



Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 10:16 AM JST

PDB ID : 23PX / pdb_000023px
EMDB ID : EMD-69160
Title : YghJ protein zymogen-like autoinhibited state
Authors : Gu, J.K.; Zhang, M.H.
Deposited on : 2026-02-12
Resolution : 3.01 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.dev133
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) : 2.50

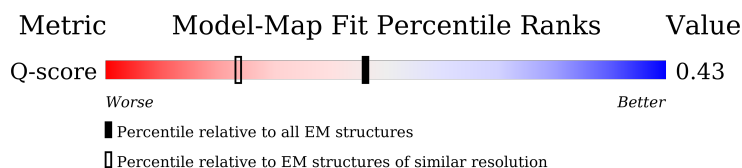
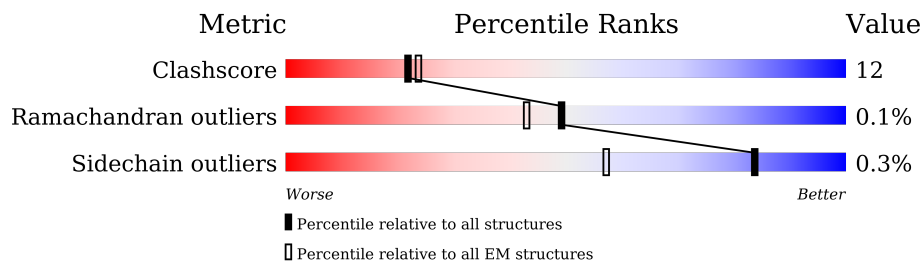
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 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	13882 (2.51 - 3.51)

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	1520	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10819 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 Putative lipoprotein AcfD homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1391	Total	C	N	O	S	0	0
			10818	6796	1828	2152	42		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	

L1370	L1371	M372	L1373	Q1375	D1385	K1388	W1389	Y1390	F1399	W1409	L1414	L1417	K1418	V1424	S1425	L1426	W1439	A1442	T1445	V1453	E1460	F1461	W1465	N1466	P1467	A1471	P1475	E1483	D1498	L1499	E1507	T1508	L1509	S1518	ALA	GLU							
T1251	Y1252	H1260	R1261	L1268	S1269	S1275	G1276	Y1277	P1278	V1279	M1280	S1288	L1296	E1304	H1307	N1308	V1316	V1322	A1323	N1324	N1325	L1329	N1330	M1331	G1332	D1333	Y1334	Y1335	M1339	D1345	L1346	T1347	V1348	A1349	P1350	L1353	Q1359	L1360	W1361	A1362	R1363	G1364	D1368
R1131	K1145	V1148	G1151	L1154	Y1155	L1156	S1167	F1170	T1171	G1172	V1173	Y1179	K1180	D1181	D1187	L1188	A1192	P1193	E1196	L1197	E1198	F1202	V1203	Y1204	T1205	T1206	P1207	K1208	W1209	N1210	E1221	D1226	L1227	F1230	M1234	D1241	D1244	G1245	R1248	M1249	F1250		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	291422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.905	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	231.56001, 231.56001, 231.56001	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/11065	0.43	7/15031 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	763	PRO	N-CA-CB	-10.88	91.82	103.25
1	A	1276	GLY	CA-C-O	-6.78	117.57	122.45
1	A	1277	TYR	N-CA-C	-5.87	105.62	113.25
1	A	1277	TYR	N-CA-CB	5.59	120.65	110.08
1	A	777	GLY	CA-C-N	-5.52	115.08	121.71
1	A	777	GLY	C-N-CA	-5.52	115.08	121.71
1	A	1025	PRO	N-CD-CG	-5.40	97.32	103.80

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	10818	0	10347	246	0
2	A	1	0	0	0	0
All	All	10819	0	10347	246	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 12.

