



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:05 PM UTC

PDB ID : 6L53 / pdb_00006l53
EMDB ID : EMD-0836
Title : Structure of SMG1
Authors : Xu, Y.; Qi, Y.
Deposited on : 2019-10-22
Resolution : 3.63 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

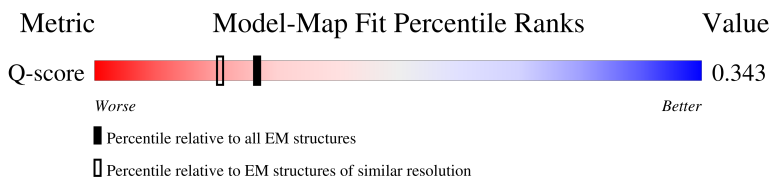
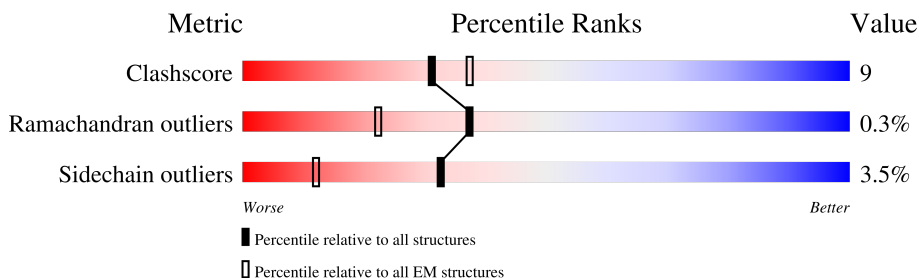
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.63 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	11696 (3.13 - 4.13)

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

Mol	Chain	Length	Quality of chain
1	A	3661	<p>42% 10% • 47%</p>

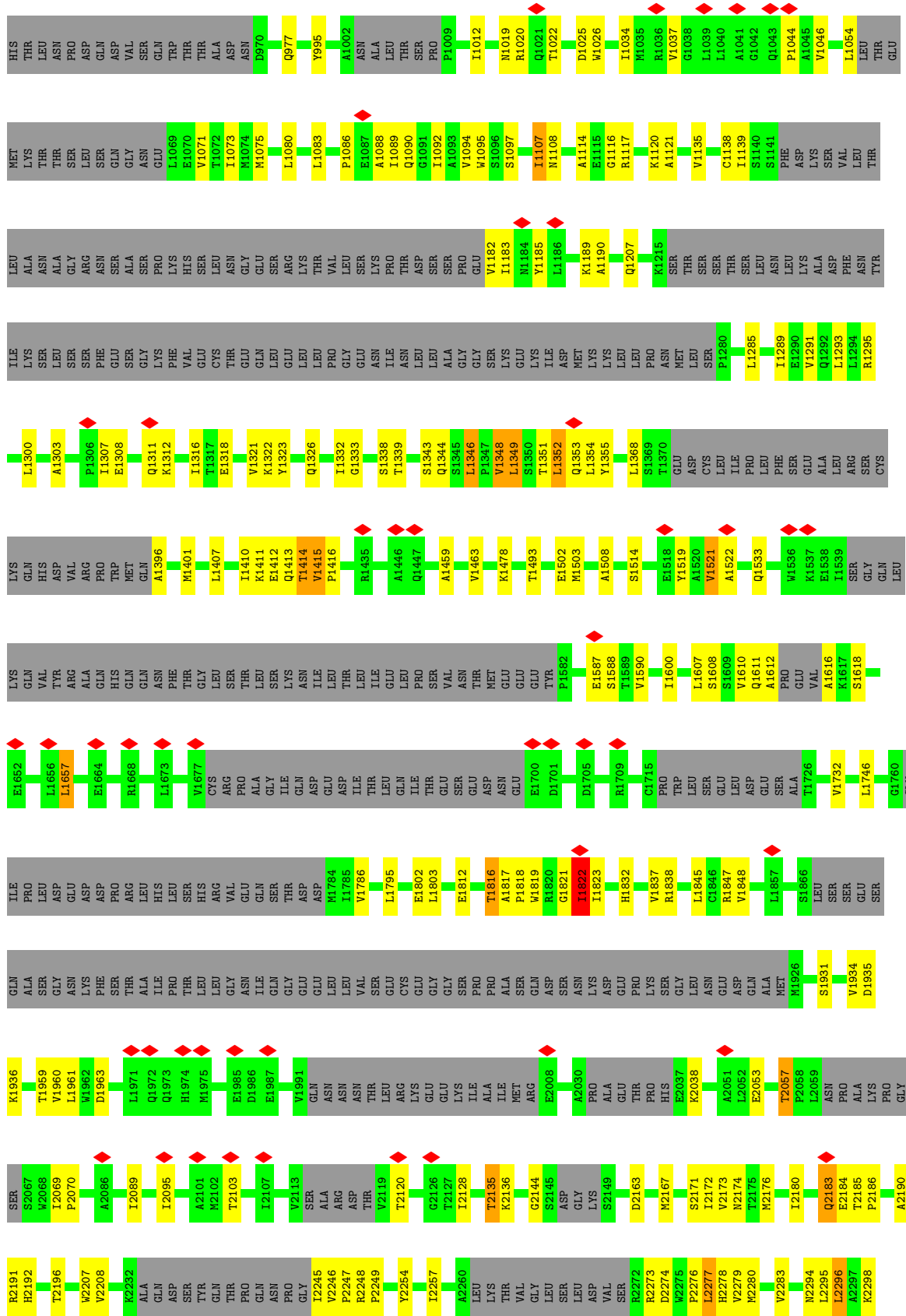
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13991 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 Serine/threonine-protein kinase SMG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1935	13991	8824	2394	2701	72	0	0



PRO	SER	THR	VAL	PRO	GLY	THR	GLY	LYS	SER	VAL	ALA	CYS	SER	PRO	LYS	LYS	ALA	VAL	ARG	ASP	PRO	LYS	THR	GLY	LYS	ALA	VAL	GLN	GLU	ARG	13606		
																																	13627
																																	13641
																																	13661

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42688	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	49.033	Depositor
Minimum map value	-22.818	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	A	0.13	0/14180	0.42	13/19326 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	489	CYS	CA-C-N	8.02	136.13	121.70
1	A	489	CYS	C-N-CA	8.02	136.13	121.70
1	A	2277	LEU	CA-C-N	6.65	133.67	121.70
1	A	2277	LEU	C-N-CA	6.65	133.67	121.70
1	A	675	HIS	CA-C-N	6.46	133.32	121.70
1	A	675	HIS	C-N-CA	6.46	133.32	121.70
1	A	3627	PRO	N-CA-CB	6.35	110.03	102.60
1	A	1019	ASN	CA-C-N	5.88	132.28	121.70
1	A	1019	ASN	C-N-CA	5.88	132.28	121.70
1	A	2365	LEU	CA-C-N	5.40	131.42	121.70
1	A	2365	LEU	C-N-CA	5.40	131.42	121.70
1	A	2183	GLN	CA-C-N	5.02	130.73	121.70
1	A	2183	GLN	C-N-CA	5.02	130.73	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1089	ILE	Peptide
1	A	1657	LEU	Peptide
1	A	901	ILE	Peptide

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	13991	0	13246	239	0
All	All	13991	0	13246	239	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 9.

