



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 03:04 AM UTC

PDB ID : 9LG9 / pdb_00009lg9
EMDB ID : EMD-63058
Title : bovine ABCC1 bound to GSSG
Authors : Sun, P.P.; Liu, K.X.; Gao, P.
Deposited on : 2025-01-10
Resolution : 3.56 Å(reported)

This is a Full wwPDB EM Validation 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

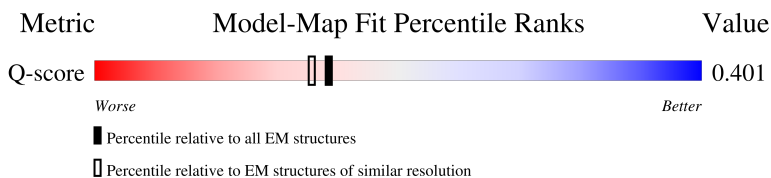
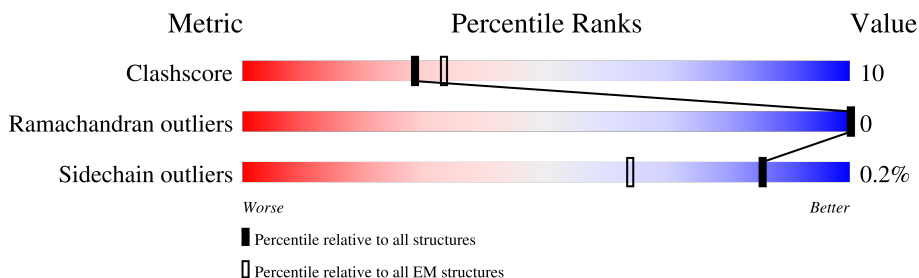
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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	12750 (3.06 - 4.06)

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	1558	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10647 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.

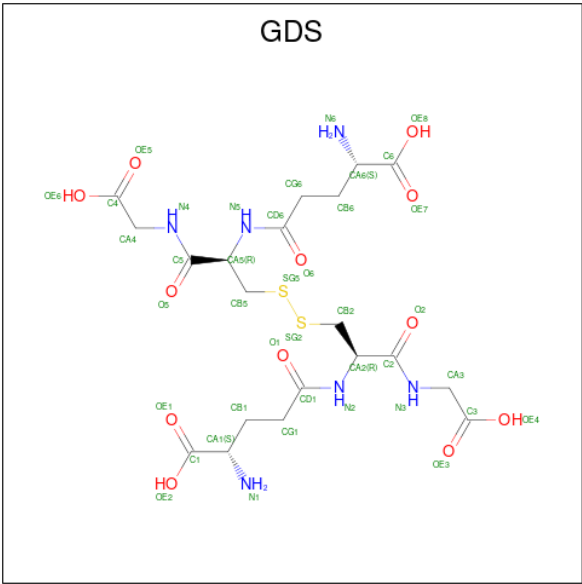
- Molecule 1 is a protein called Multidrug resistance-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1336	Total	C	N	O	S	0	0
			10607	6902	1759	1890	56		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1531	LYS	-	expression tag	UNP Q8HXQ5
A	1532	LEU	-	expression tag	UNP Q8HXQ5
A	1533	GLY	-	expression tag	UNP Q8HXQ5
A	1534	SER	-	expression tag	UNP Q8HXQ5
A	1535	GLU	-	expression tag	UNP Q8HXQ5
A	1536	ASN	-	expression tag	UNP Q8HXQ5
A	1537	LEU	-	expression tag	UNP Q8HXQ5
A	1538	TYR	-	expression tag	UNP Q8HXQ5
A	1539	PHE	-	expression tag	UNP Q8HXQ5
A	1540	GLN	-	expression tag	UNP Q8HXQ5
A	1541	GLY	-	expression tag	UNP Q8HXQ5
A	1542	GLY	-	expression tag	UNP Q8HXQ5
A	1543	SER	-	expression tag	UNP Q8HXQ5
A	1544	GLY	-	expression tag	UNP Q8HXQ5
A	1545	GLY	-	expression tag	UNP Q8HXQ5
A	1546	SER	-	expression tag	UNP Q8HXQ5
A	1547	GLY	-	expression tag	UNP Q8HXQ5
A	1548	HIS	-	expression tag	UNP Q8HXQ5
A	1549	HIS	-	expression tag	UNP Q8HXQ5
A	1550	HIS	-	expression tag	UNP Q8HXQ5
A	1551	HIS	-	expression tag	UNP Q8HXQ5
A	1552	HIS	-	expression tag	UNP Q8HXQ5
A	1553	HIS	-	expression tag	UNP Q8HXQ5
A	1554	HIS	-	expression tag	UNP Q8HXQ5
A	1555	HIS	-	expression tag	UNP Q8HXQ5
A	1556	HIS	-	expression tag	UNP Q8HXQ5
A	1557	HIS	-	expression tag	UNP Q8HXQ5
A	1558	HIS	-	expression tag	UNP Q8HXQ5

- Molecule 2 is OXIDIZED GLUTATHIONE DISULFIDE (CCD ID: GDS) (formula: C₂₀H₃₂N₆O₁₂S₂) (labeled as "Ligand of Interest" by depositor).

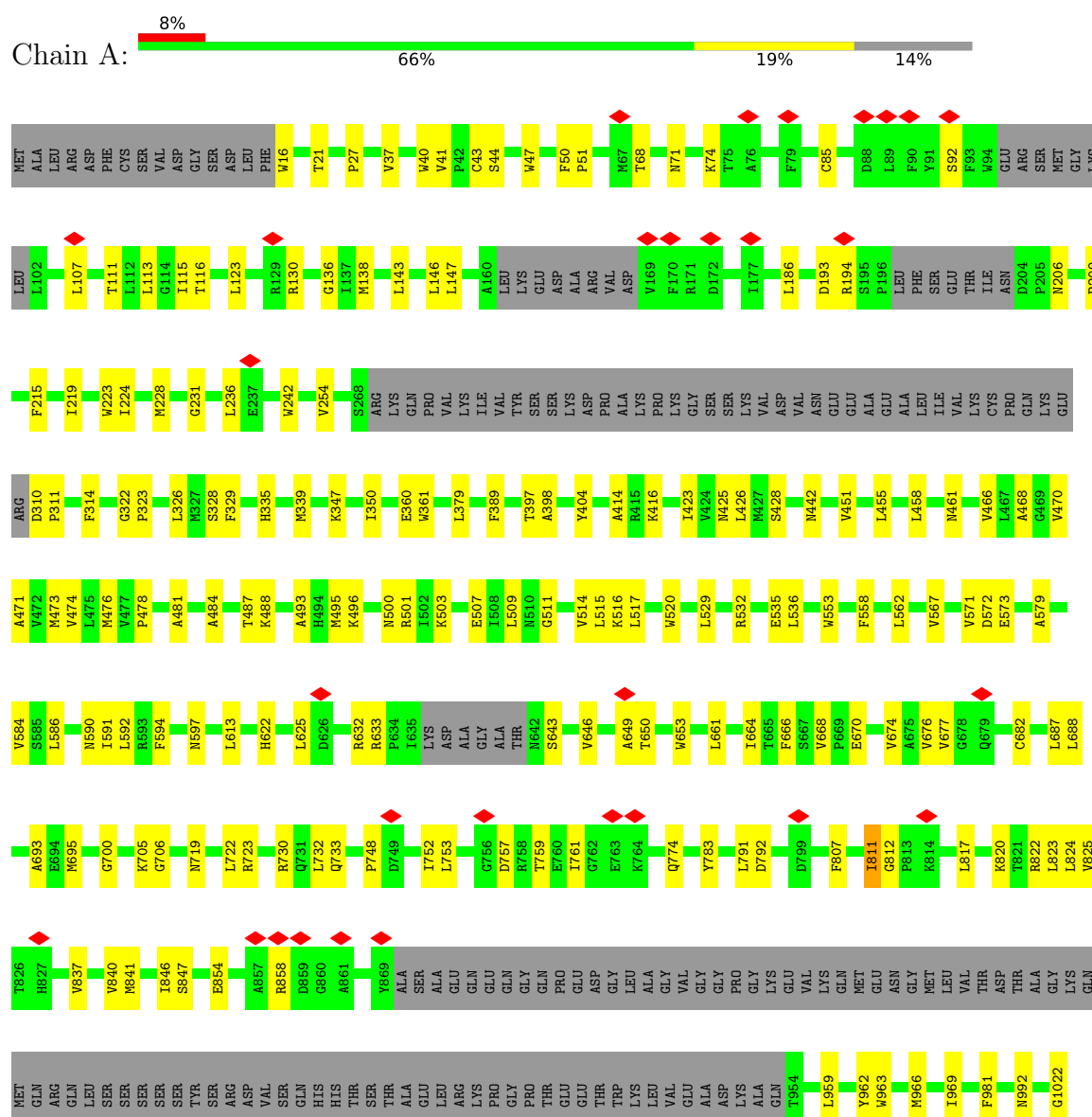


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	40	20	6	12	2	0

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: Multidrug resistance-associated protein 1



