



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 06:14 PM UTC

PDB ID : 7MWF / pdb_00007mwf
EMDB ID : EMD-22430
Title : HUWE1 in map with focus on interface
Authors : Hunkeler, M.; Fischer, E.S.
Deposited on : 2021-05-16
Resolution : 3.30 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

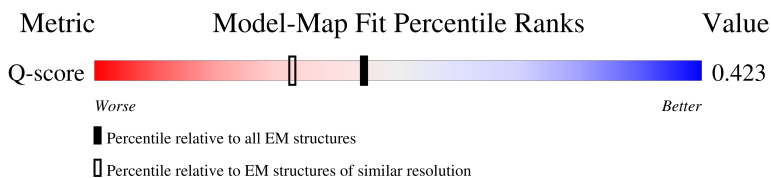
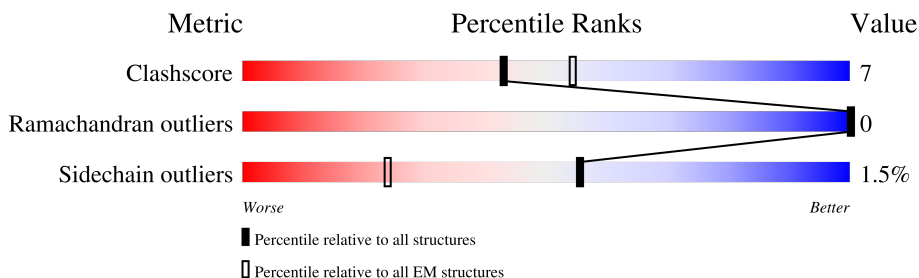
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	4411	18% 45% 9% 45%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38719 atoms, of which 19554 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 E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2427	Total	C	H	N	O	S	0	0
			38719	12225	19554	3292	3528	120		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	MET	-	expression tag	UNP Q7Z6Z7
A	-35	ASP	-	expression tag	UNP Q7Z6Z7
A	-34	TYR	-	expression tag	UNP Q7Z6Z7
A	-33	LYS	-	expression tag	UNP Q7Z6Z7
A	-32	ASP	-	expression tag	UNP Q7Z6Z7
A	-31	ASP	-	expression tag	UNP Q7Z6Z7
A	-30	ASP	-	expression tag	UNP Q7Z6Z7
A	-29	ASP	-	expression tag	UNP Q7Z6Z7
A	-28	LYS	-	expression tag	UNP Q7Z6Z7
A	-27	LEU	-	expression tag	UNP Q7Z6Z7
A	-26	ALA	-	expression tag	UNP Q7Z6Z7
A	-25	ALA	-	expression tag	UNP Q7Z6Z7
A	-24	ALA	-	expression tag	UNP Q7Z6Z7
A	-23	ASN	-	expression tag	UNP Q7Z6Z7
A	-22	SER	-	expression tag	UNP Q7Z6Z7
A	-21	SER	-	expression tag	UNP Q7Z6Z7
A	-20	ILE	-	expression tag	UNP Q7Z6Z7
A	-19	ASP	-	expression tag	UNP Q7Z6Z7
A	-18	LEU	-	expression tag	UNP Q7Z6Z7
A	-17	ILE	-	expression tag	UNP Q7Z6Z7
A	-16	SER	-	expression tag	UNP Q7Z6Z7
A	-15	THR	-	expression tag	UNP Q7Z6Z7
A	-14	SER	-	expression tag	UNP Q7Z6Z7
A	-13	LEU	-	expression tag	UNP Q7Z6Z7
A	-12	TYR	-	expression tag	UNP Q7Z6Z7
A	-11	LYS	-	expression tag	UNP Q7Z6Z7
A	-10	LYS	-	expression tag	UNP Q7Z6Z7
A	-9	ALA	-	expression tag	UNP Q7Z6Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q7Z6Z7
A	-7	PHE	-	expression tag	UNP Q7Z6Z7
A	-6	LYS	-	expression tag	UNP Q7Z6Z7
A	-5	GLY	-	expression tag	UNP Q7Z6Z7
A	-4	THR	-	expression tag	UNP Q7Z6Z7
A	-3	ASN	-	expression tag	UNP Q7Z6Z7
A	-2	SER	-	expression tag	UNP Q7Z6Z7
A	-1	VAL	-	expression tag	UNP Q7Z6Z7
A	0	ASP	-	expression tag	UNP Q7Z6Z7







D4329	R4330	S4331	T4332	D4333	R4334	L4335	P4336	S4337	A4338	H4339	T4340	C4341	F4342	M4343	Q4344	L4345	D4346	L4347	P4348	A4349	Y4350	E4351	S4352	F4353	E4354	K4355	L4356	R4357	H4358	M4359	L4360	L4361	L4362	A4363	T4364	GLN	GLU	CYS	SER	GLU	GLY	PHE	GLY	LEU	ALA														
H4269	K4270	Y4271	Q4272	S4273	M4274	S4275	I4276	Q4277	I4278	Q4279	W4280	F4281	W4282	R4283	A4284	L4285	R4286	S4287	F4288	D4289	Q4290	A4291	D4292	R4293	A4294	K4295	F4296	L4297	Q4298	F4299	V4300	T4301	G4302	T4303	S4304	K4305	V4306	P4307	L4308	Q4309	G4310	F4311	A4312	A4313	L4314	E4315	G4316	M4317	N4318	G4319	I4320	Q4321	K4322	F4323	Q4324	I4325	H4326	R4327	D4328
L4209	V4210	C4211	Q4212	M4213	R4214	M4215	T4216	G4217	A4218	I4219	R4220	K4221	Q4222	L4223	A4224	A4225	F4226	L4227	E4228	G4229	F4230	Y4231	E4232	I4233	I4234	P4235	K4236	R4237	L4238	I4239	S4240	I4241	F4242	T4243	E4244	Q4245	E4246	L4247	E4248	L4249	L4250	I4251	S4252	G4253	L4254	P4255	T4256	I4257	D4258	I4259	D4260	D4261	L4262	K4263	S4264	N4265	T4266	E4267	Y4268
E4149	D4150	Y4151	H4152	F4153	Y4154	Q4155	G4156	L4157	V4158	Y4159	L4160	L4161	E4162	H4163	D4164	V4165	S4166	T4167	L4168	G4169	Y4170	D4171	L4172	T4173	F4174	S4175	T4176	E4177	V4178	Q4179	E4180	F4181	G4182	V4183	C4184	E4185	V4186	R4187	D4188	L4189	K4190	PRO	ASN	GLY	ALA	ASN	ILE	LEU	V4198	T4199	E4200	E4201	H4202	K4203	K4204	E4205	Y4206	V4207	H4208

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	125477	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; standard correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.68	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.139	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	300.3, 300.3, 300.3	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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	0.26	0/19509	0.51	1/26411 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1598	ILE	N-CA-C	-8.28	101.62	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19165	19554	19539	257	0
All	All	19165	19554	19539	257	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 7.

