



Full wwPDB EM Validation Report ⓘ

Jul 8, 2024 – 06:06 PM EDT

PDB ID : 8GHA
EMDB ID : EMD-40029
Title : Hir3 Arm/Tail, Hir2 WD40, C-terminal Hpc2
Authors : Kim, H.J.; Murakami, K.
Deposited on : 2023-03-09
Resolution : 6.80 Å(reported)
Based on initial model : .

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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

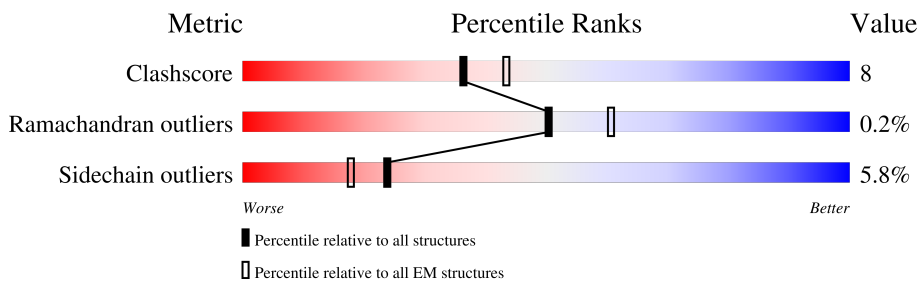
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	E	625	
2	D	1648	
3	B	875	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9783 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 Histone promoter control protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	126	1012	651	162	198	1	0	0

- Molecule 2 is a protein called Histone transcription regulator 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	705	5762	3724	946	1068	24	0	0

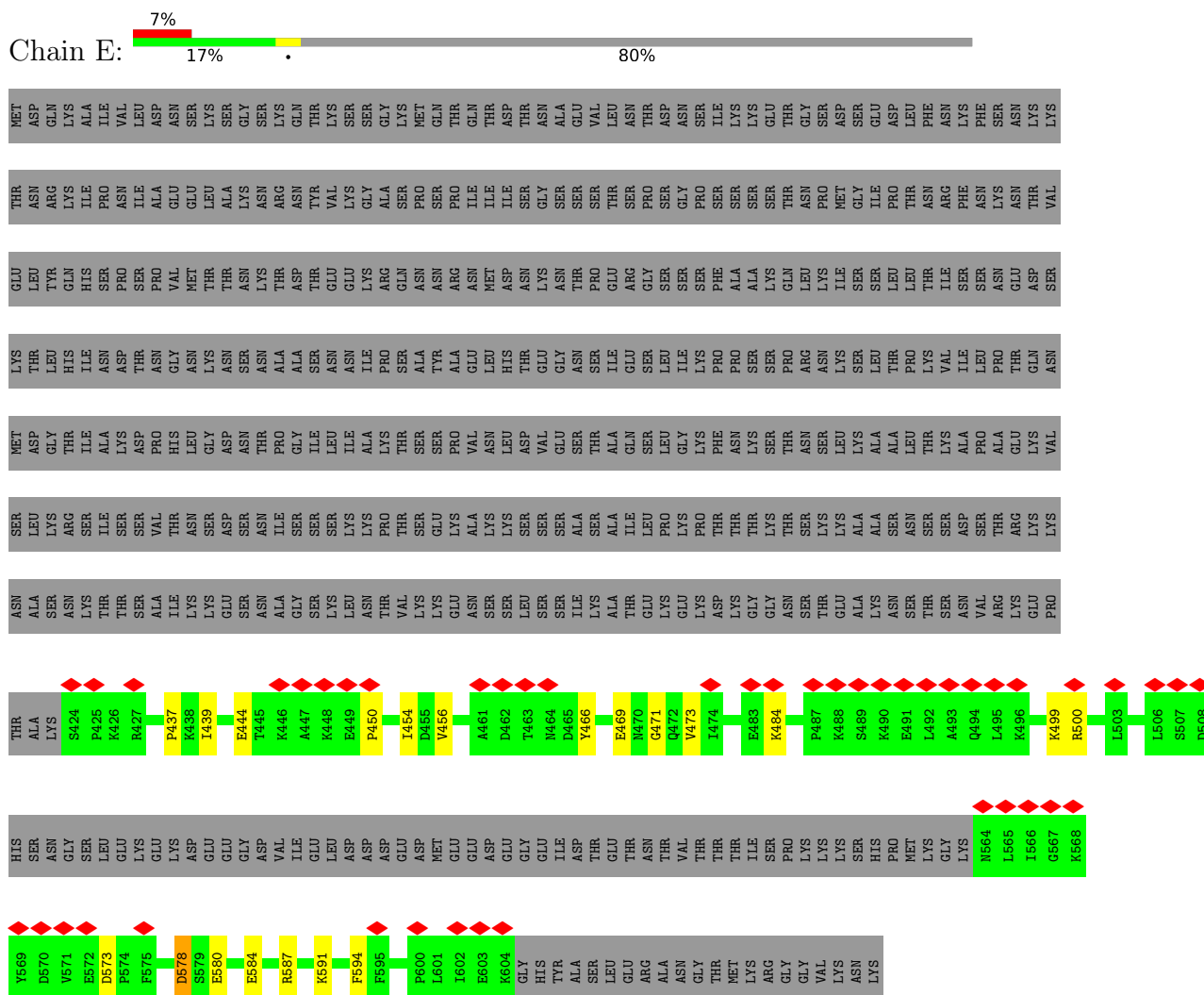
- Molecule 3 is a protein called Protein HIR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	381	3009	1921	505	570	13	0	0

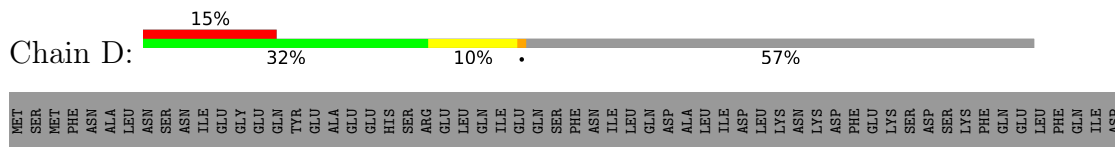
3 Residue-property plots

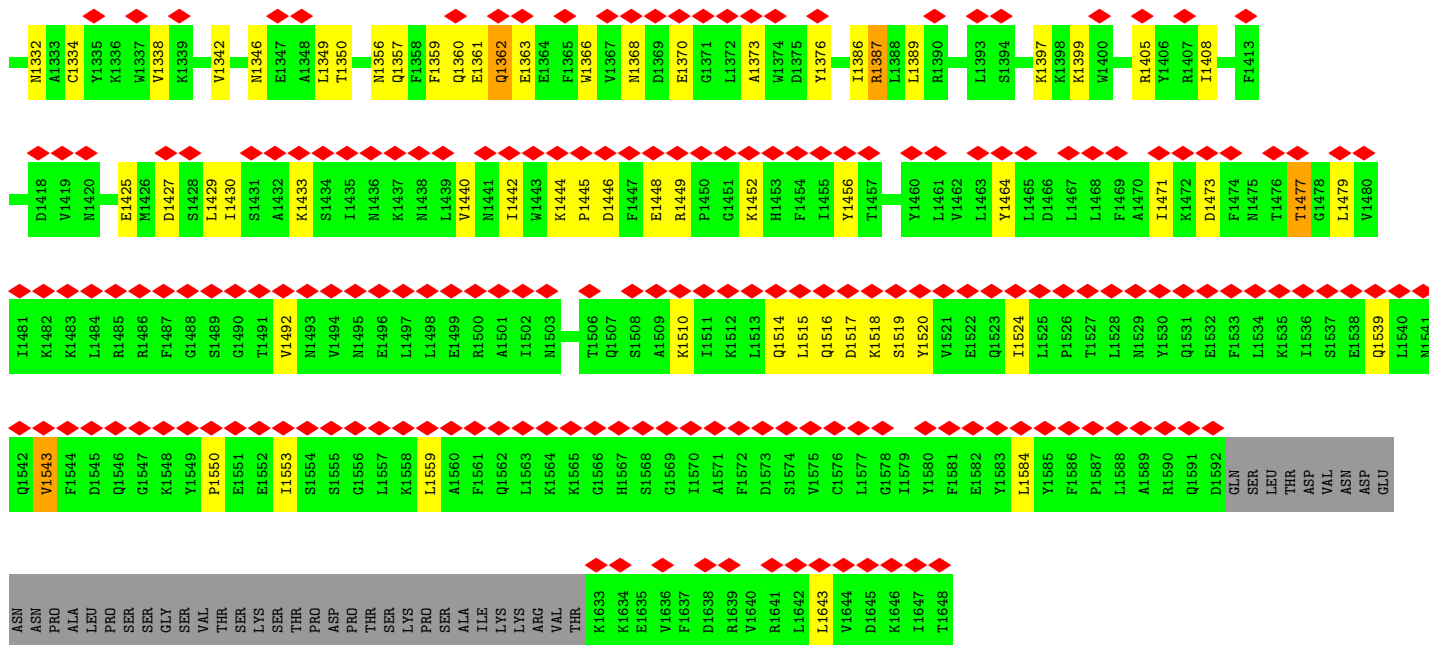
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Histone promoter control protein 2