All (239) 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:1338:SER:H	1:A:1339:THR:HA	1.51	0.76
1:A:2277:LEU:H	1:A:2278:HIS:HB3	1.49	0.75
1:A:361:LEU:HA	1:A:401:LEU:HD21	1.68	0.74
1:A:108:LEU:H	1:A:113:VAL:HG21	1.53	0.72
1:A:1307:ILE:HB	1:A:2306:THR:HG21	1.72	0.71
1:A:2276:PRO:HB2	1:A:2279:VAL:HB	1.72	0.70
1:A:147:SER:H	1:A:149:LEU:HD23	1.56	0.69
1:A:1022:THR:HB	1:A:1415:VAL:H	1.60	0.67
1:A:1092:ILE:HA	1:A:1095:TRP:HB3	1.76	0.67
1:A:2191:ARG:HG3	1:A:2351:VAL:HG12	1.77	0.67
1:A:803:ARG:HG3	1:A:805:GLN:HG2	1.79	0.65
1:A:2389:GLU:HG3	1:A:2394:LEU:HD22	1.78	0.64
1:A:2296:LEU:HB3	1:A:2383:LEU:HD21	1.78	0.63
1:A:995:TYR:HB2	1:A:1012:ILE:HG21	1.80	0.63
1:A:637:THR:H	1:A:638:VAL:HA	1.63	0.62
1:A:1114:ALA:HA	1:A:1117:ARG:HE	1.65	0.62
1:A:1207:GLN:HG3	1:A:1285:LEU:HD22	1.82	0.62
1:A:1349:LEU:HD12	1:A:1354:LEU:HD22	1.82	0.62
1:A:894:ASP:N	1:A:895:LYS:HA	2.16	0.60
1:A:1587:GLU:N	1:A:1588:SER:HA	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2276:PRO:N	1:A:2277:LEU:HA	2.17	0.60
1:A:656:HIS:H	1:A:660:ILE:HD11	1.68	0.59
1:A:2089:ILE:HG21	1:A:2128:ILE:HD11	1.85	0.59
1:A:2186:PRO:O	1:A:2319:ARG:NH1	2.35	0.59
1:A:492:CYS:O	1:A:565:TYR:OH	2.20	0.59
1:A:421:GLY:O	1:A:425:THR:N	2.34	0.58
1:A:1338:SER:N	1:A:1339:THR:HA	2.16	0.58
1:A:388:VAL:HG13	1:A:389:PRO:HD3	1.86	0.58
1:A:752:PHE:HB2	1:A:762:LYS:HZ3	1.68	0.58
1:A:1960:VAL:N	1:A:1961:LEU:HA	2.18	0.58
1:A:675:HIS:HB2	1:A:676:ASP:HB2	1.86	0.58
1:A:395:LEU:HB3	1:A:396:PRO:HD3	1.84	0.58
1:A:2365:LEU:HA	1:A:2366:ARG:HB3	1.85	0.58
1:A:277:MET:SD	1:A:277:MET:N	2.77	0.57
1:A:637:THR:N	1:A:638:VAL:HA	2.19	0.57
1:A:866:ILE:HD13	1:A:1295:ARG:HE	1.68	0.57
1:A:1080:LEU:HD13	1:A:1083:LEU:HD12	1.87	0.57
1:A:2327:VAL:HG22	1:A:2404:ARG:HH21	1.70	0.57
1:A:1832:HIS:O	1:A:1838:ARG:NH2	2.38	0.57
1:A:1963:ASP:OD1	1:A:1963:ASP:N	2.38	0.57
1:A:1351:THR:O	1:A:1355:TYR:N	2.36	0.57
1:A:143:TYR:N	1:A:144:SER:HA	2.20	0.56
1:A:649:VAL:HG11	1:A:667:THR:HB	1.88	0.56
1:A:1116:GLY:O	1:A:1120:LYS:NZ	2.36	0.56
1:A:602:PHE:N	1:A:603:ASN:HA	2.22	0.55
1:A:2388:VAL:HG23	1:A:2393:ARG:HD3	1.87	0.55
1:A:114:THR:O	1:A:134:ARG:NH2	2.38	0.55
1:A:1816:THR:HG21	1:A:1819:TRP:HB3	1.88	0.55
1:A:341:GLY:HA2	1:A:344:GLN:HE22	1.70	0.55
1:A:2245:ILE:N	1:A:2246:VAL:HA	2.21	0.55
1:A:117:GLU:HB2	1:A:134:ARG:HH21	1.72	0.55
1:A:295:LYS:HA	1:A:297:VAL:HG23	1.88	0.55
1:A:236:ILE:HG23	1:A:260:LEU:HD12	1.88	0.54
1:A:322:LEU:HA	1:A:325:TRP:HB2	1.90	0.54
1:A:2332:GLY:HA3	1:A:2359:PHE:N	2.23	0.54
1:A:552:VAL:O	1:A:556:LYS:NZ	2.32	0.54
1:A:2365:LEU:HA	1:A:2366:ARG:CB	2.38	0.54
1:A:1333:GLY:O	1:A:1396:ALA:N	2.41	0.54
1:A:2053:GLU:O	1:A:2057:THR:OG1	2.25	0.54
1:A:1338:SER:HB3	1:A:1401:MET:HE2	1.88	0.54
1:A:2385:VAL:HG22	1:A:2386:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HG13	1:A:177:GLN:HG3	1.89	0.54
1:A:1412:GLU:HA	1:A:1413:GLN:C	2.33	0.54
1:A:2247:PRO:HD2	1:A:2249:PRO:HD3	1.91	0.53
1:A:91:ASN:ND2	1:A:95:GLY:O	2.41	0.53
1:A:1291:VAL:HG13	1:A:1295:ARG:HH12	1.73	0.53
1:A:111:ASN:O	1:A:115:SER:OG	2.25	0.53
1:A:1090:GLN:O	1:A:1092:ILE:N	2.39	0.53
1:A:1138:CYS:SG	1:A:1139:ILE:N	2.82	0.53
1:A:2332:GLY:HA3	1:A:2359:PHE:H	1.74	0.52
1:A:2335:ASP:OD1	1:A:2337:HIS:NE2	2.42	0.52
1:A:648:ILE:HA	1:A:714:LEU:HD12	1.92	0.52
1:A:409:VAL:HG13	1:A:453:LEU:HG	1.92	0.52
1:A:845:LEU:HD12	1:A:922:GLN:HE22	1.74	0.52
1:A:117:GLU:HG3	1:A:130:THR:HB	1.91	0.52
1:A:904:ASN:HB3	1:A:906:LEU:HD22	1.92	0.51
1:A:1054:LEU:HB3	1:A:1415:VAL:HG21	1.92	0.51
1:A:1533:GLN:HA	1:A:1607:LEU:HD22	1.93	0.51
1:A:2173:VAL:HA	1:A:2176:MET:HE2	1.93	0.51
1:A:866:ILE:HA	1:A:868:PHE:H	1.76	0.51
