Full wwPDB EM Validation Report (i)

Mar 20, 2024 – 12:12 AM JST

PDB ID	:	6KIQ
EMDB ID	:	EMD-9997
Title	:	Complex of yeast cytoplasmic dynein MTBD-High and MT with DTT
Authors	:	Komori, Y.; Nishida, N.; Shimada, I.; Kikkawa, M.
Deposited on	:	2019-07-19
Resolution	:	3.62 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 (i) 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 (i)) were used in the production of this report:

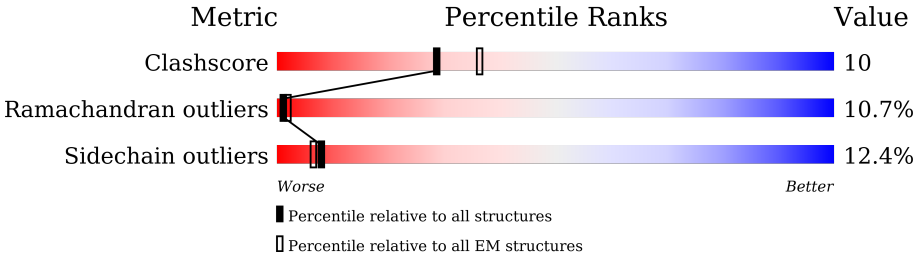
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.62 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	a	412	57% 30% 11% •
2	b	426	63% 28% 8% •
3	M	130	23% 82% 13% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15093 atoms, of which 7444 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 Alpha tubulin.

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

- Molecule 2 is a protein called Tubulin beta chain.

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

- Molecule 3 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	M	130	2134	679	1065	184	197	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

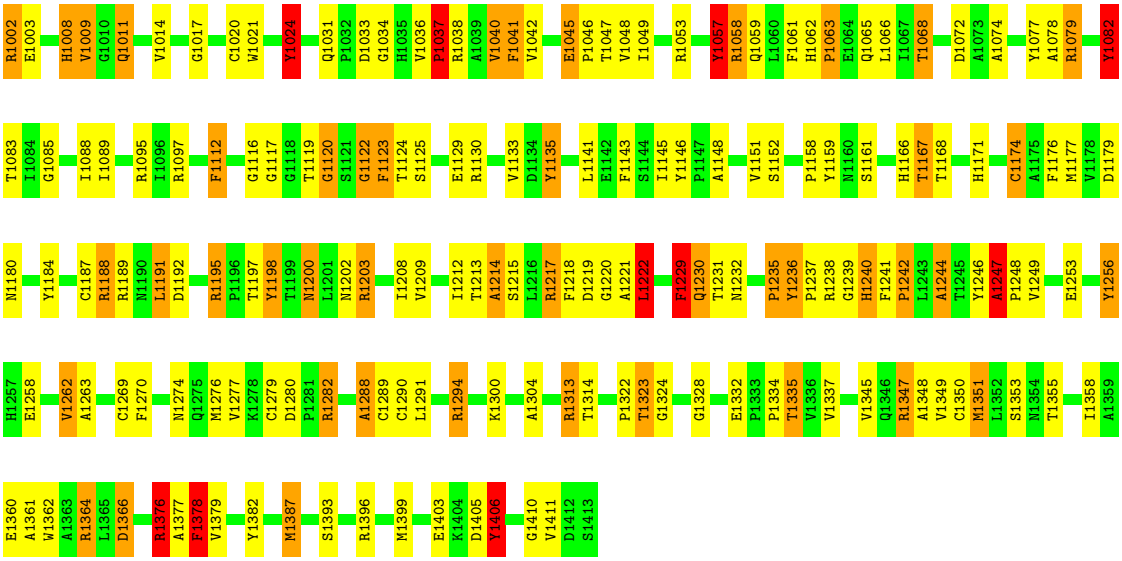
Chain	Residue	Modelled	Actual	Comment	Reference
M	3101	CYS	ILE	engineered mutation	UNP P36022
M	3222	CYS	VAL	engineered mutation	UNP P36022

3 Residue-property plots (i)

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.

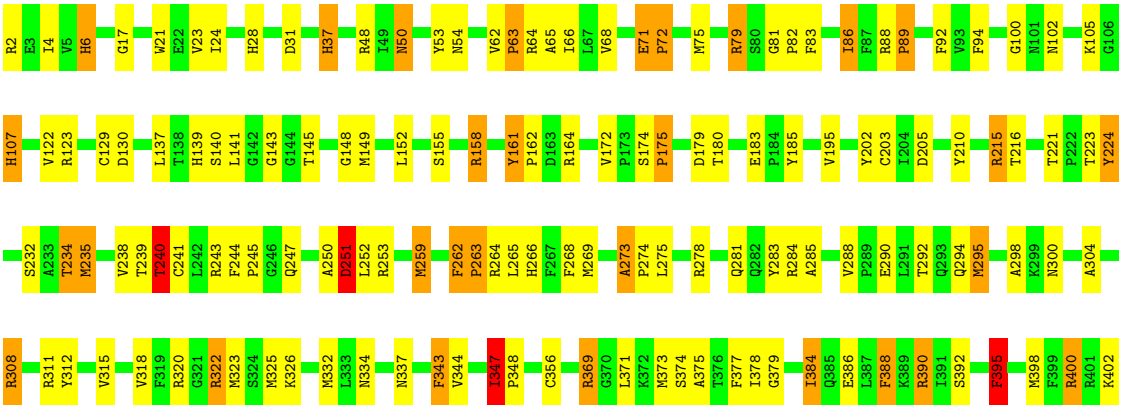
- Molecule 1: Alpha tubulin

Chain a: 57% 30% 11%



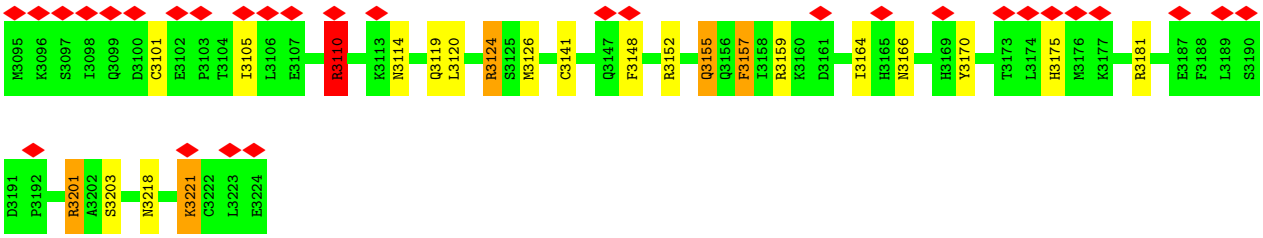
- Molecule 2: Tubulin beta chain

Chain b: 63% 28% 8%



• Molecule 3: Dynein heavy chain, cytoplasmic

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7519°, rise=9.2219 Å, axial sym=C1	Depositor
Number of segments used	32666	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 ($e^-/Å^2$)	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	0.898	Depositor
Minimum map value	-0.367	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.125	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 (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	1.75	32/3302 (1.0%)	2.08	105/4485 (2.3%)
2	b	1.69	18/3427 (0.5%)	2.04	98/4642 (2.1%)
3	M	0.92	0/1092	1.45	9/1472 (0.6%)
All	All	1.63	50/7821 (0.6%)	1.99	212/10599 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	46
2	b	0	33
3	M	0	4
All	All	0	83

