



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 02:51 pm GMT

PDB ID : 6YAI
EMDB ID : EMD-10754
Title : Clathrin with bound beta2 appendage of AP2
Authors : Kovtun, O.; Kane Dickson, V.; Kelly, B.T.; Owen, D.; Briggs, J.A.G.
Deposited on : 2020-03-12
Resolution : 9.20 Å(reported)
Based on initial models : 1E42, 6SCT, 1XI4

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

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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.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) : 2.31.3

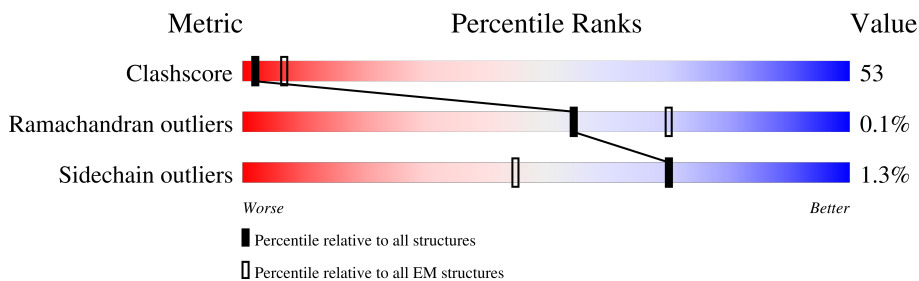
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.20 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 ≥ 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	1630	
1	B	1630	
1	E	1630	
1	H	1630	
1	J	1630	
1	K	1630	
1	L	1630	
1	M	1630	

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Mol	Chain	Length	Quality of chain
2	F	233	 82% 14%
3	C	1630	 5% 24% 69%
4	D	229	 14% 31% 55%
4	I	229	 13% 13% 75%
4	N	229	 14% 21% 65%
4	O	229	 10% 16% 74%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 35282 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 Clathrin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	726	5740	3660	981	1066	33	0	0
1	M	518	4213	2681	725	787	20	0	0
1	A	379	3168	2037	528	584	19	0	0
1	B	468	3744	2357	652	717	18	0	0
1	J	165	1379	875	227	269	8	0	0
1	K	257	2150	1377	358	404	11	0	0
1	L	548	4458	2843	757	838	20	0	0
1	H	236	1928	1239	327	353	9	0	0

- Molecule 2 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	233	1844	1189	307	337	11	0	0

- Molecule 3 is a protein called Clathrin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	513	4133	2645	706	762	20	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	871	THR	GLU	conflict	UNP C0MHR2

- Molecule 4 is a protein called Clathrin light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	104	Total 875	C 539	N 165	O 168	S 3	0	0
4	O	59	Total 514	C 312	N 101	O 101		0	0
4	I	58	Total 468	C 291	N 86	O 88	S 3	0	0
4	N	80	Total 668	C 412	N 123	O 130	S 3	0	0

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: Clathrin heavy chain



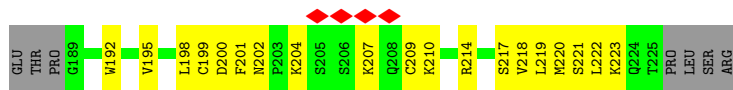
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T1585	W1521	V1455	K1392	P1329	K1264	GLY	GLY	GLN	VAL	ARG	GLU	ASP	SER	THR	ASP	GLN	ASP	ASP	ASN
A1586	K1522	Q1456	D1393	K1330	E1265	ASP	ARG	ALA	VAL	ASN	VAL	VAL	LEU	GLU	GLN	THR	VAL	VAL	GLN
W1587	K1523	N1457	I1394	K1331	F1266	ARG	VAL	ALA	VAL	ASN	ASN	VAL	LEU	GLU	GLN	ASP	ASP	ASP	THR
R1588	S1524	H1458	I1395	M1332	R1267	CYS	THR	THR	LEU	ASN	THR	GLY	VAL	VAL	ASP	VAL	CYS	THR	PHE
H1589	V1525	T1396	I1396	L1333	L1268	TYR	THR	GLN	LEU	ASN	LEU	LEU	VAL	VAL	ASP	VAL	LEU	LEU	HIS
E1590	E1526	N1460	K1397	E1334	A1269	ASP	ASP	SER	GLU	LEU	ARG	TYR	VAL	VAL	LEU	VAL	ARG	LEU	THR
L1591	L1527	H1461	V1398	H1335	Q1270	GLU	GLY	HIS	GLU	LEU	ARG	TYR	VAL	VAL	VAL	HIS	ARG	ARG	TYR
M1592	C1528	A1399	A1399	L1336	I1276	LYS	ILE	ILE	ILE	LEU	PRO	CYS	VAL	VAL	ALA	PHE	ALA	ALA	ASP
D1593	N1400	E1337	N1400	E1337	I1276	TYR	GLY	GLY	THR	THR	LEU	LEU	GLU	GLU	TYR	TYR	TYR	ALA	ARG
F1594	K1530	V1463	V1401	L1338	H1279	TYR	ASN	ASN	ASN	ALA	ASP	LYS	LYS	LYS	LEU	LEU	LEU	ALA	HIS
D1591	D1531	S1466	E1402	F1339	A1280	ASP	GLU	LEU	ASP	ILE	GLN	ARG	ASP	ASN	ASN	ALA	ALA	ALA	HIS
M1592	S1532	I1463	I1403	ALA	D1281	ALA	VAL	VAL	ARG	LYS	VAL	PRO	PRO	ARG	ASN	ASN	ASN	ALA	ALA
L1533	L1533	M1469	Y1404	R1342	E1282	LYS	VAL	VAL	ARG	ALA	VAL	HIS	HIS	ARG	ASN	ASN	ASN	ALA	ILE
Y1598	Y1594	L1470	Y1405	V1343	L1283	LYS	TYR	TYR	TYR	ASP	GLN	VAL	LEU	LEU	LEU	CYS	GLN	GLN	GLN
F1599	K1535	F1471	R1406	M1344	E1284	LEU	TYR	TYR	TYR	ASP	THR	VAL	LEU	LEU	LEU	CYS	GLN	GLN	GLN
E1600	L1536	I1472	I1407	I1345	E1284	LEU	GLU	GLU	GLU	ARG	THR	ALA	LEU	LEU	LEU	GLN	GLN	GLN	GLN
Q1601	A1537	T1473	I1408	P1346	E1285	TYR	PHE	PHE	PHE	THR	THR	ALA	LEU	LEU	LEU	LYS	LYS	LYS	LYS
M1538	M1538	E1474	Q1409	K1347	L1286	ASN	MET	ALA	VAL	ARG	VAL	VAL	VAL	TYR	TYR	GLY	GLY	GLY	GLY
Q1539	Q1539	E1475	F1410	V1348	I1287	ASN	ALA	GLU	GLU	VAL	SER	ALA	ALA	PRO	ILE	LEU	LEU	LEU	ALA
Y1540	Y1540	D1476	L1411	L1349	M1288	VAL	ARG	ARG	ARG	MET	GLU	TYR	TYR	TRP	TRP	GLU	GLU	GLU	GLY
A1541	A1541	Y1477	L1412	R1350	Y1289	SER	LYS	LYS	LYS	LEU	THR	GLU	GLU	LEU	LEU	ILE	ILE	ILE	ILE
S1542	S1542	Q1478	E1413	R1351	Y1290	ASN	ASN	ASN	ASN	TYR	THR	GLN	GLU	GLU	TYR	TYR	TYR	TYR	CYS
E1543	E1543	A1479	F1414	A1352	Q1291	PHE	ALA	ALA	ALA	ILE	ASP	GLY	ALA	ALA	VAL	VAL	VAL	VAL	VAL
S1544	L1480	L1480	K1415	E1353	D1292	GLY	PRO	PRO	PRO	ARG	PRO	GLN	GLN	GLN	ARG	ARG	ARG	ARG	ARG
K1545	K1545	R1481	K1415	Q1354	R1293	ARG	ALA	ALA	ALA	ARG	GLU	CYS	CYS	CYS	LYS	LYS	LYS	LYS	ALA
D1546	D1546	T1482	L1418	A1355	Y1294	LEU	SER	SER	SER	LEU	GLU	ASP	VAL	VAL	VAL	VAL	VAL	VAL	VAL
T1547	T1547	L1419	L1419	H1356	Y1295	ALA	ALA	ALA	ALA	LEU	TRP	ASP	VAL	VAL	VAL	VAL	VAL	VAL	VAL
E1548	E1548	Y1487	N1420	H1357	F1296	SER	VAL	VAL	VAL	ASP	VAL	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
L1549	L1549	D1488	D1421	L1357	E1297	THR	GLU	GLN	GLN	TYR	VAL	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL
A1550	A1550	M1489	L1422	A1359	E1298	LEU	THR	THR	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR
L1553	L1553	F1490	L1423	E1360	L1299	VAL	GLU	GLU	GLU	ALA	VAL	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
L1554	L1554	D1491	M1424	H1361	I1300	HIS	LEU	LEU	LEU	PRO	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
W1556	W1556	M1492	L1425	V1362	T1301	LEU	LEU	LEU	LEU	ILE	ALA	CYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA
F1557	F1557	I1493	L1426	F1363	M1302	GLY	GLY	GLY	GLY	ILE	PHE	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
L1558	L1558	S1494	L1426	L1364	L1303	GLU	GLU	GLU	GLU	ALA	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
Q1559	Q1559	A1496	R1429	Y1365	E1304	TYR	TYR	TYR	TYR	GLN	LEU	THR	THR	THR	THR	THR	THR	THR	THR
E1560	E1560	Q1497	L1430	D1366	A1305	ALA	ALA	ALA	ALA	LYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
E1561	E1561	R1498	H1432	K1367	A1306	ALA	ALA	ALA	ALA	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR
K1562	K1562	L1499	T1433	Y1368	L1307	VAL	VAL	VAL	VAL	ILE	THR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
R1563	R1563	E1500	R1434	E1370	G1308	ASP	ASP	ASP	ASP	LEU	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
E1564	E1564	K1501	A1435	Y1371	L1309	GLY	GLY	GLY	GLY	GLU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
C1565	C1565	H1502	V1436	D1372	E1310	ALA	ALA	ALA	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
F1566	F1566	E1503	N1437	M1373	R1311	ARG	ARG	ARG	ARG	PHE	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
F1567	F1567	L1504	Y1438	R1311	A1312	LYS	LYS	LYS	LYS	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
C1569	C1569	R1508	F1439	I1376	M1314	ALA	ALA	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L1570	L1570	K1441	S1440	T1377	G1315	PHE	PHE	PHE	PHE	ILE	PHE	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
F1571	F1571	R1509	K1442	M1378	M1316	ILE	ILE	ILE	ILE	ALA	ALA	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
Y1574	Y1574	I1510	K1443	M1380	F1317	ASN	ASN	ASN	ASN	ALA	ALA	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
D1575	D1575	A1511	Q1444	H1381	T1318	GLY	GLY	GLY	GLY	PHE	PHE	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
L1576	L1576	I1512	L1445	D1384	E1319	VAL	VAL	VAL	VAL	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
L1577	L1577	Y1513	L1445	A1385	L1320	PRO	PRO	PRO	PRO	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
K1576	K1576	F1514	Q1449	M1386	A1321	ASN	ASN	ASN	ASN	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
G1577	G1577	L1515	P1450	K1387	L1323	ASN	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D1580	D1580	M1517	Y1451	G1388	Y1324	HIS	HIS	HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
Y1579	Y1579	M1518	L1452	E1389	K1326	ILE	ILE	ILE	ILE	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET
D1580	D1580	M1519	R1453	K1326	D1262	GLN	GLN	GLN	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

