



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 09:19 PM UTC

PDB ID : 9JN2 / pdb\_00009jn2  
EMDB ID : EMD-61619  
Title : Multidrug resistance-associated protein 2 in complex with AMP-PNP in active state  
Authors : Chen, D.D.; Zhao, P.  
Deposited on : 2024-09-22  
Resolution : 3.44 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.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

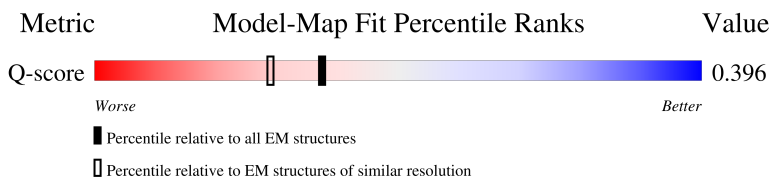
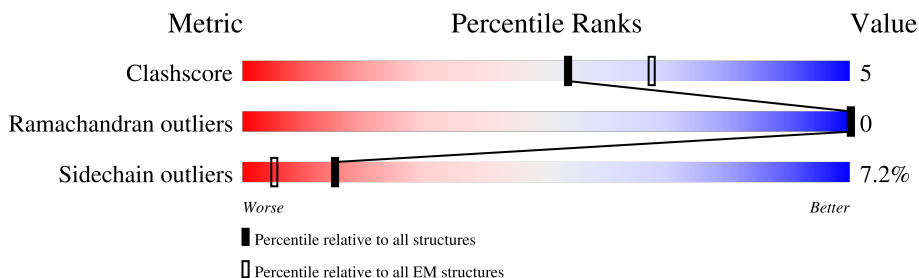
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.44 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	13877 ( 2.94 - 3.94 )

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	1545	<div> <div>24%</div> <div>75%</div> <div>14%</div> <div>9%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11156 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.

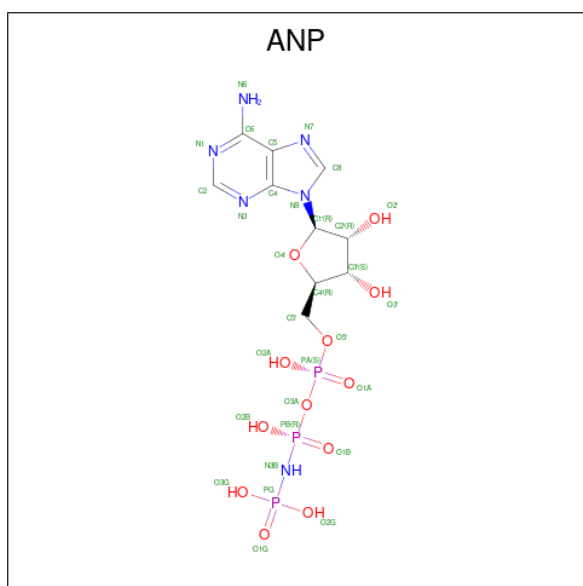
- Molecule 1 is a protein called ATP-binding cassette sub-family C member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1400	Total	C	N	O	S	0	0
			11123	7219	1842	2005	57		

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Mg	0
			2	2	

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

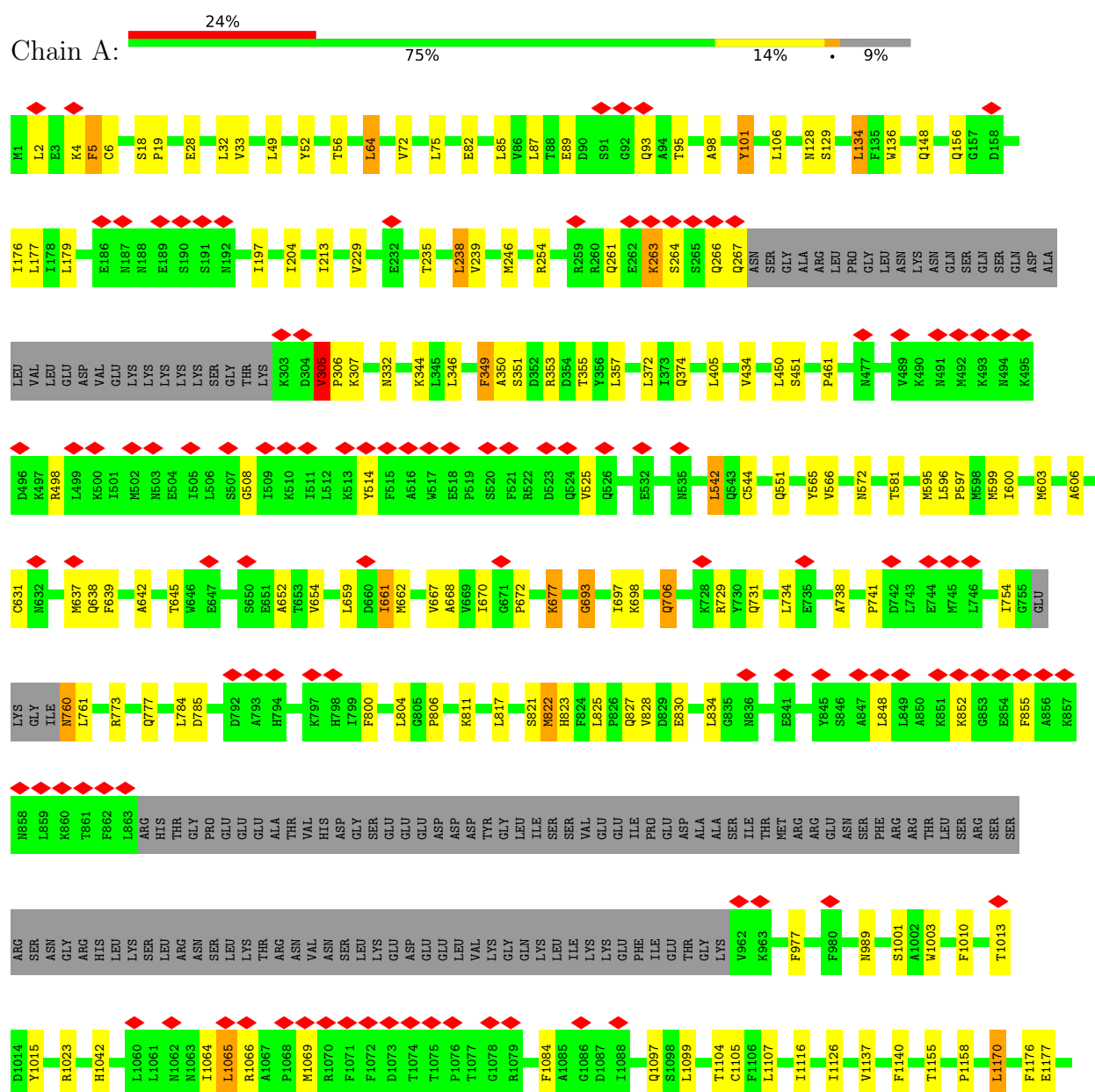


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-binding cassette sub-family C member 2



PHE	H1485	G1425	I1365	Y1305	L1207
	C1486	L1426	A1366	Q1306	R1210
	T1487	S1427	S1367	V1307	L1211
	V1488	H1428	I1368	R1308	F1221
	I1489	E1429	G1369	Y1309	L1224
	T1490	V1430	L1370	R1310	M1225
	I1491	T1431	H1371	P1311	M1226
	A1492	E1432	D1372	E1312	V1227
	H1493	A1433	L1373	L1313	
	R1494	G1434	R1374	D1314	L1233
	L1495	G1435	E1375	L1315	D1236
	H1496	N1436	K1376	V1316	F1240
	T1497	L1437	L1377	L1317	V1241
	I1498	S1438	T1378	R1318	L1242
	M1499	I1439	I1379	G1319	T1251
	D1500	G1440	I1380	I1320	
	S1501	Q1441	P1381	T1321	L1255
	D1502	R1442	Q1382	C1322	V1256
	K1503	Q1443	D1383	D1323	R1257
	V1504	L1444	P1384	I1324	
	M1505	L1445	I1385	G1325	E1270
	V1506	G1446	L1386	S1326	R1271
	L1507	L1447	F1387	M1327	
	D1508	G1448	S1388	E1328	E1274
	M1509	R1449	G1389	K1329	Y1275
	G1510	A1450	S1390	I1330	T1276
	K1511	L1451	L1391	G1331	K1277
	I1512	L1452	R1392	V1332	V1278
	I1513	R1453	M1393	V1333	E1279
	E1514	K1454	M1394	G1334	M1280
	C1515	S1455	L1395	R1335	E1281
	G1516	K1456	D1396	A1282	P1283
	S1517	I1457	P1397	T1336	W1284
	P1518	L1458	F1398	G1337	V1285
	E1519	V1459	M1399	G1338	T1286
	E1520	L1460	N1400	G1339	D1287
	L1521	D1461	Y1401	K1340	K1288
	L1522	E1462		S1341	R1289
	Q1523	A1463		L1343	P1291
	I1524	T1464		T1344	P1292
	P1525	A1465		N1345	D1293
	G1526	A1466		C1346	W1294
	P1527	V1467		L1347	P1295
	F1528	D1468		F1348	S1296
	Y1529	L1469		R1349	K1297
	F1530	E1470		I1350	G1298
	M1531	T1471		L1351	K1299
	A1532	D1472		E1352	I1300
	K1533	N1473		A1353	Q1301
	E1534	L1474		A1354	F1302
	A1535	I1475		G1355	N1303
	G1536	Q1476		K1416	A1304
	I1537	T1477		S1417	
	GLU	T1478		F1418	
	ASN	I1479		V1419	
	VAL	Q1480		A1420	
	ASN	N1481		S1421	
	SER	THR		L1422	
	LYS	E1482		G1362	
		F1483		V1363	
		A1484		D1364	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111169	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.354	Depositor
Minimum map value	-0.957	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	256.80002, 256.80002, 256.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MG

