



Full wwPDB EM Validation Report ⓘ

Sep 23, 2025 – 02:16 PM JST

PDB ID : 9LG8 / pdb_00009lg8
EMDB ID : EMD-63057
Title : bovine ABCC1 bound to estrogen sulfate and GSH
Authors : Sun, P.P.; Liu, K.X.; Gao, P.
Deposited on : 2025-01-10
Resolution : 3.55 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

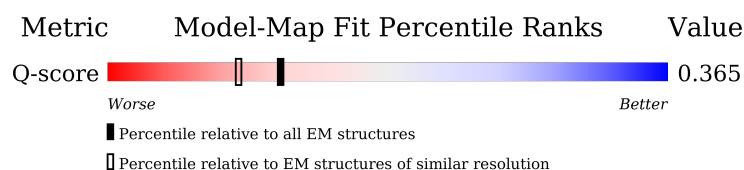
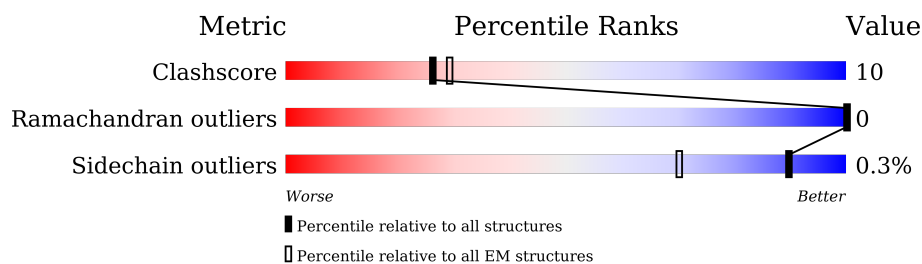
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12819 (3.05 - 4.05)

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 3 unique types of molecules in this entry. The entry contains 10600 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.

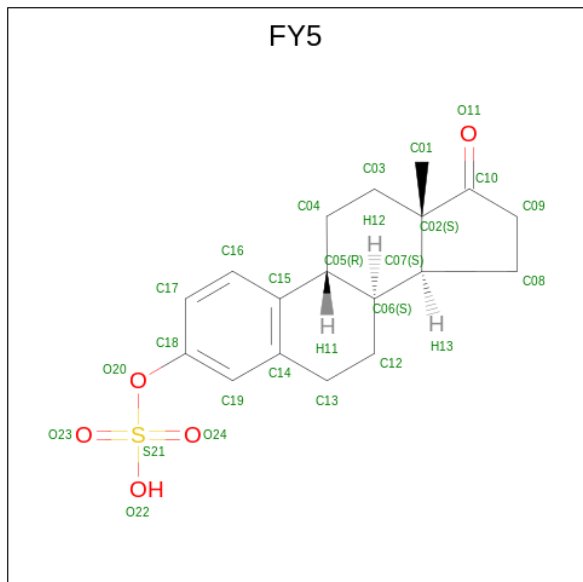
- Molecule 1 is a protein called Multidrug resistance-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1329	Total	C	N	O	S	0	0
			10556	6872	1751	1877	56		

There are 28 discrepancies between the modelled and reference sequences:

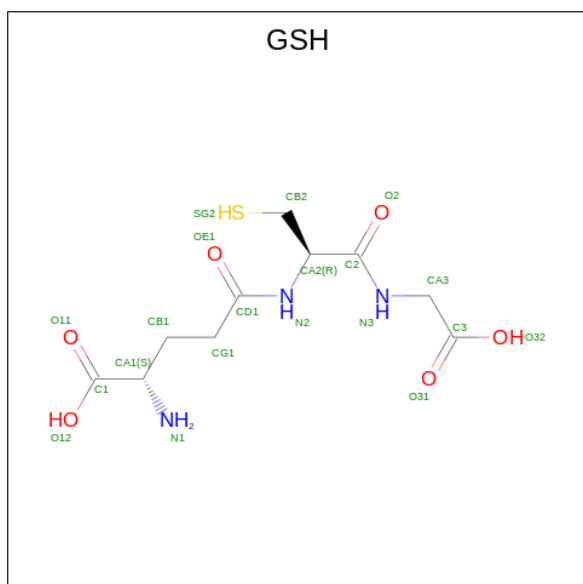
Chain	Residue	Modelled	Actual	Comment	Reference
A	1531	LYS	-	expression tag	UNP Q8HXQ5
A	1532	LEU	-	expression tag	UNP Q8HXQ5
A	1533	GLY	-	expression tag	UNP Q8HXQ5
A	1534	SER	-	expression tag	UNP Q8HXQ5
A	1535	GLU	-	expression tag	UNP Q8HXQ5
A	1536	ASN	-	expression tag	UNP Q8HXQ5
A	1537	LEU	-	expression 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 estrone 3-sulfate (CCD ID: FY5) (formula: $C_{18}H_{22}O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	S	0
			24	18	5	1	

- Molecule 3 is GLUTATHIONE (CCD ID: GSH) (formula: $C_{10}H_{17}N_3O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			20	10	3	6	1	

GLY	VAL	L1387	H1311	G1230	V1072	GLU
SER	ASP	Q1392	I1312	S1236	N1073	ALA
GLU	LEU	Y1393	N1313	V1239	R1074	ASP
ASN	E1462	S1394	V1314	Y1242	K1077	LYS
LEU	D1465	D1395	D1317	L1243	E1078	ALA
TYR	D1472	S1401	E1320	W1244	D1083	GLN
PHE	F1475	L1402	K1321	R1248		THR
GLN	D1476	E1403	G1323	M1249		GLY
GLY	L1481	H1406	R1327	M1253		GLN
GLY	T1482	L1407	T1328	E1254	Y957	
SER	I1483	K1408	G1329	T1255	K958	
GLY	A1484	G1409	A1330	N1256	L959	
HIS	H1485	F1410	G1331	V1257	S960	
HIS	R1486	V1411	K1332	A1259	Y961	
HIS	L1487	S1412	T1336	V1260	Y962	
HIS	N1488	A1413	L1337	E1261		
HIS	T1489	L1414	R1341	R1262	Y965	
HIS	I1490	P1415	I1342	L1263	K966	
HIS	R1495	D1416	A1346	K1264	K967	
HIS	V1496	N1419	E1347	E1265	L971	
HIS	I1497	H1420	G1348	E1270	F981	
HIS	D1500	E1421	E1349	K1271	K1140	
HIS	K1501	C1422	I1351	I1277	K1150	
HIS	G1502	A1423	I1352	Q1278	V1157	
HIS	E1503	E1424	D1353	D1279	S1162	
HIS	T1504	G1425	D1354	M1280	R1165	
HIS	Q1505	G1426	D1355	A1281	A1166	
HIS	E1506	E1427	N1356	P1282	F1167	
HIS	W1507	N1428	I1357	W1286	D1178	
HIS	G1508	L1429	A1358	P1287	L1179	
HIS	S1509	S1430	K1359	V1289	K1180	
HIS	P1510	V1431	I1360	E1293	V1181	
HIS	S1511	G1432	G1361	F1294	Q1185	
HIS	D1512	Q1433	L1362	R1295	S1033	
HIS	L1513	R1434	H1363	G1298	M1034	
HIS	L1514	Q1435	D1364	L1299	A1035	
HIS	GLN	G1438	L1365	Y1301	V1036	
HIS	GLN	R1441	R1366	ARG	S1037	
HIS	ARG	A1442	T1370	R1300	I1038	
HIS	GLY		I1371	Y1301	A1043	
HIS	PHE	R1445	I1372	GLU	L1047	
HIS	TYR		P1373	ASP	R1057	
HIS	SER		Q1374	LEU	F1062	
HIS	MET	K1448	D1375	D1306	T1066	
HIS	ALA	I1449	P1376	D1307	G1069	
HIS	LYS	L1450	V1377	L1307	N1070	
HIS	ASP	V1451	L1378	V1308	L1071	
HIS	SER	L1452	S1382	L1309		
HIS	GLY	D1453	L1383	K1310		
HIS	LEU	E1454	R1384			
HIS	VAL	A1455				
HIS	LYS	THR				
HIS	LEU	ALA				
HIS		ALA				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111086	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)	200	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	1.093	Depositor
Minimum map value	-0.680	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.134	Depositor
Map size (Å)	320.0, 320.0, 320.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: GSH, FY5

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	0.47	0/10792	0.66	2/14650 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1289	VAL	N-CA-C	-6.47	107.56	113.71
1	A	441	ILE	N-CA-C	-5.24	105.43	110.72

