



Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 08:16 AM EST

PDB ID : 7MWE
EMDB ID : EMD-22429
Title : HUWE1 in map with focus on WWE
Authors : Hunkeler, M.; Fischer, E.S.
Deposited on : 2021-05-16
Resolution : 3.40 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

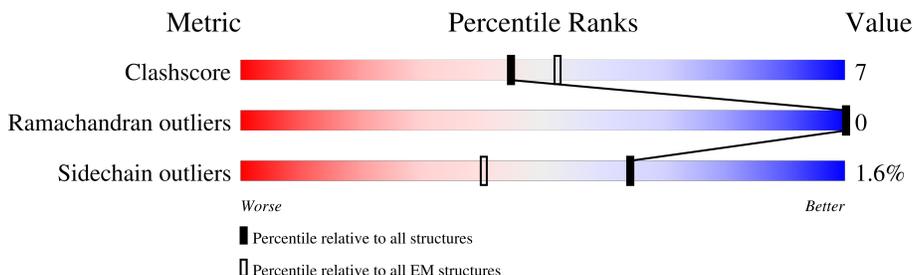
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4411	

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	
			Total	C	H	N	O			S
1	A	2427	38719	12225	19554	3292	3528	120	0	0

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

D4346	R4286	F4226	Y4106	L4046	V3986	THR	GLU	T3730	E3651	ASP
L4347	S4287	L4227	F4107	Y4047	D3987	PRO	GLN	S3731	GLN	GLY
P4348	F4288	E4228	K4108	I4048	Y3988	ALA	ALA	K3732	ALA	GLY
A4349	D4289	G4229	F4109	V4049	I3989	PRO	THR	L3852	ARG	SER
Y4350	Q4290	F4230	V4110	F4050	R3990	SER	SER	L3853	ALA	SER
E4351	A4291	Y4170	G4111	E4051	V3991	LEU	GLU	R3741	ALA	THR
S4352	D4292	L4172	R4112	G4052	L3992	ASP	SER	D3751	CYS	ASP
F4353	R4293	T4173	I4113	E4053	D3993	PRO	GLN	T3751	THR	PHE
E4354	A4294	F4174	V4114	E4054	F3994	PHE	SER	D3752	LEU	LYS
K4355	K4295	S4175	A4115	G4055	V3995	PHE	GLU	M3859	LEU	MET
L4356	F4296	T4176	K4116	Q4056	V3996	SER	ALA	K3855	SER	VAL
R4357	L4297	E4177	D4057	D4057	K3997	ARG	SER	K3865	ASP	SER
H4358	Q4298	V4178	A4058	A4058	R3998	GLU	VAL	E3868	GLY	GLY
M4359	F4299	Q4179	Y4119	A4059	R3999	PRO	ARG	E3869	LEU	LEU
L4360	V4300	E4180	D4120	G4060	K3999	SER	ARG	S3870	PRO	PRO
L4361	T4301	F4181	M4121	L4061	F4001	MET	GLU	H3871	GLU	GLY
L4362	G4302	G4182	R4122	L4062	R4002	HIS	SER	D3872	THR	GLN
A4363	S4304	V4183	L4123	R4063	Q4003	ILE	ASP	H3873	GLY	GLN
I4364	K4305	C4184	L4124	E4064	A4004	SER	MET	H3874	PRO	PRO
V4306	F4306	E4185	E4126	W4065	L4005	LEU	ASP	A3875	GLY	GLN
V4307	V4307	V4186	C4126	W4065	E4006	PRO	ASP	V3876	LEU	THR
L4308	L4308	R4187	Y4127	W4067	R4007	LEU	ASP	L3877	LEU	THR
L4309	D4309	D4188	F4128	I4068	L4008	LEU	THR	F3887	GLY	THR
Q4309	L4249	L4189	T4129	I4069	D4009	PRO	ASP	L3888	GLY	THR
G4310	L4250	K4190	R4130	S4070	R4007	ASP	ALA	V3889	ALA	ASP
F4311	I4251	ASN	S4131	R4071	L4010	GLN	ALA	T3892	GLN	ASP
A4312	S4252	GLY	F4132	E4072	G4011	THR	ASP	E3893	ASP	SER
A4313	G4253	ALA	Y4133	M4073	L4012	GLN	THR	R3957	THR	ARG
L4314	L4254	ASN	K4134	F4074	R4013	GLU	ALA	F3958	GLN	PHE
E4315	P4255	ILE	H4135	N4075	K4014	SER	ALA	A3959	ALA	MET
G4316	T4256	LEU	I4136	W4076	E4015	LYS	VAL	L3960	VAL	ALA
M4317	I4257	V4198	L4137	M4077	D4016	PRO	ARG	R3964	ALA	ARG
M4318	D4258	T4199	C4138	Y4078	M4017	ASP	THR	V3965	ALA	GLY
Q4319	I4259	E4200	K4139	A4079	V4019	ASP	THR	L3966	ALA	VAL
I4320	D4260	E4201	S4140	F4081	H4020	ASP	THR	R3967	ALA	VAL
Q4321	D4261	M4202	V4141	L4080	V4021	THR	ALA	Q3968	ALA	VAL
K4322	L4262	K4203	R4142	F4082	R4022	GLU	GLY	I3969	ALA	VAL
F4323	K4263	K4204	Y4143	T4083	R4023	SER	LYS	L3970	ALA	VAL
Q4324	S4264	E4205	T4144	S4084	D4024	ALA	ALA	R3971	ALA	VAL
I4325	M4265	V4207	D4145	P4085	H4025	ILE	ALA	Q3972	ALA	VAL
H4326	T4266	H4208	M4146	P4086	V4026	HIS	ILE	S3973	ALA	VAL
R4327	E4267	E4147	E4147	D4087	F4027	LYS	ARG	T3974	ALA	VAL
D4328	L4269	S4148	S4148	R4088	E4028	ASP	ASP	T3975	ALA	VAL
D4329	C4211	E4149	E4149	V4089	D4029	GLU	GLY	H3976	ALA	VAL
R4330	F4330	D4150	D4150	T4090	S4030	PRO	PRO	L3977	ALA	VAL
S4331	K4331	Y4151	Y4151	Y4091	Y4031	PRO	PRO	A3978	ALA	VAL
T4332	Q4272	M4213	H4152	T4092	R4032	SER	SER	D3979	ALA	VAL
D4333	S4273	R4214	F4153	T4093	E4033	GLN	GLN	G3980	ALA	VAL
M4334	M4274	M4215	Y4154	I4094	L4034	LEU	LEU	F3981	ALA	VAL
L4335	S4275	T4216	Q4155	P4095	H4035	ALA	ALA	A3983	ALA	VAL
P4336	I4276	G4217	G4156	S4096	R4036	ILE	ILE	V3984	ALA	VAL
S4337	I4277	I4219	L4157	S4097	K4037	HIS	HIS	L3985	ALA	VAL
A4338	I4278	R4220	V4158	H4098	S4038	ARG	ARG	P4039	ALA	VAL
H4339	Q4279	K4221	Y4159	C4099	E4040	PRO	PRO	E4041	ALA	VAL
T4340	W4280	F4221	L4160	N4100	E4042	PRO	PRO	M4042	ALA	VAL
C4341	F4281	Q4222	L4161	N4102	M4043	PRO	PRO	K4043	ALA	VAL
F4342	W4282	L4223	E4162	N4103	M4044	PRO	PRO	I4044	ALA	VAL
M4343	R4283	A4224	M4163	H4103	R4045	LEU	LEU	R4045	ALA	VAL
Q4344	A4284	A4225	D4164	L4104	R4045	SER	SER		ALA	VAL
L4345	L4285		V4165	S4105		LEU	LEU		ALA	VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85184	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	0.101	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0165	Depositor
Map size (\AA)	300.3, 300.3, 300.3	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.32	0/19509	0.55	0/26411