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	269	MET	C-N	-8.38	1.18	1.34
2	b	21	TRP	NE1-CE2	-7.97	1.27	1.37
1	a	1350	CYS	CB-SG	-7.86	1.68	1.82
2	b	63	PRO	CA-C	-7.46	1.38	1.52
1	a	1241	PHE	C-N	-7.23	1.20	1.34
2	b	17	GLY	CA-C	-6.71	1.41	1.51
2	b	273	ALA	C-N	-6.61	1.21	1.34
1	a	1235	PRO	CA-C	-6.51	1.39	1.52
1	a	1328	GLY	CA-C	-6.51	1.41	1.51
1	a	1248	PRO	N-CD	-6.44	1.38	1.47
2	b	6	HIS	CB-CG	-6.38	1.38	1.50
2	b	274	PRO	N-CD	-6.38	1.39	1.47
1	a	1045	GLU	C-N	-6.36	1.22	1.34
1	a	1262	VAL	CA-CB	-6.28	1.41	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	432	TYR	CB-CG	-6.21	1.42	1.51
1	a	1024	TYR	CA-C	-6.18	1.36	1.52
1	a	1289	CYS	CB-SG	-6.18	1.71	1.82
1	a	1112	PHE	CB-CG	-6.16	1.40	1.51
1	a	1406	TYR	CB-CG	-6.12	1.42	1.51
1	a	1120	GLY	CA-C	-6.11	1.42	1.51
1	a	1014	VAL	CA-CB	-6.05	1.42	1.54
2	b	89	PRO	CA-C	-5.99	1.40	1.52
1	a	1024	TYR	CB-CG	-5.98	1.42	1.51
2	b	202	TYR	CB-CG	-5.83	1.43	1.51
1	a	1037	PRO	CA-C	-5.76	1.41	1.52
2	b	62	VAL	CA-CB	-5.73	1.42	1.54
1	a	1349	VAL	CA-CB	-5.54	1.43	1.54
2	b	379	GLY	CA-C	-5.51	1.43	1.51
1	a	1324	GLY	CA-C	-5.50	1.43	1.51
1	a	1174	CYS	CB-SG	-5.49	1.72	1.81
1	a	1020	CYS	CB-SG	-5.46	1.73	1.81
1	a	1017	GLY	CA-C	-5.42	1.43	1.51
2	b	244	PHE	CB-CG	-5.40	1.42	1.51
1	a	1242	PRO	N-CD	-5.28	1.40	1.47
1	a	1256	TYR	CB-CG	-5.28	1.43	1.51
1	a	1242	PRO	CA-C	-5.26	1.42	1.52
1	a	1176	PHE	CB-CG	-5.25	1.42	1.51
2	b	161	TYR	CB-CG	-5.24	1.43	1.51
2	b	343	PHE	CB-CG	-5.23	1.42	1.51
2	b	148	GLY	CA-C	-5.21	1.43	1.51
1	a	1146	TYR	CB-CG	-5.20	1.43	1.51
1	a	1350	CYS	CA-C	-5.18	1.39	1.52
1	a	1042	VAL	CA-CB	-5.16	1.44	1.54
1	a	1135	TYR	CB-CG	-5.14	1.44	1.51
1	a	1122	GLY	CA-C	-5.14	1.43	1.51
1	a	1063	PRO	CA-C	-5.13	1.42	1.52
2	b	53	TYR	CB-CG	-5.13	1.44	1.51
1	a	1082	TYR	CB-CG	-5.07	1.44	1.51
2	b	72	PRO	N-CD	-5.07	1.40	1.47
1	a	1036	VAL	CA-CB	-5.03	1.44	1.54