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	0.92	0/11358	1.26	16/15400 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1010	PHE	CB-CA-C	-7.48	98.59	111.45
1	A	351	SER	N-CA-C	-6.76	105.16	113.41
1	A	1176	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	693	GLY	CA-C-O	-6.53	117.72	122.23
1	A	106	LEU	N-CA-C	-5.87	104.88	111.28
1	A	349	PHE	N-CA-C	-5.77	102.92	110.53
1	A	1491	ILE	CA-C-O	-5.73	117.65	122.63
1	A	305	VAL	N-CA-C	-5.45	101.79	107.84
1	A	1069	MET	N-CA-C	-5.43	105.47	111.71
1	A	75	LEU	N-CA-C	-5.41	105.38	111.28
1	A	461	PRO	CB-CA-C	-5.40	104.18	111.85
1	A	72	VAL	N-CA-C	-5.23	104.52	111.05
1	A	1176	PHE	CB-CA-C	-5.12	101.89	110.19
1	A	134	LEU	N-CA-C	-5.08	107.75	114.31
1	A	101	TYR	CB-CA-C	-5.05	102.30	110.79
1	A	1240	PHE	CB-CA-C	5.03	119.41	110.85

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11123	0	11383	116	0
2	A	2	0	0	0	0
3	A	31	0	13	1	0
All	All	11156	0	11396	117	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 5.

All (117) 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:434:VAL:HG21	1:A:606:ALA:HB2	1.57	0.85
1:A:1305:TYR:HA	1:A:1355:GLY:HA3	1.69	0.74
1:A:544:CYS:HB3	1:A:1042:HIS:HB3	1.71	0.72
1:A:637:MET:HE3	1:A:661:ILE:HG13	1.71	0.71
1:A:254:ARG:HG3	1:A:306:PRO:HG3	1.73	0.70
1:A:645:THR:HB	1:A:652:ALA:HA	1.77	0.66
1:A:1333:VAL:HG22	1:A:1498:ILE:HG13	1.79	0.65
1:A:706:GLN:HG2	1:A:785:ASP:OD2	1.98	0.64
1:A:1335:ARG:HB2	1:A:1493:HIS:HB2	1.81	0.61
1:A:754:ILE:HA	1:A:760:ASN:HD21	1.64	0.61
1:A:852:LYS:HA	1:A:855:PHE:HB3	1.84	0.60
1:A:1295:PRO:HA	1:A:1457:ILE:HD11	1.85	0.58
1:A:1295:PRO:HD3	1:A:1376:LYS:HD2	1.84	0.58
1:A:1360:ILE:HG12	1:A:1368:ILE:HD11	1.85	0.57
1:A:1284:TRP:HB3	1:A:1371:HIS:CG	2.40	0.56
1:A:1291:PRO:HD3	1:A:1360:ILE:HG21	1.87	0.56
1:A:263:LYS:O	1:A:267:GLN:HG3	2.07	0.55
1:A:1329:LYS:HB2	1:A:1502:ASP:H	1.72	0.54
1:A:1411:GLU:HB2	1:A:1416:LYS:HD2	1.90	0.54
1:A:1308:ARG:HB3	1:A:1315:LEU:HA	1.90	0.53
1:A:1064:ILE:HG13	1:A:1084:PHE:HE2	1.74	0.53
1:A:1462:GLU:HG2	1:A:1492:ALA:HA	1.90	0.53
1:A:1305:TYR:HB3	1:A:1320:ILE:HB	1.90	0.53
1:A:264:SER:HA	1:A:267:GLN:CD	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518:PRO:HA	1:A:1521:LEU:HD12	1.92	0.52
1:A:1406:ILE:HG12	1:A:1452:LEU:HD21	1.92	0.52
1:A:1409:ALA:HA	1:A:1412:LEU:HD12	1.92	0.51
1:A:1333:VAL:H	1:A:1506:VAL:HG22	1.76	0.51
1:A:344:LYS:HB2	1:A:581:THR:HG21	1.93	0.51
1:A:1299:LYS:HA	1:A:1324:ILE:HG22	1.93	0.51
1:A:1359:ILE:HG13	1:A:1360:ILE:HG13	1.92	0.50
1:A:2:LEU:HB3	1:A:5:PHE:HB3	1.92	0.50
1:A:1317:LEU:HD23	1:A:1510:GLY:HA2	1.94	0.50
1:A:1451:LEU:HD22	1:A:1482:GLU:HG3	1.93	0.50
1:A:93:GLN:HG3	1:A:95:THR:H	1.77	0.50
1:A:596:LEU:N	1:A:597:PRO:HD2	2.27	0.50
1:A:667:VAL:HG22	1:A:830:GLU:HB3	1.93	0.49
1:A:595:MET:HB3	1:A:599:MET:HE2	1.93	0.49
1:A:773:ARG:O	1:A:777:GLN:HG2	2.11	0.49
1:A:264:SER:O	1:A:267:GLN:HB2	2.12	0.48
1:A:28:GLU:HA	1:A:32:LEU:HD12	1.94	0.48
1:A:566:VAL:HG21	1:A:1003:TRP:HZ2	1.78	0.48
1:A:18:SER:HB3	1:A:19:PRO:HD2	1.96	0.48
1:A:806:PRO:O	1:A:811:LYS:HB3	2.13	0.48
1:A:305:VAL:HG22	1:A:306:PRO:HD2	1.94	0.47
1:A:1358:ILE:HG23	1:A:1362:GLY:HA3	1.96	0.47
1:A:668:ALA:HB2	1:A:828:VAL:HG21	1.96	0.47
1:A:332:ASN:HD22	1:A:374:GLN:HG3	1.79	0.47
1:A:822:MET:HA	1:A:825:LEU:HG	1.96	0.47
1:A:1116:ILE:HG12	1:A:1241:VAL:HG13	1.97	0.47
1:A:235:THR:O	1:A:239:VAL:HG23	2.15	0.46
1:A:1306:GLN:HB3	1:A:1315:LEU:HD22	1.98	0.46
1:A:349:PHE:O	1:A:350:ALA:HB3	2.16	0.46
1:A:637:MET:HG2	1:A:697:ILE:HG22	1.98	0.46
1:A:1294:TRP:N	1:A:1295:PRO:HD2	2.31	0.46
1:A:1514:GLU:HB3	1:A:1521:LEU:HD13	1.97	0.46
1:A:405:LEU:HD23	1:A:1170:LEU:HD11	1.98	0.46
1:A:631:CYS:HA	1:A:698:LYS:HG3	1.97	0.46
1:A:1105:CYS:HB2	1:A:1255:LEU:HD13	1.98	0.45
1:A:213:ILE:CG2	1:A:1140:PHE:HB3	2.47	0.45
1:A:1137:VAL:HG12	1:A:1207:LEU:HD12	1.99	0.45
1:A:266:GLN:O	1:A:267:GLN:C	2.59	0.45
1:A:372:LEU:HD23	1:A:372:LEU:HA	1.81	0.45
1:A:677:LYS:H	1:A:677:LYS:HG3	1.49	0.45
1:A:1226:MET:HA	1:A:1233:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:CD2	1:A:98:ALA:HB3	2.52	0.44
1:A:98:ALA:HA	1:A:101:TYR:HD1	1.82	0.44
1:A:542:LEU:HD12	1:A:542:LEU:HA	1.70	0.44
1:A:136:TRP:HB2	1:A:179:LEU:HD13	1.99	0.44
1:A:305:VAL:O	1:A:307:LYS:HG2	2.18	0.44
1:A:1378:THR:HB	1:A:1457:ILE:O	2.17	0.44
1:A:661:ILE:CG2	1:A:667:VAL:HG21	2.48	0.44
1:A:800:PHE:CD1	1:A:804:LEU:HB2	2.52	0.44
1:A:1305:TYR:HD2	1:A:1355:GLY:HA3	1.83	0.44
1:A:1294:TRP:HA	1:A:1297:LYS:HG2	2.01	0.43
1:A:1371:HIS:C	1:A:1373:LEU:H	2.25	0.43
1:A:1211:LEU:HD23	1:A:1211:LEU:HA	1.83	0.43
1:A:514:TYR:HD2	1:A:1379:ILE:HG21	1.84	0.43
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.87	0.43
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.67	0.43
3:A:1602:ANP:H8	3:A:1602:ANP:O1A	2.18	0.43
1:A:1064:ILE:HD13	1:A:1064:ILE:HA	1.94	0.42
1:A:238:LEU:HA	1:A:238:LEU:HD12	1.72	0.42
1:A:1242:LEU:HD13	1:A:1242:LEU:HA	1.84	0.42
1:A:1065:LEU:HD13	1:A:1065:LEU:HA	1.88	0.42
1:A:1415:LEU:HA	1:A:1415:LEU:HD22	1.81	0.42
1:A:508:GLY:HA3	1:A:1387:PHE:HE1	1.84	0.42
1:A:672:PRO:HD2	1:A:834:LEU:O	2.20	0.42
1:A:1224:LEU:HD12	1:A:1224:LEU:HA	1.92	0.42
1:A:1226:MET:HE3	1:A:1241:VAL:HG11	2.02	0.42
1:A:642:ALA:HA	1:A:693:GLY:HA3	2.00	0.42
1:A:1348:PHE:HD1	1:A:1374:ARG:HG2	1.84	0.42
1:A:49:LEU:HD23	1:A:52:TYR:HD2	1.84	0.42
1:A:1003:TRP:HA	1:A:1023:ARG:HD3	2.02	0.42
1:A:85:LEU:O	1:A:89:GLU:HG3	2.20	0.41
1:A:661:ILE:HG22	1:A:667:VAL:HG21	2.02	0.41
1:A:1107:LEU:HD23	1:A:1107:LEU:HA	1.92	0.41
1:A:1155:THR:O	1:A:1158:PRO:HD2	2.20	0.41
1:A:1302:PHE:HB2	1:A:1322:CYS:H	1.85	0.41
1:A:738:ALA:O	1:A:741:PRO:HD2	2.20	0.41
1:A:1348:PHE:HB3	1:A:1374:ARG:HE	1.85	0.41
1:A:1371:HIS:C	1:A:1373:LEU:N	2.77	0.41
1:A:1430:VAL:HG12	1:A:1434:GLY:HA2	2.01	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.85	0.41
1:A:566:VAL:HG21	1:A:1003:TRP:CZ2	2.55	0.41
1:A:1099:LEU:HD23	1:A:1099:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1395:LEU:HD23	1:A:1449:ARG:HG2	2.02	0.41
1:A:1519:GLU:H	1:A:1519:GLU:HG3	1.54	0.41
1:A:450:LEU:HD23	1:A:450:LEU:HA	1.95	0.41
1:A:498:ARG:HG3	1:A:525:VAL:HG13	2.03	0.41
1:A:565:TYR:CZ	1:A:572:ASN:HB3	2.56	0.41
1:A:821:SER:HB3	1:A:823:HIS:CD2	2.56	0.41
1:A:1347:LEU:O	1:A:1373:LEU:HD21	2.21	0.41
1:A:1221:PHE:O	1:A:1225:MET:HG2	2.21	0.41
1:A:1504:VAL:HG23	1:A:1518:PRO:HD3	2.03	0.40
1:A:1155:THR:C	1:A:1158:PRO:HD2	2.46	0.40
1:A:639:PHE:HB2	1:A:659:LEU:H	1.85	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	1392/1545 (90%)	1378 (99%)	14 (1%)	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	1242/1372 (90%)	1153 (93%)	89 (7%)	13 39

