WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 05:55 AM JST

PDB ID	:	6KIO
EMDB ID	:	EMD-9996
Title	:	Complex of yeast cytoplasmic dynein MTBD-High and MT without DTT
Authors	:	Komori, Y.; Nishida, N.; Shimada, I.; Kikkawa, M.
Deposited on	:	2019-07-19
Resolution	:	3.94 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 3.94 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.
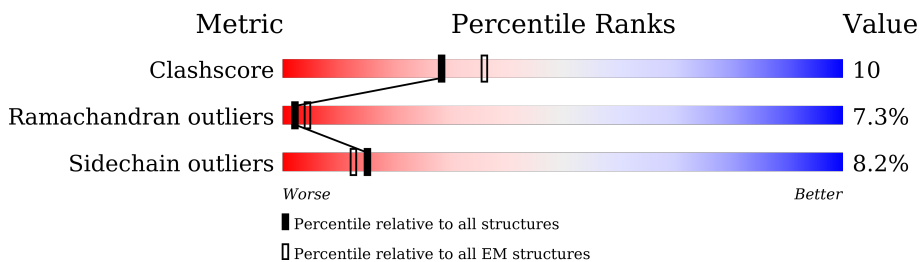
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	b	426	69% 25% 6%
2	M	130	38% / 81% 18% •
3	a	412	71% 22% 5% •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 15091 atoms, of which 7442 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 Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	b	426	Total	C	H	N	O	S	0	0
			6584	2105	3232	575	647	25		

- Molecule 2 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	130	Total	C	H	N	O	S	0	0
			2132	679	1063	184	197	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	3101	CYS	ILE	engineered mutation	UNP P36022
M	3222	CYS	VAL	engineered mutation	UNP P36022

- Molecule 3 is a protein called Tubulin alpha-1A chain.

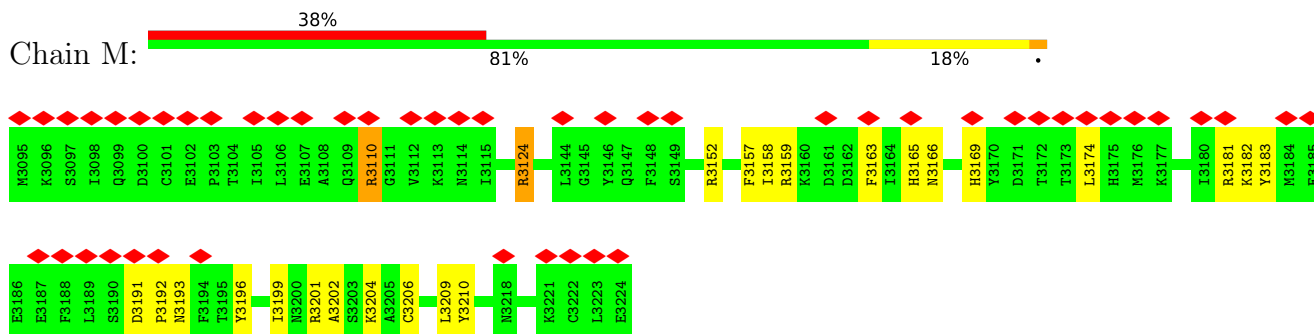| Mol	Chain	Residues	Atoms						AltConf	Trace
3	a	412	Total	C	H	N	O	S	0	0
			6375	2043	3147	551	614	20		

3 Residue-property plots ⓘ

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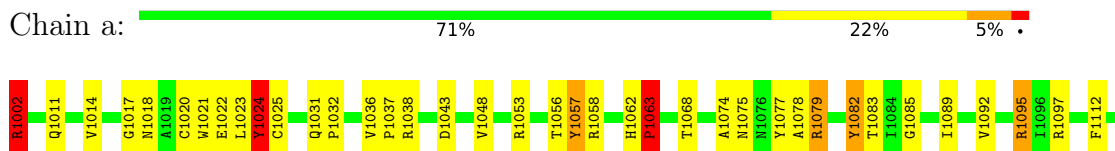
• Molecule 1: Tubulin beta chain

Chain b:

69%   25%   6%
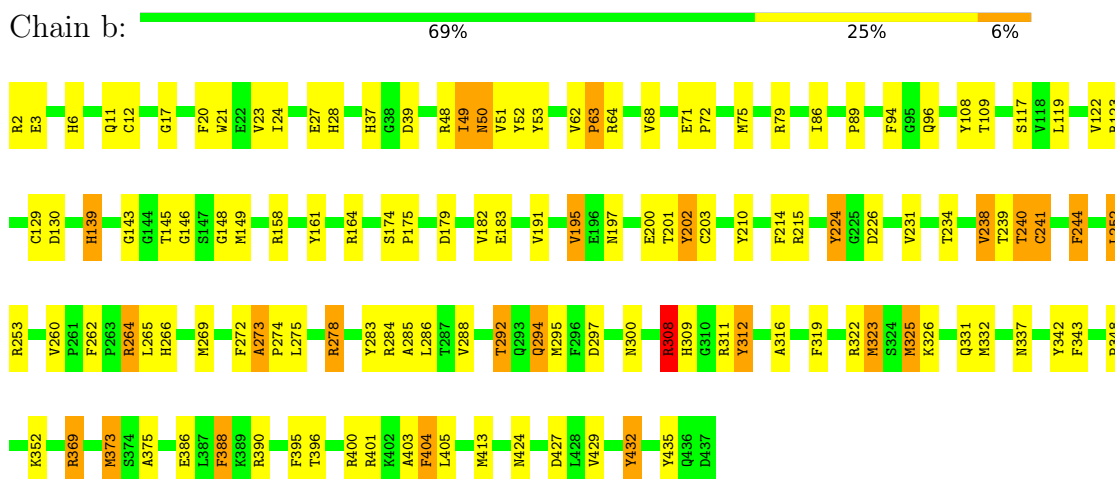
• Molecule 2: Dynein heavy chain, cytoplasmic

Chain M:

38%

81%   18%   •

• Molecule 3: Tubulin alpha-1A chain

Chain a:

71%   22%   5%   •

G1117 G1118 T1119 G1122 F1123 L1126 L1127 M1128 E1129 R1130 Y1135 Y1146 P1147 A1148 S1152 V1156 E1157 P1158 Y1159 M1177 V1178 D1179 Y1184 C1187 R1188 R1189 N1190 L1191 R1195 Y1198 T1199 N1200 L1201 N1202 R1203 I1212 T1213 A1214 R1217 F1229 Q1230 V1234 P1235 Y1236 P1237

R1238 G1239 H1240 F1241 A1247 P1248 Y1256 H1257 E1258 Q1259 V1262 A1263 C1269 M1276 V1277 R1282 Y1286 M1287 A1288 C1289 K1300 A1304 I1315 P1322 T1323 G1324 G1328 I1329 N1330 Y1331 E1332 P1333 P1334 V1337 A1343 K1344 V1345 Q1346 R1347 A1348 V1349 C1350 M1351 E1360 A1361