● Molecule 1: Clathrin heavy chain

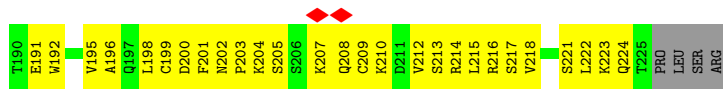
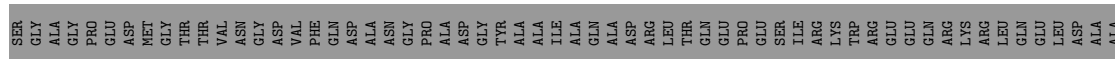
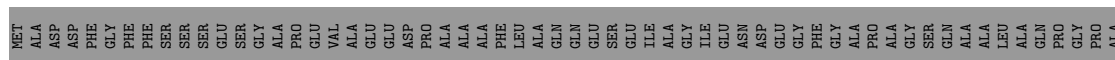
THR	GLY	PHE	K1441	M1379	H1313	A1240	A1176	P1105	T1038	P969	ASP	SER	THR	SER	PHE	GLU	GLU
GLU	ALA	ARG	V1442	M1380	M1314	V1241	L1177	A1106	R1039	L970	SER	THR	THR	ASP	ASP	ASP	ASP
THR	CYS	ARG	K1443	H1381	G1315	G1242	A1179	V1107	V1040	1971	VAL	GLN	ASP	GLN	GLN	GLN	GLN
THR	LEU	ILE	P1382	M1316	M1316	G1243	K1179	M1108	Y1043	D972	VAL	VAL	VAL	ASP	PRO	LEU	LEU
THR	PHE	ALA	L1445	T1383	F1317	A1244	N1181	S1109	I1044	Q973	GLY	THR	THR	HIS	THR	THR	THR
CYS	THR	ALA	P1446	D1384	T1318	R1245	M1181	Q1110	N1045	Y974	VAL	VAL	VAL	CYS	VAL	LEU	LEU
CYS	THR	TYR	L1447	A1385	E1319	K1246	H1182	L1111	N1046	Y975	VAL	VAL	VAL	LEU	VAL	ARG	ARG
TYR	LEU	LEU	V1448	W1386	I1322	A1247	L1183	A1112	R1046	Q976	VAL	GLU	GLU	ARG	HIS	ARG	ARG
ASP	PHE	PHE	K1449	K1387	I1322	M1248	A1184	K1113	L1047	Y977	VAL	VAL	VAL	ALA	ALA	ALA	ALA
LEU	LYS	LYS	E1388	L1323	L1323	S1249	E1185	A1114	Y1050	Y978	GLU	GLU	GLU	LEU	LEU	LEU	LEU
LEU	GLY	GLY	P1450	G1389	Y1324	T1250	L1186	Q1115	D1051	Y978	LEU	LEU	LEU	LEU	LEU	LEU	LEU
ARG	ASN	ASN	L1452	Q1390	S1325	R1251	E1187	L1116	D1051	Y978	ARG	ARG	ARG	ILE	ILE	ILE	ILE
PRO	ASN	ASN	R1453	F1391	K1326	T1252	F1188	Q1117	D1051	Y978	ASN	ASN	ASN	ALA	ALA	ALA	ALA
ASP	ARG	ARG	S1454	K1392	F1327	W1253	F1189	K1118	ARG	Y978	ASN	ASN	ASN	ALA	ALA	ALA	ALA
V1455	VAL	TRP	V1455	D1393	K1328	K1254	I1190	G1119	D1054	Y984	PRO	PRO	PRO	ALA	ALA	ALA	ALA
VAL	VAL	LYS	I1394	P1329	P1329	E1254	N1195	G1119	I1055	Y984	HIS	HIS	HIS	ILE	ILE	ILE	ILE
LEU	LEU	GLN	T1395	K1330	K1330	E1255	N1195	W1120	I1056	Y986	LEU	LEU	LEU	ALA	ALA	ALA	ALA
GLU	GLU	SER	T1396	K1331	K1331	A1259	I1198	V1121	A1056	Y986	LEU	LEU	LEU	CYS	CYS	CYS	CYS
THR	VAL	VAL	K1397	R1332	R1332	D1262	Q1200	E1123	I1057	Y987	GLN	GLN	GLN	LYS	LYS	LYS	LYS
ALA	ALA	GLU	V1398	R1333	R1333	G1263	Q1200	A1124	D1058	Y988	VAL	VAL	VAL	GLY	GLY	GLY	GLY
TRP	LEU	LEU	A1399	E1334	E1334	G1263	Q1200	A1125	S1061	Y990	ALA	ALA	ALA	GLN	GLN	GLN	GLN
ARG	CYS	ARG	M1400	H1335	H1335	G1264	V1201	Y1128	F1065	Y992	GLY	GLY	GLY	LYS	LYS	LYS	LYS
HIS	LYS	LYS	V1401	L1336	L1336	E1265	G1202	T1129	E1066	Y993	GLU	GLU	GLU	VAL	VAL	VAL	VAL
ASN	ASN	ASN	L1470	E1337	E1337	F1266	D1203	I1129	E1067	Y994	GLY	GLY	GLY	VAL	VAL	VAL	VAL
F1471	ASN	ASN	L1403	L1338	L1338	B1267	R1204	K1130	E1068	Y995	GLN	GLN	GLN	VAL	VAL	VAL	VAL
I1472	SER	SER	Y1404	R1342	R1342	Q1270	C1205	A1131	A1068	Y996	LYS	LYS	LYS	ARG	ARG	ARG	ARG
ASP	ASP	ASP	Y1405	R1343	R1343	M1271	Y1206	S1136	F1069	Y997	VAL	VAL	VAL	ALA	ALA	ALA	ALA
ASP	GLU	TYR	R1406	M1344	M1344	M1271	D1207	A1070	I1071	Y997	HIS	HIS	HIS	ILE	ILE	ILE	ILE
ALA	ALA	ASP	L1407	L1344	L1344	H1279	E1208	A1070	F1072	L1000	GLU	GLU	GLU	LYS	LYS	LYS	LYS
PRO	PRO	ALA	Q1409	I1345	I1345	H1279	E1208	A1070	I1071	L1000	TYR	TYR	TYR	CYS	CYS	CYS	CYS
TYR	TYR	MET	F1410	P1346	P1346	D1281	D1208	E1139	F1073	N1001	ARG	ARG	ARG	GLU	GLU	GLU	GLU
PHE	GLN	GLN	Y1411	L1349	L1349	D1281	M1210	V1140	K1073	N1001	LEU	LEU	LEU	GLN	GLN	GLN	GLN
ILE	ILE	ILE	L1412	R1350	R1350	E1282	Y1211	A1144	K1074	N1002	PRO	PRO	PRO	VAL	VAL	VAL	VAL
GLN	GLN	GLN	L1413	L1350	L1350	E1283	D1212	M1145	F1076	N1003	VAL	VAL	VAL	ALA	ALA	ALA	ALA
VAL	VAL	VAL	F1414	A1351	A1351	E1284	A1214	E1006	D1076	N1005	THR	THR	THR	ASP	ASP	ASP	ASP
MET	SER	SER	K1415	E1352	E1352	E1285	K1215	M1149	S1080	L1006	THR	THR	THR	ASP	ASP	ASP	ASP
ILE	ILE	ILE	P1416	Q1354	Q1354	L1287	L1216	W1150	A1081	L1007	ASN	ASN	ASN	GLY	GLY	GLY	GLY
ASP	ASP	ASP	L1417	L1357	L1357	M1288	L1217	E1151	E1082	L1008	ALA	ALA	ALA	GLY	GLY	GLY	GLY
LYS	LYS	LYS	L1418	L1357	L1357	M1288	Y1218	E1152	V1082	E1009	LEU	LEU	LEU	GLY	GLY	GLY	GLY
TYR	TYR	TYR	L1419	W1358	W1358	Y1289	N1219	L1153	V1082	K1010	LEU	LEU	LEU	VAL	VAL	VAL	VAL
ASP	ASP	ASP	M1420	A1359	A1359	Y1290	M1220	V1154	V1084	I1011	LEU	LEU	LEU	LYS	LYS	LYS	LYS
VAL	VAL	VAL	D1421	E1360	E1360	Q1291	V1221	K1155	V1084	I1011	LEU	LEU	LEU	LYS	LYS	LYS	LYS
ASP	ASP	ASP	L1422	L1361	L1361	D1292	S1222	Y1156	L1085	I1012	VAL	VAL	VAL	PHE	PHE	PHE	PHE
ASP	ASP	ASP	L1423	V1362	V1362	Y1295	A1228	L1157	I1086	R950	THR	THR	THR	PHE	PHE	PHE	PHE
ASN	ASN	ASN	L1426	F1363	F1363	F1296	F1224	Q1158	H1088	R1022	ASP	ASP	ASP	GLU	GLU	GLU	GLU
LEU	LEU	LEU	L1430	L1364	L1364	F1296	G1225	M1159	I1089	M1022	GLU	GLU	GLU	ALA	ALA	ALA	ALA
LEU	LEU	LEU	L1431	L1364	L1364	E1297	R1226	A1160	G1090	M1024	LYS	LYS	LYS	LYS	LYS	LYS	LYS
LEU	LEU	LEU	D1432	Y1365	Y1365	E1298	L1227	R1161	G1090	Q1025	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ALA	ALA	ALA	R1429	D1366	D1366	L1299	A1228	K1162	N1091	Q1025	VAL	VAL	VAL	PHE	PHE	PHE	PHE
ALA	ALA	ALA	L1430	D1366	D1366	L1300	S1229	K1163	L1092	L1027	THR	THR	THR	THR	THR	THR	THR
GLN	GLN	GLN	D1431	E1369	E1369	T1301	T1230	A1164	R1094	L1028	GLN	GLN	GLN	GLN	GLN	GLN	GLN
ARG	ARG	ARG	H1432	E1370	E1370	M1302	L1231	R1165	A1095	L1028	LEU	LEU	LEU	LEU	LEU	LEU	LEU
LEU	LEU	LEU	T1433	Y1371	Y1371	L1303	V1232	E1166	Y1096	I1029	VAL	VAL	VAL	PRO	PRO	PRO	PRO
ARG	ARG	ARG	R1434	D1372	D1372	E1304	H1233	S1167	E1097	L1030	LEU	LEU	LEU	LEU	LEU	LEU	LEU
LYS	LYS	LYS	A1435	M1373	M1373	A1305	H1234	L1234	F1098	T1031	ARG	ARG	ARG	ILE	ILE	ILE	ILE
HIS	HIS	HIS	V1436	A1374	A1374	G1235	G1235	E1170	A1098	L1033	VAL	VAL	VAL	VAL	VAL	VAL	VAL
GLU	GLU	GLU	M1437	L1375	L1375	L1309	E1236	T1171	E1100	K1034	ARG	ARG	ARG	VAL	VAL	VAL	VAL
LEU	LEU	LEU	F1438	I1376	I1376	E1310	Y1237	T1171	E1100	K1034	GLY	GLY	GLY	VAL	VAL	VAL	VAL
ILE	ILE	ILE	F1439	T1377	T1377	R1311	Q1238	I1174	R1101	D1036	VAL	VAL	VAL	CYS	CYS	CYS	CYS
GLU	GLU	GLU	S1440	M1378	M1378	A1312	A1239	F1175	C1102	R1037	ARG	ARG	ARG	ASP	ASP	ASP	ASP