GLN	R1441	Q1374	H1311	L1202	I1023
GLN	A1442	D1375	I1312	E1203	I1027
ARG	L1443	E1376	N1313	C1204	
GLY	L1444	V1377	V1314	N1207	I1041
LEU	R1445	L1378			
PHE		L1379	D1317	F1216	S1044
TYR	K1448	S1380	G1318		R1045
SER	I1449	G1381	G1319	I1219	R1046
MET	L1450	S1382	E1320	S1220	L1047
ALA		L1383	L1321	R1221	H1048
LYS	D1453	R1384	V1322	L1231	L1049
ASP	E1454	M1385	G1323		
SER	A1455	N1386	I1324	R1057	
GLY	THR	L1387	V1325	Y1236	
LEU	ALA	D1388	G1326	Q1238	I1060
VAL	ALA	P1389	R1327		S1061
LEU	ASP		T1328	V1247	
GLY	LEU	Q1392	G1329	A1269	R1065
SER	E1462	Y1393	A1330	L1263	L1071
GLU		S1394	G1331	K1264	
ASN	D1465	D1395	K1332	E1265	R1074
LEU		E1396	S1333		F1075
TYR		E1397	S1334	K1271	E1078
PHE	R1472		L1335		
GLN	T1473	L1401	T1336	P1274	G1095
GLY	Q1474	L1402	L1337		
SER	F1475	E1403	G1338	Q1278	F1098
GLY	D1476	L1404	L1339	D1279	
SER	D1477	H1405	F1340		A1103
GLY		H1406	R1341	P1282	Y1132
	L1481	L1407	I1342	P1283	
HIS		K1408	K1343	K1284	S1148
HIS	H1485	G1409	E1344	D1285	P1149
HIS	R1486	F1410	S1345	W1286	V1150
HIS	L1487	V1411	A1346	P1287	V1151
HIS	L1488	S1412	E1347	Q1288	E1156
HIS	T1489	A1413	G1348	V1289	T1157
HIS	I1490	L1414	E1349	G1290	
HIS	M1491	P1415	I1350	R1291	R1175
	D1492	D1416	I1351	V1292	
	T1493	K1417	I1352	E1293	D1178
	T1494	L1418	D1353	F1294	
	R1495	N1419	D1354		Y1181
		H1420	I1355	G1298	Q1185
	L1499	E1421	M1356	L1299	
	D1500	C1422	I1357	R1300	Y1189
	K1501	A1423	A1358	P1190	
	G1502	E1424	K1359	Y1301	S1191
	E1503	G1425	I1360	ARG	I1192
	I1504	G1426	G1361	GLU	
	Q1505	E1427	L1362	ASP	W1197
	E1506	N1428	H1363	LEU	L1198
	W1507	L1429	D1364	D1306	
	G1508	S1430	L1365	L1307	A1199
	S1509		R1366	V1308	
	P1510	Q1433	F1367	K1310	
	S1511	R1434	T1370		
	D1512	G1435	I1371		
	L1513	L1436			
	L1514				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105909	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.355	Depositor
Minimum map value	-0.863	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.16	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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: GDS

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	0.40	0/10844	0.59	1/14723 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1289	VAL	N-CA-C	-6.39	107.64	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10607	0	10826	205	0
2	A	40	0	28	3	0
All	All	10647	0	10854	205	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 10.