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19165	19554	19539	262	0
All	All	19165	19554	19539	262	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 (262) 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:4023:ARG:O	1:A:4023:ARG:NH1	2.13	0.82
1:A:1109:LEU:HD22	1:A:1138:THR:HG22	1.63	0.81
1:A:4082:ARG:NH1	1:A:4094:ASN:OD1	2.20	0.75
1:A:1134:SER:O	1:A:1138:THR:HG23	1.87	0.73
1:A:1825:ARG:NH1	1:A:2081:SER:OG	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1510:VAL:O	1:A:1514:ILE:HG23	1.88	0.73
1:A:1829:GLU:OE2	1:A:2082:TYR:OH	2.07	0.73
1:A:2663:MET:O	1:A:2667:VAL:HG23	1.89	0.72
1:A:125:SER:OG	1:A:127:ASP:OD1	2.09	0.70
1:A:2691:GLU:OE1	1:A:2694:ARG:NH1	2.27	0.67
1:A:1762:CYS:SG	1:A:1778:THR:OG1	2.54	0.66
1:A:4324:GLN:NE2	1:A:4342:PHE:O	2.27	0.65
1:A:1507:THR:O	1:A:1509:THR:HG23	1.97	0.65
1:A:2227:ARG:NH2	1:A:3184:GLU:OE1	2.30	0.65
1:A:3993:ASP:OD1	1:A:3994:PHE:N	2.31	0.64
1:A:1498:ALA:O	1:A:1516:GLN:NE2	2.31	0.63
1:A:1682:LEU:HD11	1:A:2668:SER:HB3	1.80	0.63
1:A:1579:THR:OG1	1:A:1770:VAL:O	2.16	0.63
1:A:3851:LEU:HD13	1:A:3851:LEU:O	2.00	0.62
1:A:669:HIS:ND1	1:A:4054:GLU:OE1	2.32	0.62
1:A:1826:HIS:NE2	1:A:2654:GLU:OE2	2.33	0.62
1:A:1671:GLU:N	1:A:1671:GLU:OE2	2.33	0.61
1:A:1655:ARG:HE	1:A:1655:ARG:HA	1.66	0.61
1:A:1664:THR:O	1:A:1872:ARG:NH2	2.35	0.60
1:A:1626:ARG:NH1	1:A:1920:ASN:OD1	2.32	0.59
1:A:3454:LEU:HD11	1:A:3585:VAL:HG11	1.86	0.58
1:A:1165:ALA:O	1:A:1169:THR:HG23	2.04	0.58
1:A:4216:THR:O	1:A:4220:ARG:N	2.37	0.58
1:A:785:THR:HG22	1:A:785:THR:O	2.04	0.58
1:A:3292:ALA:HB1	1:A:3327:GLN:HB3	1.86	0.58
1:A:1539:GLU:OE2	1:A:1539:GLU:N	2.37	0.58
1:A:2069:SER:OG	1:A:2125:ASP:OD1	2.12	0.58
1:A:4270:LYS:HB2	1:A:4327:ARG:HB2	1.85	0.57
1:A:157:THR:OG1	1:A:158:PRO:HD3	2.04	0.57
1:A:664:ASP:OD2	1:A:783:ASN:ND2	2.36	0.56
1:A:1817:THR:OG1	1:A:1818:PRO:HD3	2.04	0.56
1:A:3726:MET:O	1:A:3730:THR:HG23	2.06	0.56
1:A:4040:GLU:OE2	1:A:4040:GLU:N	2.38	0.56
1:A:4358:HIS:O	1:A:4362:LEU:HD13	2.05	0.55
1:A:3963:ARG:NE	1:A:3990:ARG:O	2.36	0.55
1:A:425:GLN:O	1:A:429:VAL:HG23	2.07	0.54
1:A:1232:ASN:OD1	1:A:1233:PHE:N	2.41	0.54
1:A:3292:ALA:CB	1:A:3327:GLN:HB3	2.38	0.54
1:A:786:THR:HG22	1:A:786:THR:O	2.07	0.53
1:A:1862:LEU:O	1:A:1866:GLU:OE2	2.26	0.53
1:A:1151:HIS:NE2	1:A:1218:SER:OG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4112:ARG:NH2	1:A:4232:GLU:OE1	2.41	0.53
1:A:359:LEU:HB3	1:A:360:PRO:HD3	1.91	0.52
1:A:1521:PRO:O	1:A:1524:SER:OG	2.23	0.52
1:A:968:GLN:O	1:A:972:GLN:HG2	2.10	0.52
1:A:3988:TYR:O	1:A:3991:VAL:HG22	2.09	0.52
1:A:528:ILE:HD12	1:A:531:VAL:HG21	1.92	0.52
1:A:1655:ARG:HA	1:A:1655:ARG:NE	2.25	0.52
1:A:66:ALA:O	1:A:70:GLN:NE2	2.37	0.52
1:A:4147:GLU:OE1	1:A:4340:THR:N	2.42	0.52
1:A:437:ASP:OD1	1:A:517:LYS:HE2	2.10	0.51
1:A:4269:HIS:NE2	1:A:4324:GLN:OE1	2.44	0.51
1:A:258:PHE:HA	1:A:261:ILE:HG22	1.92	0.51
1:A:4300:VAL:HG23	1:A:4301:THR:HG23	1.93	0.51
1:A:1822:LEU:O	1:A:1826:HIS:ND1	2.44	0.51
1:A:4248:GLU:OE1	1:A:4298:GLN:NE2	2.33	0.51
1:A:1882:PRO:O	1:A:1886:THR:HG23	2.11	0.50
1:A:1939:PRO:HD2	1:A:1942:ILE:HD12	1.93	0.50
1:A:3876:VAL:HG21	1:A:3965:VAL:CG1	2.41	0.50
1:A:1771:ASP:OD1	1:A:1772:PRO:HD2	2.12	0.50
1:A:3989:ILE:HG21	1:A:4241:ILE:O	2.11	0.50
1:A:611:LEU:O	1:A:617:GLY:HA3	2.12	0.50
1:A:263:LEU:CD2	1:A:3294:LEU:HD21	2.42	0.50
1:A:355:TYR:O	1:A:364:ARG:NH2	2.45	0.49
1:A:2217:LEU:HD21	1:A:2253:LEU:HD21	1.93	0.49
1:A:1512:GLU:O	1:A:1516:GLN:HB3	2.12	0.49
1:A:1770:VAL:HG23	1:A:1771:ASP:H	1.76	0.49
1:A:372:ASP:OD1	1:A:373:PRO:HD2	2.12	0.49
1:A:1254:LYS:NZ	1:A:1435:GLU:OE2	2.43	0.49
1:A:4271:TYR:CD2	1:A:4278:ILE:HD11	2.48	0.49
1:A:1768:VAL:HG23	1:A:1768:VAL:O	2.12	0.49
1:A:1597:ALA:O	1:A:1598:ILE:C	2.51	0.49
1:A:1620:PHE:HZ	1:A:1863:GLY:HA2	1.78	0.49
1:A:236:PRO:HG3	1:A:265:HIS:CD2	2.48	0.49
1:A:1875:GLY:HA2	1:A:2667:VAL:HG22	1.95	0.48
1:A:144:ARG:HD2	1:A:145:SER:HB2	1.96	0.48
1:A:1137:PHE:CZ	1:A:1141:MET:SD	3.06	0.48
1:A:2117:LEU:HG	1:A:2178:ALA:HB1	1.94	0.48
1:A:3970:LEU:HD22	1:A:3977:LEU:HD12	1.94	0.48
1:A:4131:SER:HA	1:A:4141:VAL:HG12	1.95	0.48
1:A:153:SER:O	1:A:153:SER:OG	2.29	0.48
1:A:550:TYR:HB3	1:A:554:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:O	1:A:186:LEU:HD23	2.12	0.48
1:A:1661:GLN:O	1:A:1665:MET:N	2.46	0.48
1:A:1591:ASP:OD1	1:A:1784:ARG:NH1	2.47	0.48
1:A:911:ARG:NH2	1:A:1065:GLU:OE1	2.46	0.48
1:A:1132:ILE:CD1	1:A:1197:GLU:HG2	2.44	0.48
1:A:3598:LEU:HD13	1:A:3741:ARG:HD2	1.95	0.48
1:A:3887:PHE:CD2	1:A:3982:PHE:HE1	2.31	0.48
1:A:1535:LEU:HD23	1:A:1538:GLU:OE1	2.14	0.48
1:A:856:GLU:N	1:A:857:PRO:HD2	2.29	0.48
1:A:1180:VAL:HG12	1:A:1181:PRO:O	2.14	0.47
1:A:1621:ASP:O	1:A:1625:GLY:N	2.46	0.47
1:A:4271:TYR:CE1	1:A:4327:ARG:HG3	2.50	0.47
1:A:522:PRO:O	1:A:523:ALA:HB3	2.13	0.47
1:A:950:VAL:HG13	1:A:966:PHE:HE1	1.79	0.47
1:A:1775:LEU:HA	1:A:1778:THR:HG22	1.96	0.47
1:A:4048:ILE:HG13	1:A:4065:TRP:CG	2.50	0.47
1:A:567:PHE:O	1:A:4057:ASP:OD2	2.32	0.47
1:A:2176:LEU:O	1:A:2180:MET:HG2	2.15	0.47
1:A:3602:ALA:O	1:A:3606:LEU:HG	2.14	0.47
1:A:4271:TYR:CZ	1:A:4327:ARG:HG3	2.49	0.47
1:A:416:ILE:O	1:A:416:ILE:HG22	2.14	0.47
1:A:873:GLU:OE2	1:A:890:THR:HA	2.14	0.47
1:A:1265:TYR:O	1:A:1269:MET:SD	2.73	0.47
1:A:3853:LEU:O	1:A:3857:TRP:CD1	2.68	0.47
1:A:4157:LEU:HD21	1:A:4210:VAL:HG11	1.97	0.46
1:A:409:MET:SD	1:A:436:VAL:HG13	2.55	0.46
1:A:427:THR:O	1:A:430:THR:HG22	2.16	0.46
1:A:3219:ARG:HG2	1:A:3223:ILE:HD12	1.98	0.46
1:A:3985:LEU:HD11	1:A:3992:LEU:HD21	1.98	0.46
1:A:88:GLN:O	1:A:92:LEU:HD13	2.16	0.46
1:A:1622:ASP:OD2	1:A:1863:GLY:HA3	2.16	0.46
1:A:2212:ILE:HG13	1:A:2213:ILE:N	2.31	0.46
1:A:4134:LYS:O	1:A:4138:GLY:N	2.49	0.46
1:A:1886:THR:HG22	1:A:2670:VAL:HG13	1.98	0.46
1:A:183:CYS:HA	1:A:274:LEU:HD21	1.96	0.46
1:A:456:PHE:CD1	1:A:511:MET:HG3	2.51	0.46
1:A:974:LEU:HD12	1:A:1045:ARG:HG2	1.98	0.46
1:A:3639:GLY:N	1:A:3859:MET:HE1	2.31	0.46
1:A:974:LEU:HD11	1:A:1048:GLN:HG3	1.97	0.46
1:A:1866:GLU:OE2	1:A:1866:GLU:N	2.48	0.46
1:A:1253:ILE:HG23	1:A:1273:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1584:THR:HG22	1:A:1774:THR:HA	1.98	0.45
1:A:1849:GLY:HA2	1:A:1864:SER:HB3	1.98	0.45