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	10556	0	10783	211	0
2	A	24	0	0	0	0
3	A	20	0	15	3	0
All	All	10600	0	10798	212	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 (212) 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:451:VAL:HA	1:A:592:LEU:HD11	1.58	0.86
1:A:371:PHE:HB2	1:A:1211:LEU:HB2	1.64	0.80
1:A:388:CYS:HB3	1:A:439:THR:HA	1.69	0.74
1:A:674:VAL:HG22	1:A:837:VAL:HB	1.70	0.73
1:A:244:LEU:HD11	1:A:1185:GLN:HB2	1.69	0.73
1:A:674:VAL:HB	1:A:823:LEU:HD22	1.73	0.70
1:A:539:LEU:HD21	1:A:1083:ASP:HB2	1.79	0.65
1:A:331:PHE:HB3	1:A:384:TYR:HB2	1.79	0.63
1:A:124:ILE:HG23	1:A:138:MET:HE2	1.81	0.63
1:A:1323:GLY:HA3	1:A:1490:ILE:HD11	1.81	0.62
1:A:331:PHE:HD1	1:A:380:VAL:HG13	1.64	0.61
1:A:1286:TRP:HE1	1:A:1355:ILE:HB	1.67	0.60
1:A:382:HIS:CE1	1:A:1199:ALA:HB1	2.38	0.58
1:A:592:LEU:O	1:A:596:LEU:HB2	2.04	0.57
1:A:1352:ILE:HD13	1:A:1449:ILE:HD12	1.86	0.57
1:A:1376:PRO:HG3	1:A:1435:GLN:HA	1.86	0.57
1:A:556:THR:HG21	1:A:597:ASN:HD21	1.70	0.57
1:A:134:SER:HB2	1:A:215:PHE:H	1.69	0.57
1:A:1402:LEU:HD13	1:A:1411:VAL:HG21	1.87	0.56
1:A:332:LYS:HE3	1:A:446:SER:HB2	1.88	0.56
1:A:353:VAL:HG11	1:A:1229:VAL:HG21	1.87	0.56
1:A:1336:THR:HG22	1:A:1451:VAL:HG11	1.87	0.56
1:A:1322:VAL:HG22	1:A:1495:ARG:HB2	1.86	0.56
1:A:1378:LEU:HD22	1:A:1434:ARG:HG2	1.88	0.56
1:A:649:ALA:HA	1:A:700:GLY:HA3	1.86	0.56
1:A:522:LEU:HG	1:A:1363:HIS:HE1	1.71	0.55
1:A:664:ILE:HG13	1:A:846:ILE:HG12	1.89	0.55
1:A:643:SER:HB2	1:A:670:GLU:HG2	1.89	0.54
1:A:425:ASN:HA	1:A:428:SER:HB3	1.89	0.54
1:A:345:ILE:HG21	1:A:370:LEU:HB2	1.88	0.54
1:A:1286:TRP:HB3	1:A:1287:PRO:HD3	1.90	0.54
1:A:682:CYS:SG	1:A:841:MET:HG3	2.48	0.53
1:A:553:TRP:CE3	1:A:597:ASN:HB2	2.44	0.53
1:A:1202:LEU:HD12	1:A:1244:ASN:HA	1.91	0.53
1:A:1078:GLU:HG2	1:A:1263:LEU:HD21	1.90	0.53
1:A:340:PHE:CZ	1:A:450:GLN:HA	2.44	0.53
1:A:599:LEU:HB3	1:A:600:PRO:HD3	1.90	0.53
1:A:981:PHE:HZ	1:A:1095:GLY:HA2	1.74	0.52
1:A:1003:ILE:HD12	1:A:1003:ILE:H	1.73	0.52
1:A:1286:TRP:CD1	1:A:1355:ILE:HD12	2.45	0.52
1:A:396:LYS:HD3	1:A:1185:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:GLU:HG3	1:A:1259:ALA:HB1	1.92	0.51
1:A:214:SER:O	1:A:218:ARG:N	2.44	0.51
1:A:607:VAL:O	1:A:610:SER:HB3	2.11	0.51
1:A:1341:ARG:NH2	1:A:1360:ILE:O	2.44	0.51
1:A:674:VAL:HA	1:A:837:VAL:O	2.11	0.51
1:A:334:VAL:O	1:A:338:MET:HG2	2.11	0.51
1:A:381:LEU:HD21	3:A:1602:GSH:HG13	1.92	0.51
1:A:646:VAL:HG11	1:A:664:ILE:HG22	1.92	0.51
1:A:253:VAL:HG12	1:A:398:ALA:HB2	1.92	0.51
1:A:967:LYS:HG2	1:A:971:LEU:HD21	1.92	0.51
1:A:1294:PHE:O	1:A:1313:ASN:HA	2.10	0.51
1:A:493:ALA:O	1:A:496:LYS:HB3	2.11	0.50
1:A:998:TRP:HB2	1:A:1014:ARG:HD2	1.93	0.50
1:A:1317:ASP:HB2	1:A:1320:GLU:HG3	1.92	0.50
1:A:1382:SER:HB2	1:A:1419:ASN:HA	1.92	0.50
1:A:1239:VAL:HA	1:A:1242:TYR:HB2	1.94	0.50
1:A:1384:ARG:HH12	1:A:1395:ASP:HA	1.76	0.50
1:A:840:VAL:HG13	1:A:847:SER:O	2.12	0.50
1:A:27:PRO:HB3	1:A:361:TRP:CZ2	2.47	0.50
1:A:134:SER:HB3	1:A:214:SER:HA	1.94	0.50
1:A:723:ARG:HD2	1:A:757:ASP:OD2	2.12	0.50
1:A:1070:ASN:O	1:A:1074:ARG:HG2	2.12	0.49
1:A:653:TRP:CE2	1:A:695:MET:HE3	2.47	0.49
1:A:499:ASP:O	1:A:503:LYS:HG3	2.13	0.49
1:A:556:THR:N	1:A:557:PRO:HD2	2.27	0.49
1:A:723:ARG:HH22	1:A:732:LEU:HD13	1.76	0.49
1:A:817:LEU:O	1:A:822:ARG:NH2	2.45	0.49
1:A:399:VAL:O	1:A:403:VAL:HG23	2.13	0.49
1:A:1062:PHE:O	1:A:1066:THR:HG22	2.12	0.49
1:A:1057:ARG:CB	1:A:1271:LYS:HD2	2.43	0.49
1:A:784:CYS:HG	1:A:1167:PHE:HD2	1.60	0.48
1:A:981:PHE:CZ	1:A:1095:GLY:HA2	2.47	0.48
1:A:403:VAL:HG13	1:A:619:PHE:CE2	2.48	0.48
1:A:1387:LEU:HD23	1:A:1441:ARG:HG2	1.94	0.48
1:A:1383:LEU:HD13	1:A:1420:HIS:HB3	1.95	0.48
1:A:753:LEU:HD13	1:A:759:THR:HG21	1.95	0.48
1:A:1078:GLU:OE2	1:A:1262:ARG:HB2	2.14	0.48
1:A:1236:SER:O	1:A:1239:VAL:HG12	2.14	0.48
1:A:1140:LYS:HE2	1:A:1255:THR:HG21	1.95	0.48
1:A:1370:THR:HG23	1:A:1450:LEU:HD13	1.96	0.48
1:A:564:THR:HG21	1:A:589:PHE:HZ	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LEU:HD22	1:A:1166:ALA:CB	2.44	0.47
1:A:1362:LEU:O	1:A:1365:LEU:HG	2.14	0.47
1:A:509:LEU:HD12	1:A:1072:VAL:HG23	1.95	0.47
1:A:748:PRO:O	1:A:752:ILE:HG22	2.14	0.47
1:A:653:TRP:CD2	1:A:695:MET:HE3	2.49	0.47
1:A:224:ILE:HA	1:A:242:TRP:HH2	1.78	0.47
1:A:532:ARG:O	1:A:535:GLU:HB2	2.14	0.47
1:A:786:SER:O	1:A:820:LYS:HD2	2.14	0.47
1:A:1092:MET:HE3	1:A:1245:TRP:HE1	1.79	0.47
1:A:50:PHE:HB3	1:A:51:PRO:HD3	1.97	0.47
1:A:1043:ALA:O	1:A:1047:LEU:HG	2.14	0.47
1:A:503:LYS:HB3	1:A:1424:GLU:OE2	2.13	0.47
1:A:985:HIS:CD2	1:A:1098:PHE:HB3	2.49	0.47
1:A:26:ASN:HB3	1:A:158:MET:HE1	1.96	0.47
1:A:43:CYS:SG	1:A:116:THR:HG21	2.54	0.47
1:A:346:LEU:HD11	1:A:1230:GLY:HA2	1.97	0.47
1:A:1282:PRO:HD3	1:A:1360:ILE:HD12	1.96	0.47
1:A:1310:LYS:HG2	1:A:1311:HIS:ND1	2.30	0.47
1:A:1317:ASP:HB2	1:A:1320:GLU:CG	2.44	0.47
1:A:340:PHE:CE2	1:A:450:GLN:HA	2.50	0.47
1:A:694:GLU:OE2	1:A:1162:SER:HA	2.15	0.47
1:A:1150:VAL:HG22	1:A:1180:LYS:HB3	1.97	0.47
1:A:411:THR:HG23	1:A:625:LEU:HD21	1.97	0.46
1:A:722:LEU:HD12	1:A:761:ILE:HG21	1.97	0.46
1:A:1387:LEU:HA	1:A:1441:ARG:HG2	1.96	0.46
1:A:1307:LEU:HB2	1:A:1310:LYS:HE2	1.97	0.46
1:A:447:ALA:N	1:A:448:PRO:HD2	2.30	0.46
1:A:1342:ILE:HA	1:A:1366:ARG:HH22	1.79	0.46
1:A:984:ASN:HD22	1:A:1025:GLN:HG2	1.80	0.46
1:A:1351:ILE:HG12	1:A:1356:ASN:HA	1.97	0.46
1:A:444:ILE:HG21	1:A:606:ILE:HD11	1.98	0.46
1:A:854:GLU:O	1:A:858:ARG:HG3	2.16	0.46
1:A:1203:GLU:O	1:A:1207:ASN:N	2.49	0.46
1:A:85:CYS:SG	1:A:113:LEU:HD22	2.56	0.46
1:A:146:LEU:HD22	1:A:186:LEU:HD22	1.98	0.46
1:A:1132:TYR:CE2	1:A:1198:LEU:HD22	2.51	0.46
1:A:40:TRP:O	1:A:44:SER:CB	2.63	0.46
1:A:340:PHE:CD2	1:A:453:LEU:HD23	2.51	0.46
1:A:661:LEU:HB3	1:A:664:ILE:HD13	1.98	0.46
1:A:385:PHE:CZ	3:A:1602:GSH:O2	2.69	0.45
3:A:1602:GSH:HG12	3:A:1602:GSH:O11	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:PHE:HB3	1:A:595:PRO:HD3	1.98	0.45
1:A:501:ARG:HD3	1:A:531:ILE:HG23	1.99	0.45
1:A:564:THR:HG21	1:A:589:PHE:CZ	2.51	0.45
1:A:673:LEU:HA	1:A:822:ARG:HG3	1.98	0.45
1:A:1206:GLY:O	1:A:1210:VAL:HG23	2.17	0.45
1:A:1351:ILE:HG23	1:A:1355:ILE:C	2.41	0.45
1:A:1253:MET:O	1:A:1257:ILE:HB	2.16	0.45
1:A:692:LEU:HD22	1:A:1166:ALA:HB2	1.98	0.45
1:A:260:ASN:HB3	1:A:316:VAL:HG13	1.99	0.45
1:A:1294:PHE:HB2	1:A:1314:VAL:HG12	1.98	0.45
1:A:822:ARG:H	1:A:822:ARG:HG2	1.48	0.45
1:A:594:PHE:HB3	1:A:595:PRO:CD	2.47	0.44
1:A:994:TRP:CZ2	1:A:1014:ARG:HD3	2.52	0.44
1:A:1181:VAL:O	1:A:1185:GLN:HG2	2.17	0.44
1:A:1298:GLY:N	1:A:1347:GLU:O	2.50	0.44
1:A:959:LEU:HA	1:A:962:TYR:HD1	1.82	0.44
1:A:27:PRO:HB3	1:A:361:TRP:CE2	2.52	0.44
1:A:958:LYS:O	1:A:961:VAL:HG12	2.18	0.44
1:A:1403:GLU:HA	1:A:1408:LYS:HB2	1.98	0.44
1:A:539:LEU:CD2	1:A:1083:ASP:HB2	2.46	0.44
1:A:1351:ILE:HG23	1:A:1355:ILE:O	2.17	0.44
1:A:1341:ARG:HH21	1:A:1362:LEU:HD23	1.83	0.44
1:A:544:TYR:O	1:A:548:VAL:HG23	2.18	0.44
1:A:688:LEU:HD12	1:A:792:ASP:HB2	2.00	0.44
1:A:1445:ARG:HG3	1:A:1445:ARG:NH1	2.32	0.43
1:A:593:ARG:NH1	1:A:1242:TYR:OH	2.44	0.43
1:A:1445:ARG:HG3	1:A:1445:ARG:HH11	1.84	0.43
1:A:1376:PRO:HB3	1:A:1438:CYS:HB2	1.99	0.43
1:A:1497:ILE:HG12	1:A:1507:TRP:CE3	2.54	0.43
1:A:558:PHE:CZ	1:A:1022:GLY:HA3	2.54	0.43
1:A:353:VAL:HG21	1:A:1229:VAL:HG11	2.01	0.43
1:A:68:THR:CG2	1:A:71:ASN:H	2.31	0.43
1:A:400:ILE:HG23	1:A:427:MET:SD	2.58	0.43
1:A:775:ARG:O	1:A:776:VAL:C	2.62	0.43
1:A:27:PRO:HB3	1:A:361:TRP:CH2	2.53	0.43
1:A:1071:LEU:HD23	1:A:1071:LEU:HA	1.88	0.43
1:A:215:PHE:O	1:A:219:ILE:HG12	2.18	0.43
1:A:1195:ASN:HB3	1:A:1248:ARG:NH2	2.34	0.43
1:A:37:VAL:O	1:A:41:VAL:HG23	2.18	0.43
1:A:490:TYR:CE2	1:A:541:LYS:HB3	2.54	0.43
1:A:747:LEU:HD23	1:A:747:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:ASN:ND2	1:A:1025:GLN:HG2	2.34	0.43
1:A:364:TYR:HA	1:A:367:THR:HG22	2.01	0.42
1:A:393:MET:HG3	1:A:1185:GLN:OE1	2.19	0.42
1:A:1034:MET:O	1:A:1038:ILE:HG12	2.19	0.42
1:A:404:TYR:HH	1:A:1157:THR:HG1	1.64	0.42
1:A:1093:PHE:HB2	1:A:1249:MET:HB3	2.00	0.42
1:A:1414:LEU:HG	1:A:1420:HIS:CG	2.55	0.42
1:A:124:ILE:CG2	1:A:138:MET:HE2	2.49	0.42
1:A:139:LEU:HD23	1:A:215:PHE:HD2	1.84	0.42
1:A:432:GLN:HE21	1:A:436:ASP:HB2	1.85	0.42
1:A:965:TYR:HB2	1:A:1260:VAL:HG11	2.01	0.42
1:A:666:PHE:HE1	1:A:687:LEU:HD11	1.85	0.42
1:A:668:VAL:HG22	1:A:674:VAL:HG21	2.00	0.42
1:A:466:VAL:O	1:A:470:VAL:HG23	2.20	0.42
1:A:630:ILE:HG12	1:A:693:ALA:HB2	2.01	0.42
1:A:1117:ILE:O	1:A:1120:PRO:HD2	2.20	0.42
1:A:1341:ARG:NH1	1:A:1358:ALA:O	2.53	0.42
1:A:193:ASP:OD1	1:A:194:ARG:N	2.48	0.41
1:A:499:ASP:O	1:A:503:LYS:NZ	2.53	0.41
1:A:534:GLU:O	1:A:537:LYS:HB3	2.20	0.41
1:A:550:THR:O	1:A:554:VAL:HG12	2.20	0.41
1:A:135:SER:HB3	1:A:138:MET:HB2	2.03	0.41
1:A:1189:TYR:HB3	1:A:1190:PRO:HD3	2.02	0.41
1:A:1299:LEU:HB3	1:A:1309:LEU:HB2	2.02	0.41
1:A:1322:VAL:O	1:A:1481:LEU:HA	2.20	0.41
1:A:40:TRP:O	1:A:44:SER:HB2	2.20	0.41
1:A:543:ALA:HB1	1:A:1037:SER:HB3	2.01	0.41
1:A:608:GLN:O	1:A:611:VAL:HG12	2.20	0.41
1:A:1032:TYR:O	1:A:1036:VAL:HG12	2.20	0.41
1:A:143:LEU:O	1:A:147:LEU:HG	2.21	0.41
1:A:408:LEU:O	1:A:1165:ARG:NH1	2.52	0.41
1:A:597:ASN:C	1:A:600:PRO:HD2	2.46	0.41
1:A:674:VAL:HB	1:A:823:LEU:CD2	2.48	0.41
1:A:1117:ILE:HG13	1:A:1212:PHE:CD2	2.55	0.41
1:A:92:SER:OG	1:A:107:LEU:HD13	2.21	0.41
1:A:412:ASN:O	1:A:416:LYS:HG2	2.21	0.41
1:A:496:LYS:HD2	1:A:496:LYS:O	2.21	0.41
1:A:553:TRP:CD1	1:A:553:TRP:C	2.98	0.41
1:A:677:VAL:HG12	1:A:840:VAL:HG23	2.02	0.41
1:A:1472:ARG:HB2	1:A:1472:ARG:CZ	2.51	0.41
1:A:43:CYS:CB	1:A:116:THR:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.86	0.40
1:A:650:THR:HA	1:A:661:LEU:O	2.21	0.40
1:A:405:ARG:NH2	1:A:1178:ASP:OD2	2.54	0.40
1:A:32:CYS:O	1:A:36:THR:HG23	2.22	0.40
1:A:1287:PRO:HB2	1:A:1448:LYS:HB2	2.04	0.40
1:A:517:LEU:HD22	1:A:1371:ILE:HG21	2.04	0.40
1:A:676:VAL:HB	1:A:825:VAL:HG22	2.03	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	1311/1558 (84%)	1272 (97%)	39 (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	1168/1358 (86%)	1165 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	ILE
1	A	593	ARG
1	A	823	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	66	GLN
1	A	432	GLN
1	A	450	GLN
1	A	590	ASN
1	A	597	ASN
1	A	642	ASN
1	A	701	HIS
1	A	718	GLN
1	A	774	GLN
1	A	984	ASN
1	A	1048	HIS
1	A	1185	GLN
1	A	1363	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
3	GSH	A	1602	-	18,19,19	0.71	0	23,24,24	0.74	0
2	FY5	A	1601	-	27,27,27	0.48	0	42,43,43	1.33	4 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GSH	A	1602	-	-	10/24/24/24	-
2	FY5	A	1601	-	-	2/5/45/45	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	FY5	C07-C02-C10	-3.49	96.59	100.59
2	A	1601	FY5	C02-C07-C06	3.10	116.45	113.12
2	A	1601	FY5	C15-C05-C06	-2.85	108.11	111.58
2	A	1601	FY5	C03-C02-C07	2.34	112.68	108.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1602	GSH	O2-C2-CA2-CB2
3	A	1602	GSH	N3-C2-CA2-CB2
3	A	1602	GSH	CG1-CD1-N2-CA2
3	A	1602	GSH	OE1-CD1-N2-CA2
3	A	1602	GSH	O31-C3-CA3-N3
3	A	1602	GSH	O32-C3-CA3-N3
3	A	1602	GSH	CA1-CB1-CG1-CD1
2	A	1601	FY5	C17-C18-O20-S21
2	A	1601	FY5	C19-C18-O20-S21
3	A	1602	GSH	OE1-CD1-CG1-CB1