R1364 L1365 D1366 Y1373 R1376 A1377 Y1382 G1390 R1396 E1407 V1411 D1412 S1413

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7561°, rise=9.20776 Å, axial sym=C1	Depositor
Number of segments used	58999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	54.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.732	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	237.6, 237.6, 237.6	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	b	1.77	21/3427 (0.6%)	1.91	77/4642 (1.7%)
2	M	0.88	0/1092	1.39	7/1472 (0.5%)
3	a	1.72	21/3302 (0.6%)	1.90	85/4485 (1.9%)
All	All	1.65	42/7821 (0.5%)	1.84	169/10599 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	20
2	M	0	5
3	a	0	16
All	All	0	41

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	269	MET	C-N	-8.05	1.19	1.34
1	b	21	TRP	NE1-CE2	-7.77	1.27	1.37
1	b	63	PRO	CA-C	-7.30	1.38	1.52
3	a	1229	PHE	CB-CG	-7.03	1.39	1.51
1	b	50	ASN	CA-C	-6.96	1.34	1.52
3	a	1112	PHE	CB-CG	-6.59	1.40	1.51
3	a	1014	VAL	CA-CB	-6.38	1.41	1.54
1	b	6	HIS	CB-CG	-6.36	1.38	1.50
3	a	1390	GLY	CA-C	-6.20	1.42	1.51
3	a	1248	PRO	N-CD	-6.19	1.39	1.47
3	a	1146	TYR	CB-CG	-6.06	1.42	1.51
1	b	244	PHE	CB-CG	-6.04	1.41	1.51
3	a	1037	PRO	CA-C	-5.94	1.41	1.52
3	a	1036	VAL	CA-CB	-5.93	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1082	TYR	CB-CG	-5.92	1.42	1.51
3	a	1017	GLY	CA-C	-5.85	1.42	1.51
3	a	1289	CYS	CB-SG	-5.78	1.72	1.81
1	b	17	GLY	CA-C	-5.75	1.42	1.51
1	b	432	TYR	CB-CG	-5.73	1.43	1.51
3	a	1324	GLY	CA-C	-5.73	1.42	1.51
3	a	1328	GLY	CA-C	-5.67	1.42	1.51
1	b	161	TYR	CB-CG	-5.66	1.43	1.51
3	a	1257	HIS	CB-CG	-5.66	1.39	1.50
3	a	1330	ASN	CA-C	-5.63	1.38	1.52
3	a	1247	ALA	C-N	-5.58	1.23	1.34
1	b	148	GLY	CA-C	-5.58	1.43	1.51
3	a	1024	TYR	CB-CG	-5.53	1.43	1.51
1	b	202	TYR	CB-CG	-5.44	1.43	1.51
3	a	1349	VAL	CA-CB	-5.44	1.43	1.54
1	b	62	VAL	CA-CB	-5.41	1.43	1.54
1	b	332	MET	CA-C	-5.40	1.39	1.52
3	a	1063	PRO	CA-C	-5.36	1.42	1.52
3	a	1097	ARG	CA-C	-5.34	1.39	1.52
1	b	50	ASN	C-N	-5.28	1.22	1.34
1	b	274	PRO	N-CD	-5.27	1.40	1.47
1	b	146	GLY	CA-C	-5.24	1.43	1.51
3	a	1241	PHE	C-N	-5.23	1.24	1.34
1	b	52	TYR	CB-CG	-5.07	1.44	1.51
1	b	201	THR	CA-CB	-5.07	1.40	1.53
1	b	234	THR	CA-C	-5.07	1.39	1.52
1	b	71	GLU	C-N	-5.05	1.24	1.34
1	b	62	VAL	C-N	-5.03	1.24	1.34