All (257) 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:2227:ARG:NH2	1:A:3184:GLU:OE1	2.12	0.82
1:A:568:GLN:O	1:A:4063:ARG:NH2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:LEU:HD22	1:A:1138:THR:HG22	1.69	0.75
1:A:1825:ARG:NH1	1:A:2081:SER:OG	2.20	0.75
1:A:1134:SER:O	1:A:1138:THR:HG23	1.87	0.73
1:A:4248:GLU:OE1	1:A:4298:GLN:NE2	2.21	0.72
1:A:1510:VAL:O	1:A:1514:ILE:HG23	1.91	0.70
1:A:4328:ASP:OD2	1:A:4330:ARG:NE	2.25	0.70
1:A:4286:ARG:O	1:A:4293:ARG:NH2	2.25	0.69
1:A:569:GLU:OE1	1:A:4063:ARG:NH1	2.25	0.68
1:A:2069:SER:OG	1:A:2125:ASP:OD2	2.07	0.68
1:A:2663:MET:O	1:A:2667:VAL:HG23	1.94	0.68
1:A:66:ALA:O	1:A:70:GLN:NE2	2.27	0.66
1:A:652:LEU:HB3	1:A:771:LEU:HD21	1.77	0.65
1:A:1826:HIS:NE2	1:A:2654:GLU:OE2	2.29	0.65
1:A:1579:THR:OG1	1:A:1770:VAL:O	2.16	0.64
1:A:1507:THR:O	1:A:1509:THR:HG23	1.97	0.63
1:A:1829:GLU:OE2	1:A:2082:TYR:OH	2.15	0.63
1:A:4082:ARG:NH1	1:A:4094:ASN:OD1	2.31	0.63
1:A:1655:ARG:HE	1:A:1655:ARG:HA	1.65	0.61
1:A:1504:THR:O	1:A:1505:SER:OG	2.12	0.61
1:A:3851:LEU:HD13	1:A:3851:LEU:O	2.01	0.61
1:A:1671:GLU:N	1:A:1671:GLU:OE2	2.34	0.60
1:A:4161:LEU:HD21	1:A:4207:VAL:HG21	1.84	0.60
1:A:1539:GLU:OE2	1:A:1539:GLU:N	2.35	0.59
1:A:1822:LEU:O	1:A:1826:HIS:ND1	2.36	0.59
1:A:157:THR:OG1	1:A:158:PRO:HD3	2.03	0.58
1:A:3292:ALA:HB1	1:A:3327:GLN:HB3	1.86	0.58
1:A:355:TYR:O	1:A:364:ARG:NH2	2.37	0.57
1:A:1817:THR:OG1	1:A:1818:PRO:HD3	2.03	0.57
1:A:785:THR:HG22	1:A:785:THR:O	2.03	0.57
1:A:4324:GLN:NE2	1:A:4342:PHE:O	2.37	0.57
1:A:4268:TYR:HH	1:A:4282:TRP:HZ2	1.53	0.56
1:A:1165:ALA:O	1:A:1169:THR:HG23	2.06	0.56
1:A:1756:THR:HG22	1:A:1794:MET:HE1	1.87	0.55
1:A:1897:LEU:HD21	1:A:2682:ARG:HG2	1.87	0.55
1:A:100:THR:HG22	1:A:104:ILE:HD13	1.89	0.55
1:A:4174:PHE:CD2	1:A:4190:LYS:HG2	2.42	0.54
1:A:425:GLN:O	1:A:429:VAL:HG23	2.07	0.54
1:A:1597:ALA:O	1:A:1598:ILE:C	2.50	0.54
1:A:181:GLU:O	1:A:191:TYR:OH	2.21	0.54
1:A:4115:ALA:HB1	1:A:4234:ILE:HG12	1.90	0.54
1:A:3721:LEU:HD12	1:A:3875:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:THR:HG22	1:A:786:THR:O	2.07	0.53
1:A:1510:VAL:HG12	1:A:1574:GLN:OE1	2.08	0.53
1:A:3726:MET:O	1:A:3730:THR:HG23	2.08	0.53
1:A:535:SER:O	1:A:538:THR:OG1	2.24	0.53
1:A:175:ASN:ND2	1:A:3327:GLN:OE1	2.43	0.52
1:A:188:MET:HE3	1:A:191:TYR:HD2	1.74	0.52
1:A:1132:ILE:HD12	1:A:1197:GLU:HG2	1.92	0.52
1:A:1762:CYS:SG	1:A:1778:THR:OG1	2.67	0.52
1:A:3873:GLN:OE1	1:A:3968:GLN:NE2	2.33	0.51
1:A:181:GLU:OE1	1:A:184:ARG:NH2	2.37	0.51
1:A:263:LEU:CD2	1:A:3294:LEU:HD21	2.41	0.51
1:A:1655:ARG:HA	1:A:1655:ARG:NE	2.25	0.51
1:A:1766:LEU:HD23	1:A:1775:LEU:HD22	1.92	0.50
1:A:4300:VAL:HG23	1:A:4301:THR:HG23	1.93	0.50
1:A:1626:ARG:NH1	1:A:1920:ASN:OD1	2.44	0.50
1:A:3638:ILE:HB	1:A:3859:MET:HE1	1.93	0.50
1:A:550:TYR:HB3	1:A:554:LEU:HD23	1.94	0.50
1:A:1151:HIS:NE2	1:A:1218:SER:OG	2.45	0.50
1:A:2117:LEU:HG	1:A:2178:ALA:HB1	1.93	0.50
1:A:359:LEU:HB3	1:A:360:PRO:HD3	1.93	0.50
1:A:2126:LYS:HG3	1:A:2127:ASP:OD1	2.12	0.50
1:A:2152:LEU:HD13	1:A:2152:LEU:C	2.37	0.50
1:A:4073:MET:HE1	1:A:4126:CYS:SG	2.52	0.50
1:A:22:LEU:HD22	1:A:39:GLN:NE2	2.27	0.50
1:A:522:PRO:O	1:A:523:ALA:HB3	2.12	0.50
1:A:1768:VAL:HG23	1:A:1768:VAL:O	2.11	0.49
1:A:372:ASP:OD1	1:A:373:PRO:HD2	2.13	0.49
1:A:1882:PRO:O	1:A:1886:THR:HG23	2.13	0.49
1:A:184:ARG:O	1:A:186:LEU:HD23	2.12	0.49
1:A:2100:GLU:OE1	1:A:2100:GLU:N	2.43	0.49
1:A:611:LEU:O	1:A:617:GLY:HA3	2.13	0.49
1:A:1584:THR:HG22	1:A:1774:THR:HA	1.95	0.49
1:A:3437:MET:HE3	1:A:3440:HIS:ND1	2.28	0.49
1:A:1771:ASP:OD1	1:A:1772:PRO:HD2	2.13	0.48
1:A:3233:SER:OG	1:A:3329:ALA:HB1	2.13	0.48
1:A:1770:VAL:HG23	1:A:1771:ASP:H	1.77	0.48
1:A:3985:LEU:HD11	1:A:3992:LEU:HD21	1.95	0.48
1:A:1615:ASN:HB3	1:A:1680:LEU:HD21	1.95	0.48
1:A:1661:GLN:O	1:A:1665:MET:N	2.46	0.48
1:A:1265:TYR:O	1:A:1269:MET:SD	2.72	0.48
1:A:1862:LEU:O	1:A:1866:GLU:OE2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:MET:HE2	1:A:524:PHE:CE1	2.49	0.47
1:A:2176:LEU:O	1:A:2180:MET:HG2	2.14	0.47
1:A:437:ASP:OD1	1:A:517:LYS:HE2	2.14	0.47
1:A:61:PHE:O	1:A:65:LEU:HG	2.14	0.47
1:A:1508:LYS:O	1:A:1509:THR:OG1	2.27	0.47
1:A:2187:MET:HE1	1:A:2253:LEU:HB2	1.95	0.47
1:A:1775:LEU:HA	1:A:1778:THR:HG22	1.96	0.47
1:A:4330:ARG:HD3	1:A:4330:ARG:N	2.30	0.47
1:A:911:ARG:NH2	1:A:1065:GLU:OE1	2.47	0.47
1:A:1502:LEU:HD13	1:A:1507:THR:CG2	2.44	0.47
1:A:1897:LEU:HD12	1:A:2685:GLU:OE2	2.13	0.47
1:A:416:ILE:O	1:A:416:ILE:HG22	2.14	0.47
1:A:1170:PHE:CE1	1:A:1252:CYS:HB3	2.50	0.47
1:A:3983:ALA:O	1:A:3986:VAL:HG13	2.14	0.47
1:A:4288:PHE:O	1:A:4293:ARG:NE	2.47	0.46
1:A:3286:LEU:HD11	1:A:3392:LEU:CD1	2.45	0.46
1:A:4142:ARG:HG2	1:A:4142:ARG:HH11	1.79	0.46
1:A:129:GLN:NE2	1:A:275:GLN:OE1	2.47	0.46
1:A:1591:ASP:OD1	1:A:1781:LEU:HA	2.15	0.46
1:A:4216:THR:O	1:A:4220:ARG:N	2.49	0.46
1:A:1875:GLY:HA2	1:A:2667:VAL:HG22	1.97	0.46
1:A:573:LEU:HD23	1:A:614:ASN:HB2	1.98	0.46
1:A:2212:ILE:HG13	1:A:2213:ILE:N	2.30	0.46
1:A:4005:LEU:O	1:A:4008:LEU:HG	2.16	0.46
1:A:4271:TYR:CG	1:A:4278:ILE:HD11	2.51	0.46
1:A:258:PHE:HA	1:A:261:ILE:HG22	1.97	0.46
1:A:1159:CYS:SG	1:A:1160:SER:N	2.89	0.46
1:A:1866:GLU:OE2	1:A:1866:GLU:N	2.48	0.46
1:A:1940:ASP:O	1:A:1944:GLU:HG3	2.16	0.46
1:A:3594:SER:O	1:A:3597:GLY:N	2.49	0.46
1:A:856:GLU:N	1:A:857:PRO:HD2	2.31	0.45
1:A:4150:ASP:OD2	1:A:4150:ASP:N	2.47	0.45
1:A:1254:LYS:O	1:A:1259:ARG:NH1	2.50	0.45
1:A:960:LEU:N	1:A:961:PRO:HD2	2.31	0.45
1:A:1886:THR:HG22	1:A:2670:VAL:HG13	1.97	0.45
1:A:3219:ARG:HG2	1:A:3223:ILE:HD12	1.98	0.45
1:A:3967:ASN:OD1	1:A:3993:ASP:N	2.43	0.45
1:A:974:LEU:C	1:A:974:LEU:HD13	2.42	0.45
1:A:3636:LYS:O	1:A:3640:THR:HG23	2.16	0.45
1:A:3892:THR:O	1:A:3893:GLU:C	2.60	0.45
1:A:4132:PHE:CE2	1:A:4136:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:ILE:HG23	1:A:1273:MET:HG3	1.98	0.45
1:A:937:LEU:HD22	1:A:1063:LEU:HD21	1.99	0.45
1:A:972:GLN:HA	1:A:972:GLN:OE1	2.17	0.45
1:A:4141:VAL:HG22	1:A:4142:ARG:N	2.32	0.45