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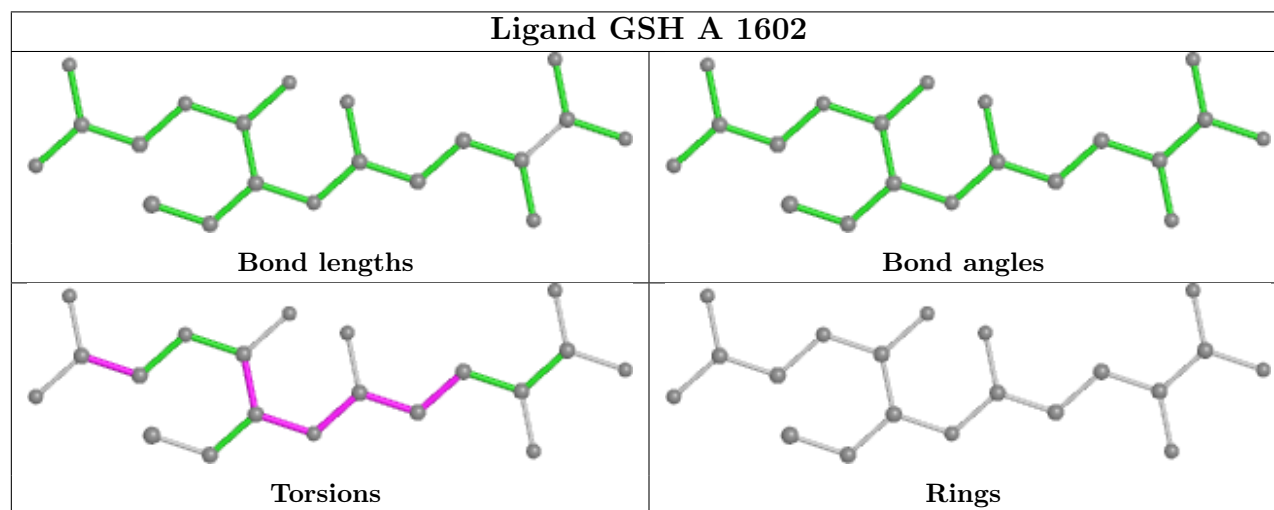
Mol	Chain	Res	Type	Atoms
3	A	1602	GSH	N2-CD1-CG1-CB1
3	A	1602	GSH	C2-CA2-N2-CD1

