



## Full wwPDB EM Validation Report ⓘ

May 20, 2023 – 04:15 pm BST

PDB ID : 7Z7N  
EMDB ID : EMD-14534  
Title : Mot1E1434Q:TBP:DNA - substrate recognition state  
Authors : Woike, S.; Eustermann, S.; Jung, J.; Wenzl, S.J.; Hagemann, G.; Bartho, J.D.;  
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Deposited on : 2022-03-16  
Resolution : 5.10 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50  
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) : 2.32.2

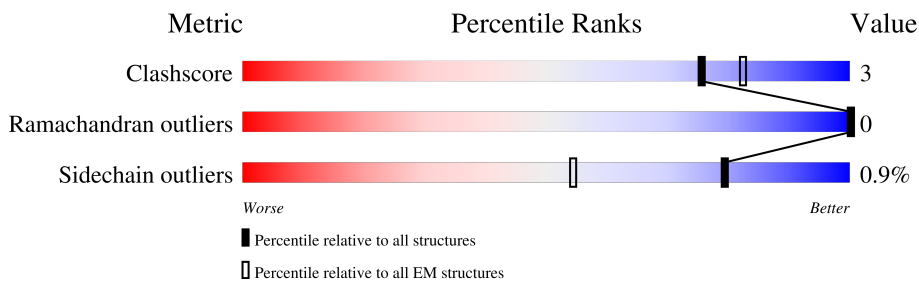
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.10 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  $\geq 3$ , 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	36	
2	B	36	
3	D	276	
4	E	1897	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25969 atoms, of which 12825 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 DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	36	1144	348	400	147	213	36	0	0

- Molecule 2 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	B	36	1135	345	403	132	219	36	0	0

- Molecule 3 is a protein called Putative tata-box binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	178	2907	919	1490	245	247	6	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP G0SAL6
D	-19	GLY	-	expression tag	UNP G0SAL6
D	-18	SER	-	expression tag	UNP G0SAL6
D	-17	SER	-	expression tag	UNP G0SAL6
D	-16	HIS	-	expression tag	UNP G0SAL6
D	-15	HIS	-	expression tag	UNP G0SAL6
D	-14	HIS	-	expression tag	UNP G0SAL6
D	-13	HIS	-	expression tag	UNP G0SAL6
D	-12	HIS	-	expression tag	UNP G0SAL6
D	-11	HIS	-	expression tag	UNP G0SAL6
D	-10	SER	-	expression tag	UNP G0SAL6
D	-9	SER	-	expression tag	UNP G0SAL6
D	-8	GLY	-	expression tag	UNP G0SAL6
D	-7	GLU	-	expression tag	UNP G0SAL6
D	-6	ASN	-	expression tag	UNP G0SAL6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	LEU	-	expression tag	UNP G0SAL6
D	-4	TYR	-	expression tag	UNP G0SAL6
D	-3	PHE	-	expression tag	UNP G0SAL6
D	-2	GLN	-	expression tag	UNP G0SAL6
D	-1	GLY	-	expression tag	UNP G0SAL6
D	0	HIS	-	expression tag	UNP G0SAL6