1:A:3605:LEU:HD22	1:A:3619:VAL:HG21	1.98	0.45
1:A:1510:VAL:HG12	1:A:1574:GLN:OE1	2.17	0.45
1:A:1940:ASP:O	1:A:1944:GLU:HG3	2.17	0.45
1:A:2108:VAL:O	1:A:2112:VAL:HG23	2.16	0.45
1:A:2659:ASP:OD1	1:A:2659:ASP:N	2.49	0.45
1:A:1132:ILE:HD12	1:A:1197:GLU:HG2	1.97	0.45
1:A:4071:ARG:NE	1:A:4071:ARG:HA	2.31	0.45
1:A:4206:TYR:O	1:A:4210:VAL:HG12	2.17	0.45
1:A:847:GLN:HB3	1:A:902:TYR:HH	1.82	0.45
1:A:1253:ILE:HG23	1:A:1273:MET:CG	2.47	0.45
1:A:1469:ILE:O	1:A:1472:ASN:O	2.34	0.45
1:A:100:THR:HG22	1:A:104:ILE:HD13	1.99	0.45
1:A:201:GLU:OE1	1:A:3297:ARG:HD3	2.17	0.45
1:A:1953:LEU:HA	1:A:2068:THR:HG22	1.99	0.45
1:A:3578:GLU:O	1:A:3582:GLN:HG3	2.17	0.45
1:A:873:GLU:OE2	1:A:889:ALA:O	2.33	0.45
1:A:698:ILE:O	1:A:763:PRO:HA	2.17	0.45
1:A:3721:LEU:HD12	1:A:3875:ALA:HB1	1.98	0.45
1:A:3851:LEU:HD12	1:A:3889:VAL:HG21	1.97	0.45
1:A:4079:ALA:O	1:A:4097:SER:HB3	2.17	0.45
1:A:263:LEU:HD21	1:A:3294:LEU:HD21	1.99	0.45
1:A:311:ASP:O	1:A:315:ILE:HG12	2.17	0.44
1:A:937:LEU:HD22	1:A:1063:LEU:HD21	1.98	0.44
1:A:3970:LEU:HD22	1:A:3977:LEU:CD1	2.48	0.44
1:A:317:ASP:OD2	1:A:317:ASP:N	2.49	0.44
1:A:614:ASN:O	1:A:615:ALA:HB3	2.18	0.44
1:A:1838:MET:SD	1:A:1877:ALA:HB1	2.58	0.44
1:A:4107:PHE:CE1	1:A:4222:GLN:HG2	2.52	0.44
1:A:120:THR:OG1	1:A:155:LYS:HE2	2.18	0.44
1:A:4280:TRP:CD1	1:A:4353:PHE:HB2	2.52	0.44
1:A:951:LEU:HD22	1:A:1049:ILE:HG23	2.00	0.43
1:A:1129:THR:HA	1:A:1132:ILE:HG22	2.00	0.43
1:A:1627:TRP:CZ3	1:A:1679:MET:HB3	2.53	0.43
1:A:1943:LYS:HD3	1:A:2088:LEU:HD11	2.00	0.43
1:A:3877:LEU:HD23	1:A:3969:ILE:HD13	1.99	0.43
1:A:4004:GLU:HB3	1:A:4238:LEU:HD11	2.00	0.43
1:A:4045:ARG:HE	1:A:4046:LEU:N	2.16	0.43
1:A:4021:VAL:HB	1:A:4026:VAL:HA	1.99	0.43
1:A:188:MET:HA	1:A:188:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ALA:HB1	1:A:376:ASP:O	2.18	0.43
1:A:142:SER:HB3	1:A:148:ILE:HD11	2.01	0.43
1:A:3286:LEU:HD11	1:A:3392:LEU:CD1	2.49	0.43
1:A:640:LEU:N	1:A:641:PRO:HD2	2.33	0.43
1:A:820:ALA:O	1:A:824:VAL:HG23	2.19	0.43
1:A:1879:CYS:SG	1:A:2663:MET:HA	2.58	0.43
1:A:2655:CYS:SG	1:A:2663:MET:HB2	2.59	0.43
1:A:3642:LEU:HD23	1:A:3642:LEU:O	2.18	0.43
1:A:4089:VAL:HB	1:A:4305:LYS:NZ	2.34	0.43
1:A:1610:LEU:HG	1:A:1682:LEU:HD23	2.00	0.43
1:A:3976:HIS:CG	1:A:4003:GLN:OE1	2.72	0.43
1:A:376:ASP:HA	1:A:377:PRO:HD3	1.86	0.42
1:A:644:ARG:HG2	1:A:644:ARG:HH11	1.84	0.42
1:A:1682:LEU:HD13	1:A:2672:VAL:CG2	2.49	0.42
1:A:3636:LYS:O	1:A:3640:THR:HG23	2.19	0.42
1:A:4014:LYS:NZ	1:A:4043:LYS:O	2.50	0.42
1:A:258:PHE:O	1:A:261:ILE:HG22	2.19	0.42
1:A:4189:LEU:N	1:A:4189:LEU:CD2	2.83	0.42
1:A:1195:THR:HG22	1:A:1195:THR:O	2.18	0.42
1:A:157:THR:O	1:A:161:THR:HG23	2.19	0.42
1:A:248:SER:O	1:A:248:SER:OG	2.35	0.42
1:A:949:THR:HG21	1:A:1129:THR:HG23	2.00	0.42
1:A:1447:CYS:O	1:A:1451:LEU:HG	2.18	0.42
1:A:4042:MET:SD	1:A:4112:ARG:HD3	2.60	0.42
1:A:3182:ASP:OD1	1:A:3182:ASP:N	2.50	0.42
1:A:186:LEU:HB3	1:A:190:LYS:HB2	2.01	0.42
1:A:972:GLN:HA	1:A:972:GLN:OE1	2.20	0.42
1:A:1139:SER:HB3	1:A:1140:PRO:HD3	2.01	0.42
1:A:4189:LEU:O	1:A:4209:LEU:HD21	2.19	0.42
1:A:61:PHE:O	1:A:65:LEU:HG	2.19	0.42
1:A:367:ILE:HG23	1:A:415:VAL:HG22	2.01	0.42
1:A:648:SER:O	1:A:648:SER:OG	2.33	0.42
1:A:3970:LEU:HD21	1:A:3982:PHE:CD2	2.55	0.42
1:A:20:ARG:HA	1:A:23:ILE:HD12	2.01	0.42
1:A:2117:LEU:N	1:A:2118:PRO:HD2	2.35	0.42
1:A:1770:VAL:HG23	1:A:1771:ASP:N	2.35	0.42
1:A:2152:LEU:HD13	1:A:2152:LEU:C	2.40	0.42
1:A:3298:THR:HG22	1:A:3325:HIS:CE1	2.55	0.42
1:A:4080:LEU:HA	1:A:4107:PHE:CZ	2.55	0.42
1:A:4134:LYS:HB3	1:A:4139:LYS:O	2.20	0.42
1:A:186:LEU:HD12	1:A:190:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:ILE:HG21	1:A:866:GLY:HA3	2.01	0.42
1:A:974:LEU:C	1:A:974:LEU:HD13	2.40	0.42
1:A:1825:ARG:NH1	1:A:2081:SER:HG	2.15	0.42
1:A:1943:LYS:O	1:A:1947:TYR:CG	2.73	0.42
1:A:3458:SER:HA	1:A:3604:VAL:HG22	2.01	0.42
1:A:4083:THR:HA	1:A:4090:THR:O	2.20	0.42
1:A:4324:GLN:HG3	1:A:4344:GLN:HA	2.01	0.41
1:A:99:PHE:CE1	1:A:103:LEU:HD21	2.54	0.41
1:A:847:GLN:OE1	1:A:902:TYR:OH	2.37	0.41
1:A:1584:THR:OG1	1:A:1585:PRO:HD3	2.20	0.41
1:A:4107:PHE:HA	1:A:4110:VAL:HG12	2.01	0.41
1:A:4129:THR:HG22	1:A:4130:ARG:N	2.35	0.41
1:A:4216:THR:HG23	1:A:4223:LEU:HD22	2.02	0.41
1:A:1680:LEU:HD23	1:A:1681:THR:N	2.35	0.41
1:A:2089:ILE:HG21	1:A:2135:PHE:HZ	1.86	0.41
1:A:4131:SER:HB3	1:A:4145:ASP:OD2	2.21	0.41
1:A:1535:LEU:O	1:A:1539:GLU:OE2	2.39	0.41
1:A:4089:VAL:O	1:A:4305:LYS:NZ	2.54	0.41
1:A:521:ASP:OD1	1:A:522:PRO:HD2	2.20	0.41
1:A:528:ILE:HD12	1:A:531:VAL:CG2	2.50	0.41
1:A:2169:SER:O	1:A:2172:LYS:HB3	2.20	0.41
1:A:1828:ILE:HD13	1:A:1942:ILE:HG23	2.03	0.41
1:A:2691:GLU:O	1:A:2695:LYS:HD3	2.20	0.41
1:A:3233:SER:OG	1:A:3329:ALA:HB1	2.21	0.41
1:A:440:THR:HA	1:A:443:ASP:O	2.21	0.41
1:A:1170:PHE:CE1	1:A:1252:CYS:HB3	2.56	0.41
1:A:1253:ILE:O	1:A:1257:TRP:N	2.54	0.41
1:A:1580:PRO:HB3	1:A:1582:TRP:NE1	2.36	0.41
1:A:1824:LEU:O	1:A:1828:ILE:HG12	2.20	0.41
1:A:4042:MET:HG3	1:A:4112:ARG:HD3	2.03	0.41
1:A:4045:ARG:HH21	1:A:4046:LEU:HB2	1.86	0.41
1:A:1867:ILE:HG23	1:A:1868:ASN:N	2.36	0.41
1:A:3598:LEU:HD22	1:A:3741:ARG:NE	2.36	0.41
1:A:3967:ASN:OD1	1:A:3993:ASP:N	2.51	0.41
1:A:1502:LEU:CD1	1:A:1509:THR:HA	2.51	0.40
1:A:1885:PHE:HD1	1:A:2670:VAL:HG11	1.86	0.40
1:A:2099:SER:OG	1:A:2102:ILE:HG12	2.21	0.40
1:A:3963:ARG:NH2	1:A:3992:LEU:O	2.54	0.40
1:A:17:ALA:O	1:A:20:ARG:N	2.54	0.40
1:A:764:ILE:HG13	1:A:765:PRO:HD2	2.04	0.40
1:A:1626:ARG:HD2	1:A:1920:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4034:LEU:HA	1:A:4037:LYS:CG	2.52	0.40
1:A:1619:TRP:CZ2	1:A:1628:CYS:SG	3.14	0.40
1:A:779:SER:O	1:A:783:ASN:HB2	2.21	0.40
1:A:1451:LEU:HD11	1:A:1532:LEU:HD22	2.02	0.40
1:A:4005:LEU:HD13	1:A:4238:LEU:HD23	2.04	0.40
1:A:4317:MET:HB2	1:A:4341:CYS:HB2	2.04	0.40
1:A:154:ASP:OD1	1:A:155:LYS:N	2.53	0.40
1:A:359:LEU:HD13	1:A:359:LEU:C	2.42	0.40
1:A:2117:LEU:O	1:A:2129:PRO:HB3	2.21	0.40
1:A:2146:THR:HB	1:A:2150:VAL:HG23	2.03	0.40
1:A:3443:ILE:HD13	1:A:3449:LEU:HD13	2.04	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%)	2312 (98%)	57 (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%)	2115 (98%)	34 (2%)	62 81

