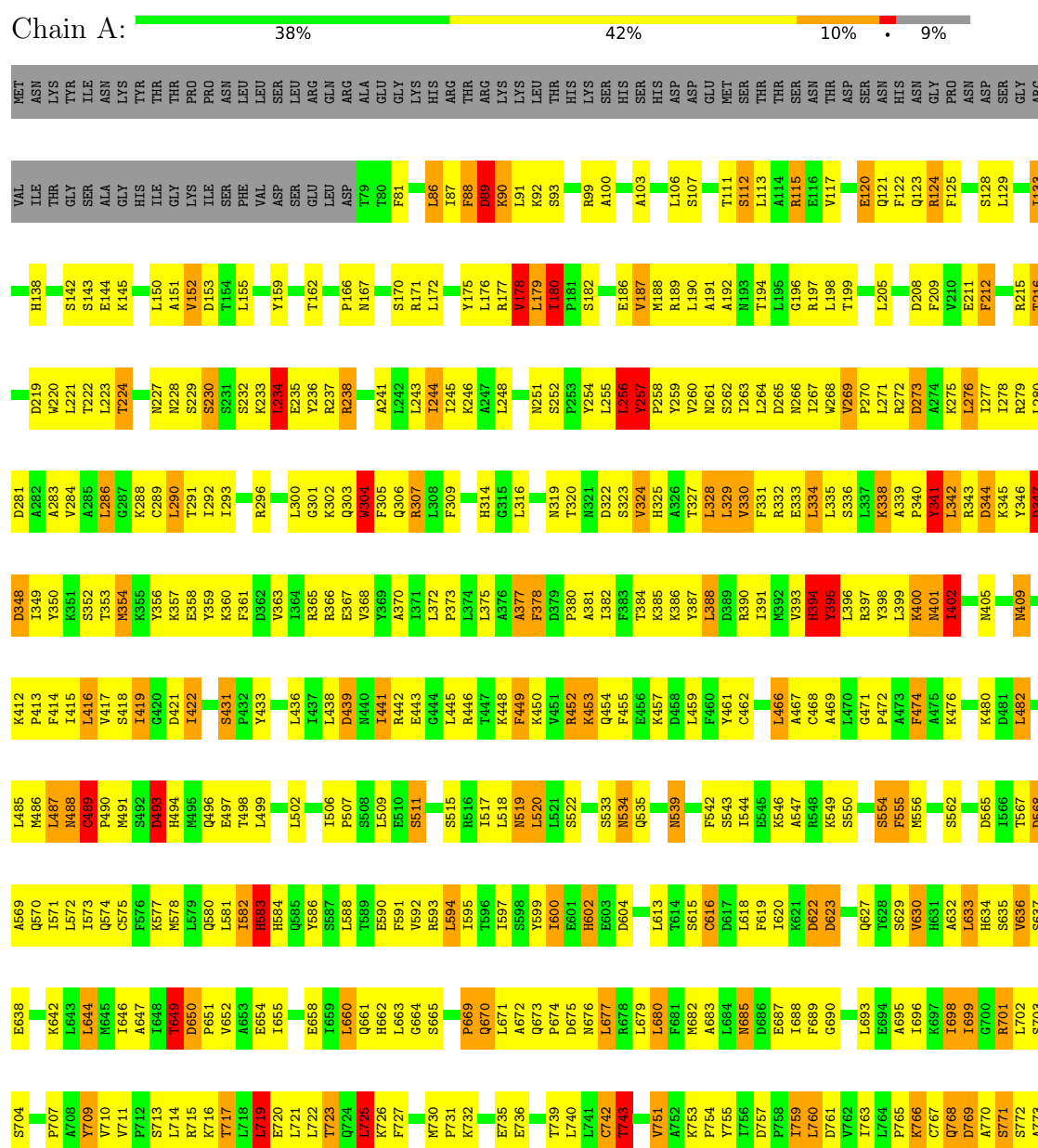
- Molecule 5 is a protein called Target of rapamycin complex 2 subunit AVO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	S	0	0
			1171	739	187	242	3		
5	J	146	Total	C	N	O	S	0	0
			1171	739	187	242	3		