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	PHE
1	A	6	CYS
1	A	33	VAL
1	A	56	THR
1	A	64	LEU
1	A	82	GLU
1	A	87	LEU
1	A	128	ASN
1	A	129	SER
1	A	134	LEU
1	A	148	GLN
1	A	156	GLN
1	A	176	ILE
1	A	197	ILE
1	A	204	ILE
1	A	229	VAL
1	A	238	LEU
1	A	246	MET
1	A	261	GLN
1	A	263	LYS
1	A	305	VAL
1	A	346	LEU
1	A	353	ARG
1	A	355	THR
1	A	451	SER
1	A	542	LEU
1	A	551	GLN
1	A	600	ILE
1	A	603	MET
1	A	638	GLN
1	A	654	VAL
1	A	661	ILE
1	A	662	MET
1	A	670	ILE
1	A	677	LYS
1	A	706	GLN
1	A	729	ARG

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Mol	Chain	Res	Type
1	A	731	GLN
1	A	734	LEU
1	A	760	ASN
1	A	761	LEU
1	A	784	LEU
1	A	817	LEU
1	A	822	MET
1	A	827	GLN
1	A	848	LEU
1	A	977	PHE
1	A	989	ASN
1	A	1001	SER
1	A	1013	THR
1	A	1015	TYR
1	A	1065	LEU
1	A	1066	ARG
1	A	1097	GLN
1	A	1104	THR
1	A	1126	ILE
1	A	1170	LEU
1	A	1177	GLU
1	A	1210	ARG
1	A	1227	VAL
1	A	1236	ASP
1	A	1242	LEU
1	A	1251	THR
1	A	1257	ARG
1	A	1274	GLU
1	A	1279	GLU
1	A	1285	VAL
1	A	1294	TRP
1	A	1300	ILE
1	A	1305	TYR
1	A	1312	GLU
1	A	1315	LEU
1	A	1316	VAL
1	A	1318	ARG
1	A	1324	ILE
1	A	1336	THR
1	A	1358	ILE
1	A	1365	ILE
1	A	1367	SER

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	1373	LEU
1	A	1379	ILE
1	A	1415	LEU
1	A	1452	LEU
1	A	1470	GLU
1	A	1482	GLU
1	A	1493	HIS
1	A	1512	ILE
1	A	1519	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	146	GLN
1	A	156	GLN
1	A	245	HIS
1	A	261	GLN
1	A	332	ASN
1	A	341	GLN
1	A	447	GLN
1	A	551	GLN
1	A	577	GLN
1	A	629	HIS
1	A	638	GLN
1	A	658	ASN
1	A	690	ASN
1	A	706	GLN
1	A	711	GLN
1	A	731	GLN
1	A	823	HIS
1	A	827	GLN
1	A	1054	ASN
1	A	1057	HIS
1	A	1062	ASN
1	A	1193	ASN
1	A	1301	GLN
1	A	1414	HIS
1	A	1436	ASN
1	A	1443	GLN
1	A	1496	HIS

### 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 ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	ANP	A	1602	-	33,33,33	1.11	5 (15%)	45,52,52	0.87	3 (6%)

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	ANP	A	1602	-	-	8/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1602	ANP	PG-O1G	3.32	1.51	1.46
3	A	1602	ANP	PB-O1B	3.05	1.50	1.46
3	A	1602	ANP	PB-O2B	-2.29	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1602	ANP	PG-O3G	-2.14	1.51	1.56
3	A	1602	ANP	PG-O2G	-2.08	1.51	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1602	ANP	O2B-PB-O1B	4.01	118.47	109.87
3	A	1602	ANP	O2G-PG-O1G	-2.02	108.37	113.45
3	A	1602	ANP	O3G-PG-O1G	-2.01	108.41	113.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1602	ANP	PB-N3B-PG-O1G
3	A	1602	ANP	PA-O3A-PB-O1B
3	A	1602	ANP	PA-O3A-PB-O2B
3	A	1602	ANP	C5'-O5'-PA-O1A
3	A	1602	ANP	C3'-C4'-C5'-O5'
3	A	1602	ANP	O4'-C4'-C5'-O5'
3	A	1602	ANP	PG-N3B-PB-O3A
3	A	1602	ANP	C4'-C5'-O5'-PA