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	283	TYR	CB-CG-CD2	-17.05	110.77	121.00
1	b	283	TYR	CB-CG-CD1	16.93	131.16	121.00
2	M	3181	ARG	NE-CZ-NH1	14.34	127.47	120.30
3	a	1217	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	b	264	ARG	NE-CZ-NH1	13.71	127.15	120.30
3	a	1002	ARG	NE-CZ-NH1	13.69	127.14	120.30
1	b	2	ARG	NE-CZ-NH2	-13.05	113.78	120.30
3	a	1217	ARG	NE-CZ-NH1	12.68	126.64	120.30
3	a	1195	ARG	NE-CZ-NH1	12.17	126.38	120.30
3	a	1203	ARG	NE-CZ-NH1	12.12	126.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1053	ARG	NE-CZ-NH1	12.04	126.32	120.30
3	a	1282	ARG	NE-CZ-NH1	11.39	126.00	120.30
3	a	1238	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	b	342	TYR	CB-CG-CD1	-11.21	114.28	121.00
1	b	79	ARG	NE-CZ-NH1	10.91	125.76	120.30
1	b	278	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	b	215	ARG	NE-CZ-NH1	10.17	125.38	120.30
3	a	1097	ARG	NE-CZ-NH1	10.02	125.31	120.30
3	a	1188	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	b	390	ARG	NE-CZ-NH1	9.65	125.12	120.30
3	a	1082	TYR	CB-CG-CD2	-9.54	115.28	121.00
1	b	253	ARG	NE-CZ-NH2	-9.38	115.61	120.30
3	a	1373	TYR	CB-CG-CD1	-9.30	115.42	121.00
1	b	253	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	b	388	PHE	CB-CG-CD1	-9.19	114.37	120.80
3	a	1038	ARG	NE-CZ-NH1	9.14	124.87	120.30
3	a	1203	ARG	NE-CZ-NH2	-8.86	115.87	120.30
2	M	3159	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	b	79	ARG	NE-CZ-NH2	-8.70	115.95	120.30
3	a	1097	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	b	400	ARG	NE-CZ-NH1	8.45	124.52	120.30
3	a	1058	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	b	37	HIS	CA-CB-CG	-8.41	99.30	113.60
1	b	49	ILE	C-N-CA	8.39	142.67	121.70
1	b	149	MET	CG-SD-CE	-8.29	86.93	100.20
3	a	1146	TYR	CB-CG-CD1	-8.28	116.03	121.00
1	b	240	THR	N-CA-CB	8.27	126.02	110.30
1	b	278	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	b	308	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	b	214	PHE	N-CA-CB	-8.13	95.97	110.60
3	a	1376	ARG	NE-CZ-NH1	8.08	124.34	120.30
3	a	1130	ARG	NE-CZ-NH1	8.03	124.31	120.30
3	a	1276	MET	CG-SD-CE	-7.96	87.46	100.20
1	b	308	ARG	NE-CZ-NH2	-7.95	116.32	120.30
3	a	1347	ARG	NE-CZ-NH1	7.83	124.22	120.30
3	a	1364	ARG	NE-CZ-NH1	7.83	124.21	120.30
3	a	1269	CYS	CA-CB-SG	-7.79	99.98	114.00
1	b	123	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	b	342	TYR	CB-CG-CD2	7.65	125.59	121.00
3	a	1031	GLN	CA-C-N	7.60	138.37	117.10
1	b	224	TYR	CB-CG-CD2	-7.50	116.50	121.00
3	a	1247	ALA	CA-C-N	7.47	138.02	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1366	ASP	CB-CG-OD1	7.45	125.00	118.30
3	a	1057	TYR	N-CA-CB	7.32	123.78	110.60
2	M	3110	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	a	1256	TYR	CA-CB-CG	-7.13	99.85	113.40
3	a	1189	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	b	231	VAL	CA-CB-CG2	-6.92	100.52	110.90
3	a	1289	CYS	CA-CB-SG	-6.90	101.59	114.00
1	b	6	HIS	N-CA-CB	-6.83	98.31	110.60
3	a	1238	ARG	NE-CZ-NH1	6.75	123.68	120.30
3	a	1364	ARG	CB-CA-C	-6.75	96.89	110.40
2	M	3193	ASN	CA-CB-CG	-6.70	98.67	113.40
3	a	1200	ASN	CA-CB-CG	-6.59	98.90	113.40
3	a	1256	TYR	CA-C-N	-6.53	102.83	117.20
1	b	404	PHE	CB-CG-CD2	-6.47	116.27	120.80
3	a	1130	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	b	388	PHE	CB-CG-CD2	6.42	125.30	120.80
1	b	325	MET	CG-SD-CE	-6.41	89.95	100.20
1	b	432	TYR	CA-CB-CG	-6.35	101.33	113.40
1	b	401	ARG	NE-CZ-NH1	6.35	123.47	120.30
3	a	1351	MET	CG-SD-CE	-6.33	90.08	100.20
1	b	413	MET	CG-SD-CE	-6.32	90.10	100.20
1	b	241	CYS	CA-CB-SG	-6.27	102.72	114.00
3	a	1112	PHE	CB-CG-CD2	-6.26	116.42	120.80
1	b	252	LEU	N-CA-C	6.25	127.88	111.00
3	a	1229	PHE	CB-CA-C	-6.18	98.04	110.40
1	b	273	ALA	CA-C-N	6.17	134.38	117.10
1	b	297	ASP	CB-CG-OD1	6.17	123.85	118.30
3	a	1119	THR	CA-CB-CG2	-6.16	103.78	112.40
1	b	429	VAL	CA-CB-CG2	-6.14	101.69	110.90
1	b	51	VAL	N-CA-C	6.12	127.53	111.00
1	b	48	ARG	NE-CZ-NH1	6.11	123.36	120.30
3	a	1396	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	a	1146	TYR	CB-CA-C	6.02	122.44	110.40
1	b	343	PHE	CA-CB-CG	-6.00	99.50	113.90
3	a	1343	ALA	N-CA-C	5.99	127.18	111.00
1	b	203	CYS	CA-CB-SG	-5.97	103.25	114.00
3	a	1177	MET	CG-SD-CE	-5.97	90.64	100.20
1	b	226	ASP	CA-CB-CG	-5.97	100.27	113.40
3	a	1247	ALA	N-CA-C	5.93	127.01	111.00
3	a	1159	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	b	75	MET	CG-SD-CE	-5.90	90.76	100.20
3	a	1259	GLN	N-CA-C	-5.89	95.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	244	PHE	CB-CG-CD1	-5.88	116.68	120.80
1	b	292	THR	CA-CB-CG2	-5.80	104.28	112.40
1	b	197	ASN	CA-CB-CG	-5.80	100.64	113.40
3	a	1024	TYR	CB-CA-C	5.78	121.96	110.40
3	a	1032	PRO	C-N-CA	5.76	136.10	121.70
1	b	52	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	b	309	HIS	CA-CB-CG	-5.73	103.85	113.60
3	a	1351	MET	CA-CB-CG	5.72	123.03	113.30
3	a	1079	ARG	NE-CZ-NH2	-5.71	117.44	120.30
3	a	1156	VAL	CA-CB-CG1	-5.71	102.34	110.90
3	a	1257	HIS	CA-CB-CG	-5.66	103.97	113.60
3	a	1236	TYR	N-CA-C	-5.65	95.76	111.00
3	a	1135	TYR	CB-CG-CD2	-5.64	117.61	121.00
2	M	3152	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	b	432	TYR	CB-CG-CD1	-5.62	117.63	121.00
3	a	1095	ARG	NE-CZ-NH1	5.61	123.11	120.30
3	a	1234	VAL	CA-CB-CG1	-5.60	102.50	110.90
1	b	191	VAL	CA-CB-CG2	-5.60	102.50	110.90
3	a	1373	TYR	CA-CB-CG	-5.55	102.85	113.40
1	b	264	ARG	CD-NE-CZ	5.51	131.31	123.60
3	a	1247	ALA	O-C-N	-5.51	110.64	121.10
1	b	27	GLU	N-CA-CB	-5.50	100.70	110.60
3	a	1187	CYS	CA-CB-SG	-5.49	104.11	114.00
3	a	1128	MET	CG-SD-CE	-5.48	91.43	100.20
1	b	269	MET	CG-SD-CE	-5.47	91.44	100.20
3	a	1031	GLN	O-C-N	-5.46	110.72	121.10
3	a	1092	VAL	CA-CB-CG2	-5.45	102.72	110.90
3	a	1343	ALA	N-CA-CB	-5.44	102.48	110.10
2	M	3196	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	b	275	LEU	N-CA-CB	-5.41	99.58	110.40
3	a	1020	CYS	N-CA-CB	-5.40	100.89	110.60
1	b	48	ARG	CG-CD-NE	-5.39	100.48	111.80
1	b	405	LEU	N-CA-CB	-5.39	99.62	110.40
3	a	1195	ARG	NE-CZ-NH2	-5.37	117.61	120.30
3	a	1198	TYR	CB-CG-CD2	-5.36	117.78	121.00
3	a	1198	TYR	CB-CG-CD1	5.35	124.21	121.00
3	a	1361	ALA	N-CA-CB	-5.35	102.61	110.10
1	b	2	ARG	NH1-CZ-NH2	5.35	125.28	119.40
3	a	1286	TYR	CA-CB-CG	-5.34	103.24	113.40
1	b	319	PHE	CB-CA-C	-5.33	99.73	110.40
3	a	1159	TYR	CB-CG-CD2	5.33	124.20	121.00
1	b	68	VAL	CA-CB-CG2	-5.29	102.96	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	1382	TYR	CB-CG-CD1	-5.28	117.83	121.00
3	a	1043	ASP	N-CA-CB	5.22	120.00	110.60
1	b	62	VAL	CA-CB-CG1	-5.22	103.07	110.90
3	a	1112	PHE	CA-CB-CG	-5.22	101.37	113.90
3	a	1229	PHE	N-CA-CB	5.21	119.98	110.60
3	a	1152	SER	N-CA-CB	5.21	118.31	110.50
1	b	130	ASP	CB-CG-OD1	5.20	122.98	118.30
3	a	1195	ARG	O-C-N	-5.20	111.22	121.10
3	a	1024	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	b	316	ALA	O-C-N	-5.18	114.42	122.70
3	a	1198	TYR	O-C-N	-5.17	114.42	122.70
1	b	53	TYR	CB-CG-CD2	-5.16	117.90	121.00
3	a	1002	ARG	NH1-CZ-NH2	-5.16	113.72	119.40
1	b	396	THR	CA-CB-CG2	-5.16	105.17	112.40
1	b	323	MET	CG-SD-CE	-5.15	91.96	100.20
1	b	240	THR	CB-CA-C	-5.13	97.74	111.60
1	b	238	VAL	CG1-CB-CG2	-5.13	102.69	110.90
3	a	1349	VAL	CB-CA-C	-5.12	101.67	111.40
1	b	253	ARG	CG-CD-NE	-5.12	101.04	111.80
1	b	108	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	b	164	ARG	CG-CD-NE	-5.11	101.06	111.80
1	b	202	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	b	337	ASN	CA-CB-CG	-5.09	102.19	113.40
3	a	1014	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	b	375	ALA	CB-CA-C	-5.08	102.48	110.10
1	b	129	CYS	C-N-CA	5.08	134.39	121.70
3	a	1347	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	M	3201	ARG	NE-CZ-NH2	5.06	122.83	120.30
3	a	1396	ARG	NE-CZ-NH1	5.05	122.82	120.30
3	a	1023	LEU	C-N-CA	5.04	134.29	121.70
3	a	1038	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	b	200	GLU	CB-CA-C	-5.01	100.37	110.40
1	b	312	TYR	CB-CG-CD1	-5.01	118.00	121.00