### 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: Serine/threonine-protein kinase TOR2



GLU	V1742	K1670	R1591	A1520	E1428	A1348	F1280	K1205	I1128	V1060	Q984	ASP	V774
VAL	Y1743	Q1671	I1592	L1523	Y1429	L1351	S1281	R1206	L1129	P1061	L985	E914	A775
TYR	L1744	L1672	R1593	L1524	M1430	H1352	C1282	Y1207	M1130	I1062	T854	Y915	T777
	L1745	F1675	L1594	V1525	K1433	K1353	V1285	D1209	R1134	R1063	L855	T918	L779
	D1750	M1679	V1526	T1526	L1434	K1354	Y1286	Q1212	E1135	I1064	K993	Y919	K780
N1751	N1751		E1527	R1435	E1286	V1355	E1287	V1213	L1136	L1065	Q994	V920	V761
N1813	N1752		L1528	S1436	Q1288	V1356	Q1288	V1214	T1137	S1067	R997	R921	R861
L1814	T1752		L1529	L1437	T1289	E1357	T1289	K1215	L1138	L1068	P998	N922	E784
H1815	Y1753		E1534	Y1438	L1359	F1358	S1290	L1216	A1139	V1069	H999	N923	G863
H1816	K1755		S1535	L1439	L1359	L1359	L1291	P1217	T1140	T1070	T864		V768
	V1819	LEU	A1539	L1440			Y1291		M1141	F1071	V865	I927	K791
	P1820	ASP	P1602				Y1292		M1142	E1001	R866	L928	E792
P1821	K1603	PRO	K1603				E1293	Q1220	T1143	G1072	R867	N929	M793
A1822	A1606	ASN	L1446	L1447	T1366	T1366	D1294	I1221	L1144	P1073	L867	D930	T794
I1823	Q1607	ASN	S1447	S1447	I1367	I1367	LEU	I1222	S1145		I1003	P931	R795
K1824	Q1608	ASN	L1448	L1449	E1368	A1369	ILE	L1223		E1076	G869		W796
G1825	R1609	ILE	A1546	L1449	A1369	L1370	GLN	K1224	L1148	D1077	ILE		L797
F1826	R1610	ALA	Q1547	E1452	L1370	L1371	ALA		L1149	Y1078	LEU		K798
F1827	K1611	GLN	K1453	K1453	I1371		LEU	W1227	Q1150	S1079	GLY		E799
	F1612	SER			S1372			Y1228	F1151	E1077	ALA		L800
H1828	F1613	VAL	T1456	T1456	I1373		CYS	C1229	L1151	M1082	ASP		M801
S1829	A1613	VAL	A1550	A1550	I1373		LYS	S1230	G1152	P1083	PRO		I804
I1830	E1551	PRO	L1458	A1457	I1384	I1384	ALA	Q1231	T1153	V1087	TYR		N806
S1831	L1615	GLN	L1458	P1459	Q1385	G1385	SER	Q1232	D1154	I1085	LYS		F808
L1832	C1616	GLN	P1459	P1459	I1387	I1387	SER	K1233	F1155	V1086	GLU		Q809
	R1617	SER	M1465	M1465	Q1379	Q1391			V1157	I1007	GLU		D810
	L1621	LYS	L1556	L1556	T1380	Q1391	GLU	E1236	F1158	L1016	VAL		Q811
S1835	R1621	ARG	L1556	L1556	I1380	I1380	GLU	E1237	Y1159	L1017	THR		S812
S1837	A1622	VAL	K1557	K1557	I1387	I1387	ILE	D1237	L1166	Q1017	SER		F815
L1838	A1623	VAL	L1468	L1468	L1387	L1387	TYR	W1238	L1167	I1018	ASN		K816
Q1839	L1624	ARG	L1476	E1477	G1388	A1390	GLN		R1170	E1025	LYS		R817
L1840	A1625	HIS	E1477	E1477	I1389	Q1391	MET	L1245	S1246	S1026	SER		D818
A1841	K1626	GLN	D1480	D1480	H1389	L1396	ASN	Q1248	H1173	S1028	VAL		L821
R1843	K1627	GLY	K1490	K1490	K1389	L1396	V1320	L1249	S1174	K1029	GLN		L824
L1844	V1628	GLY	M1489	M1489	H1389	L1396	D1326	E1252	V1175	G1033	ASN		L827
	L1712	SER	K1490	K1490	K1389	L1396	D1327	S1253	D1177	E1034	ALA		V835
ASP	L1713	ASP	K1491	K1491	K1389	L1396	K1328	L1258	Q1178	R1107	PRO		L838
ALA	A1714	ALA	S1491	S1491	K1389	L1396	P1329	R1259	M1181	K1110	SER		
SER	R1715	SER	Q1492	Q1492	K1405	L1406	P1331	S1263	K1182	N1111	ILE		
SER	C1716	SER	S1493	S1493	L1406	L1406	P1330		L1183	I1112	ASP		
VAL	K1719	VAL	M1571	M1571	Q1407	L1406	P1332	V1267	L1184	N1113	ALA		
THR	A1723	THR	K1496	K1496	Q1407	L1406	P1333	Y1268	L1189	E1116	LEU		Y841
ASP	R1724	ASP	E1497	E1497	L1406	L1406	P1334	L1268	P1190	M1117	LEU		P842
ILE	V1725	ILE	L1502	L1502	K1405	L1406	P1334	S1263	T1191	E1117	MET		E843
ASN	V1725	ASN	L1503	L1503	L1406	L1406	P1334	L1268	N1192	R1120	GLN		L844
GLY	K1730	GLY	C1504	C1504	L1406	L1406	P1334	L1268	L1193	F1045	GLY		L845
MET	A1731	MET	F1510	F1510	Q1407	L1406	P1334	L1268	L1193	W1122	VAL		G846
ILE	R1732	ILE	R1511	R1511	L1406	L1406	P1334	L1268	L1193	Q1123	SER		I847
ASN	P1729	ASN	K1582	K1582	L1406	L1406	P1334	L1268	L1193	L1050	PRO		L848
GLY	K1730	GLY	K1583	K1583	L1406	L1406	P1334	L1268	L1193	L1050	SER		L849
THR	A1731	THR	L1584	L1584	L1406	L1406	P1334	L1268	L1193	Q1054	ASN		N850
ASN	N1735	ASN	L1585	L1585	L1406	L1406	P1334	L1268	L1193	L1050			
ASN	P1736	ASN	L1586	L1586	L1406	L1406	P1334	L1268	L1193	L1050			
PHE	P1736	PHE	D1587	D1587	L1406	L1406	P1334	L1268	L1193	L1050			
ASP	I1739	ASP	E1588	E1588	L1406	L1406	P1334	L1268	L1193	L1050			
ALA	L1740	ALA	F1518	F1518	L1406	L1406	P1334	L1268	L1193	L1050			
LYS	G1741	LYS	L1669	L1669	L1406	L1406	P1334	L1268	L1193	L1050			

Q1879	V1950	L2035	R2107	W2178	E2254	E2327	V2404	P2470
L1880	S1951	N2036	P2108	W2181	R2255	V2328	Q2405	F2471
I1881	E1952	Q2037	R2109	S2182	R2256	I2331	E2406	W2472
S1882	E1953	K2038	K2110	T2257	L2257	E2332	T2407	
L1883	L1954	W2040	F2111	T2183	T2258	G2333	E2408	
I1884	I1955	D2049	C2112	T2184	T2259	G2334	H2411	
H1885	R1956	Y2043	C2113	T2185	T2260	S2334		
Q1886	M1957	N2044	K2114	W2186	R2261	F2335	A2414	
	A1958		G2115	V2187	S2262	R2336	L2415	
			D2117	L2188	L2263	T2337	R2416	
				L2189	A2264	C2339		
				R2190	M2265	E2340	R2419	
				E2191	S2267	W2341		
				H2192	T2268	V2342	L2422	
				E2193	T2269		V2423	
				E2194			V2424	
							K2425	
							R2426	
							L2427	
							T2428	
							D2429	
							K2430	
							L2431	
							T2432	
							G2433	
							N2434	
							D2435	
							L2436	
							R2437	
							L2438	
							F2439	
							N2440	
							D2441	
							L2442	
							D2443	
							V2444	
							L2445	
							T2446	
							Q2447	
							V2448	
							D2449	
							K2450	
							L2451	
							T2452	
							Q2453	
							Q2454	
							A2455	
							T2456	
							S2457	
							V2458	
							E2459	
							C2462	
							Y2465	
							L2466	
							T2467	
							W2468	
							C2469	