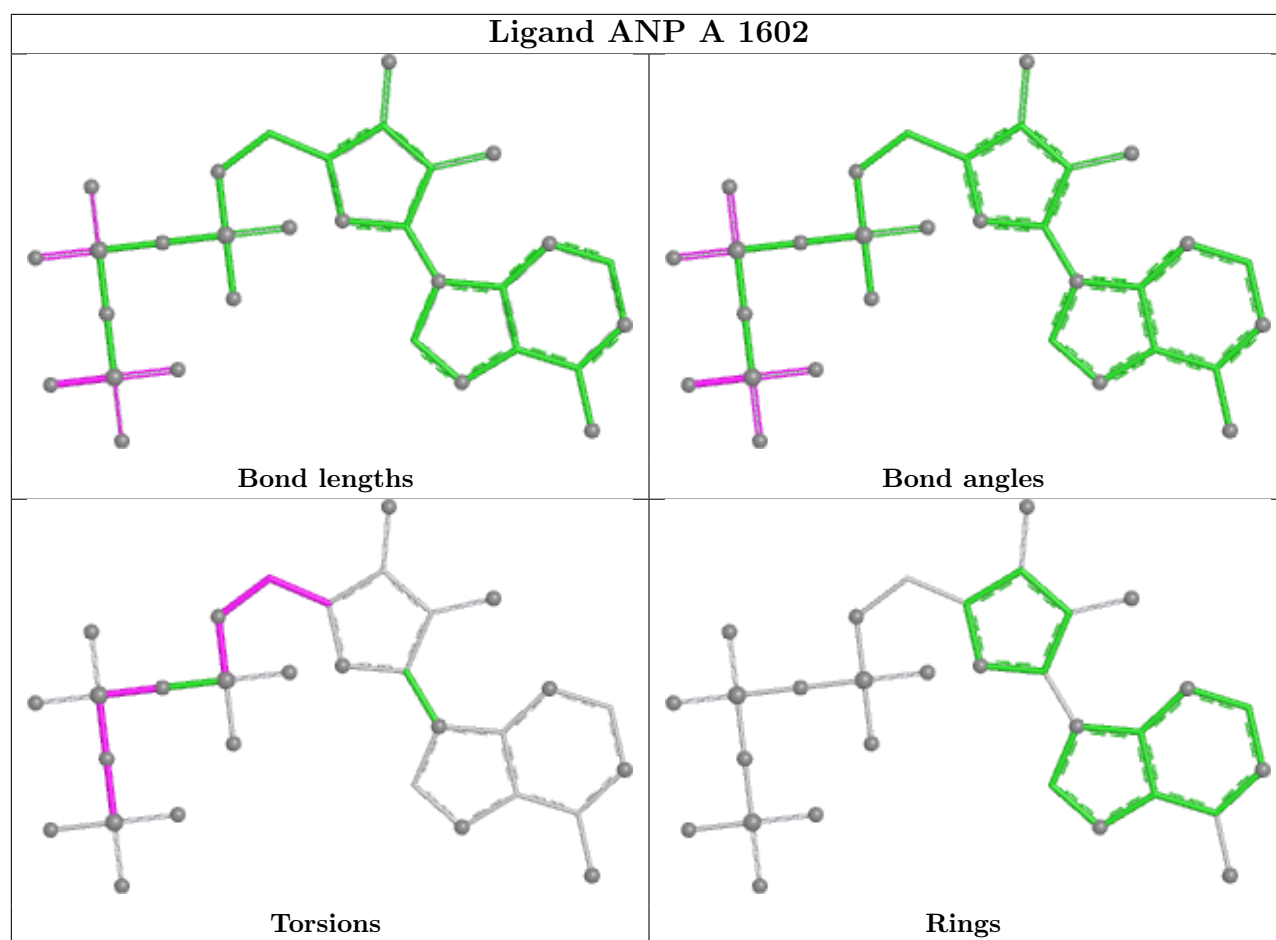
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

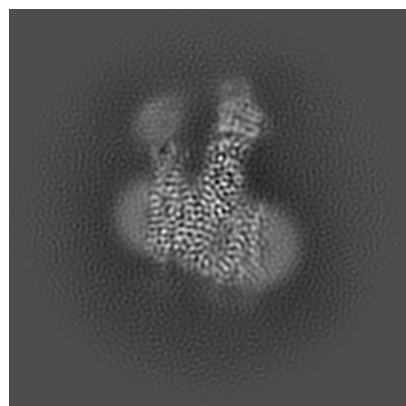
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61619. These allow visual inspection of the internal detail of the map and identification of artifacts.

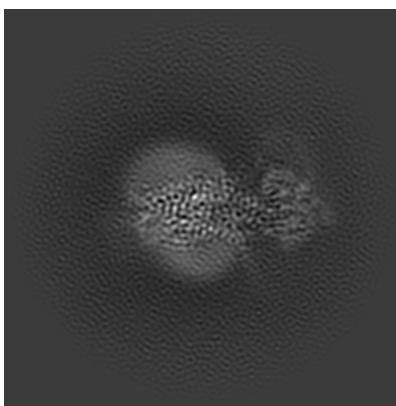
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

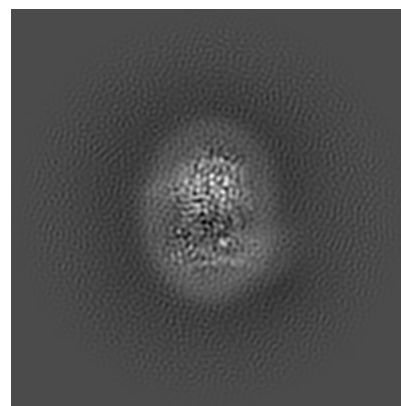
#### 6.1.1 Primary map



X

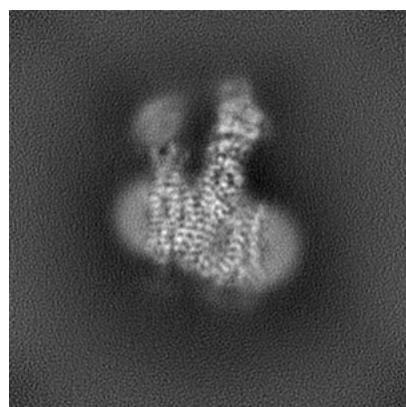


Y

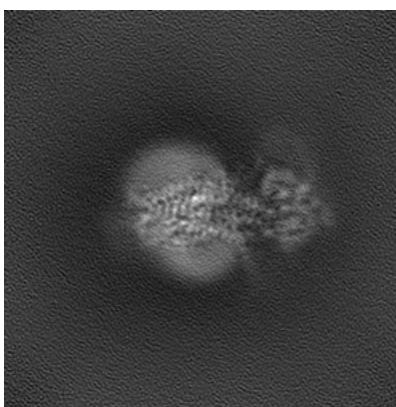


Z

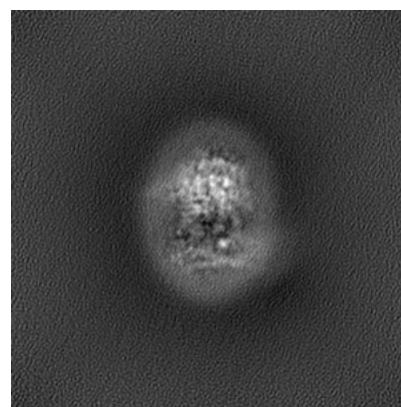
#### 6.1.2 Raw map



X



Y

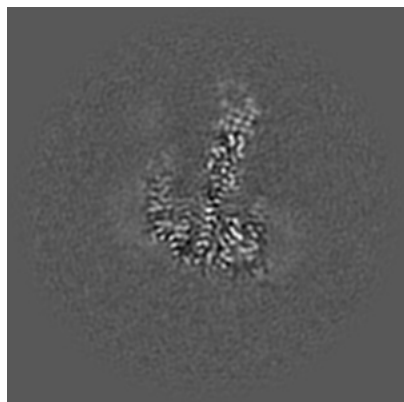


Z

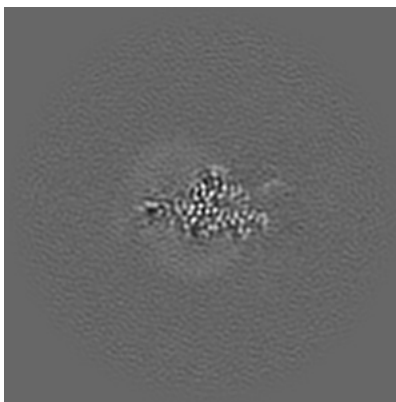
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