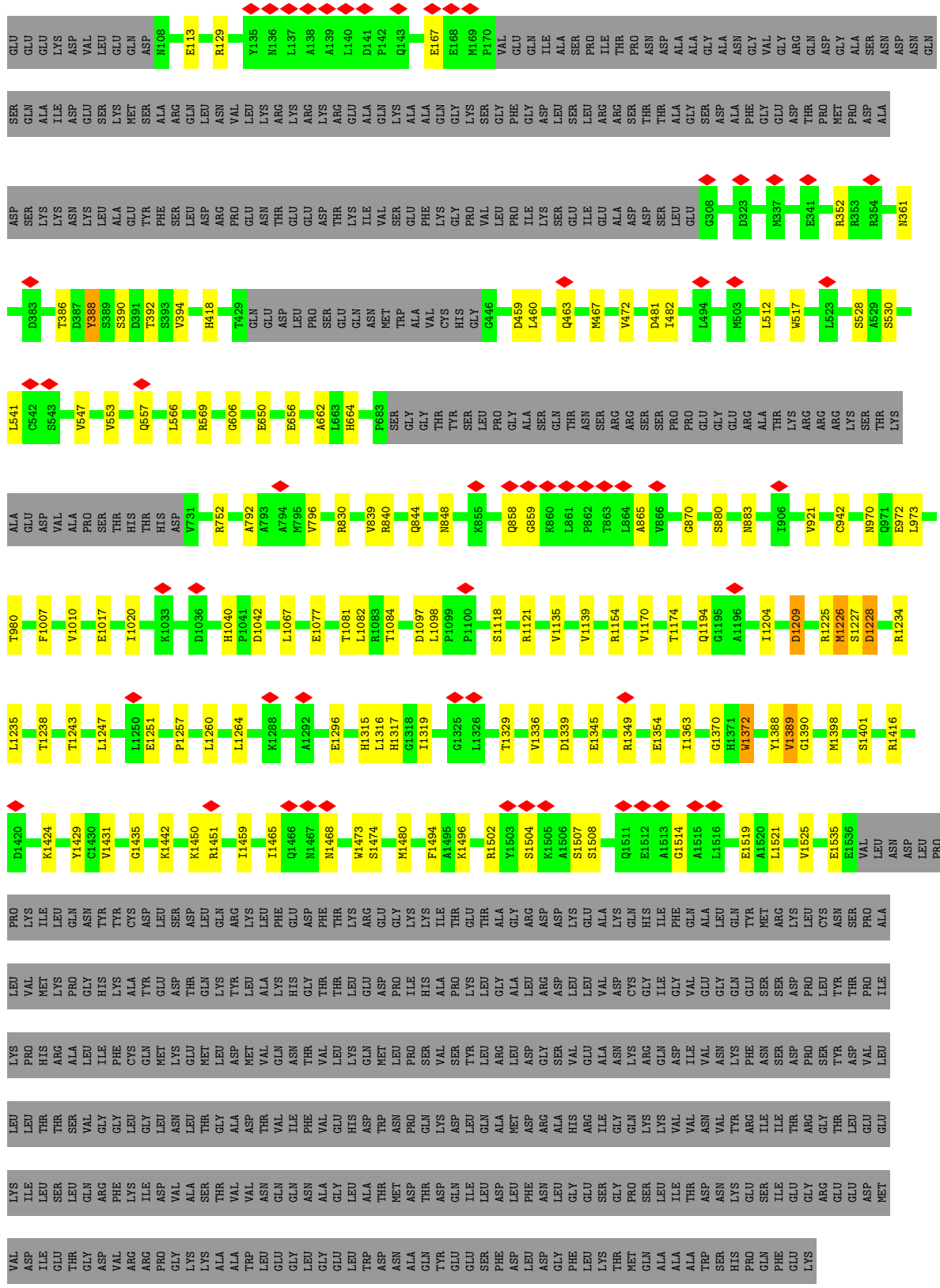
- Molecule 4 is a protein called Helicase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	E	1306	20783	6520	10532	1807	1872	52	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1434	GLN	GLU	engineered mutation	UNP G0S6C0
E	1887	ALA	-	expression tag	UNP G0S6C0
E	1888	ALA	-	expression tag	UNP G0S6C0
E	1889	ALA	-	expression tag	UNP G0S6C0
E	1890	TRP	-	expression tag	UNP G0S6C0
E	1891	SER	-	expression tag	UNP G0S6C0
E	1892	HIS	-	expression tag	UNP G0S6C0
E	1893	PRO	-	expression tag	UNP G0S6C0
E	1894	GLN	-	expression tag	UNP G0S6C0
E	1895	PHE	-	expression tag	UNP G0S6C0
E	1896	GLU	-	expression tag	UNP G0S6C0
E	1897	LYS	-	expression tag	UNP G0S6C0





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.056	Depositor
Minimum map value	-0.471	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.219	Depositor
Map size (Å)	296.52002, 296.52002, 296.52002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	1.63	0/836	2.37	60/1289 (4.7%)
2	B	1.63	0/818	2.31	53/1259 (4.2%)
3	D	2.01	37/1444 (2.6%)	1.73	14/1945 (0.7%)
4	E	0.70	25/10441 (0.2%)	0.76	10/14151 (0.1%)
All	All	1.06	62/13539 (0.5%)	1.22	137/18644 (0.7%)

