



## Full wwPDB EM Validation Report ⓘ

Sep 23, 2025 – 02:35 PM JST

PDB ID : 9LG7 / pdb\_00009lg7  
EMDB ID : EMD-63056  
Title : bovine ABCC1 bound to 2'3'-CDAS (in the presence of GSH)  
Authors : Sun, P.P.; Liu, K.X.; Gao, P.  
Deposited on : 2025-01-10  
Resolution : 3.64 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

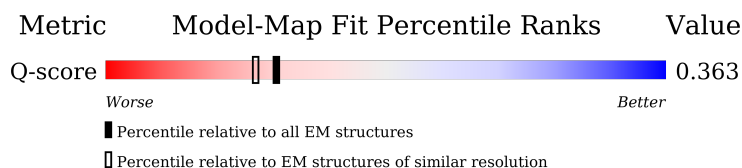
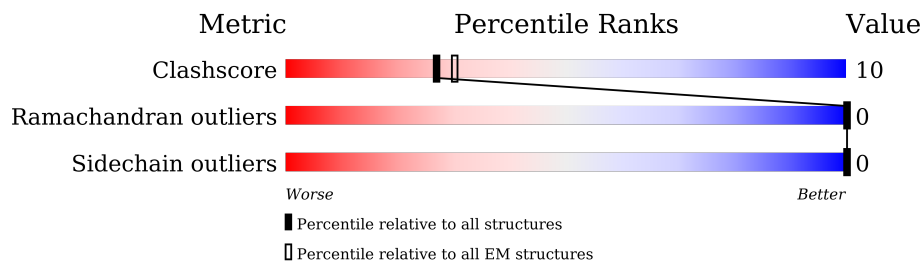
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.64 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	11633 ( 3.14 - 4.14 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1558	<div> <div>14%</div> <div>66%</div> <div>20%</div> <div>14%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10679 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.

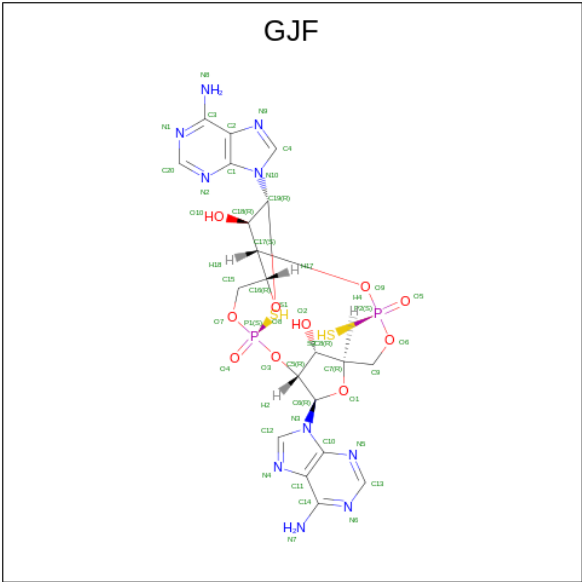
- Molecule 1 is a protein called Multidrug resistance-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1338	Total	C	N	O	S	0	0
			10635	6925	1761	1893	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 (1 {R},3 {S},6 {R},8 {R},9 {R},10 {S},12 {S},15 {R},17 {R},18 {R})-8,17-bis(6-aminopurin-9-yl)-3,12-bis(oxidanylidene)-3,12-bis(sulfanyl)-2,4,7,11,13,16-hexaoxa-3 $\lambda$ ^5,12 $\lambda$ ^5-diphosphatricyclo[13.2.1.0^6,10]octadecane-9,18-diol (CCD ID: GJF) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>10</sub>P<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

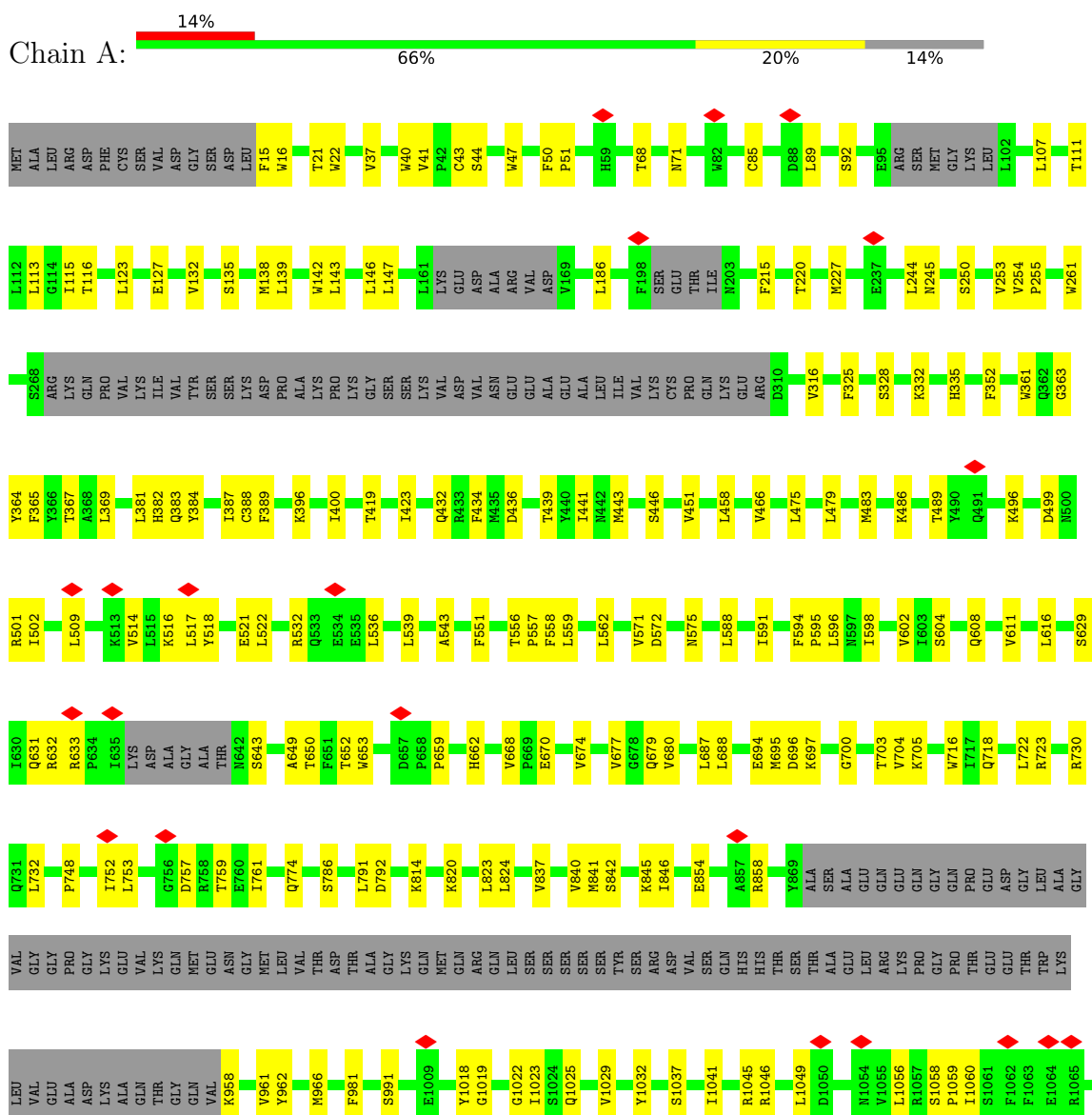


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			44	20	10	10	2	2	

### 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



SER	I1483	N1419	I1357	Y1297	R1196	V1072
	GLY	H1420	A1358	G1298	W1197	M1073
GLY	A1484	H1420	A1358	G1298	L1198	R1074
SER	E1485	E1421	I1359	L1299	A1199	
GLY	R1486	C1422	I1360	R1300	V1200	K1077
HIS	L1487	C1423	G1361	Y1301	R1201	E1078
HIS	N1488	E1424	H1363	ARG	L1202	L1079
HIS	I1489	G1425	D1364	ASP	E1203	D1080
HIS	I1490	G1426	L1365	LEU	L1216	F1081
HIS		E1427	R1366	D1306	F1216	V1083
HIS	M1491	N1428	F1367	L1307	R1221	P1087
HIS	D1492	L1429	K1368	V1308	L1228	G1088
HIS	V1493	S1430	I1369	L1309		V1089
HIS	T1494	V1431	T1370	K1310	S1236	I1090
HIS	R1495	C1432	T1371	H1311	V1239	M1092
	V1496	Q1433	I1372	I1312	V1247	F1093
	I1497	R1434	P1373	N1313	R1248	M1094
	V1498	Q1435	Q1374	V1314	M1249	
	L1499	V1437	D1375	T1315		F1098
	D1500	C1438	P1376	I1316	M1253	G1102
	M1501		V1377	D1317		
	G1502	R1441	L1378	G1318	E1281	I1105
	E1503			G1319	R1262	T1111
	I1504	L1444	G1381	E1320	L1263	
	Q1505	R1445	S1382	K1321	Y1266	Q1129
	E1506	K1446	L1383	V1322	S1267	
	W1507	T1447	M1385	G1323	E1268	V1133
	G1508	K1448	M1386	I1324	T1269	S1146
	S1509	I1449	L1387	V1325	E1270	P1149
	P1510	L1450	D1388	I1326	K1271	V1150
	S1511	V1451	S1391	G1327	E1272	Y1151
	D1512	L1452	Q1392	T1328		
	L1513	E1453	Y1393	G1329	W1275	L1158
	L1514	E1454	S1394	A1330	Q1276	L1159
	GLN	A1455	E1395	G1331	I1277	G1160
GLN	GLN	THR	E1396	G1332	Q1278	V1161
ARG	ARG	ALA	E1397	S1333	D1279	I1164
GLY	GLY	ALA	V1398	S1334	M1280	R1165
LEU	LEU	VAL	W1399	L1335	A1281	Q1170
PHE	PHE	ASP		L1336	P1282	F1173
TYR	TYR	LEU	T1400	T1337	P1283	D1178
SER	SER	E1462	S1401	G1338	K1284	V1181
MET	MET	T1463	L1402	L1339	D1285	
ALA	ALA	D1464	E1403	L1340	W1286	M1184
ASP	ASP	D1465	A1405	R1341	P1287	Q1185
LYS	LYS	D1466	I1407	I1342	Q1288	
SER	SER	I1467	H1406	K1343	V1289	P1190
GLY	GLY	Q1468	L1408	E1344	G1290	
LEU	LEU	S1469	G1409	S1345	R1291	
VAL	VAL		F1410	A1346	V1292	
LEU	LEU		V1411	A1347	E1293	
ASN	ASN	F1475	S1412	G1348	F1294	
LEU	LEU	D1476	A1413	E1349	R1296	
TVR	TVR	D1477	L1414	I1350	D1296	
PHE	PHE	D1477	P1415	I1351		
GLN	GLN	C1478	D1416	I1352		
GLY	GLY		K1417	D1353		
			L1418	D1354		
				I1355		
				M1356		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146406	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	3.482	Depositor
Minimum map value	-2.150	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.42	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: GJF