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	3110	ARG	Sidechain
2	M	3124	ARG	Sidechain
2	M	3157	PHE	Sidechain
2	M	3183	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	M	3210	TYR	Sidechain
3	a	1002	ARG	Sidechain
3	a	1024	TYR	Sidechain
3	a	1079	ARG	Sidechain
3	a	1095	ARG	Sidechain
3	a	1123	PHE	Sidechain
3	a	1130	ARG	Sidechain
3	a	1146	TYR	Sidechain
3	a	1184	TYR	Sidechain
3	a	1195	ARG	Sidechain
3	a	1198	TYR	Sidechain
3	a	1236	TYR	Sidechain
3	a	1257	HIS	Sidechain
3	a	1286	TYR	Sidechain
3	a	1347	ARG	Sidechain
3	a	1364	ARG	Sidechain
3	a	1373	TYR	Sidechain
1	b	139	HIS	Sidechain
1	b	20	PHE	Sidechain
1	b	202	TYR	Sidechain
1	b	210	TYR	Sidechain
1	b	224	TYR	Sidechain
1	b	244	PHE	Sidechain
1	b	262	PHE	Sidechain
1	b	264	ARG	Sidechain
1	b	272	PHE	Sidechain
1	b	28	HIS	Sidechain
1	b	311	ARG	Sidechain
1	b	312	TYR	Sidechain
1	b	322	ARG	Sidechain
1	b	369	ARG	Sidechain
1	b	388	PHE	Sidechain
1	b	404	PHE	Sidechain
1	b	432	TYR	Sidechain
1	b	435	TYR	Sidechain
1	b	49	ILE	Mainchain
1	b	64	ARG	Sidechain

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	b	3352	3232	3229	0	0
2	M	1069	1063	1060	7	0
3	a	3228	3147	3144	0	0
All	All	7649	7442	7433	7	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 10.

All (7) 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)
2:M:3174:LEU:HD23	2:M:3174:LEU:H	1.68	0.57
2:M:3158:ILE:HG22	2:M:3163:PHE:CE1	2.44	0.52
2:M:3199:ILE:O	2:M:3202:ALA:HB3	2.19	0.42
2:M:3165:HIS:O	2:M:3169:HIS:CG	2.73	0.42
2:M:3191:ASP:HA	2:M:3192:PRO:HD3	1.93	0.41
2:M:3124:ARG:HA	2:M:3158:ILE:HD12	2.03	0.41
2:M:3182:LYS:HA	2:M:3182:LYS:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	b	424/426 (100%)	304 (72%)	88 (21%)	32 (8%)	1	15
2	M	128/130 (98%)	112 (88%)	16 (12%)	0	100	100
3	a	410/412 (100%)	297 (72%)	75 (18%)	38 (9%)	0	11
All	All	962/968 (99%)	713 (74%)	179 (19%)	70 (7%)	2	16

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	50	ASN
1	b	174	SER
1	b	183	GLU
1	b	240	THR
1	b	252	LEU
1	b	265	LEU
1	b	285	ALA
1	b	286	LEU
1	b	288	VAL
1	b	294	GLN
3	a	1057	TYR
3	a	1082	TYR
3	a	1083	THR
3	a	1214	ALA
3	a	1229	PHE
3	a	1235	PRO
3	a	1377	ALA
1	b	23	VAL
1	b	24	ILE
1	b	96	GLN
1	b	109	THR
1	b	238	VAL
1	b	284	ARG
1	b	295	MET
3	a	1085	GLY
3	a	1117	GLY
3	a	1191	LEU
3	a	1213	THR
3	a	1239	GLY
3	a	1263	ALA
3	a	1288	ALA
3	a	1332	GLU
3	a	1360	GLU
3	a	1361	ALA
1	b	3	GLU
1	b	239	THR
1	b	266	HIS
1	b	273	ALA
1	b	369	ARG
1	b	386	GLU
1	b	403	ALA
3	a	1074	ALA

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Mol	Chain	Res	Type
3	a	1212	ILE
3	a	1304	ALA
3	a	1347	ARG
1	b	143	GLY
1	b	308	ARG
1	b	395	PHE
3	a	1024	TYR
3	a	1077	TYR
3	a	1078	ALA
3	a	1123	PHE
3	a	1262	VAL
1	b	195	VAL
1	b	373	MET
3	a	1063	PRO
3	a	1122	GLY
3	a	1237	PRO
3	a	1247	ALA
1	b	424	ASN
3	a	1195	ARG
3	a	1089	ILE
3	a	1157	GLU
1	b	175	PRO
1	b	348	PRO
3	a	1277	VAL
3	a	1322	PRO
3	a	1148	ALA
3	a	1411	VAL
3	a	1345	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	367/367 (100%)	336 (92%)	31 (8%)	11	38
2	M	120/120 (100%)	116 (97%)	4 (3%)	38	62
3	a	347/347 (100%)	314 (90%)	33 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	834/834 (100%)	766 (92%)	68 (8%)	15	38