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	17
2	B	0	13
All	All	0	30

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	253	ARG	CZ-NH1	-7.70	1.23	1.33
3	D	186	ARG	CZ-NH1	-7.65	1.23	1.33
4	E	129	ARG	CZ-NH1	-7.59	1.23	1.33
4	E	1451	ARG	CZ-NH1	-7.55	1.23	1.33
4	E	1502	ARG	CZ-NH1	-7.55	1.23	1.33
3	D	122	ARG	CZ-NH1	-7.55	1.23	1.33
3	D	235	ARG	CZ-NH1	-7.54	1.23	1.33
3	D	105	ARG	CZ-NH1	-7.53	1.23	1.33
3	D	94	ARG	CZ-NH1	-7.52	1.23	1.33
3	D	122	ARG	CZ-NH2	-7.27	1.23	1.33
4	E	1451	ARG	CZ-NH2	-7.23	1.23	1.33
3	D	253	ARG	CZ-NH2	-7.22	1.23	1.33
4	E	1502	ARG	CZ-NH2	-7.21	1.23	1.33
3	D	186	ARG	CZ-NH2	-7.19	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	129	ARG	CZ-NH2	-7.11	1.23	1.33
3	D	105	ARG	CZ-NH2	-7.08	1.23	1.33
3	D	235	ARG	CZ-NH2	-7.06	1.23	1.33
3	D	94	ARG	CZ-NH2	-7.04	1.23	1.33
3	D	154	TYR	CD2-CE2	-5.99	1.30	1.39
3	D	200	TYR	CD2-CE2	-5.87	1.30	1.39
3	D	200	TYR	CD1-CE1	-5.72	1.30	1.39
3	D	154	TYR	CD1-CE1	-5.63	1.30	1.39
3	D	210	TYR	CD2-CE2	-5.61	1.30	1.39
4	E	1435	GLY	N-CA	-5.58	1.37	1.46
3	D	210	TYR	CD1-CE1	-5.57	1.30	1.39
3	D	109	TYR	CD1-CE1	-5.45	1.31	1.39
4	E	388	TYR	CD2-CE2	-5.44	1.31	1.39
4	E	1372	TRP	CD1-NE1	-5.44	1.28	1.38
3	D	177	GLY	N-CA	-5.44	1.37	1.46
3	D	239	TYR	CD2-CE2	-5.43	1.31	1.39
3	D	109	TYR	CD2-CE2	-5.42	1.31	1.39
3	D	117	VAL	CB-CG2	-5.40	1.41	1.52
4	E	1370	GLY	N-CA	-5.38	1.38	1.46
4	E	1514	GLY	N-CA	-5.37	1.38	1.46
3	D	239	TYR	CD1-CE1	-5.36	1.31	1.39
4	E	1473	TRP	CD1-NE1	-5.34	1.28	1.38
3	D	207	GLY	N-CA	-5.30	1.38	1.46
4	E	388	TYR	CD1-CE1	-5.28	1.31	1.39
4	E	1390	GLY	N-CA	-5.27	1.38	1.46
4	E	1474	SER	CB-OG	-5.23	1.35	1.42
3	D	134	GLY	N-CA	-5.20	1.38	1.46
3	D	199	SER	CB-OG	-5.18	1.35	1.42
4	E	1507	SER	CB-OG	-5.16	1.35	1.42
4	E	16	SER	CB-OG	-5.15	1.35	1.42
4	E	1504	SER	CB-OG	-5.15	1.35	1.42
3	D	233	LYS	CE-NZ	-5.10	1.36	1.49
4	E	1496	LYS	CE-NZ	-5.09	1.36	1.49
3	D	171	LYS	CE-NZ	-5.09	1.36	1.49
3	D	148	LYS	CE-NZ	-5.08	1.36	1.49
4	E	1401	SER	CB-OG	-5.08	1.35	1.42
4	E	1508	SER	CB-OG	-5.07	1.35	1.42
3	D	166	LYS	CE-NZ	-5.06	1.36	1.49
3	D	198	SER	CB-OG	-5.06	1.35	1.42
3	D	142	LYS	CE-NZ	-5.05	1.36	1.49
3	D	182	LYS	CE-NZ	-5.04	1.36	1.49
4	E	1424	LYS	CE-NZ	-5.03	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1431	VAL	CB-CG2	-5.03	1.42	1.52
4	E	1450	LYS	CE-NZ	-5.03	1.36	1.49
3	D	98	LYS	CE-NZ	-5.02	1.36	1.49
3	D	112	LYS	CE-NZ	-5.01	1.36	1.49
3	D	214	LYS	CE-NZ	-5.01	1.36	1.49
4	E	1442	LYS	CE-NZ	-5.00	1.36	1.49