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	0.51	0/10874	0.69	0/14763

There are no bond length outliers.

There are no bond angle outliers.

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	10635	0	10851	209	0
2	A	44	0	0	1	0
All	All	10679	0	10851	209	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 (209) 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:543:ALA:HB1	1:A:1037:SER:HB3	1.73	0.70
1:A:382:HIS:NE2	1:A:1199:ALA:HB1	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:VAL:HG23	1:A:595:PRO:HB2	1.78	0.66
1:A:389:PHE:HE1	1:A:439:THR:HB	1.63	0.64
1:A:981:PHE:CE1	1:A:1094:MET:HG2	2.34	0.63
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	0.62
1:A:1111:THR:HG21	1:A:1216:PHE:HB3	1.81	0.62
1:A:558:PHE:CZ	1:A:1022:GLY:HA3	2.34	0.61
1:A:138:MET:O	1:A:142:TRP:CD1	2.54	0.61
1:A:1341:ARG:NH1	1:A:1357:ILE:O	2.35	0.60
1:A:716:TRP:CH2	1:A:1164:ILE:HD11	2.37	0.60
1:A:517:LEU:HB3	1:A:1371:ILE:HG21	1.83	0.60
1:A:718:GLN:NE2	1:A:1173:PHE:HZ	2.00	0.60
1:A:522:LEU:HD21	1:A:1275:TRP:HZ3	1.67	0.59
1:A:1286:TRP:HE1	1:A:1355:ILE:HB	1.67	0.59
1:A:516:LYS:HG3	1:A:1060:ILE:HD11	1.85	0.59
1:A:139:LEU:HD23	1:A:215:PHE:HD2	1.69	0.58
1:A:396:LYS:NZ	1:A:1184:ASN:OD1	2.38	0.57
1:A:127:GLU:HG2	1:A:132:VAL:HG21	1.85	0.57
1:A:1299:LEU:HB3	1:A:1309:LEU:HB2	1.84	0.57
1:A:1082:VAL:HG21	1:A:1263:LEU:HD12	1.86	0.57
1:A:364:TYR:O	1:A:367:THR:HG22	2.05	0.56
1:A:632:ARG:HA	1:A:704:VAL:O	2.05	0.56
1:A:1402:LEU:HD13	1:A:1411:VAL:HG21	1.87	0.56
1:A:649:ALA:HA	1:A:700:GLY:HA3	1.86	0.56
1:A:1199:ALA:O	1:A:1203:GLU:HG2	2.04	0.56
1:A:458:LEU:HB3	1:A:466:VAL:HG21	1.86	0.56
1:A:325:PHE:HE2	1:A:441:ILE:HD13	1.71	0.56
1:A:21:THR:O	1:A:361:TRP:CH2	2.58	0.56
1:A:539:LEU:HD21	1:A:1083:ASP:HB2	1.86	0.56
1:A:558:PHE:CE1	1:A:1022:GLY:HA3	2.41	0.56
1:A:1352:ILE:HD13	1:A:1449:ILE:HD12	1.86	0.55
1:A:629:SER:HA	1:A:697:LYS:HE3	1.88	0.55
1:A:1092:MET:HG3	1:A:1249:MET:HG3	1.88	0.55
1:A:383:GLN:O	1:A:387:ILE:HG12	2.07	0.55
1:A:571:VAL:O	1:A:572:ASP:OD1	2.23	0.55
1:A:135:SER:HB3	1:A:138:MET:HB2	1.89	0.55
1:A:643:SER:HB2	1:A:670:GLU:HG2	1.89	0.55
1:A:227:MET:HE1	1:A:1190:PRO:HB3	1.88	0.54
1:A:718:GLN:NE2	1:A:1173:PHE:CZ	2.76	0.54
1:A:791:LEU:HD12	1:A:824:LEU:HD12	1.89	0.54
1:A:594:PHE:HD2	2:A:1601:GJF:C1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:VAL:HG22	1:A:1165:ARG:HE	1.73	0.54
1:A:496:LYS:HB2	1:A:496:LYS:NZ	2.23	0.54
1:A:382:HIS:HD2	1:A:1200:VAL:HG13	1.73	0.54
1:A:123:LEU:HD23	1:A:138:MET:SD	2.49	0.53
1:A:1298:GLY:N	1:A:1347:GLU:O	2.42	0.53
1:A:250:SER:HA	1:A:253:VAL:HG22	1.91	0.52
1:A:1382:SER:HB2	1:A:1419:ASN:HA	1.92	0.52
1:A:687:LEU:HD23	1:A:688:LEU:HD23	1.91	0.52
1:A:400:ILE:HG21	1:A:1181:VAL:HG21	1.92	0.52
1:A:652:THR:HG22	1:A:659:PRO:HA	1.91	0.52
1:A:1337:LEU:HD22	1:A:1342:ILE:HG13	1.90	0.52
1:A:1317:ASP:HB2	1:A:1320:GLU:HG3	1.92	0.52
1:A:1286:TRP:HB3	1:A:1287:PRO:HD3	1.93	0.51
1:A:1378:LEU:HD22	1:A:1434:ARG:HG2	1.93	0.51
1:A:1286:TRP:CD1	1:A:1355:ILE:HD12	2.45	0.51
1:A:514:VAL:HG13	1:A:518:TYR:CE1	2.46	0.51
1:A:1386:ASN:HB3	1:A:1441:ARG:HH11	1.76	0.51
1:A:21:THR:O	1:A:361:TRP:HH2	1.95	0.50
1:A:588:LEU:HD23	1:A:591:ILE:HD11	1.92	0.50
1:A:1294:PHE:O	1:A:1313:ASN:HA	2.10	0.50
1:A:139:LEU:HD23	1:A:215:PHE:CD2	2.47	0.50
1:A:1077:LYS:HE2	1:A:1077:LYS:HA	1.94	0.50
1:A:1236:SER:O	1:A:1239:VAL:HG12	2.12	0.50
1:A:1384:ARG:HH12	1:A:1395:ASP:HA	1.77	0.50
1:A:15:PHE:HD1	1:A:16:TRP:HB2	1.74	0.50
1:A:653:TRP:CE2	1:A:695:MET:HE3	2.47	0.50
1:A:962:TYR:O	1:A:966:MET:HG3	2.12	0.50
1:A:716:TRP:CD2	1:A:1160:GLY:HA3	2.47	0.50
1:A:250:SER:HB3	1:A:1178:ASP:OD2	2.12	0.49
1:A:723:ARG:HD2	1:A:757:ASP:OD2	2.12	0.49
1:A:723:ARG:HH22	1:A:732:LEU:HD13	1.76	0.49
1:A:92:SER:OG	1:A:107:LEU:HG	2.12	0.49
1:A:436:ASP:O	1:A:439:THR:HG22	2.13	0.48
1:A:753:LEU:HD13	1:A:759:THR:HG21	1.95	0.48
1:A:517:LEU:HB3	1:A:1371:ILE:CG2	2.43	0.48
1:A:653:TRP:CD2	1:A:695:MET:HE3	2.48	0.48
1:A:536:LEU:HD12	1:A:1045:ARG:HD3	1.94	0.48
1:A:786:SER:O	1:A:820:LYS:HD2	2.14	0.48
1:A:352:PHE:CE2	1:A:363:GLY:HA3	2.48	0.48
1:A:677:VAL:O	1:A:840:VAL:HA	2.14	0.48
1:A:556:THR:HB	1:A:557:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:ARG:O	1:A:1200:VAL:HG22	2.13	0.47
1:A:1282:PRO:HD3	1:A:1360:ILE:HD12	1.96	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:748:PRO:O	1:A:752:ILE:HG22	2.14	0.47
1:A:841:MET:HG3	1:A:846:ILE:HD13	1.95	0.47
1:A:1310:LYS:HG2	1:A:1311:HIS:ND1	2.30	0.47
1:A:1351:ILE:HG12	1:A:1356:ASN:HA	1.97	0.47
1:A:43:CYS:SG	1:A:116:THR:HG21	2.54	0.47
1:A:518:TYR:HD2	1:A:1445:ARG:HH12	1.62	0.47
1:A:1383:LEU:HD13	1:A:1420:HIS:HB3	1.95	0.47
1:A:1387:LEU:HA	1:A:1441:ARG:HG2	1.97	0.47
1:A:22:TRP:O	1:A:361:TRP:HZ3	1.98	0.47
1:A:89:LEU:HD13	1:A:111:THR:OG1	2.15	0.46
1:A:367:THR:HG21	1:A:1215:LEU:CD1	2.45	0.46
1:A:1362:LEU:O	1:A:1365:LEU:HG	2.14	0.46
1:A:40:TRP:O	1:A:44:SER:CB	2.64	0.46
1:A:50:PHE:HB3	1:A:51:PRO:HD3	1.97	0.46
1:A:352:PHE:O	1:A:1221:ARG:NH2	2.48	0.46
1:A:1403:GLU:HA	1:A:1408:LYS:HB2	1.98	0.46
1:A:1059:PRO:HD3	1:A:1271:LYS:HA	1.98	0.46
1:A:1299:LEU:HD11	1:A:1343:LYS:HB2	1.97	0.46
1:A:1351:ILE:HG23	1:A:1355:ILE:C	2.41	0.46