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	SER
1	A	344	SER
1	A	850	SER
1	A	1121	THR
1	A	1489	TRP
1	A	1537	PHE
1	A	1591	ASP
1	A	1870	ILE
1	A	1911	PHE
1	A	1922	VAL
1	A	1933	SER
1	A	2105	ASP
1	A	2114	ASP
1	A	2144	SER
1	A	2185	THR
1	A	2239	MET
1	A	2643	SER
1	A	2662	SER
1	A	3284	SER
1	A	3288	VAL
1	A	3302	GLN
1	A	3609	SER
1	A	3619	VAL
1	A	3725	SER
1	A	3732	LYS
1	A	3870	SER
1	A	3984	VAL
1	A	4006	GLU
1	A	4013	ARG
1	A	4071	ARG
1	A	4183	VAL
1	A	4189	LEU
1	A	4327	ARG
1	A	4358	HIS

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	39	GLN
1	A	136	ASN
1	A	260	HIS
1	A	356	HIS
1	A	1258	ASN
1	A	1516	GLN
1	A	3206	HIS
1	A	3302	GLN
1	A	3976	HIS
1	A	4056	GLN
1	A	4135	HIS
1	A	4272	GLN
1	A	4343	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

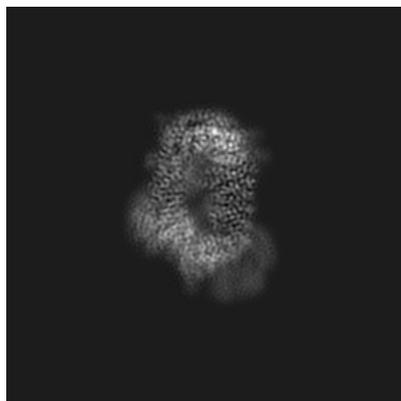
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22429. These allow visual inspection of the internal detail of the map and identification of artifacts.

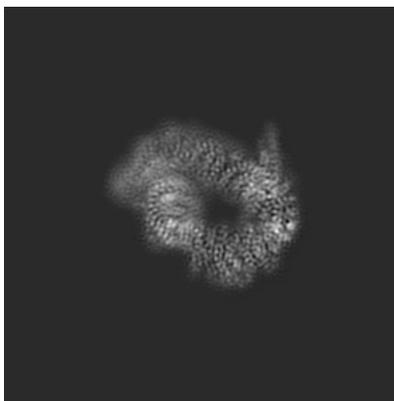
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