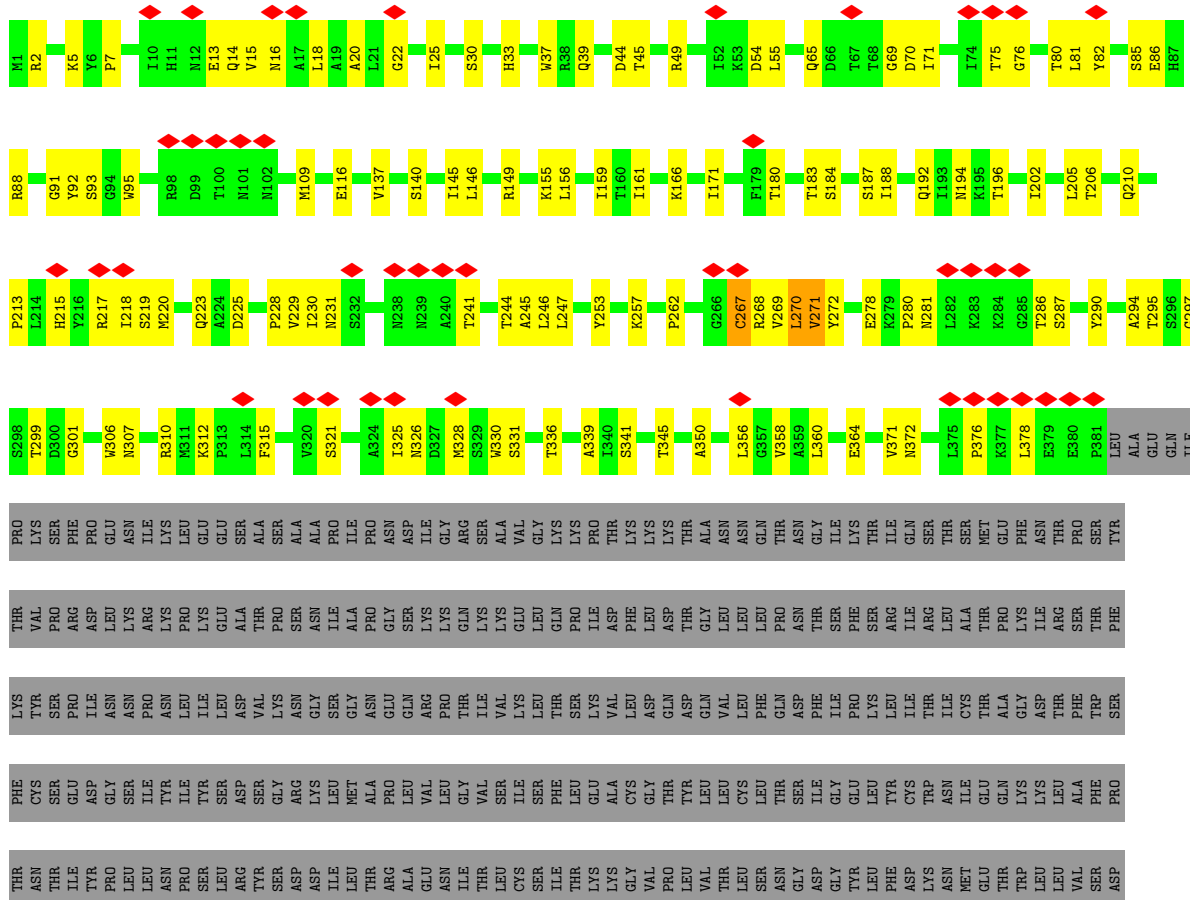
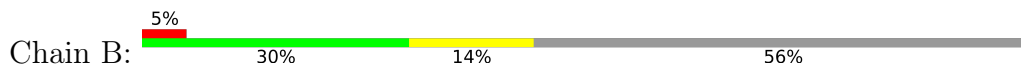


- Molecule 2: Histone transcription regulator 3





• Molecule 3: Protein HIR2



GLY TRP TRP
 ASN ARG ALA
 TYR GLY TYR
 SER GLN SER
 TYR TRP ASP
 THR THR THR
 ASN THR ASP

LEU ASN ARG
 LYS GLY MET
 TYR ILE MET
 ASN LYS ASP
 LEU TRP ASP
 ARG PHE ASP
 THR THR THR
 ILE TRP TYR
 LEU MET LYS
 SER GLY PHE
 ALA GLY ASN
 MET THR ASP
 SER GLU PHE
 ILE ASN VAL
 THR SER LEU
 SER HIS ASN
 LEU ILE ILE
 ASN GLU ASN
 GLY ASN ILE
 ILE VAL SER
 LEU ILE ILE
 ILE ILE ILE
 LYS ILE ARG
 ASP LEU ASP
 ASN GLU ASN
 ALA GLN SER
 PRO GLY ILE
 GLY ASP PHE
 ARG LYS ARG
 ASN LEU LEU
 LEU LYS LYS
 ILE ILE LEU
 ILE ILE ILE
 LEU LEU ILE
 ILE ILE ILE
 LEU ILE ILE
 ARG ARG GLN
 VAL VAL VAL
 THR ARG VAL
 THR THR THR
 ASP THR ASP
 ARG ILE ARG

ARG LEU SER
 LEU GLU MET
 TYR MET ASP
 ASP ARG LEU
 ASN ASP PHE
 VAL PHE GLN
 THR TRP LEU
 TYR TYR ASP
 ASP ASP LEU
 PRO LEU ILE
 SER ILE GLY
 THR THR GLY
 GLY ALA PHE
 ALA PHE ALA
 ASP ASP LYS
 LYS PHE LYS
 ARG ARG LYS
 ASN ASN LEU
 LEU LEU LYS
 LEU LYS LYS
 ILE ILE ILE
 LEU LEU ILE
 ILE ILE ILE
 LEU ILE ILE
 ILE ILE ILE
 LEU ILE ILE
 ARG ARG GLN
 VAL VAL VAL
 THR ARG VAL
 THR THR THR
 ASP THR ASP
 ARG ILE ARG

TYR
 ALA
 LYS
 GLU
 MET
 ASN
 ILE
 ILE
 SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	639629	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	217.6, 217.6, 217.6	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.27	0/1032	0.43	0/1397
2	D	0.29	0/5887	0.48	0/7948
3	B	0.30	0/3070	0.51	0/4168
All	All	0.29	0/9989	0.48	0/13513

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	E	1012	0	1019	15	0
2	D	5762	0	5786	90	0
3	B	3009	0	3053	69	0
All	All	9783	0	9858	165	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 8.