1:A:1438:CYS:HA	1:A:1441:ARG:HD2	1.98	0.46
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.83	0.46
1:A:604:SER:O	1:A:608:GLN:HG3	2.16	0.46
1:A:608:GLN:O	1:A:611:VAL:HG12	2.16	0.46
1:A:722:LEU:HD12	1:A:761:ILE:HG21	1.97	0.46
1:A:85:CYS:SG	1:A:113:LEU:HD22	2.56	0.46
1:A:688:LEU:HD12	1:A:792:ASP:HB2	1.98	0.46
1:A:679:GLN:O	1:A:680:VAL:C	2.58	0.45
1:A:981:PHE:HB2	1:A:1032:TYR:CD1	2.50	0.45
1:A:146:LEU:HD22	1:A:186:LEU:HD22	1.98	0.45
1:A:443:MET:HA	1:A:446:SER:HB3	1.98	0.45
1:A:254:VAL:N	1:A:255:PRO:HD2	2.32	0.45
1:A:551:PHE:HA	1:A:1029:VAL:CG1	2.47	0.45
1:A:991:SER:OG	1:A:1018:TYR:HE1	2.00	0.45
1:A:1307:LEU:HB2	1:A:1310:LYS:HE2	1.97	0.45
1:A:539:LEU:HD23	1:A:1041:ILE:HG13	1.99	0.45
1:A:981:PHE:HZ	1:A:1098:PHE:HB2	1.81	0.45
1:A:1102:GLY:HA2	1:A:1105:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1294:PHE:HB2	1:A:1314:VAL:HG12	1.98	0.45
1:A:694:GLU:OE2	1:A:1165:ARG:NH1	2.50	0.45
1:A:854:GLU:O	1:A:858:ARG:HG3	2.16	0.45
1:A:501:ARG:HG3	1:A:501:ARG:HH11	1.82	0.45
1:A:1351:ILE:HG23	1:A:1355:ILE:O	2.17	0.45
1:A:1445:ARG:HG3	1:A:1445:ARG:NH1	2.32	0.44
1:A:486:LYS:O	1:A:489:THR:OG1	2.23	0.44
1:A:1046:ARG:HG2	1:A:1046:ARG:HH11	1.82	0.44
1:A:451:VAL:CG2	1:A:595:PRO:HB2	2.46	0.44
1:A:1019:GLY:O	1:A:1023:ILE:HG12	2.18	0.44
1:A:138:MET:O	1:A:142:TRP:HD1	1.99	0.44
1:A:68:THR:CG2	1:A:71:ASN:H	2.31	0.44
1:A:361:TRP:O	1:A:365:PHE:CB	2.66	0.43
1:A:432:GLN:NE2	1:A:1151:TYR:OH	2.51	0.43
1:A:551:PHE:HA	1:A:1029:VAL:HG12	2.00	0.43
1:A:1025:GLN:O	1:A:1029:VAL:HG23	2.17	0.43
1:A:499:ASP:O	1:A:502:ILE:HG22	2.18	0.43
1:A:509:LEU:HD12	1:A:1072:VAL:HG22	2.00	0.43
1:A:517:LEU:HD13	1:A:1371:ILE:HD13	2.00	0.43
1:A:650:THR:HB	1:A:662:HIS:O	2.18	0.43
1:A:37:VAL:O	1:A:41:VAL:HG23	2.18	0.43
1:A:244:LEU:HD11	1:A:1185:GLN:HB2	1.99	0.43
1:A:668:VAL:HG22	1:A:674:VAL:HG21	2.00	0.43
1:A:419:THR:O	1:A:423:ILE:HG13	2.19	0.43
1:A:1087:PRO:O	1:A:1090:ILE:HG22	2.18	0.43
1:A:1129:GLN:O	1:A:1133:VAL:HG12	2.18	0.43
1:A:1388:ASP:OD2	1:A:1393:TYR:N	2.43	0.43
1:A:572:ASP:HB2	1:A:575:ASN:ND2	2.34	0.42
1:A:814:LYS:HE2	1:A:814:LYS:HB2	1.83	0.42
1:A:1497:ILE:HG12	1:A:1507:TRP:CE3	2.54	0.42
1:A:382:HIS:HE2	1:A:1199:ALA:HB1	1.83	0.42
1:A:633:ARG:HB2	1:A:705:LYS:HG3	2.01	0.42
1:A:1074:ARG:NH2	1:A:1266:TYR:OH	2.51	0.42
1:A:1181:VAL:O	1:A:1185:GLN:HG2	2.19	0.42
1:A:521:GLU:HB3	1:A:1056:LEU:HD23	2.01	0.42
1:A:631:GLN:HG3	1:A:703:THR:HG23	1.99	0.42
1:A:1170:GLN:H	1:A:1170:GLN:HG2	1.67	0.42
1:A:1089:VAL:HG12	1:A:1253:MET:SD	2.59	0.42
1:A:479:LEU:O	1:A:483:MET:HG2	2.19	0.42
1:A:434:PHE:HE2	1:A:616:LEU:HD12	1.84	0.42
1:A:688:LEU:HD21	1:A:823:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:MET:HE3	1:A:1249:MET:HA	2.01	0.42
1:A:1414:LEU:HG	1:A:1420:HIS:CG	2.55	0.42
1:A:40:TRP:O	1:A:44:SER:HB2	2.20	0.42
1:A:536:LEU:CD1	1:A:1045:ARG:HD3	2.50	0.42
1:A:335:HIS:CD2	1:A:381:LEU:HD13	2.55	0.41
1:A:598:ILE:HG12	1:A:602:VAL:HG23	2.02	0.41
1:A:842:SER:N	1:A:845:LYS:O	2.53	0.41
1:A:47:TRP:HZ2	1:A:115:ILE:HG22	1.85	0.41
1:A:1228:LEU:HD23	1:A:1228:LEU:HA	1.88	0.41
1:A:1300:ARG:HB2	1:A:1346:ALA:HB2	2.01	0.41
1:A:1322:VAL:O	1:A:1481:LEU:HA	2.21	0.41
1:A:43:CYS:CB	1:A:116:THR:HG21	2.51	0.41
1:A:143:LEU:O	1:A:147:LEU:HG	2.21	0.41
1:A:475:LEU:HD12	1:A:475:LEU:HA	1.85	0.41
1:A:981:PHE:CZ	1:A:1098:PHE:HB2	2.55	0.41
1:A:1198:LEU:HD12	1:A:1198:LEU:HA	1.82	0.41
1:A:1445:ARG:HG3	1:A:1445:ARG:HH11	1.84	0.41
1:A:261:TRP:HE3	1:A:316:VAL:HG21	1.86	0.41
1:A:389:PHE:CE1	1:A:439:THR:HB	2.48	0.41
1:A:1299:LEU:HD23	1:A:1334:SER:HB3	2.01	0.41
1:A:730:ARG:HB2	1:A:730:ARG:HH11	1.85	0.41
1:A:1146:SER:O	1:A:1149:PRO:HD2	2.21	0.41
1:A:1049:LEU:HA	1:A:1049:LEU:HD23	1.83	0.41
1:A:1058:SER:HA	1:A:1271:LYS:HA	2.03	0.41
1:A:1202:LEU:HD11	1:A:1247:VAL:HG21	2.03	0.41
1:A:135:SER:O	1:A:139:LEU:HB2	2.20	0.41
1:A:328:SER:OG	1:A:384:TYR:HD1	2.04	0.41
1:A:332:LYS:HD2	1:A:332:LYS:HA	1.89	0.41
1:A:532:ARG:NH1	1:A:1079:LEU:HD21	2.35	0.41
1:A:559:LEU:HD12	1:A:559:LEU:HA	1.88	0.41
1:A:674:VAL:HG22	1:A:837:VAL:HB	2.01	0.41
1:A:696:ASP:OD1	1:A:696:ASP:C	2.64	0.41
1:A:958:LYS:O	1:A:961:VAL:HG22	2.21	0.41
1:A:1280:MET:HE2	1:A:1280:MET:HB3	1.92	0.41
1:A:220:THR:HG22	1:A:1201:ARG:HH12	1.85	0.41
1:A:325:PHE:HE1	1:A:388:CYS:SG	2.44	0.40
1:A:596:LEU:HA	1:A:596:LEU:HD12	1.86	0.40
1:A:1282:PRO:HB2	1:A:1286:TRP:HB2	2.04	0.40
1:A:1297:TYR:HB3	1:A:1312:ILE:HB	2.03	0.40
1:A:245:ASN:OD1	1:A:245:ASN:N	2.54	0.40
1:A:558:PHE:CZ	1:A:562:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:GLN:HA	1:A:774:GLN:HE21	1.85	0.40
1:A:1158:LEU:HD23	1:A:1158:LEU:HA	1.93	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	1320/1558 (85%)	1280 (97%)	40 (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	1177/1358 (87%)	1177 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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Mol	Chain	Res	Type
1	A	383	GLN
1	A	500	ASN
1	A	622	HIS
1	A	718	GLN
1	A	774	GLN
1	A	1010	HIS
1	A	1025	GLN
1	A	1138	GLN
1	A	1207	ASN
1	A	1363	HIS
1	A	1386	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	GJF	A	1601	-	39,50,50	2.28	13 (33%)	46,78,78	2.19	6 (13%)