All (246) 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:524:LEU:CD1	1:A:806:TYR:OH	1.66	1.40
1:A:524:LEU:HD11	1:A:806:TYR:OH	1.25	1.10
1:A:524:LEU:HD12	1:A:806:TYR:OH	1.54	1.05
1:A:524:LEU:HD11	1:A:806:TYR:CZ	1.94	1.02
1:A:825:GLU:OE2	1:A:834:ARG:NH2	2.06	0.87
1:A:527:ILE:HD11	1:A:802:VAL:HG21	1.56	0.85
1:A:1083:MET:O	1:A:1261:ARG:NH2	2.14	0.79
1:A:1322:VAL:HG21	1:A:1369:ARG:HB2	1.64	0.79
1:A:1088:LEU:HD23	1:A:1173:VAL:HG21	1.65	0.78
1:A:1086:THR:HG22	1:A:1088:LEU:HD13	1.69	0.75
1:A:1268:ILE:HG22	1:A:1280:MET:HE2	1.70	0.73
1:A:1202:PHE:HD2	1:A:1227:LEU:HD22	1.53	0.72
1:A:289:GLY:O	1:A:371:ARG:NH2	2.24	0.71
1:A:466:VAL:HG13	1:A:902:LEU:HD11	1.72	0.70
1:A:356:SER:O	1:A:364:ARG:NH2	2.24	0.70
1:A:416:GLN:NE2	1:A:419:GLU:OE1	2.28	0.67
1:A:532:SER:HB2	1:A:795:ILE:HD12	1.78	0.65
1:A:778:ILE:HD11	1:A:881:ARG:HD2	1.79	0.65
1:A:199:LYS:HE3	1:A:1345:ASP:HA	1.79	0.65
1:A:1099:LYS:NZ	1:A:1101:ASN:OD1	2.26	0.64
1:A:452:VAL:HA	1:A:455:LYS:HG2	1.79	0.64
1:A:167:LYS:NZ	1:A:209:ASP:OD1	2.30	0.64
1:A:458:GLY:HA3	1:A:465:SER:HA	1.80	0.63
1:A:941:SER:OG	1:A:944:ASP:OD2	2.11	0.63
1:A:243:VAL:HG11	1:A:1025:PRO:HG2	1.81	0.63
1:A:799:THR:HG23	1:A:801:GLU:H	1.63	0.62
1:A:1020:MET:HE2	1:A:1049:VAL:HG22	1.82	0.62
1:A:1069:ILE:HD13	1:A:1156:ILE:HG13	1.81	0.62
1:A:781:TYR:HD2	1:A:821:ALA:HB2	1.64	0.62
1:A:681:PHE:HD2	1:A:698:ALA:HB1	1.65	0.61
1:A:383:GLU:OE2	1:A:1269:SER:OG	2.18	0.61
1:A:1210:ASN:ND2	1:A:1288:SER:OG	2.30	0.61
1:A:164:SER:OG	1:A:166:ASP:OD1	2.18	0.61
1:A:243:VAL:HG21	1:A:1025:PRO:HB2	1.82	0.61
1:A:765:GLY:HA2	1:A:772:GLN:HB3	1.83	0.61
1:A:1248:ARG:NH1	1:A:1252:TYR:OH	2.34	0.61
1:A:1110:VAL:HG11	1:A:1148:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:OG1	1:A:364:ARG:NH1	2.34	0.61
1:A:524:LEU:HD11	1:A:806:TYR:CE1	2.36	0.61
1:A:1230:PHE:HD1	1:A:1331:MET:HE2	1.64	0.61
1:A:488:GLN:NE2	1:A:754:LEU:O	2.34	0.60
1:A:1333:ASP:OD2	1:A:1409:TRP:NE1	2.30	0.60
1:A:1372:MET:HE1	1:A:1467:PRO:HB3	1.84	0.60
1:A:482:THR:HG21	1:A:581:TRP:HH2	1.66	0.60
1:A:698:ALA:HB2	1:A:727:GLU:OE2	2.02	0.60
1:A:347:ASN:ND2	1:A:387:LEU:O	2.35	0.59
1:A:1507:GLU:HG2	1:A:1508:THR:HG23	1.85	0.59
1:A:204:LEU:HD13	1:A:219:VAL:HG12	1.84	0.58
1:A:391:ASN:OD1	1:A:406:ASN:ND2	2.36	0.58
1:A:506:ASP:OD1	1:A:545:THR:N	2.33	0.58
1:A:1359:GLN:OE1	1:A:1466:ASN:ND2	2.31	0.58
1:A:136:ASN:OD1	1:A:159:GLN:NE2	2.36	0.58
1:A:156:GLU:HB3	1:A:168:LYS:HD2	1.84	0.58
1:A:1179:TYR:OH	1:A:1221:GLU:OE1	2.22	0.57
1:A:628:THR:HG22	1:A:677:ILE:HB	1.86	0.57
1:A:1203:VAL:HG13	1:A:1261:ARG:HD3	1.85	0.57
1:A:1375:GLN:NE2	1:A:1509:ILE:HG12	2.19	0.57
1:A:927:GLU:OE2	1:A:1034:THR:OG1	2.22	0.57
1:A:1304:GLU:HA	1:A:1307:HIS:HD2	1.68	0.57
1:A:186:GLU:O	1:A:187:GLN:HG2	2.04	0.57
1:A:965:GLU:HB3	1:A:968:LYS:HD3	1.85	0.56
1:A:262:GLU:OE1	1:A:942:SER:OG	2.18	0.56
1:A:457:TRP:CZ3	1:A:902:LEU:HB2	2.40	0.56
1:A:1098:ILE:HD12	1:A:1170:PHE:HD2	1.71	0.56
1:A:1362:ALA:HB1	1:A:1471:ALA:HB2	1.88	0.56
1:A:1095:GLU:OE2	1:A:1097:THR:OG1	2.23	0.55
1:A:1040:ARG:HG2	1:A:1047:ILE:HD12	1.88	0.55
1:A:499:PRO:HB3	1:A:549:PRO:HG3	1.89	0.55
1:A:961:SER:OG	1:A:963:ARG:NH1	2.40	0.55
1:A:130:THR:HG21	1:A:201:PHE:HD2	1.70	0.55
1:A:1101:ASN:ND2	1:A:1167:SER:OG	2.34	0.55
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.72	0.54
1:A:724:LEU:HD21	1:A:726:MET:HE3	1.88	0.54
1:A:1083:MET:HE3	1:A:1277:TYR:CD2	2.43	0.54
1:A:130:THR:HG21	1:A:201:PHE:CD2	2.42	0.54
1:A:1098:ILE:HD12	1:A:1170:PHE:CD2	2.43	0.54
1:A:484:ASN:HA	1:A:761:ASN:HD22	1.73	0.54
1:A:392:GLY:HA2	1:A:404:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:MET:HG2	1:A:657:ILE:HG22	1.90	0.53
1:A:1418:LYS:NZ	1:A:1426:ASN:OD1	2.33	0.53
1:A:553:LEU:HD21	1:A:560:LYS:HB2	1.90	0.53
1:A:982:ASN:OD1	1:A:989:TYR:HB2	2.09	0.53
1:A:1275:SER:HB3	1:A:1304:GLU:OE2	2.08	0.53
1:A:288:ALA:HB3	1:A:365:VAL:HG22	1.91	0.53
1:A:95:THR:HG22	1:A:101:ARG:HA	1.91	0.53
1:A:192:PHE:CE2	1:A:198:SER:HB2	2.44	0.53
1:A:1347:THR:HG23	1:A:1348:VAL:HG13	1.91	0.53
1:A:1148:VAL:HG12	1:A:1151:GLY:H	1.74	0.52
1:A:1261:ARG:HB2	1:A:1278:PRO:HA	1.90	0.52
1:A:1020:MET:HE1	1:A:1038:LEU:HA	1.90	0.52
1:A:1278:PRO:O	1:A:1280:MET:HG3	2.09	0.52
1:A:926:HIS:NE2	1:A:1029:MET:O	2.43	0.52
1:A:1333:ASP:OD1	1:A:1339:MET:HB3	2.10	0.52
1:A:1244:ASP:OD1	1:A:1245:GLY:N	2.42	0.52
1:A:1372:MET:HE2	1:A:1465:TRP:HB3	1.92	0.51
1:A:542:ASP:OD1	1:A:543:THR:N	2.43	0.51
1:A:634:TYR:HB2	1:A:696:LEU:HD11	1.93	0.51
1:A:711:THR:OG1	1:A:743:ARG:NH2	2.36	0.51
1:A:310:SER:O	1:A:313:GLU:HG2	2.10	0.51
1:A:1198:GLU:HG3	1:A:1203:VAL:HB	1.92	0.51
1:A:199:LYS:HZ3	1:A:1348:VAL:H	1.57	0.51
1:A:1316:VAL:HA	1:A:1442:ALA:HB3	1.93	0.51
1:A:1067:GLU:HB2	1:A:1170:PHE:HE1	1.75	0.51
1:A:1361:TRP:CZ3	1:A:1369:ARG:HB3	2.46	0.51
1:A:175:VAL:HG13	1:A:190:LEU:HD13	1.92	0.50
1:A:1203:VAL:CG1	1:A:1261:ARG:HD3	2.41	0.50
1:A:455:LYS:HB2	1:A:463:TYR:CD2	2.46	0.50
1:A:1261:ARG:HB2	1:A:1277:TYR:O	2.11	0.50
1:A:1353:LEU:HD21	1:A:1465:TRP:CE2	2.47	0.50
1:A:1230:PHE:CD1	1:A:1331:MET:HE2	2.45	0.50
1:A:1187:ASP:OD1	1:A:1188:LEU:N	2.44	0.50
1:A:1324:ASN:OD1	1:A:1325:ASN:N	2.44	0.50
1:A:199:LYS:NZ	1:A:1348:VAL:HG22	2.27	0.49
1:A:769:ARG:HB2	1:A:772:GLN:NE2	2.27	0.49
1:A:1202:PHE:HE1	1:A:1260:HIS:HD1	1.60	0.49
1:A:1097:THR:HB	1:A:1171:THR:OG1	2.13	0.49
1:A:482:THR:HG21	1:A:581:TRP:CH2	2.47	0.49
1:A:682:GLU:OE1	1:A:702:LYS:HB3	2.12	0.49
1:A:95:THR:N	1:A:153:PHE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:H	1:A:187:GLN:HA	1.77	0.49
1:A:199:LYS:HZ3	1:A:1348:VAL:HG22	1.77	0.49
1:A:450:GLN:NE2	1:A:454:ASN:OD1	2.45	0.49
1:A:327:VAL:HG11	1:A:334:ILE:HD13	1.94	0.49
1:A:1375:GLN:HE22	1:A:1509:ILE:HG12	1.77	0.49