All (165) 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)
3:B:215:HIS:H	3:B:268:ARG:HH21	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1452:LYS:O	2:D:1456:TYR:HB2	1.97	0.64
3:B:71:ILE:HA	3:B:85:SER:HA	1.80	0.63
2:D:1182:LYS:NZ	2:D:1189:ASP:OD2	2.31	0.62
2:D:956:GLN:NE2	2:D:960:CYS:SG	2.71	0.61
2:D:1189:ASP:N	2:D:1189:ASP:OD1	2.31	0.61
2:D:1281:SER:O	2:D:1285:ASN:ND2	2.33	0.61
2:D:1539:GLN:O	2:D:1543:VAL:HB	2.01	0.60
3:B:95:TRP:HA	3:B:109:MET:HG2	1.83	0.60
3:B:267:CYS:HA	3:B:297:GLY:HA2	1.84	0.60
2:D:1362:GLN:OE1	2:D:1387:ARG:NH2	2.35	0.59
2:D:952:LEU:HA	2:D:955:LYS:HE2	1.85	0.59
3:B:65:GLN:NE2	3:B:69:GLY:O	2.35	0.59
2:D:1270:LYS:HD2	2:D:1278:LEU:HD21	1.85	0.58
3:B:271:VAL:HG23	3:B:294:ALA:HB3	1.86	0.58
2:D:1304:LYS:HG2	2:D:1308:GLN:HE22	1.69	0.58
1:E:499:LYS:NZ	1:E:573:ASP:O	2.37	0.58
2:D:940:LYS:O	2:D:944:GLN:NE2	2.37	0.57
3:B:187:SER:HA	3:B:206:THR:HA	1.85	0.57
3:B:217:ARG:HB3	3:B:269:VAL:HG13	1.84	0.57
3:B:280:PRO:HA	3:B:287:SER:HA	1.85	0.57
2:D:1430:ILE:HG12	2:D:1440:VAL:HG22	1.85	0.57
2:D:1356:ASN:HA	2:D:1359:PHE:HB2	1.86	0.57
3:B:192:GLN:NE2	3:B:376:PRO:O	2.33	0.57
3:B:44:ASP:HB3	3:B:49:ARG:HB2	1.87	0.56
1:E:473:VAL:HB	3:B:315:PHE:HB2	1.88	0.56
2:D:1110:ASP:N	2:D:1110:ASP:OD1	2.39	0.55
3:B:2:ARG:HB2	3:B:350:ALA:HB3	1.87	0.55
2:D:949:ASP:N	2:D:949:ASP:OD1	2.39	0.55
2:D:1114:ARG:HA	2:D:1117:LYS:HD2	1.89	0.55
2:D:928:ASP:OD1	2:D:928:ASP:N	2.40	0.55
2:D:1180:TYR:O	2:D:1185:ARG:NH2	2.39	0.55
2:D:960:CYS:HG	2:D:976:HIS:CD2	2.25	0.55
1:E:578:ASP:OD1	1:E:578:ASP:N	2.40	0.54
3:B:225:ASP:N	3:B:225:ASP:OD1	2.39	0.54
3:B:247:LEU:HD13	3:B:253:TYR:HB3	1.88	0.54
2:D:1059:THR:HA	2:D:1177:SER:HB2	1.89	0.54
2:D:1520:TYR:HA	2:D:1524:ILE:HD12	1.90	0.54
2:D:1188:ASP:N	2:D:1188:ASP:OD1	2.39	0.54
1:E:471:GLY:O	3:B:310:ARG:NH2	2.36	0.53
2:D:955:LYS:HA	2:D:966:ILE:HD12	1.90	0.53
1:E:500:ARG:NH1	2:D:1252:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:ILE:HA	1:E:454:ILE:HG12	1.92	0.52
3:B:45:THR:HG21	3:B:55:LEU:HD22	1.91	0.52
2:D:1269:ILE:O	2:D:1273:ASP:N	2.43	0.52
3:B:183:THR:HG1	3:B:187:SER:HG	1.55	0.51
2:D:969:ASP:N	2:D:969:ASP:OD1	2.43	0.51
3:B:5:LYS:HE3	3:B:345:THR:HG21	1.93	0.51
3:B:328:MET:HA	3:B:339:ALA:HA	1.91	0.51
2:D:939:GLU:OE1	2:D:961:ARG:NH1	2.41	0.51
2:D:1128:GLU:HA	2:D:1131:ILE:HD12	1.92	0.50
3:B:192:GLN:HB2	3:B:202:ILE:HD13	1.93	0.50
3:B:229:VAL:N	3:B:245:ALA:O	2.39	0.50
2:D:1188:ASP:HA	2:D:1191:LYS:HD2	1.93	0.50
2:D:1250:ASN:O	2:D:1254:SER:OG	2.30	0.50
1:E:587:ARG:HD3	2:D:1243:ILE:HG21	1.92	0.50
2:D:1357:GLN:O	2:D:1360:GLN:NE2	2.44	0.50
2:D:912:GLU:O	2:D:916:SER:OG	2.27	0.50
3:B:219:SER:H	3:B:270:LEU:HD23	1.76	0.50
2:D:1389:LEU:HD13	2:D:1408:ILE:HG13	1.92	0.50
2:D:1058:HIS:O	2:D:1063:ALA:N	2.44	0.50
3:B:228:PRO:HG3	3:B:272:TYR:HE1	1.76	0.50
3:B:229:VAL:HB	3:B:245:ALA:HB3	1.94	0.50
3:B:295:THR:OG1	3:B:306:TRP:NE1	2.36	0.49
3:B:16:ASN:HA	3:B:326:ASN:HD22	1.77	0.49
2:D:1087:SER:O	2:D:1091:SER:OG	2.27	0.49
2:D:1304:LYS:O	2:D:1308:GLN:NE2	2.45	0.49
3:B:15:VAL:O	3:B:326:ASN:ND2	2.45	0.49
2:D:1368:ASN:ND2	2:D:1370:GLU:OE2	2.46	0.49
2:D:1187:ILE:HG22	2:D:1191:LYS:HE3	1.95	0.49
3:B:325:ILE:HD13	3:B:341:SER:HB3	1.94	0.49
3:B:137:VAL:HB	3:B:146:LEU:HB2	1.94	0.48
3:B:7:PRO:HA	3:B:345:THR:HA	1.95	0.48
3:B:81:LEU:HB3	3:B:92:TYR:HB2	1.94	0.48
2:D:1127:PHE:HA	2:D:1130:TRP:HD1	1.78	0.48
3:B:326:ASN:N	3:B:326:ASN:OD1	2.46	0.48
2:D:1473:ASP:O	2:D:1477:THR:OG1	2.32	0.48
2:D:963:HIS:NE2	2:D:978:THR:O	2.37	0.47
2:D:1150:ASP:OD1	2:D:1150:ASP:N	2.42	0.47
2:D:1218:SER:HA	2:D:1244:THR:HA	1.96	0.47
2:D:1260:ASN:O	2:D:1264:SER:OG	2.28	0.47
3:B:278:GLU:N	3:B:358:VAL:O	2.46	0.47
2:D:1399:LYS:HA	2:D:1399:LYS:HD2	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:GLU:HA	1:E:450:PRO:HB3	1.96	0.46
3:B:149:ARG:HB2	3:B:156:LEU:HD21	1.97	0.46
2:D:968:SER:HB3	2:D:971:PHE:HB2	1.98	0.46
2:D:1444:LYS:HG3	2:D:1448:GLU:HB3	1.97	0.46
3:B:146:LEU:HD22	3:B:155:LYS:HE3	1.98	0.46
3:B:20:ALA:HA	3:B:25:ILE:HA	1.98	0.46
3:B:271:VAL:HB	3:B:330:TRP:CD1	2.50	0.46
2:D:1040:SER:O	2:D:1044:ASN:ND2	2.49	0.45
2:D:1363:GLU:HA	2:D:1366:TRP:CD1	2.51	0.45
1:E:594:PHE:HD1	3:B:262:PRO:HG3	1.80	0.45
2:D:946:ILE:HA	2:D:994:TYR:HE2	1.81	0.45
2:D:1143:ASP:HA	2:D:1147:TRP:HD1	1.81	0.45
3:B:223:GLN:O	3:B:372:ASN:ND2	2.47	0.45
3:B:281:ASN:N	3:B:286:THR:O	2.48	0.45
3:B:310:ARG:HH21	3:B:312:LYS:HB2	1.81	0.45
2:D:1198:ASP:O	2:D:1202:SER:OG	2.32	0.45
2:D:1247:SER:OG	2:D:1250:ASN:ND2	2.50	0.45
3:B:22:GLY:O	3:B:39:GLN:NE2	2.49	0.45
3:B:210:GLN:HB3	3:B:231:ASN:HB3	1.99	0.45
2:D:1405:ARG:NH1	2:D:1425:GLU:O	2.42	0.45
3:B:171:ILE:N	3:B:180:THR:O	2.46	0.45
2:D:1006:TYR:HE2	2:D:1132:LEU:HD21	1.82	0.45
3:B:215:HIS:O	3:B:268:ARG:NE	2.50	0.45
2:D:925:HIS:HA	2:D:976:HIS:HA	1.99	0.44
2:D:1298:ASN:O	2:D:1302:VAL:N	2.42	0.44
1:E:437:PRO:HB3	1:E:456:VAL:HG13	1.98	0.44
2:D:1248:ASP:HA	2:D:1251:ILE:HD12	1.99	0.44
3:B:80:THR:HA	3:B:93:SER:HA	2.00	0.44
2:D:960:CYS:SG	2:D:976:HIS:NE2	2.83	0.44
2:D:1072:ASN:N	2:D:1076:GLN:OE1	2.51	0.44
3:B:75:THR:OG1	3:B:76:GLY:N	2.51	0.44
3:B:360:LEU:HD13	3:B:364:GLU:HG2	2.00	0.44
2:D:959:TRP:NE1	2:D:973:PRO:HB3	2.33	0.44
3:B:37:TRP:HZ3	3:B:55:LEU:HG	1.83	0.44
3:B:230:ILE:HA	3:B:244:THR:HA	2.00	0.43
1:E:580:GLU:OE2	2:D:1250:ASN:ND2	2.51	0.43
3:B:13:GLU:OE2	3:B:33:HIS:ND1	2.51	0.43
3:B:301:GLY:HA3	3:B:321:SER:H	1.83	0.43
2:D:1159:ASP:OD1	2:D:1242:LYS:NZ	2.45	0.43
2:D:1427:ASP:OD1	2:D:1464:TYR:OH	2.34	0.43
3:B:194:ASN:ND2	3:B:196:THR:OG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1349:LEU:HD12	2:D:1368:ASN:HA	2.01	0.43
3:B:218:ILE:HG23	3:B:270:LEU:HD22	2.00	0.43
3:B:290:TYR:OH	3:B:356:LEU:O	2.27	0.43
2:D:1047:LEU:HA	2:D:1170:LEU:HD13	2.00	0.42
3:B:166:LYS:O	3:B:184:SER:N	2.51	0.42
1:E:466:TYR:OH	3:B:307:ASN:ND2	2.50	0.42
2:D:1074:GLU:H	2:D:1074:GLU:HG3	1.59	0.42
2:D:1028:PRO:HG2	2:D:1118:ASN:HB3	2.01	0.42
2:D:1373:ALA:HB3	2:D:1376:TYR:HD2	1.84	0.42
3:B:82:TYR:HA	3:B:91:GLY:HA2	2.01	0.42
3:B:331:SER:N	3:B:336:THR:O	2.45	0.42
2:D:1515:LEU:HD23	2:D:1515:LEU:HA	1.91	0.42
2:D:1550:PRO:HD2	2:D:1553:ILE:HD12	2.01	0.42
2:D:1299:CYS:HA	2:D:1302:VAL:HB	2.01	0.42
2:D:1517:ASP:HA	2:D:1520:TYR:CE2	2.55	0.41
2:D:948:ASN:HA	2:D:951:PHE:HB3	2.02	0.41
2:D:1035:ILE:HG23	2:D:1038:ARG:HH22	1.84	0.41
2:D:1148:THR:HG21	2:D:1151:LYS:HE3	2.01	0.41
2:D:1288:LYS:HA	2:D:1288:LYS:HD2	1.88	0.41
2:D:1334:CYS:O	2:D:1338:VAL:HB	2.20	0.41
2:D:1517:ASP:C	2:D:1519:SER:H	2.24	0.41
3:B:188:ILE:N	3:B:205:LEU:O	2.51	0.41
2:D:989:LEU:O	2:D:993:THR:OG1	2.32	0.41
2:D:942:LEU:HD22	2:D:950:SER:HB2	2.02	0.41
2:D:1038:ARG:HB2	3:B:213:PRO:HB2	2.03	0.41
2:D:1361:GLU:OE1	2:D:1387:ARG:NE	2.49	0.41
1:E:584:GLU:HG3	1:E:587:ARG:NH2	2.34	0.41
2:D:915:TRP:O	2:D:919:THR:OG1	2.31	0.41
3:B:88:ARG:HG2	3:B:116:GLU:HG3	2.03	0.41
2:D:956:GLN:HE22	2:D:959:TRP:HD1	1.69	0.41
2:D:1584:LEU:HD13	2:D:1643:LEU:HD13	2.03	0.41
1:E:439:ILE:HD12	1:E:484:LYS:HD2	2.03	0.40
1:E:469:GLU:HG2	3:B:310:ARG:HG2	2.03	0.40
3:B:14:GLN:H	3:B:30:SER:HB3	1.86	0.40
3:B:307:ASN:HB3	3:B:310:ARG:HB2	2.03	0.40
3:B:75:THR:HG23	3:B:82:TYR:HB2	2.02	0.40
2:D:1433:LYS:HA	2:D:1479:LEU:HD13	2.03	0.40
2:D:1510:LYS:O	2:D:1514:GLN:HA	2.22	0.40
3:B:145:ILE:HD12	3:B:159:ILE:HB	2.03	0.40
3:B:246:LEU:HD12	3:B:257:LYS:HB2	2.03	0.40
2:D:1346:ASN:O	2:D:1350:THR:OG1	2.29	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	E	122/625 (20%)	118 (97%)	4 (3%)	0	100	100
2	D	701/1648 (42%)	681 (97%)	18 (3%)	2 (0%)	41	77
3	B	379/875 (43%)	365 (96%)	14 (4%)	0	100	100
All	All	1202/3148 (38%)	1164 (97%)	36 (3%)	2 (0%)	50	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1518	LYS
2	D	1445	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	114/557 (20%)	112 (98%)	2 (2%)	59	77
2	D	642/1528 (42%)	594 (92%)	48 (8%)	13	38
3	B	343/790 (43%)	329 (96%)	14 (4%)	30	55
All	All	1099/2875 (38%)	1035 (94%)	64 (6%)	24	45