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	GJF	A	1601	-	-	12/18/62/62	0/6/7/7

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	GJF	P2-O9	5.58	1.66	1.57
2	A	1601	GJF	O1-C6	4.68	1.47	1.41
2	A	1601	GJF	O8-C19	4.19	1.46	1.41
2	A	1601	GJF	P2-O6	4.01	1.64	1.57
2	A	1601	GJF	C18-C17	-3.80	1.44	1.52
2	A	1601	GJF	C18-C19	-3.40	1.48	1.53
2	A	1601	GJF	P1-O7	3.25	1.63	1.57
2	A	1601	GJF	P1-O3	3.25	1.63	1.57
2	A	1601	GJF	C3-N8	3.14	1.45	1.34
2	A	1601	GJF	C14-N7	3.01	1.45	1.34
2	A	1601	GJF	C8-C5	-2.84	1.46	1.52
2	A	1601	GJF	O8-C16	2.82	1.51	1.45
2	A	1601	GJF	C17-C16	-2.51	1.46	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	GJF	O6-P2-O9	7.34	122.74	102.22
2	A	1601	GJF	O3-P1-O7	6.56	120.56	102.22
2	A	1601	GJF	N5-C13-N6	-4.95	120.95	128.68
2	A	1601	GJF	N2-C20-N1	-4.38	121.83	128.68
2	A	1601	GJF	O8-C19-C18	-4.29	100.65	106.93
2	A	1601	GJF	O1-C7-C8	-2.27	100.62	105.11

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	GJF	O1-C7-C9-O6
2	A	1601	GJF	C5-O3-P1-O7
2	A	1601	GJF	C17-O9-P2-O5
2	A	1601	GJF	C17-O9-P2-O6

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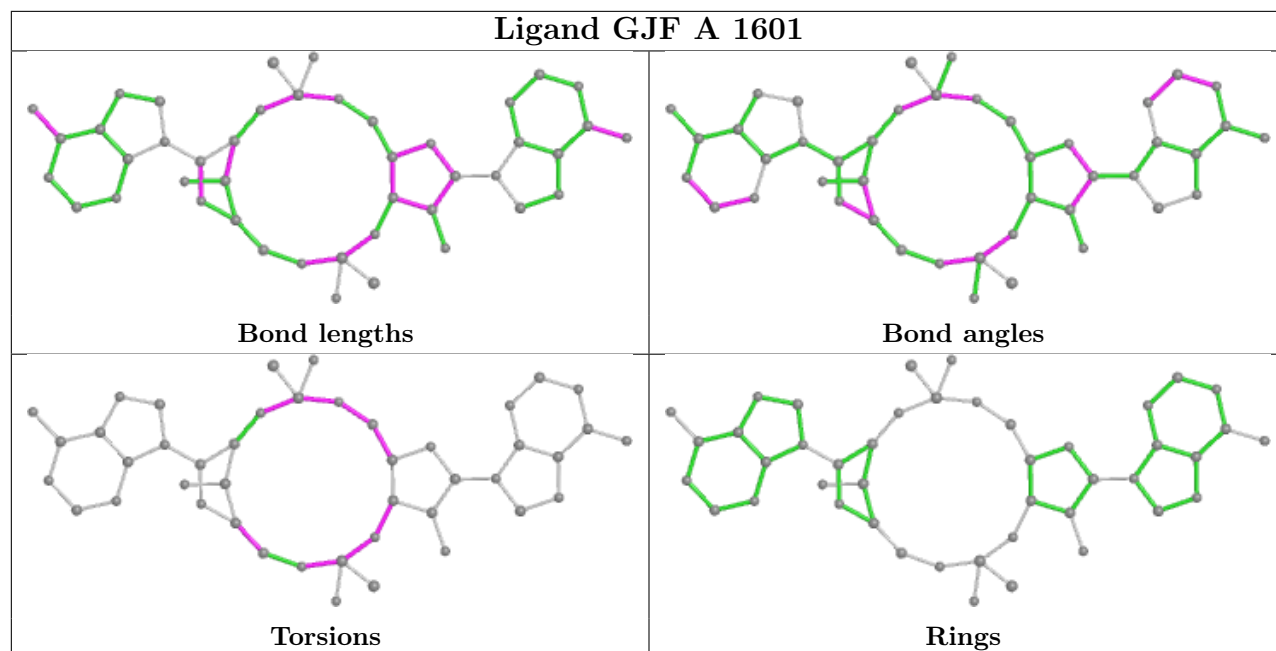
Mol	Chain	Res	Type	Atoms
2	A	1601	GJF	C16-C17-O9-P2
2	A	1601	GJF	C8-C7-C9-O6
2	A	1601	GJF	O7-C15-C16-C17
2	A	1601	GJF	C5-O3-P1-O4
2	A	1601	GJF	O7-C15-C16-O8
2	A	1601	GJF	C16-C15-O7-P1
2	A	1601	GJF	C9-O6-P2-O5
2	A	1601	GJF	C15-O7-P1-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	GJF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

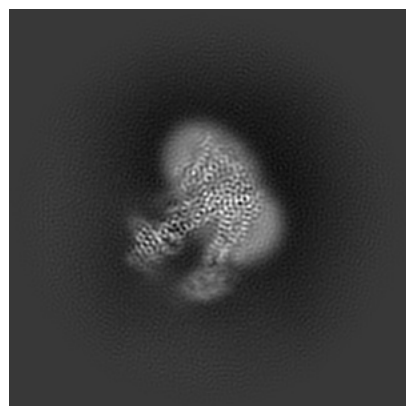
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63056. These allow visual inspection of the internal detail of the map and identification of artifacts.

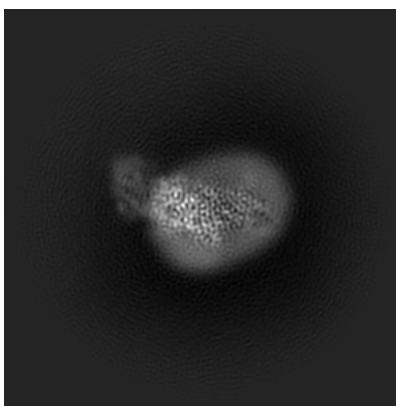
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

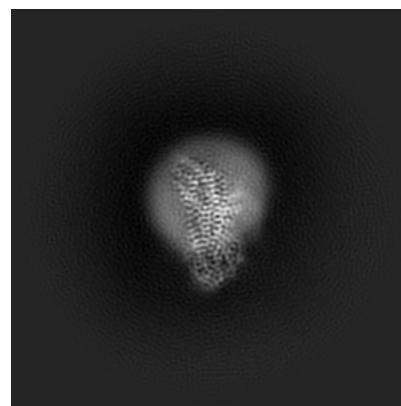
#### 6.1.1 Primary map



X

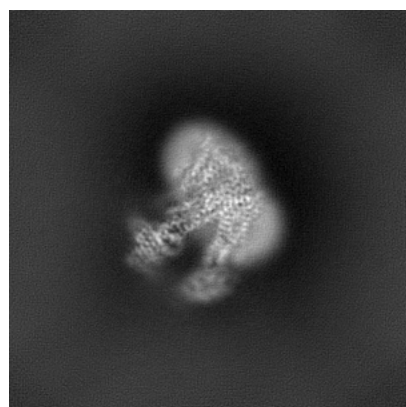


Y

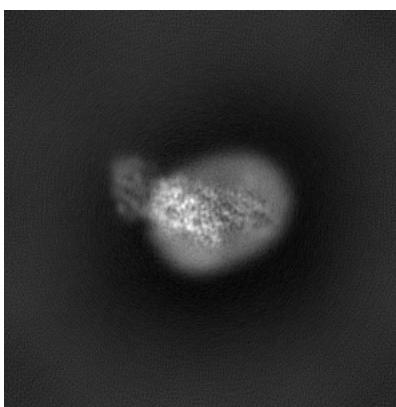


Z

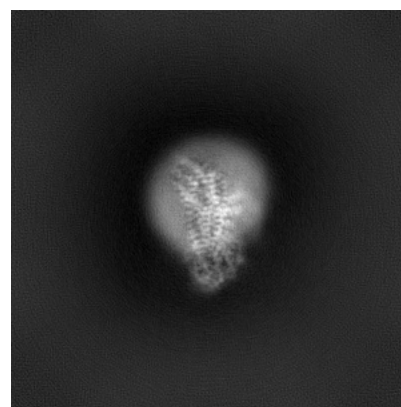
#### 6.1.2 Raw map



X



Y

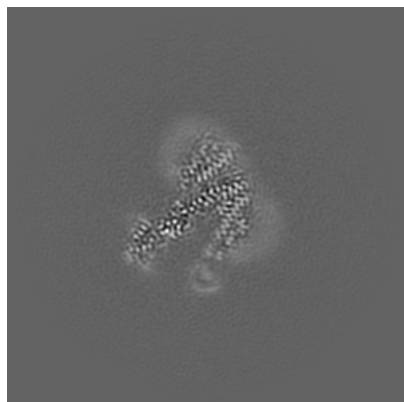


Z

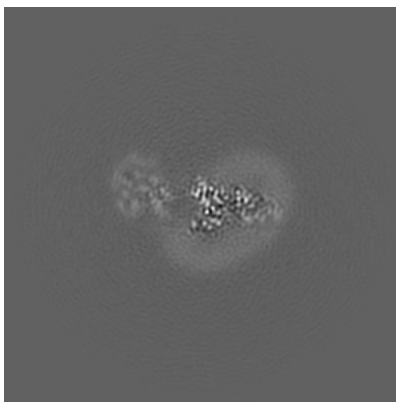
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