1:A:1249:MET:SD	1:A:1252:TYR:HB3	2.53	0.48
1:A:1329:LEU:HD22	1:A:1339:MET:HB2	1.94	0.48
1:A:566:ASN:OD1	1:A:567:PRO:HD2	2.14	0.48
1:A:472:PHE:HB2	1:A:566:ASN:ND2	2.29	0.48
1:A:916:LEU:HD21	1:A:955:TRP:CD2	2.49	0.48
1:A:1275:SER:HB2	1:A:1308:ASN:OD1	2.13	0.48
1:A:1364:GLY:HA3	1:A:1368:ASP:OD2	2.14	0.48
1:A:252:LEU:HD13	1:A:265:TYR:CE2	2.49	0.48
1:A:1202:PHE:HE1	1:A:1260:HIS:ND1	2.13	0.47
1:A:529:GLU:HG3	1:A:531:PRO:HD2	1.97	0.47
1:A:1498:ASP:N	1:A:1498:ASP:OD1	2.45	0.47
1:A:949:TYR:HD2	1:A:950:GLN:HE21	1.61	0.47
1:A:1349:ALA:N	1:A:1350:PRO:HD2	2.30	0.47
1:A:694:ILE:HD13	1:A:730:MET:HE1	1.96	0.47
1:A:1026:LEU:HG	1:A:1126:LEU:HB3	1.97	0.47
1:A:1399:PHE:CZ	1:A:1417:ARG:HD2	2.50	0.47
1:A:381:ILE:HD11	1:A:385:ILE:HD12	1.96	0.46
1:A:1079:PHE:CD1	1:A:1308:ASN:HB3	2.49	0.46
1:A:1085:SER:HA	1:A:1155:TYR:HD1	1.80	0.46
1:A:1126:LEU:HD21	1:A:1130:PRO:HD3	1.97	0.46
1:A:304:ASN:O	1:A:304:ASN:ND2	2.32	0.46
1:A:1276:GLY:O	1:A:1277:TYR:C	2.58	0.46
1:A:452:VAL:HG21	1:A:498:PHE:CE1	2.50	0.46
1:A:945:LEU:HD21	1:A:1029:MET:HA	1.97	0.46
1:A:170:ASN:OD1	1:A:212:PRO:HA	2.16	0.46
1:A:1498:ASP:O	1:A:1499:LEU:HD23	2.15	0.46
1:A:1115:ASP:OD1	1:A:1131:ARG:HG2	2.15	0.46
1:A:779:TRP:NE1	1:A:840:GLU:OE2	2.49	0.46
1:A:777:GLY:N	1:A:840:GLU:OE1	2.49	0.45
1:A:551:ILE:HG12	1:A:564:ILE:HG23	1.97	0.45
1:A:617:LYS:HB2	1:A:620:ALA:HB3	1.99	0.45
1:A:1399:PHE:HZ	1:A:1417:ARG:HD2	1.81	0.45
1:A:1277:TYR:HB3	1:A:1278:PRO:HD3	1.99	0.45
1:A:1414:LEU:HD23	1:A:1453:VAL:HG13	1.97	0.45
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.78	0.45
1:A:1077:LYS:HG3	1:A:1250:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:ASP:OD2	1:A:1296:LEU:HG	2.16	0.45
1:A:429:ASP:OD1	1:A:429:ASP:N	2.44	0.45
1:A:460:ASP:C	1:A:462:ASN:H	2.25	0.45
1:A:609:ARG:NH1	1:A:614:ASP:HA	2.32	0.45
1:A:769:ARG:HB2	1:A:772:GLN:HE22	1.82	0.44
1:A:1078:TRP:CH2	1:A:1276:GLY:HA2	2.51	0.44
1:A:1095:GLU:OE2	1:A:1145:LYS:HG2	2.17	0.44
1:A:958:ASN:O	1:A:1040:ARG:NH1	2.50	0.44
1:A:471:VAL:HB	1:A:898:THR:HB	1.99	0.44
1:A:791:LEU:HD13	1:A:793:TYR:CZ	2.52	0.44
1:A:952:MET:HE2	1:A:952:MET:HB2	1.81	0.44
1:A:279:LEU:HD22	1:A:317:PHE:CE1	2.53	0.44
1:A:174:LEU:HB2	1:A:215:PHE:HE2	1.82	0.44
1:A:1192:ALA:O	1:A:1208:LYS:HD2	2.18	0.44
1:A:455:LYS:HB2	1:A:463:TYR:CE2	2.53	0.44
1:A:785:PRO:HD3	1:A:819:GLU:OE1	2.17	0.44
1:A:1234:MET:HE3	1:A:1250:PHE:CD2	2.52	0.44
1:A:274:LEU:HD13	1:A:1475:PRO:HG2	2.00	0.43
1:A:1196:GLU:HA	1:A:1204:TYR:O	2.18	0.43
1:A:1202:PHE:HE2	1:A:1230:PHE:HD2	1.66	0.43
1:A:1371:LEU:O	1:A:1375:GLN:HG2	2.18	0.43
1:A:630:LEU:HB2	1:A:648:PHE:CD2	2.54	0.43
1:A:768:ASN:HA	1:A:820:VAL:HG21	2.00	0.43
1:A:1244:ASP:CG	1:A:1245:GLY:H	2.26	0.43
1:A:775:ALA:O	1:A:883:GLY:HA3	2.18	0.43
1:A:130:THR:HG22	1:A:202:ASP:OD1	2.19	0.43
1:A:356:SER:HB3	1:A:366:VAL:HG12	2.00	0.43
1:A:1460:GLU:HG2	1:A:1461:PHE:N	2.33	0.43
1:A:463:TYR:HB3	1:A:606:ASN:OD1	2.19	0.43
1:A:1385:ASP:HB3	1:A:1388:LYS:HE2	2.01	0.43
1:A:96:LEU:HD21	1:A:175:VAL:HG11	2.00	0.43
1:A:872:HIS:CD2	1:A:882:PRO:HD3	2.54	0.43
1:A:107:CYS:N	1:A:110:GLU:O	2.51	0.43
1:A:766:TYR:HE1	1:A:892:MET:HA	1.84	0.43
1:A:166:ASP:OD1	1:A:166:ASP:N	2.52	0.43
1:A:478:PHE:HE1	1:A:691:PRO:HB2	1.84	0.43
1:A:654:PHE:HB3	1:A:657:ILE:HD11	2.00	0.43
1:A:1005:ASP:OD1	1:A:1006:ASN:N	2.51	0.43
1:A:1483:GLU:N	1:A:1483:GLU:OE1	2.51	0.43
1:A:927:GLU:OE1	1:A:1033:LEU:HB3	2.19	0.42
1:A:484:ASN:HA	1:A:761:ASN:ND2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ASP:O	1:A:763:PRO:C	2.63	0.42
1:A:380:VAL:HA	1:A:383:GLU:OE1	2.19	0.42
1:A:1001:LYS:HA	1:A:1004:VAL:HG22	2.01	0.42
1:A:730:MET:O	1:A:755:ASN:ND2	2.53	0.42
1:A:932:THR:HB	1:A:935:ARG:HG2	2.01	0.42
1:A:986:ASN:OD1	1:A:1018:GLY:HA3	2.19	0.42
1:A:196:ILE:HG13	1:A:197:GLU:N	2.34	0.42
1:A:1024:TYR:HA	1:A:1025:PRO:HA	1.86	0.42
1:A:171:ALA:N	1:A:208:ILE:HD11	2.35	0.42
1:A:1442:ALA:HA	1:A:1445:THR:HG22	2.01	0.41
1:A:510:TRP:HZ2	1:A:873:TYR:CE2	2.37	0.41
1:A:1296:LEU:HD22	1:A:1335:TYR:CD2	2.55	0.41
1:A:1390:TYR:CE2	1:A:1424:VAL:HG21	2.55	0.41
1:A:158:ALA:HB3	1:A:161:LEU:HG	2.02	0.41
1:A:192:PHE:HB2	1:A:197:GLU:HB3	2.03	0.41
1:A:727:GLU:OE1	1:A:729:VAL:HG23	2.19	0.41
1:A:961:SER:O	1:A:963:ARG:NH1	2.53	0.41
1:A:174:LEU:HB2	1:A:215:PHE:CE2	2.55	0.41
1:A:174:LEU:HD22	1:A:215:PHE:HZ	1.85	0.41
1:A:199:LYS:NZ	1:A:1348:VAL:H	2.17	0.41
1:A:199:LYS:CE	1:A:1348:VAL:HG22	2.50	0.41
1:A:328:ARG:NH1	1:A:330:ASN:HB3	2.36	0.41
1:A:872:HIS:HB2	1:A:873:TYR:CD1	2.55	0.41
1:A:1112:LEU:HD23	1:A:1112:LEU:HA	1.83	0.41
1:A:1206:THR:HG23	1:A:1207:PRO:O	2.21	0.41
1:A:1279:VAL:HG13	1:A:1304:GLU:HG2	2.03	0.41
1:A:782:GLU:CD	1:A:881:ARG:HH22	2.29	0.41
1:A:1322:VAL:HG12	1:A:1373:TYR:HE2	1.86	0.41
1:A:624:MET:O	1:A:657:ILE:HA	2.21	0.41
1:A:771:ARG:HD2	1:A:873:TYR:HD2	1.86	0.41
1:A:1065:VAL:HG21	1:A:1088:LEU:HD21	2.02	0.41
1:A:931:ARG:HH12	1:A:1008:MET:HG2	1.86	0.41
1:A:1026:LEU:HD11	1:A:1126:LEU:HD23	2.03	0.41
1:A:1241:ASP:HA	1:A:1249:MET:HE2	2.02	0.41
1:A:193:SER:O	1:A:194:SER:OG	2.29	0.41
1:A:1180:LYS:C	1:A:1181:ASP:OD1	2.64	0.40
1:A:328:ARG:HH12	1:A:330:ASN:HB3	1.87	0.40
1:A:940:LEU:HB3	1:A:944:ASP:OD1	2.21	0.40
1:A:1108:VAL:HG13	1:A:1154:ILE:HG23	2.03	0.40
1:A:327:VAL:HB	1:A:339:LEU:HD23	2.02	0.40
1:A:542:ASP:OD1	1:A:543:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:GLY:HA3	1:A:1193:PRO:HG3	2.03	0.40
1:A:348:ILE:HD13	1:A:348:ILE:HA	1.95	0.40
1:A:628:THR:HG21	1:A:648:PHE:CE2	2.57	0.40
1:A:1048:LYS:NZ	1:A:1093:GLN:OE1	2.45	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	1381/1520 (91%)	1321 (96%)	58 (4%)	2 (0%)	48 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	763	PRO
1	A	772	GLN