1:A:1879:CYS:SG	1:A:2663:MET:HA	2.57	0.45
1:A:1939:PRO:HD2	1:A:1942:ILE:HD12	1.99	0.45
1:A:144:ARG:HD2	1:A:145:SER:HB2	1.98	0.45
1:A:974:LEU:HD11	1:A:1048:GLN:HB2	1.99	0.45
1:A:968:GLN:O	1:A:972:GLN:HG2	2.17	0.45
1:A:3736:GLN:NE2	1:A:3878:VAL:O	2.37	0.45
1:A:3853:LEU:O	1:A:3857:TRP:CD1	2.70	0.45
1:A:4174:PHE:CZ	1:A:4206:TYR:HB2	2.52	0.45
1:A:2117:LEU:O	1:A:2129:PRO:HB3	2.18	0.44
1:A:88:GLN:O	1:A:92:LEU:HD13	2.18	0.44
1:A:311:ASP:O	1:A:315:ILE:HG12	2.17	0.44
1:A:3602:ALA:O	1:A:3606:LEU:HG	2.16	0.44
1:A:2659:ASP:OD1	1:A:2659:ASP:N	2.51	0.44
1:A:456:PHE:CD1	1:A:511:MET:HG3	2.52	0.44
1:A:1137:PHE:CZ	1:A:1141:MET:SD	3.10	0.44
1:A:1180:VAL:HG12	1:A:1181:PRO:O	2.17	0.44
1:A:1132:ILE:CD1	1:A:1197:GLU:HG2	2.47	0.44
1:A:1215:VAL:HG12	1:A:1238:ALA:HB1	2.00	0.44
1:A:1621:ASP:O	1:A:1625:GLY:N	2.50	0.44
1:A:4308:LEU:HD12	1:A:4308:LEU:H	1.83	0.44
1:A:3966:LEU:HD21	1:A:3985:LEU:HD21	1.98	0.44
1:A:1620:PHE:HZ	1:A:1863:GLY:HA2	1.84	0.43
1:A:2646:THR:HG1	1:A:2649:THR:HG23	1.83	0.43
1:A:33:GLN:OE1	1:A:92:LEU:HD11	2.18	0.43
1:A:188:MET:HE3	1:A:188:MET:HA	1.99	0.43
1:A:2108:VAL:O	1:A:2112:VAL:HG23	2.18	0.43
1:A:3454:LEU:HD11	1:A:3585:VAL:HG11	1.99	0.43
1:A:4073:MET:HE3	1:A:4110:VAL:HG21	2.00	0.43
1:A:810:ASN:C	1:A:810:ASN:OD1	2.61	0.43
1:A:3196:ASP:HB3	1:A:3290:MET:HE2	2.00	0.43
1:A:666:LEU:HD23	1:A:666:LEU:C	2.43	0.43
1:A:1826:HIS:CE1	1:A:2654:GLU:OE2	2.72	0.43
1:A:2668:SER:O	1:A:2672:VAL:HG23	2.19	0.43
1:A:1469:ILE:O	1:A:1472:ASN:O	2.37	0.43
1:A:1521:PRO:O	1:A:1524:SER:OG	2.25	0.43
1:A:2253:LEU:C	1:A:2253:LEU:HD23	2.43	0.43
1:A:4142:ARG:NE	1:A:4144:THR:OG1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1867:ILE:CD1	1:A:2678:LEU:HD12	2.48	0.43
1:A:440:THR:HA	1:A:443:ASP:O	2.19	0.42
1:A:1682:LEU:HD12	1:A:1682:LEU:N	2.33	0.42
1:A:3225:SER:O	1:A:3229:ILE:HG13	2.19	0.42
1:A:3851:LEU:HD12	1:A:3889:VAL:HG21	1.99	0.42
1:A:691:LEU:HD13	1:A:764:ILE:HD11	2.00	0.42
1:A:1770:VAL:HG23	1:A:1774:THR:HB	2.01	0.42
1:A:2688:GLU:OE2	1:A:2688:GLU:HA	2.19	0.42
1:A:3876:VAL:HG21	1:A:3965:VAL:CG1	2.49	0.42
1:A:409:MET:SD	1:A:436:VAL:HG13	2.59	0.42
1:A:427:THR:O	1:A:430:THR:HG22	2.20	0.42
1:A:1195:THR:HG22	1:A:1195:THR:O	2.18	0.42
1:A:3598:LEU:HD13	1:A:3741:ARG:HD2	2.01	0.42
1:A:3600:ASP:O	1:A:3604:VAL:HG23	2.19	0.42
1:A:3988:TYR:O	1:A:3991:VAL:HG22	2.18	0.42
1:A:4151:TYR:O	1:A:4155:GLN:HG3	2.20	0.42
1:A:263:LEU:C	1:A:263:LEU:HD23	2.44	0.42
1:A:528:ILE:HD12	1:A:531:VAL:HG21	2.01	0.42
1:A:1584:THR:OG1	1:A:1585:PRO:HD3	2.19	0.42
1:A:1824:LEU:O	1:A:1828:ILE:HG12	2.18	0.42
1:A:1828:ILE:HD13	1:A:1942:ILE:HG23	2.01	0.42
1:A:3953:GLN:HG2	1:A:3954:LYS:H	1.85	0.42
1:A:773:VAL:O	1:A:777:VAL:HG23	2.19	0.42
1:A:1611:GLN:HE21	1:A:1613:ASN:H	1.68	0.42
1:A:1627:TRP:CZ3	1:A:1679:MET:HB3	2.55	0.42
1:A:3876:VAL:HG21	1:A:3965:VAL:HG13	2.01	0.42
1:A:528:ILE:HD12	1:A:531:VAL:CG2	2.50	0.42
1:A:3391:LEU:O	1:A:3395:LEU:HG	2.20	0.42
1:A:3962:HIS:O	1:A:3965:VAL:N	2.52	0.42
1:A:1139:SER:HB3	1:A:1140:PRO:HD3	2.02	0.42
1:A:1854:THR:HG21	1:A:1872:ARG:HH12	1.85	0.42
1:A:1953:LEU:HA	1:A:2068:THR:HG22	2.02	0.42
1:A:4110:VAL:O	1:A:4114:VAL:HG23	2.20	0.42
1:A:248:SER:O	1:A:248:SER:OG	2.36	0.41
1:A:376:ASP:HA	1:A:377:PRO:HD3	1.87	0.41
1:A:1680:LEU:HD23	1:A:1681:THR:N	2.35	0.41
1:A:4065:TRP:O	1:A:4068:ILE:HG13	2.20	0.41
1:A:2133:ARG:HG3	1:A:2182:ILE:HD12	2.03	0.41
1:A:4188:ASP:OD2	1:A:4188:ASP:N	2.52	0.41
1:A:369:ALA:HB1	1:A:376:ASP:O	2.20	0.41
1:A:589:LEU:HD22	1:A:604:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1756:THR:HG22	1:A:1794:MET:CE	2.50	0.41
1:A:4020:HIS:O	1:A:4033:GLU:OE1	2.38	0.41
1:A:614:ASN:O	1:A:615:ALA:HB3	2.21	0.41
1:A:779:SER:O	1:A:783:ASN:HB2	2.21	0.41
1:A:949:THR:HG21	1:A:1129:THR:HG23	2.02	0.41
1:A:2112:VAL:CG1	1:A:2132:ALA:HB1	2.50	0.41
1:A:4206:TYR:O	1:A:4210:VAL:HG12	2.21	0.41
1:A:1538:GLU:HA	1:A:1592:PHE:CZ	2.56	0.41
1:A:1611:GLN:O	1:A:1615:ASN:ND2	2.54	0.41
1:A:1463:ASP:O	1:A:1467:THR:HG23	2.21	0.41
1:A:1787:ARG:HD3	1:A:2654:GLU:OE2	2.20	0.41
1:A:2143:GLY:O	1:A:2144:SER:C	2.64	0.41
1:A:640:LEU:N	1:A:641:PRO:HD2	2.36	0.41
1:A:1148:TYR:CD1	1:A:1218:SER:HA	2.56	0.41
1:A:3985:LEU:HD12	1:A:3985:LEU:C	2.46	0.41
1:A:320:LEU:O	1:A:323:ILE:N	2.53	0.41
1:A:1535:LEU:O	1:A:1539:GLU:OE2	2.39	0.41
1:A:2089:ILE:HG21	1:A:2135:PHE:HZ	1.86	0.41
1:A:3232:ARG:NH1	1:A:3322:VAL:O	2.46	0.41
1:A:3329:ALA:HB3	1:A:3330:PRO:HD3	2.03	0.41
1:A:146:ASN:O	1:A:146:ASN:CG	2.63	0.41
1:A:618:LEU:HD23	1:A:618:LEU:O	2.20	0.41
1:A:1580:PRO:HB3	1:A:1582:TRP:NE1	2.36	0.41
1:A:1770:VAL:HG23	1:A:1771:ASP:N	2.36	0.41
1:A:3962:HIS:O	1:A:3963:ARG:C	2.63	0.41
1:A:4157:LEU:O	1:A:4161:LEU:HG	2.21	0.41
1:A:4330:ARG:HD3	1:A:4330:ARG:H	1.85	0.41
1:A:343:LEU:HD11	1:A:393:LEU:HD12	2.03	0.41
1:A:873:GLU:OE2	1:A:890:THR:HA	2.21	0.41
1:A:2217:LEU:HD21	1:A:2253:LEU:HD21	2.03	0.41
1:A:4004:GLU:OE1	1:A:4007:ARG:NE	2.53	0.41
1:A:4334:ARG:HD3	1:A:4335:LEU:O	2.21	0.41
1:A:1434:ASP:N	1:A:1434:ASP:OD2	2.54	0.40
1:A:4181:PHE:N	1:A:4181:PHE:CD1	2.87	0.40
1:A:359:LEU:HD13	1:A:359:LEU:C	2.47	0.40
1:A:4257:ILE:HD11	1:A:4297:LEU:HD22	2.03	0.40
1:A:17:ALA:O	1:A:20:ARG:N	2.54	0.40
1:A:1149:PRO:CB	1:A:1154:LEU:HD11	2.52	0.40
1:A:3182:ASP:OD1	1:A:3182:ASP:N	2.49	0.40
1:A:3595:GLU:HA	1:A:3598:LEU:HG	2.03	0.40
1:A:597:THR:CG2	1:A:600:VAL:HG23	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:LEU:HD11	1:A:1048:GLN:HG3	2.03	0.40
1:A:1099:ARG:HH22	1:A:1233:PHE:HB3	1.86	0.40
1:A:1503:THR:HG23	1:A:1504:THR:HG23	2.03	0.40
1:A:4107:PHE:CE1	1:A:4222:GLN:HG2	2.56	0.40
1:A:4107:PHE:HA	1:A:4110:VAL:HG12	2.02	0.40
1:A:157:THR:O	1:A:161:THR:HG23	2.22	0.40
1:A:1531:LEU:HD23	1:A:1531:LEU:O	2.21	0.40
1:A:3859:MET:HA	1:A:3862:GLU:HG2	2.02	0.40
1:A:4207:VAL:HA	1:A:4210:VAL:HG12	2.03	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	2369/4411 (54%)	2310 (98%)	59 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2149/3839 (56%)	2116 (98%)	33 (2%)	57 72