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	202	TYR	CB-CG-CD2	-17.62	110.43	121.00
2	b	202	TYR	CB-CG-CD1	14.59	129.75	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	284	ARG	NE-CZ-NH1	14.45	127.53	120.30
1	a	1079	ARG	NE-CZ-NH1	13.85	127.23	120.30
2	b	123	ARG	NE-CZ-NH1	13.85	127.22	120.30
1	a	1198	TYR	CB-CG-CD1	12.54	128.53	121.00
2	b	53	TYR	CB-CG-CD2	-12.03	113.78	121.00
1	a	1229	PHE	CB-CG-CD1	-11.80	112.54	120.80
2	b	48	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	a	1217	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	a	1347	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	a	1347	ARG	NE-CZ-NH2	-11.17	114.71	120.30
2	b	224	TYR	CB-CG-CD2	10.92	127.55	121.00
2	b	283	TYR	CB-CG-CD2	-10.85	114.49	121.00
2	b	283	TYR	CB-CG-CD1	10.80	127.48	121.00
3	M	3159	ARG	NE-CZ-NH1	10.77	125.69	120.30
1	a	1282	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	a	1203	ARG	NE-CZ-NH1	10.41	125.51	120.30
2	b	215	ARG	NE-CZ-NH1	10.38	125.49	120.30
2	b	53	TYR	CB-CG-CD1	10.07	127.04	121.00
2	b	158	ARG	NE-CZ-NH2	-10.07	115.27	120.30
2	b	390	ARG	NE-CZ-NH1	10.06	125.33	120.30
2	b	407	TRP	N-CA-CB	9.88	128.38	110.60
2	b	164	ARG	NE-CZ-NH1	9.79	125.20	120.30
3	M	3181	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	a	1002	ARG	NE-CZ-NH1	9.57	125.09	120.30
2	b	140	SER	N-CA-CB	9.44	124.66	110.50
1	a	1189	ARG	NE-CZ-NH1	9.44	125.02	120.30
2	b	407	TRP	CA-CB-CG	9.33	131.42	113.70
1	a	1198	TYR	CB-CG-CD2	-9.29	115.43	121.00
1	a	1214	ALA	N-CA-CB	9.19	122.96	110.10
1	a	1406	TYR	CB-CG-CD2	-9.11	115.53	121.00
1	a	1215	SER	N-CA-CB	-9.01	96.98	110.50
1	a	1058	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	a	1053	ARG	NE-CZ-NH1	8.88	124.74	120.30
2	b	388	PHE	CB-CG-CD1	-8.86	114.60	120.80
1	a	1095	ARG	NE-CZ-NH1	8.85	124.72	120.30
2	b	395	PHE	CB-CG-CD1	-8.72	114.69	120.80
2	b	278	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	a	1229	PHE	CB-CG-CD2	8.51	126.76	120.80
2	b	224	TYR	CB-CG-CD1	-8.48	115.91	121.00
3	M	3124	ARG	NE-CZ-NH1	8.36	124.48	120.30
2	b	161	TYR	CB-CG-CD2	-8.32	116.01	121.00
1	a	1364	ARG	CB-CA-C	-8.31	93.78	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	3152	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	a	1143	PHE	CB-CG-CD1	8.20	126.54	120.80
2	b	37	HIS	CA-CB-CG	-8.18	99.70	113.60
1	a	1217	ARG	NE-CZ-NH2	-8.17	116.22	120.30
2	b	268	PHE	CB-CG-CD2	8.14	126.50	120.80
1	a	1195	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	b	240	THR	N-CA-CB	8.07	125.64	110.30
1	a	1215	SER	CB-CA-C	-8.03	94.85	110.10
1	a	1231	THR	CA-CB-CG2	-8.02	101.17	112.40
1	a	1282	ARG	NE-CZ-NH2	-7.93	116.33	120.30
2	b	273	ALA	CA-C-N	7.93	139.29	117.10
1	a	1130	ARG	NE-CZ-NH1	7.78	124.19	120.30
3	M	3201	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	a	1364	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	b	308	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	a	1247	ALA	CA-C-N	7.49	138.07	117.10
1	a	1079	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	b	158	ARG	NE-CZ-NH1	7.47	124.03	120.30
3	M	3124	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	a	1269	CYS	CA-CB-SG	-7.31	100.84	114.00
2	b	268	PHE	CB-CG-CD1	-7.23	115.74	120.80
1	a	1313	ARG	NE-CZ-NH1	7.22	123.91	120.30
2	b	102	ASN	N-CA-CB	-7.16	97.71	110.60
2	b	264	ARG	NE-CZ-NH1	7.05	123.83	120.30
2	b	375	ALA	CB-CA-C	-7.03	99.55	110.10
1	a	1072	ASP	CB-CG-OD1	6.96	124.56	118.30
2	b	247	GLN	N-CA-C	-6.95	92.25	111.00
1	a	1290	CYS	O-C-N	-6.85	111.74	122.70
2	b	388	PHE	CB-CG-CD2	6.80	125.56	120.80
1	a	1020	CYS	N-CA-CB	-6.79	98.38	110.60
2	b	375	ALA	N-CA-CB	-6.79	100.60	110.10
2	b	123	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	a	1143	PHE	CB-CG-CD2	-6.74	116.08	120.80
1	a	1350	CYS	CA-CB-SG	-6.69	101.95	114.00
1	a	1057	TYR	N-CA-CB	6.67	122.61	110.60
1	a	1011	GLN	N-CA-CB	6.65	122.56	110.60
1	a	1347	ARG	CB-CA-C	-6.63	97.15	110.40
2	b	259	MET	CG-SD-CE	-6.62	89.60	100.20
1	a	1351	MET	CG-SD-CE	-6.62	89.60	100.20
1	a	1393	SER	N-CA-CB	-6.57	100.64	110.50
2	b	369	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	a	1294	ARG	NE-CZ-NH2	-6.55	117.03	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	318	VAL	O-C-N	-6.54	112.24	122.70
2	b	235	MET	CG-SD-CE	-6.53	89.76	100.20
1	a	1095	ARG	N-CA-CB	6.48	122.27	110.60
2	b	322	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	a	1289	CYS	CA-CB-SG	-6.43	102.42	114.00
2	b	79	ARG	NE-CZ-NH1	6.43	123.51	120.30
2	b	407	TRP	CB-CG-CD2	6.39	134.91	126.60
1	a	1095	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	a	1222	LEU	N-CA-C	-6.31	93.96	111.00
1	a	1300	LYS	N-CA-CB	-6.30	99.26	110.60
1	a	1040	VAL	O-C-N	-6.27	112.67	122.70
2	b	215	ARG	NE-CZ-NH2	-6.25	117.18	120.30
2	b	50	ASN	CB-CA-C	-6.23	97.93	110.40
1	a	1218	PHE	CB-CA-C	-6.22	97.95	110.40
2	b	262	PHE	N-CA-C	-6.22	94.22	111.00
2	b	308	ARG	N-CA-CB	-6.22	99.41	110.60
2	b	273	ALA	O-C-N	-6.21	109.31	121.10
1	a	1203	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	b	318	VAL	N-CA-CB	-6.17	97.93	111.50
1	a	1378	PHE	CB-CG-CD2	-6.16	116.49	120.80
1	a	1376	ARG	N-CA-CB	6.15	121.66	110.60
2	b	243	ARG	NE-CZ-NH2	6.14	123.37	120.30
2	b	284	ARG	N-CA-CB	6.12	121.62	110.60
1	a	1387	MET	N-CA-C	-6.12	94.49	111.00
1	a	1159	TYR	CB-CG-CD2	6.09	124.66	121.00
1	a	1042	VAL	CA-CB-CG2	-6.09	101.77	110.90
1	a	1079	ARG	N-CA-CB	-6.09	99.64	110.60
1	a	1382	TYR	CB-CG-CD1	-6.03	117.38	121.00
2	b	253	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	a	1082	TYR	CB-CG-CD2	-6.00	117.40	121.00
2	b	374	SER	N-CA-CB	-5.99	101.52	110.50
1	a	1244	ALA	O-C-N	-5.98	113.13	122.70
1	a	1291	LEU	CB-CG-CD1	5.97	121.15	111.00
2	b	161	TYR	CA-CB-CG	-5.94	102.12	113.40
2	b	308	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	a	1231	THR	N-CA-C	5.92	126.97	111.00
2	b	75	MET	CG-SD-CE	-5.91	90.74	100.20
1	a	1141	LEU	CB-CA-C	-5.87	99.04	110.20
1	a	1288	ALA	N-CA-CB	5.85	118.29	110.10
3	M	3110	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	a	1112	PHE	CB-CG-CD2	-5.83	116.72	120.80
2	b	203	CYS	CA-CB-SG	-5.83	103.50	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	356	CYS	CA-CB-SG	-5.83	103.50	114.00
1	a	1058	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	a	1405	ASP	CB-CG-OD2	5.78	123.50	118.30
2	b	48	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	a	1024	TYR	N-CA-CB	5.77	120.98	110.60
1	a	1068	THR	CB-CA-C	-5.77	96.03	111.60
1	a	1350	CYS	CB-CA-C	-5.77	98.87	110.40
1	a	1072	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	a	1188	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	a	1348	ALA	N-CA-CB	-5.69	102.13	110.10
1	a	1009	VAL	CA-CB-CG2	5.69	119.43	110.90
1	a	1232	ASN	CB-CA-C	-5.69	99.03	110.40
1	a	1247	ALA	CA-C-O	-5.65	108.23	120.10
2	b	284	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	b	232	SER	CB-CA-C	-5.59	99.48	110.10
3	M	3126	MET	CG-SD-CE	-5.58	91.28	100.20
2	b	432	TYR	CA-CB-CG	-5.57	102.82	113.40
2	b	88	ARG	N-CA-CB	5.57	120.62	110.60
2	b	378	ILE	O-C-N	-5.56	113.75	123.20
2	b	234	THR	N-CA-CB	5.54	120.82	110.30
2	b	65	ALA	CB-CA-C	-5.51	101.83	110.10
2	b	6	HIS	CB-CA-C	-5.50	99.41	110.40
2	b	243	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	a	1353	SER	CB-CA-C	-5.46	99.73	110.10
2	b	243	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	a	1198	TYR	CA-CB-CG	5.44	123.73	113.40
1	a	1177	MET	CG-SD-CE	-5.43	91.50	100.20
2	b	251	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	a	1116	GLY	C-N-CA	5.43	133.69	122.30
1	a	1200	ASN	CA-CB-CG	-5.42	101.46	113.40
2	b	347	ILE	N-CA-C	-5.42	96.37	111.00
1	a	1335	THR	C-N-CA	5.41	135.22	121.70
1	a	1376	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	a	1041	PHE	CB-CG-CD2	-5.39	117.03	120.80
2	b	332	MET	CG-SD-CE	-5.38	91.60	100.20
1	a	1176	PHE	CA-CB-CG	-5.37	101.01	113.90
2	b	6	HIS	N-CA-C	5.37	125.50	111.00
2	b	275	LEU	CB-CA-C	-5.35	100.03	110.20
2	b	320	ARG	NE-CZ-NH2	5.35	122.97	120.30
2	b	155	SER	N-CA-CB	5.34	118.51	110.50
1	a	1130	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	a	1202	ASN	CB-CG-OD1	5.34	132.28	121.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	241	CYS	CA-CB-SG	-5.33	104.40	114.00
2	b	292	THR	CA-CB-CG2	-5.33	104.94	112.40
1	a	1291	LEU	O-C-N	-5.32	114.18	122.70
1	a	1061	PHE	N-CA-C	-5.32	96.64	111.00
1	a	1379	VAL	CA-CB-CG2	-5.32	102.93	110.90
1	a	1079	ARG	CD-NE-CZ	-5.30	116.18	123.60
2	b	404	PHE	CB-CG-CD2	-5.30	117.09	120.80
2	b	392	SER	N-CA-CB	5.29	118.44	110.50
1	a	1180	ASN	CB-CA-C	5.27	120.94	110.40
3	M	3155	GLN	CB-CG-CD	5.25	125.25	111.60
1	a	1053	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	a	1366	ASP	CB-CA-C	5.24	120.88	110.40
2	b	54	ASN	N-CA-C	-5.23	96.88	111.00
2	b	395	PHE	CB-CG-CD2	5.23	124.46	120.80
1	a	1376	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	b	175	PRO	N-CA-CB	-5.22	96.85	102.60
2	b	300	ASN	CA-CB-CG	-5.22	101.91	113.40
1	a	1095	ARG	CG-CD-NE	-5.21	100.85	111.80
2	b	295	MET	CG-SD-CE	-5.21	91.86	100.20
2	b	337	ASN	CA-CB-CG	-5.20	101.95	113.40
2	b	315	VAL	CA-C-N	5.19	128.62	117.20
1	a	1270	PHE	CA-CB-CG	-5.18	101.47	113.90
1	a	1289	CYS	O-C-N	-5.17	114.43	122.70
1	a	1008	HIS	CA-C-N	5.16	128.56	117.20
1	a	1203	ARG	CB-CA-C	-5.16	100.09	110.40
1	a	1167	THR	CA-CB-CG2	5.15	119.61	112.40
2	b	68	VAL	CA-CB-CG2	-5.15	103.18	110.90
2	b	337	ASN	CB-CA-C	-5.14	100.11	110.40
2	b	251	ASP	N-CA-CB	5.13	119.83	110.60
2	b	205	ASP	CB-CA-C	-5.12	100.16	110.40
1	a	1314	THR	C-N-CA	5.10	134.45	121.70
2	b	221	THR	CA-CB-CG2	-5.10	105.26	112.40
2	b	152	LEU	CB-CA-C	-5.09	100.53	110.20
1	a	1209	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	a	1066	LEU	N-CA-C	-5.08	97.29	111.00
2	b	273	ALA	N-CA-C	5.05	124.63	111.00
2	b	384	ILE	O-C-N	-5.05	114.62	122.70
2	b	205	ASP	CB-CG-OD1	-5.04	113.76	118.30
2	b	215	ARG	CB-CA-C	-5.04	100.31	110.40
1	a	1130	ARG	CB-CA-C	-5.04	100.33	110.40
2	b	202	TYR	CB-CA-C	-5.02	100.36	110.40
1	a	1276	MET	CG-SD-CE	-5.01	92.18	100.20

There are no chirality outliers.