1:A:2280:MET:HA	1:A:2283:VAL:HG12	1.93	0.50
1:A:1821:GLY:O	1:A:1823:ILE:N	2.44	0.50
1:A:1657:LEU:HD23	1:A:1657:LEU:H	1.75	0.50
1:A:602:PHE:H	1:A:603:ASN:HA	1.76	0.50
1:A:1094:VAL:O	1:A:1097:SER:OG	2.19	0.50
1:A:149:LEU:O	1:A:187:LYS:NZ	2.30	0.50
1:A:1323:TYR:HA	1:A:1326:GLN:HG2	1.93	0.50
1:A:120:SER:HA	1:A:122:GLN:HE22	1.77	0.50
1:A:184:VAL:HG12	1:A:186:VAL:HB	1.94	0.49
1:A:300:ILE:HD11	1:A:302:LEU:HB2	1.93	0.49
1:A:927:SER:OG	1:A:977:GLN:NE2	2.45	0.49
1:A:419:ILE:HG21	1:A:442:ALA:H	1.77	0.49
1:A:1935:ASP:OD1	1:A:1936:LYS:N	2.44	0.49
1:A:2247:PRO:N	1:A:2248:ARG:HA	2.27	0.49
1:A:1120:LYS:HB3	1:A:1121:ALA:HB2	1.93	0.49
1:A:1182:VAL:HG22	1:A:1291:VAL:HG11	1.94	0.49
1:A:148:ARG:HA	1:A:153:LEU:HD22	1.95	0.49
1:A:1931:SER:HA	1:A:1934:VAL:HG12	1.95	0.48
1:A:154:ARG:HD2	1:A:157:THR:HB	1.95	0.48
1:A:127:ALA:HB1	1:A:131:LYS:HE3	1.94	0.48
1:A:771:GLU:HA	1:A:773:VAL:HG13	1.95	0.48
1:A:773:VAL:HA	1:A:774:ASN:HA	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2254:TYR:HA	1:A:2257:ILE:HG22	1.94	0.48
1:A:390:PRO:HB2	1:A:391:PRO:HD3	1.96	0.48
1:A:2183:GLN:HA	1:A:2184:GLU:C	2.39	0.48
1:A:672:CYS:SG	1:A:673:THR:N	2.87	0.47
1:A:487:GLU:HA	1:A:488:ASN:C	2.39	0.47
1:A:335:LEU:HA	1:A:336:THR:HA	1.60	0.47
1:A:274:GLN:HA	1:A:275:LEU:HA	1.48	0.47
1:A:1189:LYS:HA	1:A:1190:ALA:HA	1.61	0.47
1:A:891:GLN:HE22	1:A:2298:LYS:HB3	1.80	0.47
1:A:1818:PRO:HG3	1:A:1848:VAL:HG23	1.96	0.47
1:A:2374:ARG:HH22	1:A:3641:ILE:HA	1.80	0.47
1:A:858:HIS:CD2	1:A:860:GLN:HB2	2.50	0.47
1:A:1293:LEU:HD13	1:A:1322:LYS:HD2	1.97	0.47
1:A:807:VAL:HA	1:A:808:HIS:HA	1.56	0.47
1:A:1786:VAL:HG11	1:A:2172:ILE:HD12	1.97	0.47
1:A:143:TYR:H	1:A:144:SER:HA	1.80	0.47
1:A:199:VAL:HG23	1:A:200:LEU:HD12	1.96	0.47
1:A:845:LEU:HD11	1:A:883:LEU:HD11	1.96	0.47
1:A:1610:VAL:HA	1:A:1611:GLN:HA	1.50	0.47
1:A:433:LEU:HD21	1:A:471:MET:HE2	1.96	0.46
1:A:489:CYS:CB	1:A:490:GLN:HB2	2.46	0.46
1:A:550:GLN:HB3	1:A:609:PHE:HB2	1.97	0.46
1:A:166:LEU:HG	1:A:167:ALA:H	1.80	0.46
1:A:2120:THR:HB	1:A:2144:GLY:HA3	1.97	0.46
1:A:2365:LEU:HB3	1:A:2367:VAL:HB	1.96	0.46
1:A:1608:SER:O	1:A:1618:SER:OG	2.23	0.46
1:A:1318:GLU:HA	1:A:1321:VAL:HG12	1.97	0.46
1:A:1802:GLU:HA	1:A:1803:LEU:HA	1.63	0.46
1:A:554:SER:HA	1:A:612:ILE:HD13	1.97	0.46
1:A:1412:GLU:HB3	1:A:1416:PRO:HD2	1.97	0.46
1:A:1343:SER:HA	1:A:1344:GLN:CB	2.46	0.46
1:A:1346:LEU:HD22	1:A:1349:LEU:HG	1.97	0.46
1:A:333:PRO:HA	1:A:342:TRP:HZ3	1.80	0.46
1:A:1845:LEU:HA	1:A:1848:VAL:HG12	1.97	0.46
1:A:336:THR:HA	1:A:342:TRP:HZ2	1.80	0.46
1:A:398:LEU:O	1:A:401:LEU:N	2.43	0.46
1:A:2163:ASP:O	1:A:2167:MET:HG2	2.16	0.46
1:A:435:ARG:HG2	1:A:436:VAL:H	1.80	0.46
1:A:1086:PRO:HA	1:A:1090:GLN:HA	1.98	0.45
1:A:1090:GLN:C	1:A:1092:ILE:H	2.24	0.45
1:A:1746:LEU:HD13	1:A:1795:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2391:VAL:HG12	1:A:2392:PHE:H	1.82	0.45
1:A:107:GLU:HG2	1:A:108:LEU:HD13	1.99	0.45
1:A:675:HIS:H	1:A:676:ASP:HB2	1.80	0.45
1:A:2277:LEU:N	1:A:2278:HIS:HB3	2.25	0.45
1:A:771:GLU:HA	1:A:772:ASP:C	2.42	0.45
1:A:864:ASP:HA	1:A:865:VAL:HA	1.63	0.45
1:A:1025:ASP:OD1	1:A:1026:TRP:N	2.42	0.45
1:A:1348:VAL:HG23	1:A:1349:LEU:H	1.81	0.45
1:A:1182:VAL:HA	1:A:1183:ILE:HA	1.72	0.45
1:A:1346:LEU:HB3	1:A:1349:LEU:HD23	1.98	0.45
1:A:1411:LYS:C	1:A:1413:GLN:HB2	2.42	0.45
1:A:1300:LEU:HD21	1:A:1316:ILE:HG13	1.99	0.45
1:A:1508:ALA:HB1	1:A:1600:ILE:HG13	1.98	0.45
1:A:1071:VAL:HG13	1:A:1073:ILE:H	1.82	0.45
1:A:2135:THR:HA	1:A:2136:LYS:HA	1.57	0.44
1:A:275:LEU:HB2	1:A:276:VAL:HA	1.99	0.44
1:A:356:PHE:HB3	1:A:360:LEU:HD22	1.99	0.44
1:A:1034:ILE:HG23	1:A:1075:MET:HE1	1.99	0.44
1:A:2180:ILE:HG21	1:A:2403:MET:HE3	1.99	0.44