• Molecule 1: Clathrin heavy chain

ALA	ASN	VAL	GLY	ARG	LEU	VAL	L858	Q797	C736	R676	I613	V550	Q490	Y430	L363
ASN	ASN	VAL	GLU	MET	SER	ALA	L859	K798	K737	Q677	A614	D551	C491	E431	L364
HIS	VAL	ASP	GLU	GLU	GLU	TYR	P860	T800	T739	M678	Q615	V552	F492	S432	F365
PHE	GLU	VAL	GLU	GLU	THR	TYR	R861	R801	G738	L679	L616	F553	A493	L433	R366
ASP	LEU	ASP	ASN	ASP	ASP	ARG	L862	R802	Q740	Q680	E617	M554	E494	E434	K367
GLY	PRO	ASP	GLY	ASP	PRO	ASN	A864	R803	K742	I681	E618	E555	T495	L435	R368
VAL	ALA	ARG	R865	R804	GLU	CYS	R866	R804	E743	C682	Q621	Y556	G496	C436	F369
THR	ALA	ARG	T871	R805	GLU	ASP	H867	R806	V744	Q684	L622	L588	V498	R438	A370
THR	ALA	ASP	C870	R807	VAL	VAL	H867	R807	R745	A686	L623	I589	K500	L371	L371
VAL	THR	ASP	T871	R808	VAL	VAL	H867	R808	R746	A686	Q624	Q560	L440	L371	L371
THR	THR	ASP	R870	R809	THR	THR	H867	R809	I747	S687	R625	M625	I501	Q441	M376
VAL	VAL	ALA	R871	R810	THR	THR	H867	R810	C748	K688	A626	C562	V502	Q442	M376
THR	VAL	ALA	T871	R811	VAL	ASN	H867	R811	R749	Y689	L627	Q561	L503	R438	E379
THR	VAL	ALA	T871	R812	VAL	VAL	H867	R812	E750	H690	E628	Y504	Y504	A380	A380
THR	VAL	ALA	T871	R813	VAL	CYS	H867	R813	S751	E691	A629	A505	A505	K445	A380
THR	VAL	ALA	T871	R814	VAL	THR	H867	R814	R692	Q692	F630	L567	K506	Q446	V383
THR	VAL	ALA	T871	R815	VAL	ASN	H867	R815	C753	L693	T631	D568	K507	L447	A384
THR	VAL	ALA	T871	R816	VAL	ASN	H867	R816	Y754	S694	D632	A569	V508	L448	A387
THR	VAL	ALA	T871	R817	VAL	SER	H867	R817	D755	T695	L633	L570	G509	E449	A387
THR	VAL	ALA	T871	R818	VAL	LEU	H867	R818	P756	Q696	B634	L570	G509	E449	A387
THR	VAL	ALA	T871	R819	VAL	LEU	H867	R819	E757	Q696	B634	L570	G509	E449	A387
THR	VAL	ALA	T871	R820	VAL	LEU	H867	R820	R758	S697	D635	R571	Y510	K450	P388
THR	VAL	ALA	T871	R821	VAL	LEU	H867	R821	R759	L698	L636	N572	T511	W451	K389
THR	VAL	ALA	T871	R822	VAL	LEU	H867	R822	V759	L698	L636	N572	T511	W451	K389
THR	VAL	ALA	T871	R823	VAL	LEU	H867	R823	K760	I699	K637	R574	P512	L452	G390
THR	VAL	ALA	T871	R824	VAL	LEU	H867	R824	N761	E700	R638	P575	D513	K453	I391
THR	VAL	ALA	T871	R825	VAL	LEU	H867	R825	F762	L701	R638	P575	D513	K453	I391
THR	VAL	ALA	T871	R826	VAL	LEU	H867	R826	E763	F702	V641	S576	I515	R454	R393
THR	VAL	ALA	T871	R827	VAL	LEU	H867	R827	S825	E702	V641	S576	I515	R454	R393
THR	VAL	ALA	T871	R828	VAL	LEU	H867	R828	E826	F703	H642	E577	F516	K456	T394
THR	VAL	ALA	T871	R829	VAL	LEU	H867	R829	E827	S704	H643	P579	L518	E458	D396
THR	VAL	ALA	T871	R830	VAL	LEU	H867	R830	E828	R705	H644	L580	R519	E459	T397
THR	VAL	ALA	T871	R831	VAL	LEU	H867	R831	E829	K706	L645	Q581	N520	S460	I398
THR	VAL	ALA	T871	R832	VAL	LEU	H867	R832	K767	S707	L646	T582	E521	E461	R399
THR	VAL	ALA	T871	R833	VAL	LEU	H867	R833	R830	F708	M647	R583	M522	E462	R400
THR	VAL	ALA	T871	R834	VAL	LEU	H867	R834	T769	E709	P648	L584	R523	L463	F401
THR	VAL	ALA	T871	R835	VAL	LEU	H867	R835	R771	G710	P649	L585	I524	L464	Q402
THR	VAL	ALA	T871	R836	VAL	LEU	H867	R836	Q771	L711	W650	E586	S525	D465	S403
THR	VAL	ALA	T871	R837	VAL	LEU	H867	R837	L772	L712	W650	M587	P526	L466	V404
THR	VAL	ALA	T871	R838	VAL	LEU	H867	R838	P773	Y713	M653	Y588	D527	V467	P405
THR	VAL	ALA	T871	R839	VAL	LEU	H867	R839	L774	F714	Y684	L589	Q528	K468	A406
THR	VAL	ALA	T871	R840	VAL	LEU	H867	R840	L775	L715	P655	M590	G529	S469	Q407
THR	VAL	ALA	T871	R841	VAL	LEU	H867	R841	L776	G656	H591	H591	Q530	V470	P408
THR	VAL	ALA	T871	R842	VAL	LEU	H867	R842	L777	G716	G656	A592	Q531	D471	P409
THR	VAL	ALA	T871	R843	VAL	LEU	H867	R843	L778	S717	L658	P593	F532	P472	G409
THR	VAL	ALA	T871	R844	VAL	LEU	H867	R844	C778	L718	L659	Q594	A533	T473	Q410
THR	VAL	ALA	T871	R845	VAL	LEU	H867	R845	D779	W719	V680	Q594	Q534	L474	T411
THR	VAL	ALA	T871	R846	VAL	LEU	H867	R846	R780	R720	B661	D597	M535	A475	S412
THR	VAL	ALA	T871	R847	VAL	LEU	H867	R847	F781	F721	E661	D597	M535	A475	P413
THR	VAL	ALA	T871	R848	VAL	LEU	H867	R848	D782	S722	D662	I598	V537	L476	P413
THR	VAL	ALA	T871	R849	VAL	LEU	H867	R849	F783	Q723	L663	I599	V537	L476	P413
THR	VAL	ALA	T871	R850	VAL	LEU	H867	R850	V784	L664	L600	I600	V537	L476	P413
THR	VAL	ALA	T871	R851	VAL	LEU	H867	R851	H785	R725	E665	I600	V537	L476	P413
THR	VAL	ALA	T871	R852	VAL	LEU	H867	R852	D786	D726	G686	I600	V537	L476	P413
THR	VAL	ALA	T871	R853	VAL	LEU	H867	R853	L787	W727	L687	I600	V537	L476	P413
THR	VAL	ALA	T871	R854	VAL	LEU	H867	R854	Y790	V728	L604	Q603	E540	L480	F418
THR	VAL	ALA	T871	R855	VAL	LEU	H867	R855	Y791	H728	M604	M604	E541	R481	G419
THR	VAL	ALA	T871	R856	VAL	LEU	H867	R856	Y792	F729	F605	F605	P542	A482	I420
THR	VAL	ALA	T871	R857	VAL	LEU	H867	R857	Y793	K730	T606	T606	L543	M483	L421
THR	VAL	ALA	T871	R858	VAL	LEU	H867	R858	Y794	R731	H607	H607	A544	V484	Q424
THR	VAL	ALA	T871	R859	VAL	LEU	H867	R859	Y795	I732	G608	G608	D545	P485	Q425
THR	VAL	ALA	T871	R860	VAL	LEU	H867	R860	Y796	I733	D609	D609	I546	M486	Q426
THR	VAL	ALA	T871	R861	VAL	LEU	H867	R861	Y797	Q733	A610	A610	I547	K487	L427
THR	VAL	ALA	T871	R862	VAL	LEU	H867	R862	Y798	A734	M674	M674	Q548	V488	K428
THR	VAL	ALA	T871	R863	VAL	LEU	H867	R863	Y799	A735	I675	H612	I549	I489	K428