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	578	ASP
1	E	591	LYS
2	D	905	GLU
2	D	916	SER
2	D	918	HIS
2	D	927	CYS
2	D	936	ASP
2	D	944	GLN
2	D	949	ASP
2	D	969	ASP
2	D	976	HIS
2	D	981	VAL
2	D	998	LEU
2	D	1015	LYS
2	D	1016	GLN
2	D	1037	SER
2	D	1091	SER
2	D	1110	ASP
2	D	1119	ASP
2	D	1125	ASN
2	D	1148	THR
2	D	1186	THR
2	D	1188	ASP
2	D	1189	ASP
2	D	1202	SER
2	D	1214	LYS
2	D	1229	LEU
2	D	1249	PHE
2	D	1254	SER
2	D	1264	SER
2	D	1275	VAL
2	D	1284	TYR
2	D	1304	LYS
2	D	1305	TYR
2	D	1332	ASN
2	D	1342	VAL
2	D	1362	GLN
2	D	1386	ILE
2	D	1387	ARG
2	D	1397	LYS
2	D	1429	LEU
2	D	1442	ILE
2	D	1446	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	1449	ARG
2	D	1471	ILE
2	D	1477	THR
2	D	1492	VAL
2	D	1516	GLN
2	D	1543	VAL
2	D	1559	LEU
3	B	18	LEU
3	B	54	ASP
3	B	70	ASP
3	B	86	GLU
3	B	140	SER
3	B	161	ILE
3	B	220	MET
3	B	241	THR
3	B	267	CYS
3	B	270	LEU
3	B	271	VAL
3	B	299	THR
3	B	371	VAL
3	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	476	ASN
2	D	953	GLN
2	D	1020	ASN
2	D	1044	ASN
2	D	1118	ASN
2	D	1250	ASN
2	D	1332	ASN
2	D	1368	ASN
2	D	1516	GLN
3	B	39	GLN
3	B	40	GLN
3	B	65	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

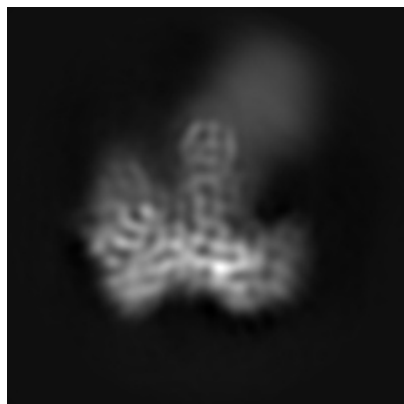
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40029. These allow visual inspection of the internal detail of the map and identification of artifacts.

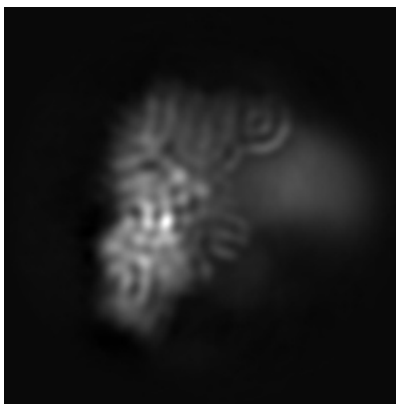
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