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	SER
1	A	571	SER
1	A	672	THR
1	A	959	SER
1	A	1121	THR
1	A	1210	VAL
1	A	1442	THR
1	A	1500	LEU
1	A	1524	SER
1	A	1558	ILE
1	A	1596	THR
1	A	1870	ILE
1	A	2127	ASP
1	A	2144	SER
1	A	2169	SER
1	A	2185	THR
1	A	2235	SER
1	A	2239	MET
1	A	2250	LEU
1	A	2643	SER
1	A	2662	SER
1	A	3284	SER
1	A	3288	VAL
1	A	3303	ILE
1	A	3584	SER
1	A	3615	THR
1	A	3619	VAL
1	A	3870	SER
1	A	3984	VAL
1	A	4036	ARG
1	A	4183	VAL
1	A	4308	LEU
1	A	4330	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	319	GLN
1	A	356	HIS
1	A	568	GLN

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Mol	Chain	Res	Type
1	A	625	GLN
1	A	669	HIS
1	A	859	HIS
1	A	924	GLN
1	A	1255	ASN
1	A	1569	GLN
1	A	1574	GLN
1	A	1611	GLN
1	A	1613	ASN
1	A	3972	GLN
1	A	4269	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

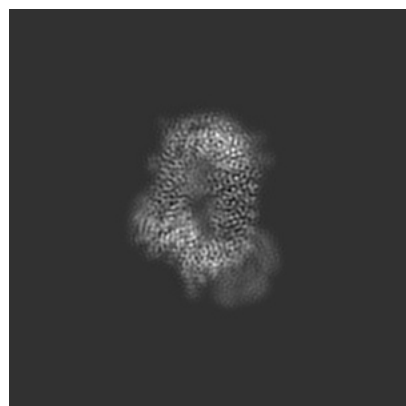
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22430. These allow visual inspection of the internal detail of the map and identification of artifacts.

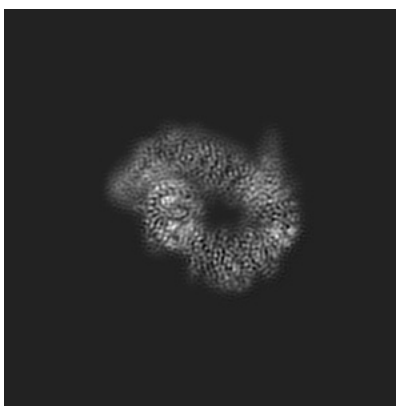
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

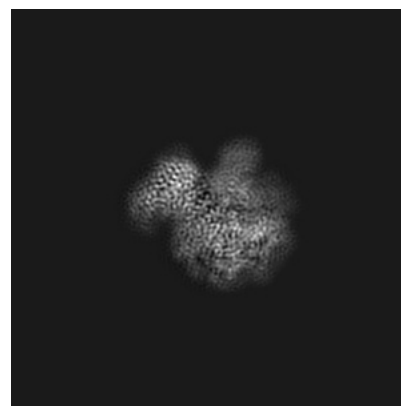
6.1.1 Primary map



X

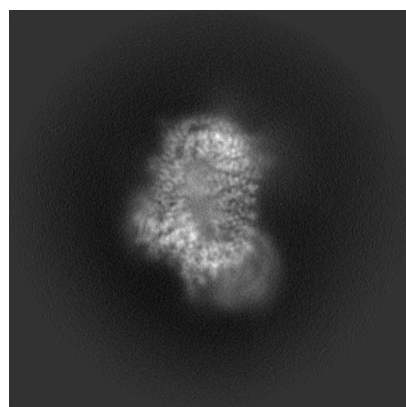


Y

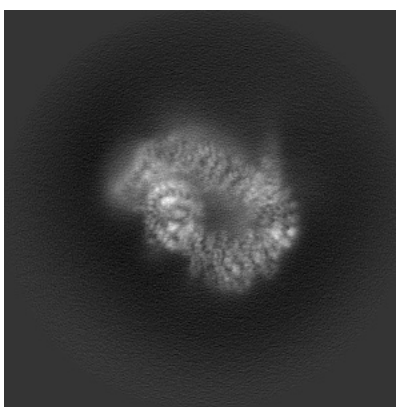


Z

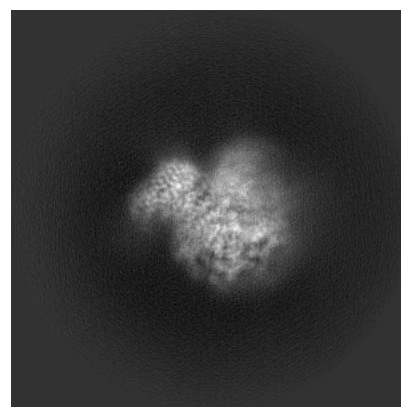
6.1.2 Raw map



X



Y

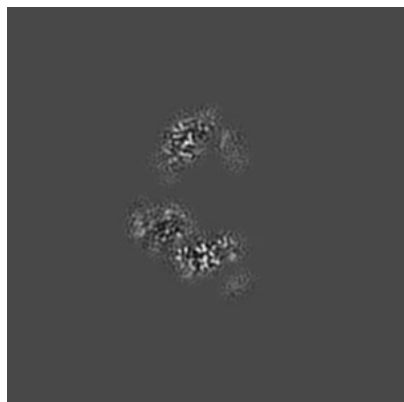


Z

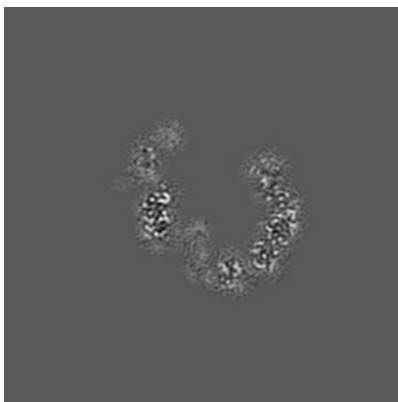
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