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	1170/1284 (91%)	1166 (100%)	4 (0%)	86 90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	763	PRO
1	A	776	THR
1	A	1026	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	382	ASN
1	A	406	ASN
1	A	450	GLN
1	A	488	GLN
1	A	708	GLN
1	A	755	ASN
1	A	760	ASN
1	A	761	ASN
1	A	772	GLN
1	A	1210	ASN
1	A	1375	GLN
1	A	1383	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

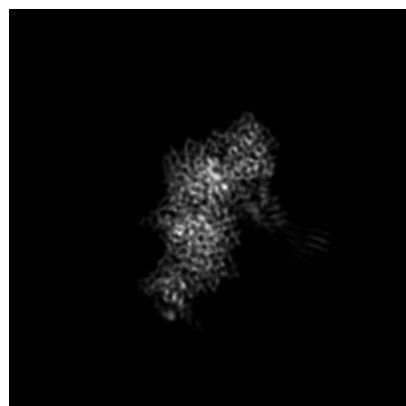
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69160. These allow visual inspection of the internal detail of the map and identification of artifacts.

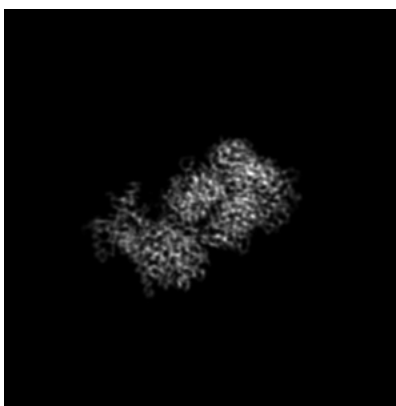
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