1:A:2207:TRP:CD1	1:A:2208:VAL:HG12	2.51	0.44
1:A:635:SER:HB2	1:A:636:PRO:HD3	1.99	0.44
1:A:479:ILE:HG23	1:A:480:THR:HG23	1.99	0.44
1:A:2069:ILE:HB	1:A:2070:PRO:HD3	2.00	0.44
1:A:1812:GLU:O	1:A:1847:ARG:NH2	2.41	0.43
1:A:2171:SER:HA	1:A:2192:HIS:HE1	1.83	0.43
1:A:191:ASN:ND2	1:A:222:CYS:SG	2.89	0.43
1:A:2273:ARG:N	1:A:2274:ASP:HA	2.32	0.43
1:A:391:PRO:HB3	1:A:459:CYS:SG	2.58	0.43
1:A:244:ALA:HB2	1:A:257:TYR:HE1	1.83	0.43
1:A:464:LEU:H	1:A:464:LEU:HD23	1.81	0.43
1:A:491:THR:HB	1:A:492:CYS:HA	2.00	0.43
1:A:1352:LEU:HA	1:A:1353:GLN:HA	1.57	0.43
1:A:246:ASP:HA	1:A:247:GLU:HA	1.59	0.43
1:A:248:VAL:HG22	1:A:249:LYS:H	1.84	0.43
1:A:1020:ARG:O	1:A:1022:THR:N	2.48	0.43
1:A:1088:ALA:HB2	1:A:1352:LEU:HD12	2.01	0.43
1:A:1478:LYS:HE2	1:A:1493:THR:HA	1.99	0.43
1:A:114:THR:HG22	1:A:134:ARG:HG3	2.00	0.42
1:A:107:GLU:HA	1:A:108:LEU:HA	1.65	0.42
1:A:216:CYS:HB3	1:A:266:LYS:HE2	2.00	0.42
1:A:2342:LEU:HB2	1:A:2351:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:SER:HA	1:A:612:ILE:HG21	2.01	0.42
1:A:846:ARG:NH2	1:A:921:ALA:O	2.52	0.42
1:A:417:SER:N	1:A:418:PRO:HD2	2.34	0.42
1:A:474:HIS:CE1	1:A:549:TYR:HE1	2.37	0.42
1:A:771:GLU:N	1:A:772:ASP:HB3	2.34	0.42
1:A:1107:ILE:HA	1:A:1108:ASN:HA	1.57	0.42
1:A:550:GLN:HA	1:A:553:LEU:HB2	2.01	0.42
1:A:1303:ALA:O	1:A:1308:GLU:HB2	2.19	0.42
1:A:295:LYS:HE2	1:A:299:CYS:HB2	2.02	0.42
1:A:363:GLN:NE2	1:A:367:ASP:OD1	2.53	0.42
1:A:2174:ASN:ND2	1:A:2190:ALA:O	2.47	0.42
1:A:619:THR:HA	1:A:620:THR:HA	1.73	0.42
1:A:675:HIS:H	1:A:676:ASP:C	2.28	0.42
1:A:2276:PRO:CD	1:A:2277:LEU:HA	2.50	0.42
1:A:2294:ASN:HB2	1:A:2298:LYS:HG2	2.01	0.42
1:A:2327:VAL:HG22	1:A:2404:ARG:NH2	2.34	0.42
1:A:805:GLN:HG3	1:A:806:LEU:H	1.85	0.41
1:A:1832:HIS:CD2	1:A:1837:VAL:HG21	2.55	0.41
1:A:347:GLU:N	1:A:348:PRO:HD2	2.35	0.41
1:A:280:LEU:HD23	1:A:283:ILE:HD12	2.02	0.41
1:A:554:SER:HB2	1:A:608:LYS:HE3	2.01	0.41
1:A:733:THR:HA	1:A:734:TRP:HA	1.69	0.41
1:A:2038:LYS:HA	1:A:2095:ILE:HD12	2.02	0.41
1:A:1959:THR:HA	1:A:1960:VAL:HA	1.79	0.41
1:A:2295:LEU:HB2	1:A:2379:ILE:HG21	2.03	0.41
1:A:321:ILE:C	1:A:325:TRP:HD1	2.28	0.41
1:A:900:THR:OG1	1:A:903:ARG:HA	2.21	0.41
1:A:1086:PRO:O	1:A:1088:ALA:N	2.54	0.41
1:A:1407:LEU:HD23	1:A:1410:ILE:HD12	2.01	0.41
1:A:1521:VAL:HA	1:A:1522:ALA:HA	1.65	0.41
1:A:188:GLN:HG3	1:A:226:SER:HB3	2.03	0.41
1:A:207:LEU:HA	1:A:208:GLN:C	2.46	0.41
1:A:1612:ALA:O	1:A:1616:ALA:N	2.53	0.41
1:A:1822:ILE:H	1:A:1822:ILE:HG13	1.47	0.41
1:A:835:HIS:CE1	1:A:836:THR:HG23	2.55	0.41
1:A:1207:GLN:HG2	1:A:1289:ILE:HD11	2.03	0.41
1:A:1311:GLN:HA	1:A:1312:LYS:HA	1.74	0.41
1:A:2387:GLY:C	1:A:2391:VAL:HG21	2.45	0.41
1:A:115:SER:OG	1:A:116:PRO:HD3	2.20	0.41
1:A:122:GLN:HE21	1:A:122:GLN:HB2	1.73	0.41
1:A:337:GLN:HA	1:A:338:GLN:HA	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:LEU:O	1:A:759:LYS:N	2.53	0.41
1:A:1514:SER:HB2	1:A:1519:TYR:HA	2.03	0.41
1:A:2336:ARG:HH21	1:A:2340:ASN:HB3	1.86	0.41
1:A:733:THR:HG21	1:A:770:VAL:HG22	2.03	0.40
1:A:1502:GLU:HA	1:A:1503:MET:HA	1.72	0.40
1:A:231:LYS:HG3	1:A:232:ILE:HD12	2.01	0.40
1:A:360:LEU:HD11	1:A:364:PHE:CG	2.56	0.40
1:A:655:VAL:HG13	1:A:807:VAL:HG21	2.02	0.40
1:A:1401:MET:HE3	1:A:1401:MET:HB3	1.97	0.40
1:A:1414:THR:HA	1:A:1415:VAL:HA	1.67	0.40
1:A:2246:VAL:HB	1:A:2247:PRO:C	2.46	0.40
1:A:295:LYS:HA	1:A:297:VAL:N	2.36	0.40
1:A:1459:ALA:O	1:A:1463:VAL:HG23	2.21	0.40
1:A:1816:THR:H	1:A:1817:ALA:HB2	1.87	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	1879/3661 (51%)	1689 (90%)	185 (10%)	5 (0%)	36 64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1822	ILE
1	A	902	PRO
1	A	151	ASN
1	A	901	ILE
1	A	1044	PRO