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	DT	O4'-C1'-N1	11.74	116.22	108.00
1	A	31	DA	N1-C6-N6	-10.68	112.19	118.60
1	A	27	DA	N1-C6-N6	-9.80	112.72	118.60
2	B	11	DA	N1-C6-N6	-9.72	112.77	118.60
1	A	32	DA	N1-C6-N6	-8.84	113.30	118.60
2	B	9	DA	C5-C6-N1	8.24	121.82	117.70
1	A	21	DC	N3-C2-O2	-8.12	116.22	121.90
3	D	239	TYR	CB-CG-CD2	7.99	125.80	121.00
1	A	30	DA	N1-C6-N6	-7.89	113.87	118.60
2	B	31	DC	N3-C2-O2	-7.88	116.38	121.90
1	A	36	DC	N3-C2-O2	-7.78	116.45	121.90
1	A	32	DA	C5-C6-N1	7.70	121.55	117.70
2	B	17	DC	N3-C2-O2	-7.70	116.51	121.90
1	A	29	DA	N1-C6-N6	-7.65	114.01	118.60
2	B	34	DC	N3-C2-O2	-7.61	116.58	121.90
3	D	200	TYR	CB-CG-CD2	7.58	125.55	121.00
1	A	11	DC	N3-C2-O2	-7.55	116.61	121.90
1	A	29	DA	C5-C6-N1	7.53	121.46	117.70
1	A	17	DA	C5-C6-N1	7.47	121.44	117.70
1	A	30	DA	C5-C6-N1	7.41	121.40	117.70
1	A	4	DC	N3-C2-O2	-7.40	116.72	121.90
1	A	13	DC	N3-C2-O2	-7.39	116.73	121.90
2	B	14	DC	N3-C2-O2	-7.35	116.76	121.90
2	B	29	DC	N3-C2-O2	-7.29	116.80	121.90
2	B	11	DA	C5-C6-N1	7.24	121.32	117.70
1	A	18	DT	O4'-C1'-N1	7.24	113.06	108.00
2	B	15	DC	N3-C2-O2	-7.21	116.85	121.90
2	B	19	DA	C5-C6-N1	7.21	121.30	117.70
1	A	28	DT	N3-C2-O2	-7.17	118.00	122.30
1	A	16	DC	N3-C2-O2	-7.09	116.93	121.90
1	A	1	DC	N3-C2-O2	-7.06	116.96	121.90
1	A	31	DA	C5-C6-N1	7.03	121.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	DC	N3-C2-O2	-7.03	116.98	121.90
2	B	23	DC	N3-C2-O2	-7.01	116.99	121.90
1	A	27	DA	C4-C5-C6	-6.94	113.53	117.00
2	B	2	DC	N3-C2-O2	-6.92	117.05	121.90
1	A	25	DC	N3-C2-O2	-6.91	117.06	121.90
1	A	34	DG	O4'-C1'-N9	6.91	112.83	108.00
2	B	3	DC	N3-C2-O2	-6.90	117.07	121.90
1	A	31	DA	C4-C5-C6	-6.88	113.56	117.00
3	D	235	ARG	CD-NE-CZ	6.82	133.15	123.60
4	E	1416	ARG	NE-CZ-NH1	6.79	123.70	120.30
4	E	1502	ARG	CD-NE-CZ	6.77	133.08	123.60
1	A	9	DC	N3-C2-O2	-6.75	117.17	121.90
4	E	129	ARG	CD-NE-CZ	6.74	133.04	123.60
1	A	27	DA	C5-C6-N1	6.70	121.05	117.70
4	E	1451	ARG	CD-NE-CZ	6.69	132.96	123.60
2	B	27	DC	N3-C2-O2	-6.62	117.26	121.90
1	A	24	DC	N3-C2-O2	-6.61	117.28	121.90
2	B	4	DC	N3-C2-O2	-6.56	117.31	121.90
2	B	11	DA	C4-C5-C6	-6.54	113.73	117.00
2	B	30	DC	N3-C2-O2	-6.53	117.33	121.90
2	B	22	DC	N3-C2-O2	-6.52	117.34	121.90
1	A	21	DC	N1-C2-O2	6.49	122.80	118.90
1	A	17	DA	N1-C6-N6	-6.48	114.71	118.60
1	A	32	DA	C4-C5-C6	-6.46	113.77	117.00
2	B	35	DC	N3-C2-O2	-6.39	117.43	121.90
1	A	18	DT	C6-C5-C7	-6.35	119.09	122.90
1	A	29	DA	C4-C5-C6	-6.31	113.85	117.00
1	A	17	DA	C4-C5-C6	-6.30	113.85	117.00
1	A	5	DC	N3-C2-O2	-6.29	117.50	121.90
1	A	11	DC	C1'-O4'-C4'	-6.28	103.82	110.10
2	B	18	DC	N3-C2-O2	-6.24	117.53	121.90
3	D	119	MET	CA-CB-CG	6.22	123.88	113.30
4	E	1389	VAL	C-N-CA	6.19	135.31	122.30
1	A	10	DG	N1-C6-O6	-6.13	116.22	119.90
2	B	9	DA	N1-C6-N6	-6.12	114.93	118.60
1	A	18	DT	N3-C2-O2	-6.12	118.63	122.30
1	A	20	DG	N1-C6-O6	-6.10	116.24	119.90