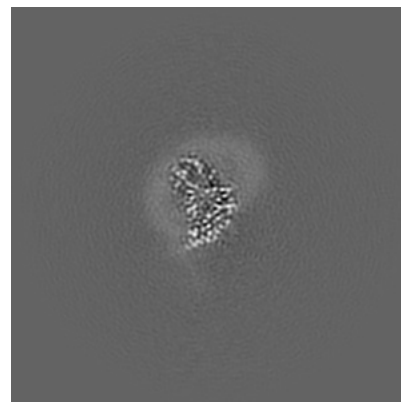
### 6.2.1 Primary map



X Index: 160

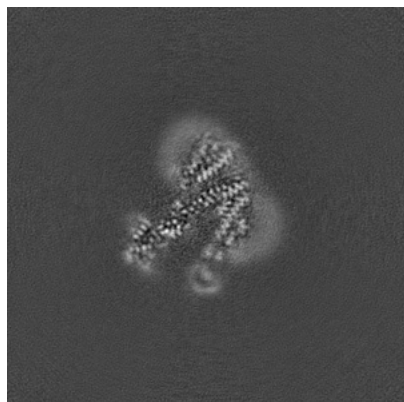


Y Index: 160

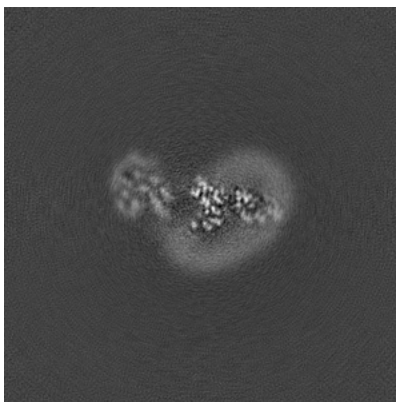


Z Index: 160

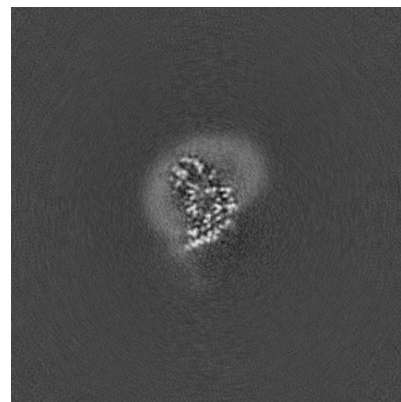
### 6.2.2 Raw map



X Index: 160



Y Index: 160

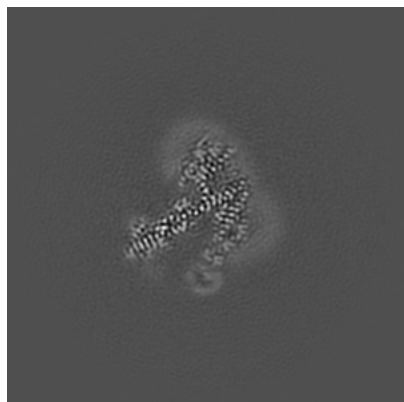


Z Index: 160

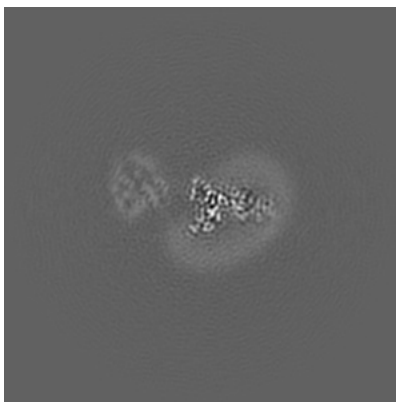
The images above show central slices of the map in three orthogonal directions.

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

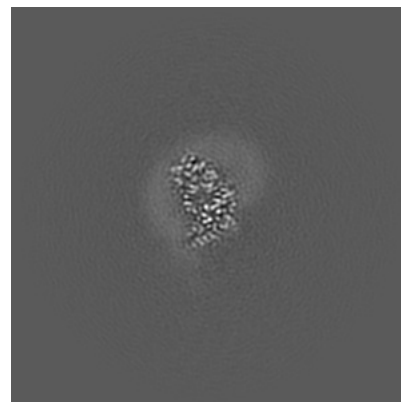
### 6.3.1 Primary map



X Index: 163

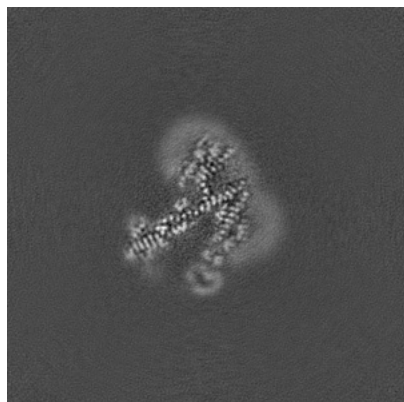


Y Index: 157

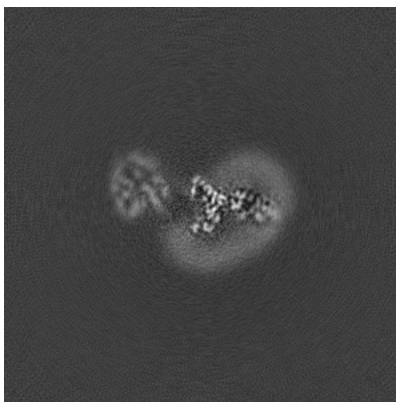


Z Index: 162

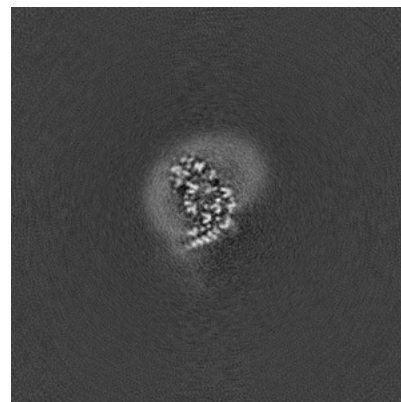
### 6.3.2 Raw map



X Index: 163



Y Index: 158

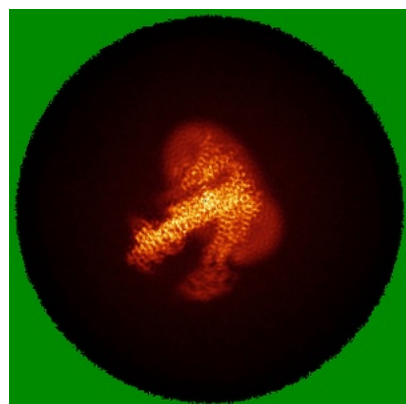


Z Index: 161

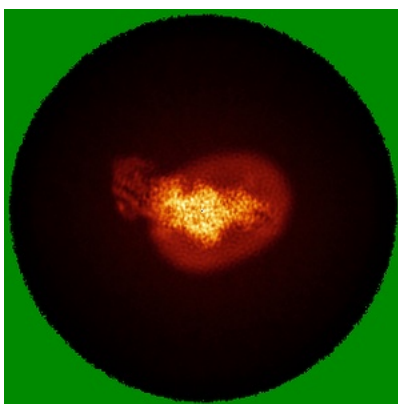
The images above show the largest variance slices of the map in three orthogonal directions.