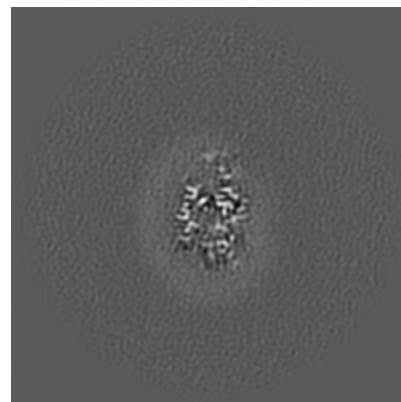
### 6.2.1 Primary map



X Index: 120

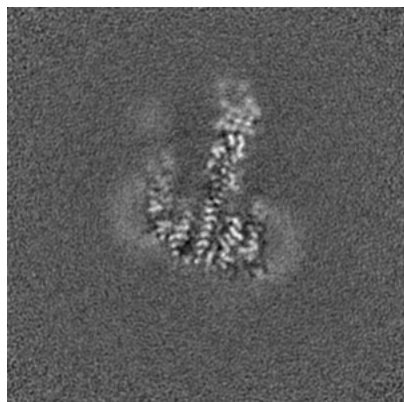


Y Index: 120

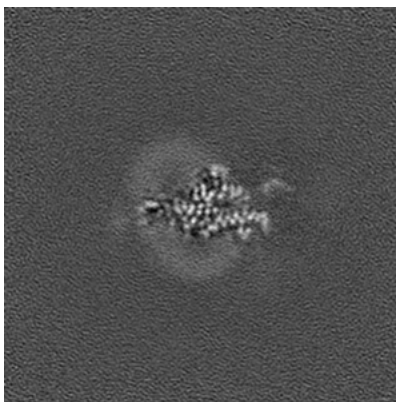


Z Index: 120

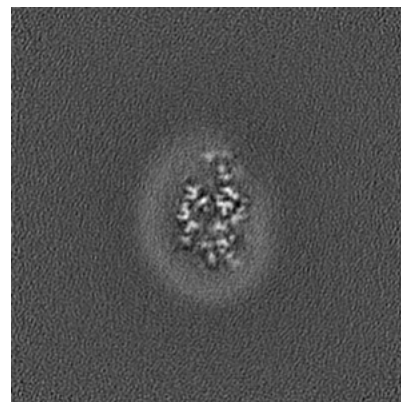
### 6.2.2 Raw map



X Index: 120



Y Index: 120

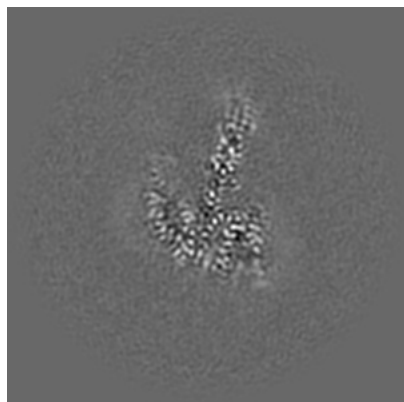


Z Index: 120

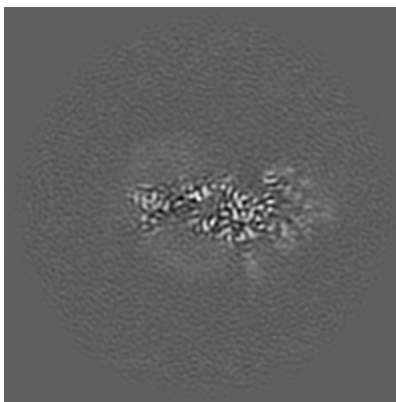
The images above show central slices of the map in three orthogonal directions.

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

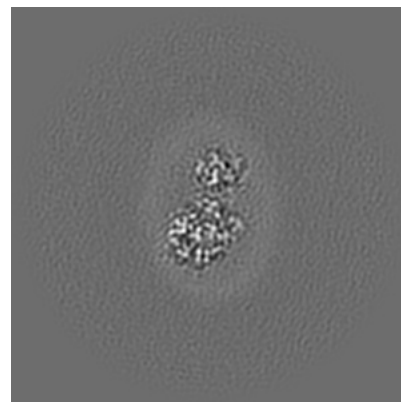
### 6.3.1 Primary map



X Index: 122

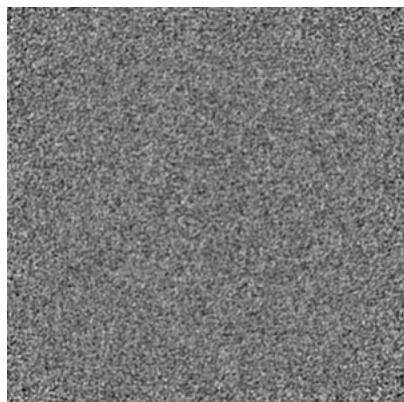


Y Index: 130

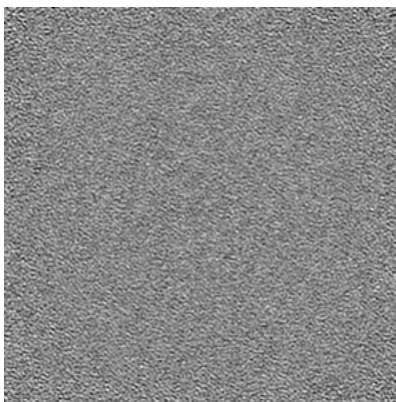


Z Index: 107

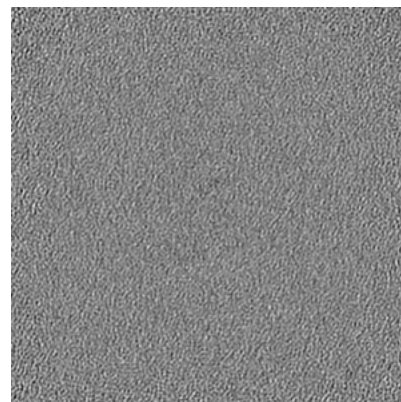
### 6.3.2 Raw map



X Index: 0



Y Index: 0



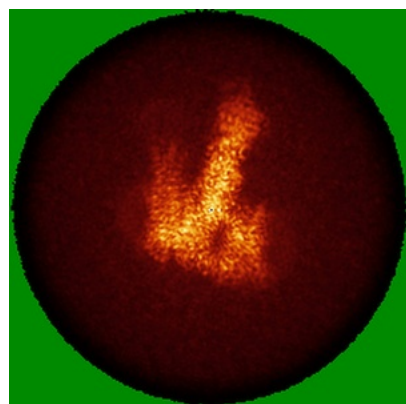
Z Index: 0

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

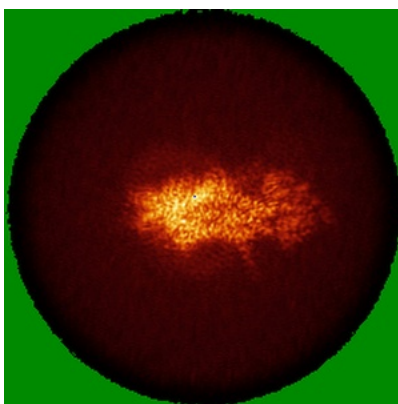


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

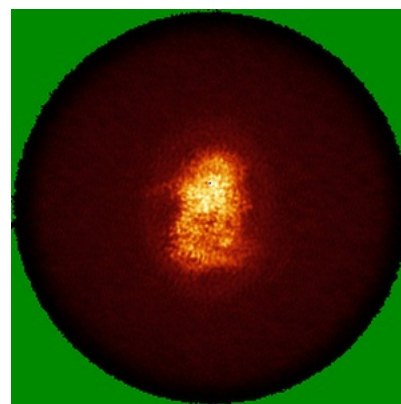
### 6.4.1 Primary map



X

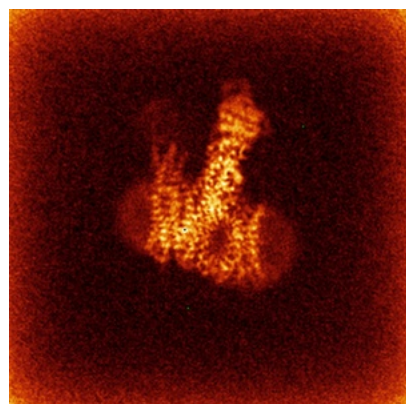


Y

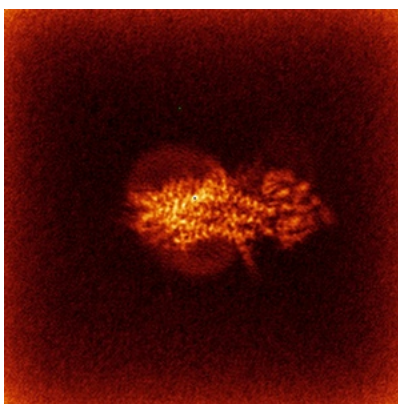


Z

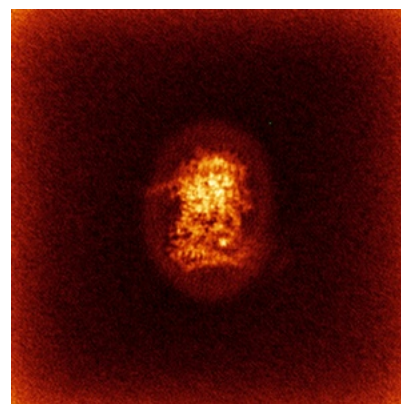
### 6.4.2 Raw map



X



Y

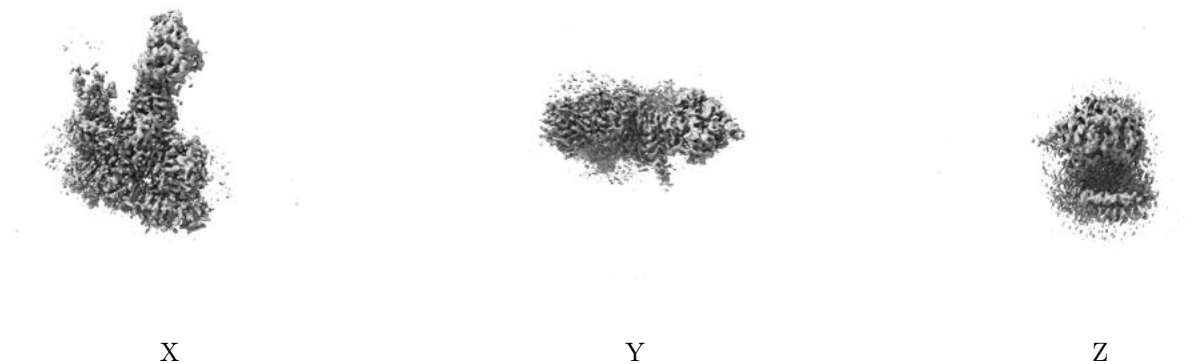


Z

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.