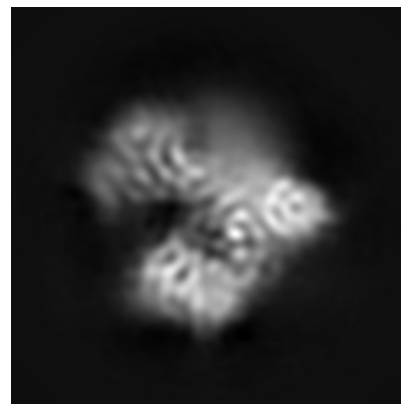
6.1.1 Primary map



X

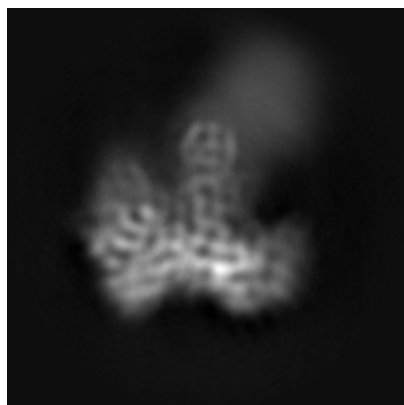


Y

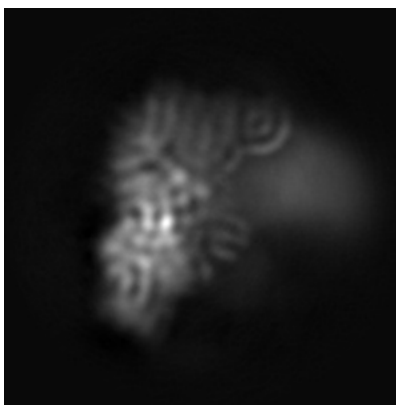


Z

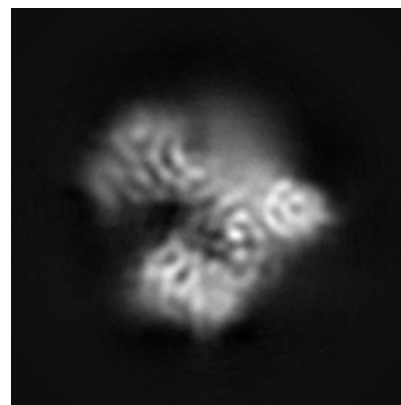
6.1.2 Raw map



X



Y

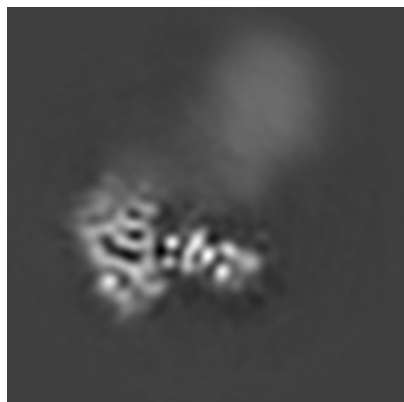


Z

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

6.2 Central slices [i](#)

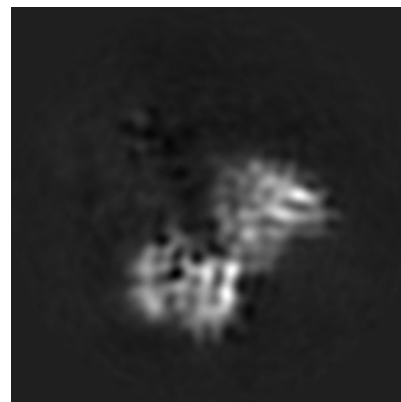
6.2.1 Primary map



X Index: 80

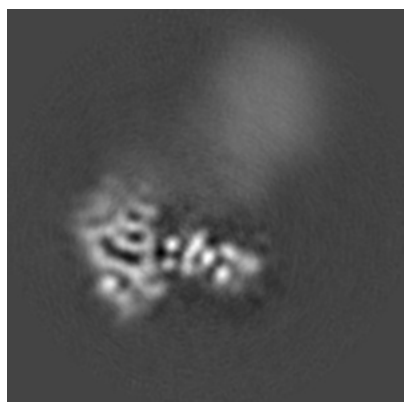


Y Index: 80

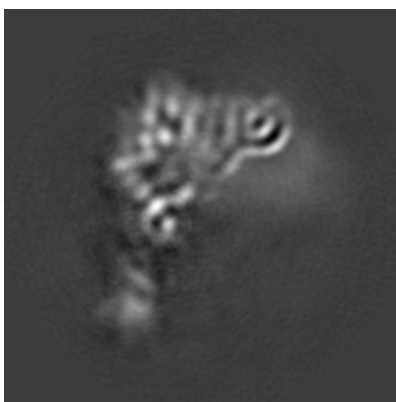


Z Index: 80

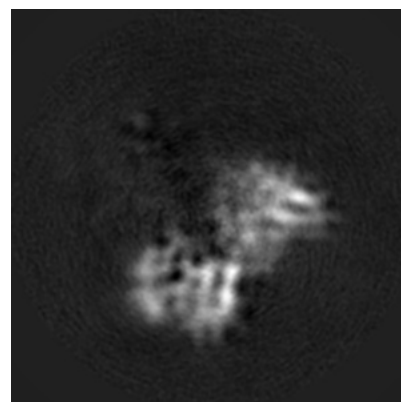
6.2.2 Raw map



X Index: 80



Y Index: 80

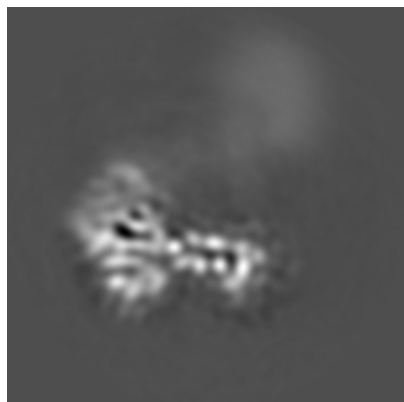


Z Index: 80

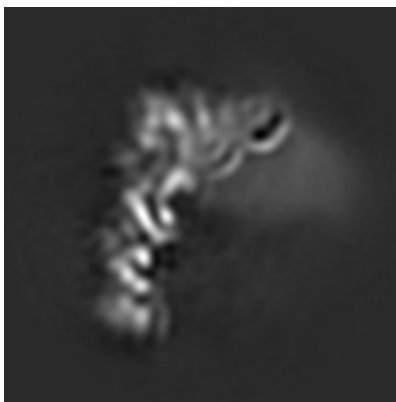
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 74

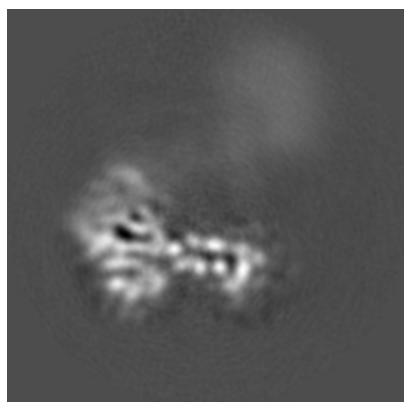


Y Index: 85

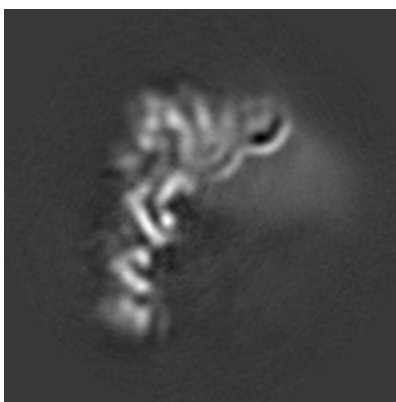


Z Index: 56

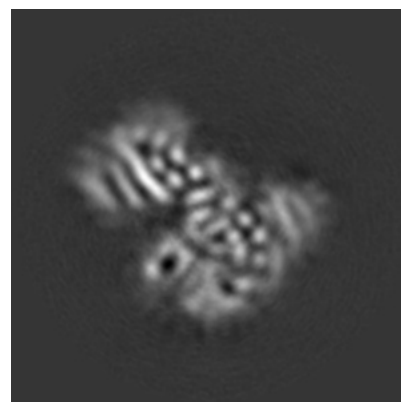
6.3.2 Raw map



X Index: 74



Y Index: 84

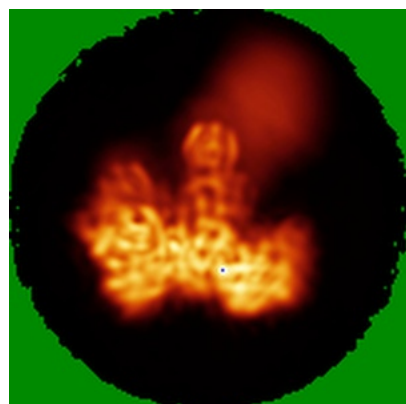


Z Index: 56

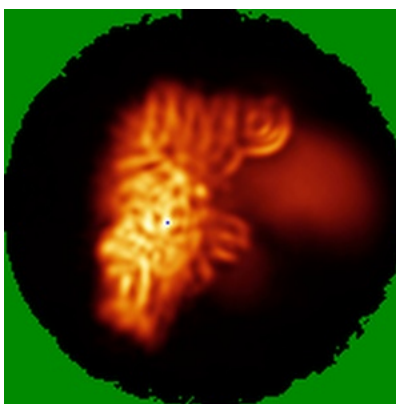
The images above show the largest variance slices of the map in three orthogonal directions.

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

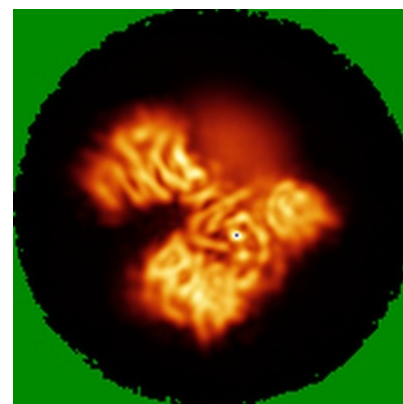
6.4.1 Primary map



X

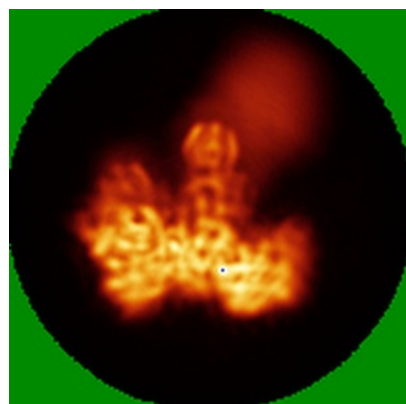


Y

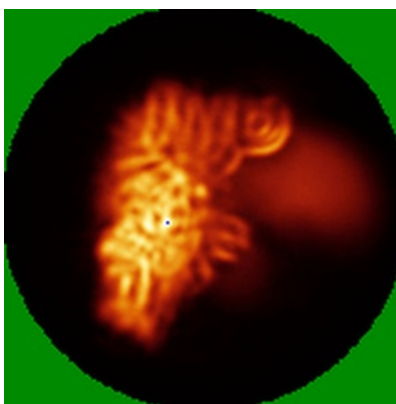


Z

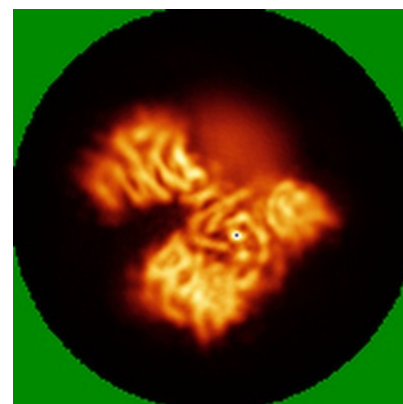
6.4.2 Raw map



X



Y

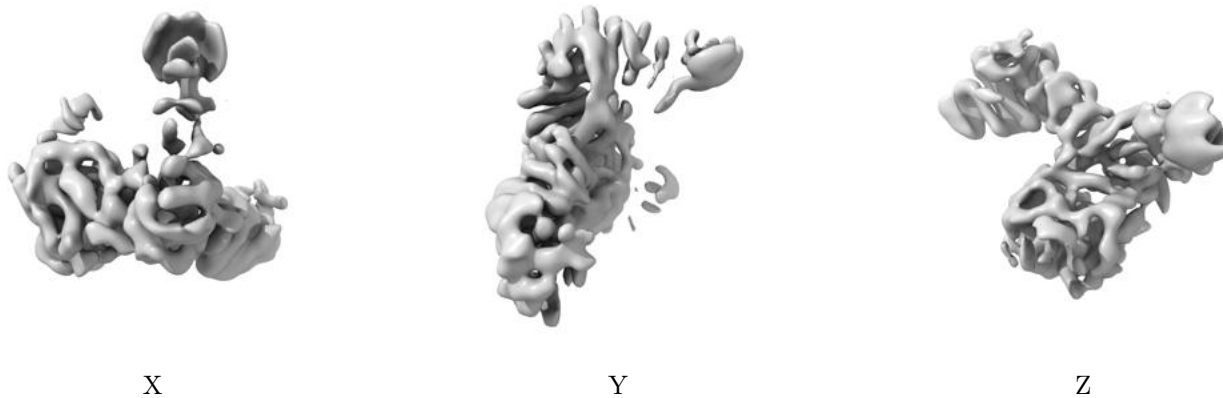


Z

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.