• Molecule 4: Clathrin light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	12076	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction in no-vaCTF with by multiplication	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	6500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.641	Depositor
Minimum map value	-0.445	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	284.8, 284.8, 284.8	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.78, 1.78, 1.78	Depositor

5 Model quality i

5.1 Standard geometry i

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	0/3240	0.49	0/4375
1	B	0.32	0/3810	0.49	1/5160 (0.0%)
1	E	1.25	7/5858 (0.1%)	0.53	2/7941 (0.0%)
1	H	0.27	0/1965	0.45	0/2659
1	J	0.29	0/1405	0.43	0/1892
1	K	0.29	0/2196	0.45	0/2966
1	L	0.31	0/4547	0.47	0/6158
1	M	0.33	0/4294	0.47	0/5820
2	F	0.81	0/1886	0.99	7/2562 (0.3%)
3	C	1.34	9/4211 (0.2%)	0.98	22/5700 (0.4%)
4	D	0.30	0/887	0.44	0/1183
4	I	0.26	0/473	0.44	0/631
4	N	0.25	0/677	0.39	0/904
4	O	0.28	0/520	0.42	0/692
All	All	0.75	16/35969 (0.0%)	0.59	32/48643 (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
1	B	0	1
3	C	0	9
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	83	LYS	CD-CE	75.02	3.38	1.51
3	C	364	PHE	CE2-CZ	35.66	2.05	1.37
3	C	364	PHE	CE1-CZ	35.12	2.04	1.37
3	C	364	PHE	CD2-CE2	32.77	2.04	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	111	TRP	CE3-CZ3	32.02	1.92	1.38

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	536	LEU	CB-CG-CD1	-11.20	91.96	111.00
3	C	457	LEU	CB-CG-CD1	-9.96	94.07	111.00
3	C	713	TYR	CA-CB-CG	-9.38	95.58	113.40
3	C	364	PHE	CB-CG-CD2	-8.90	114.57	120.80
3	C	698	LEU	CA-CB-CG	8.21	134.19	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	364	PHE	Sidechain
3	C	531	GLN	Peptide
3	C	571	LYS	Peptide
3	C	622	LEU	Peptide
3	C	647	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3168	0	3118	333	0
1	B	3744	0	3703	342	0
1	E	5740	0	5756	802	0
1	H	1928	0	1947	148	0
1	J	1379	0	1333	106	0
1	K	2150	0	2117	174	0
1	L	4458	0	4413	375	0
1	M	4213	0	4209	435	0
2	F	1844	0	1849	73	0
3	C	4133	0	4168	852	0
4	D	875	0	872	88	0
4	I	468	0	474	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	668	0	657	56	0
4	O	514	0	508	40	0
All	All	35282	0	35124	3741	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 53.

The worst 5 of 3741 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:E:111:TRP:CE3	1:E:111:TRP:CZ3	1.92	1.56
3:C:742:LYS:HE2	1:H:641:VAL:CG1	1.30	1.54
3:C:364:PHE:CD1	3:C:364:PHE:CE1	2.03	1.47
3:C:742:LYS:CE	1:H:641:VAL:HG11	1.45	1.47
3:C:364:PHE:CE1	3:C:364:PHE:CZ	2.04	1.46

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	377/1630 (23%)	328 (87%)	49 (13%)	0	100	100
1	B	466/1630 (29%)	398 (85%)	67 (14%)	1 (0%)	47	81
1	E	724/1630 (44%)	610 (84%)	114 (16%)	0	100	100
1	H	234/1630 (14%)	204 (87%)	29 (12%)	1 (0%)	34	72
1	J	163/1630 (10%)	145 (89%)	18 (11%)	0	100	100
1	K	255/1630 (16%)	229 (90%)	25 (10%)	1 (0%)	34	72
1	L	546/1630 (34%)	466 (85%)	80 (15%)	0	100	100
1	M	516/1630 (32%)	433 (84%)	83 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	231/233 (99%)	228 (99%)	3 (1%)	0	100	100
3	C	508/1630 (31%)	424 (84%)	82 (16%)	2 (0%)	34	72
4	D	100/229 (44%)	91 (91%)	9 (9%)	0	100	100
4	I	54/229 (24%)	50 (93%)	4 (7%)	0	100	100
4	N	76/229 (33%)	71 (93%)	5 (7%)	0	100	100
4	O	57/229 (25%)	53 (93%)	4 (7%)	0	100	100
All	All	4307/15819 (27%)	3730 (87%)	572 (13%)	5 (0%)	54	86

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	674	ASN
1	K	1594	PHE
3	C	438	PRO
1	B	855	LEU
1	H	773	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/1437 (24%)	338 (99%)	4 (1%)	71	83
1	B	407/1437 (28%)	403 (99%)	4 (1%)	76	86
1	E	629/1437 (44%)	627 (100%)	2 (0%)	92	95
1	H	219/1437 (15%)	219 (100%)	0	100	100
1	J	150/1437 (10%)	149 (99%)	1 (1%)	84	90
1	K	236/1437 (16%)	234 (99%)	2 (1%)	81	89
1	L	482/1437 (34%)	477 (99%)	5 (1%)	76	86
1	M	471/1437 (33%)	463 (98%)	8 (2%)	60	78
2	F	204/209 (98%)	196 (96%)	8 (4%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	457/1437 (32%)	441 (96%)	16 (4%)	36	59
4	D	96/184 (52%)	95 (99%)	1 (1%)	76	86
4	I	53/184 (29%)	53 (100%)	0	100	100
4	N	74/184 (40%)	74 (100%)	0	100	100
4	O	55/184 (30%)	55 (100%)	0	100	100
All	All	3875/13878 (28%)	3824 (99%)	51 (1%)	70	81

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	762	PHE
1	A	1535	LYS
1	L	1397	LYS
1	M	843	ASP
1	M	927	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1460	ASN
1	B	1142	GLN
4	N	150	ASN
1	L	1313	HIS
1	A	1492	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
3	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	870:CYS	C	871:THR	N	7.18
1	C	659:SER	C	660:VAL	N	3.20

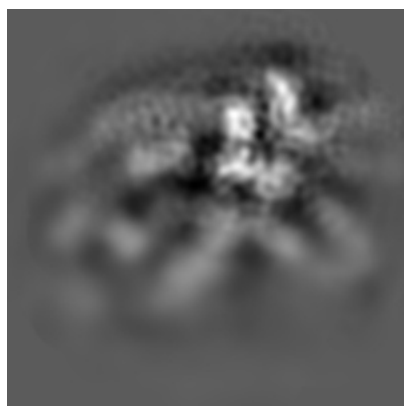
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10754. These allow visual inspection of the internal detail of the map and identification of artifacts.