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

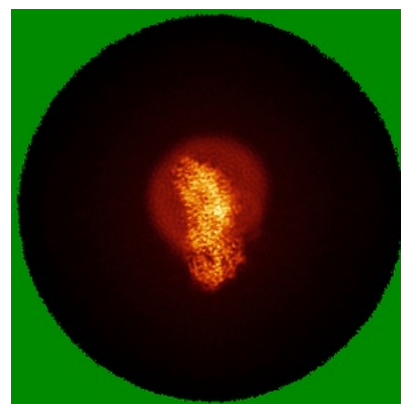
### 6.4.1 Primary map



X

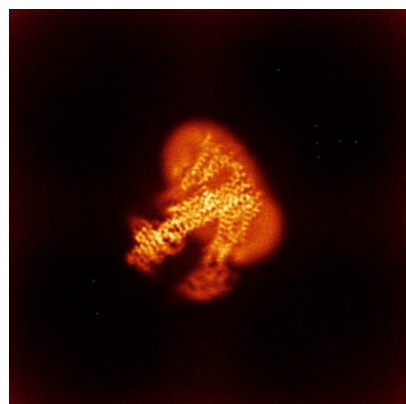


Y

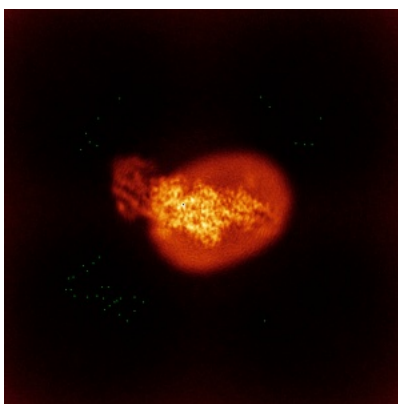


Z

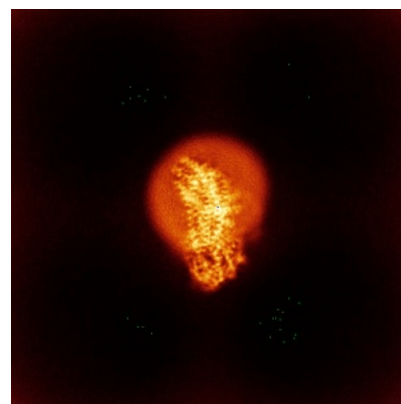
### 6.4.2 Raw map



X



Y

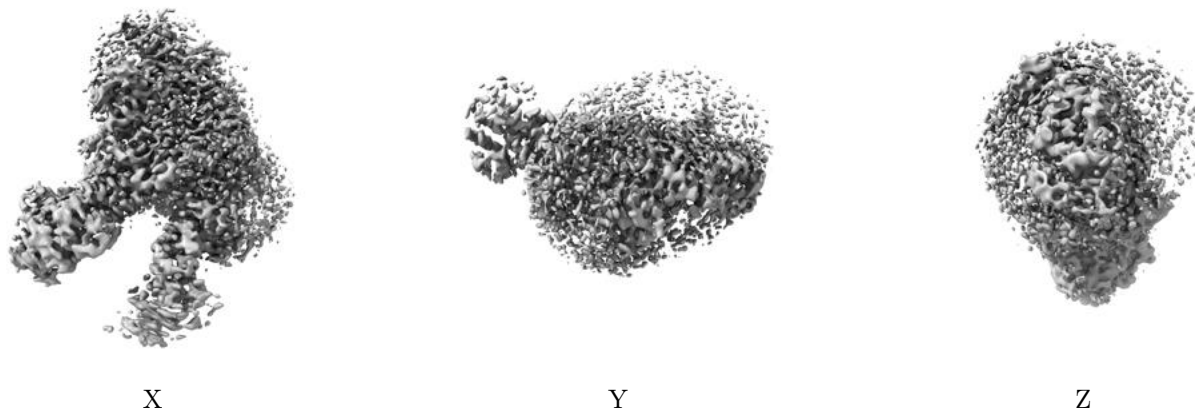


Z

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.

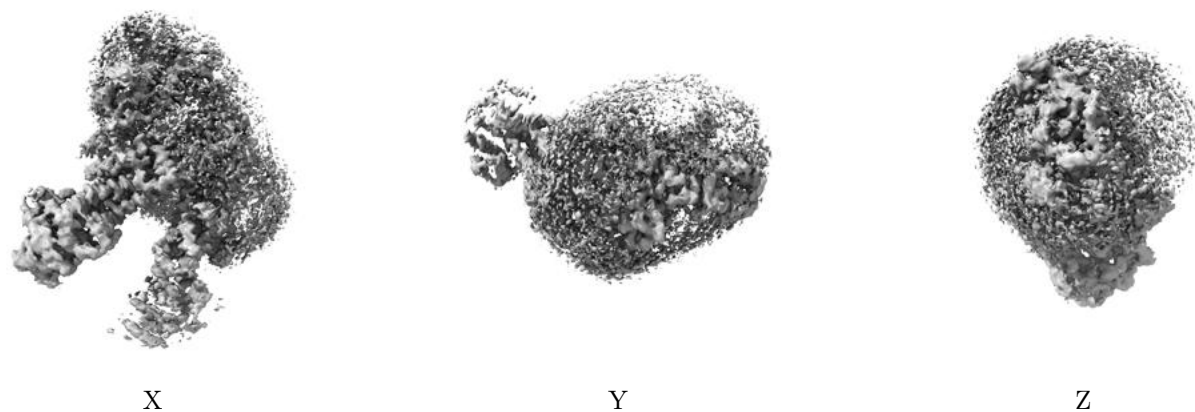
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. 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.

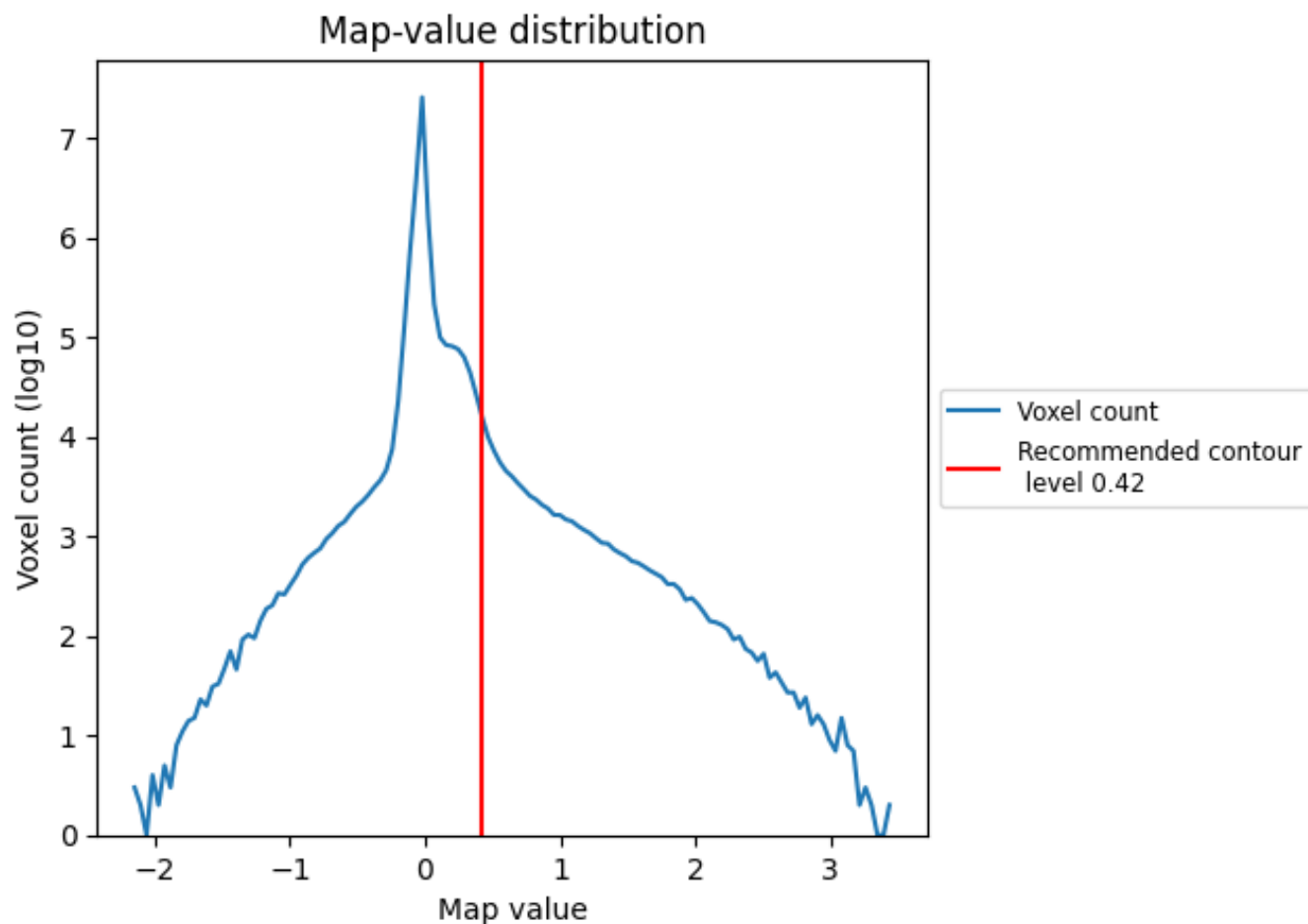
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

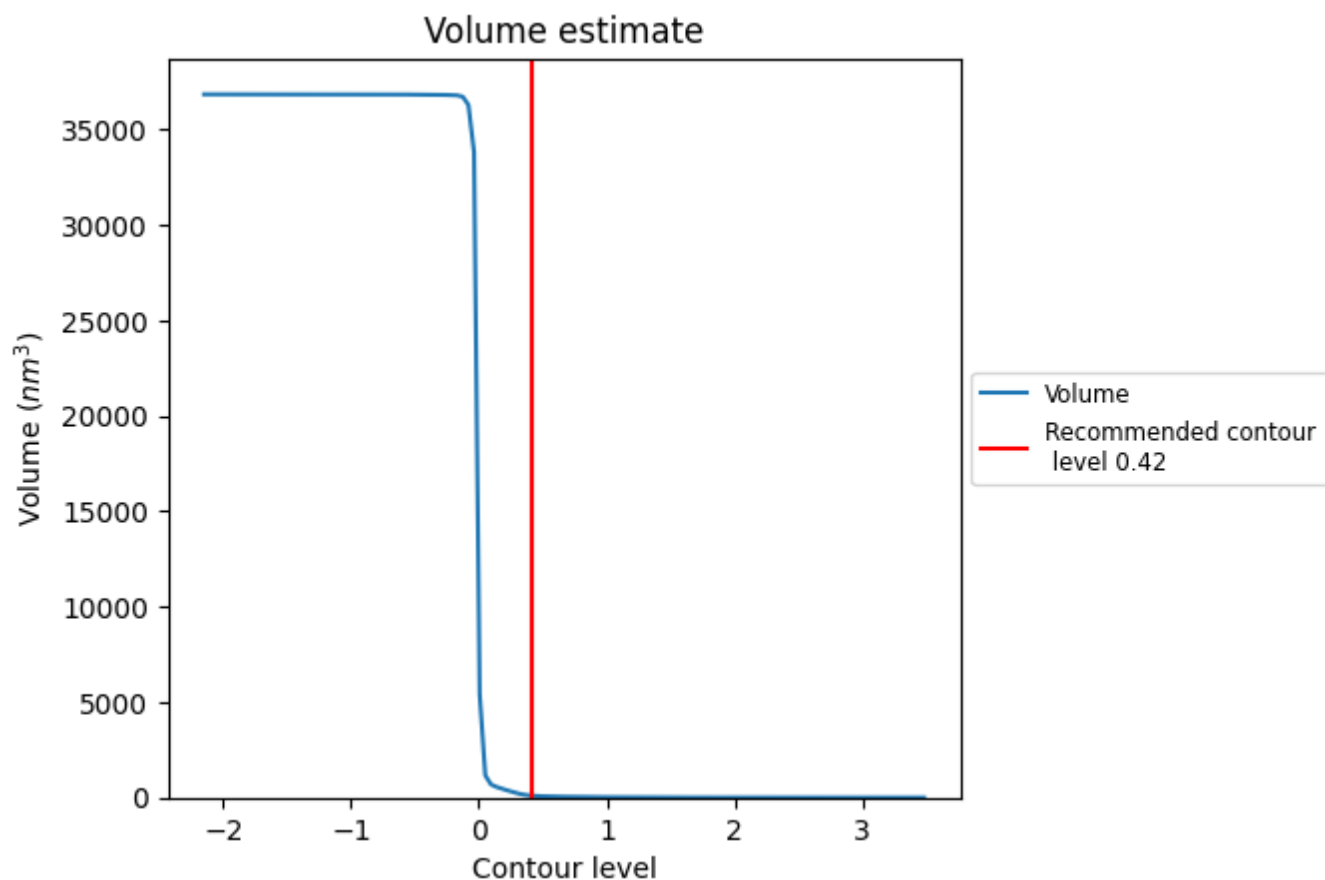
This section contains the results of statistical analysis of the map.