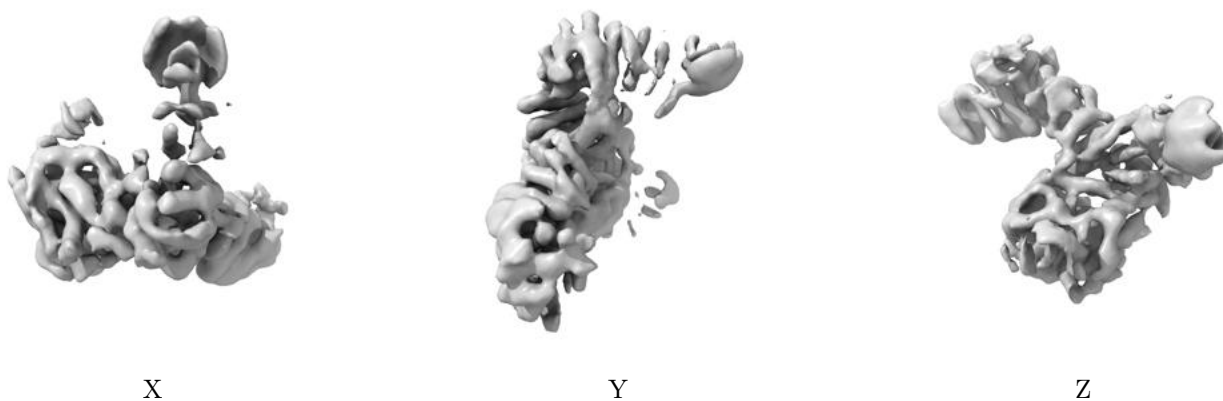
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

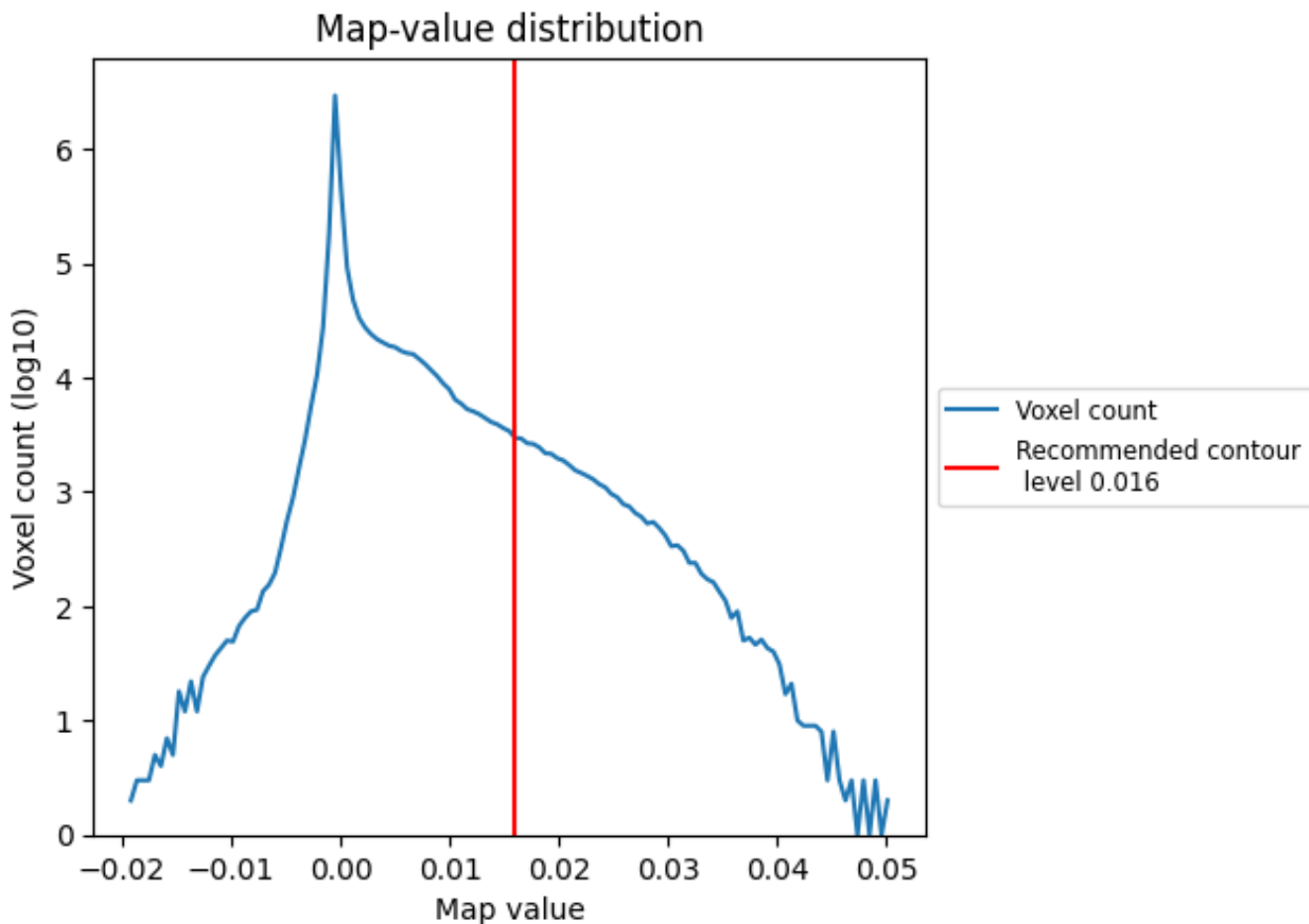
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

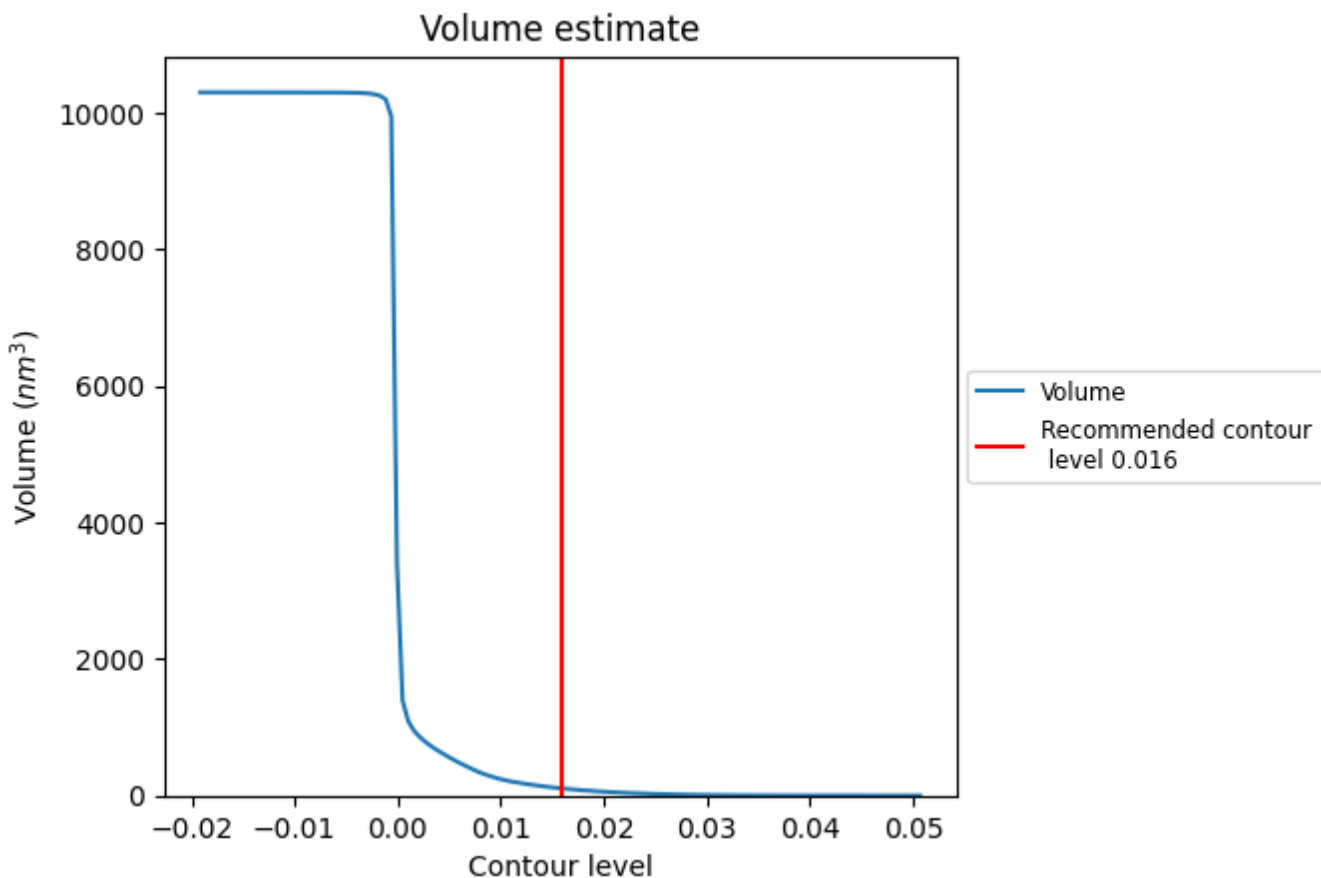
This section contains the results of statistical analysis of the map.