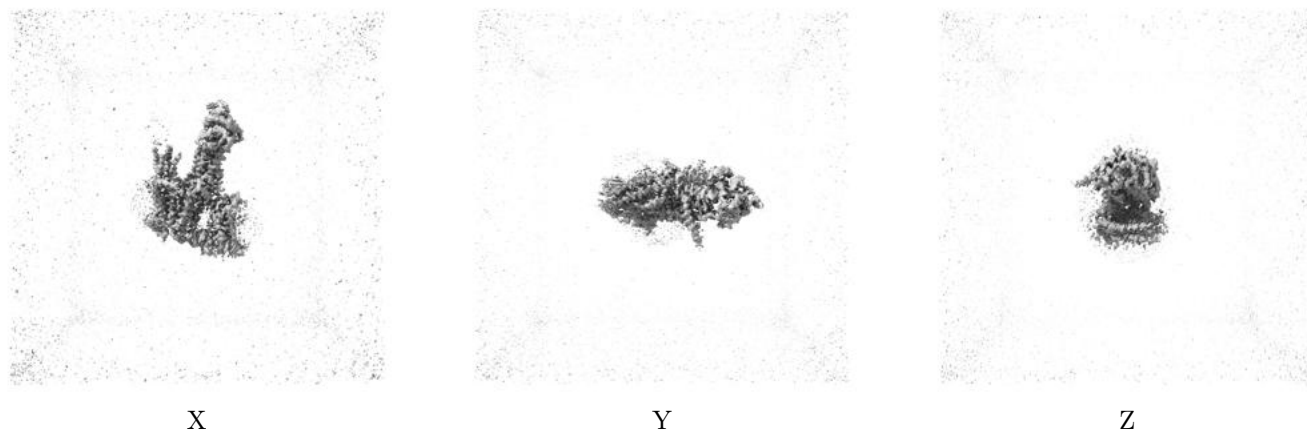
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. 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.

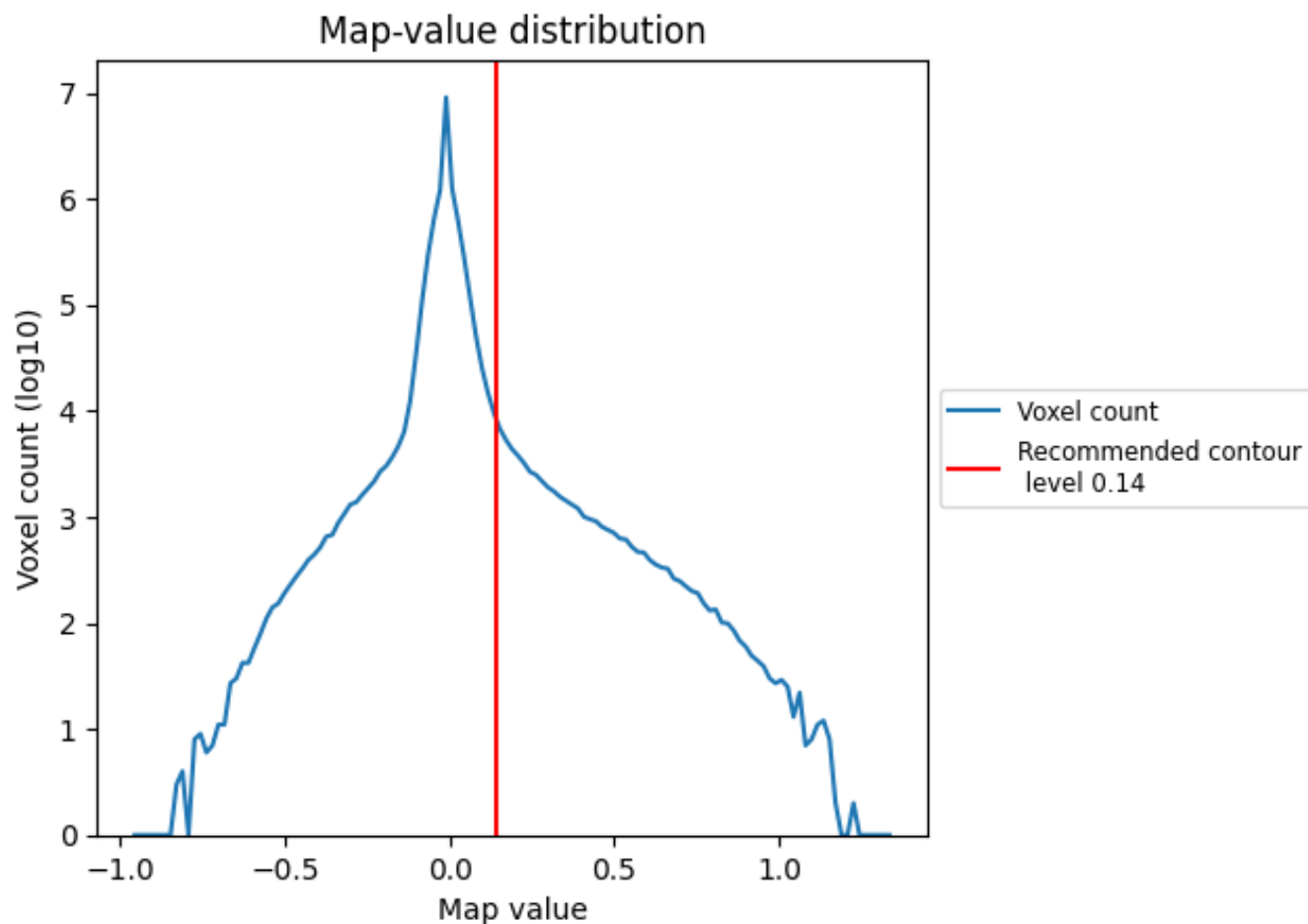
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

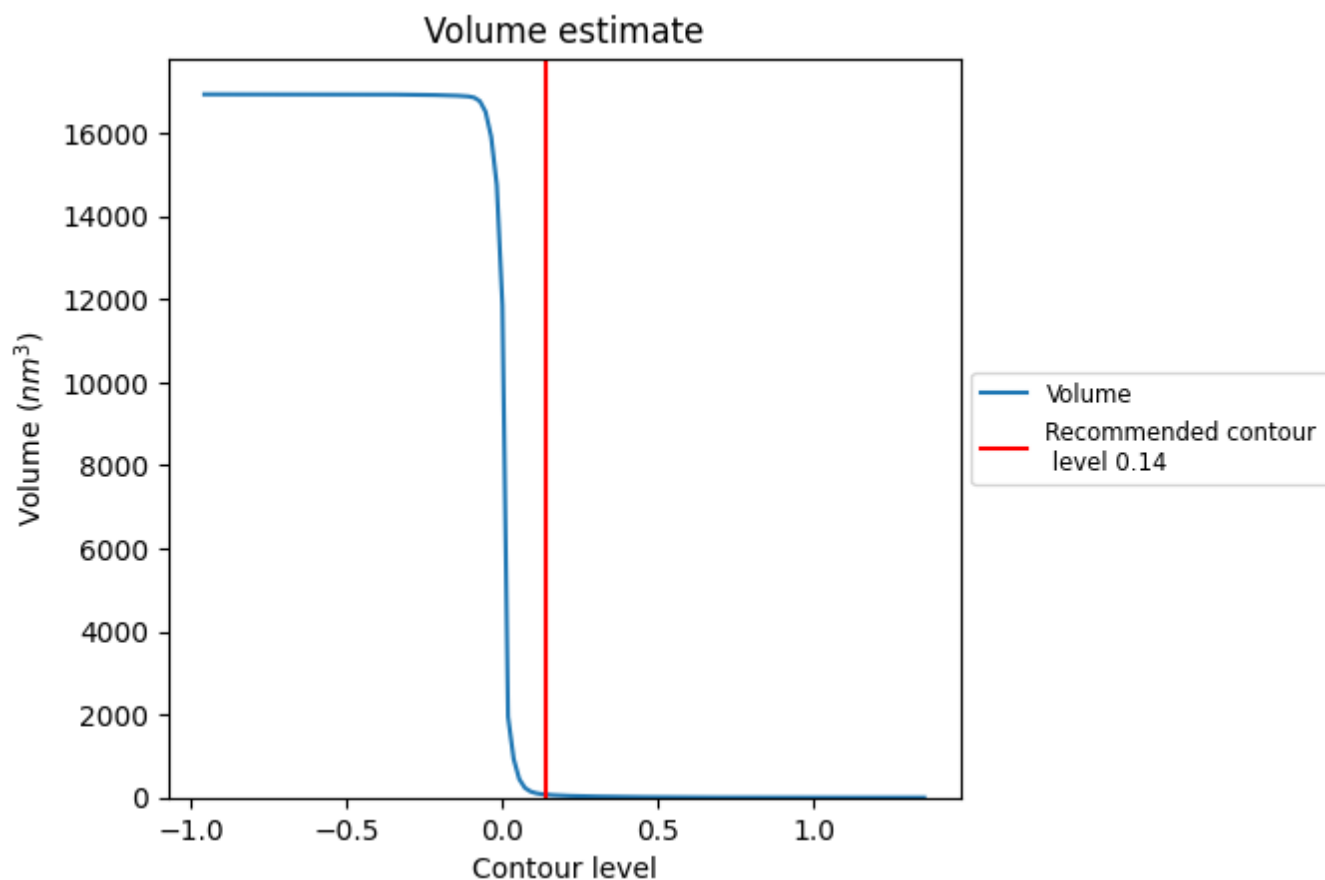
This section contains the results of statistical analysis of the map.