• Molecule 1: Serine/threonine-protein kinase TOR2

Chain C:  38% 43% 9% 9%

MET	VAL	L137	F213		N228	L156		K276
ASN	ILE	I138	E214		N229	I157		L277
LYS	THR	H139	W215		S230			I278
TYR	GLY	G140	V216		S231			I279
ILE	SER		R217		S232			R280
ASN	ALA	S143	T218		S233			L281
LYS	GLY	S144	C218		K234			D282
THR	ILE	E145	D220		L235			K283
THR	GLY	K146	W221		E236			A284
LYS	LYS	I150	L222		Y237			V285
PRO	THR	L151	T223		R238			L287
PRO	ILE	L152	T224		G239			G288
ASN	SER	W153	T225		L291			K289
LEU	PHE				L294			G290
LEU	VAL				R297			
LEU	ASP				D298			
SER	SER				P299			
LEU	GLU				A300			
ARG	LEU				L301			
GLN	ASP				G302			
ARG	THR				R303			
ALA	THR				Q304			
GLY	LYS				W305			
GLY	LYS				F306			
LYS	LYS				Q307			
LEU	LEU				L308			
THR	THR				L309			
HIS	HIS				F310			
ARG	THR				Q311			
THR	LYS				L312			
LYS	LYS				T314			
LEU	LEU				H315			
THR	HIS				G316			
HIS	ASP				L317			
ASP	ASP				N320			
GLU	GLU				T321			
GLU	GLU				L322			
MET	SER				P323			
SER	THR				S324			
THR	THR				Y325			
SER	SER				L326			
ASN	ASN				L327			
THR	THR				L328			
ASP	ASP				L329			
THR	THR				L330			
ASP	ASP				V331			
ASP	ASP				F332			
THR	THR				R333			
GLY	GLY				E334			
ASN	ASN				L335			
PRO	PRO				L336			
ASN	ASN				S337			
ASP	ASP				L338			
SER	SER				K339			
GLY	GLY							
ARG	ARG							



ALA	LEU	SER	SER	SER	GLU	ASN	PRO	PRO	GLU	GLU	ILE	TVR	GLN	MET	LEU	LEU	ASN	L1321	L1321	V1322	E1323	F1324	H1327	L1332	F1333	I1334	G1340	G1341	G1342	A1343	Q1344	H1347	A1348	F1349	A1350	K1351	Y1355	K1356	E1357	E1358	E1359	F1360	P1364	K1365	T1368	I1369	E1370	A1371	L1372	E1373	S1374	I1375	T1382					
P1218	V1219	M1220	Q1221	M1222	K1225	M1226	C1230	C1231	D1238	W1239	Q1240	E1241	W1242	I1243	R1244	R1245	L1246	S1247	I1248	Q1249	L1259	S1260	S1261	C1262	S1263	S1264	V1268	Y1269	A1273	R1274	E1275	L1276	F1281	C1284	W1285	V1286	E1287	L1288	S1291	Y1292	Q1293	E1294	D1295	LEU	ILE	GLN	ALA	LEU	CYS	LYS								
E1136	L1137	T1138	K1139	A1140	T1141	M1142	N1143	T1144	L1145	L1148	L1149	L1150	Q1151	L1152	G1153	T1154	P1161	V1162	K1165	A1166	L1167	R1171	Q1172	Q1173	H1174	S1175	V1176	Y1177	D1178	M1182	K1183	L1184	L1185	C1189	T1192	M1193	I1194	I1195	F1196	D1197	P1203	E1204	R1205	V1208	Q1213	W1214	L1215	K1216										
L1066	K1067	S1068	L1069	V1070	P1074	M1075	Y1079	S1080	H1081	L1082	I1083	M1084	L1085	I1086	V1087	V1088	R1089	M1090	Y1093	S1094	S1097	L1098	S1099	Q1100	L1101	S1102	L1103	I1104	T1105	L1106	G1107	R1108	L1109	K1111	M1112	I1113	M1114	E1117	M1118	S1119	S1120	R1121	Q1124	A1125	L1126	V1127	R1128	I1129	L1130	D1134	R1135							
H1000	V1001	K1002	E1003	I1004	Y1005	G1006	V1007	I1008	R1009	E1010	F1011	F1012	P1013	I1014	P1015	L1016	L1017	Q1018	I1019	T1020	I1021	I1022	I1025	E1026	S1027	I1028	S1029	K1030	A1031	L1032	E1033	G1034	E1035	R1038	E1042	T1043	L1044	T1045	F1046	F1047	L1048	D1049	I1050	N1053	S1056	N1057	K1058	R1059	K1060	V1061	P1062	I1063	R1064	I1065				
L929	L934	H938	T939	Q943	M946	H947	I948	F949	Q950	N951	L952	G953	L954	R955	C956	V957	F959	D961	Q962	L963	L964	P965	L968	L969	V970	M971	P976	S977	Q978	L979	D980	F981	Y982	F983	Q984	Q985	L986	G987	S988	L989	Y990	S991	L992	V993	K994	Q995	H996	L997	R998	P999								
V866	R867	L868	T869	G870	ILE	LEU	GLY	ALA	PRO	TVR	LYS	HIS	ARG	GLU	ILE	GLU	VAL	THR	SER	ASN	LYS	SER	SER	VAL	ASN	ALA	PRO	SER	ILE	ASP	ILE	ALA	LEU	LEU	MET	GLN	GLY	VAL	SER	PRO	SER	ASN	ASP	E915	Y916	Y917	P918	T919	I922	H923	Y924	R925	M926					
K799	E800	L801	M802	R803	L804	R805	L806	F809	Q810	D811	N814	S815	F816	G817	R818	D819	L822	T823	T824	L825	G826	Q827	L828	V829	A753	K754	L757	L760	L761	D762	A684	N685	D687	E688	T689	F690	Q691	L692	Q693	L694	T697	L699	I700	G701	R702	L703	S704	S705	V706	Y710	W711	Y712						
L644	L645	M646	D404	N409	M410	S411	D412	K413	F414	F415	I416	L417	V418	S419	I420	E505	G421	D422	I423	A424	F425	L437	I438	L439	D440	I442	N441	L442	R443	E444	G445	L446	R447	L448	K449	F450	R453	K454	Q455	F456	E457	K458	D459	L460	F461	Y462	L467	A468	C469	A470	L471	V472	G473	P474	A474	F475	A476	K477
L483	C490	L491	M492	S493	D494	E498	Q499	L500	M501	I502	L503	H504	H505	I506	F507	P508	N515	S516	R517	I518	L519	N520	L521	L522	S523	L526	S527	G528	E529	K530	Q533	S534	N535	Q536	Y537	N541	Q542	P543	S544	I545	V631	H632	A633	R549	H635	T636	S636	V637	E562	D566	I567	L641	S642	Y710	W711	Y712		
A570	Q571	I572	L573	I574	Q575	C576	F577	L580	L582	L583	H584	H585	G586	G587	S588	L589	F592	L595	I596	T597	I598	S599	N601	L601	E602	H603	L603	A613	L616	C617	F620	I621	K622	D623	C626	K627	Q628	T629	S630	V631	H632	A633	L634	H635	S636	V637	E638	E639	V640	L641	S642	Y710	W711	Y712				
K401	N402	I403	D404	N409	M410	S411	D412	K413	F414	F415	I416	L417	V418	S419	I420	E505	G421	D422	I423	A424	F425	L437	I438	L439	D440	I442	N441	L442	R443	E444	G445	L446	R447	L448	K449	F450	R453	K454	Q455	F456	E457	K458	D459	L460	F461	Y462	L467	A468	C469	A470	L471	V472	G473	P474	A474	F475	A476	K477