5.3.2 Protein sidechains

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	1403/3224 (44%)	1354 (96%)	49 (4%)	32 53

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	113	VAL
1	A	115	SER
1	A	149	LEU
1	A	184	VAL
1	A	186	VAL
1	A	206	LEU
1	A	289	THR
1	A	322	LEU
1	A	336	THR
1	A	388	VAL
1	A	501	LEU
1	A	561	LEU
1	A	620	THR
1	A	655	VAL
1	A	725	GLN
1	A	770	VAL
1	A	893	LEU
1	A	906	LEU
1	A	1037	VAL
1	A	1046	VAL
1	A	1107	ILE
1	A	1135	VAL
1	A	1185	TYR
1	A	1332	ILE
1	A	1346	LEU
1	A	1348	VAL
1	A	1349	LEU
1	A	1352	LEU
1	A	1368	LEU

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Mol	Chain	Res	Type
1	A	1414	THR
1	A	1415	VAL
1	A	1521	VAL
1	A	1590	VAL
1	A	1732	VAL
1	A	1816	THR
1	A	1822	ILE
1	A	2057	THR
1	A	2103	THR
1	A	2135	THR
1	A	2185	THR
1	A	2196	THR
1	A	2296	LEU
1	A	2306	THR
1	A	2357	VAL
1	A	2367	VAL
1	A	2379	ILE
1	A	2383	LEU
1	A	2385	VAL

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	71	HIS
1	A	122	GLN
1	A	177	GLN
1	A	178	GLN
1	A	191	ASN
1	A	309	HIS
1	A	474	HIS
1	A	490	GLN
1	A	671	HIS
1	A	725	GLN
1	A	805	GLN
1	A	839	GLN
1	A	848	HIS
1	A	858	HIS
1	A	891	GLN
1	A	914	GLN
1	A	977	GLN
1	A	1204	GLN
1	A	1286	GLN

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Mol	Chain	Res	Type
1	A	1465	HIS
1	A	1799	HIS
1	A	1825	GLN
1	A	1832	HIS
1	A	2104	ASN
1	A	2229	GLN
1	A	2315	GLN
1	A	2340	ASN
1	A	2352	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

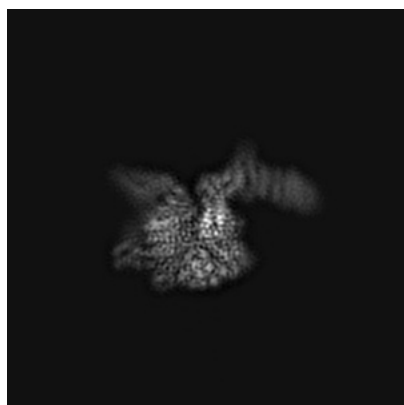
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0836. These allow visual inspection of the internal detail of the map and identification of artifacts.

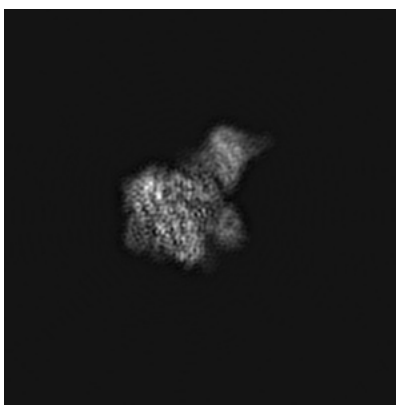
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

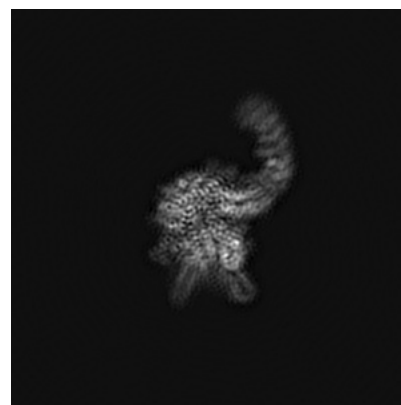
6.1.1 Primary map



X



Y

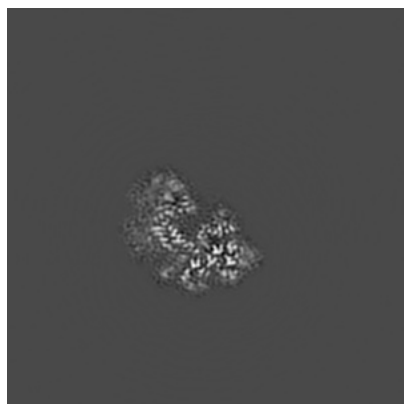


Z

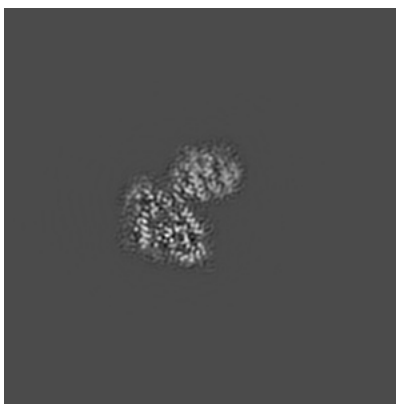
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

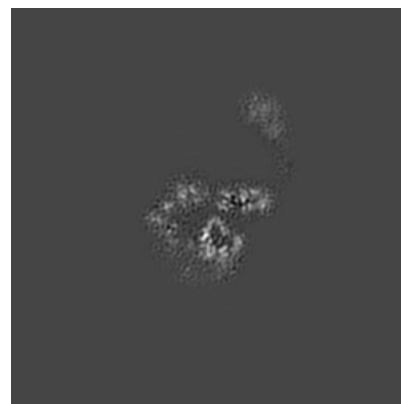
6.2.1 Primary map



X Index: 160



Y Index: 160

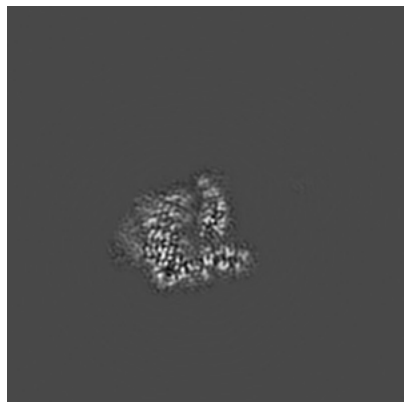


Z Index: 160

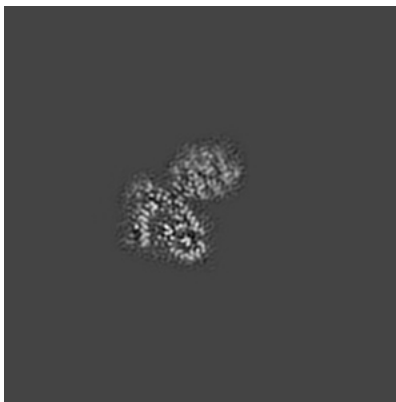
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

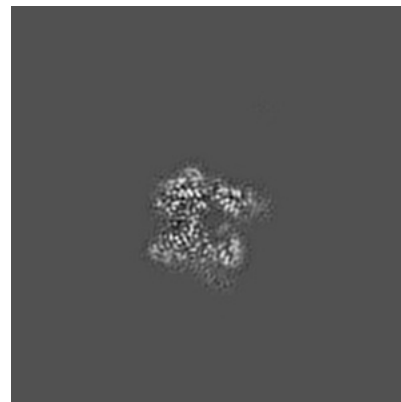
6.3.1 Primary map



X Index: 172



Y Index: 161

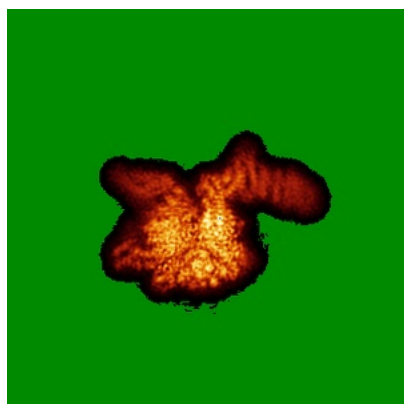


Z Index: 148

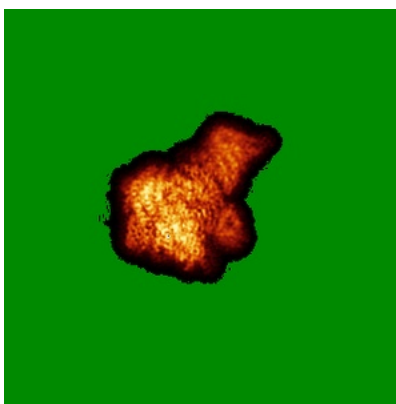
The images above show the largest variance slices of the map in three orthogonal directions.