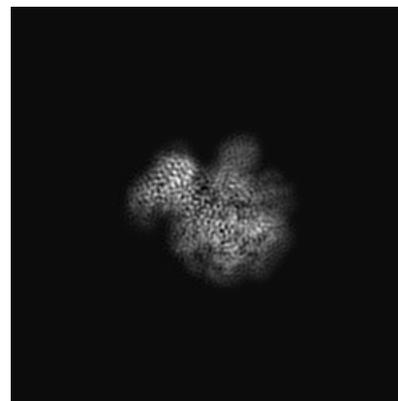
6.1.1 Primary map



X

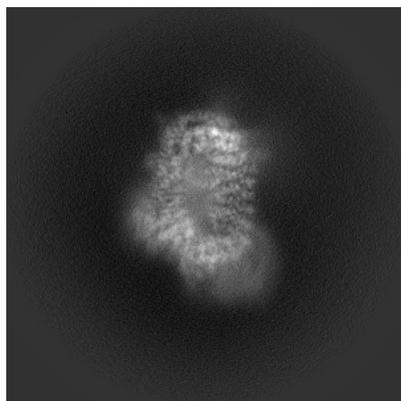


Y

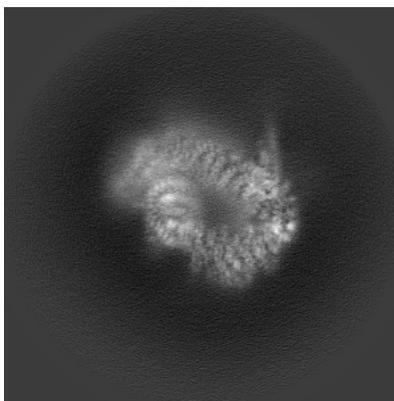


Z

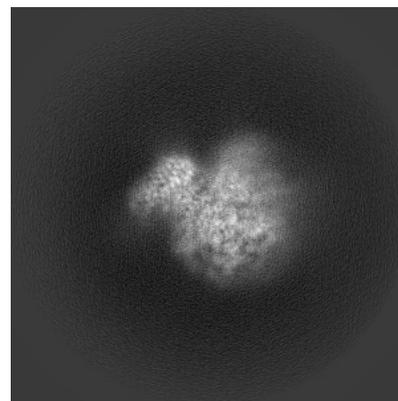
6.1.2 Raw map



X



Y

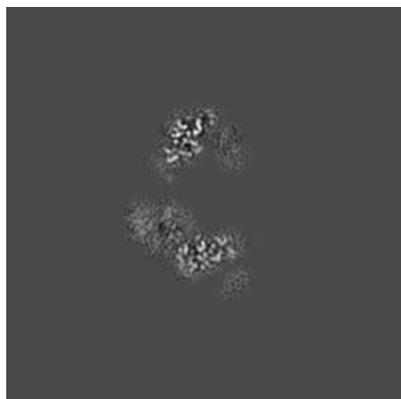


Z

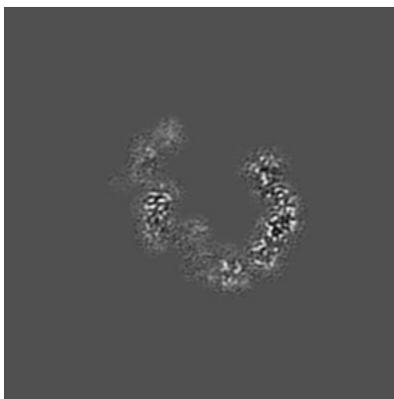
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

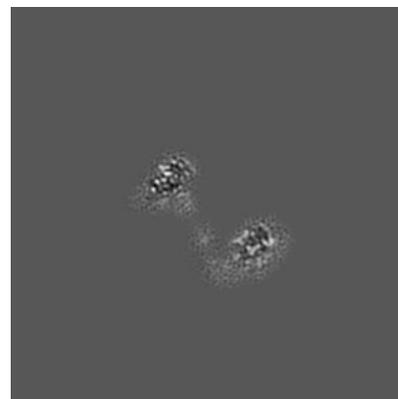
6.2.1 Primary map



X Index: 182

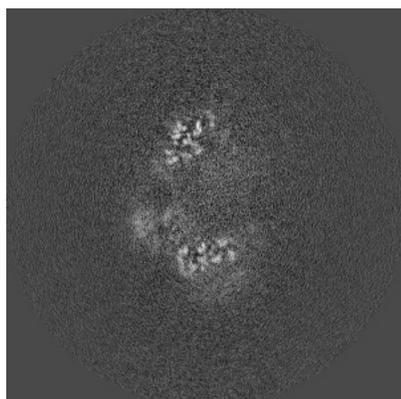


Y Index: 182

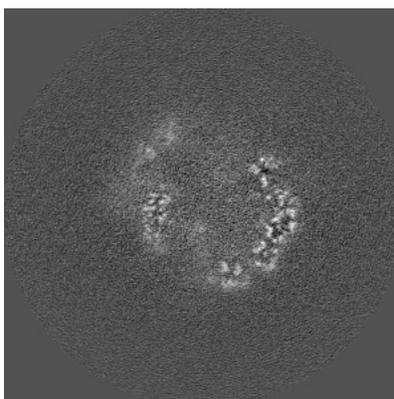


Z Index: 182

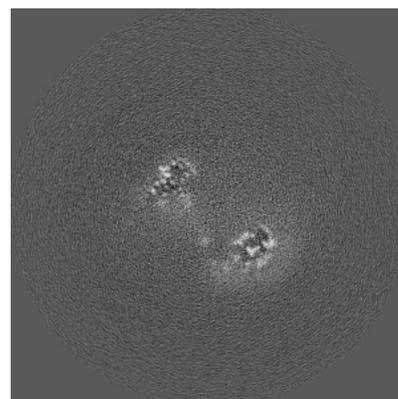
6.2.2 Raw map



X Index: 182



Y Index: 182



Z Index: 182

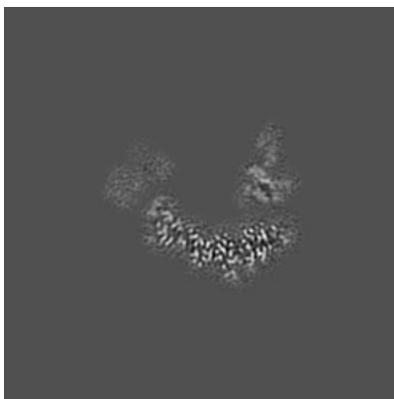
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

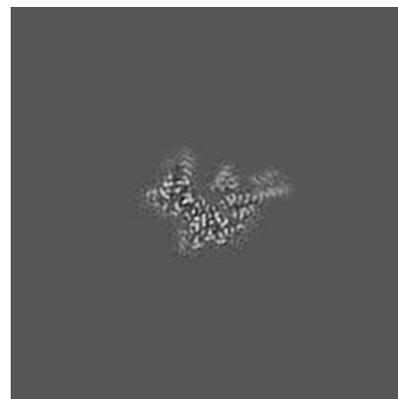
6.3.1 Primary map



X Index: 149

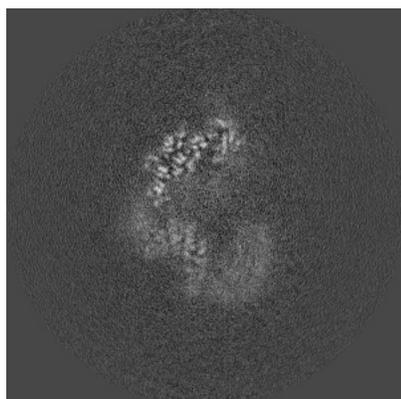


Y Index: 204

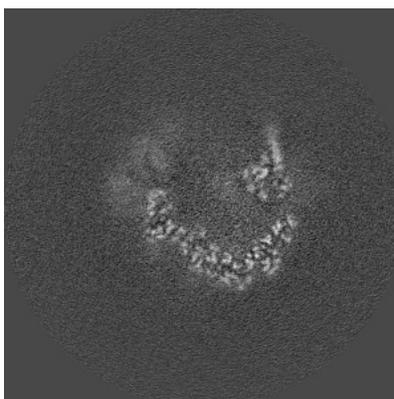


Z Index: 247

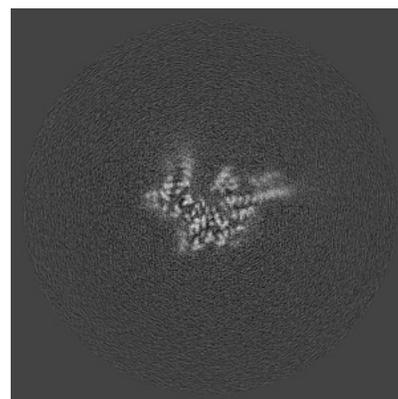
6.3.2 Raw map



X Index: 202



Y Index: 192



Z Index: 247

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

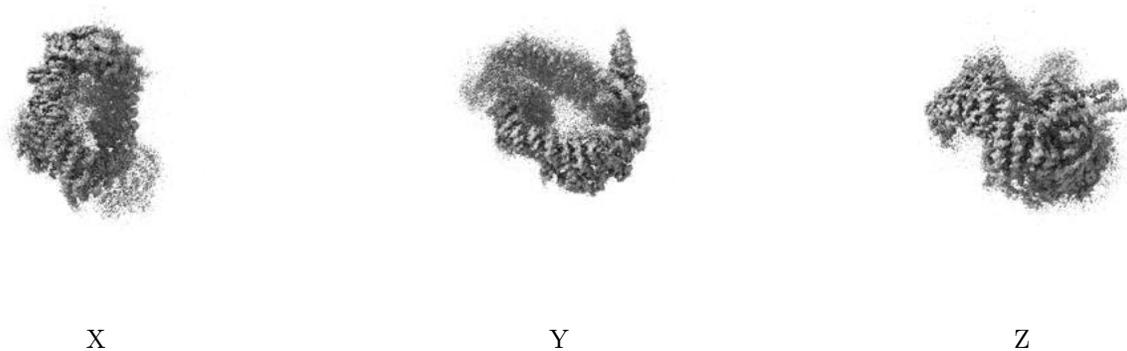
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

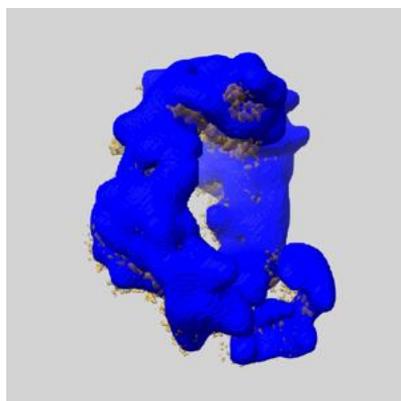
6.5 Mask visualisation [i](#)