### 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](#)

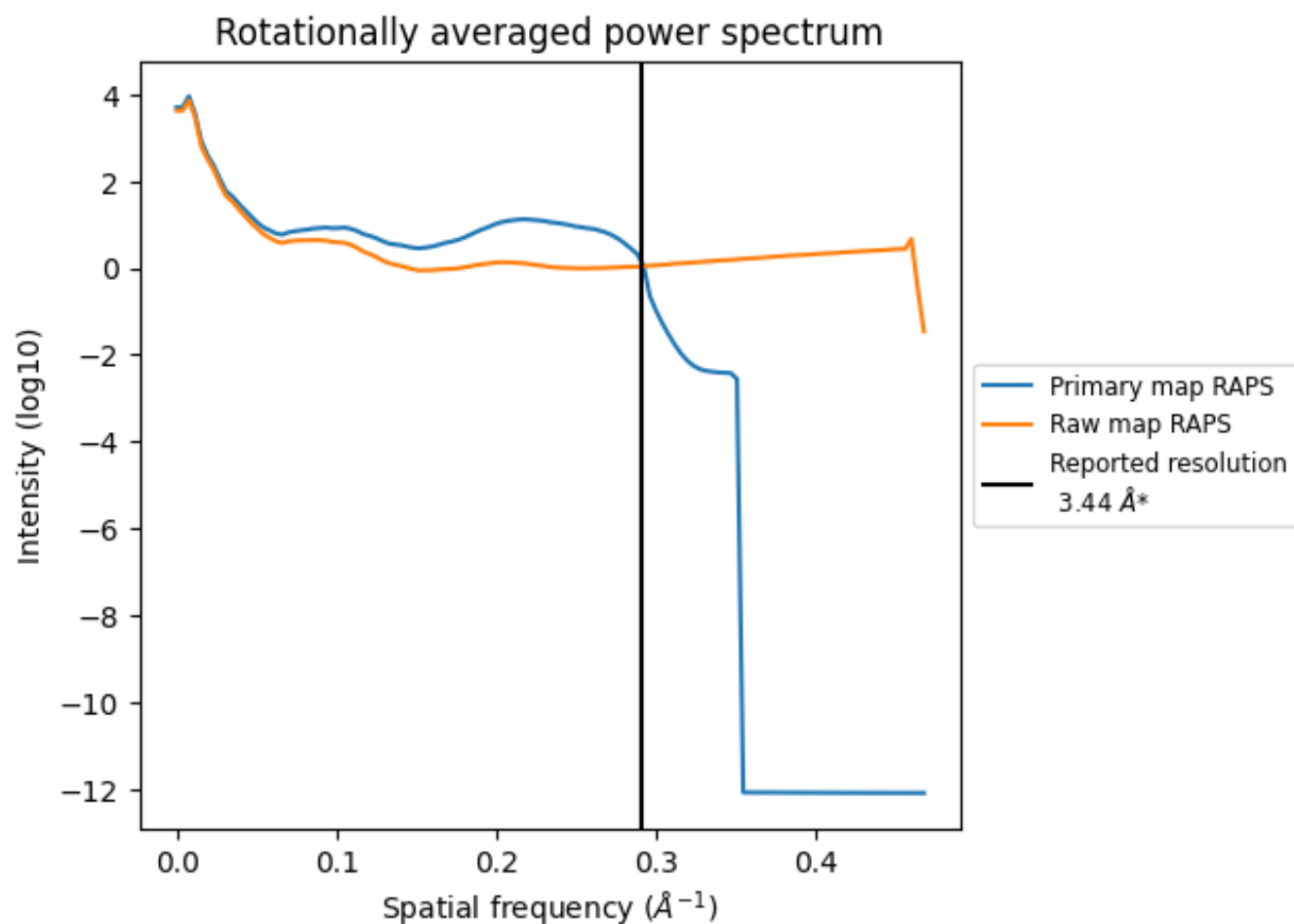


The volume at the recommended contour level is 71  $\text{nm}^3$ ; this corresponds to an approximate mass of 64 kDa.

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 ⓘ

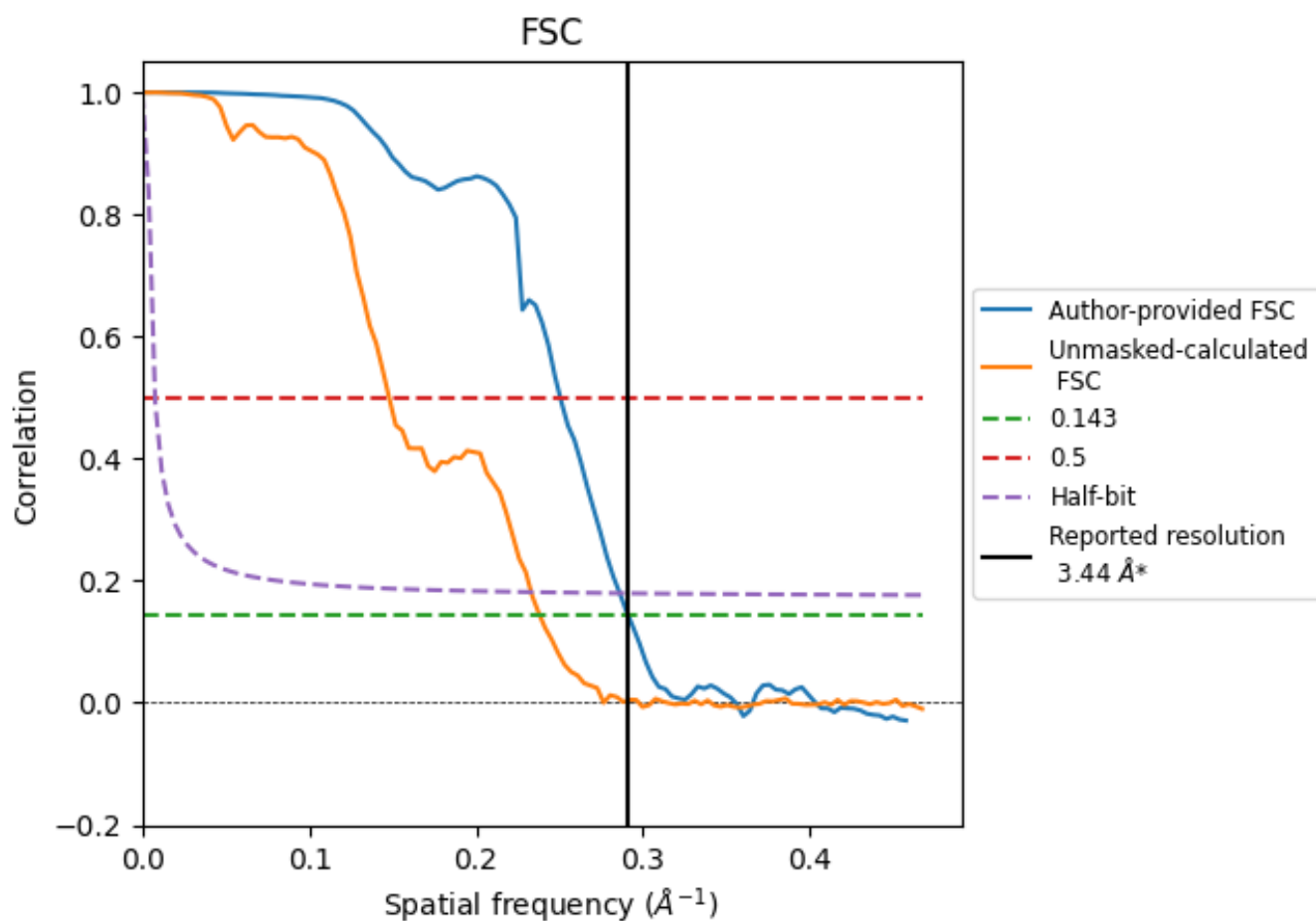


\*Reported resolution corresponds to spatial frequency of 0.291 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