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

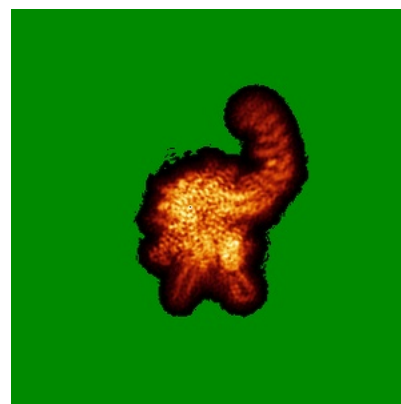
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

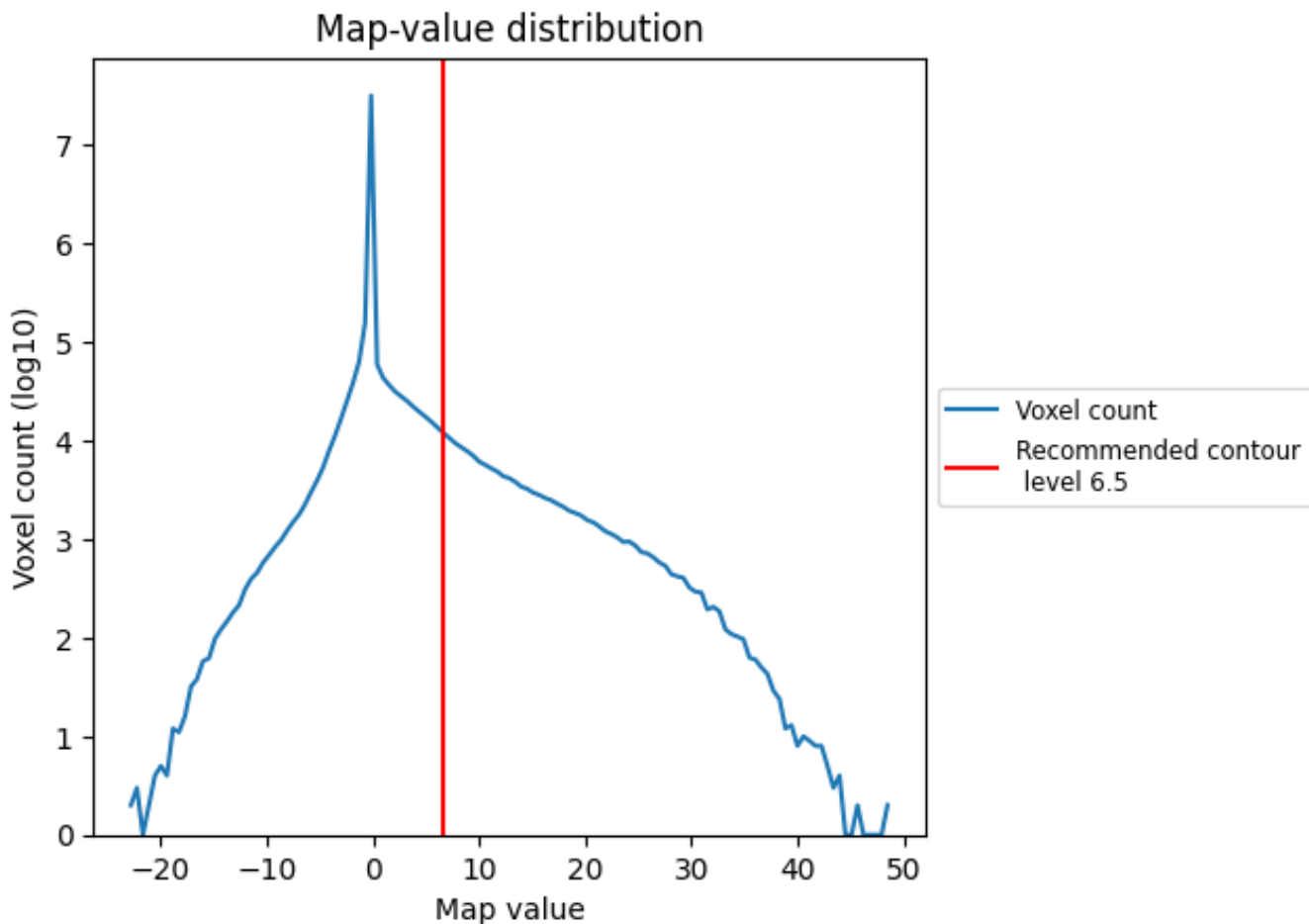
6.6 Mask visualisation

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

7 Map analysis [i](#)

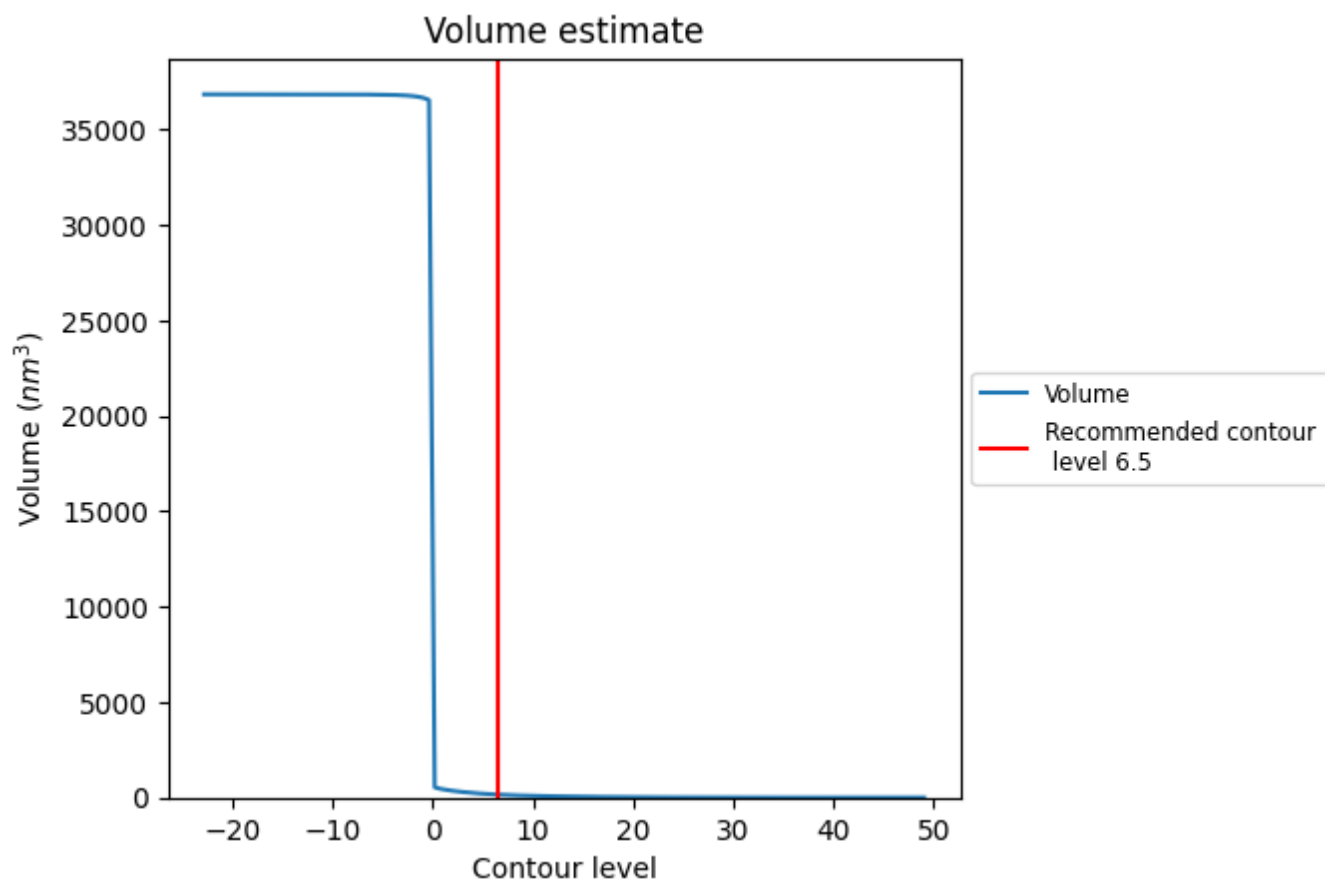
This section contains the results of statistical analysis of the map.