1	A	28	DT	C6-C5-C7	-6.10	119.24	122.90
2	B	20	DT	C6-C5-C7	-6.08	119.25	122.90
2	B	7	DT	C6-C5-C7	-6.05	119.27	122.90
2	B	28	DG	N1-C6-O6	-6.00	116.30	119.90
2	B	31	DC	N1-C2-O2	5.97	122.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	DT	O4'-C1'-N1	5.96	112.17	108.00
2	B	17	DC	O4'-C1'-N1	5.94	112.16	108.00
4	E	129	ARG	CG-CD-NE	5.93	124.26	111.80
2	B	17	DC	O4'-C1'-C2'	-5.92	101.16	105.90
1	A	2	DG	O4'-C1'-N9	5.87	112.11	108.00
3	D	244	MET	CA-CB-CG	5.86	123.27	113.30
3	D	94	ARG	CD-NE-CZ	5.79	131.71	123.60
2	B	17	DC	N1-C2-O2	5.79	122.37	118.90
1	A	33	DG	N1-C6-O6	-5.79	116.43	119.90
1	A	4	DC	N1-C2-O2	5.77	122.36	118.90
2	B	19	DA	N1-C6-N6	-5.76	115.14	118.60
3	D	154	TYR	CB-CG-CD2	5.75	124.45	121.00
2	B	34	DC	N1-C2-O2	5.69	122.31	118.90
2	B	10	DT	P-O3'-C3'	5.66	126.50	119.70
1	A	26	DT	C6-C5-C7	-5.64	119.51	122.90
2	B	30	DC	N1-C2-O2	5.61	122.26	118.90
2	B	3	DC	N1-C2-O2	5.60	122.26	118.90
2	B	6	DT	C6-C5-C7	-5.59	119.55	122.90
2	B	8	DT	C6-C5-C7	-5.58	119.55	122.90
1	A	35	DG	N1-C6-O6	-5.58	116.55	119.90
4	E	1494	PHE	CB-CG-CD2	5.58	124.70	120.80
2	B	5	DT	C6-C5-C7	-5.55	119.57	122.90
1	A	13	DC	N1-C2-O2	5.54	122.22	118.90
1	A	16	DC	N1-C2-O2	5.53	122.22	118.90
2	B	8	DT	N3-C2-O2	-5.53	118.98	122.30
1	A	24	DC	N1-C2-O2	5.53	122.22	118.90
2	B	29	DC	N1-C2-O2	5.51	122.20	118.90
2	B	10	DT	N3-C2-O2	-5.50	119.00	122.30
2	B	15	DC	N1-C2-O2	5.50	122.20	118.90
3	D	109	TYR	CB-CG-CD2	5.49	124.29	121.00
1	A	20	DG	C5-C6-N1	5.47	114.23	111.50
2	B	5	DT	N3-C2-O2	-5.44	119.04	122.30
1	A	36	DC	N1-C2-O2	5.40	122.14	118.90
1	A	2	DG	N1-C6-O6	-5.39	116.67	119.90
1	A	30	DA	C4-C5-C6	-5.37	114.31	117.00
2	B	10	DT	C6-C5-C7	-5.37	119.68	122.90
4	E	129	ARG	CA-CB-CG	5.37	125.21	113.40
3	D	105	ARG	CA-CB-CG	5.36	125.20	113.40
2	B	22	DC	N3-C4-C5	5.36	124.04	121.90
1	A	11	DC	N1-C2-O2	5.35	122.11	118.90
1	A	1	DC	N1-C2-O2	5.31	122.09	118.90
2	B	21	DG	N1-C6-O6	-5.26	116.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	DG	N1-C6-O6	-5.25	116.75	119.90
1	A	5	DC	O4'-C1'-N1	5.24	111.67	108.00
4	E	390	SER	N-CA-CB	5.24	118.37	110.50
1	A	34	DG	C1'-O4'-C4'	-5.22	104.88	110.10
2	B	22	DC	C1'-O4'-C4'	-5.21	104.89	110.10
2	B	8	DT	C5-C6-N1	-5.18	120.59	123.70
3	D	211	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	28	DT	O4'-C1'-C2'	-5.17	101.76	105.90
3	D	142	LYS	CA-CB-CG	5.16	124.74	113.40
2	B	36	DG	O4'-C1'-N9	5.15	111.60	108.00
2	B	20	DT	N3-C2-O2	-5.13	119.22	122.30
1	A	25	DC	N1-C2-O2	5.12	121.97	118.90
2	B	32	DG	N1-C6-O6	-5.12	116.83	119.90
3	D	239	TYR	CD1-CG-CD2	-5.12	112.27	117.90
2	B	12	DG	N1-C6-O6	-5.08	116.85	119.90
2	B	5	DT	C5-C6-N1	-5.07	120.66	123.70
4	E	1502	ARG	CG-CD-NE	5.07	122.45	111.80
3	D	239	TYR	CA-CB-CG	5.07	123.03	113.40
1	A	12	DC	N1-C2-O2	5.06	121.93	118.90
1	A	9	DC	N3-C4-C5	5.05	123.92	121.90
3	D	197	PHE	CB-CG-CD2	5.02	124.31	120.80