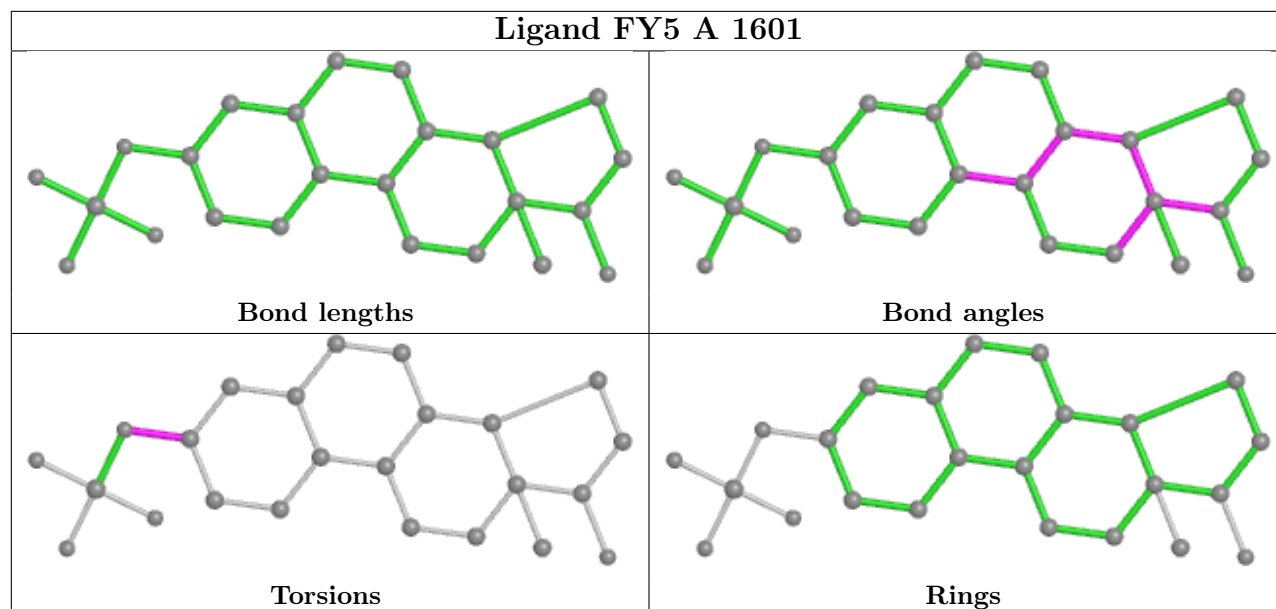
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1602	GSH	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.

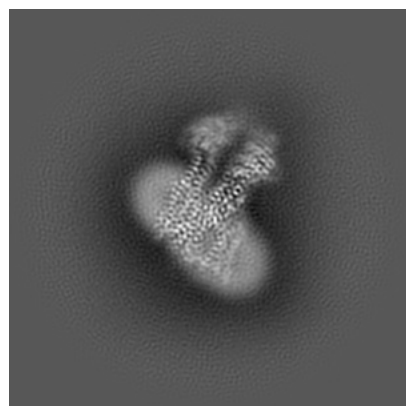
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63057. These allow visual inspection of the internal detail of the map and identification of artifacts.

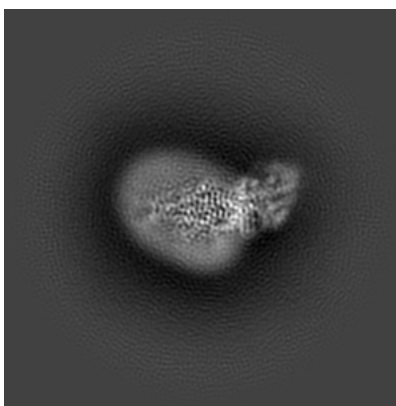
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

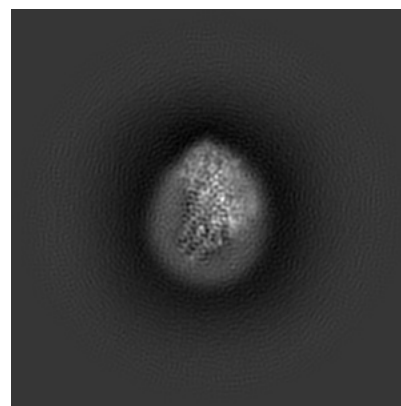
6.1.1 Primary map



X

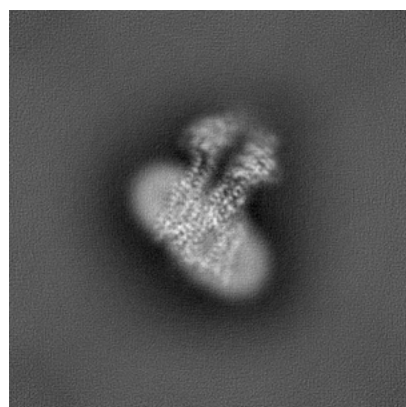


Y

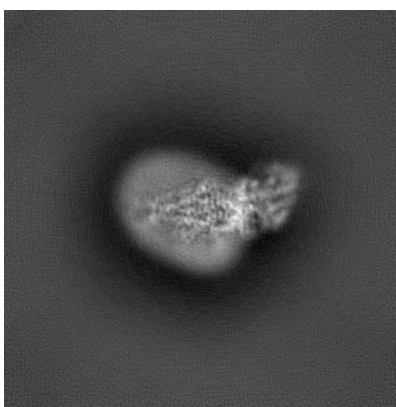


Z

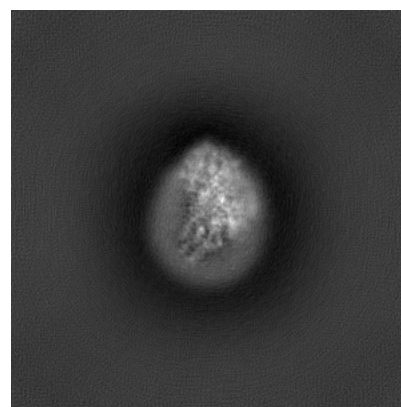
6.1.2 Raw map



X



Y

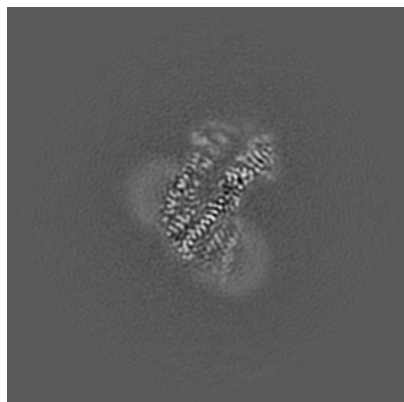


Z

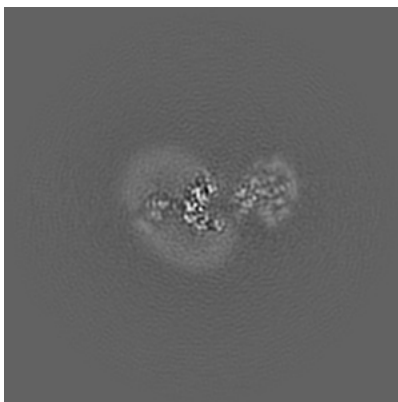
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