All (205) 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:517:LEU:HD13	1:A:1371:ILE:HD13	1.63	0.80
1:A:1060:ILE:HD12	1:A:1342:ILE:CG2	2.11	0.80
1:A:514:VAL:HG11	1:A:1377:VAL:HB	1.67	0.75
1:A:674:VAL:HG22	1:A:837:VAL:HB	1.70	0.73
1:A:1057:ARG:HH12	1:A:1274:PRO:HA	1.53	0.73
1:A:1060:ILE:HD12	1:A:1342:ILE:HG23	1.69	0.73
1:A:458:LEU:HD11	1:A:466:VAL:HG23	1.72	0.71
1:A:558:PHE:CZ	1:A:1022:GLY:HA3	2.25	0.71
1:A:520:TRP:CE2	1:A:1389:PRO:HG2	2.27	0.69
1:A:209:PRO:HB2	1:A:223:TRP:HB2	1.75	0.69
1:A:1060:ILE:CD1	1:A:1342:ILE:HG23	2.24	0.68
1:A:111:THR:O	1:A:115:ILE:HG12	1.95	0.67
1:A:1289:VAL:HG22	1:A:1318:GLY:HA3	1.79	0.64
1:A:1430:SER:HB3	1:A:1433:GLN:HG2	1.81	0.62
1:A:1323:GLY:HA3	1:A:1490:ILE:HD11	1.81	0.61
1:A:719:ASN:ND2	1:A:1156:GLU:OE2	2.33	0.61
1:A:328:SER:OG	1:A:442:ASN:ND2	2.34	0.60
1:A:1341:ARG:NH1	1:A:1357:ILE:O	2.34	0.60
1:A:27:PRO:HB3	1:A:361:TRP:CH2	2.37	0.59
1:A:206:ASN:HB3	1:A:242:TRP:HA	1.85	0.59
1:A:516:LYS:O	1:A:1366:ARG:HD3	2.02	0.58
1:A:1057:ARG:O	1:A:1271:LYS:HB3	2.03	0.58
1:A:1286:TRP:HE1	1:A:1355:ILE:HB	1.67	0.58
1:A:470:VAL:HA	1:A:473:MET:HE2	1.85	0.58
1:A:517:LEU:CD1	1:A:1371:ILE:HD13	2.33	0.58
1:A:1299:LEU:HB3	1:A:1309:LEU:HB2	1.84	0.58
1:A:649:ALA:HA	1:A:700:GLY:HA3	1.86	0.57
1:A:1337:LEU:HD22	1:A:1342:ILE:HG13	1.84	0.57
1:A:1352:ILE:HD13	1:A:1449:ILE:HD12	1.86	0.57
1:A:219:ILE:HD12	1:A:379:LEU:HD13	1.86	0.57
1:A:1402:LEU:HD13	1:A:1411:VAL:HG21	1.87	0.57
1:A:476:MET:HE2	1:A:476:MET:HA	1.86	0.56
1:A:224:ILE:HG13	1:A:242:TRP:HH2	1.69	0.56
1:A:500:ASN:HA	1:A:503:LYS:HZ2	1.69	0.56
1:A:1204:CYS:HA	1:A:1207:ASN:HB2	1.87	0.56
1:A:509:LEU:HD21	1:A:1071:LEU:HB2	1.86	0.56
1:A:532:ARG:NH1	1:A:535:GLU:OE2	2.35	0.55
1:A:791:LEU:HD12	1:A:824:LEU:HD12	1.89	0.55
1:A:314:PHE:HB2	1:A:613:LEU:HD21	1.88	0.55
1:A:404:TYR:CE1	1:A:1157:THR:HG21	2.43	0.54
1:A:123:LEU:HD23	1:A:138:MET:SD	2.47	0.54
1:A:136:GLY:HA2	1:A:215:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:TRP:CD2	2:A:1601:GDS:HB61	2.43	0.54
1:A:682:CYS:SG	1:A:841:MET:HG3	2.48	0.54
1:A:981:PHE:CZ	1:A:1095:GLY:HA2	2.42	0.54
1:A:514:VAL:HG11	1:A:1377:VAL:CB	2.37	0.54
1:A:633:ARG:NE	1:A:705:LYS:HD3	2.22	0.54
1:A:643:SER:HB2	1:A:670:GLU:HG2	1.89	0.53
1:A:536:LEU:HD22	1:A:1041:ILE:HG23	1.91	0.53
1:A:664:ILE:HG13	1:A:846:ILE:HG12	1.89	0.53
1:A:1286:TRP:HB3	1:A:1287:PRO:HD3	1.90	0.53
1:A:1178:ASP:HA	1:A:1181:VAL:HG12	1.90	0.53
1:A:1298:GLY:N	1:A:1347:GLU:O	2.42	0.53
1:A:719:ASN:HD22	1:A:1156:GLU:CD	2.17	0.52
1:A:1181:VAL:O	1:A:1185:GLN:HG2	2.10	0.52
1:A:1202:LEU:HD12	1:A:1247:VAL:HG11	1.91	0.52
1:A:959:LEU:HA	1:A:962:TYR:HD2	1.74	0.52
1:A:500:ASN:HA	1:A:503:LYS:NZ	2.25	0.51
1:A:674:VAL:HA	1:A:837:VAL:O	2.11	0.51
1:A:1382:SER:HB2	1:A:1419:ASN:HA	1.92	0.51
1:A:1286:TRP:CD1	1:A:1355:ILE:HD12	2.45	0.51
1:A:1378:LEU:HD22	1:A:1434:ARG:HG2	1.93	0.51
1:A:484:ALA:O	1:A:487:THR:OG1	2.29	0.51
1:A:1294:PHE:O	1:A:1313:ASN:HA	2.10	0.51
1:A:625:LEU:HD11	1:A:693:ALA:O	2.11	0.50
1:A:1060:ILE:HD12	1:A:1342:ILE:HG21	1.94	0.50
1:A:1384:ARG:HH12	1:A:1395:ASP:HA	1.77	0.50
1:A:723:ARG:HH22	1:A:732:LEU:HD13	1.76	0.50
1:A:646:VAL:HG11	1:A:664:ILE:HG22	1.92	0.50
1:A:653:TRP:CE2	1:A:695:MET:HE3	2.47	0.50
1:A:1198:LEU:HD21	1:A:1247:VAL:HG13	1.93	0.50
1:A:992:ASN:HB3	1:A:1231:LEU:HD11	1.94	0.50
1:A:1317:ASP:HB2	1:A:1320:GLU:HG3	1.92	0.50
1:A:1078:GLU:OE1	1:A:1259:ALA:HA	2.12	0.49
1:A:1132:TYR:CG	1:A:1198:LEU:HD22	2.47	0.49
1:A:414:ALA:HB1	1:A:622:HIS:CD2	2.47	0.49
1:A:1404:LEU:HB3	1:A:1443:LEU:HD21	1.94	0.49
1:A:753:LEU:HD13	1:A:759:THR:HG21	1.95	0.49
1:A:807:PHE:O	1:A:812:GLY:N	2.46	0.49
1:A:326:LEU:HD12	1:A:329:PHE:HE2	1.78	0.49
1:A:688:LEU:HD21	1:A:823:LEU:HD22	1.93	0.49
1:A:723:ARG:HD2	1:A:757:ASP:OD2	2.12	0.49
1:A:840:VAL:HG13	1:A:847:SER:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:GLU:HB3	1:A:1263:LEU:HD13	1.94	0.48
1:A:529:LEU:HD11	1:A:1049:LEU:HD13	1.94	0.48
1:A:1383:LEU:HD13	1:A:1420:HIS:HB3	1.95	0.48
1:A:1045:ARG:HG3	1:A:1046:ARG:N	2.29	0.48
1:A:1057:ARG:O	1:A:1271:LYS:CD	2.62	0.48
1:A:27:PRO:HB3	1:A:361:TRP:CZ2	2.48	0.48
1:A:520:TRP:CD2	1:A:1389:PRO:HG2	2.48	0.48
1:A:653:TRP:CD2	1:A:695:MET:HE3	2.48	0.48
1:A:590:ASN:ND2	1:A:1238:GLN:OE1	2.47	0.48
1:A:1175:ARG:HA	1:A:1178:ASP:OD2	2.14	0.48
1:A:495:MET:HE2	1:A:495:MET:HA	1.96	0.47
1:A:1282:PRO:HD3	1:A:1360:ILE:HD12	1.96	0.47
1:A:425:ASN:HA	1:A:428:SER:OG	2.14	0.47
1:A:50:PHE:HB3	1:A:51:PRO:HD3	1.96	0.47
1:A:43:CYS:SG	1:A:116:THR:HG21	2.54	0.47
1:A:1362:LEU:O	1:A:1365:LEU:HG	2.14	0.47
1:A:322:GLY:H	1:A:323:PRO:HD2	1.78	0.47
1:A:360:GLU:OE2	1:A:1221:ARG:NH1	2.47	0.47
1:A:471:ALA:HA	1:A:474:VAL:HG12	1.97	0.47
1:A:1317:ASP:HB2	1:A:1320:GLU:CG	2.44	0.47
1:A:1370:THR:HG23	1:A:1450:LEU:HD13	1.96	0.47
1:A:572:ASP:CG	1:A:573:GLU:H	2.23	0.47
1:A:1299:LEU:HD11	1:A:1343:LYS:HB2	1.97	0.47
1:A:1307:LEU:HB2	1:A:1310:LYS:HE2	1.97	0.47
1:A:514:VAL:HG11	1:A:1377:VAL:CG2	2.44	0.47
1:A:1074:ARG:HH12	1:A:1265:GLU:HB3	1.79	0.47
1:A:553:TRP:CE3	1:A:597:ASN:HB3	2.50	0.46
1:A:748:PRO:O	1:A:752:ILE:HG22	2.14	0.46
1:A:722:LEU:HD12	1:A:761:ILE:HG21	1.97	0.46
1:A:1061:SER:HB2	1:A:1065:ARG:HH12	1.80	0.46
1:A:1199:ALA:O	1:A:1203:GLU:HG2	2.16	0.46
1:A:40:TRP:O	1:A:44:SER:CB	2.64	0.46
1:A:228:MET:HG3	1:A:1197:TRP:CZ3	2.51	0.46
1:A:520:TRP:CH2	1:A:1386:ASN:O	2.69	0.46
1:A:1310:LYS:HG2	1:A:1311:HIS:ND1	2.29	0.46
1:A:85:CYS:SG	1:A:113:LEU:HD22	2.56	0.46
1:A:1023:ILE:O	1:A:1027:ILE:HG13	2.15	0.45
1:A:1403:GLU:HA	1:A:1408:LYS:HB2	1.98	0.45
1:A:1132:TYR:CD2	1:A:1198:LEU:HD22	2.51	0.45
1:A:1351:ILE:HG12	1:A:1356:ASN:HA	1.97	0.45
1:A:594:PHE:CD2	2:A:1601:GDS:HA1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:LEU:HB3	1:A:664:ILE:HD13	1.98	0.45
1:A:854:GLU:O	1:A:858:ARG:HG3	2.16	0.45
1:A:1294:PHE:HB2	1:A:1314:VAL:HG12	1.98	0.45
1:A:507:GLU:HG3	1:A:1379:PHE:HD1	1.82	0.45
1:A:397:THR:OG1	1:A:1185:GLN:NE2	2.50	0.45
1:A:1300:ARG:HH11	1:A:1344:GLU:HB2	1.82	0.45
1:A:1351:ILE:HG23	1:A:1355:ILE:C	2.41	0.45
1:A:1387:LEU:HA	1:A:1441:ARG:HG2	1.99	0.45
1:A:146:LEU:HD22	1:A:186:LEU:HD22	1.98	0.44
1:A:1103:ALA:HA	1:A:1235:TYR:HD2	1.81	0.44
1:A:455:LEU:HD23	1:A:458:LEU:HD21	2.00	0.44
1:A:520:TRP:CE2	1:A:1389:PRO:CG	2.99	0.44
1:A:817:LEU:HD22	1:A:820:LYS:HG3	1.99	0.44
1:A:1445:ARG:HG3	1:A:1445:ARG:NH1	2.32	0.44
1:A:350:ILE:HD13	1:A:579:ALA:HB1	2.00	0.44
1:A:231:GLY:HA2	1:A:236:LEU:HD13	1.98	0.44
1:A:1047:LEU:HD13	1:A:1263:LEU:HD23	2.00	0.44
1:A:1351:ILE:HG23	1:A:1355:ILE:O	2.17	0.44
1:A:451:VAL:HA	1:A:592:LEU:HD11	2.00	0.44
1:A:68:THR:CG2	1:A:71:ASN:H	2.31	0.43
1:A:517:LEU:HB3	1:A:1371:ILE:HG21	1.99	0.43
1:A:567:VAL:O	1:A:571:VAL:HB	2.18	0.43
1:A:1061:SER:HB2	1:A:1065:ARG:NH1	2.32	0.43
1:A:688:LEU:HD12	1:A:792:ASP:HB2	2.00	0.43
1:A:389:PHE:HB3	1:A:1192:ILE:HD12	1.99	0.43
1:A:1299:LEU:HD23	1:A:1334:SER:HB3	2.01	0.43
1:A:458:LEU:HA	1:A:461:ASN:HD22	1.84	0.43
1:A:1057:ARG:O	1:A:1271:LYS:HD2	2.18	0.43
1:A:193:ASP:OD1	1:A:194:ARG:N	2.48	0.43
1:A:1216:PHE:HA	1:A:1219:ILE:HG12	2.01	0.43
1:A:1264:LYS:HB2	1:A:1264:LYS:HE2	1.84	0.42
1:A:493:ALA:HA	1:A:496:LYS:NZ	2.34	0.42
1:A:1189:TYR:HB3	1:A:1190:PRO:HD3	2.00	0.42
1:A:511:GLY:HA3	1:A:1377:VAL:HG11	2.00	0.42
1:A:668:VAL:HG22	1:A:674:VAL:HG21	2.00	0.42
1:A:37:VAL:O	1:A:41:VAL:HG23	2.18	0.42
1:A:1198:LEU:HD11	1:A:1247:VAL:HG11	2.01	0.42
1:A:428:SER:HA	1:A:1151:TYR:CZ	2.54	0.42
1:A:677:VAL:HG12	1:A:840:VAL:HG23	2.02	0.42
1:A:558:PHE:CE1	1:A:1022:GLY:HA3	2.55	0.42
1:A:478:PRO:O	1:A:481:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:ILE:O	1:A:822:ARG:NH1	2.53	0.41
1:A:963:TRP:HA	1:A:963:TRP:CE3	2.55	0.41
1:A:1322:VAL:O	1:A:1481:LEU:HA	2.20	0.41
1:A:1436:LEU:HD13	1:A:1436:LEU:HA	1.87	0.41
1:A:666:PHE:HE1	1:A:687:LEU:HD11	1.85	0.41
1:A:981:PHE:HE1	1:A:1098:PHE:HD1	1.68	0.41
1:A:1414:LEU:HG	1:A:1420:HIS:CG	2.55	0.41
1:A:40:TRP:O	1:A:44:SER:HB2	2.20	0.41
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.85	0.41
1:A:143:LEU:O	1:A:147:LEU:HG	2.21	0.41
1:A:416:LYS:HA	1:A:416:LYS:HD3	1.85	0.41
1:A:423:ILE:O	1:A:426:LEU:HB2	2.20	0.41
1:A:1148:SER:OG	1:A:1149:PRO:HD3	2.20	0.41
1:A:43:CYS:CB	1:A:116:THR:HG21	2.51	0.41
1:A:47:TRP:HZ2	1:A:115:ILE:HG22	1.86	0.41
1:A:347:LYS:HB2	1:A:584:VAL:HG21	2.01	0.41
1:A:511:GLY:O	1:A:515:LEU:HB2	2.21	0.41
1:A:632:ARG:NH1	1:A:706:GLY:O	2.50	0.41
1:A:966:MET:O	1:A:969:ILE:HG22	2.21	0.41
1:A:74:LYS:HE3	1:A:74:LYS:HB2	1.84	0.41
1:A:487:THR:O	1:A:488:LYS:C	2.64	0.41
1:A:532:ARG:NH2	1:A:1044:SER:HB3	2.36	0.41
1:A:676:VAL:HB	1:A:825:VAL:HG22	2.03	0.41
1:A:92:SER:OG	1:A:107:LEU:HD13	2.21	0.41
1:A:339:MET:HG2	1:A:591:ILE:HD13	2.03	0.41
1:A:730:ARG:HB2	1:A:730:ARG:HH11	1.85	0.41
1:A:335:HIS:HE2	2:A:1601:GDS:C1	2.33	0.41
1:A:468:ALA:O	1:A:471:ALA:HB3	2.21	0.41
1:A:558:PHE:CZ	1:A:562:LEU:HD22	2.56	0.41
1:A:650:THR:HA	1:A:661:LEU:O	2.21	0.41
1:A:1445:ARG:HG3	1:A:1445:ARG:HH11	1.84	0.41
1:A:16:TRP:CZ3	1:A:21:THR:HG21	2.56	0.41
1:A:254:VAL:HG22	1:A:398:ALA:HA	2.02	0.41
1:A:501:ARG:NH2	1:A:1075:PHE:O	2.54	0.41
1:A:310:ASP:HB2	1:A:311:PRO:HD3	2.03	0.40
1:A:733:GLN:N	1:A:783:TYR:OH	2.53	0.40
1:A:586:LEU:HD23	1:A:586:LEU:HA	1.96	0.40
1:A:16:TRP:CH2	1:A:21:THR:HG21	2.56	0.40
1:A:322:GLY:N	1:A:323:PRO:HD2	2.36	0.40
1:A:1287:PRO:HB2	1:A:1448:LYS:HB2	2.04	0.40