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

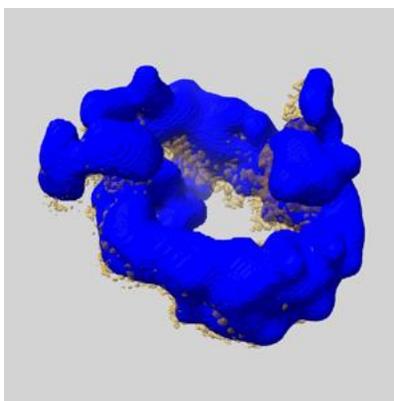
A mask typically either:

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

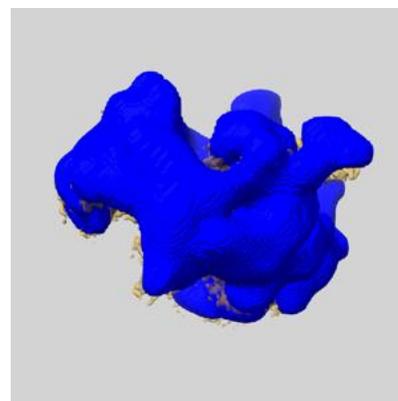
6.5.1 emd_22429_msk_1.map [i](#)



X



Y

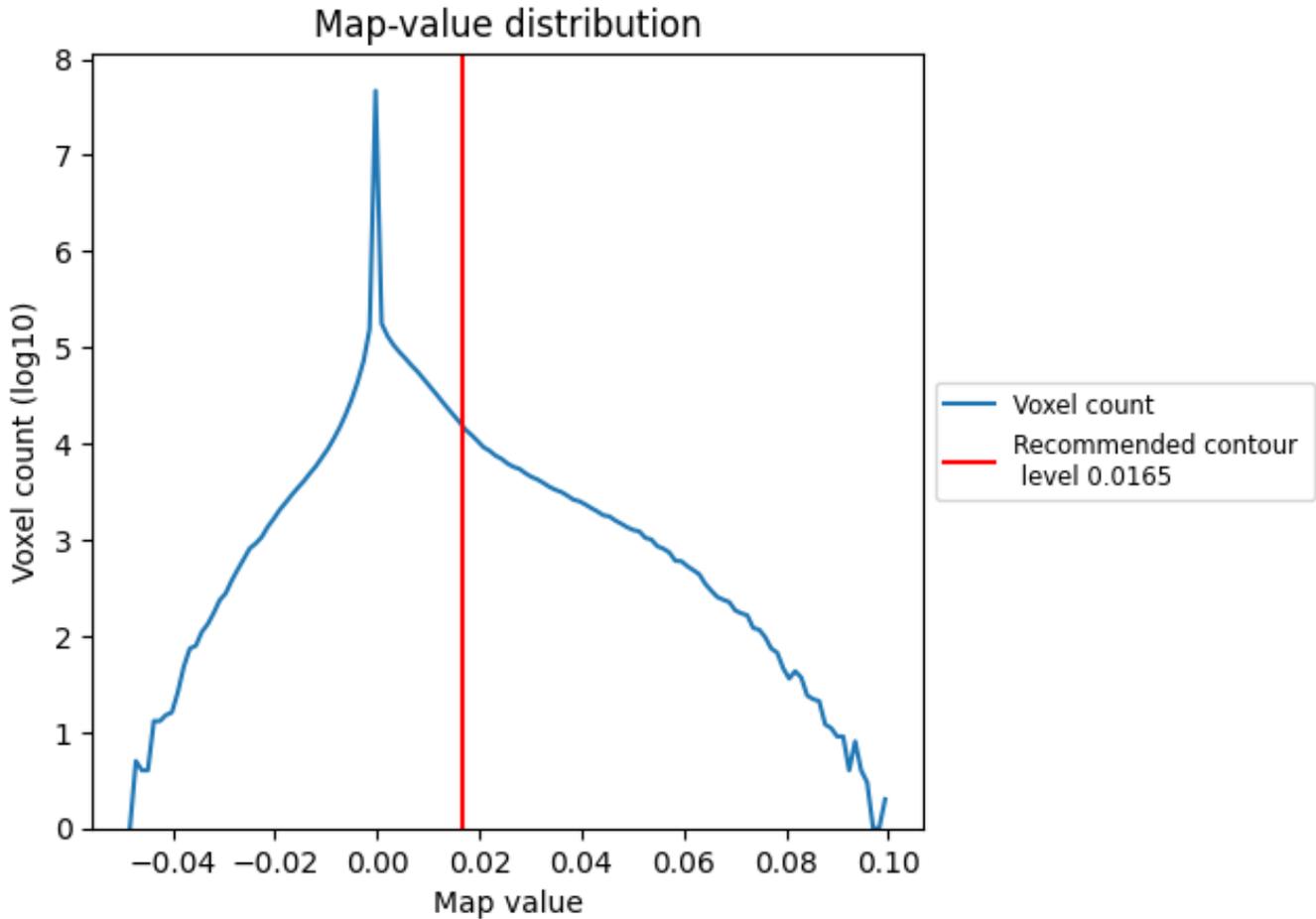


Z

7 Map analysis [i](#)

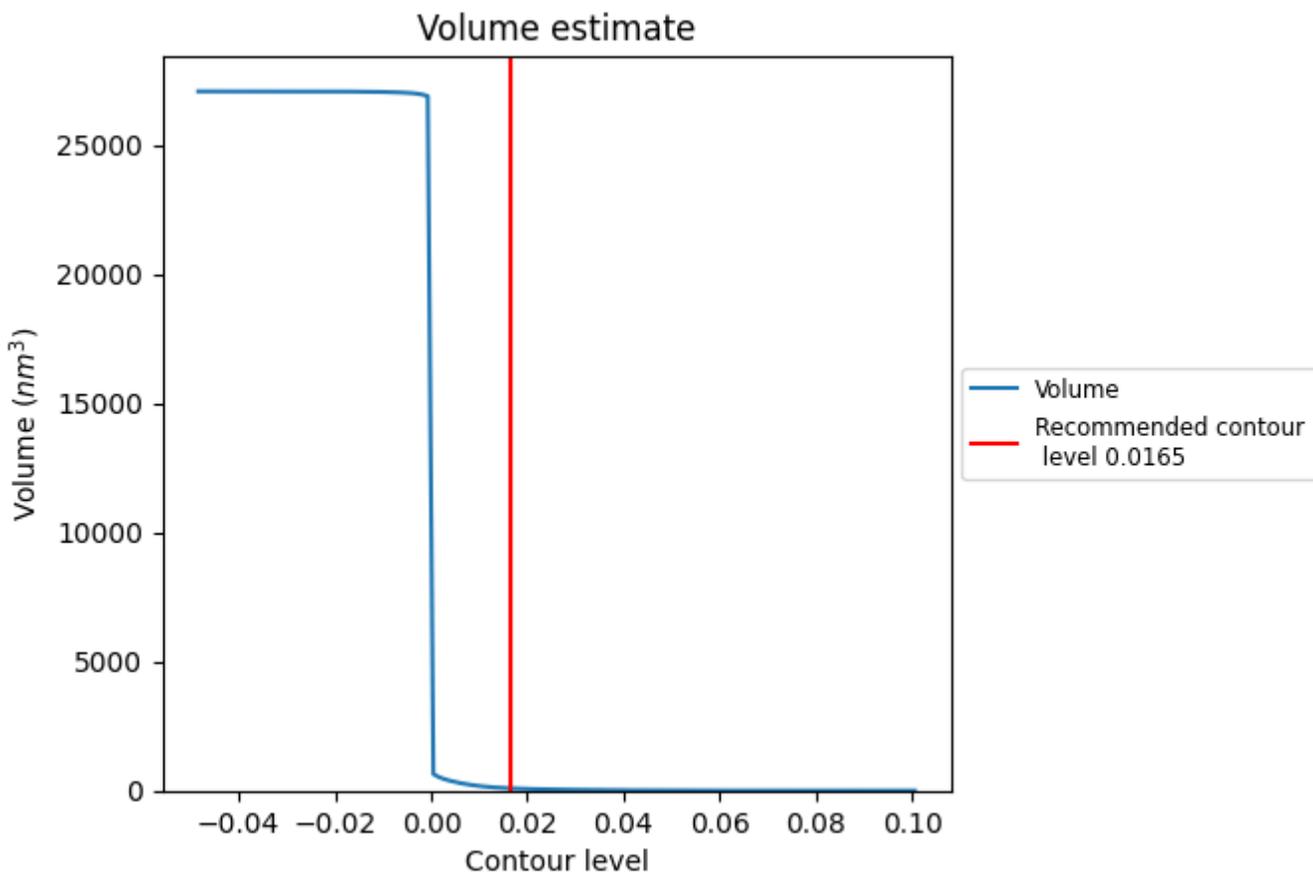
This section contains the results of statistical analysis of the map.