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	11	GLN
1	b	12	CYS
1	b	39	ASP
1	b	63	PRO
1	b	72	PRO
1	b	86	ILE
1	b	89	PRO
1	b	94	PHE
1	b	117	SER
1	b	119	LEU
1	b	122	VAL
1	b	139	HIS
1	b	145	THR
1	b	158	ARG
1	b	179	ASP
1	b	182	VAL
1	b	195	VAL
1	b	241	CYS
1	b	260	VAL
1	b	278	ARG
1	b	292	THR
1	b	294	GLN
1	b	300	ASN
1	b	308	ARG
1	b	323	MET
1	b	325	MET
1	b	326	LYS
1	b	331	GLN
1	b	352	LYS
1	b	373	MET
1	b	427	ASP
2	M	3166	ASN
2	M	3204	LYS
2	M	3206	CYS
2	M	3209	LEU
3	a	1002	ARG
3	a	1011	GLN

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Mol	Chain	Res	Type
3	a	1018	ASN
3	a	1021	TRP
3	a	1022	GLU
3	a	1024	TYR
3	a	1025	CYS
3	a	1048	VAL
3	a	1056	THR
3	a	1062	HIS
3	a	1063	PRO
3	a	1068	THR
3	a	1075	ASN
3	a	1119	THR
3	a	1126	LEU
3	a	1146	TYR
3	a	1156	VAL
3	a	1179	ASP
3	a	1195	ARG
3	a	1198	TYR
3	a	1201	LEU
3	a	1217	ARG
3	a	1230	GLN
3	a	1277	VAL
3	a	1300	LYS
3	a	1315	ILE
3	a	1334	PRO
3	a	1337	VAL
3	a	1351	MET
3	a	1366	ASP
3	a	1376	ARG
3	a	1407	GLU
3	a	1412	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	54	ASN
1	b	101	ASN
1	b	139	HIS
1	b	193	GLN
1	b	294	GLN
1	b	339	ASN
1	b	406	HIS

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Mol	Chain	Res	Type
1	b	433	GLN
3	a	1028	HIS
3	a	1075	ASN
3	a	1102	GLN

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 monosaccharides 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	b	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	269:MET	C	270:PRO	N	1.19

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-9996. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1   Orthogonal projections ⓘ

6.1.1   Primary map

| X | Y | Z |
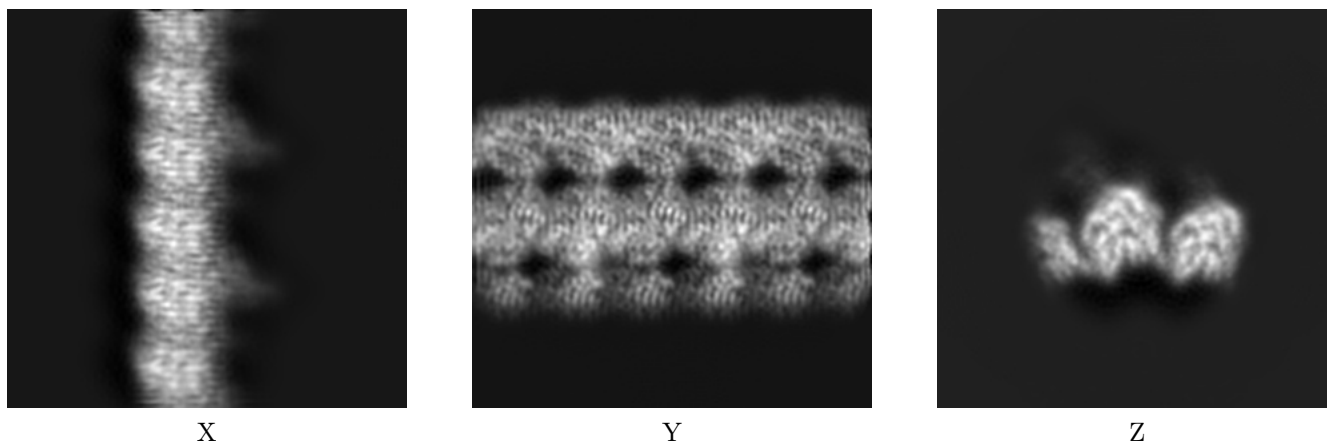
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ

6.2.1   Primary map

| X Index: 90 | Y Index: 90 | Z Index: 90 |
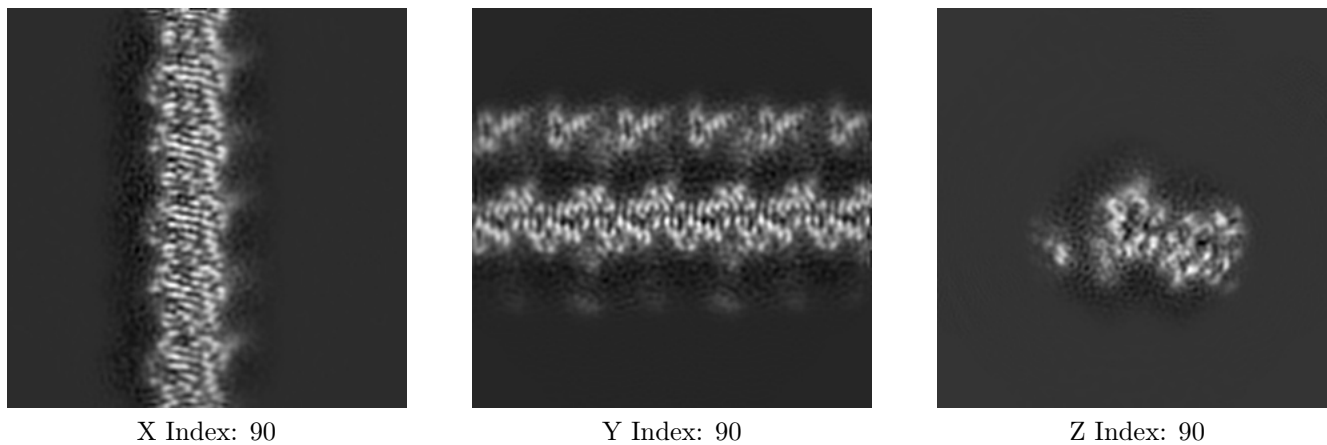
The images above show central slices of the map in three orthogonal directions.

6.3　Largest variance slices ⓘ
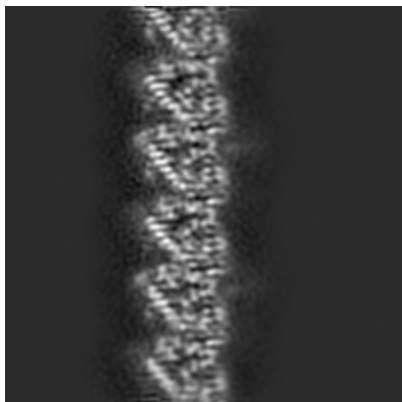
6.3.1　Primary map
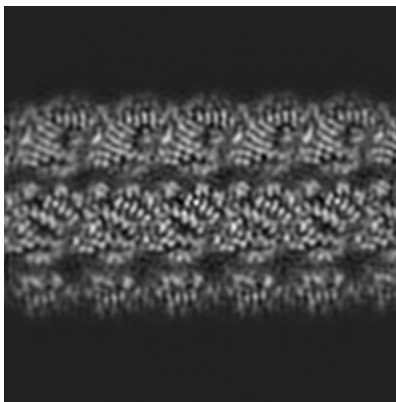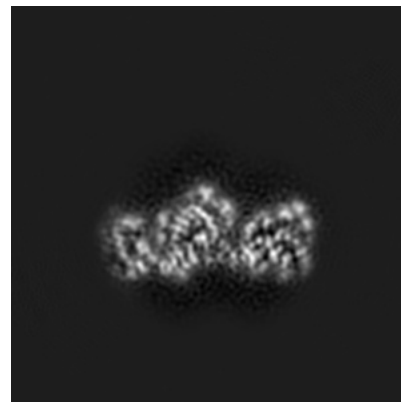
| X Index: 81 | Y Index: 75 | Z Index: 81 |