All (83) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	3110	ARG	Sidechain
3	M	3157	PHE	Sidechain
3	M	3201	ARG	Sidechain
3	M	3203	SER	Peptide
1	a	1002	ARG	Peptide
1	a	1003	GLU	Peptide
1	a	1008	HIS	Sidechain
1	a	1024	TYR	Sidechain
1	a	1037	PRO	Peptide
1	a	1038	ARG	Sidechain
1	a	1041	PHE	Sidechain
1	a	1057	TYR	Sidechain
1	a	1058	ARG	Sidechain
1	a	1059	GLN	Peptide
1	a	1074	ALA	Peptide
1	a	1079	ARG	Sidechain
1	a	1082	TYR	Sidechain
1	a	1097	ARG	Sidechain
1	a	1112	PHE	Sidechain
1	a	1119	THR	Peptide
1	a	1120	GLY	Peptide
1	a	1123	PHE	Sidechain
1	a	1135	TYR	Sidechain
1	a	1145	ILE	Peptide
1	a	1161	SER	Mainchain
1	a	1184	TYR	Sidechain
1	a	1195	ARG	Sidechain
1	a	1198	TYR	Sidechain
1	a	1203	ARG	Sidechain
1	a	1217	ARG	Sidechain
1	a	1229	PHE	Sidechain
1	a	1230	GLN	Peptide
1	a	1236	TYR	Sidechain
1	a	1238	ARG	Sidechain
1	a	1240	HIS	Peptide
1	a	1242	PRO	Peptide
1	a	1244	ALA	Mainchain
1	a	1246	TYR	Sidechain
1	a	1247	ALA	Peptide
1	a	1253	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	a	1256	TYR	Sidechain
1	a	1294	ARG	Sidechain
1	a	1313	ARG	Sidechain
1	a	1323	THR	Peptide
1	a	1335	THR	Peptide
1	a	1364	ARG	Sidechain
1	a	1378	PHE	Sidechain
1	a	1396	ARG	Sidechain
1	a	1406	TYR	Sidechain
1	a	1410	GLY	Peptide
2	b	100	GLY	Peptide
2	b	107	HIS	Peptide
2	b	129	CYS	Peptide
2	b	161	TYR	Sidechain
2	b	179	ASP	Peptide
2	b	185	TYR	Sidechain
2	b	2	ARG	Sidechain
2	b	210	TYR	Sidechain
2	b	215	ARG	Sidechain
2	b	216	THR	Peptide
2	b	259	MET	Peptide
2	b	28	HIS	Sidechain
2	b	311	ARG	Sidechain
2	b	312	TYR	Sidechain
2	b	347	ILE	Peptide
2	b	37	HIS	Sidechain
2	b	388	PHE	Sidechain
2	b	390	ARG	Sidechain
2	b	395	PHE	Sidechain
2	b	4	ILE	Peptide
2	b	400	ARG	Sidechain
2	b	402	LYS	Peptide
2	b	404	PHE	Sidechain,Peptide
2	b	408	TYR	Sidechain
2	b	415	GLU	Peptide
2	b	416	MET	Mainchain
2	b	418	PHE	Sidechain
2	b	432	TYR	Sidechain
2	b	435	TYR	Sidechain
2	b	64	ARG	Sidechain
2	b	79	ARG	Sidechain
2	b	92	PHE	Sidechain

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	3228	3147	3144	0	0
2	b	3352	3232	3229	0	0
3	M	1069	1065	1062	2	0
All	All	7649	7444	7435	2	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 (2) 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)
3:M:3157:PHE:CD2	3:M:3157:PHE:C	2.95	0.40
3:M:3101:CYS:SG	3:M:3221:LYS:HB2	2.61	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	410/412 (100%)	284 (69%)	74 (18%)	52 (13%)	0 5
2	b	424/426 (100%)	288 (68%)	88 (21%)	48 (11%)	0 6
3	M	128/130 (98%)	108 (84%)	17 (13%)	3 (2%)	6 38
All	All	962/968 (99%)	680 (71%)	179 (19%)	103 (11%)	1 7

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	1031	GLN
1	a	1057	TYR
1	a	1082	TYR
1	a	1083	THR
1	a	1117	GLY
1	a	1148	ALA
1	a	1214	ALA
1	a	1235	PRO
1	a	1236	TYR
1	a	1240	HIS
1	a	1247	ALA
1	a	1258	GLU
1	a	1277	VAL
1	a	1322	PRO
1	a	1361	ALA
1	a	1377	ALA
1	a	1378	PHE
2	b	23	VAL
2	b	72	PRO
2	b	183	GLU
2	b	239	THR
2	b	240	THR
2	b	251	ASP
2	b	252	LEU
2	b	262	PHE
2	b	263	PRO
2	b	265	LEU
2	b	273	ALA
2	b	288	VAL
2	b	294	GLN
2	b	371	LEU
1	a	1085	GLY
1	a	1151	VAL
1	a	1191	LEU
1	a	1219	ASP
1	a	1229	PHE
1	a	1230	GLN
1	a	1263	ALA
1	a	1288	ALA
1	a	1360	GLU
1	a	1376	ARG
2	b	24	ILE
2	b	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	81	GLY
2	b	86	ILE
2	b	130	ASP
2	b	143	GLY
2	b	238	VAL
2	b	245	PRO
2	b	285	ALA
2	b	295	MET
2	b	298	ALA
2	b	348	PRO
2	b	373	MET
3	M	3221	LYS
1	a	1077	TYR
1	a	1171	HIS
1	a	1212	ILE
1	a	1213	THR
1	a	1221	ALA
1	a	1222	LEU
1	a	1279	CYS
1	a	1304	ALA
1	a	1347	ARG
2	b	31	ASP
2	b	107	HIS
2	b	141	LEU
2	b	223	THR
2	b	250	ALA
2	b	304	ALA
2	b	369	ARG
2	b	386	GLU
3	M	3148	PHE
1	a	1024	TYR
1	a	1033	ASP
1	a	1078	ALA
1	a	1123	PHE
1	a	1192	ASP
1	a	1237	PRO
1	a	1239	GLY
1	a	1280	ASP
2	b	145	THR
2	b	308	ARG
2	b	344	VAL
2	b	404	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	3175	HIS
1	a	1332	GLU
2	b	82	PRO
2	b	172	VAL
2	b	180	THR
2	b	266	HIS
2	b	395	PHE
2	b	400	ARG
1	a	1262	VAL
2	b	384	ILE
2	b	424	ASN
1	a	1089	ILE
1	a	1122	GLY
1	a	1220	GLY
1	a	1358	ILE
2	b	71	GLU
1	a	1034	GLY
1	a	1411	VAL

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	347/347 (100%)	298 (86%)	49 (14%)	3 21
2	b	367/367 (100%)	325 (89%)	42 (11%)	5 29
3	M	120/120 (100%)	108 (90%)	12 (10%)	7 34
All	All	834/834 (100%)	731 (88%)	103 (12%)	8 25