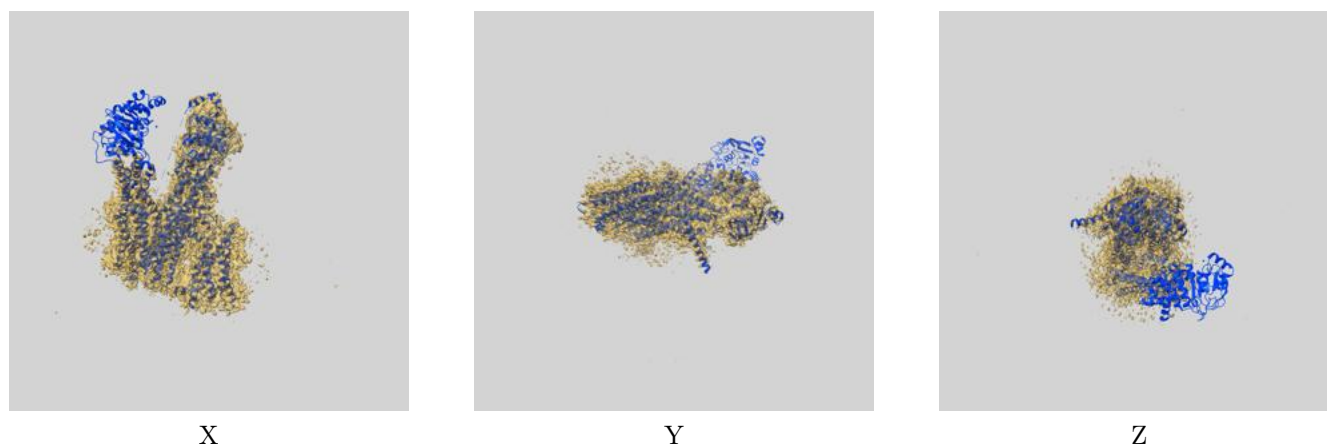
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.43	3.99	3.50
Unmasked-calculated*	4.20	6.76	4.29

\*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 4.20 differs from the reported value 3.44 by more than 10 %

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

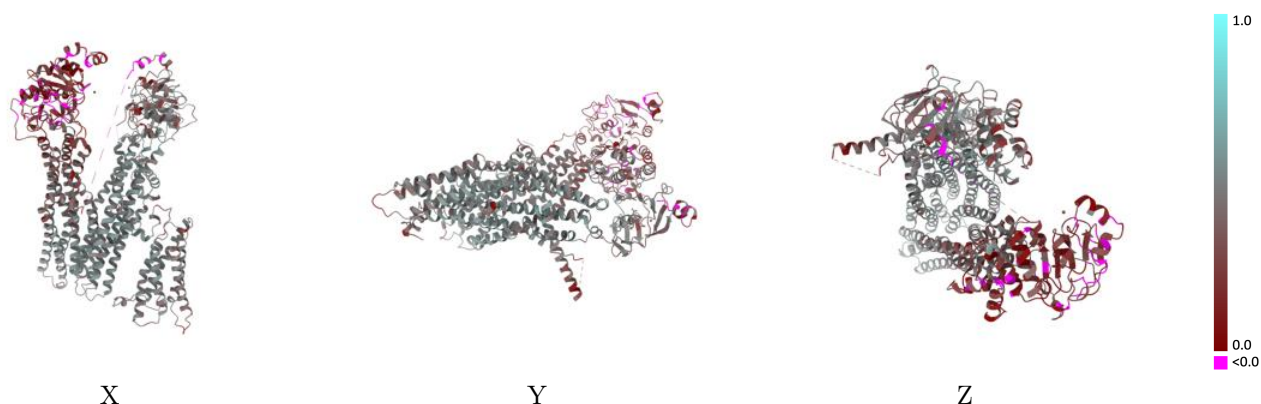
This section contains information regarding the fit between EMDB map EMD-61619 and PDB model 9JN2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



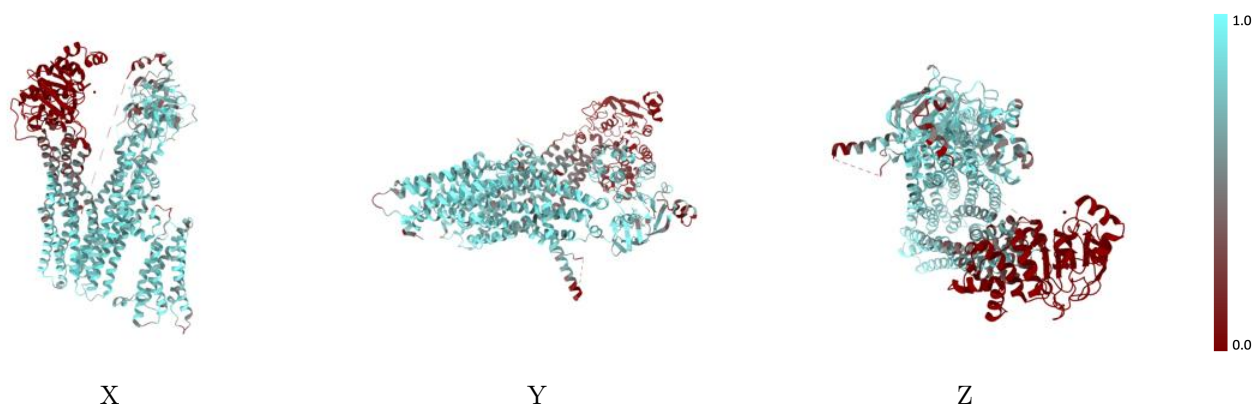
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



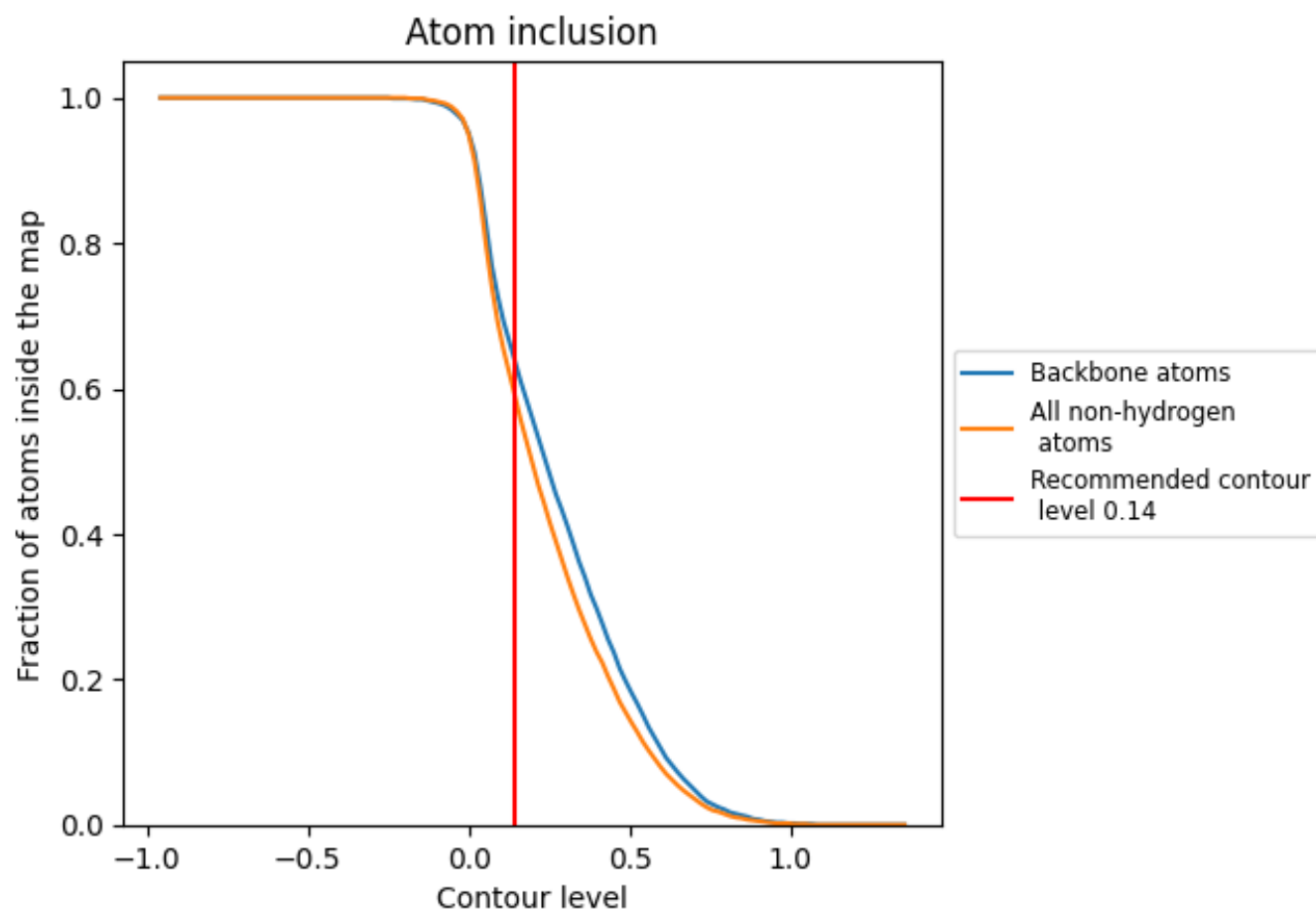
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 60% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5970	<div></div> 0.3960
A	<div></div> 0.5970	<div></div> 0.3960