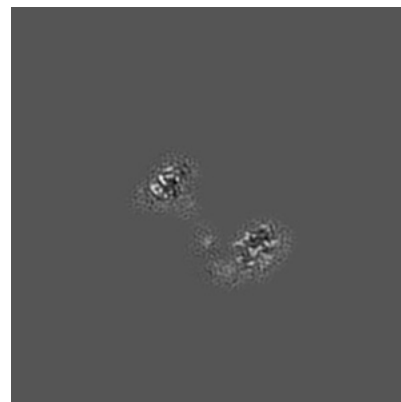
6.2.1 Primary map



X Index: 182

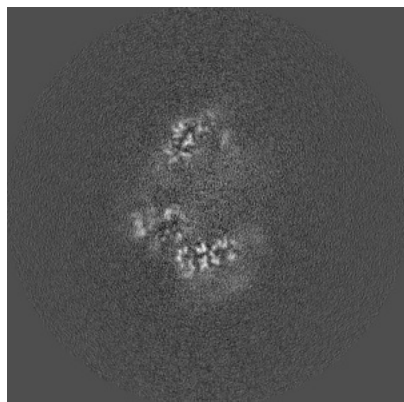


Y Index: 182

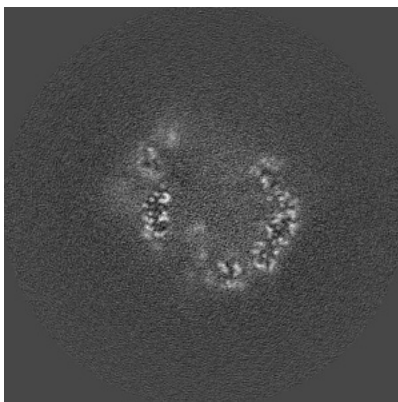


Z Index: 182

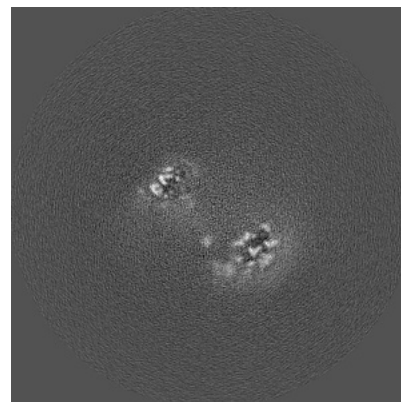
6.2.2 Raw map



X Index: 182



Y Index: 182

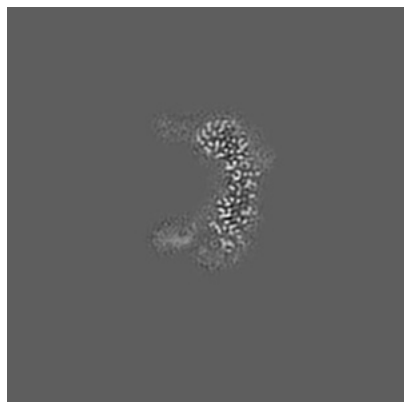


Z Index: 182

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

6.3 Largest variance slices [i](#)

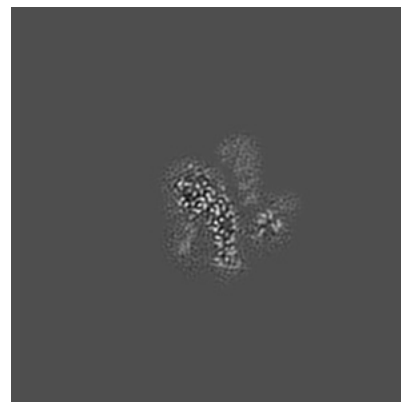
6.3.1 Primary map



X Index: 149

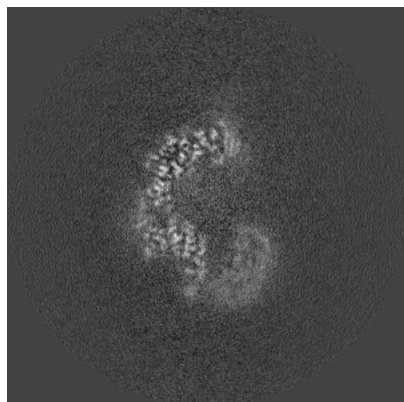


Y Index: 202

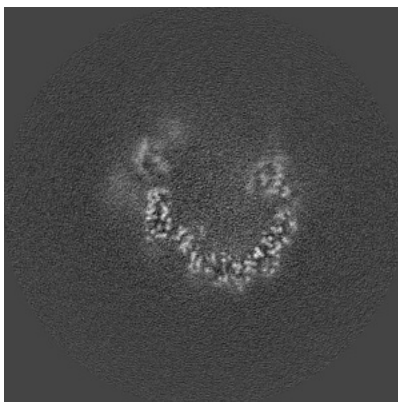


Z Index: 145

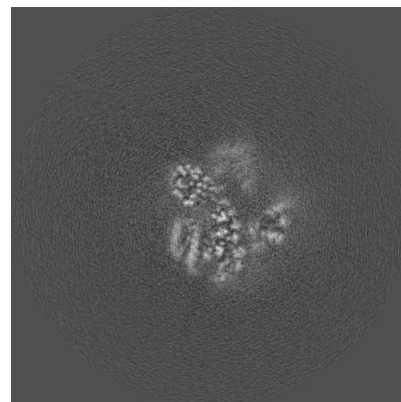
6.3.2 Raw map



X Index: 203



Y Index: 189

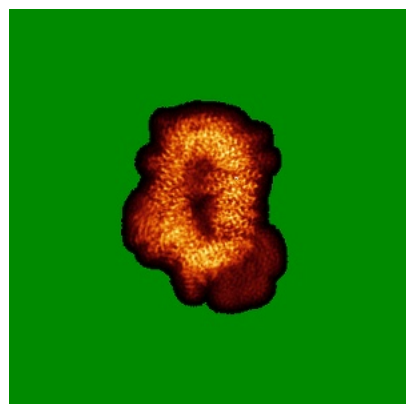


Z Index: 152

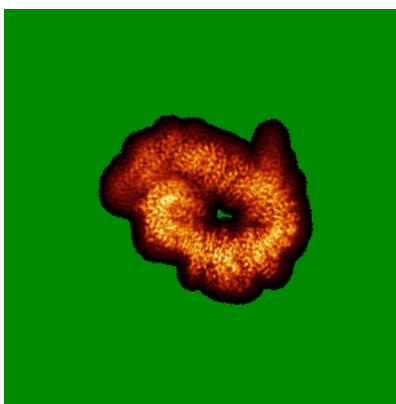
The images above show the largest variance slices of the map in three orthogonal directions.

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

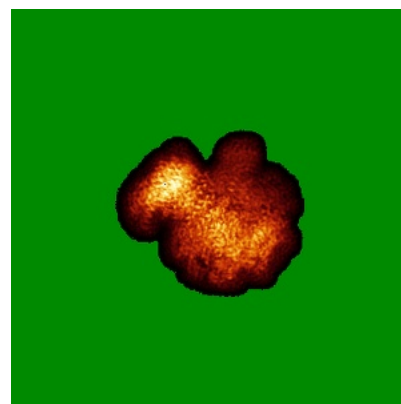
6.4.1 Primary map



X

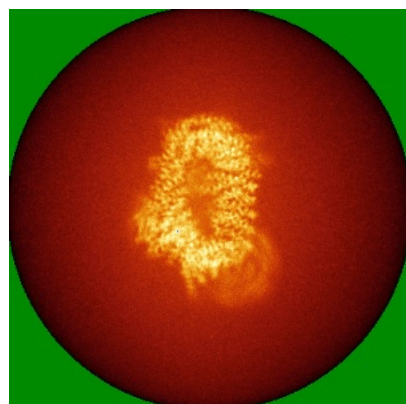


Y

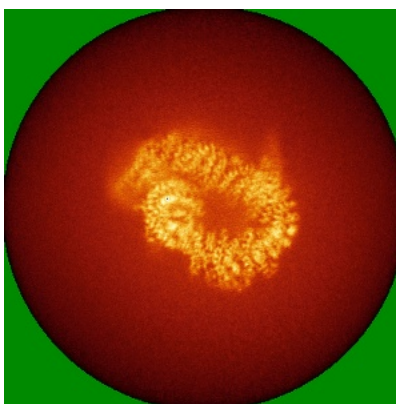


Z

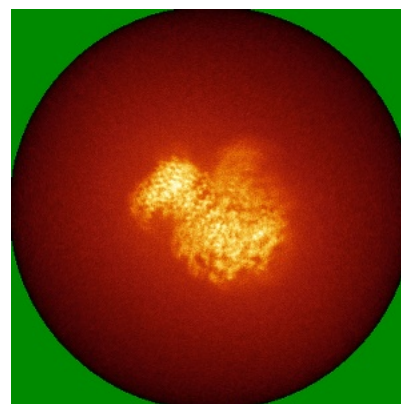
6.4.2 Raw map



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.

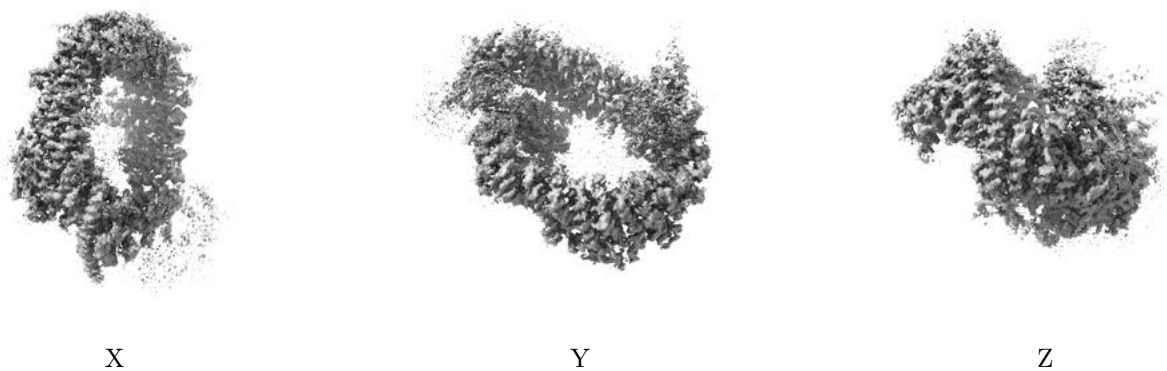
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. 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.