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	1009	VAL
1	a	1011	GLN
1	a	1021	TRP
1	a	1037	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1040	VAL
1	a	1045	GLU
1	a	1046	PRO
1	a	1047	THR
1	a	1048	VAL
1	a	1049	ILE
1	a	1062	HIS
1	a	1063	PRO
1	a	1065	GLN
1	a	1068	THR
1	a	1088	ILE
1	a	1124	THR
1	a	1125	SER
1	a	1129	GLU
1	a	1133	VAL
1	a	1152	SER
1	a	1158	PRO
1	a	1166	HIS
1	a	1167	THR
1	a	1168	THR
1	a	1174	CYS
1	a	1179	ASP
1	a	1187	CYS
1	a	1188	ARG
1	a	1191	LEU
1	a	1197	THR
1	a	1200	ASN
1	a	1208	ILE
1	a	1222	LEU
1	a	1249	VAL
1	a	1274	ASN
1	a	1282	ARG
1	a	1323	THR
1	a	1334	PRO
1	a	1337	VAL
1	a	1345	VAL
1	a	1351	MET
1	a	1355	THR
1	a	1362	TRP
1	a	1366	ASP
1	a	1376	ARG
1	a	1387	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1399	MET
1	a	1403	GLU
1	a	1406	TYR
2	b	6	HIS
2	b	63	PRO
2	b	66	ILE
2	b	71	GLU
2	b	83	PHE
2	b	86	ILE
2	b	89	PRO
2	b	94	PHE
2	b	105	LYS
2	b	122	VAL
2	b	137	LEU
2	b	139	HIS
2	b	149	MET
2	b	158	ARG
2	b	162	PRO
2	b	174	SER
2	b	175	PRO
2	b	195	VAL
2	b	224	TYR
2	b	234	THR
2	b	235	MET
2	b	240	THR
2	b	251	ASP
2	b	263	PRO
2	b	281	GLN
2	b	290	GLU
2	b	322	ARG
2	b	323	MET
2	b	325	MET
2	b	326	LYS
2	b	334	ASN
2	b	343	PHE
2	b	347	ILE
2	b	377	PHE
2	b	398	MET
2	b	404	PHE
2	b	407	TRP
2	b	415	GLU
2	b	419	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	425	MET
2	b	427	ASP
2	b	428	LEU
3	M	3105	ILE
3	M	3110	ARG
3	M	3114	ASN
3	M	3119	GLN
3	M	3120	LEU
3	M	3124	ARG
3	M	3141	CYS
3	M	3155	GLN
3	M	3164	ILE
3	M	3166	ASN
3	M	3170	TYR
3	M	3218	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	1008	HIS
1	a	1166	HIS
1	a	1180	ASN
1	a	1202	ASN
1	a	1240	HIS
1	a	1283	HIS
1	a	1367	HIS
1	a	1380	HIS
2	b	14	ASN
2	b	28	HIS
2	b	37	HIS
2	b	101	ASN
2	b	107	HIS
2	b	206	ASN
2	b	229	HIS
2	b	247	GLN
2	b	334	ASN
2	b	394	GLN
3	M	3169	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	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	1.18

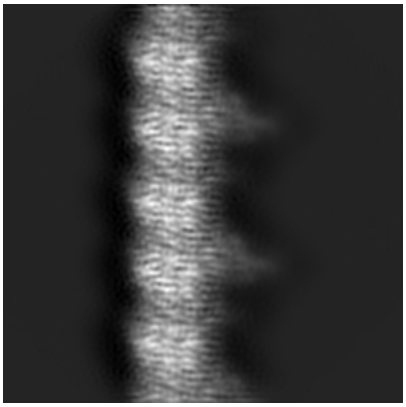
6 Map visualisation (i)

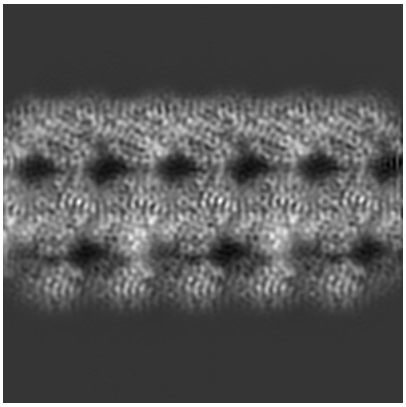
This section contains visualisations of the EMDB entry EMD-9997. These allow visual inspection of the internal detail of the map and identification of artifacts.

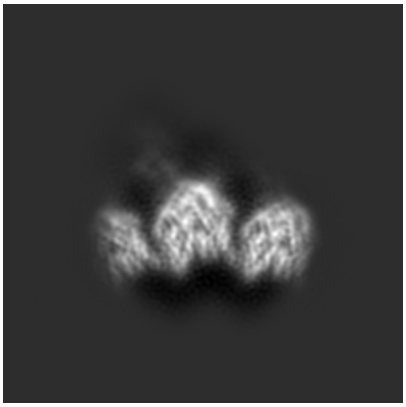
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

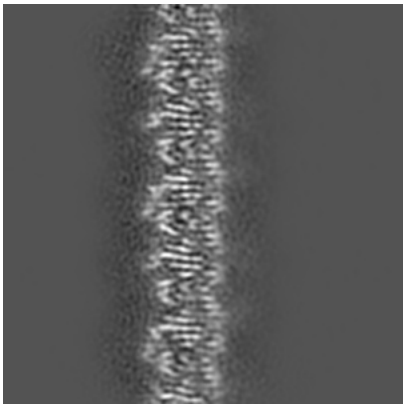

Y

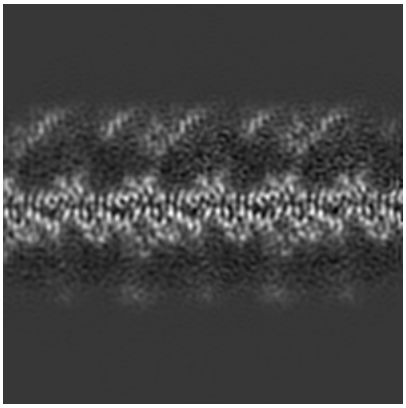

Z

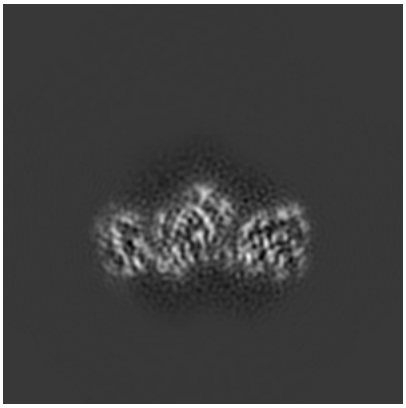
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 90

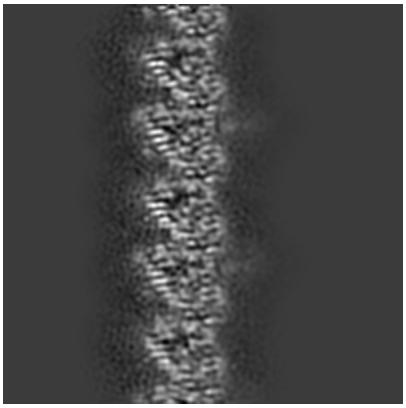

Y Index: 90

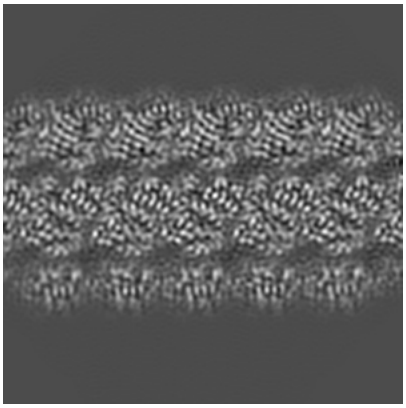

Z Index: 90

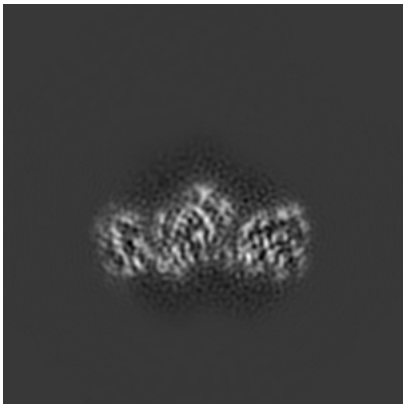
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 83