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	1318/1558 (85%)	1274 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1174/1358 (86%)	1172 (100%)	2 (0%)	87	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	774	GLN
1	A	811	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	66	GLN
1	A	351	ASN
1	A	383	GLN
1	A	461	ASN
1	A	494	HIS

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Mol	Chain	Res	Type
1	A	590	ASN
1	A	642	ASN
1	A	701	HIS
1	A	718	GLN
1	A	1008	GLN
1	A	1155	ASN
1	A	1185	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	GDS	A	1601	-	37,39,39	0.70	0	44,50,50	0.71	1 (2%)

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
2	GDS	A	1601	-	-	18/51/51/51	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	GDS	CB1-CG1-CD1	-2.81	106.79	113.06

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	GDS	CG1-CD1-N2-CA2
2	A	1601	GDS	O1-CD1-N2-CA2
2	A	1601	GDS	OE5-C4-CA4-N4
2	A	1601	GDS	OE6-C4-CA4-N4
2	A	1601	GDS	CG6-CD6-N5-CA5
2	A	1601	GDS	N6-CA6-CB6-CG6
2	A	1601	GDS	O6-CD6-N5-CA5
2	A	1601	GDS	CB2-SG2-SG5-CB5
2	A	1601	GDS	O5-C5-CA5-N5
2	A	1601	GDS	OE2-C1-CA1-N1
2	A	1601	GDS	N4-C5-CA5-N5
2	A	1601	GDS	C6-CA6-CB6-CG6
2	A	1601	GDS	CA5-CB5-SG5-SG2
2	A	1601	GDS	O2-C2-CA2-N2
2	A	1601	GDS	N3-C2-CA2-N2
2	A	1601	GDS	N2-CA2-CB2-SG2
2	A	1601	GDS	OE1-C1-CA1-CB1
2	A	1601	GDS	OE2-C1-CA1-CB1

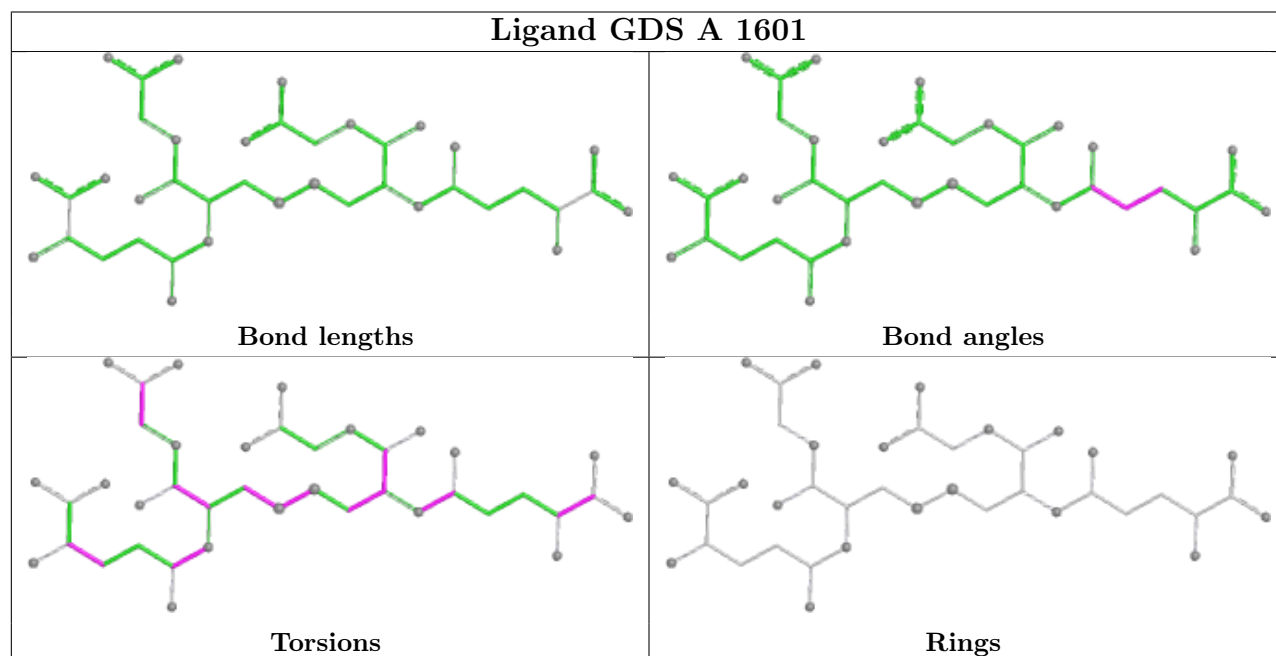
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	GDS	3	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.

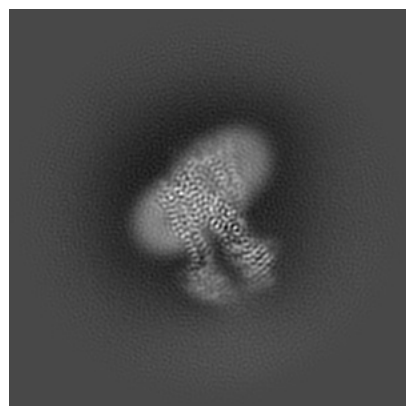
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63058. These allow visual inspection of the internal detail of the map and identification of artifacts.