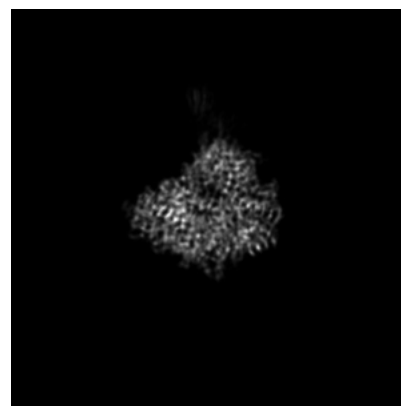
6.1.1 Primary map



X

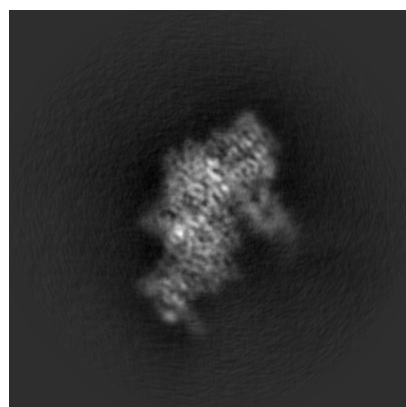


Y

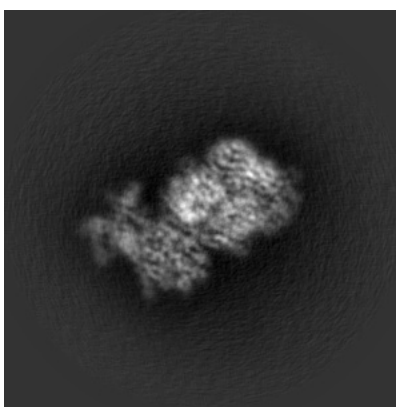


Z

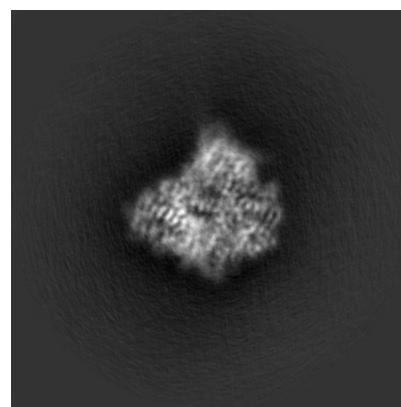
6.1.2 Raw map



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: 140

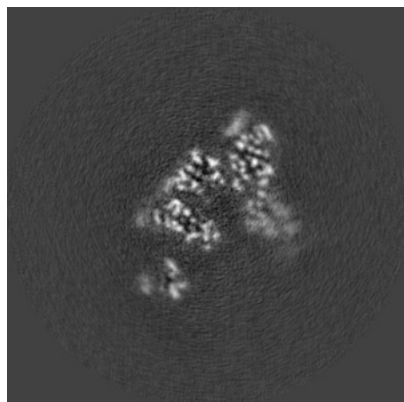


Y Index: 140

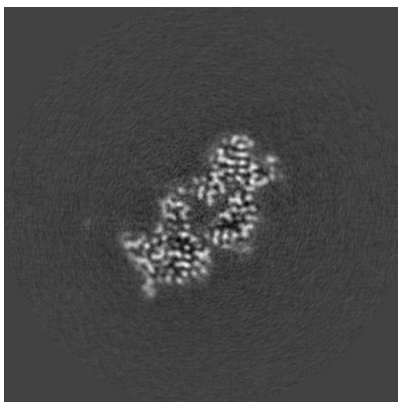


Z Index: 140

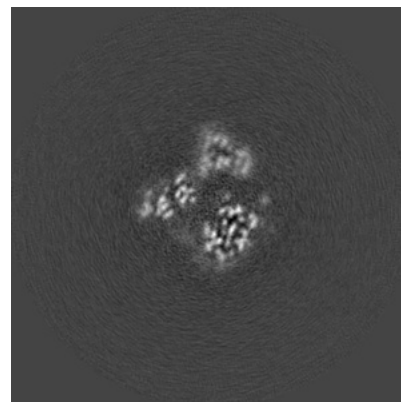
6.2.2 Raw map



X Index: 140



Y Index: 140



Z Index: 140

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: 147

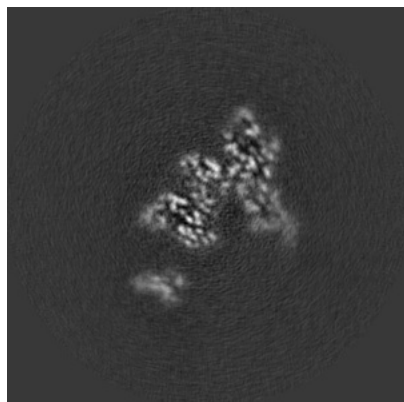


Y Index: 140

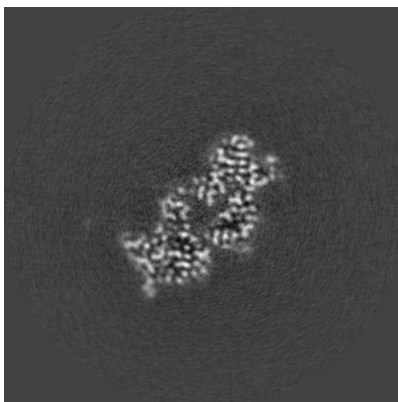


Z Index: 163

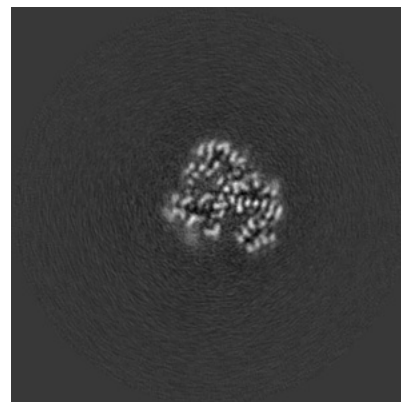
6.3.2 Raw map



X Index: 146



Y Index: 140

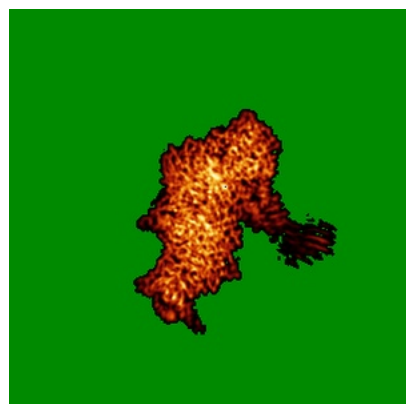


Z Index: 164

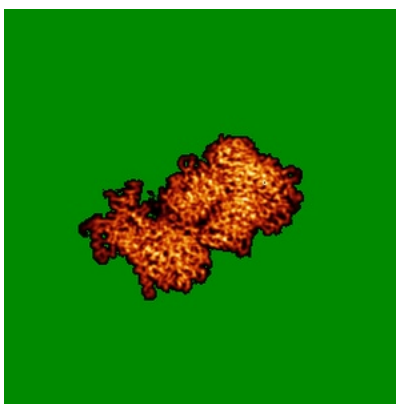
The images above show the largest variance slices of the map in three orthogonal directions.