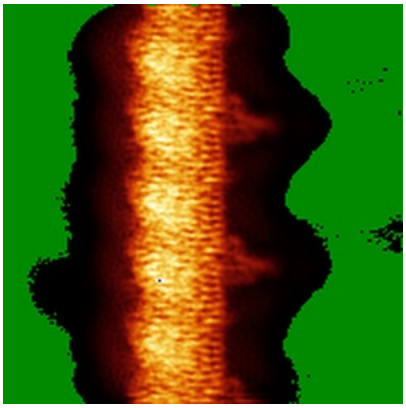

Y Index: 75

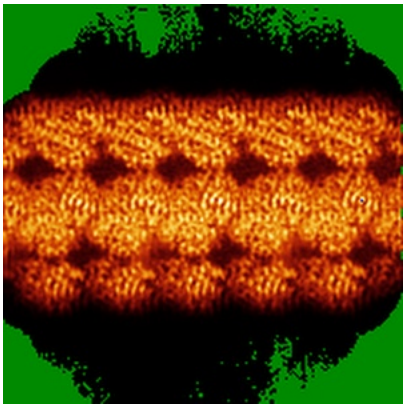

Z Index: 90

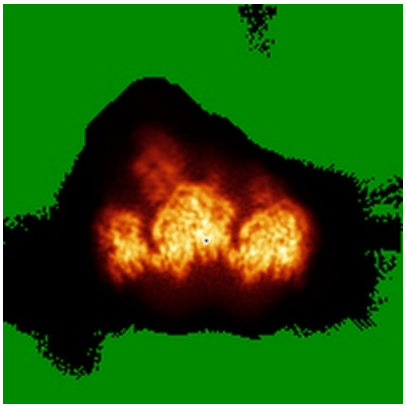
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

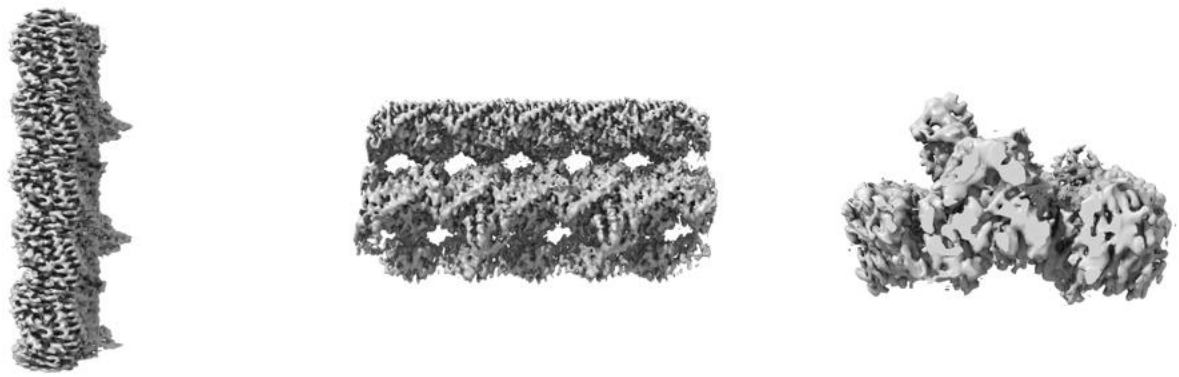

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

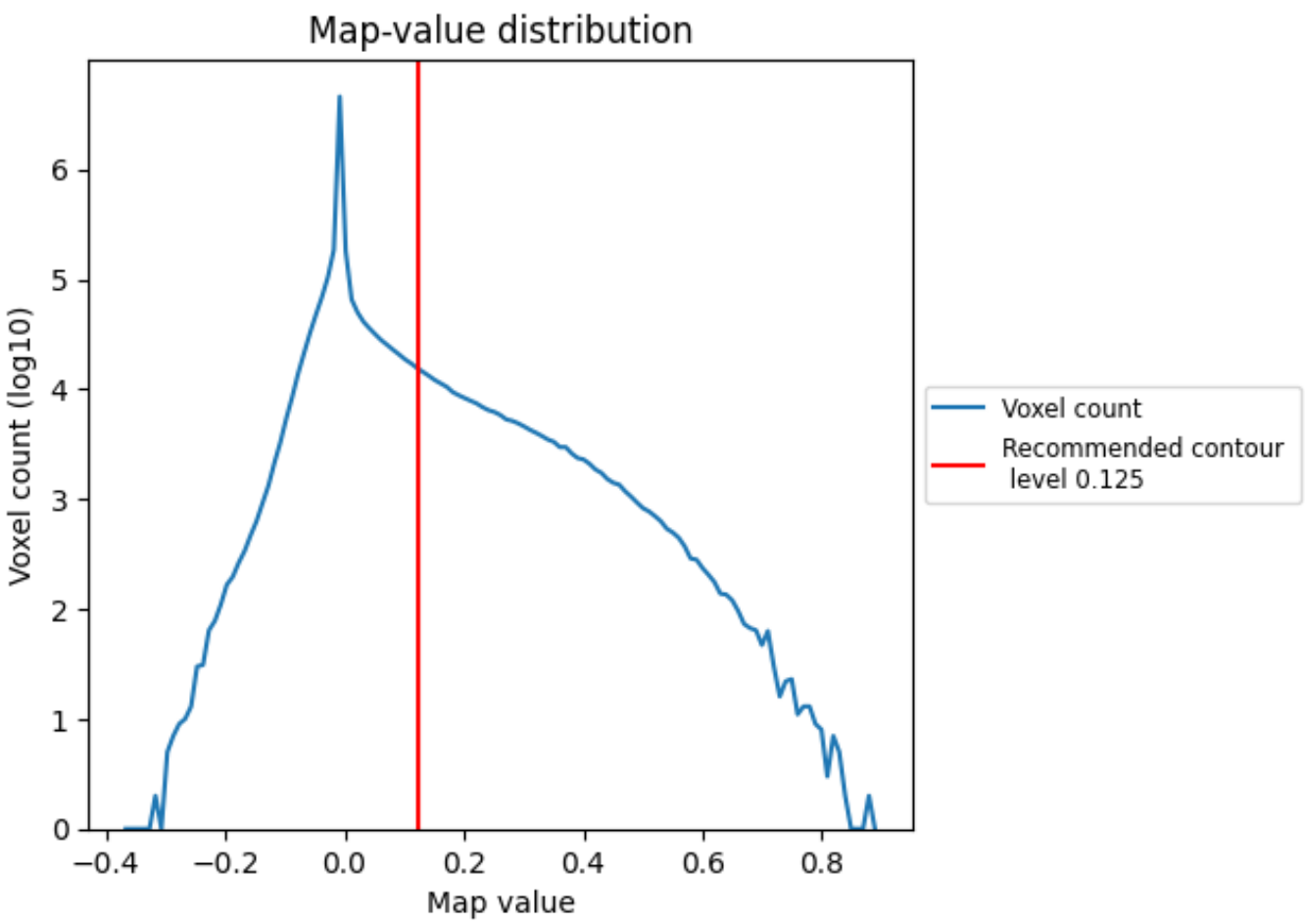
6.6 Mask visualisation (i)