- Molecule 5: Target of rapamycin complex 2 subunit AVO1

88%



VAL	VAL	LEU	VAL	VAL	LYS	LYS	SER	ARG	VAL	PRO	GLU	HIS	PHE	LYS	ILE	PHE	VAL	ARG	ARG	GLU	GLY	GLN	ASP	ASP	ILE	LYS	ARG	TYR	TYR	PHE	GLU	GLY	CYS	THR	GLU	ILE	VAL	THR	ARG	LEU	GLN	ASN	GLN	LEU	LEU	SER	ALA	ALA	TYR	ARG	MET	ASN	HIS	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	16190, 10663	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50, 47	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON II (4k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0147	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	0.60	0/18019	0.94	52/23495 (0.2%)
1	C	0.60	0/17986	0.93	40/23389 (0.2%)
2	B	0.60	0/2362	0.89	7/3108 (0.2%)
2	D	0.60	0/2353	0.93	4/3080 (0.1%)
4	G	0.48	0/715	0.68	0/918
4	H	0.49	0/718	0.87	2/927 (0.2%)
5	I	1.03	2/1165 (0.2%)	1.09	7/1526 (0.5%)
5	J	0.88	0/1160	1.01	8/1509 (0.5%)
All	All	0.62	2/44478 (0.0%)	0.93	120/57952 (0.2%)

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	1	28
1	C	0	25
2	B	0	4
2	D	0	2
5	I	0	2
5	J	0	2
All	All	1	63

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	713	LEU	N-CA	5.35	1.57	1.46
5	I	714	TYR	N-CA	5.27	1.56	1.46

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1084	MET	C-N-CD	-9.18	100.41	120.60
2	D	174	LEU	CA-CB-CG	8.54	134.94	115.30
1	A	2426	ARG	N-CA-C	7.87	132.25	111.00
2	B	106	SER	C-N-CD	-7.69	103.69	120.60
5	I	713	LEU	CA-CB-CG	7.55	132.67	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	257	TYR	CA

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	VAL	Peptide
1	A	180	ILE	Peptide
1	A	256	LEU	Peptide
1	A	257	TYR	Peptide
1	A	347	ASP	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	18186	0	18002	1077	0
1	C	18186	0	17976	1069	0
2	B	2372	0	2199	140	0
2	D	2372	0	2191	145	0
3	E	1515	0	491	15	0
3	F	1515	0	490	23	0
4	G	762	0	290	6	0
4	H	762	0	293	9	0
5	I	1171	0	1119	61	0
5	J	1171	0	1116	54	0
All	All	48012	0	44167	2571	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 28.

The worst 5 of 2571 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:A:2060:GLU:HB3	1:A:2062:GLN:HG2	1.25	1.18
1:A:841:TYR:HB2	1:A:843:GLU:HG2	1.16	1.13
1:C:983:PHE:HB3	1:C:1022:ILE:HG12	1.31	1.10
1:A:179:LEU:HD22	1:A:233:LYS:HG3	1.31	1.10
2:D:297:CYS:HA	2:D:298:VAL:HB	1.25	1.09

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	1309/2474 (53%)	872 (67%)	313 (24%)	124 (10%)	0	10
1	C	1267/2474 (51%)	849 (67%)	290 (23%)	128 (10%)	0	9
2	B	178/303 (59%)	122 (68%)	45 (25%)	11 (6%)	1	17
2	D	173/303 (57%)	113 (65%)	44 (25%)	16 (9%)	1	11
4	G	75/426 (18%)	57 (76%)	12 (16%)	6 (8%)	1	12
4	H	80/426 (19%)	43 (54%)	22 (28%)	15 (19%)	0	2
5	I	95/1176 (8%)	52 (55%)	29 (30%)	14 (15%)	0	4
5	J	88/1176 (8%)	52 (59%)	23 (26%)	13 (15%)	0	3
All	All	3265/8758 (37%)	2160 (66%)	778 (24%)	327 (10%)	1	9

5 of 327 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	112	SER
1	A	224	THR

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Mol	Chain	Res	Type
1	A	257	TYR
1	A	342	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	2029/2219 (91%)	1734 (86%)	295 (14%)	3	15
1	C	2029/2219 (91%)	1722 (85%)	307 (15%)	3	14
2	B	264/267 (99%)	229 (87%)	35 (13%)	4	18
2	D	264/267 (99%)	230 (87%)	34 (13%)	4	18
5	I	137/1066 (13%)	113 (82%)	24 (18%)	2	11
5	J	137/1066 (13%)	108 (79%)	29 (21%)	1	6
All	All	4860/7104 (68%)	4136 (85%)	724 (15%)	6	15

5 of 724 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1007	VAL
1	C	2041	TRP
1	C	1108	ARG
1	C	1004	ILE
1	C	1504	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	320	ASN
2	D	229	HIS
1	C	858	ASN
2	D	152	HIS
1	C	2284	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	567
1	A	534
3	E	90
3	F	87
2	D	75
2	B	66
4	G	45
4	H	42
5	J	31
5	I	26

The worst 5 of 1563 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	416:UNK	C	450:UNK	N	40.12
1	F	416:UNK	C	450:UNK	N	39.07

*Continued on next page...*

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	512:UNK	C	550:UNK	N	33.98
1	F	717:UNK	C	750:UNK	N	33.97
1	E	717:UNK	C	750:UNK	N	33.43

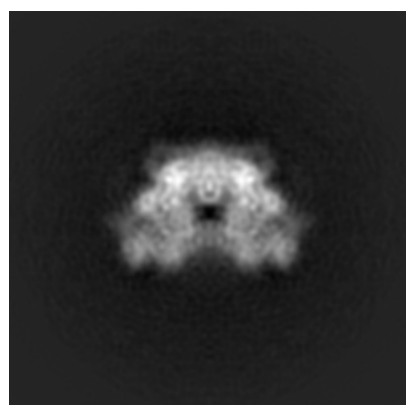
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3896. These allow visual inspection of the internal detail of the map and identification of artifacts.