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

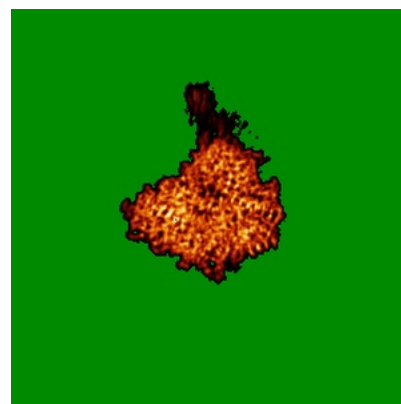
6.4.1 Primary map



X

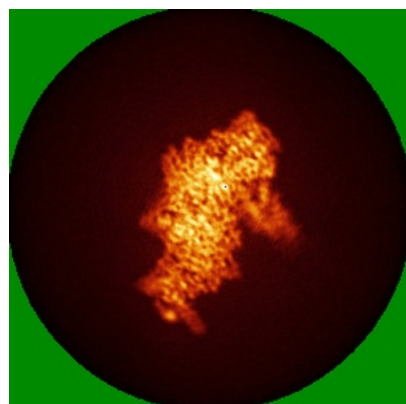


Y

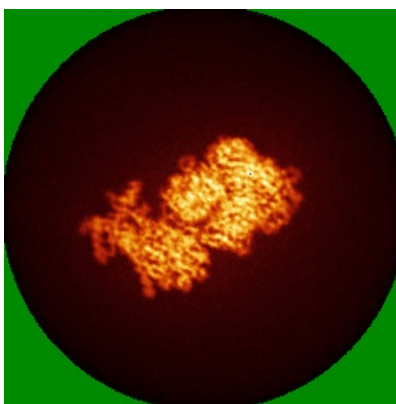


Z

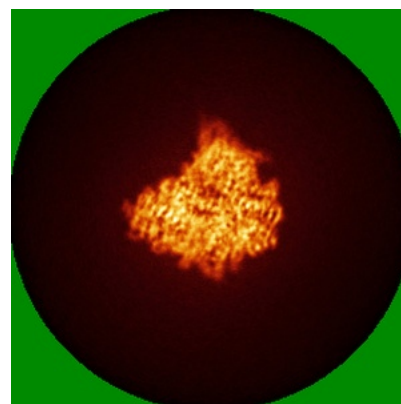
6.4.2 Raw map



X



Y

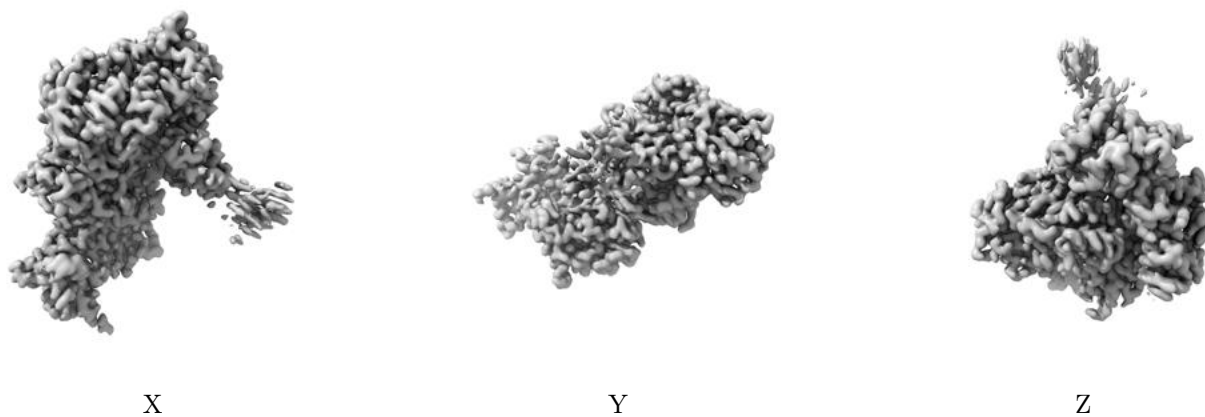


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

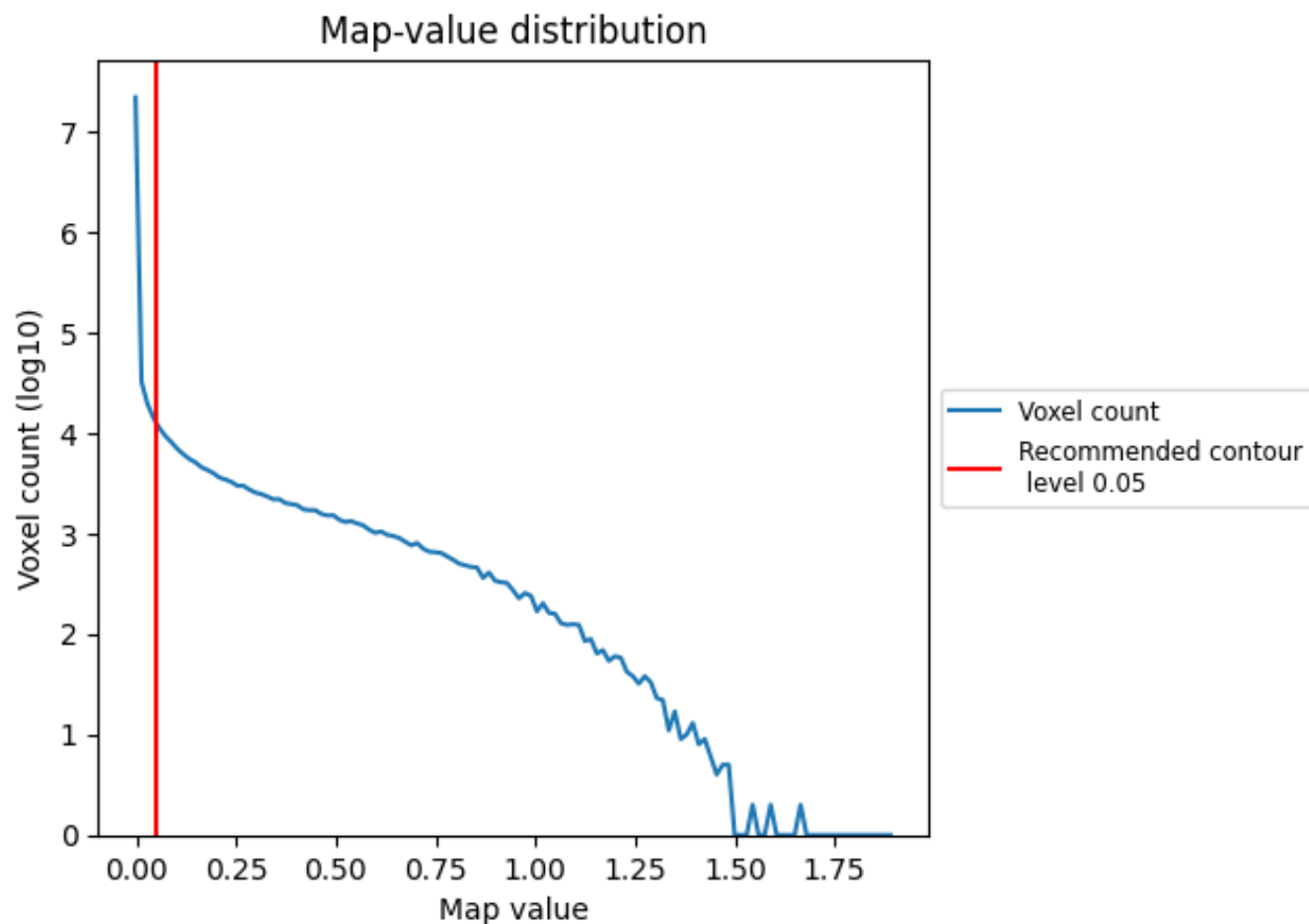
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

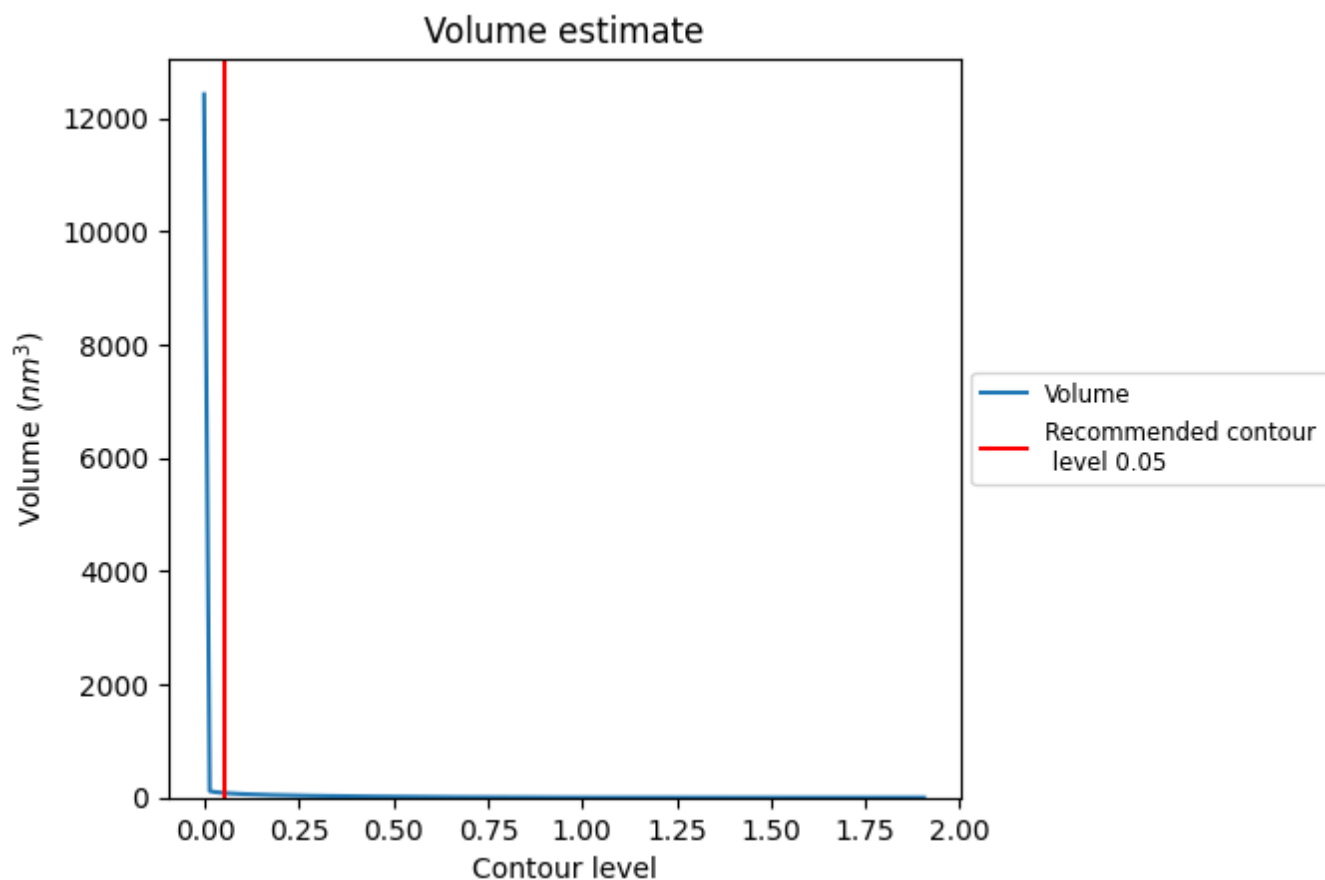
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