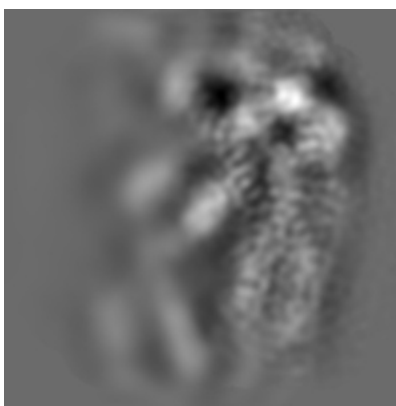
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

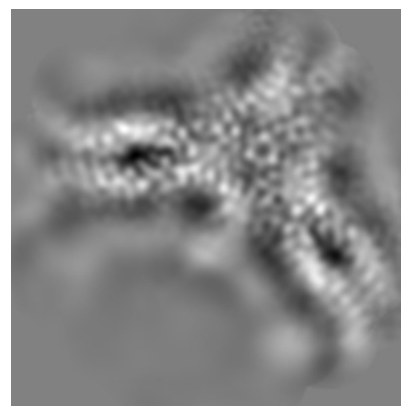
6.1.1 Primary map



X

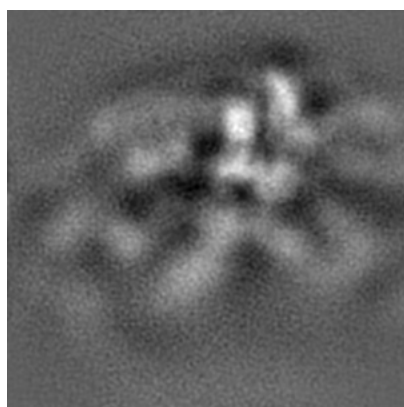


Y

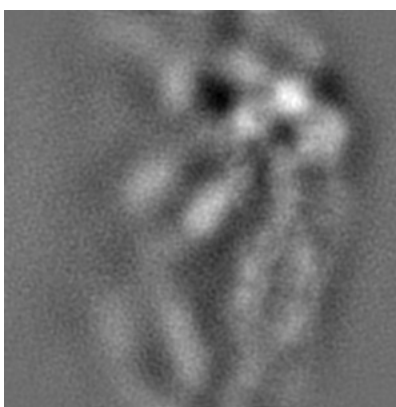


Z

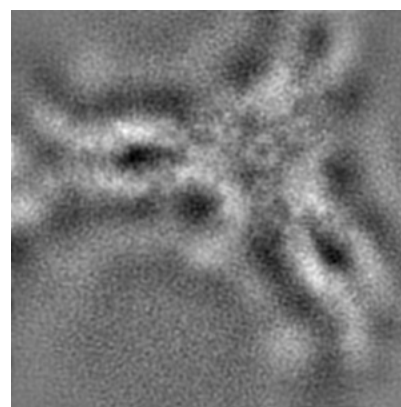
6.1.2 Raw map



X



Y

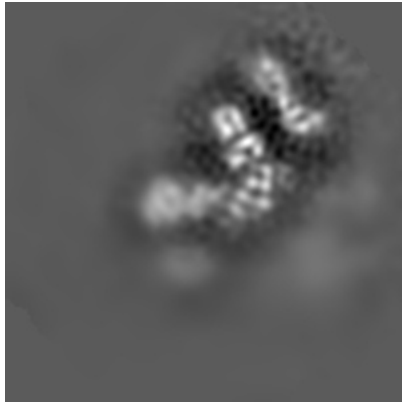


Z

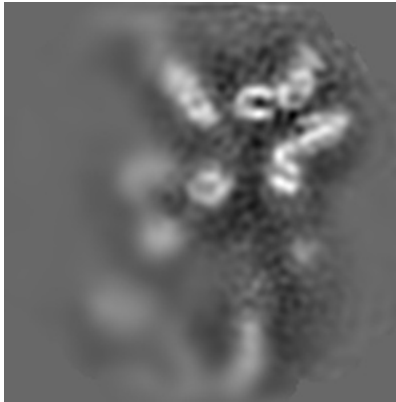
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

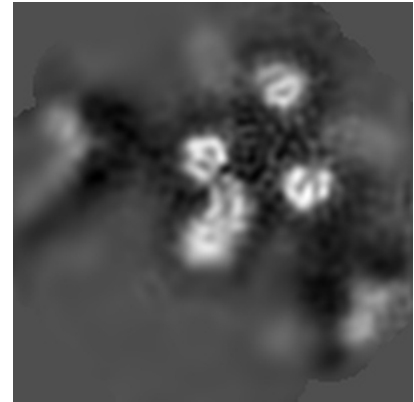
6.2.1 Primary map



X Index: 80

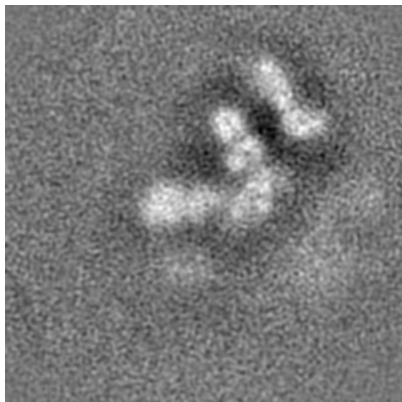


Y Index: 80

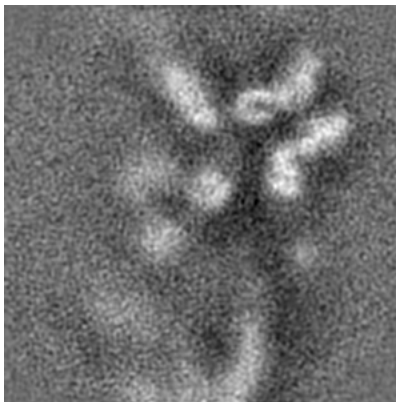


Z Index: 80

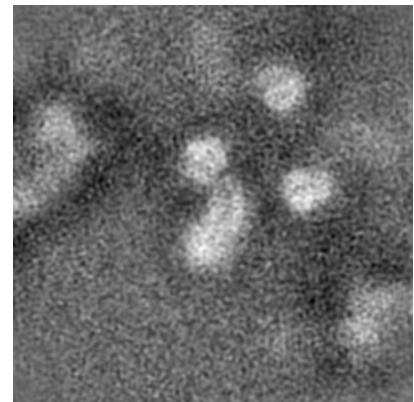
6.2.2 Raw map



X Index: 80



Y Index: 80

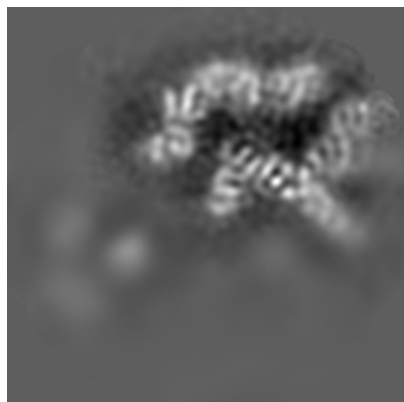


Z Index: 80

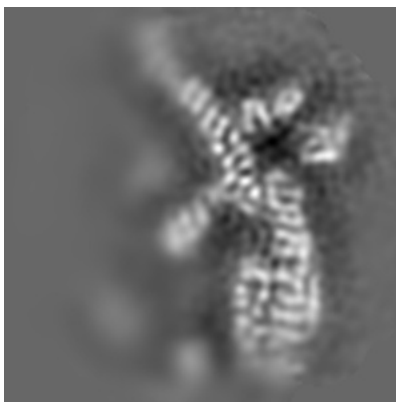
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