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.

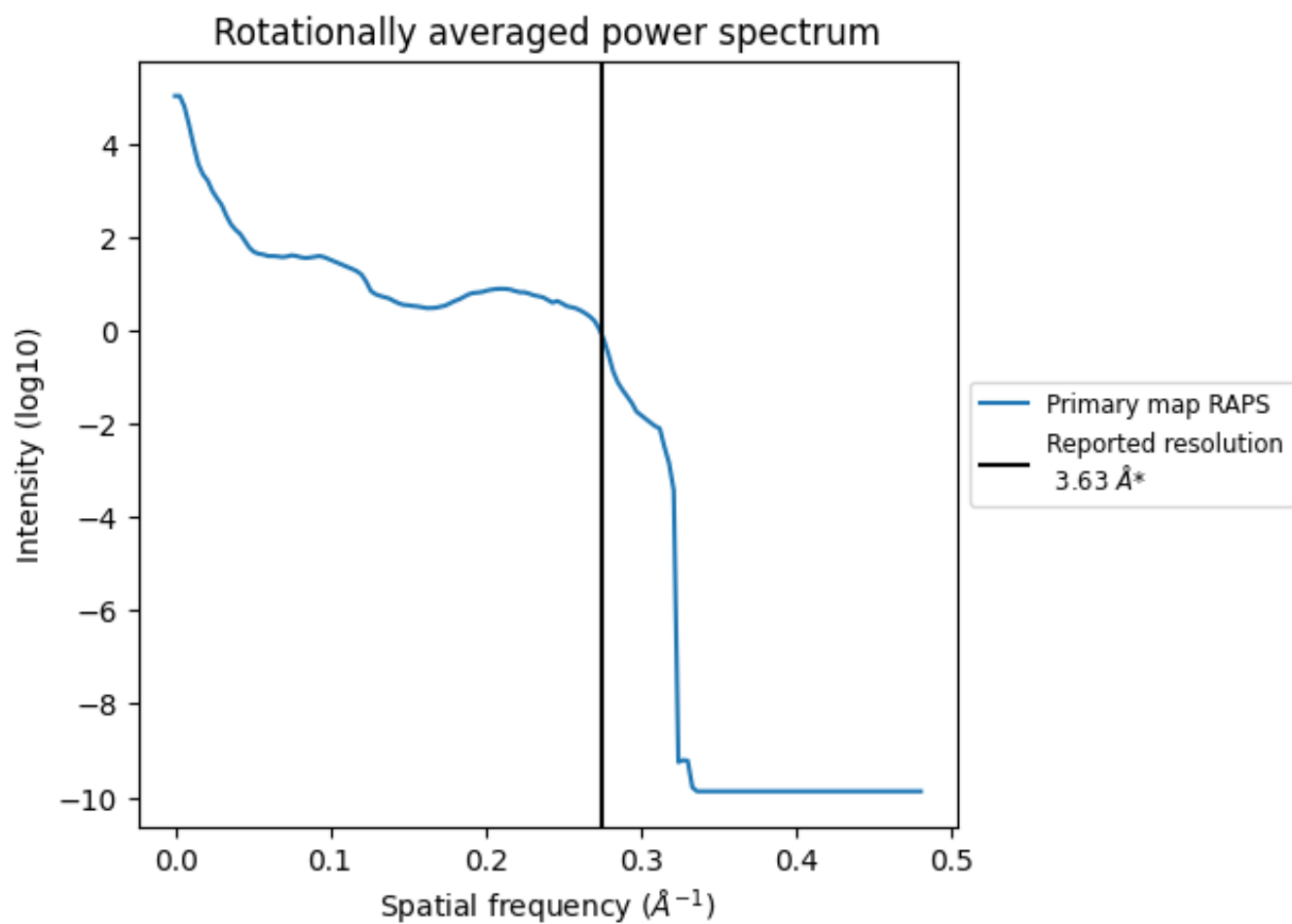
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 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 0.275 Å⁻¹

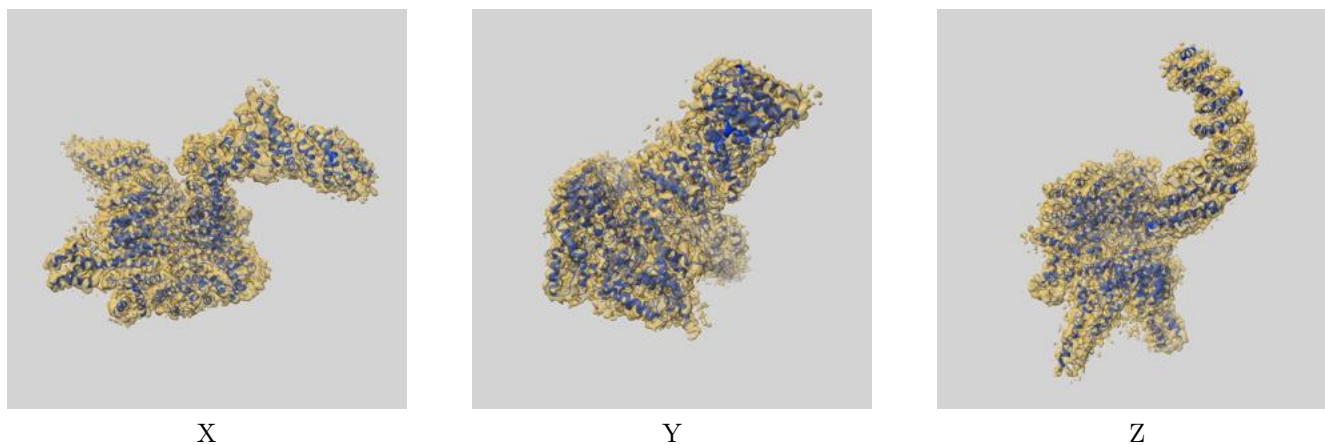
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