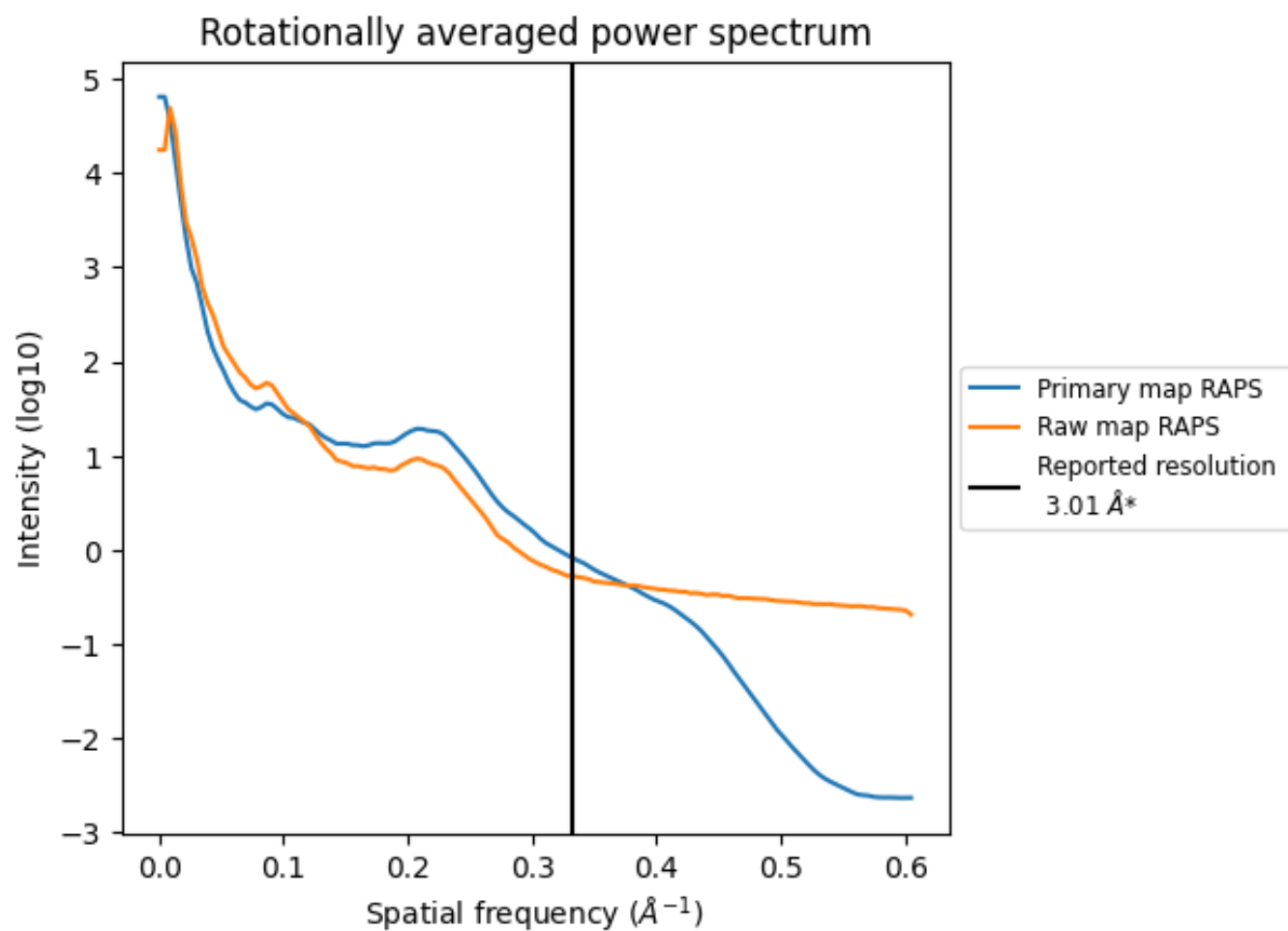
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm^3 ; this corresponds to an approximate mass of 74 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

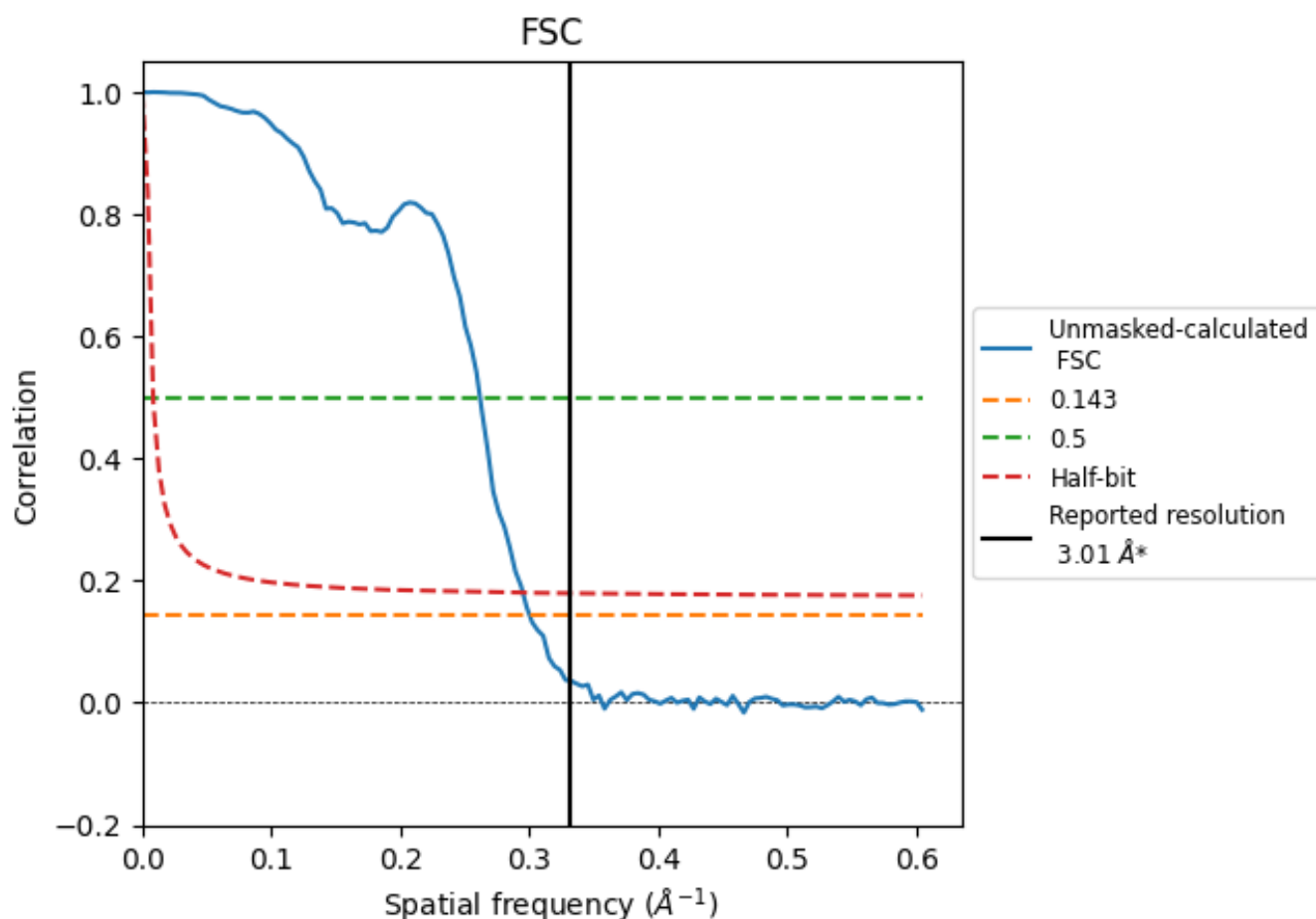


*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

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 0.332 Å⁻¹

8.2 Resolution estimates [i](#)

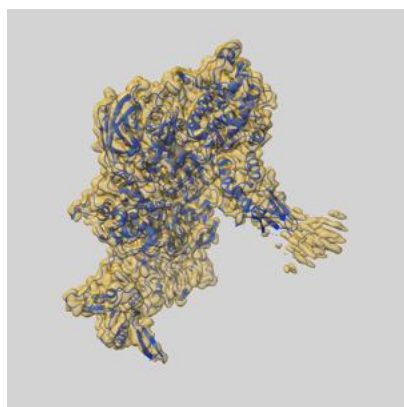
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.33	3.82	3.39

*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 3.33 differs from the reported value 3.01 by more than 10 %

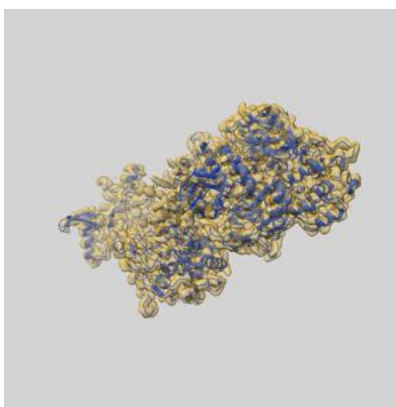
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-69160 and PDB model 23PX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