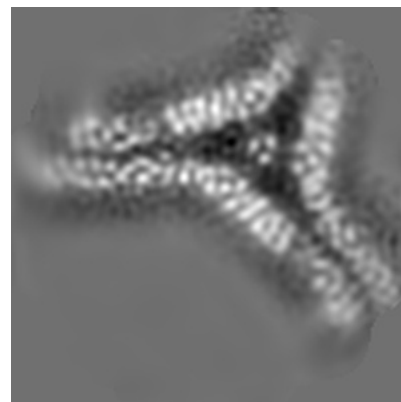
6.3.1 Primary map



X Index: 110

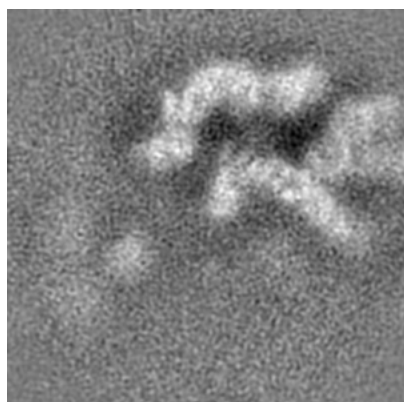


Y Index: 90



Z Index: 110

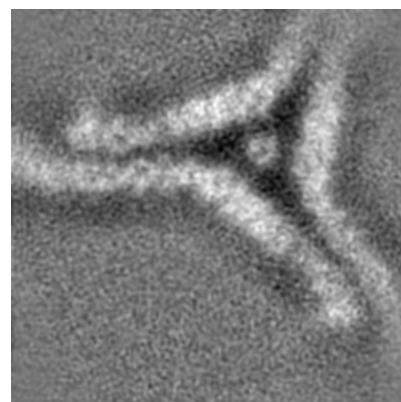
6.3.2 Raw map



X Index: 110



Y Index: 90

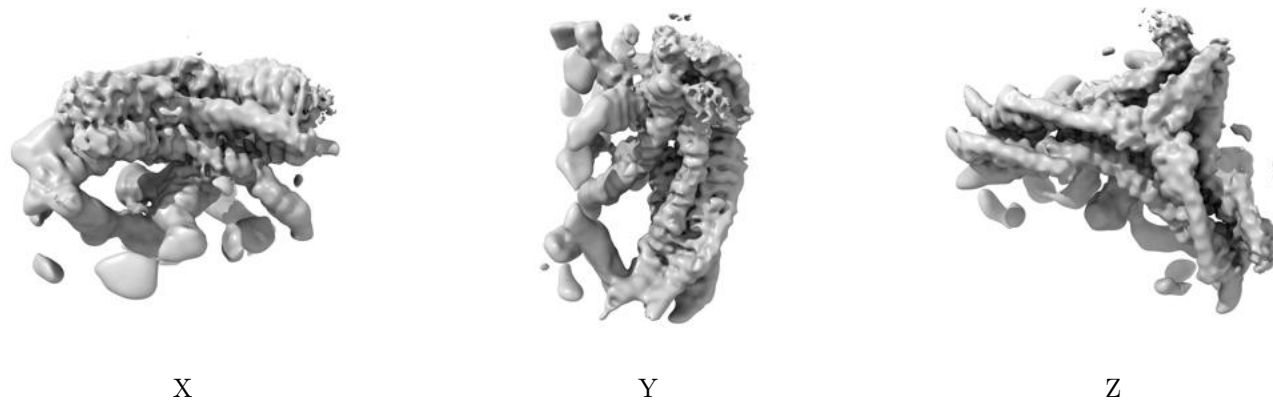


Z Index: 111

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



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

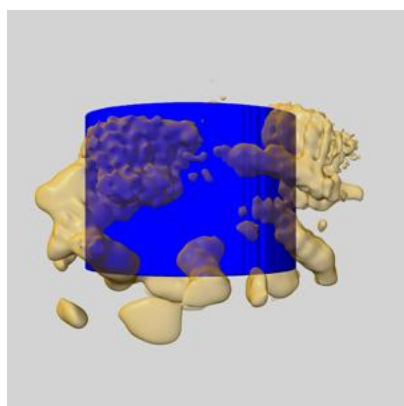
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

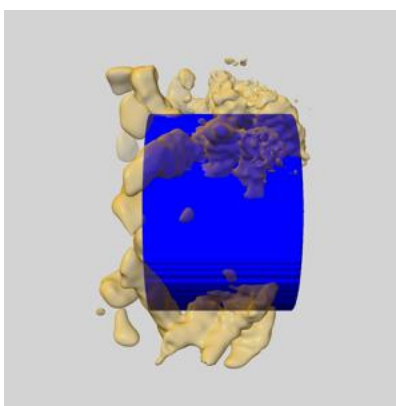
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

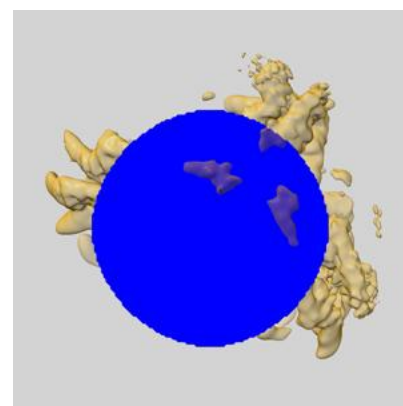
6.5.1 emd_10754_msk_1.map [i](#)



X



Y

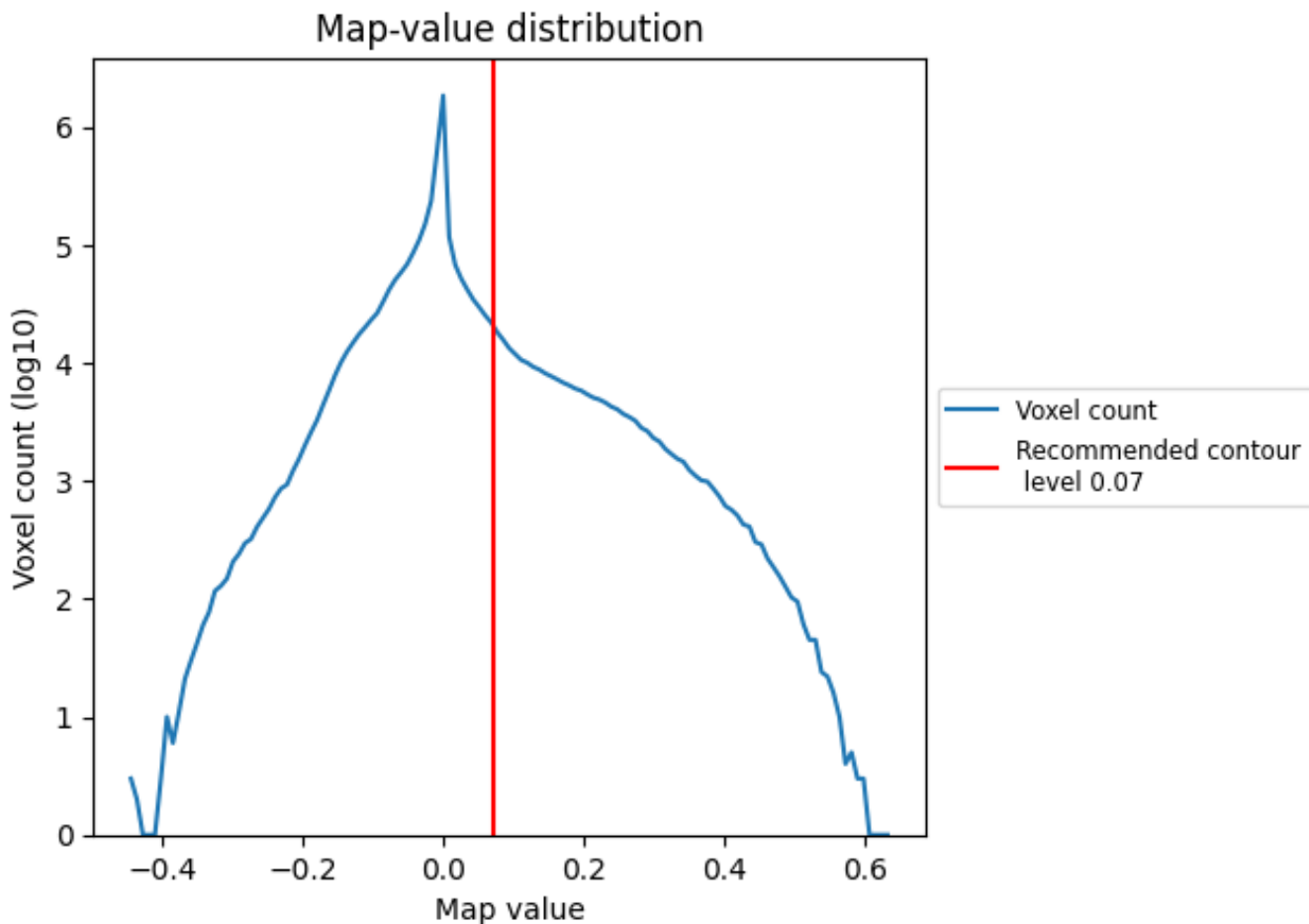


Z

7 Map analysis [i](#)

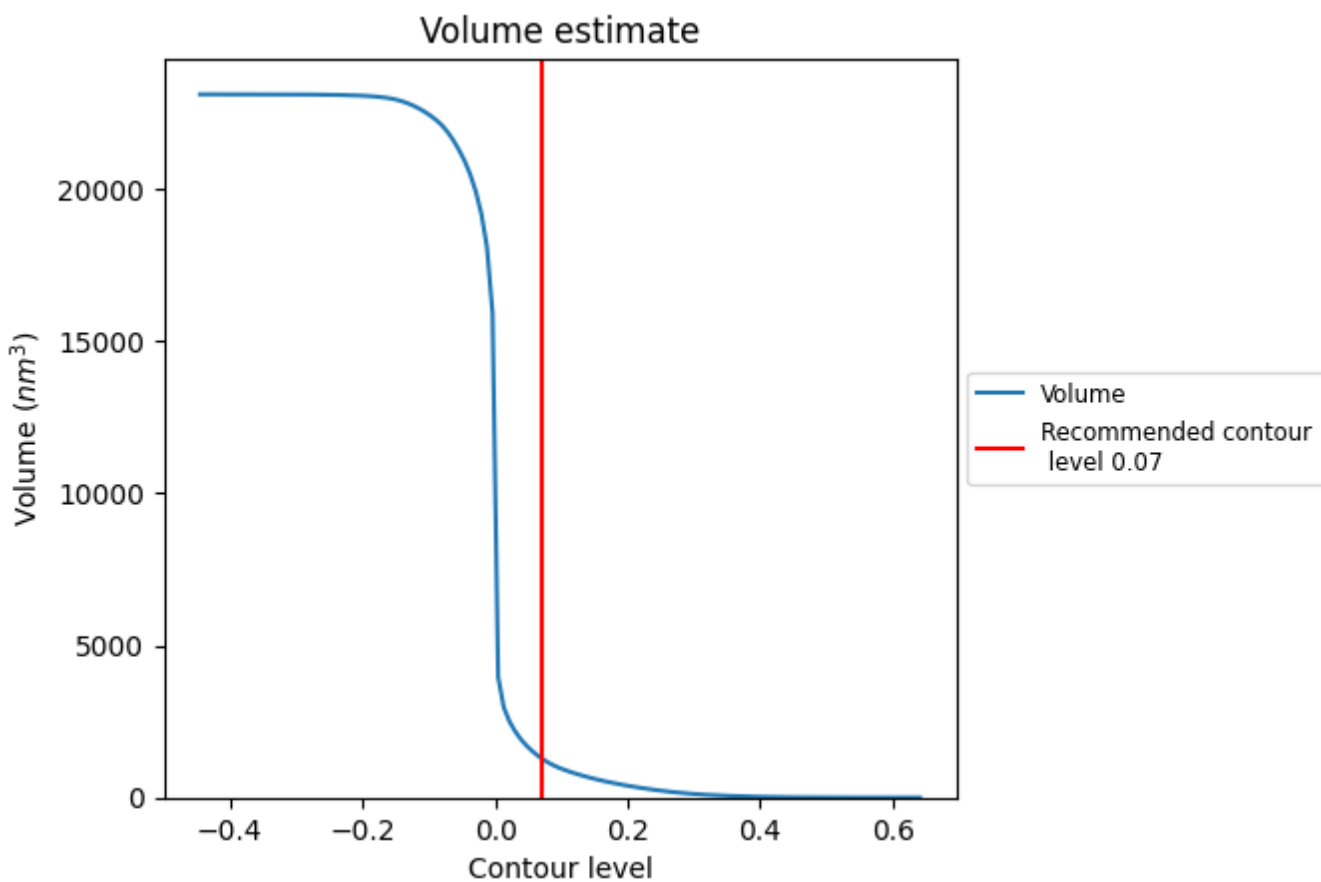
This section contains the results of statistical analysis of the map.