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.

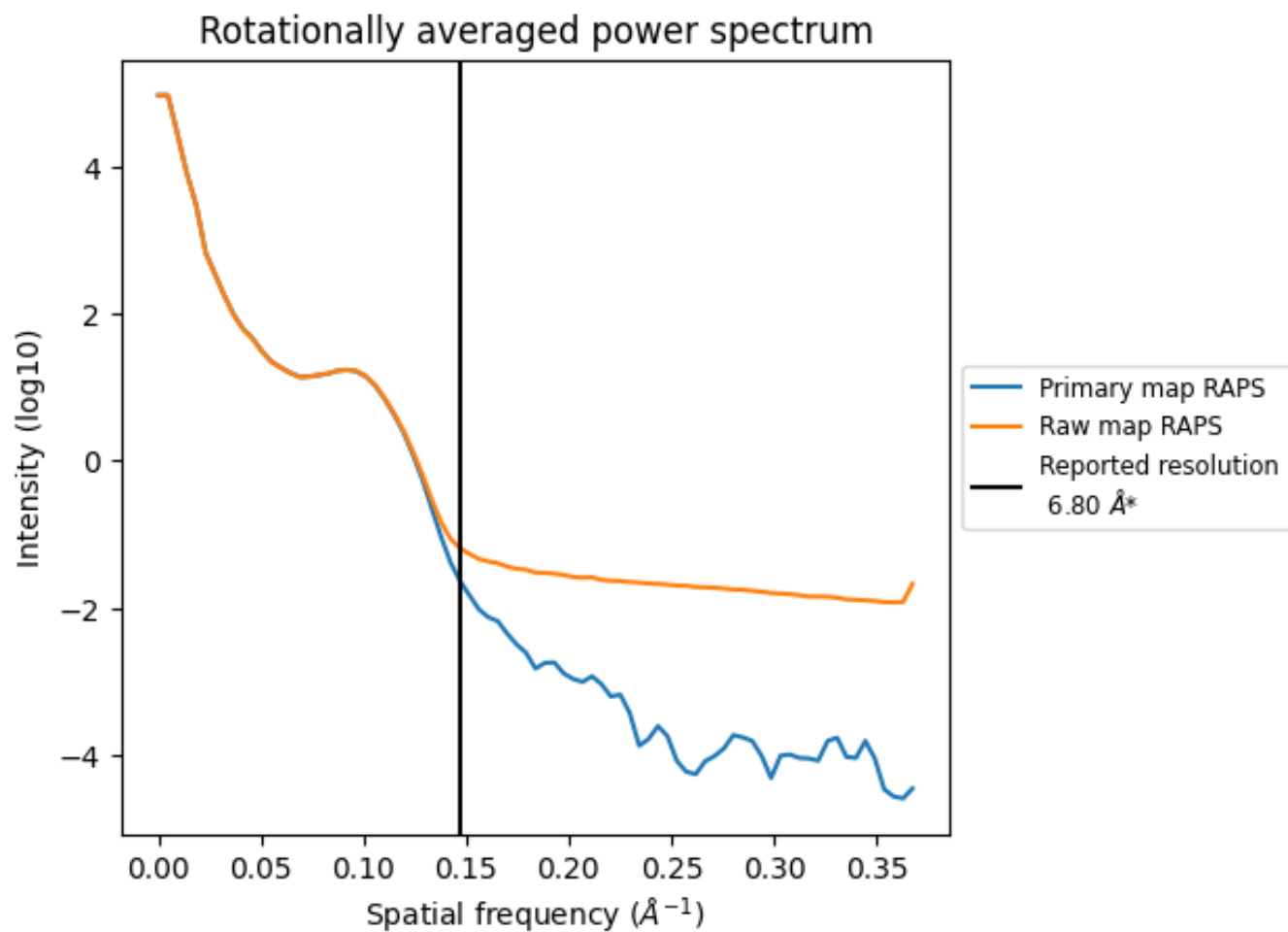
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

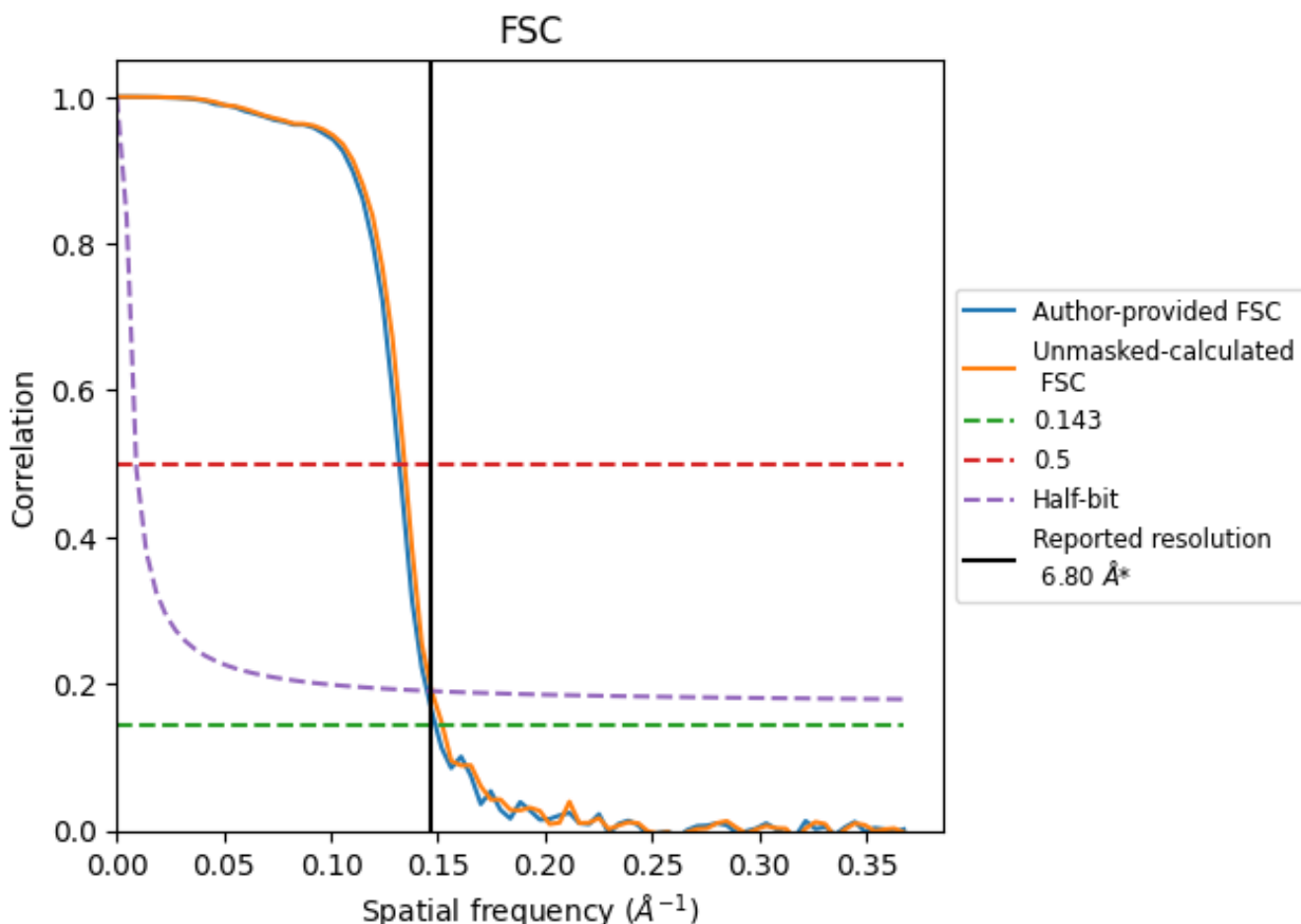


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

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 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