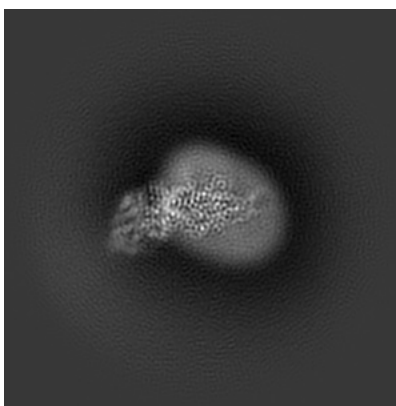
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

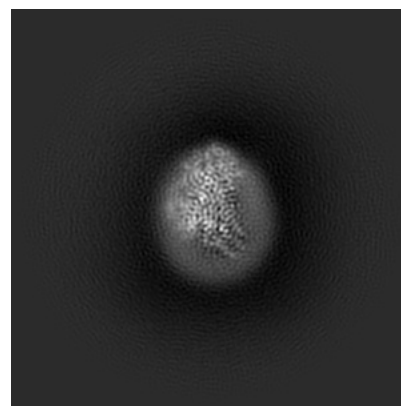
6.1.1 Primary map



X

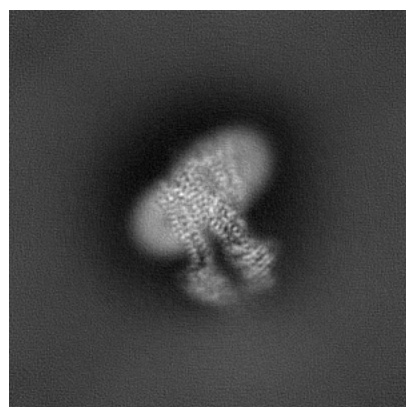


Y

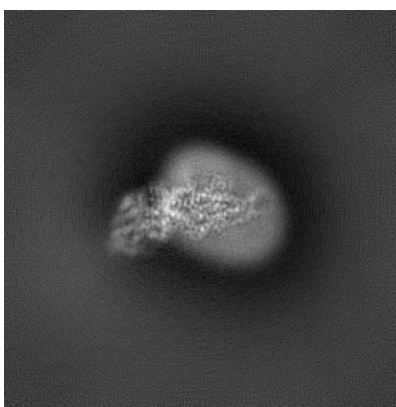


Z

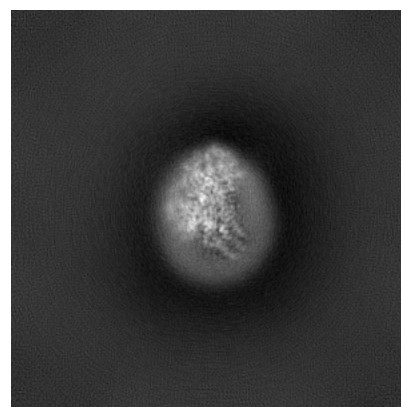
6.1.2 Raw map



X



Y

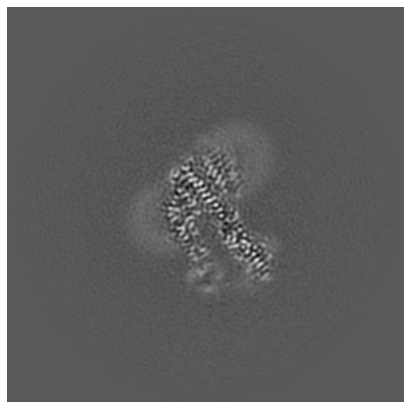


Z

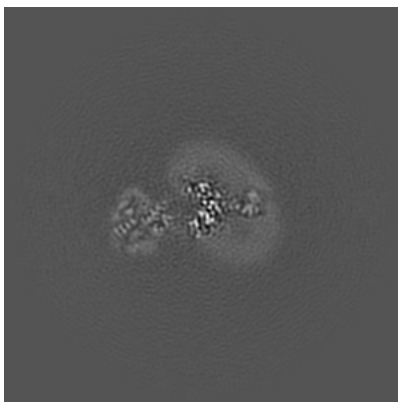
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

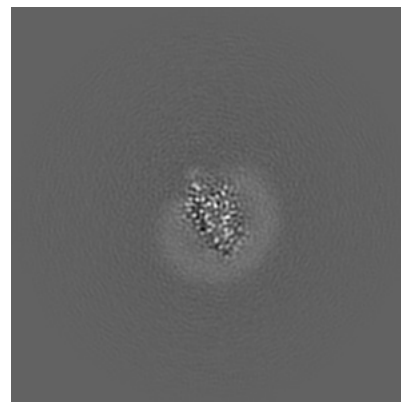
6.2.1 Primary map



X Index: 160

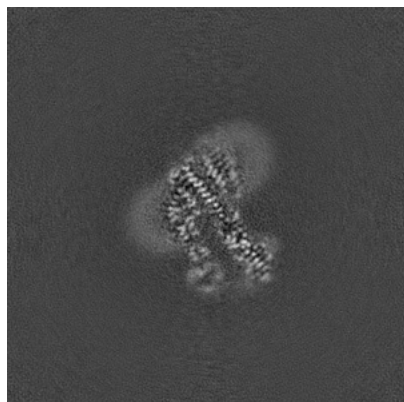


Y Index: 160

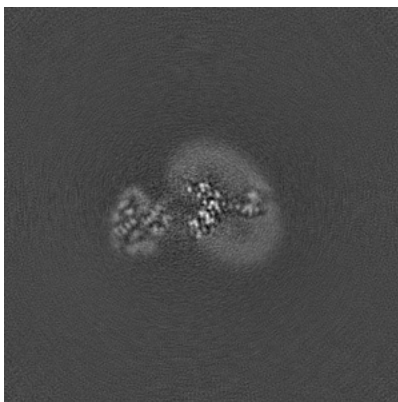


Z Index: 160

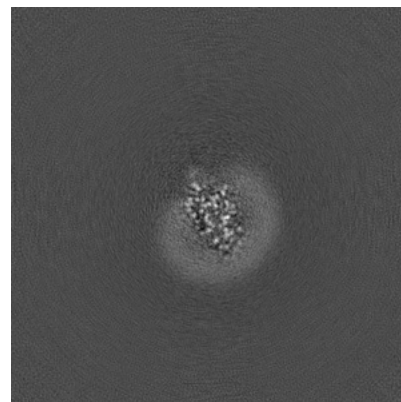
6.2.2 Raw map



X Index: 160



Y Index: 160

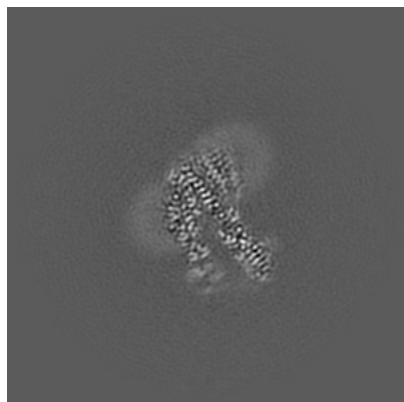


Z Index: 160

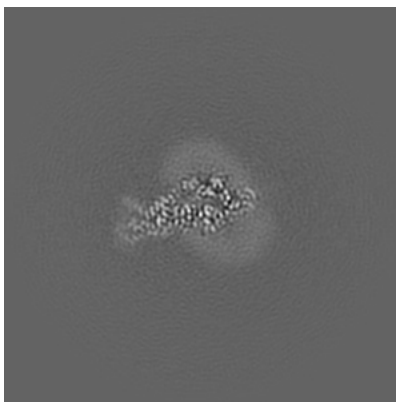
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

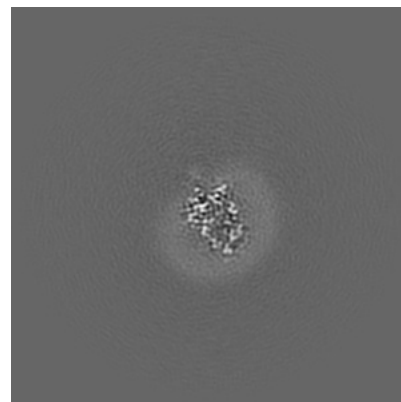
6.3.1 Primary map



X Index: 159

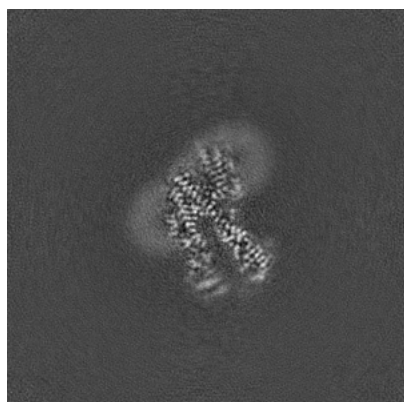


Y Index: 148

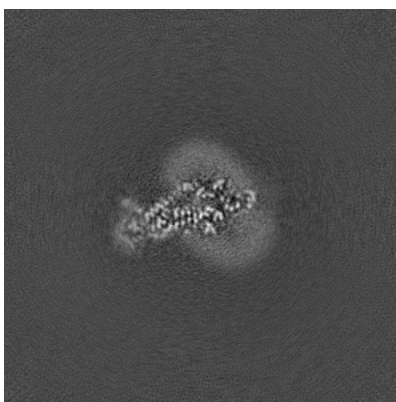


Z Index: 162

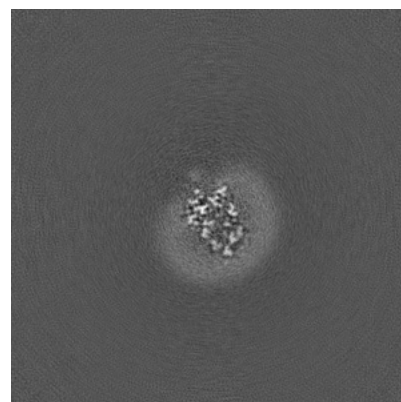
6.3.2 Raw map



X Index: 156



Y Index: 149

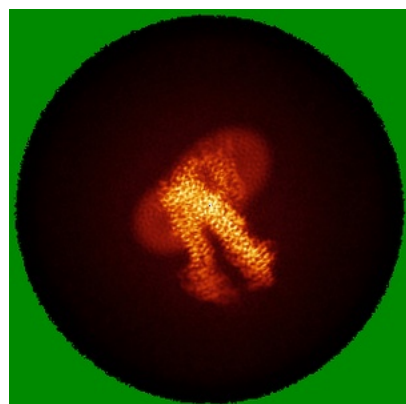


Z Index: 162

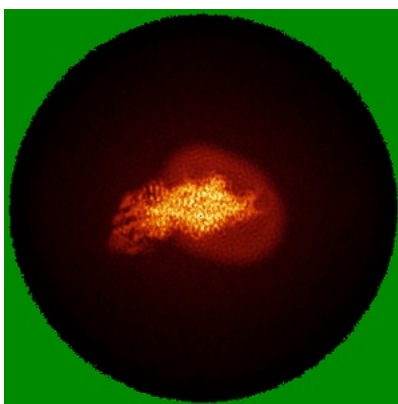
The images above show the largest variance slices of the map in three orthogonal directions.