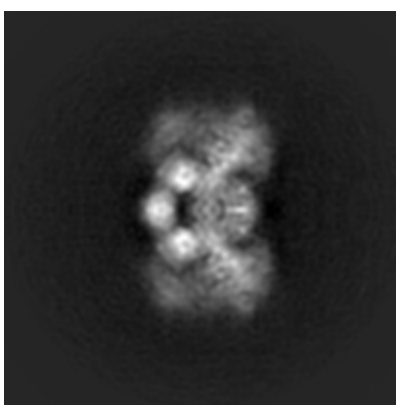
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

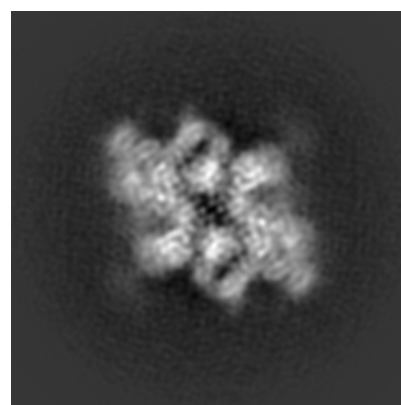
#### 6.1.1 Primary map



X



Y

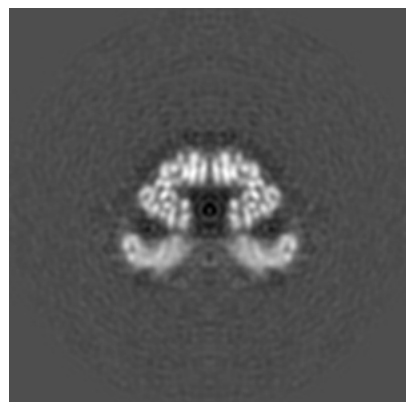


Z

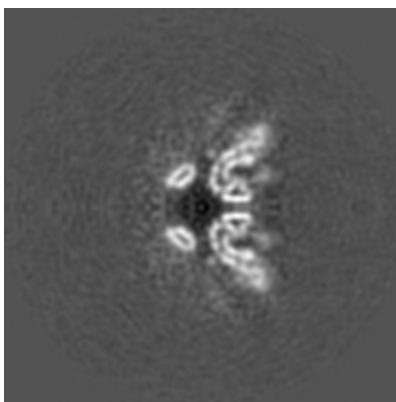
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

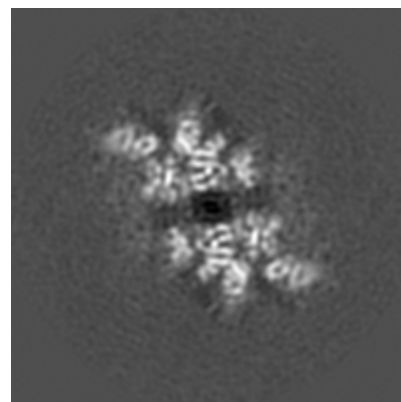
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

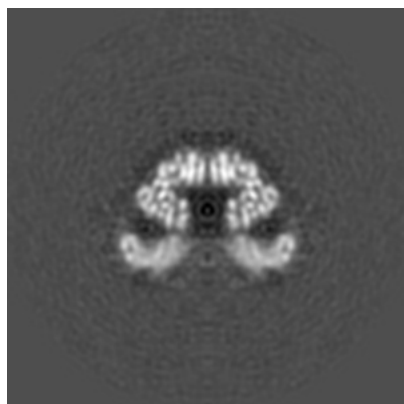


Z Index: 160

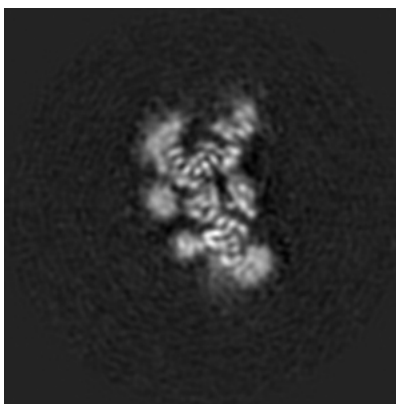
The images above show central slices of the map in three orthogonal directions.

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

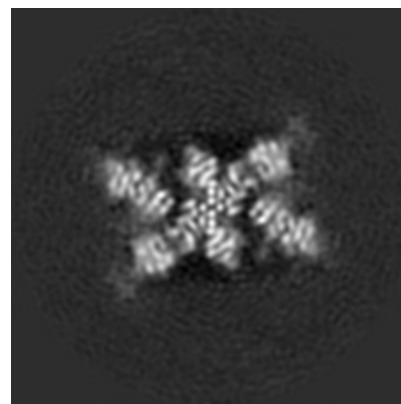
### 6.3.1 Primary map



X Index: 160



Y Index: 133

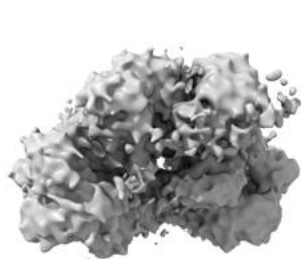


Z Index: 190

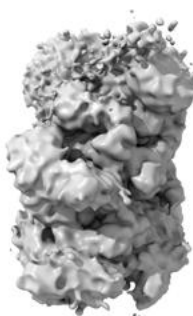
The images above show the largest variance slices of the map in three orthogonal directions.