### 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.

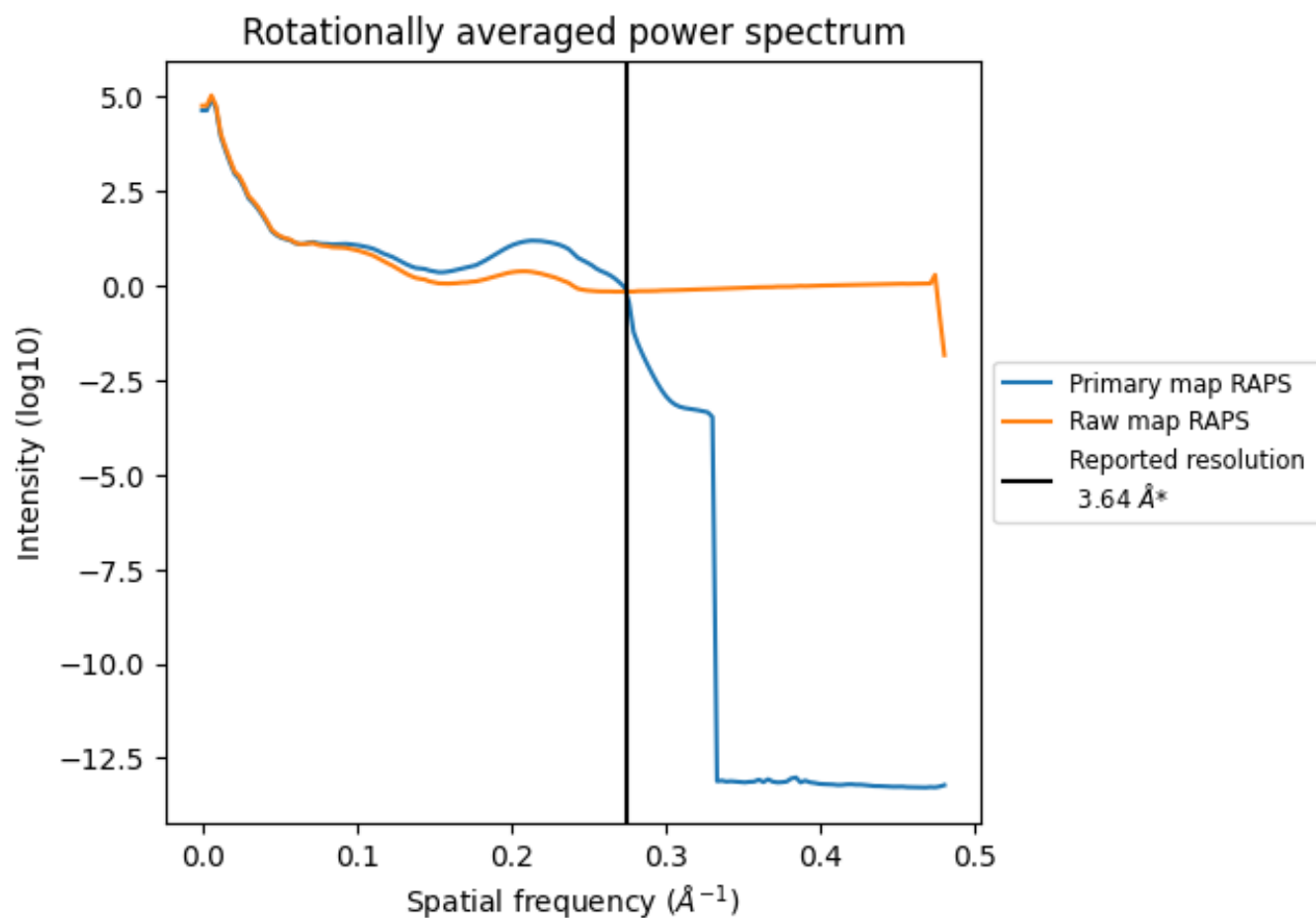
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95  $\text{nm}^3$ ; this corresponds to an approximate mass of 86 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 ⓘ