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

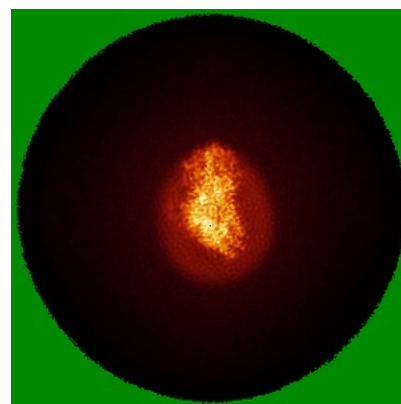
6.4.1 Primary map



X

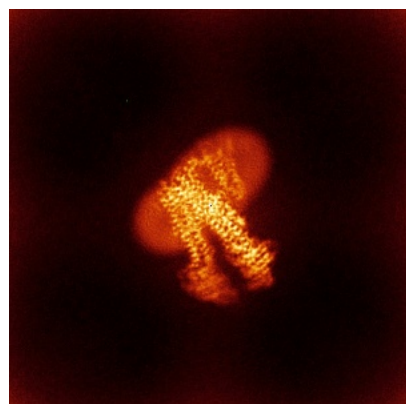


Y

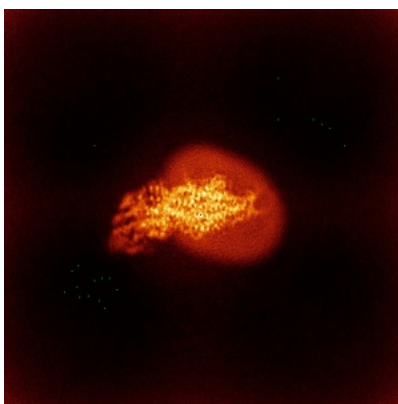


Z

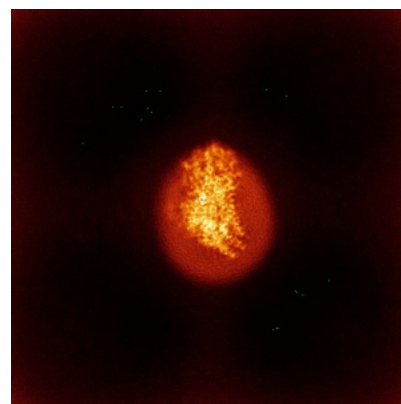
6.4.2 Raw map



X



Y

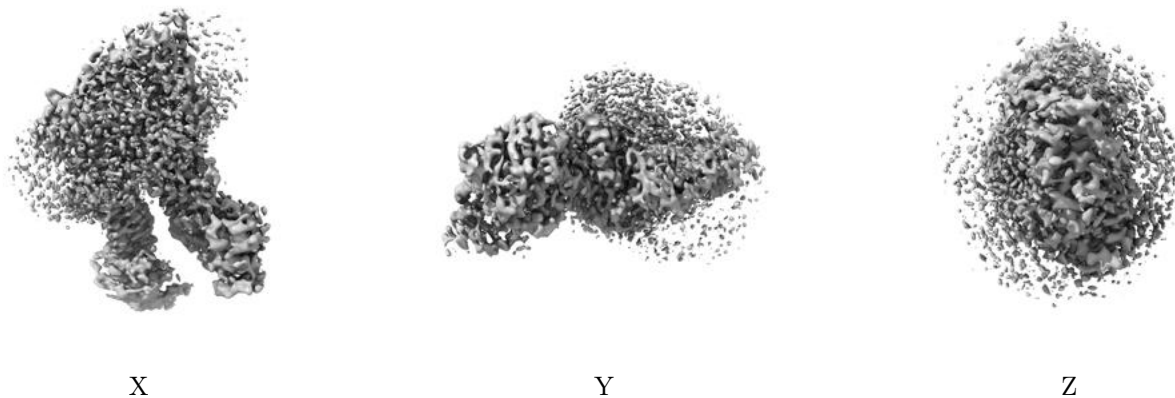


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

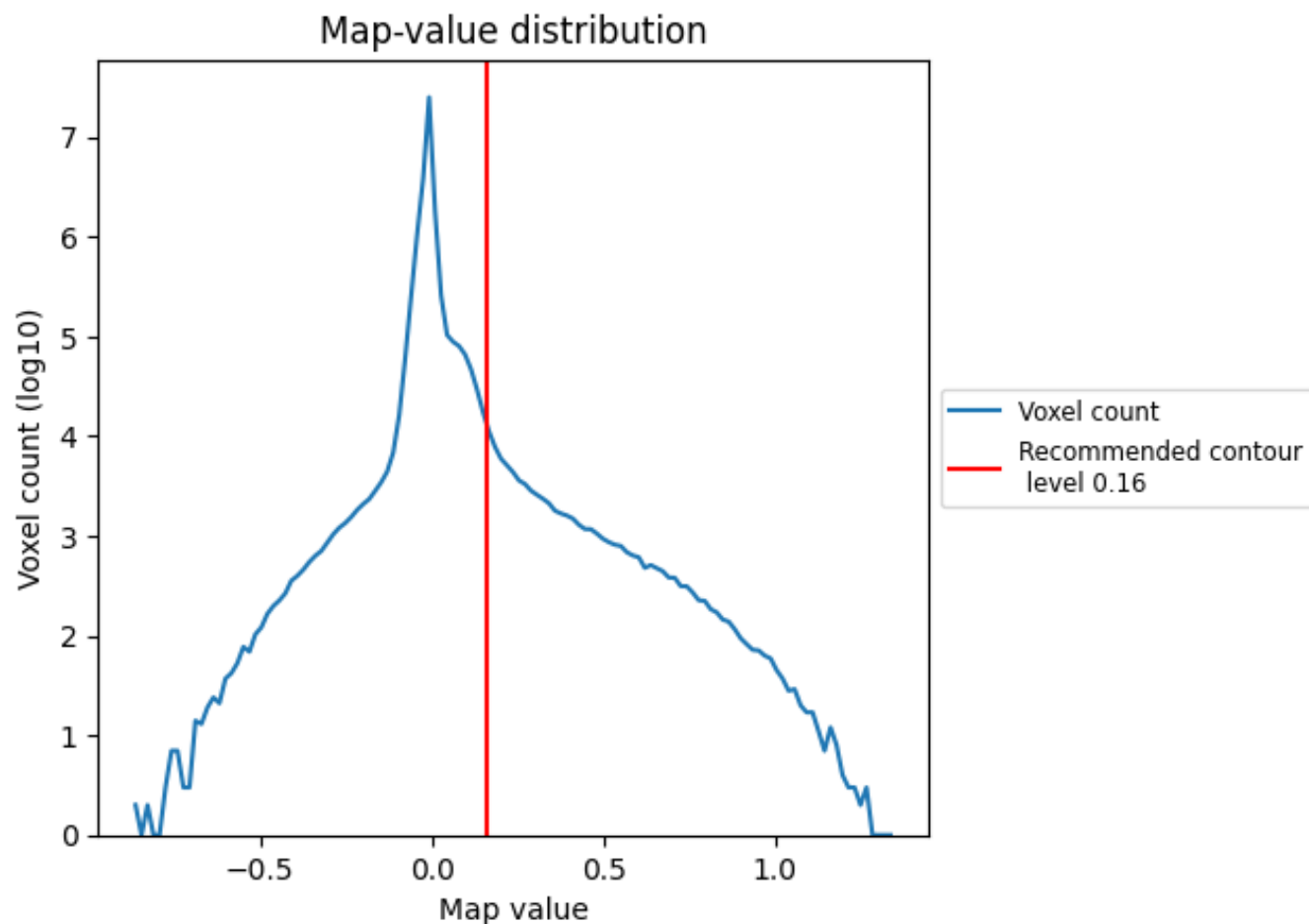
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