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

7 Map analysis (i)

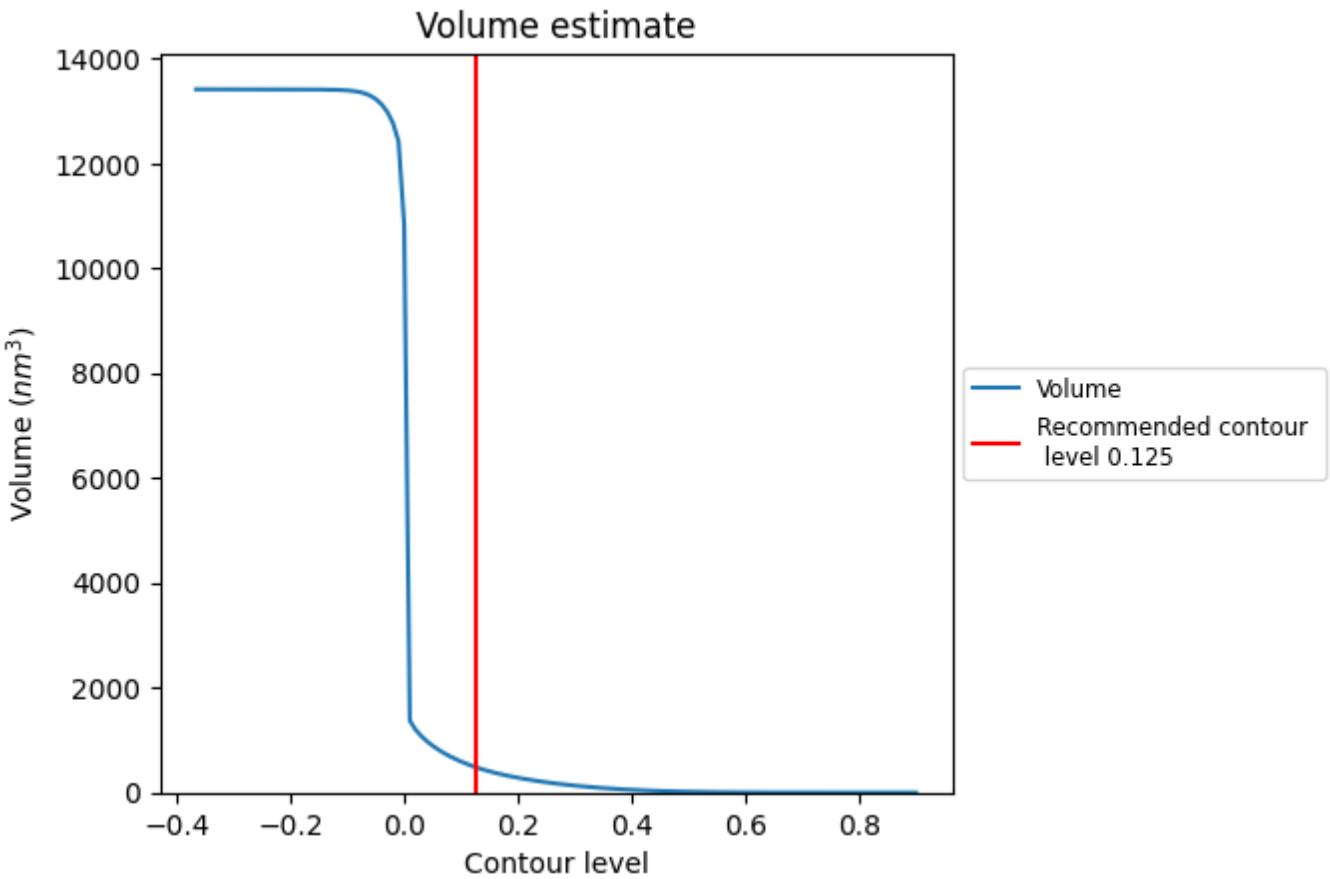
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

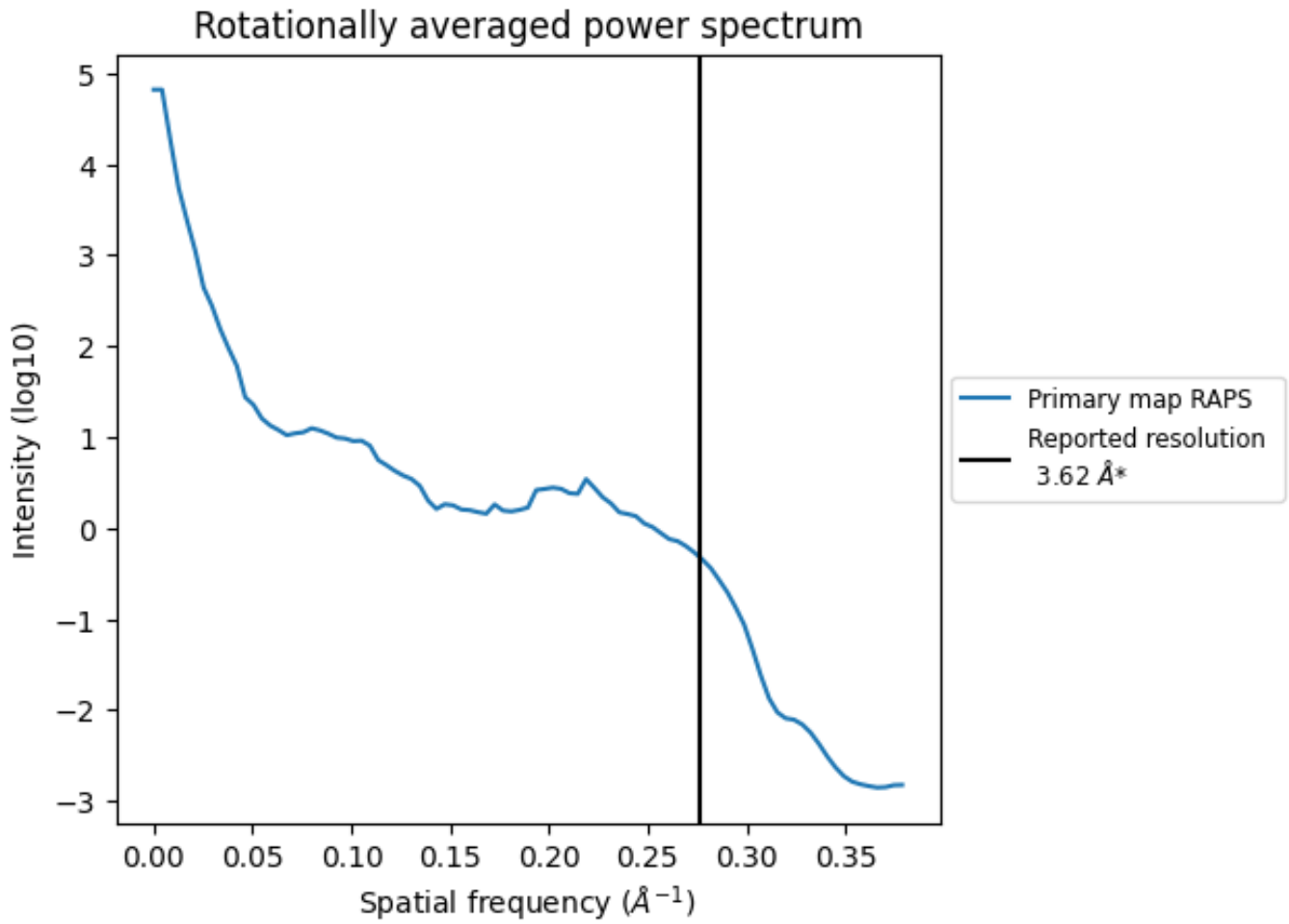
7.2 Volume estimate (i)



The volume at the recommended contour level is 484 nm^3; this corresponds to an approximate mass of 437 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 0.276 Å^{-1}

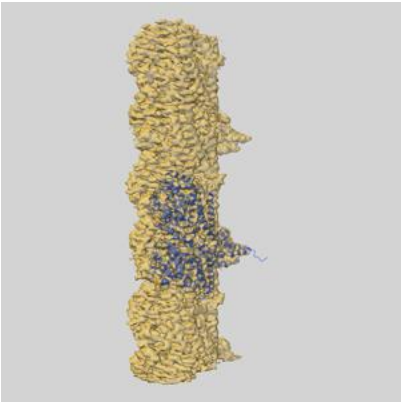
8 Fourier-Shell correlation (i)

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

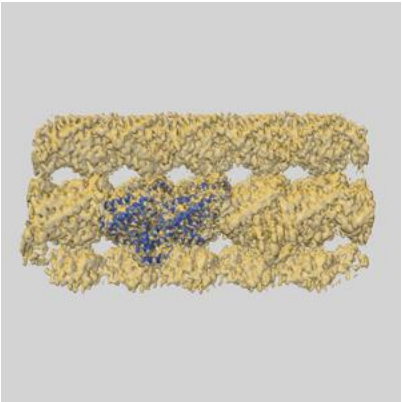
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9997 and PDB model 6KIQ. Per-residue inclusion information can be found in section 3 on page 4.