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

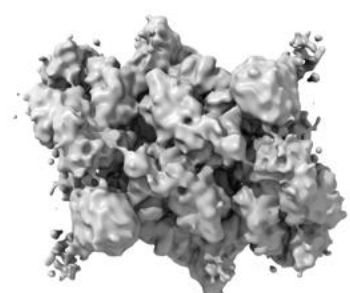
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0147. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



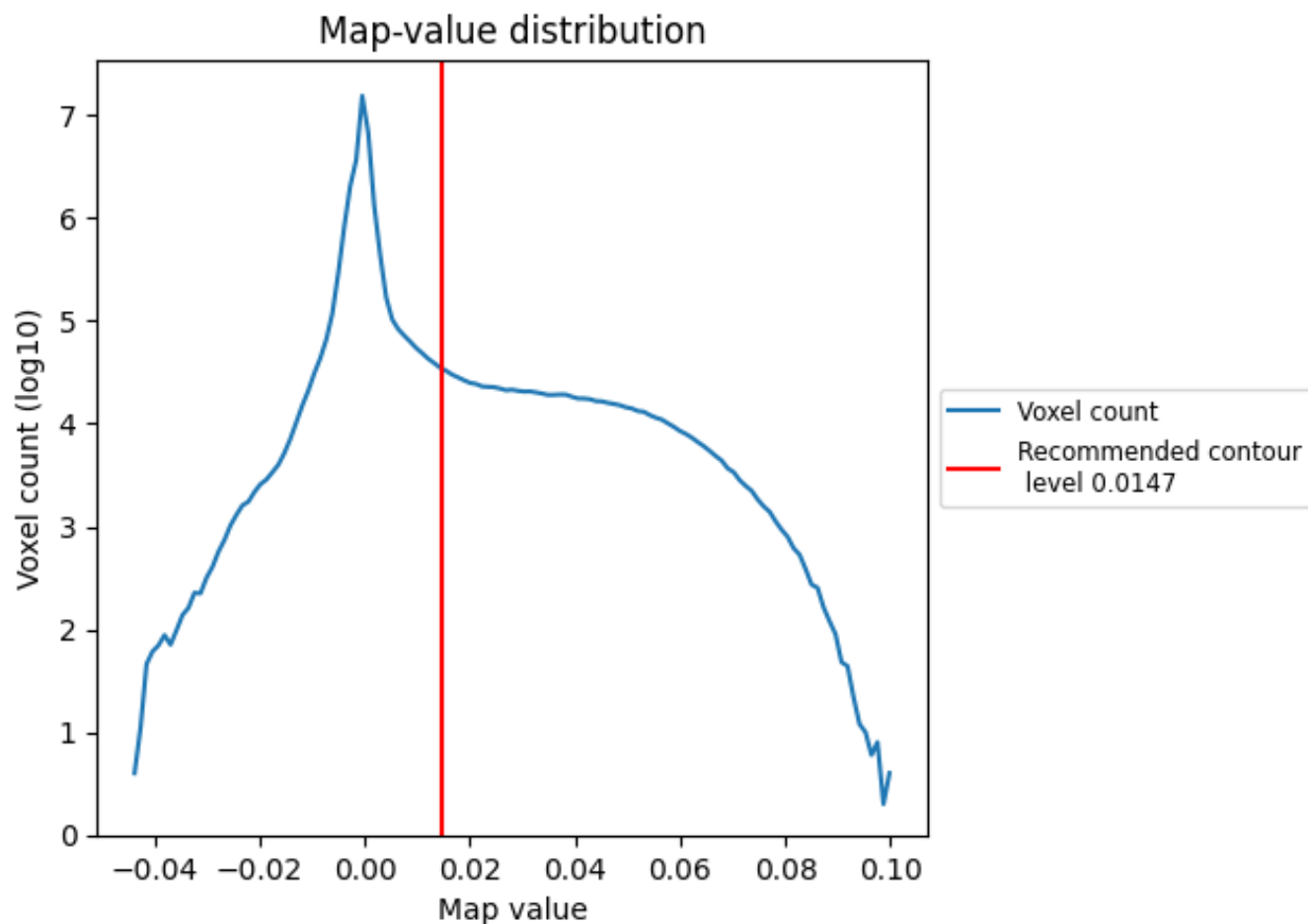
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

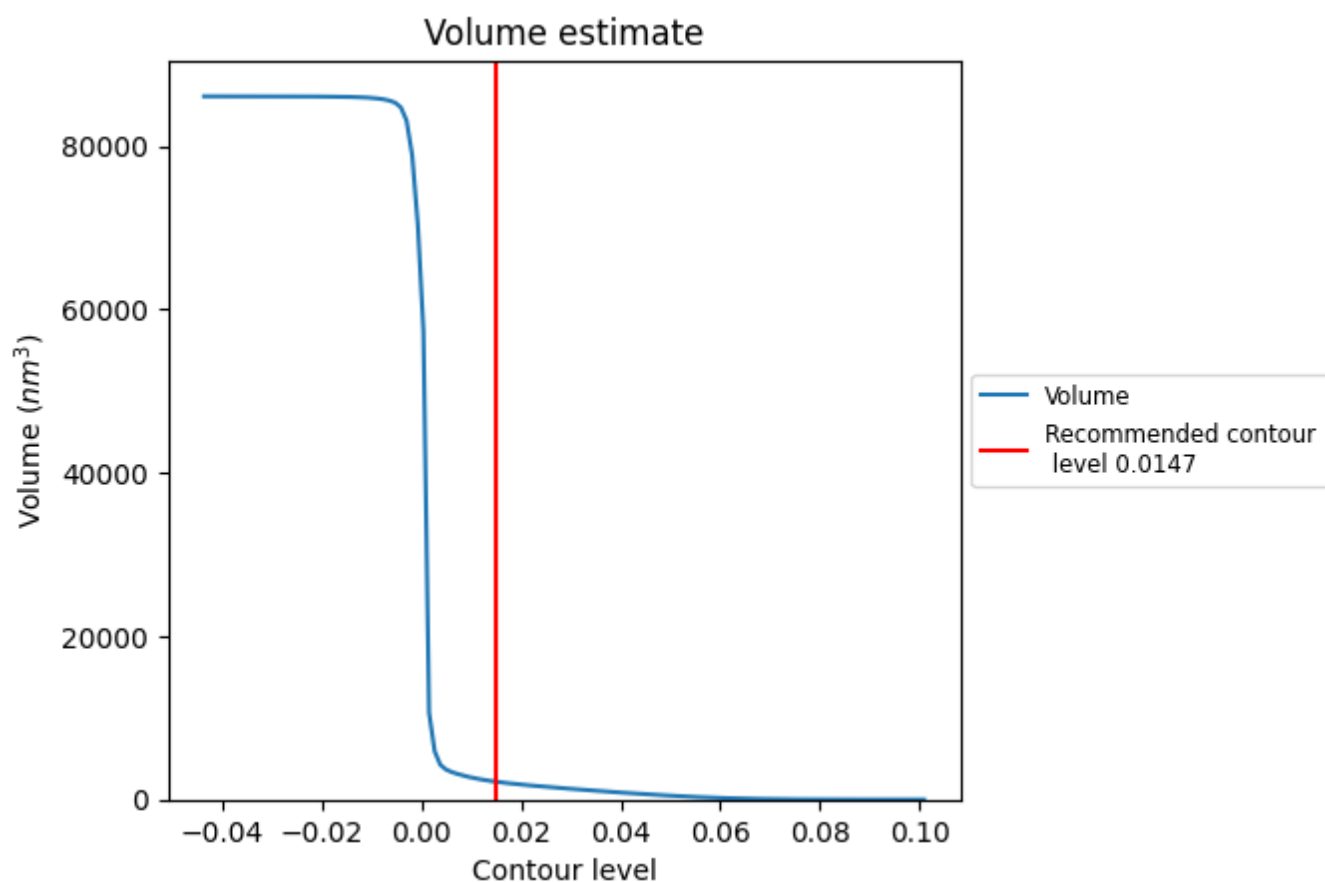
This section contains the results of statistical analysis of the map.