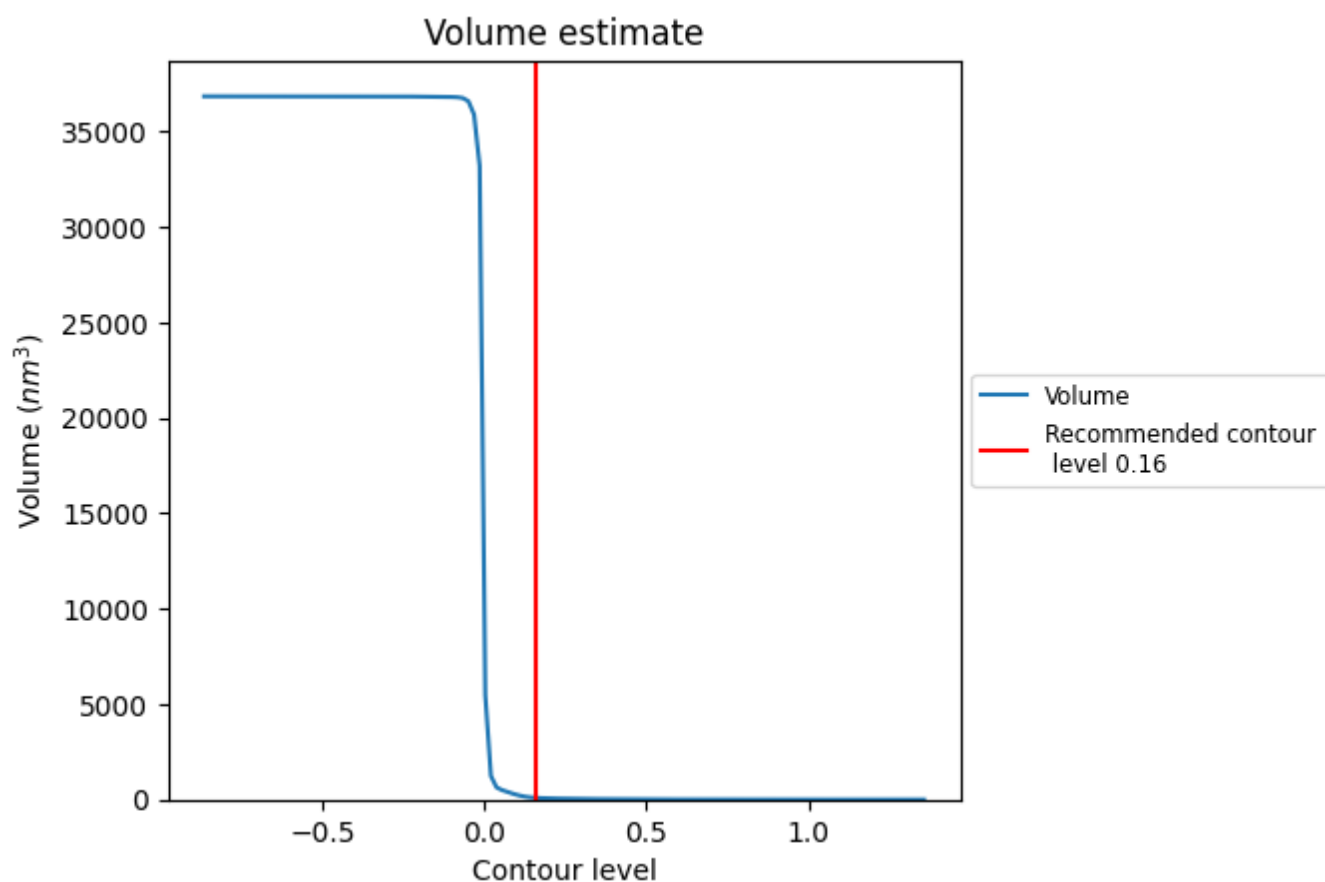
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

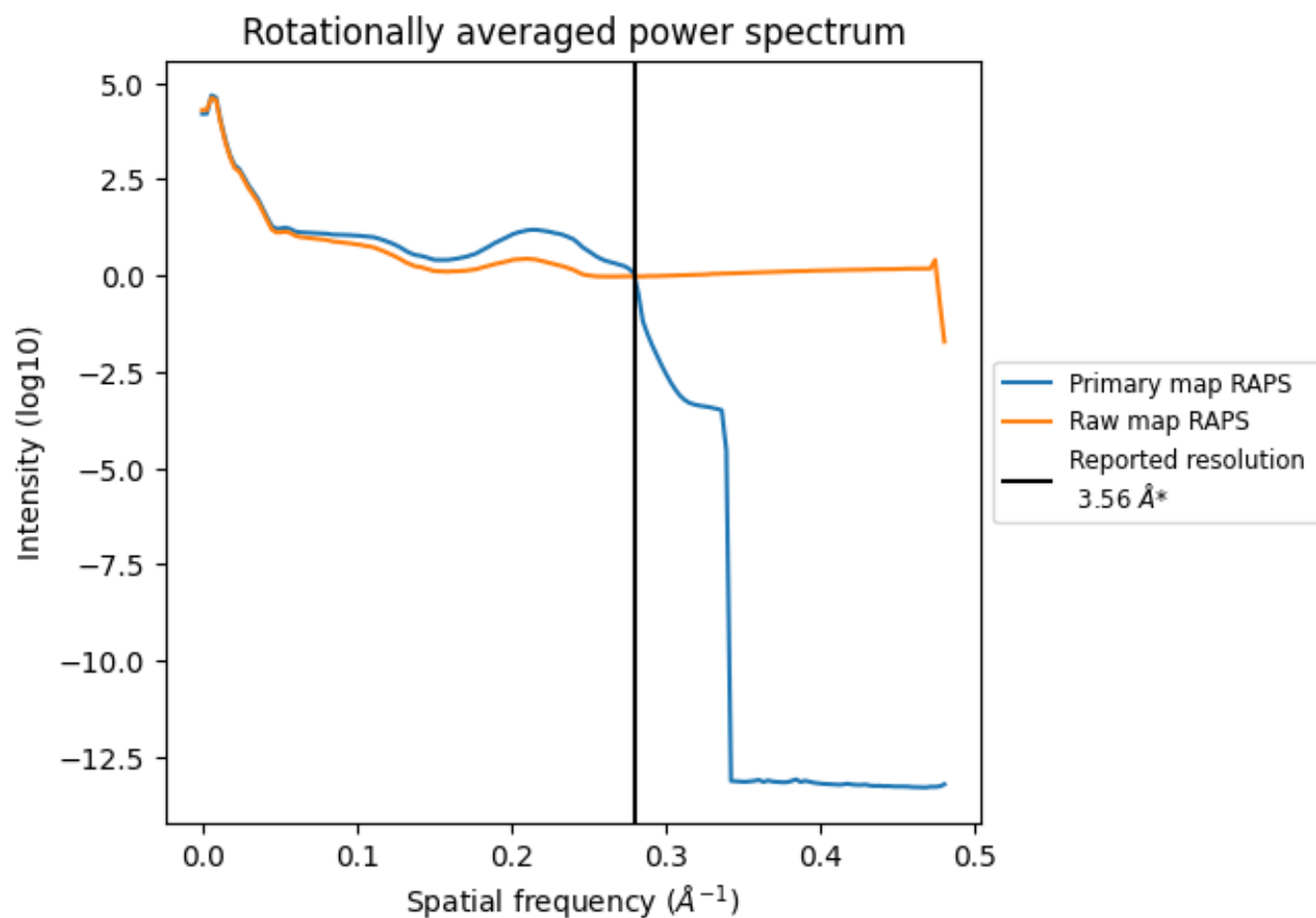
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 81 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 ⓘ