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

6.4　Orthogonal surface views ⓘ

6.4.1　Primary map

| X | Y | Z |
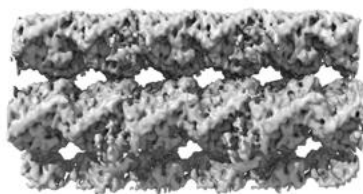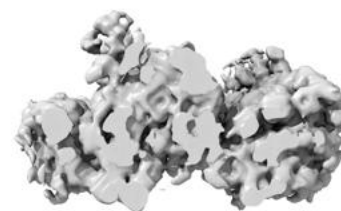
The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

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

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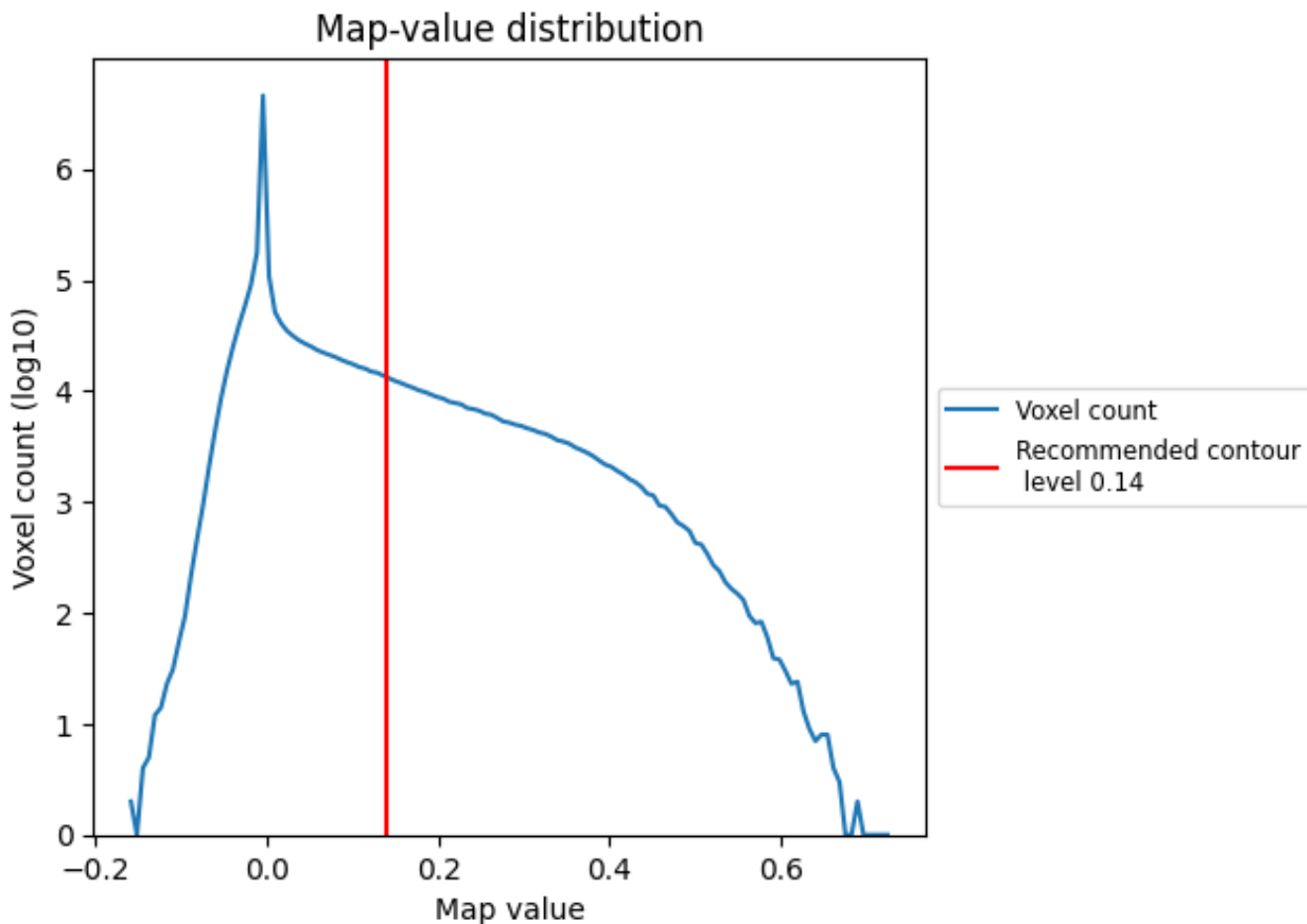
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
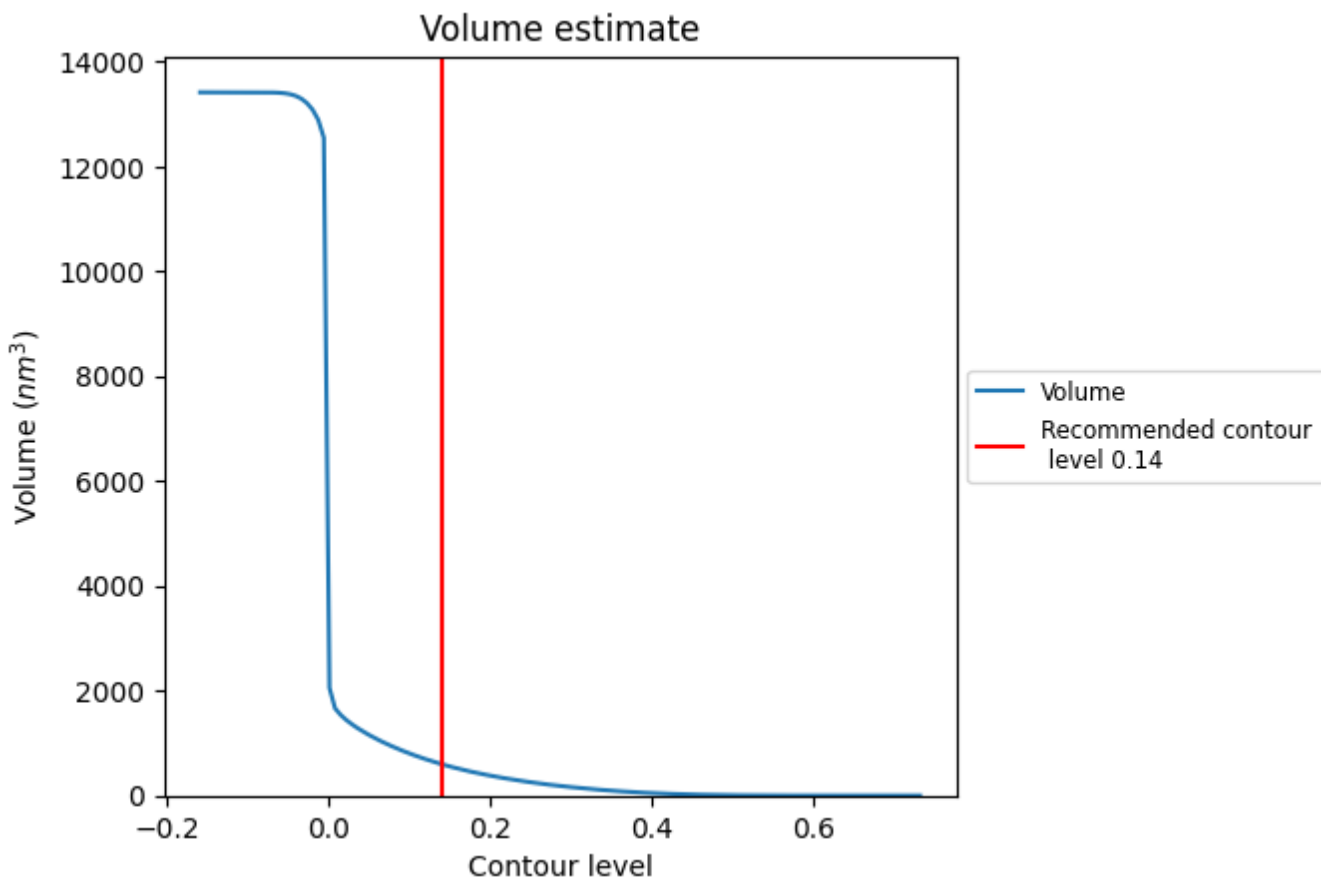
The volume at the recommended contour level is 599 nm^3; this corresponds to an approximate mass of 541 kDa.