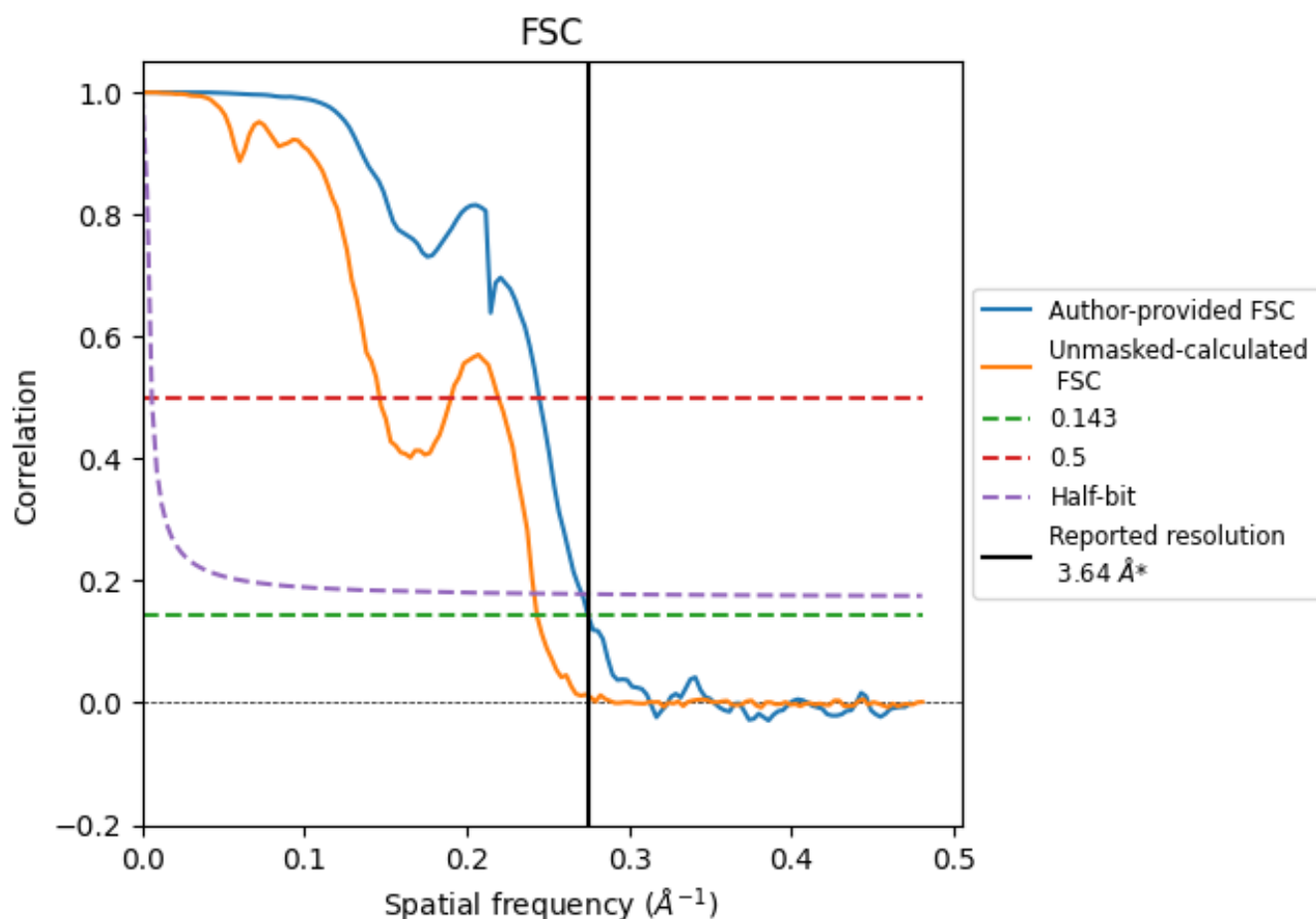


\*Reported resolution corresponds to spatial frequency of 0.275 Å<sup>-1</sup>

## 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 0.275  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

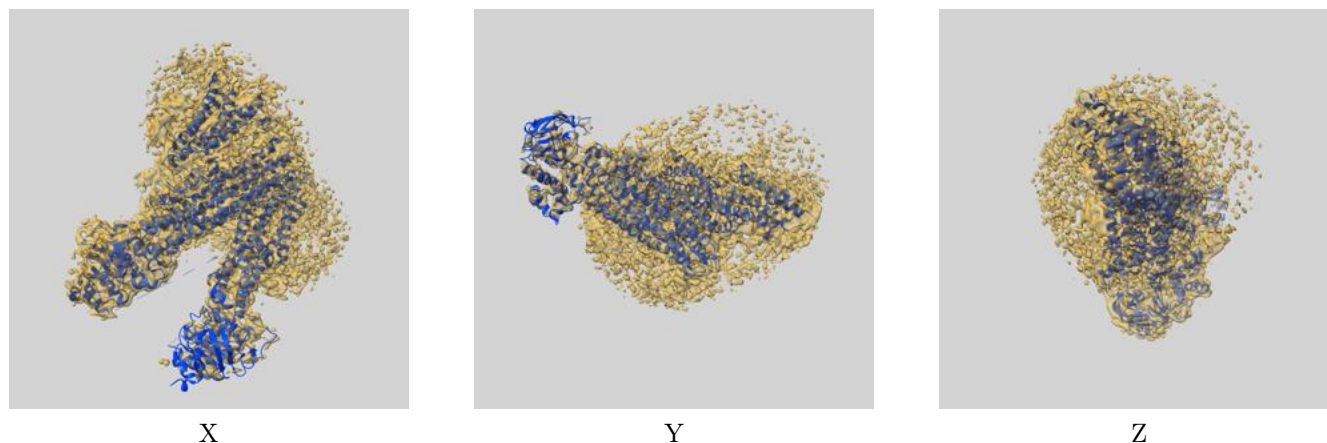
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	3.64	4.09	3.69
Unmasked-calculated*	4.11	6.83	4.14

\*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 4.11 differs from the reported value 3.64 by more than 10 %

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

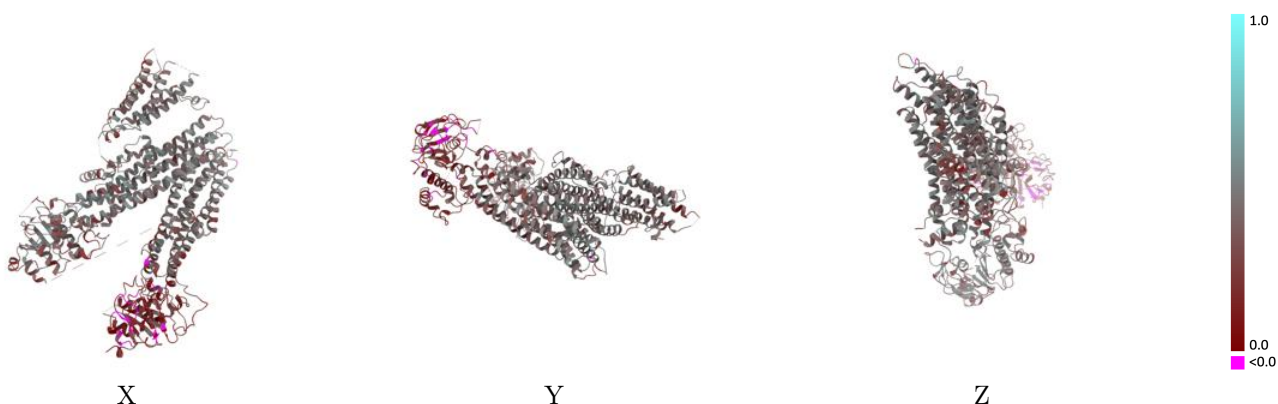
This section contains information regarding the fit between EMDB map EMD-63056 and PDB model 9LG7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



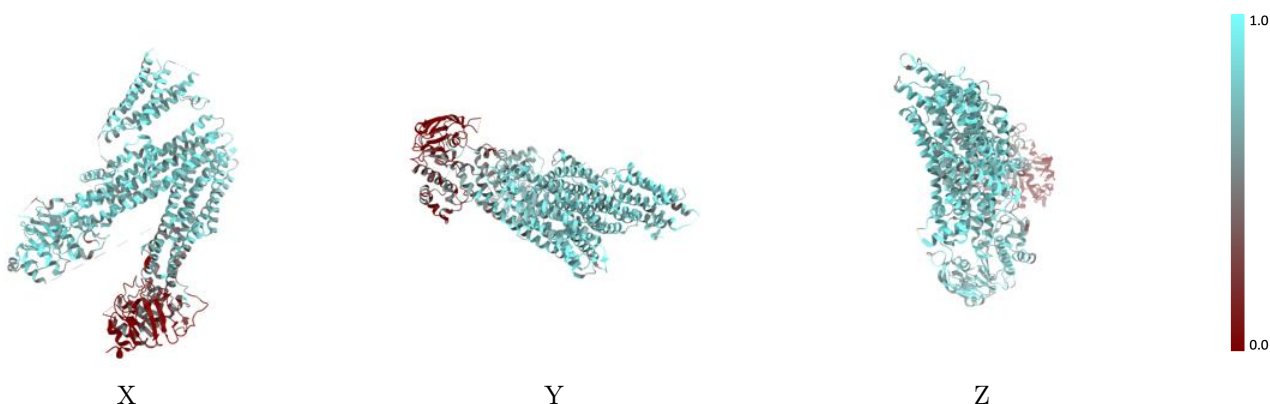
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



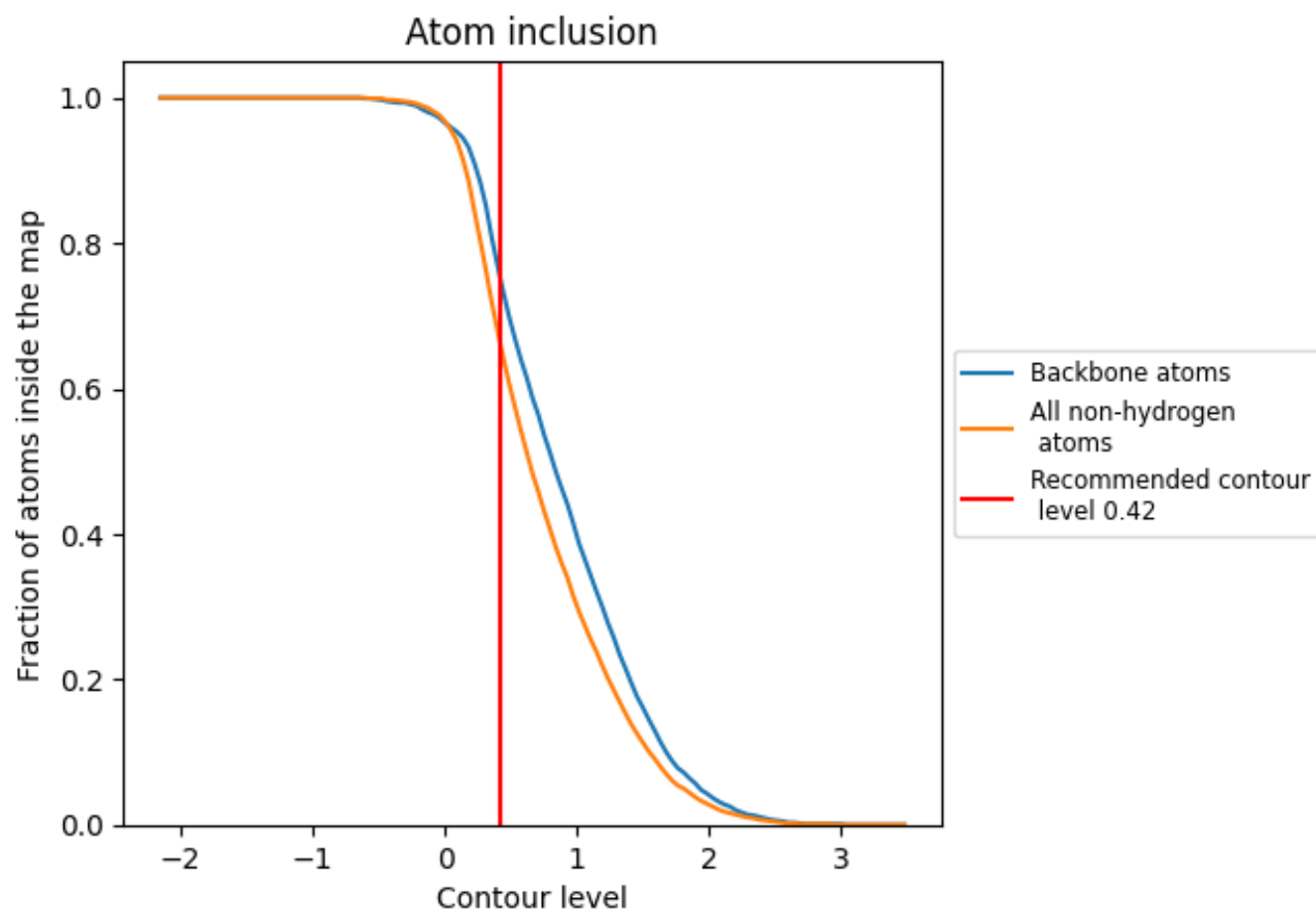
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.42).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 66% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6630	<div></div> 0.3630
A	<div></div> 0.6630	<div></div> 0.3630