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.

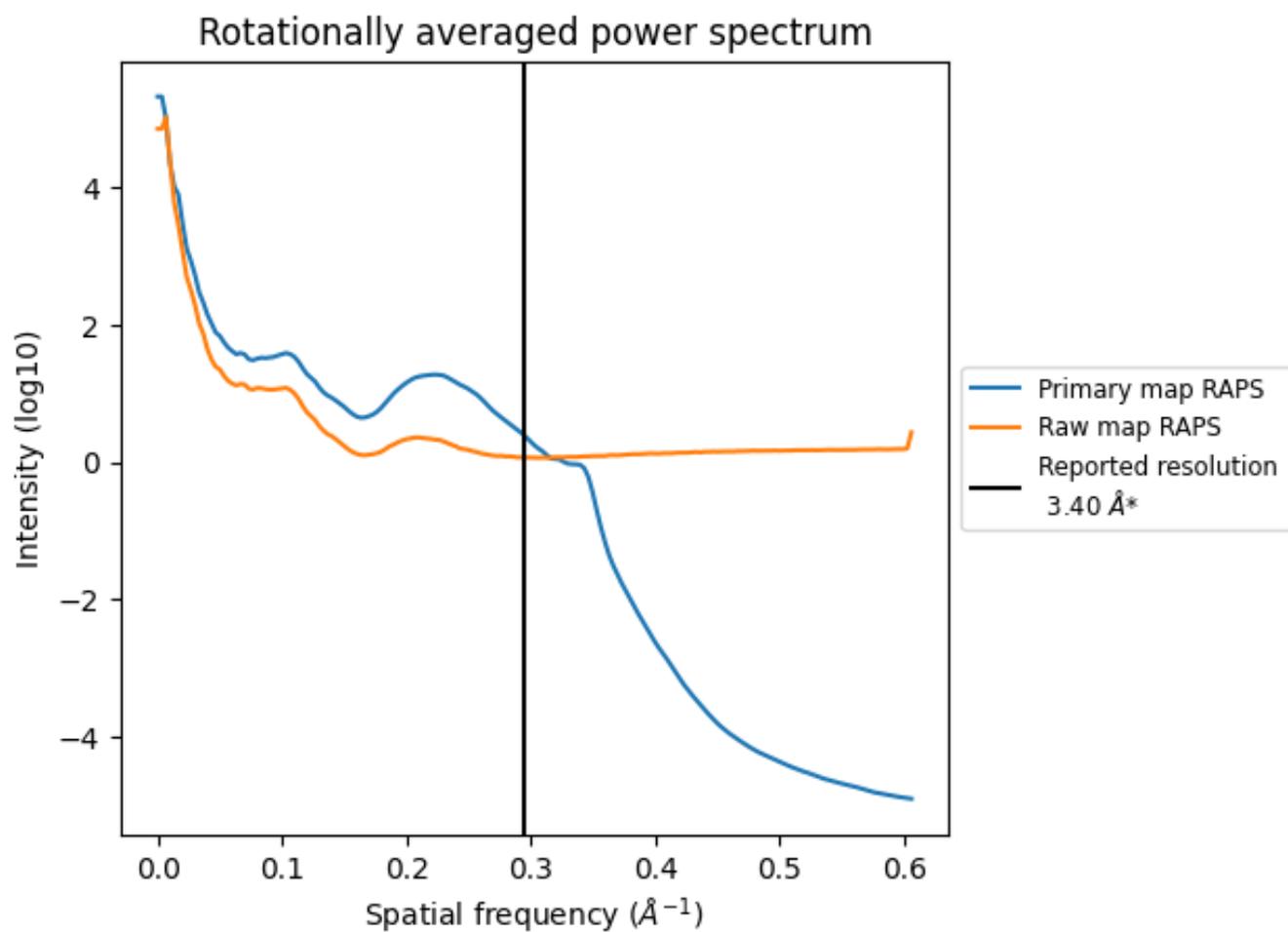
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 81 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