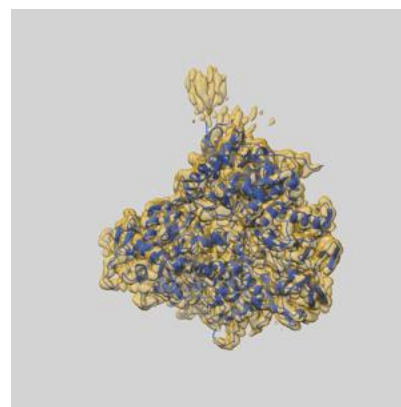
9.1 Map-model overlay [i](#)



X



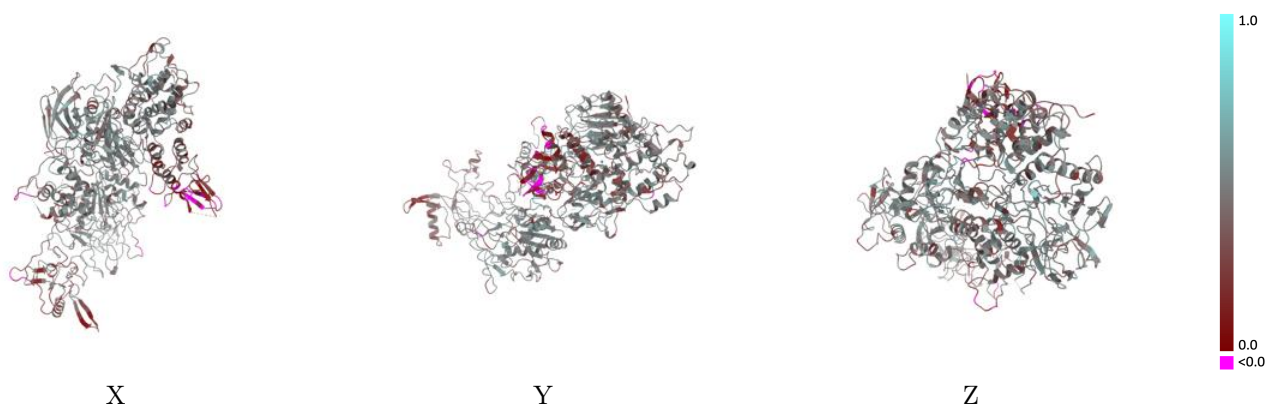
Y



Z

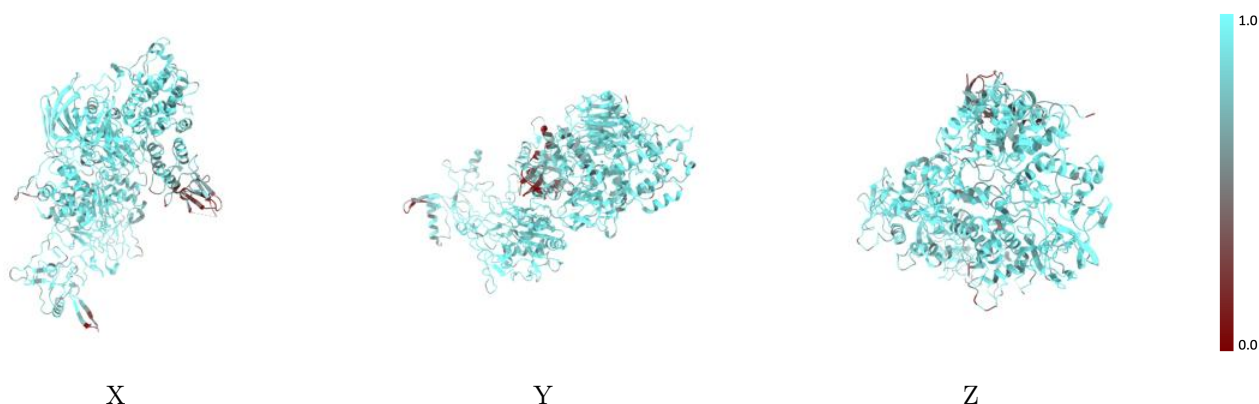
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



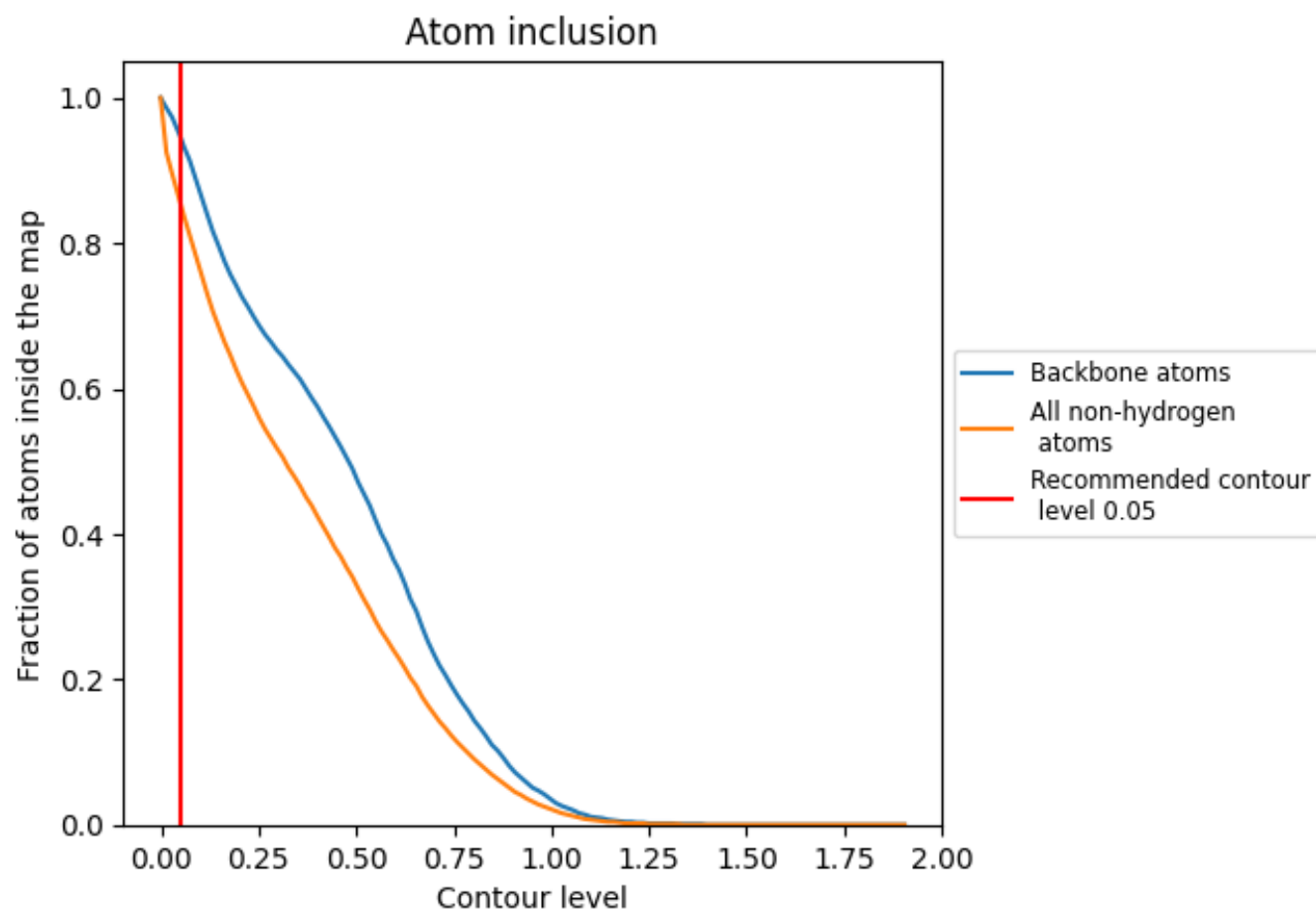
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.4300
A	0.8530	0.4300