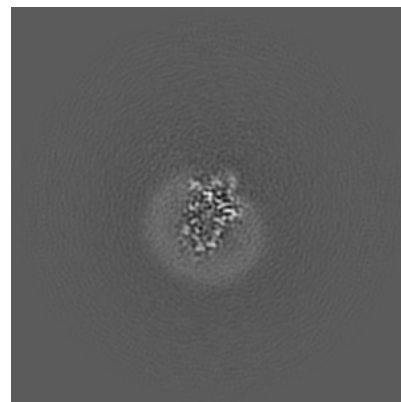
6.2.1 Primary map



X Index: 160

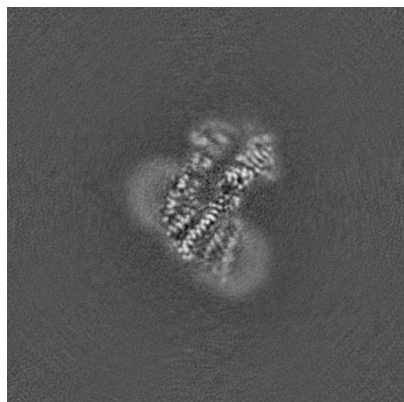


Y Index: 160

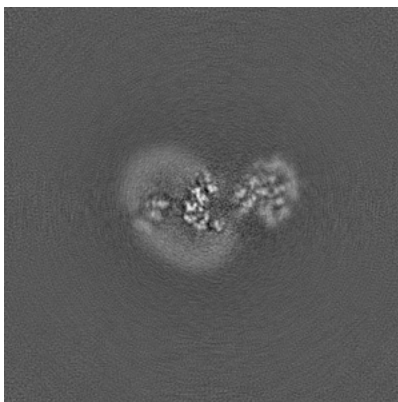


Z Index: 160

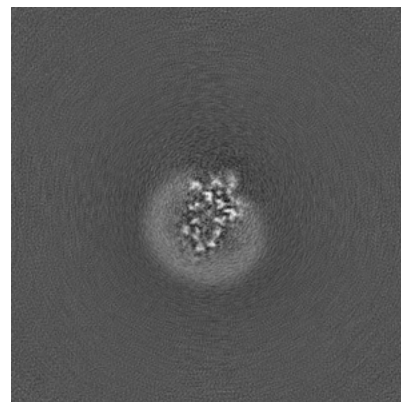
6.2.2 Raw map



X Index: 160



Y Index: 160

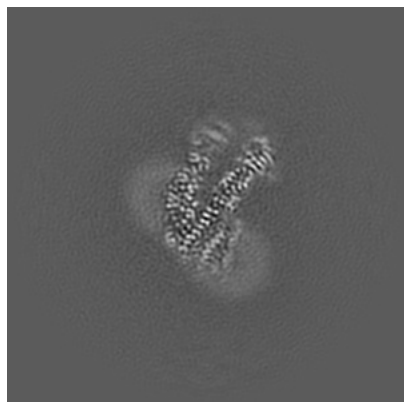


Z Index: 160

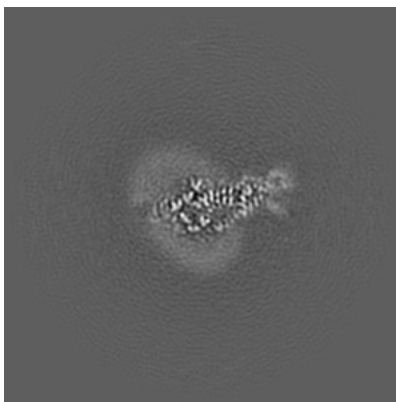
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

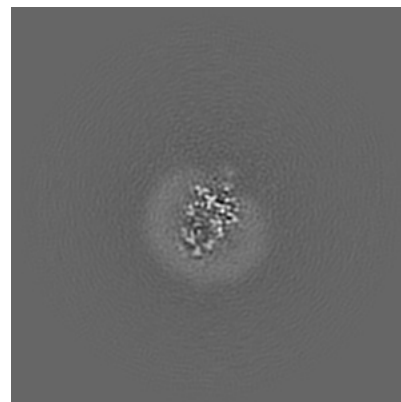
6.3.1 Primary map



X Index: 162

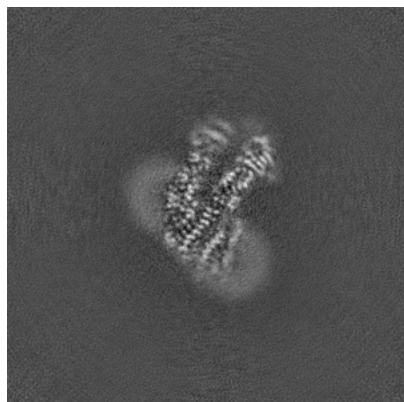


Y Index: 149

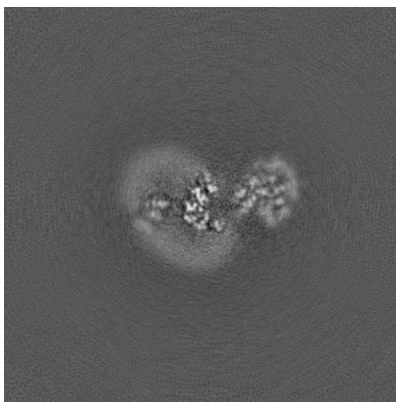


Z Index: 156

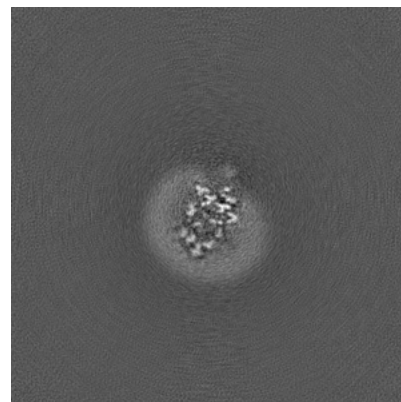
6.3.2 Raw map



X Index: 162



Y Index: 160

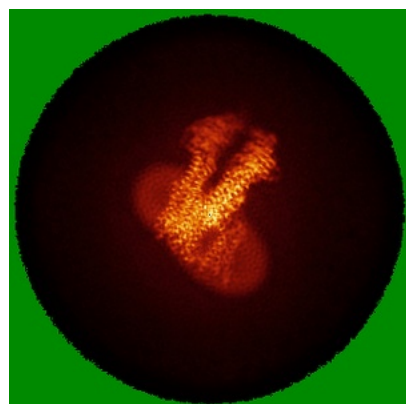


Z Index: 155

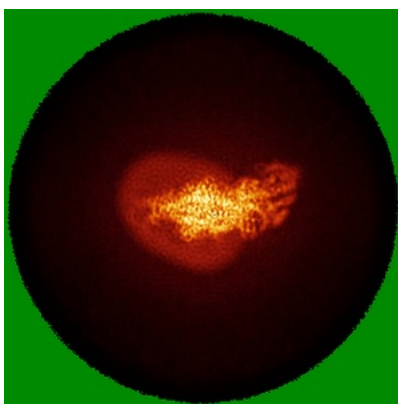
The images above show the largest variance slices of the map in three orthogonal directions.