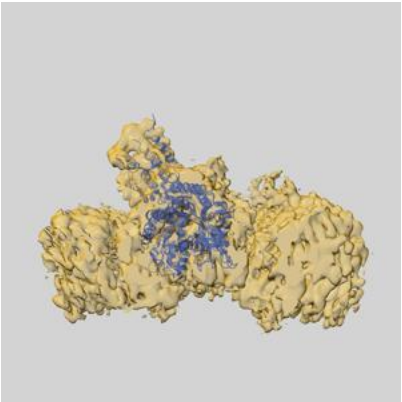
9.1 Map-model overlay (i)



X



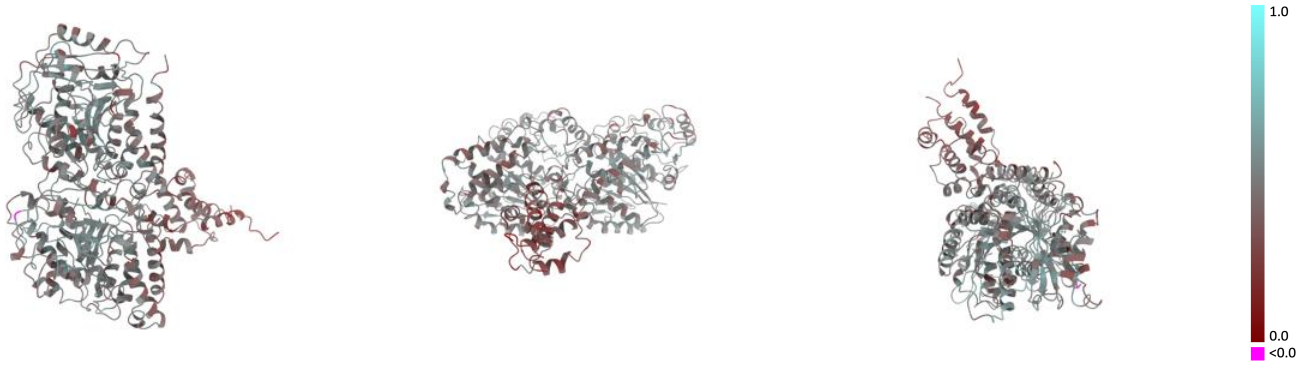
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.125 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.

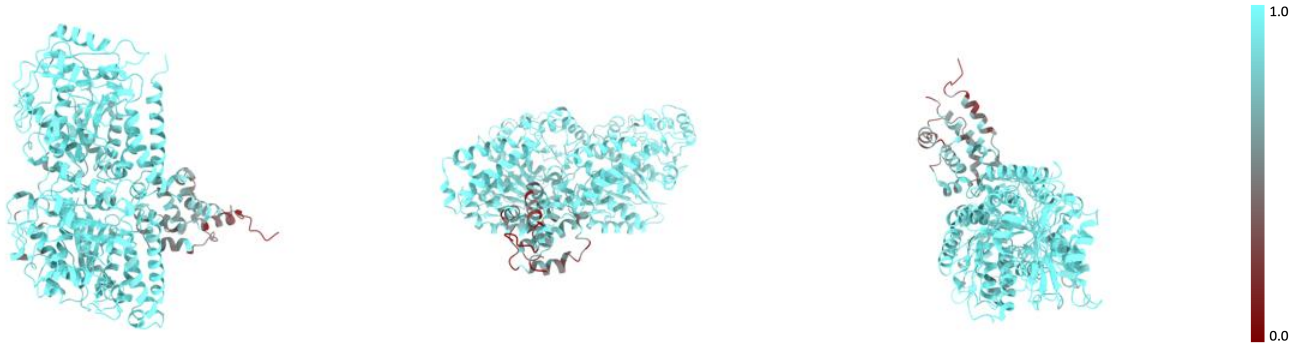
9.2 Q-score mapped to coordinate model (i)



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.

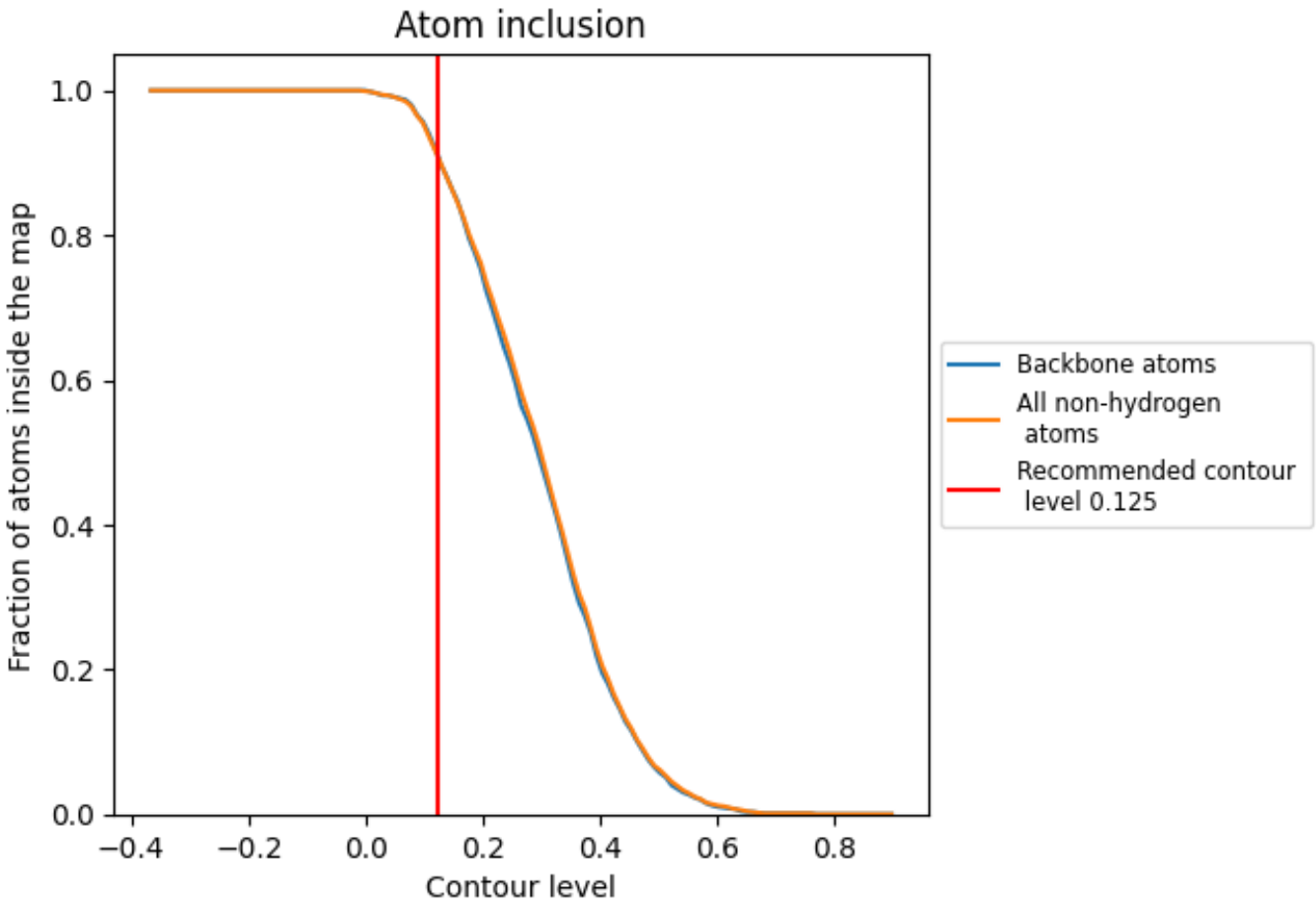
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.125).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.4550
M	0.5810	0.3210
a	0.9660	0.4790
b	0.9660	0.4730