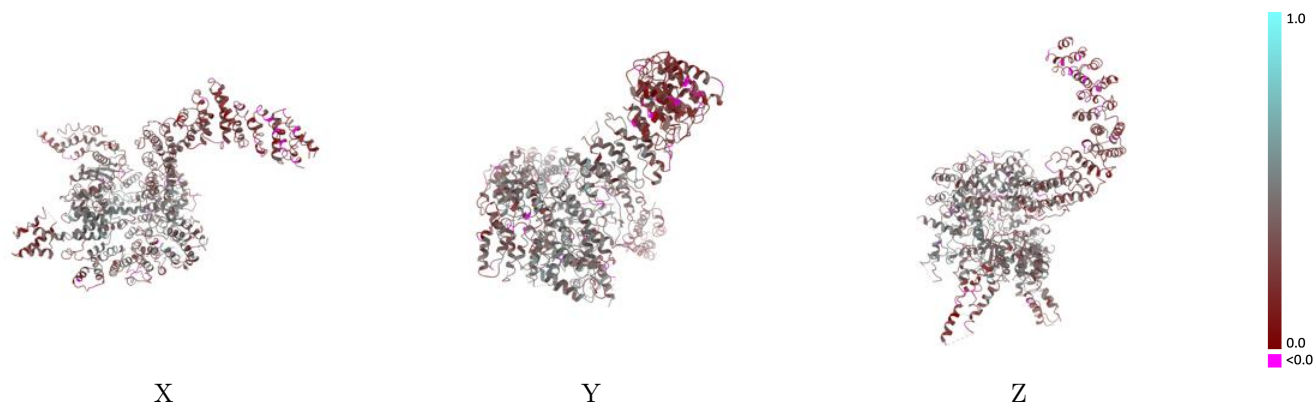
This section contains information regarding the fit between EMDB map EMD-0836 and PDB model 6L53. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



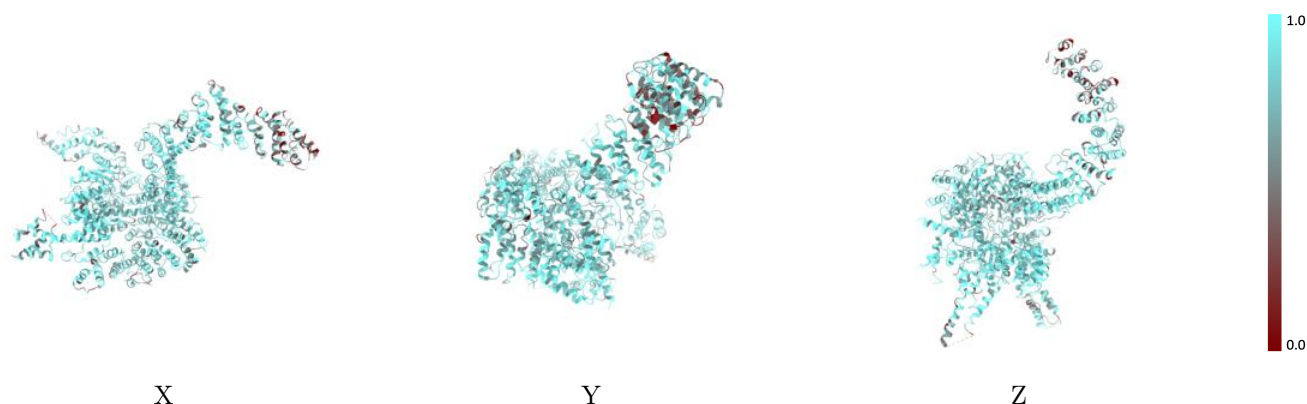
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



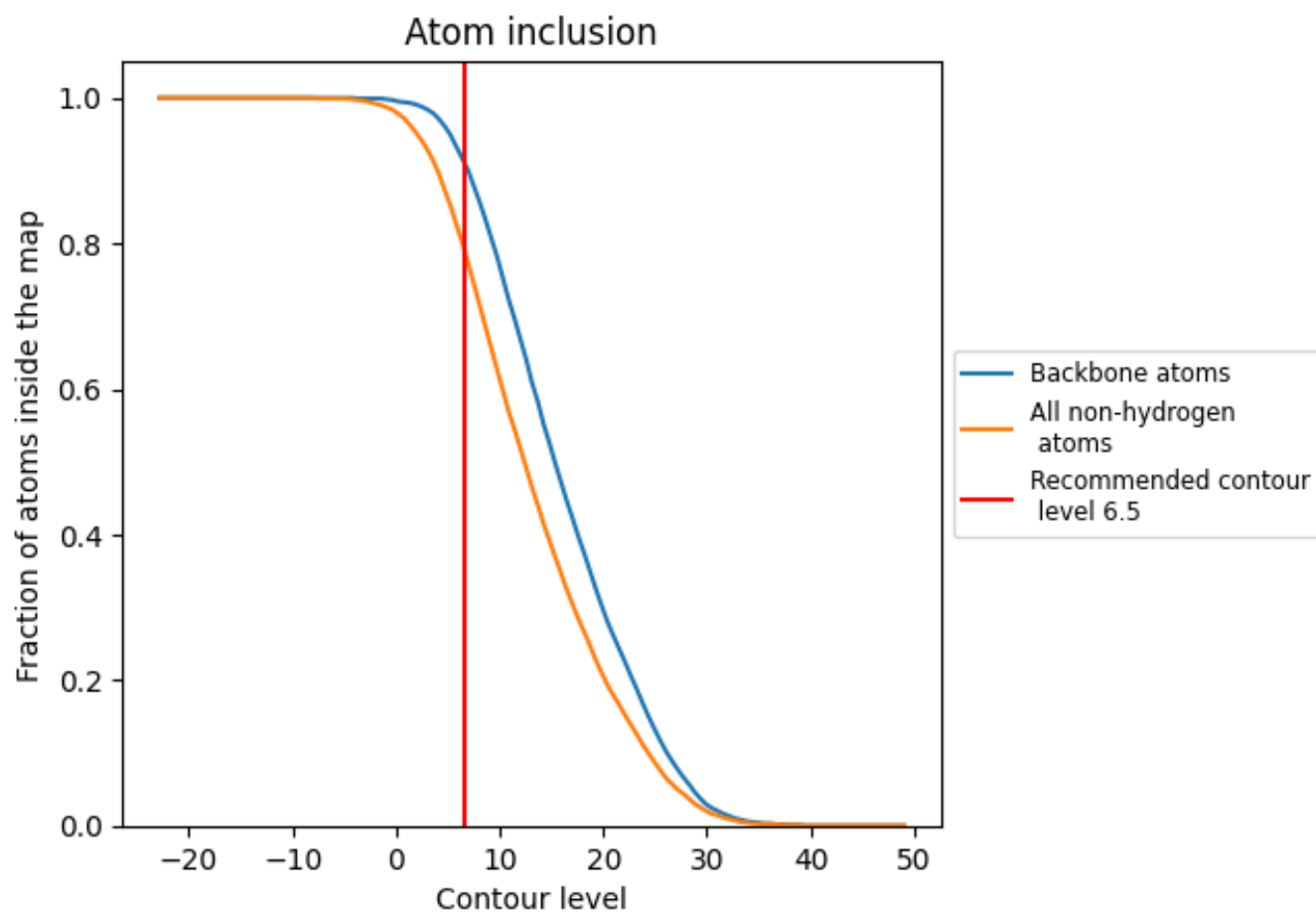
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).





9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.3430
A	 0.7950	 0.3430