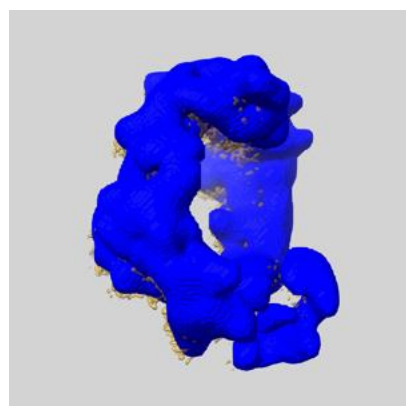
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

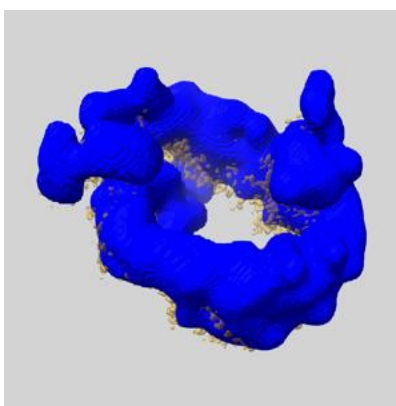
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

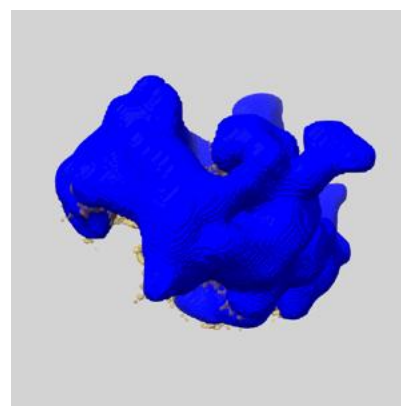
6.6.1 emd_22430_msk_1.map [i](#)



X



Y

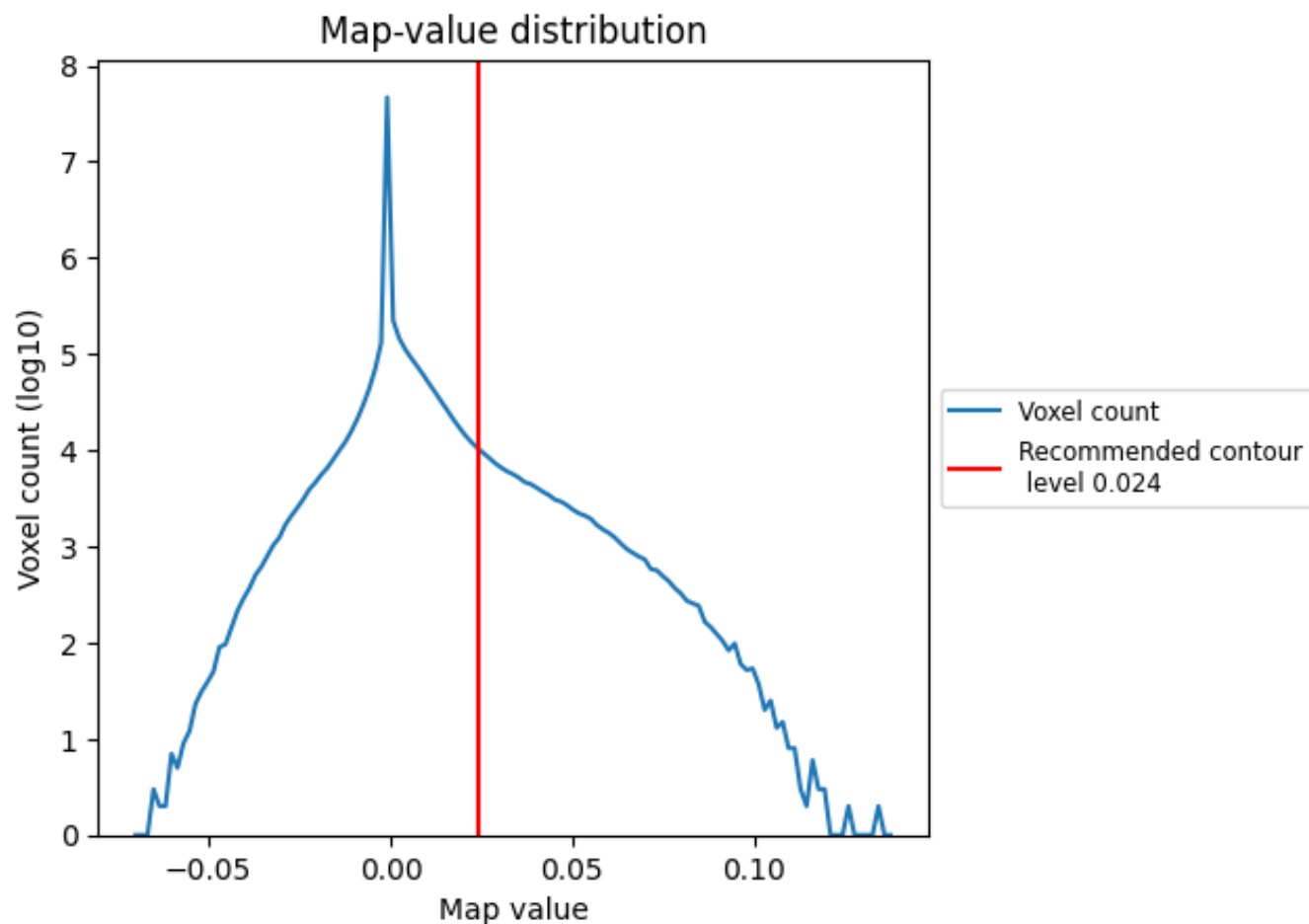


Z

7 Map analysis [i](#)

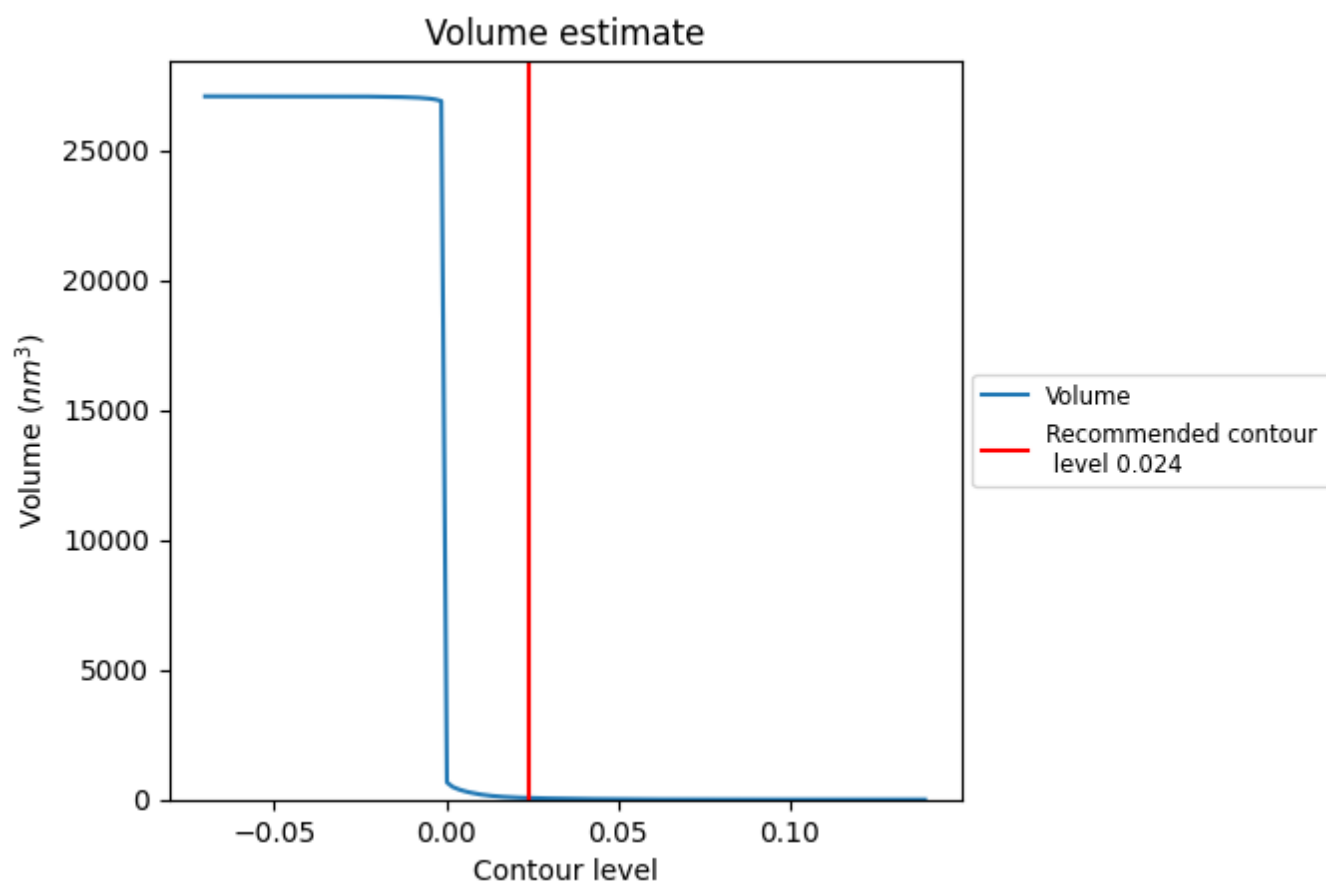
This section contains the results of statistical analysis of the map.