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

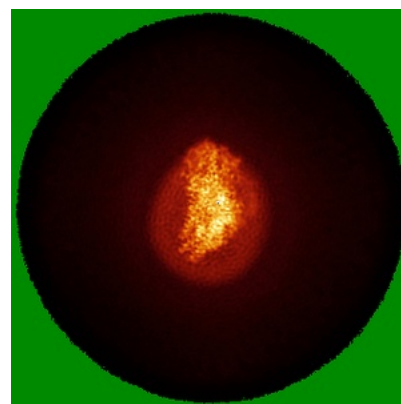
6.4.1 Primary map



X

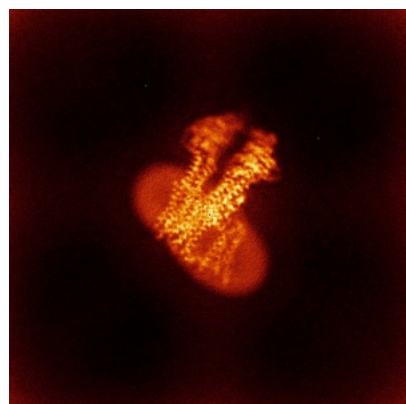


Y

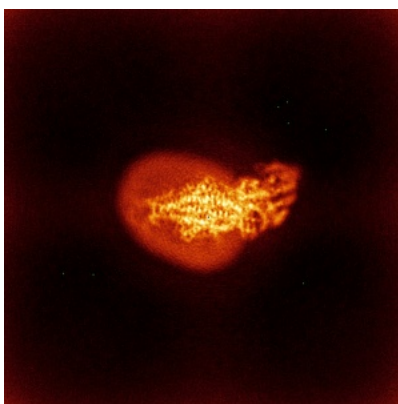


Z

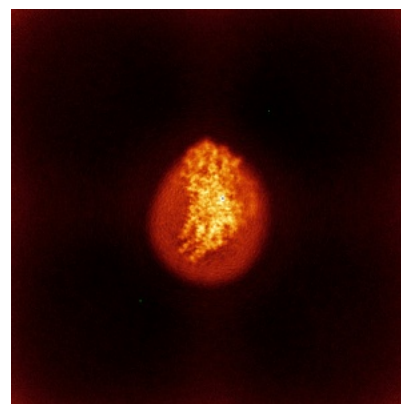
6.4.2 Raw map



X



Y

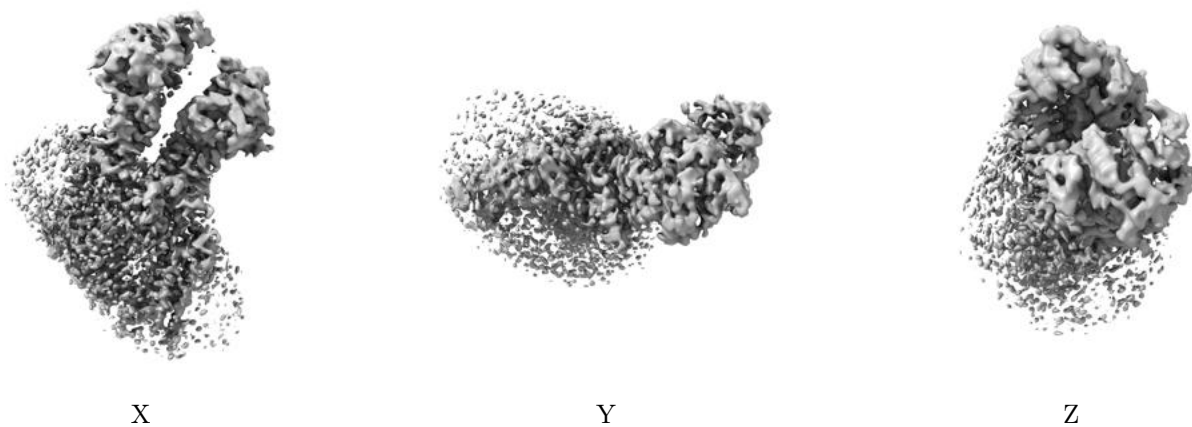


Z

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.

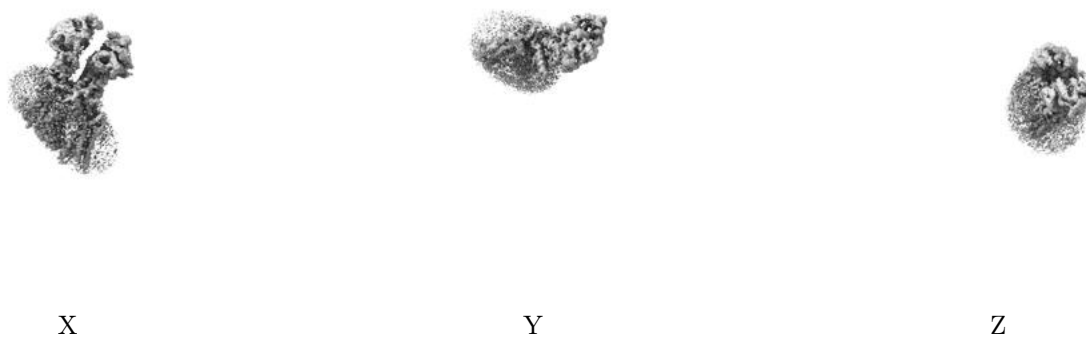
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.134. 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.

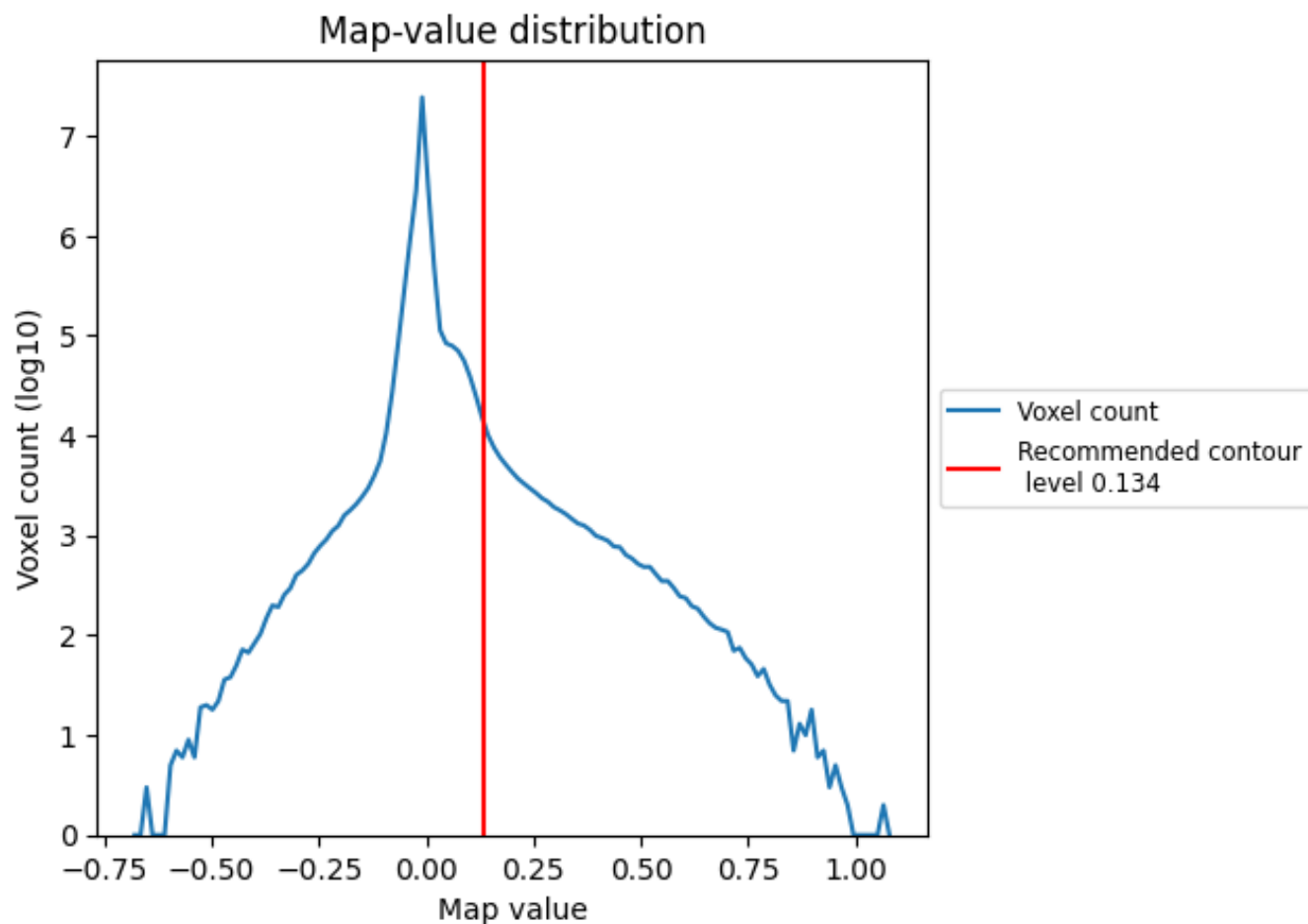
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

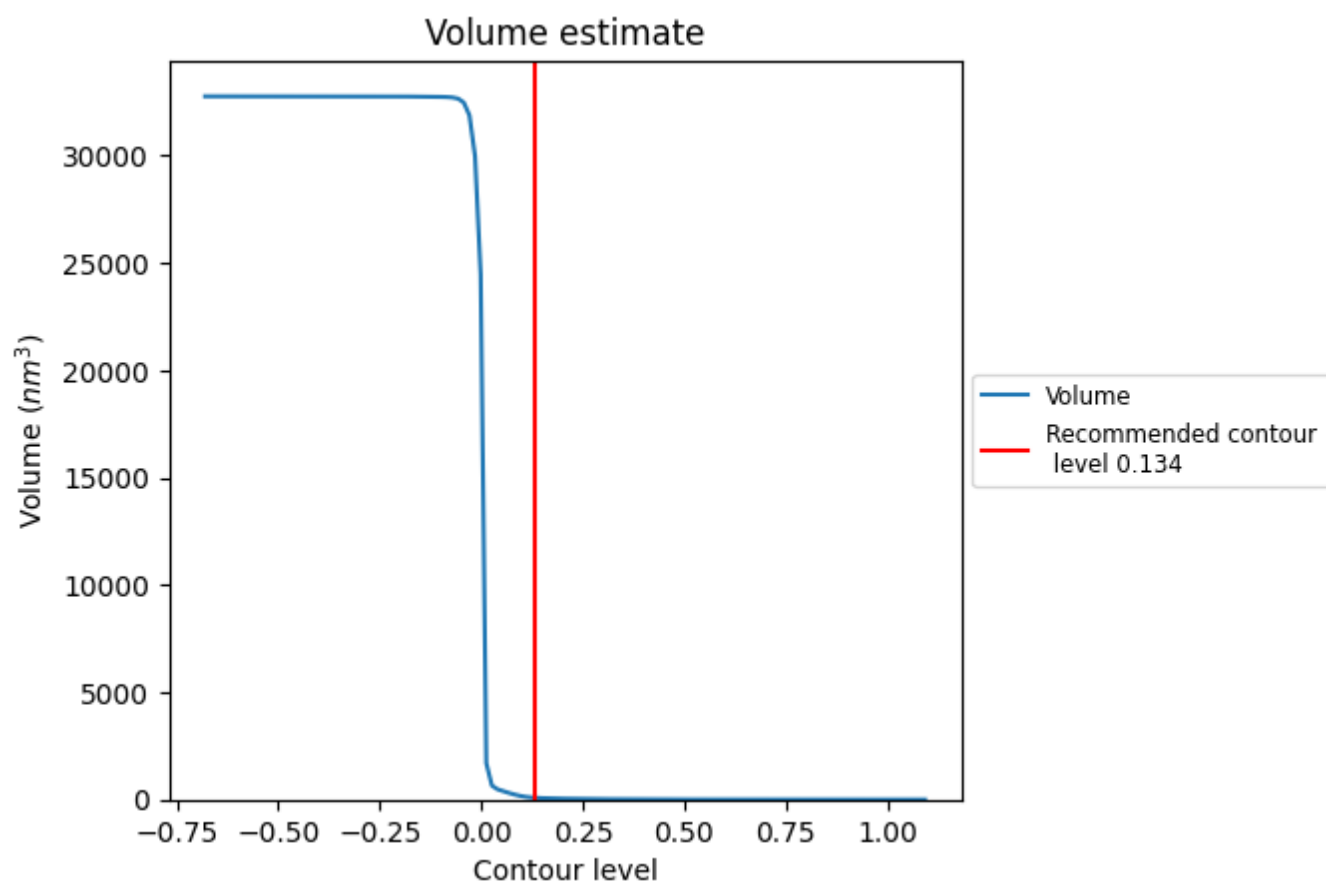
This section contains the results of statistical analysis of the map.