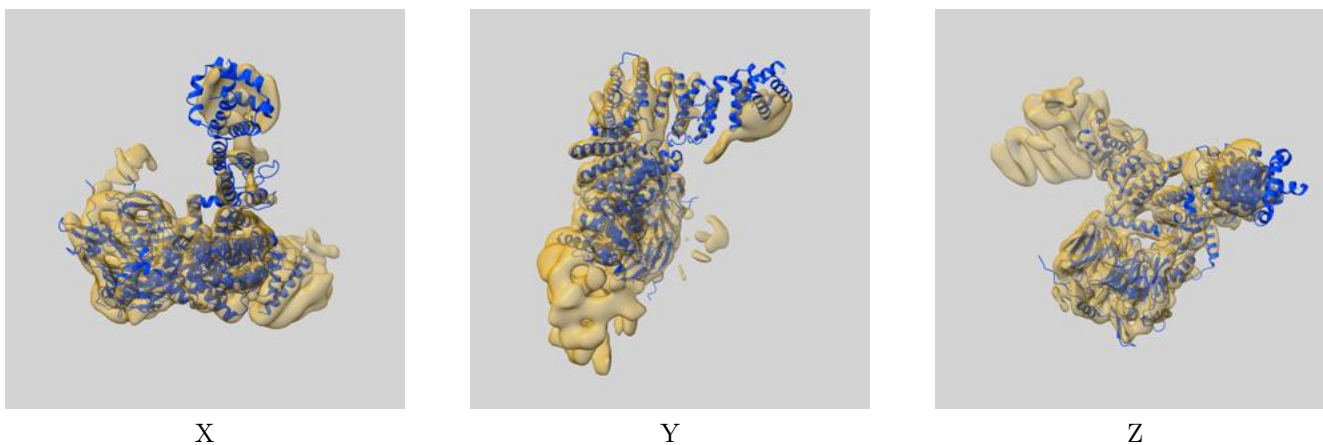
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.72	7.58	6.90
Unmasked-calculated*	6.57	7.44	6.80

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

9 Map-model fit [i](#)

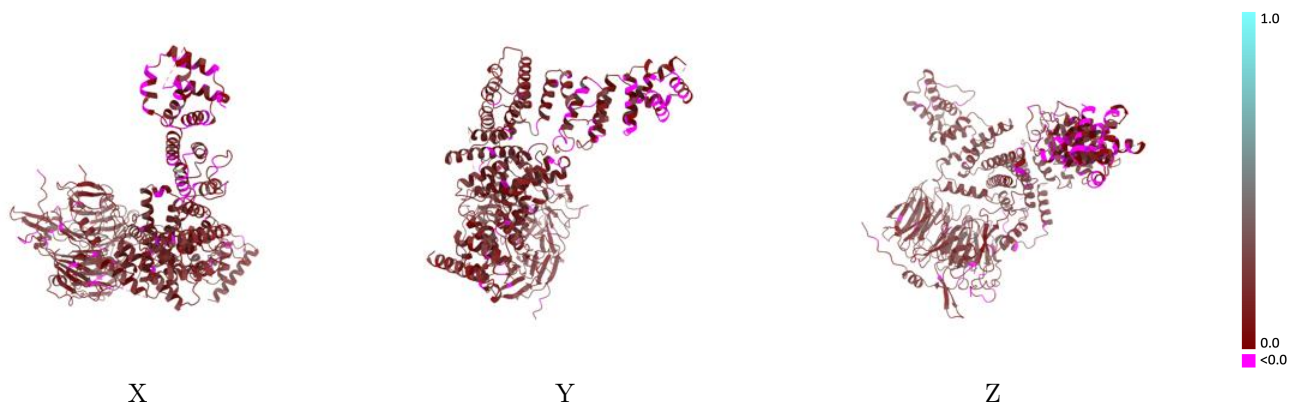
This section contains information regarding the fit between EMDB map EMD-40029 and PDB model 8GHA. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



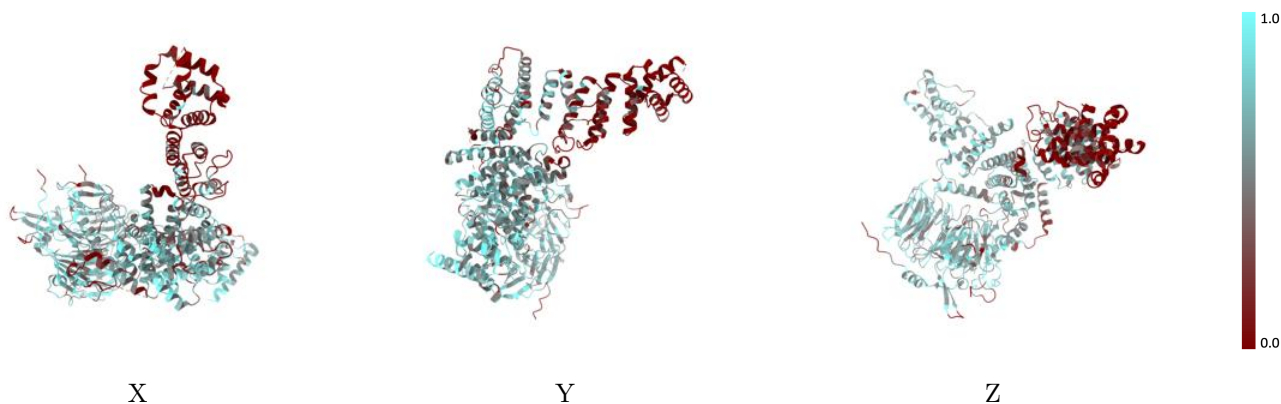
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



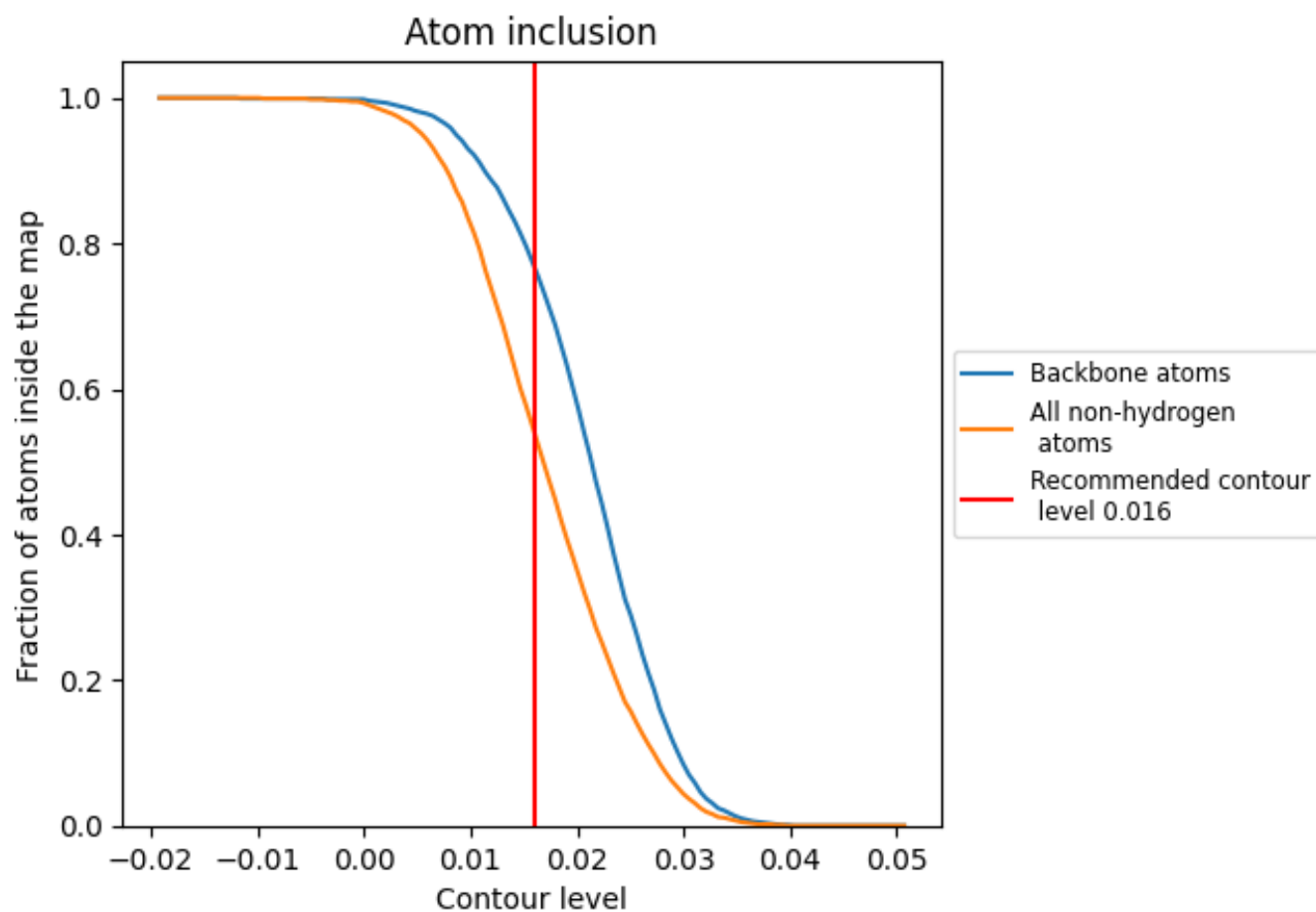
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).









9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 54% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5390	 0.1530
B	 0.6600	 0.1810
D	 0.4820	 0.1410
E	 0.5050	 0.1420