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.

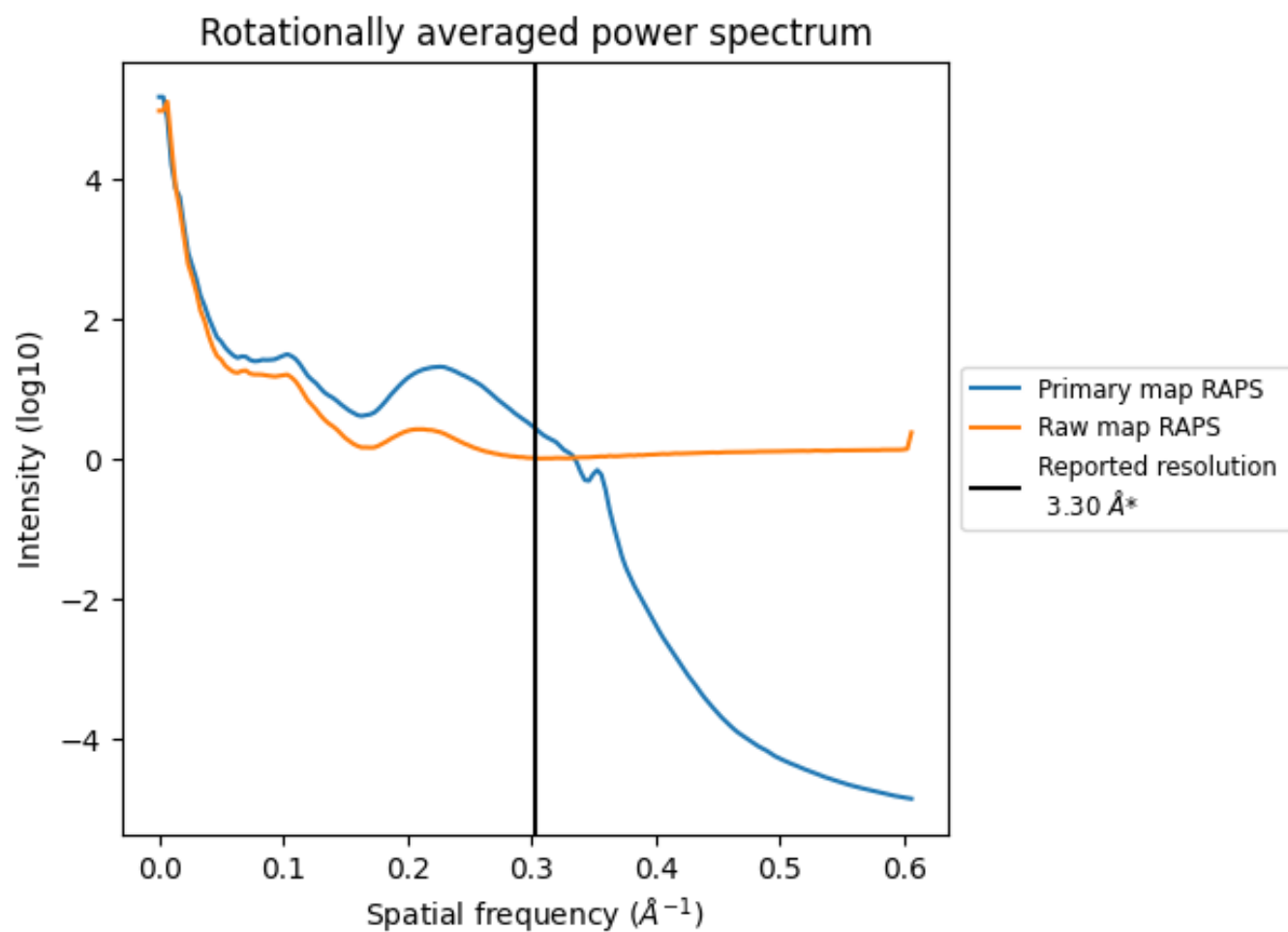
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm^3 ; this corresponds to an approximate mass of 56 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 ⓘ

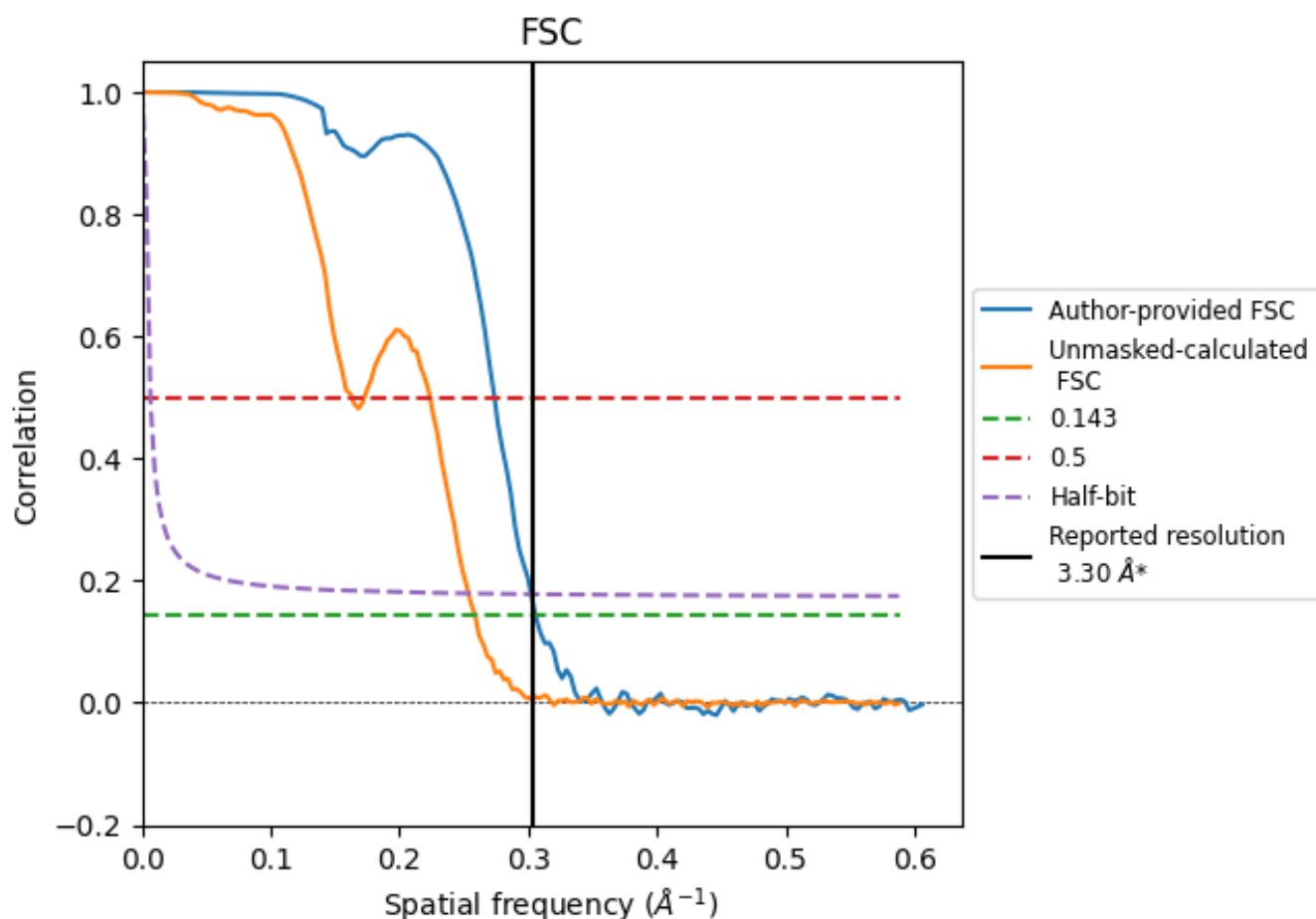


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

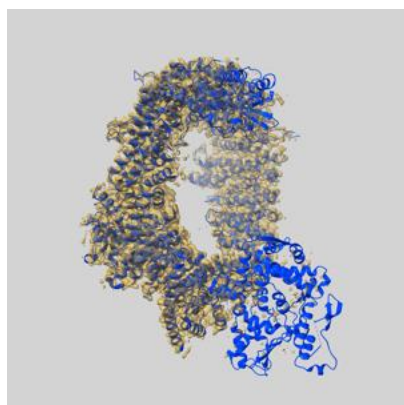
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.65	3.31
Unmasked-calculated*	3.87	6.14	3.94

*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 3.87 differs from the reported value 3.3 by more than 10 %

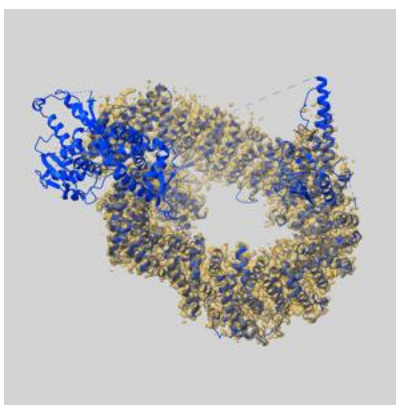
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22430 and PDB model 7MWF. Per-residue inclusion information can be found in section 3 on page 5.