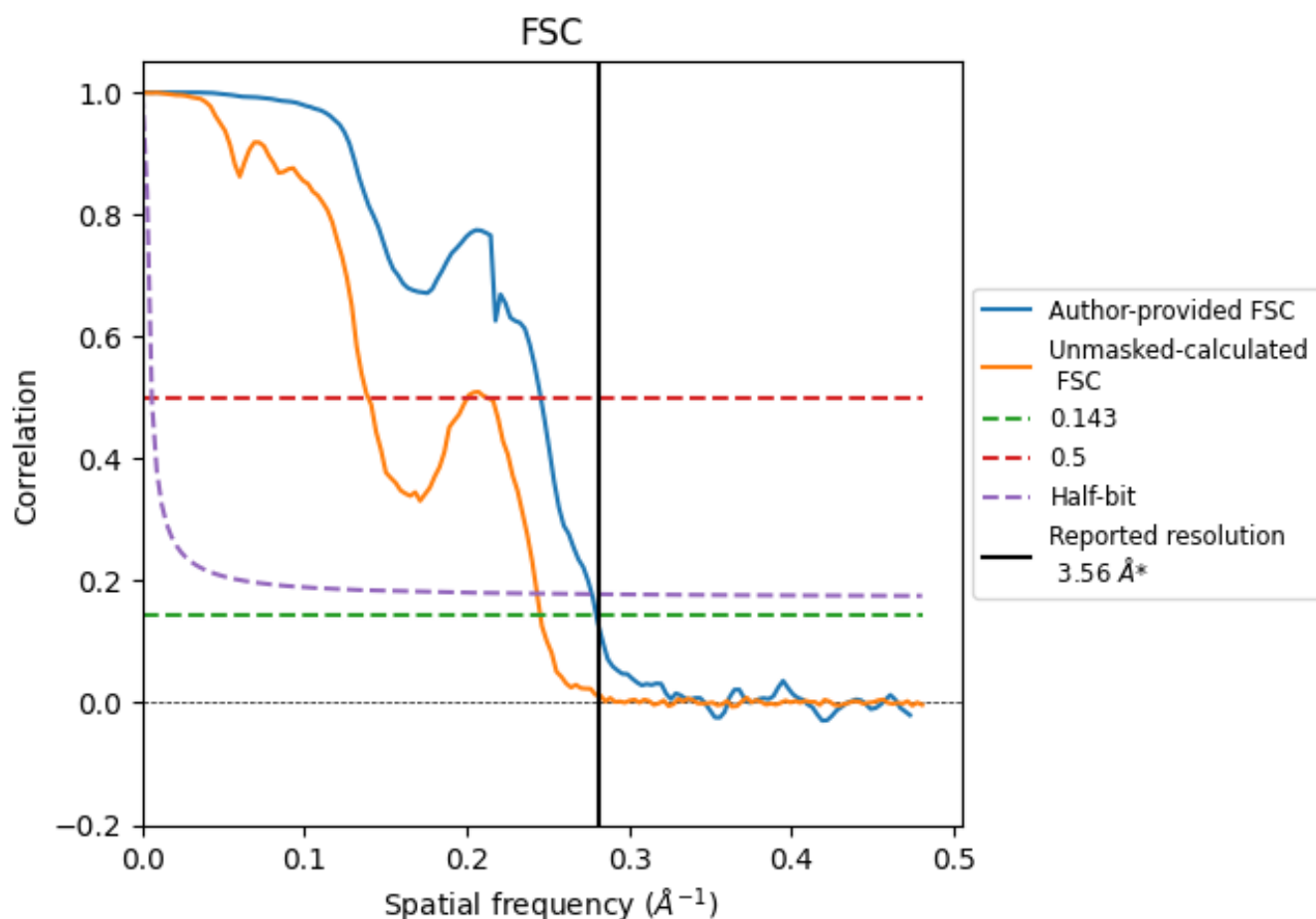


*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

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 0.281 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.57	4.07	3.61
Unmasked-calculated*	4.07	7.18	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.56 by more than 10 %

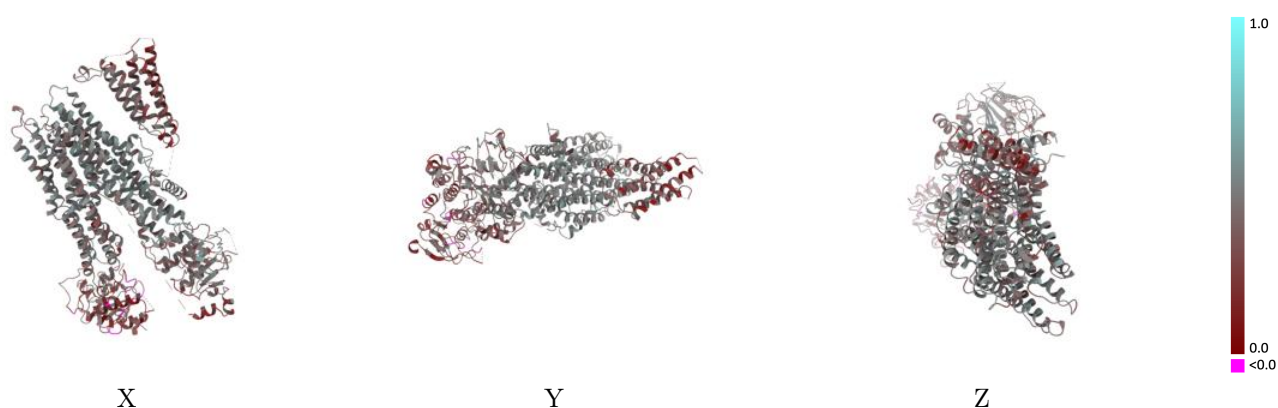
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63058 and PDB model 9LG9. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

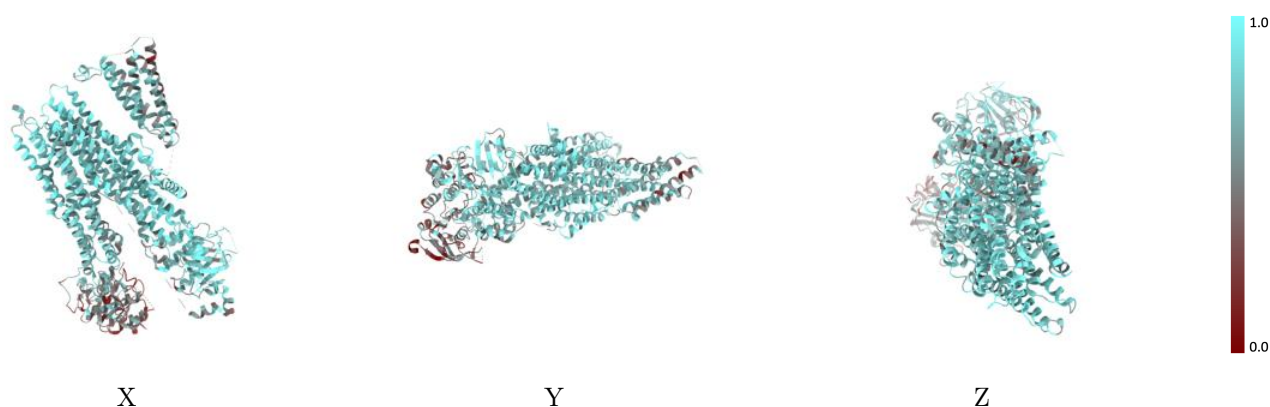
This section was not generated.

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



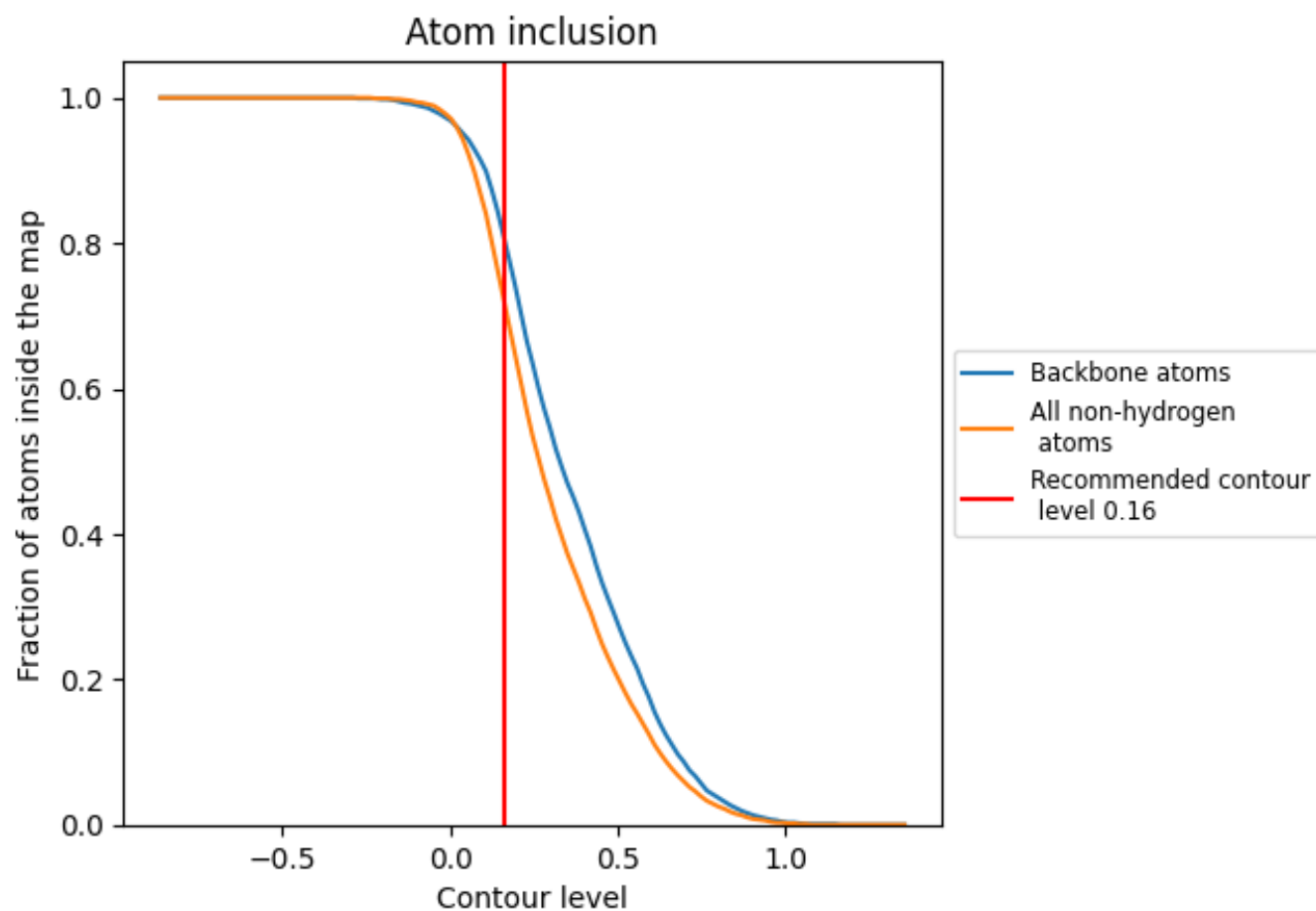
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 72% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.4010
A	0.7220	0.4010