### 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.

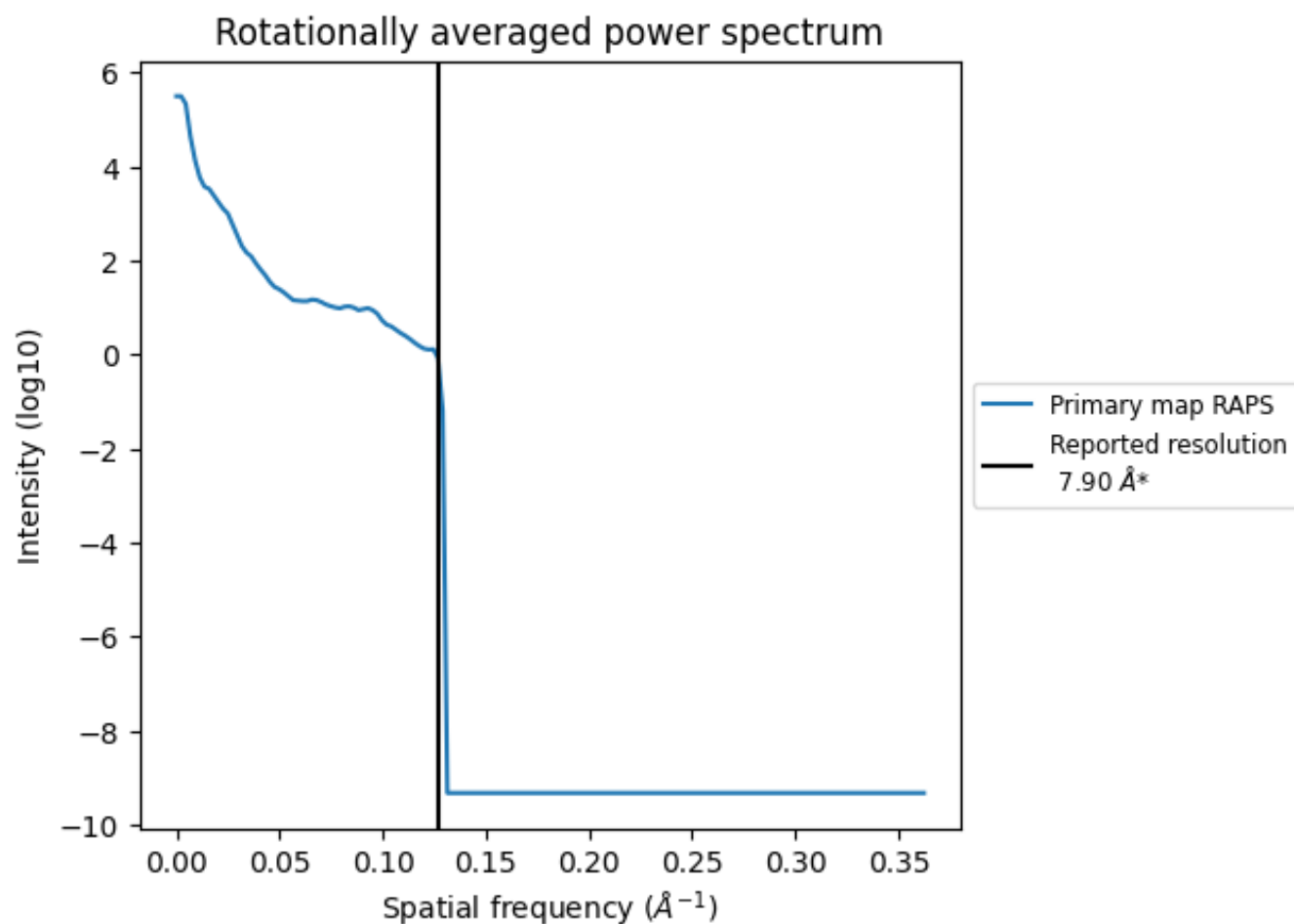
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2205 nm<sup>3</sup>; this corresponds to an approximate mass of 1992 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 0.127  $\text{\AA}^{-1}$

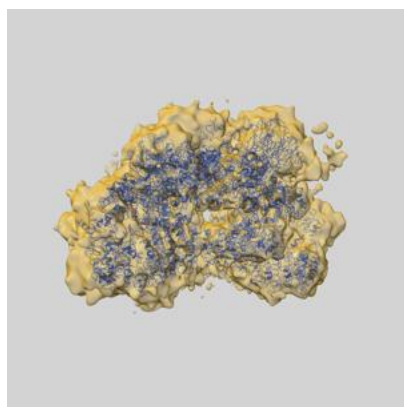
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

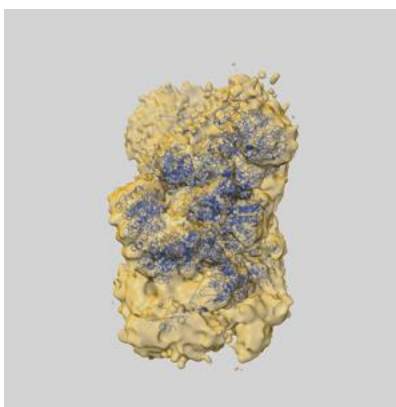
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3896 and PDB model 6EMK. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

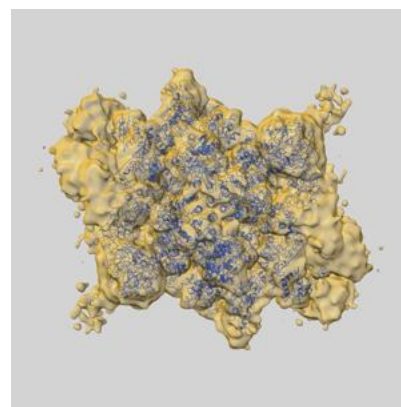
### 9.1 Map-model overlay [i](#)