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 ⓘ
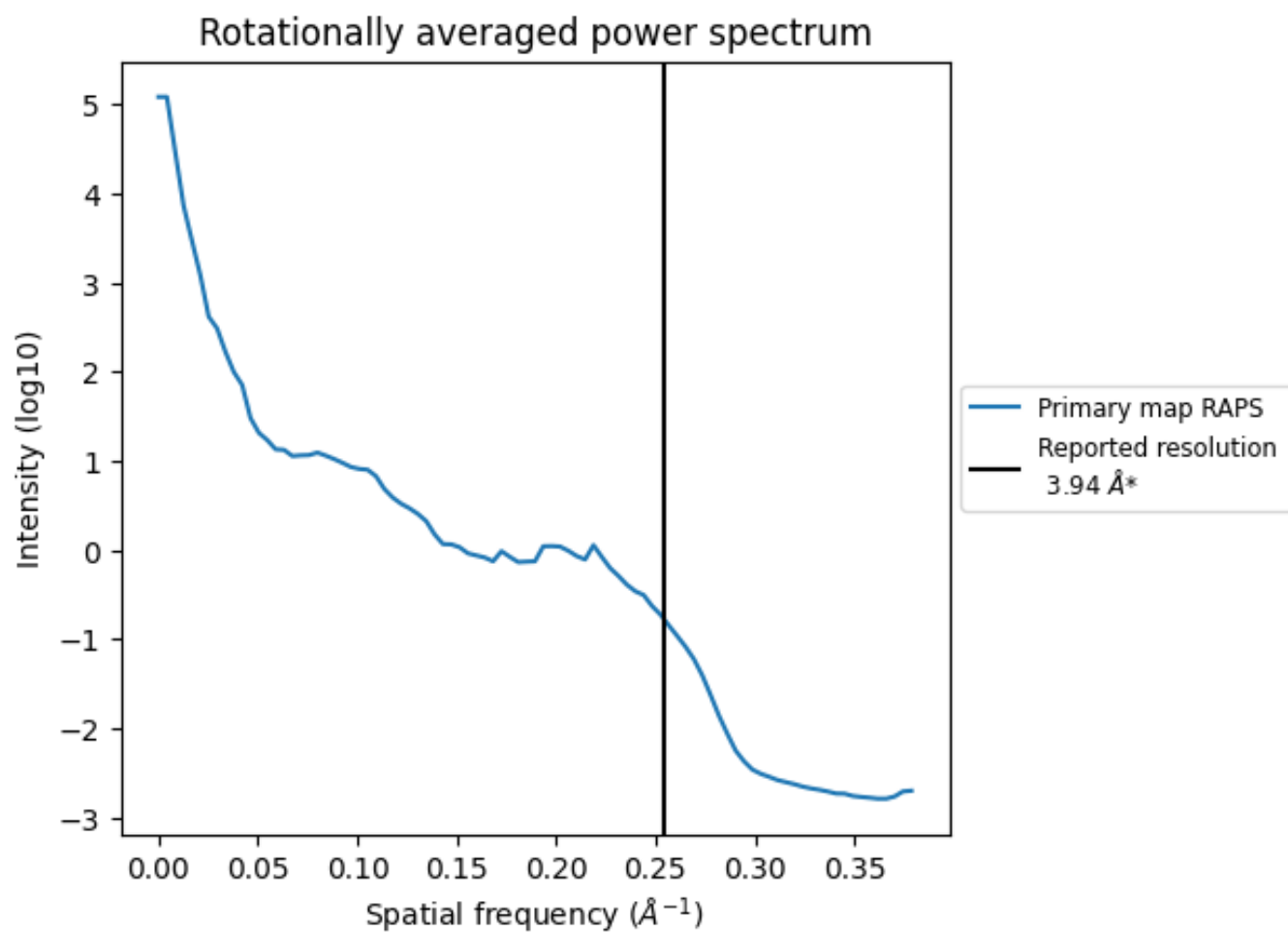
*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9996 and PDB model 6KIO. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay ⓘ