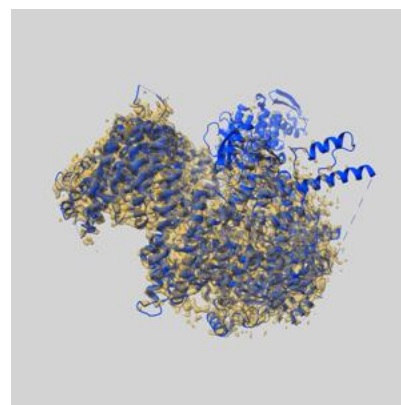
9.1 Map-model overlay [i](#)



X



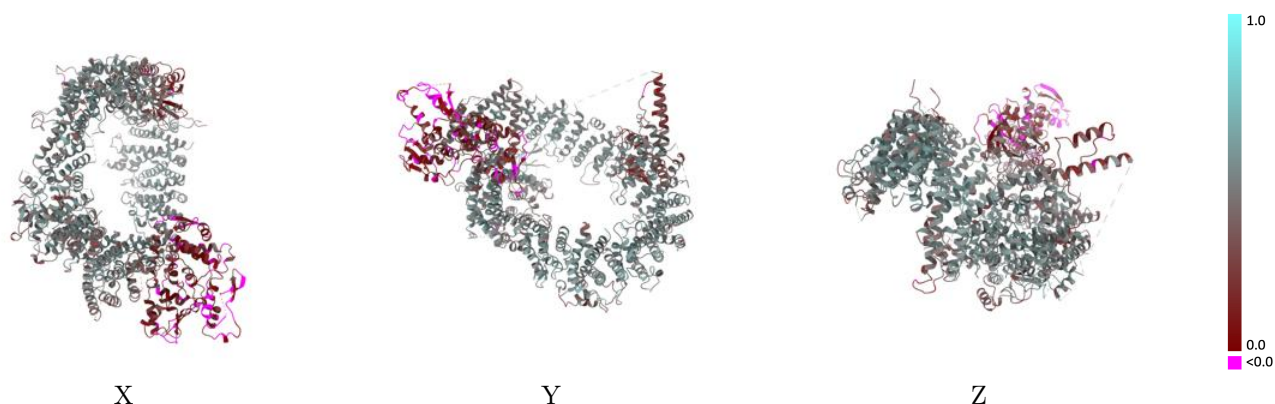
Y



Z

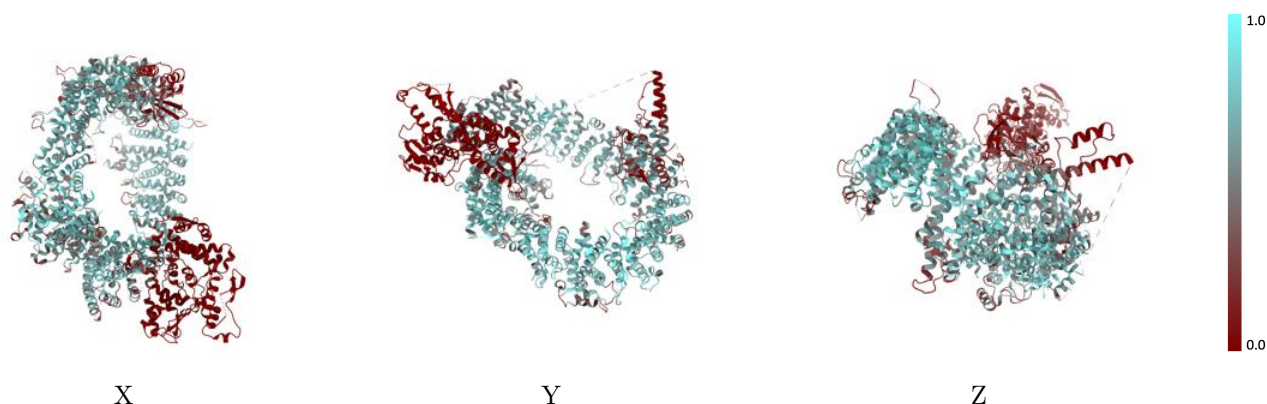
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



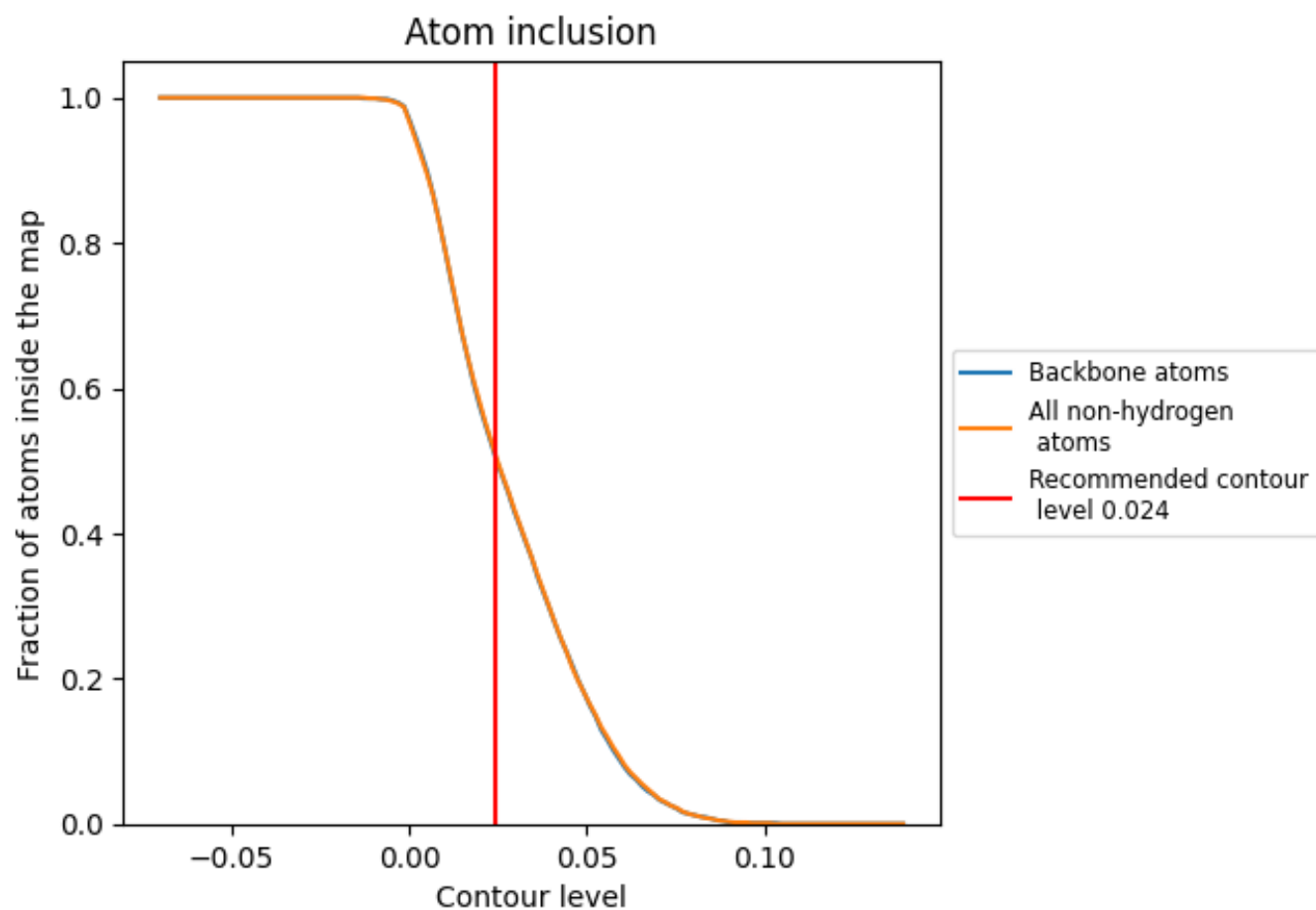
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 51% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5130	0.4230
A	0.5130	0.4230