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.

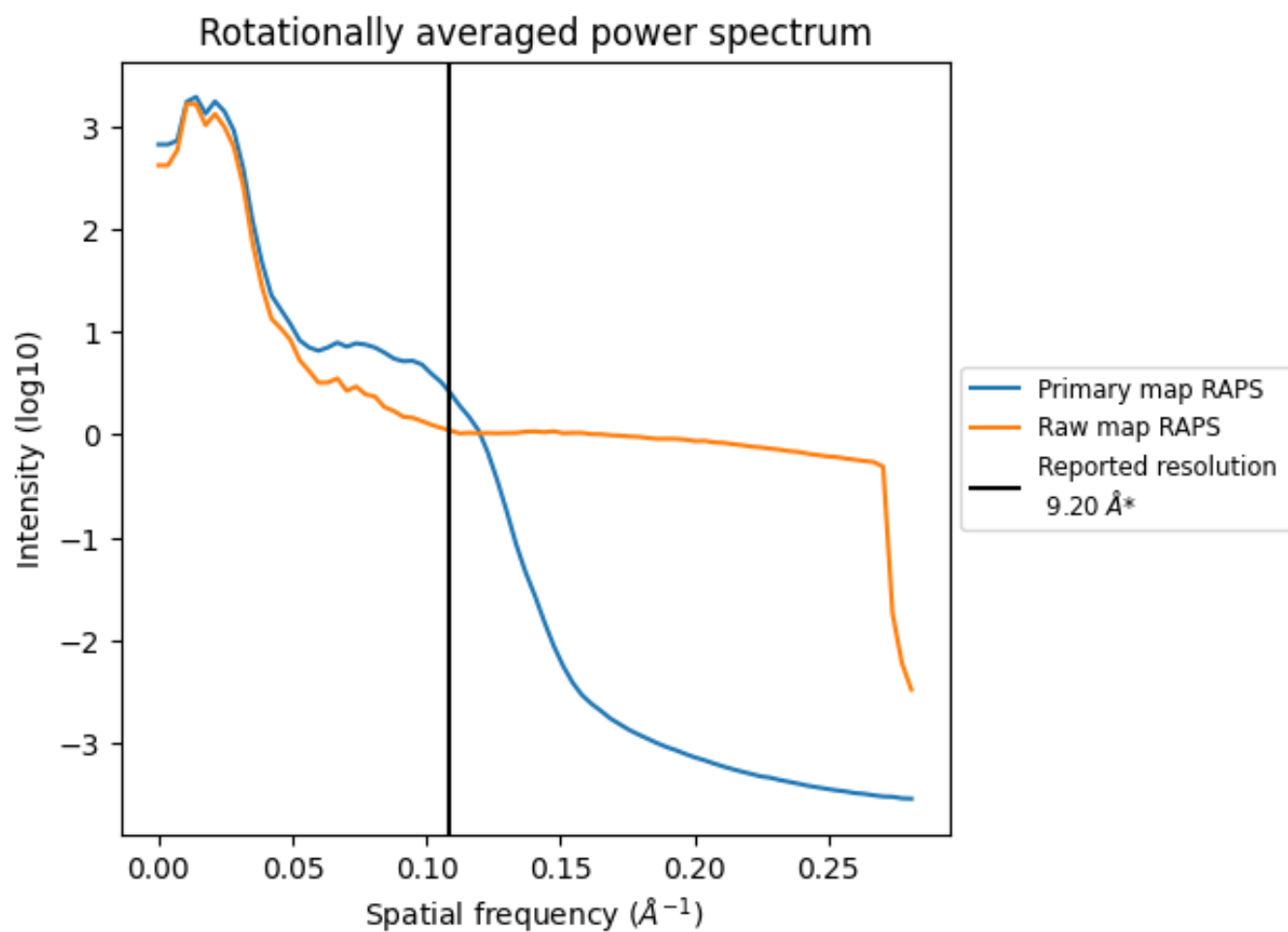
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1289 nm³; this corresponds to an approximate mass of 1164 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 [i](#)

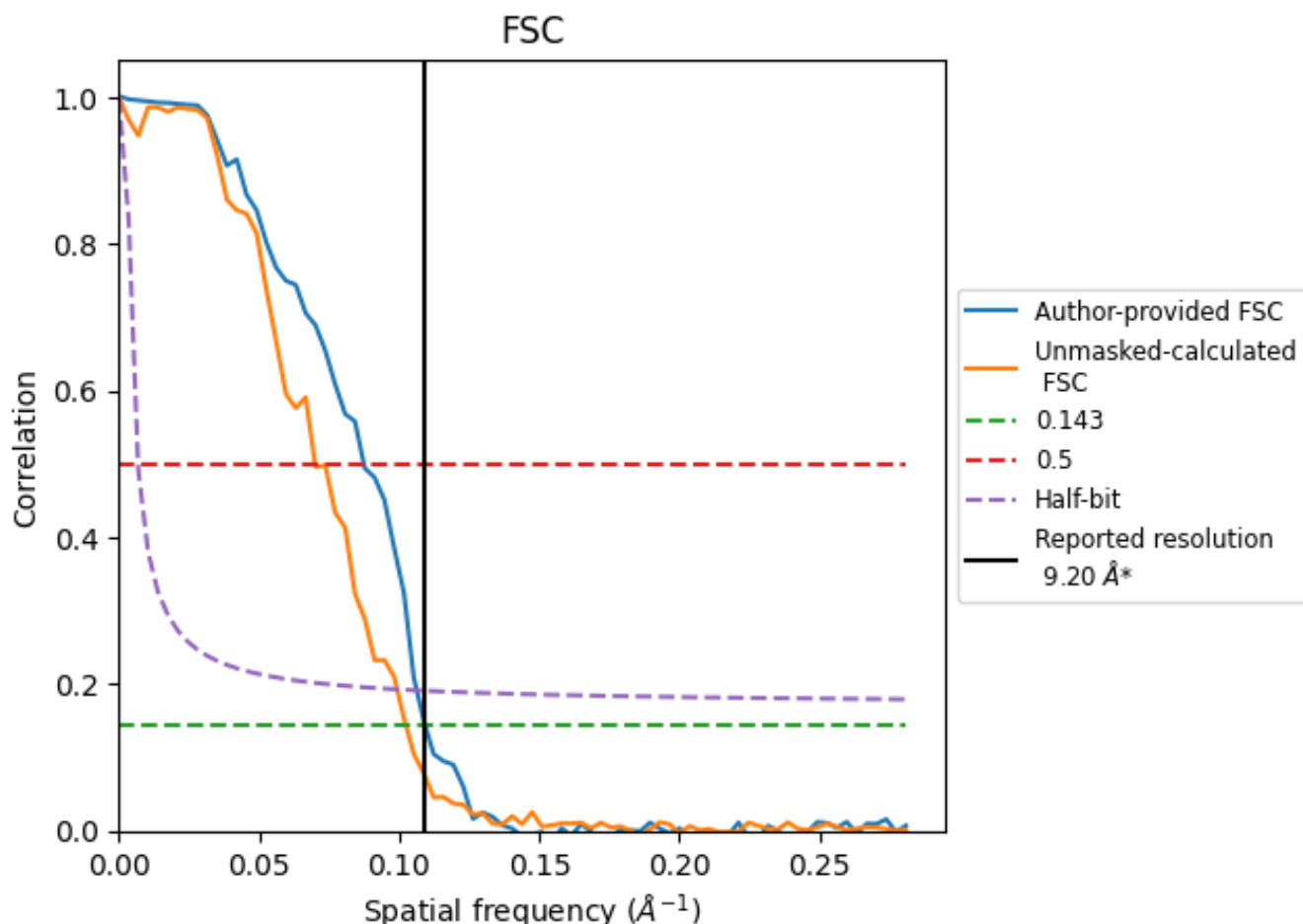


*Reported resolution corresponds to spatial frequency of 0.109 Å⁻¹

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 0.109 Å⁻¹

8.2 Resolution estimates [i](#)

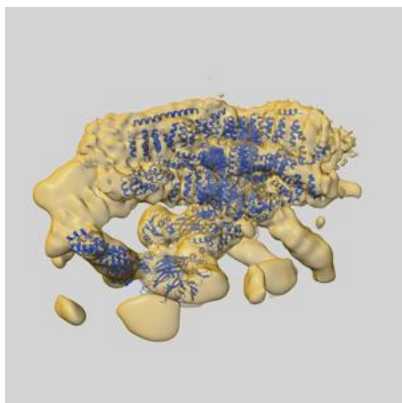
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.20	-	-
Author-provided FSC curve	9.14	11.44	9.40
Unmasked-calculated*	9.76	14.27	10.06

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

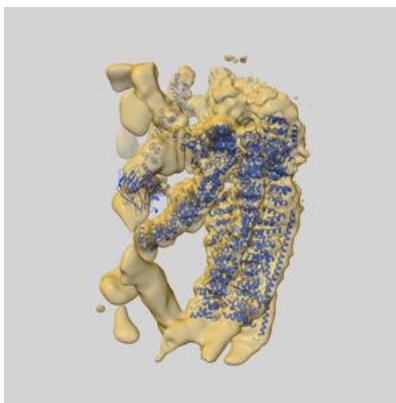
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10754 and PDB model 6YAI. Per-residue inclusion information can be found in section 3 on page 6.