X   Y   Z
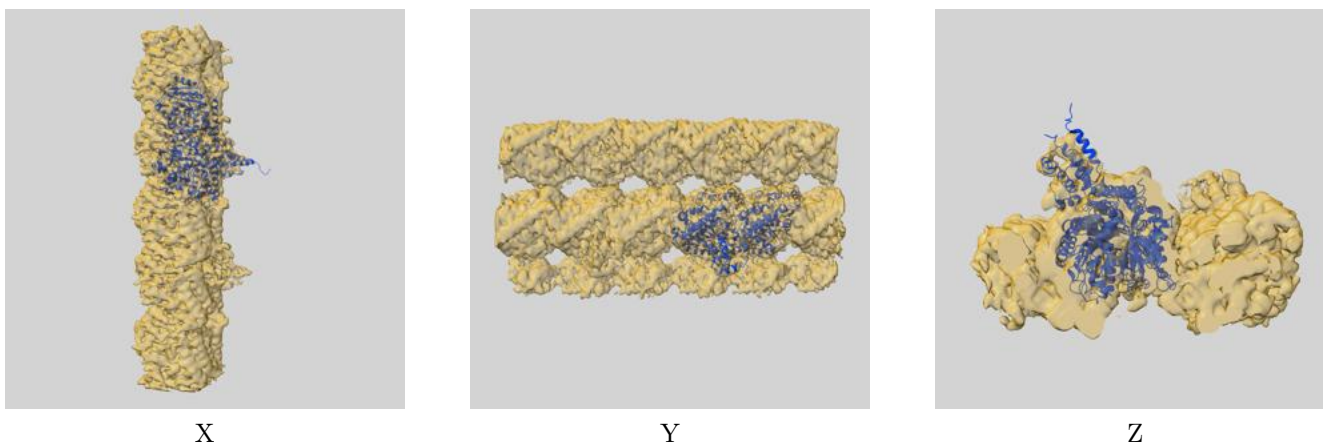
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z

The images above show the model with each residue coloured according 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 ⓘ

X   Y   Z
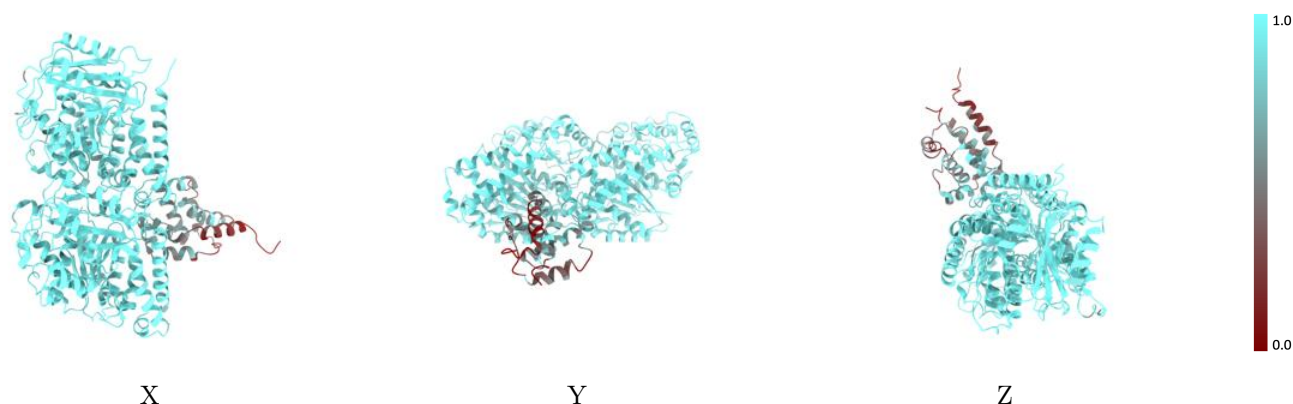
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4　Atom inclusion ⓘ
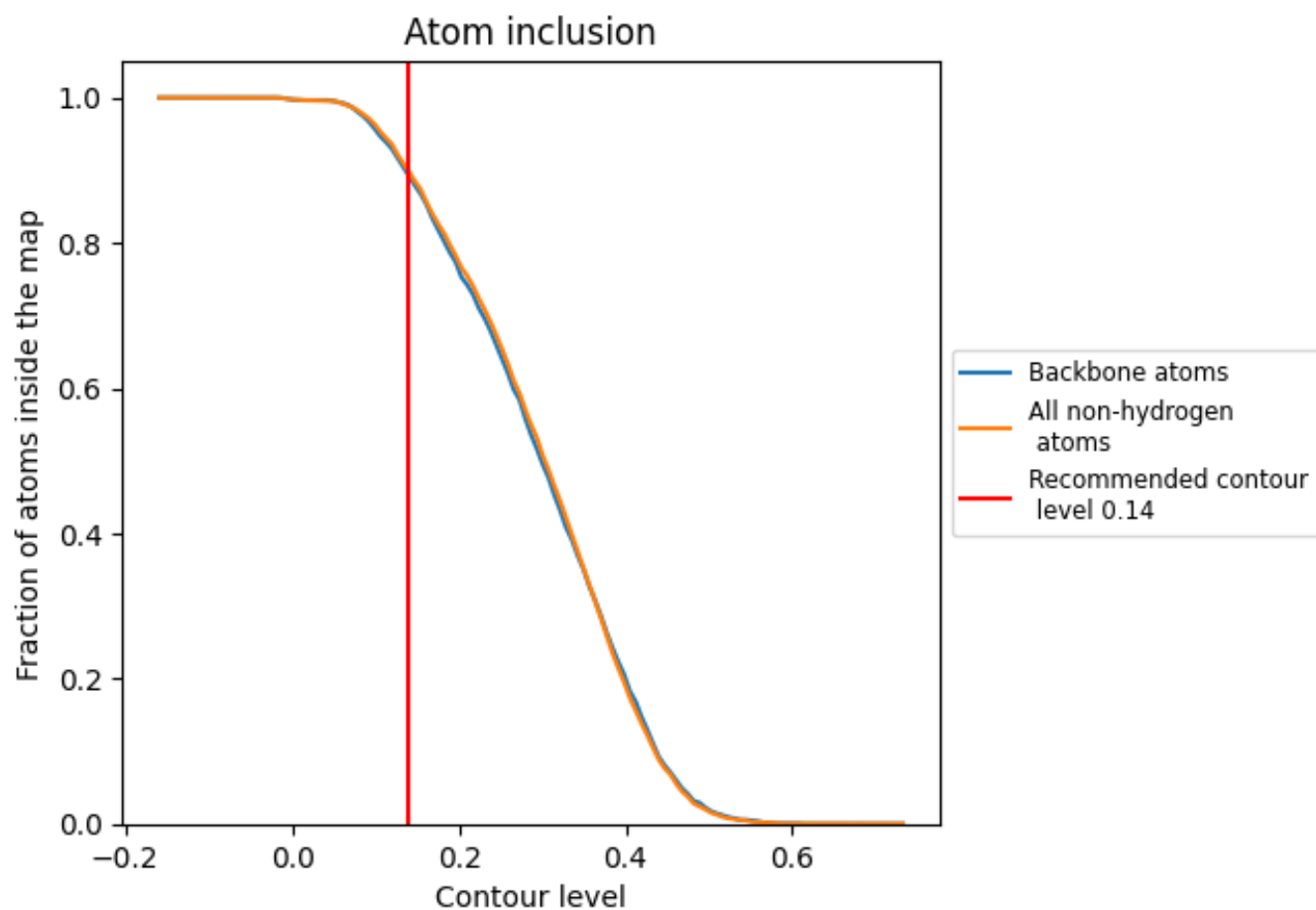
Atom inclusion

At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8984	0.4140
M	0.4857	0.2800
a	0.9665	0.4320
b	0.9772	0.4400

1.0

0.0
<0.0