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.

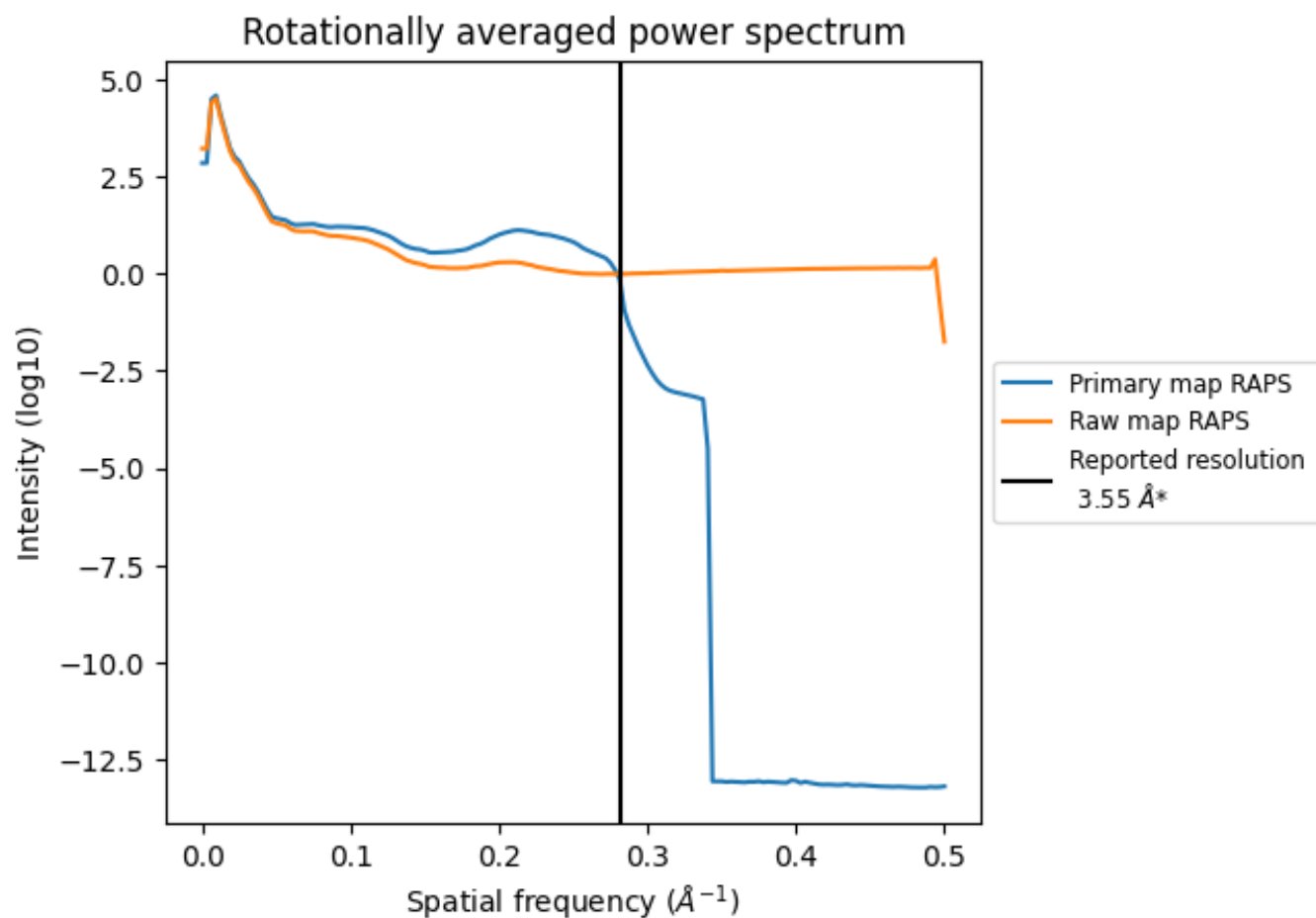
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm³; this corresponds to an approximate mass of 74 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 ⓘ