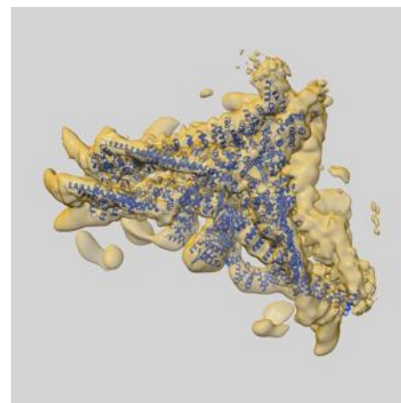
9.1 Map-model overlay [i](#)



X



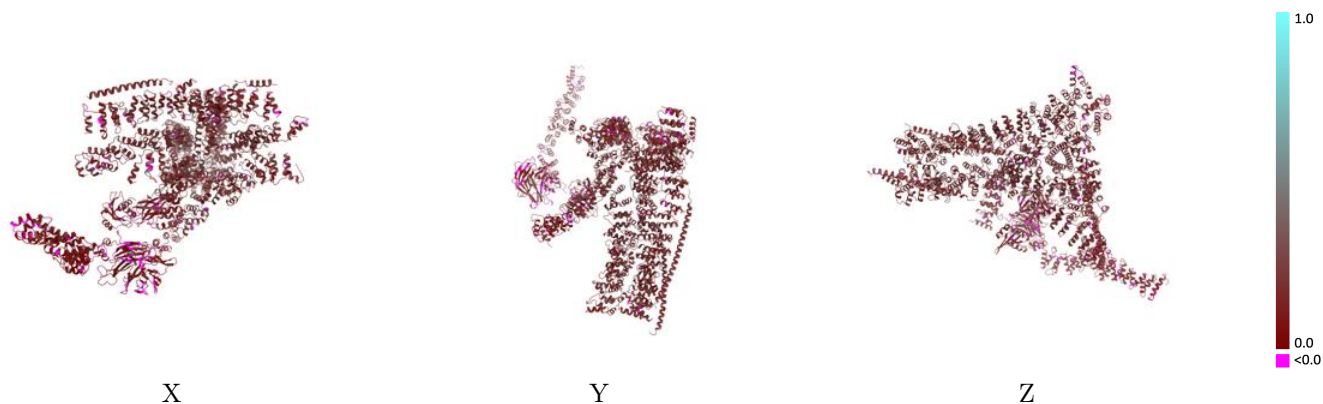
Y



Z

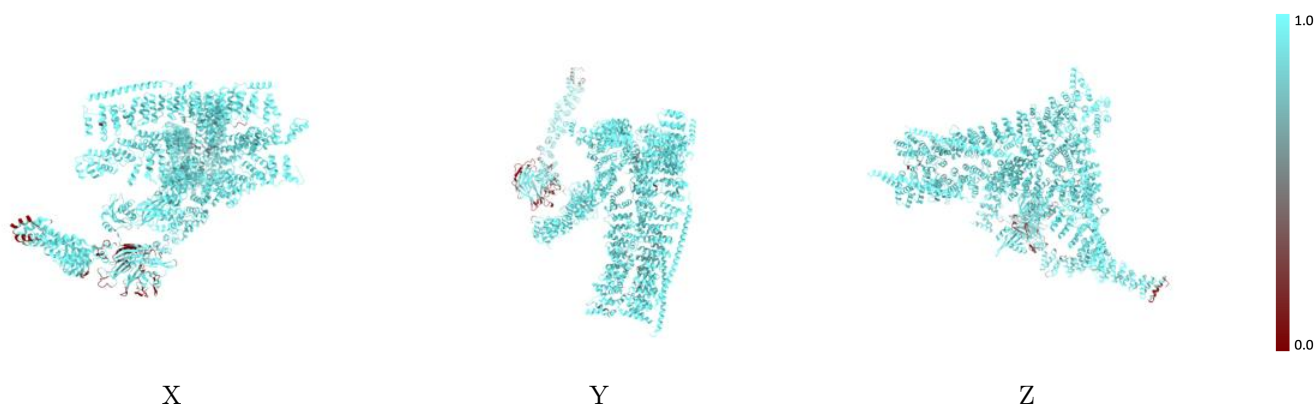
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



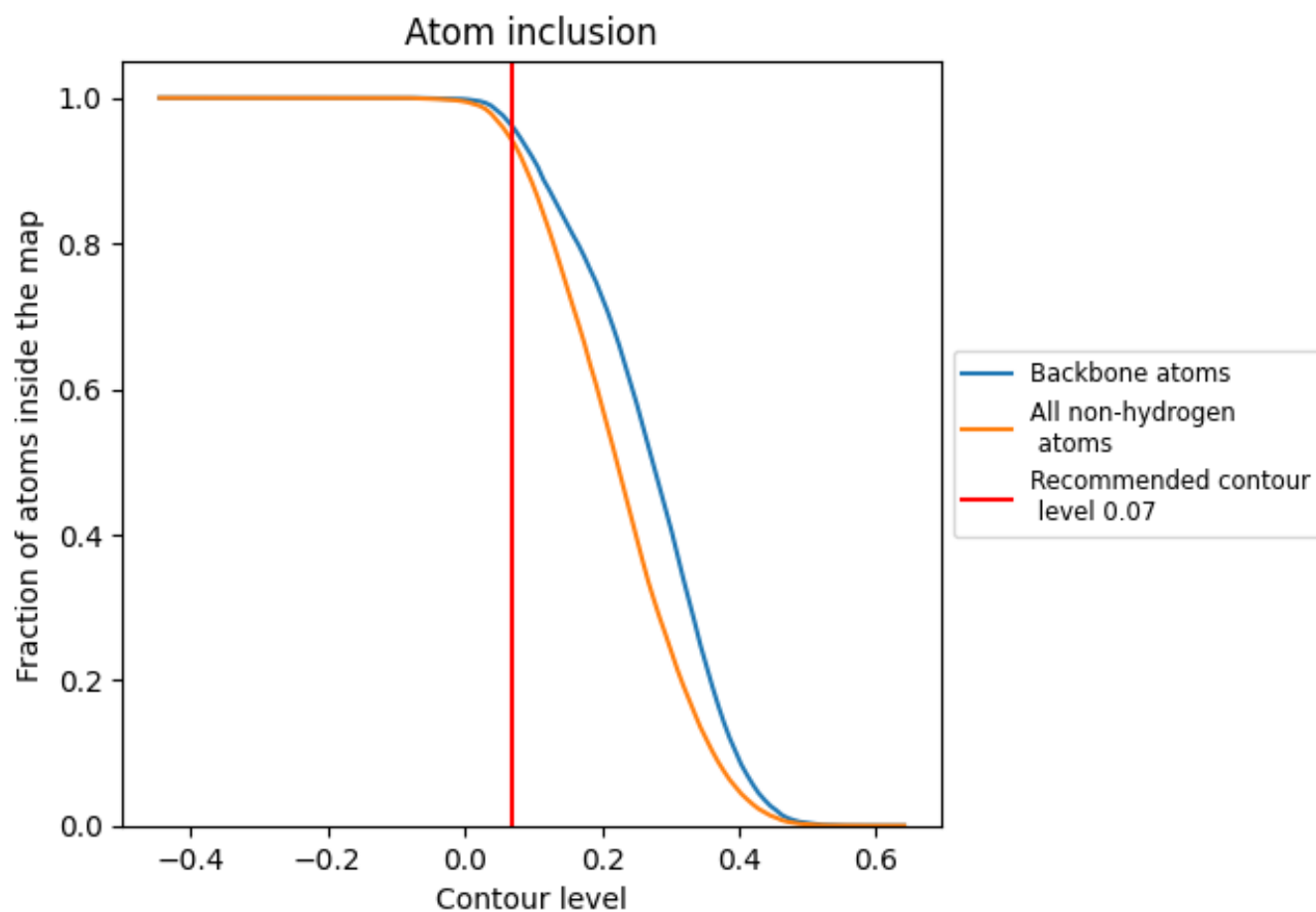
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9397	 0.1710
A	 0.9626	 0.2040
B	 0.9773	 0.2040
C	 0.9823	 0.1750
D	 0.9718	 0.2210
E	 0.7609	 0.0710
F	 0.9781	 0.1190
H	 0.9572	 0.1940
I	 0.9435	 0.2100
J	 0.9793	 0.1790
K	 0.9663	 0.1740
L	 0.9817	 0.1980
M	 0.9775	 0.2010
N	 0.9694	 0.1920
O	 0.9980	 0.2210