X



Y



Z

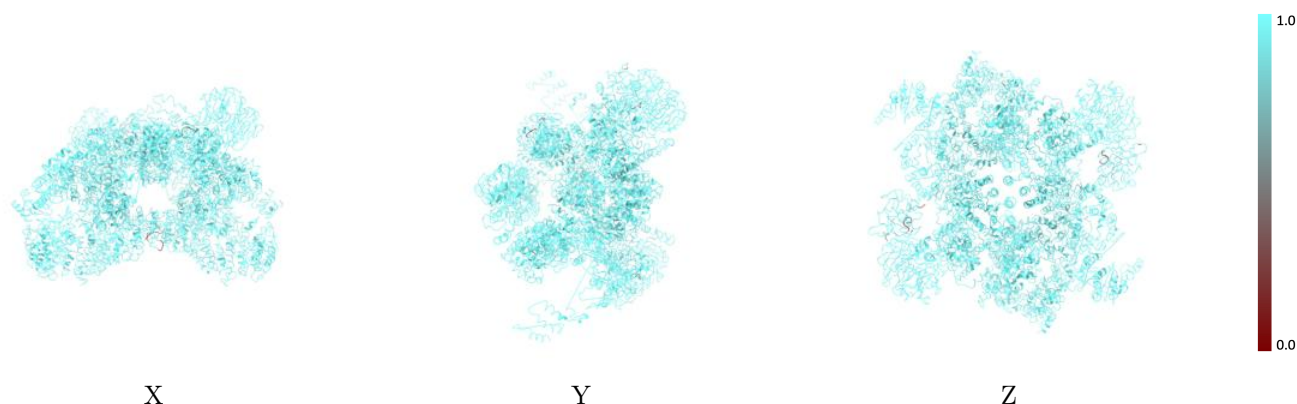
The images above show the 3D surface view of the map at the recommended contour level 0.0147 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



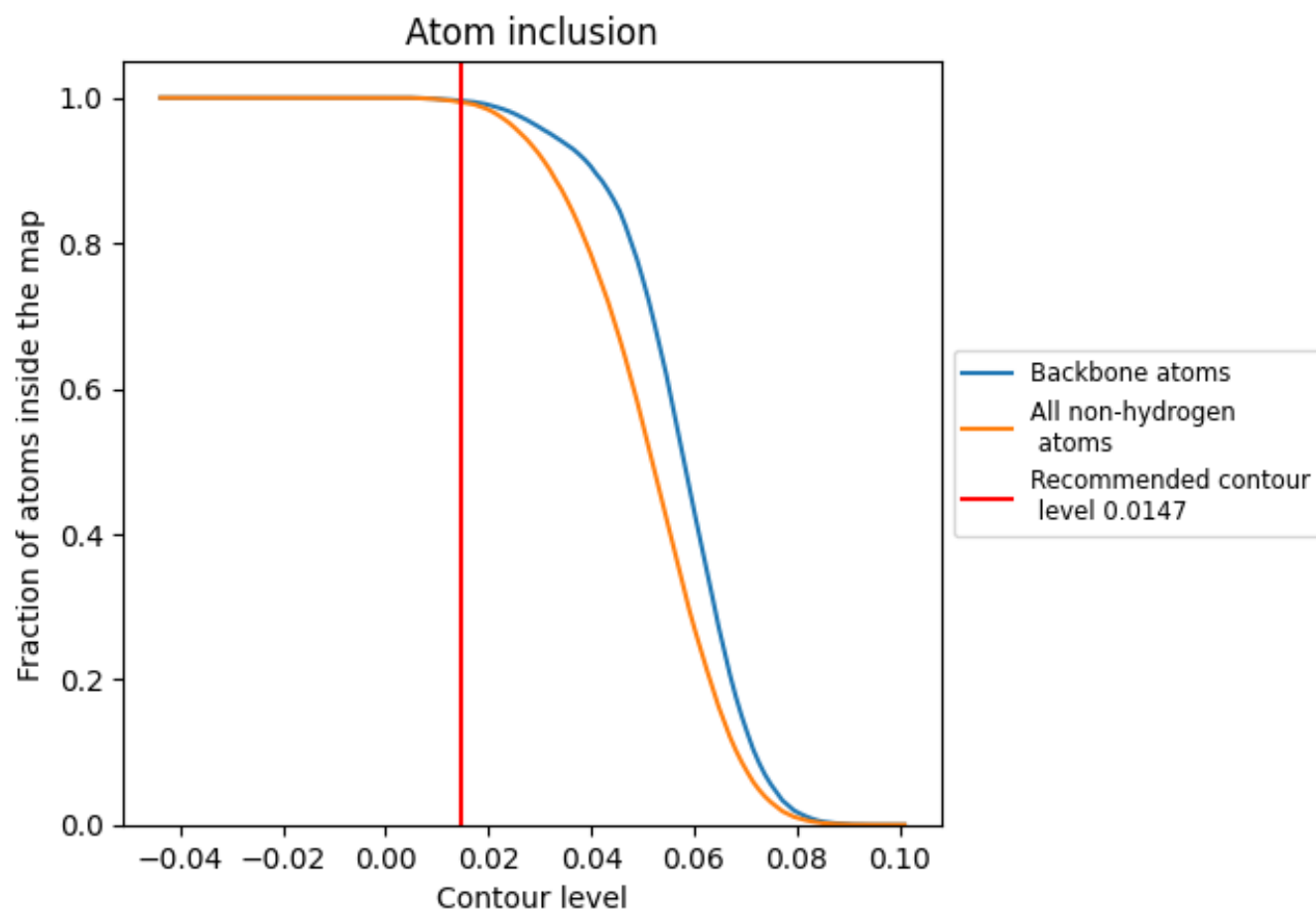
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0147).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0147) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9939</div>	<div><div></div>0.1450</div>
A	<div><div></div>0.9954</div>	<div><div></div>0.1430</div>
B	<div><div></div>1.0000</div>	<div><div></div>0.1080</div>
C	<div><div></div>0.9955</div>	<div><div></div>0.1410</div>
D	<div><div></div>1.0000</div>	<div><div></div>0.1070</div>
E	<div><div></div>1.0000</div>	<div><div></div>0.2680</div>
F	<div><div></div>1.0000</div>	<div><div></div>0.2690</div>
G	<div><div></div>1.0000</div>	<div><div></div>0.2330</div>
H	<div><div></div>1.0000</div>	<div><div></div>0.2340</div>
I	<div><div></div>0.9344</div>	<div><div></div>0.0480</div>
J	<div><div></div>0.9568</div>	<div><div></div>0.0550</div>

1.0

0.0

<0.0