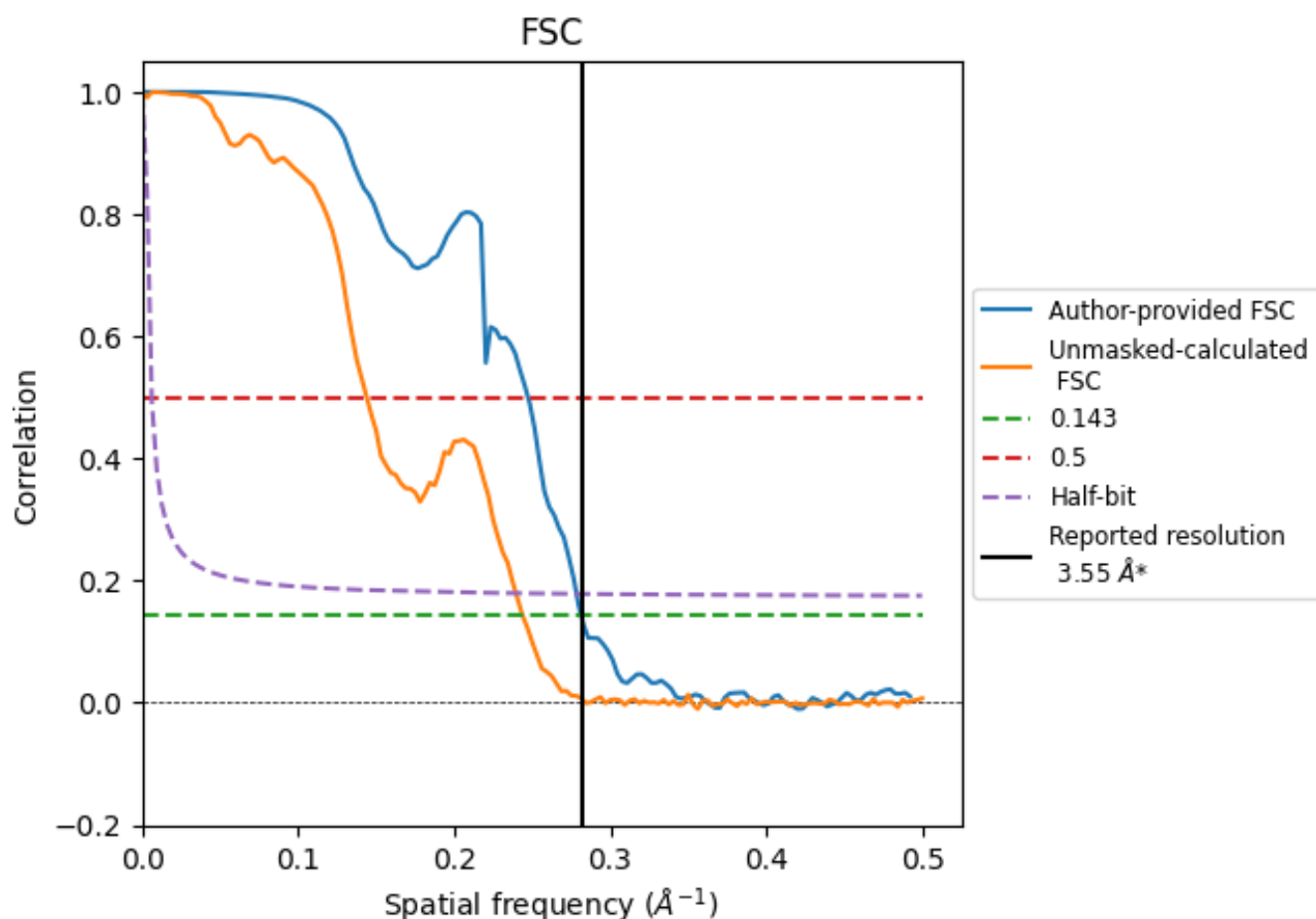


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 \AA^{-1}

8.2 Resolution estimates [i](#)

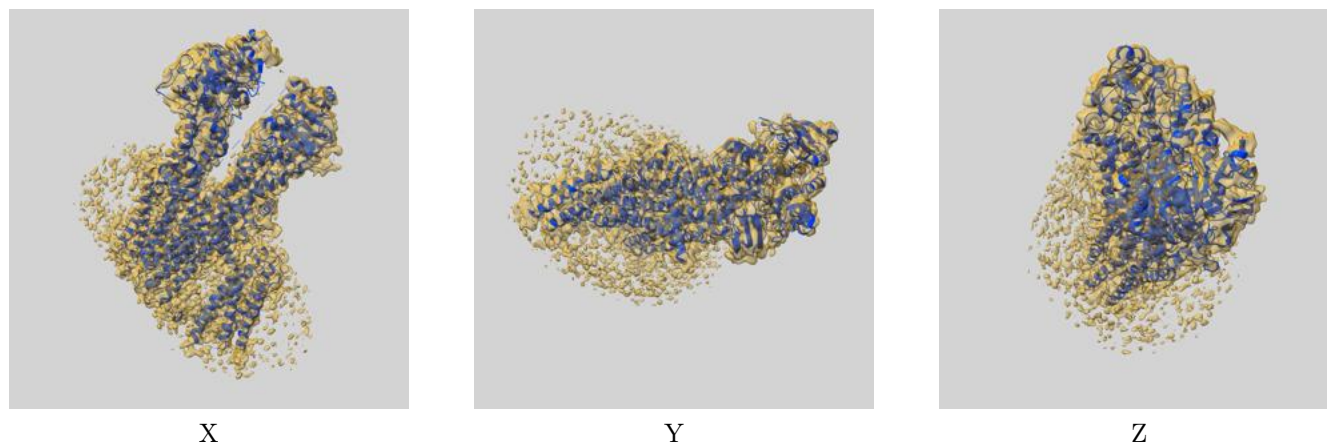
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	3.55	4.04	3.59
Unmasked-calculated*	4.10	6.96	4.17

*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 4.10 differs from the reported value 3.55 by more than 10 %

9 Map-model fit [i](#)

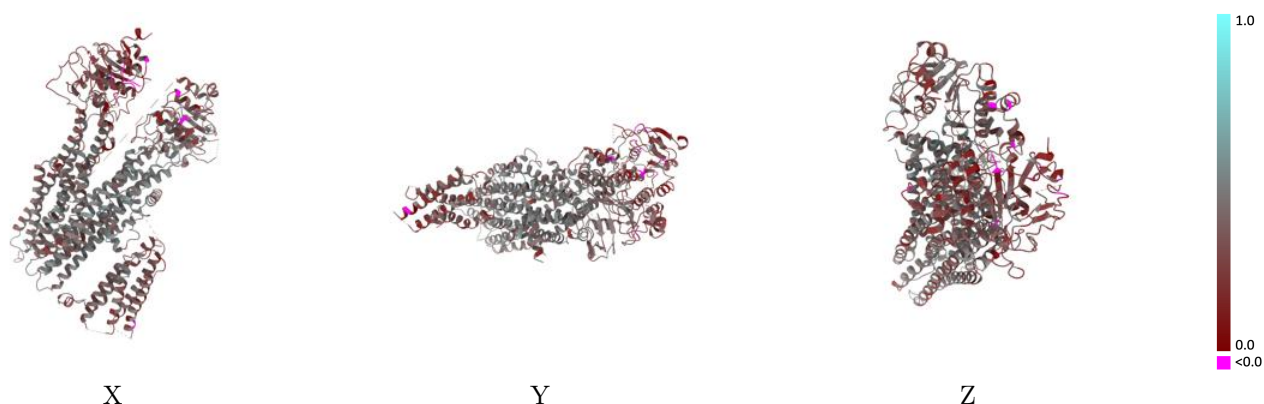
This section contains information regarding the fit between EMDB map EMD-63057 and PDB model 9LG8. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



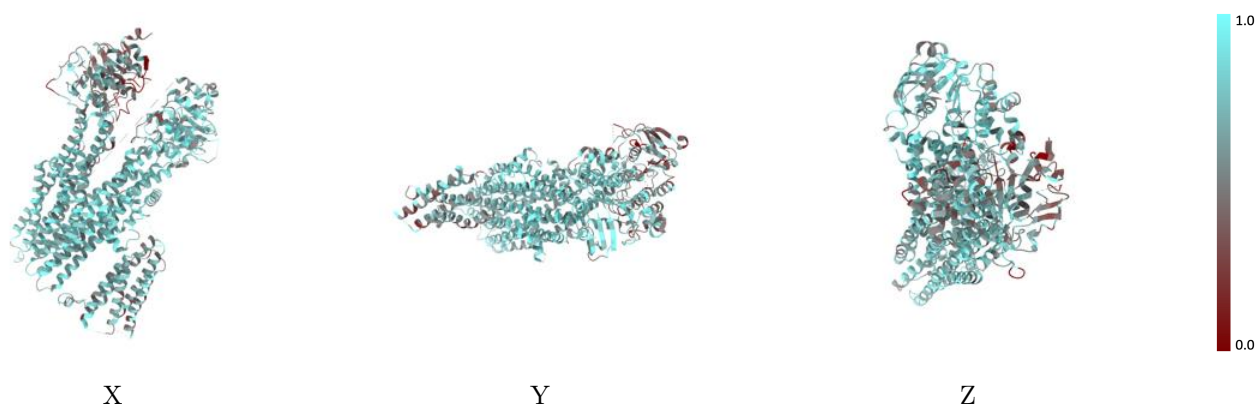
The images above show the 3D surface view of the map at the recommended contour level 0.134 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



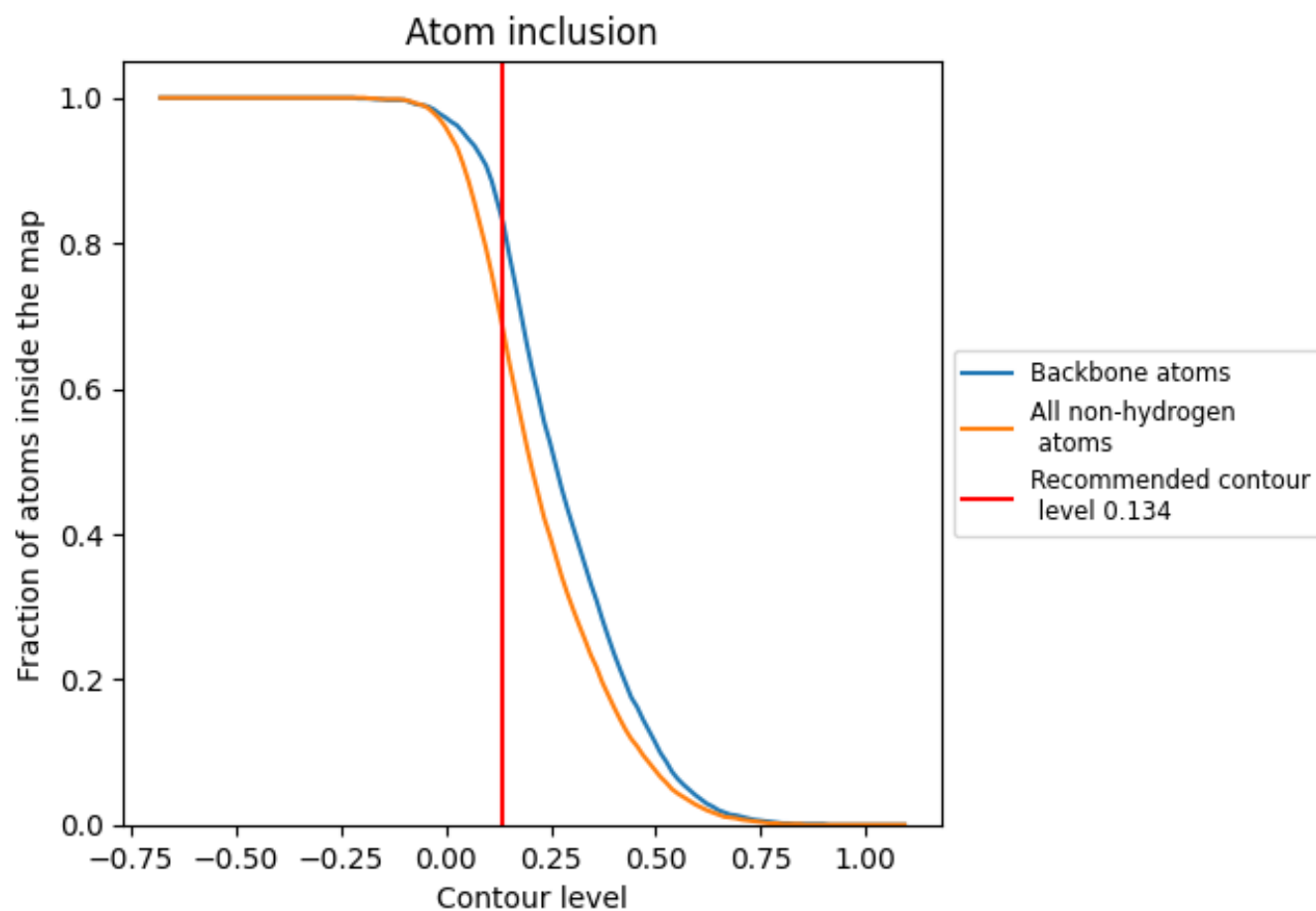
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.134).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6880	<div></div> 0.3650
A	<div></div> 0.6880	<div></div> 0.3650