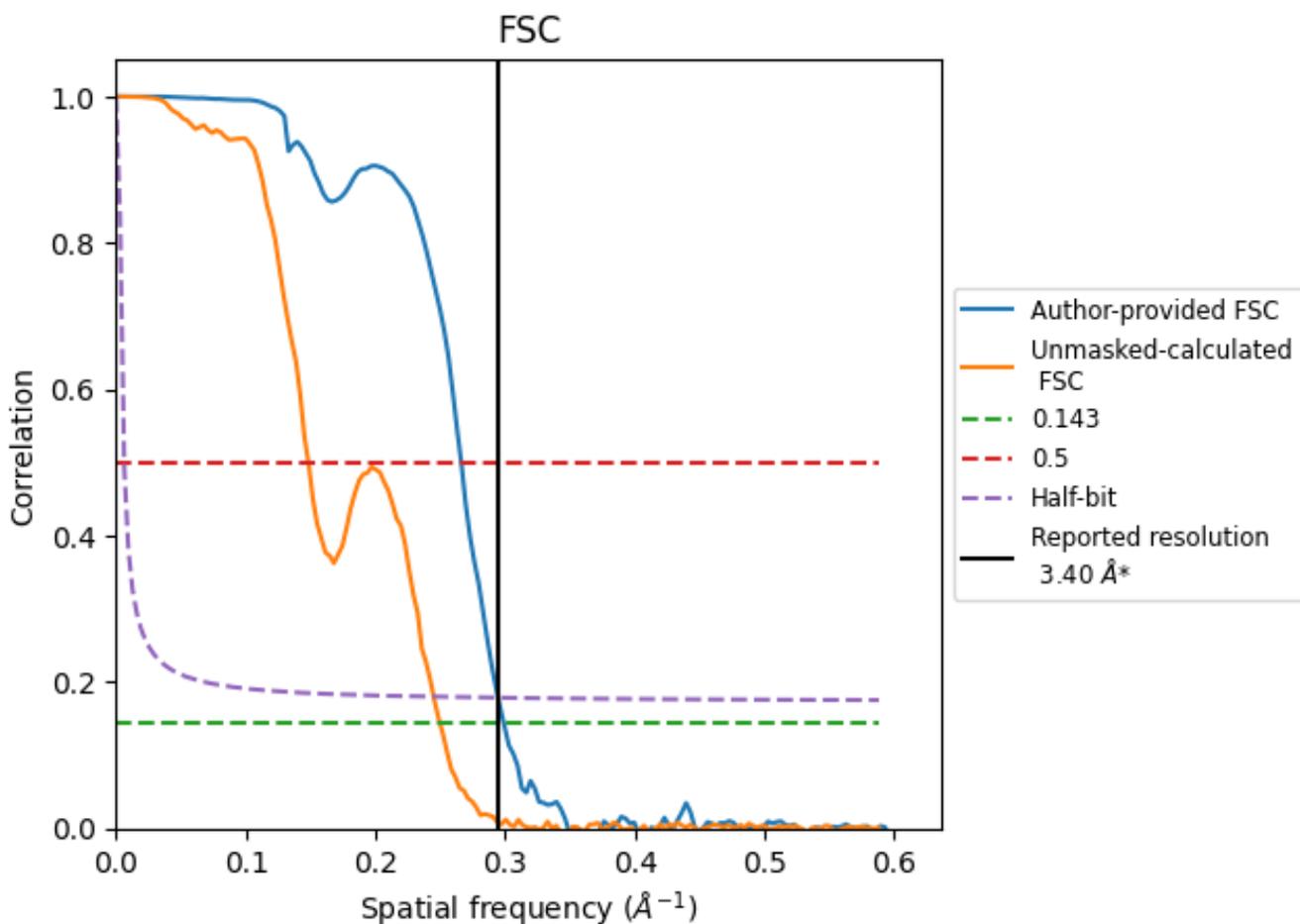


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294\AA^{-1}

8.2 Resolution estimates [i](#)

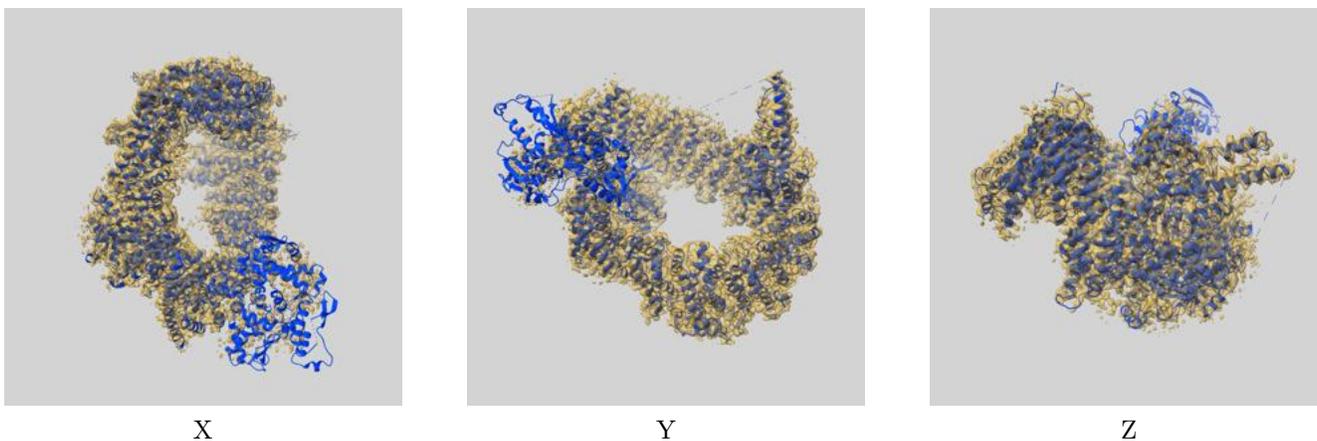
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	3.76	3.39
Unmasked-calculated*	4.00	6.74	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

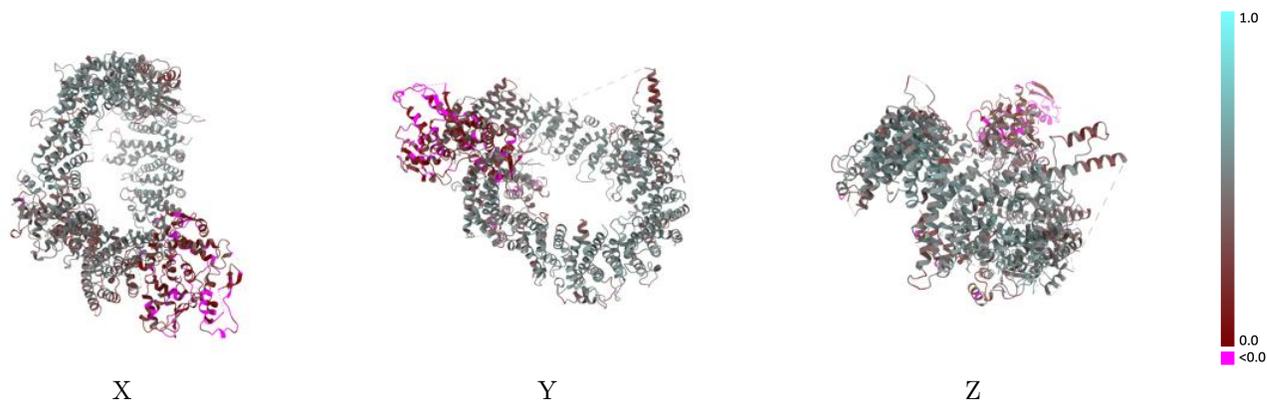
This section contains information regarding the fit between EMDB map EMD-22429 and PDB model 7MWE. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



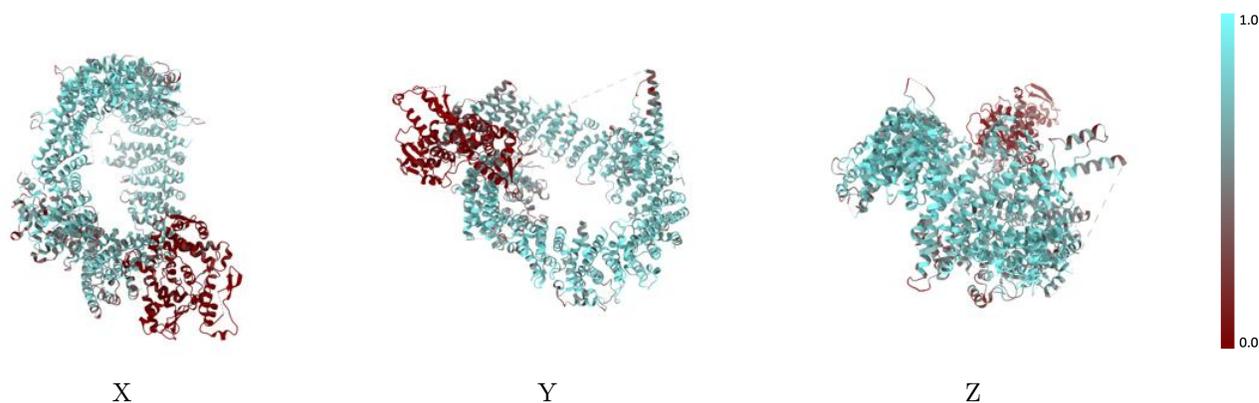
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



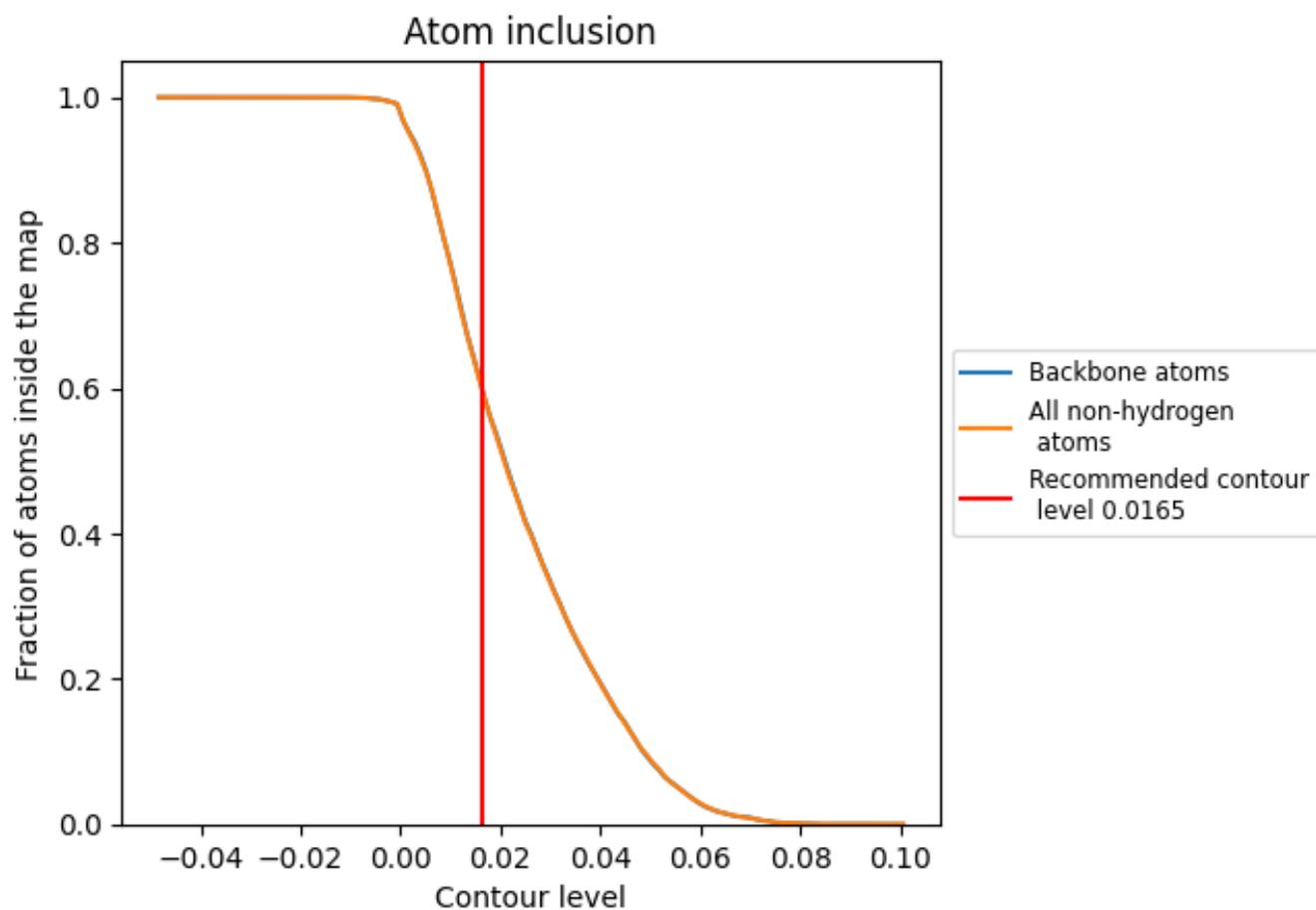
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 59% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5936	 0.4090
A	 0.5950	 0.4090