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	DG	Sidechain
1	A	12	DC	Sidechain
1	A	14	DG	Sidechain
1	A	16	DC	Sidechain
1	A	20	DG	Sidechain
1	A	22	DG	Sidechain
1	A	24	DC	Sidechain
1	A	25	DC	Sidechain
1	A	26	DT	Sidechain
1	A	27	DA	Sidechain
1	A	28	DT	Sidechain
1	A	29	DA	Sidechain
1	A	32	DA	Sidechain
1	A	34	DG	Sidechain
1	A	5	DC	Sidechain
1	A	8	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	9	DC	Sidechain
2	B	10	DT	Sidechain
2	B	11	DA	Sidechain
2	B	13	DG	Sidechain
2	B	16	DG	Sidechain
2	B	22	DC	Sidechain
2	B	24	DG	Sidechain
2	B	25	DG	Sidechain
2	B	26	DG	Sidechain
2	B	27	DC	Sidechain
2	B	32	DG	Sidechain
2	B	5	DT	Sidechain
2	B	6	DT	Sidechain
2	B	7	DT	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	744	400	400	0	0
2	B	732	403	403	0	0
3	D	1417	1490	1489	3	0
4	E	10251	10532	10526	77	0
All	All	13144	12825	12818	80	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 3.

All (80) 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)
4:E:1226:MET:O	4:E:1234:ARG:NH2	1.68	1.26
4:E:1227:SER:OG	4:E:1315:HIS:HB3	1.32	1.22
4:E:1227:SER:OG	4:E:1315:HIS:CB	2.22	0.87
4:E:1226:MET:HE2	4:E:1480:MET:SD	2.23	0.78
4:E:606:GLY:N	4:E:650:GLU:OE1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:942:CYS:SG	4:E:980:THR:OG1	2.48	0.71
4:E:830:ARG:NH1	4:E:870:GLY:O	2.26	0.68
4:E:1227:SER:HG	4:E:1315:HIS:HB3	1.55	0.68
4:E:1226:MET:O	4:E:1234:ARG:CZ	2.42	0.67
4:E:1226:MET:CE	4:E:1480:MET:SD	2.83	0.67
4:E:541:LEU:HB3	4:E:547:VAL:HG21	1.77	0.66
4:E:1251:GLU:N	4:E:1251:GLU:OE1	2.28	0.66
4:E:1339:ASP:OD2	4:E:1429:TYR:OH	2.14	0.65
4:E:13:GLU:OE2	4:E:52:HIS:NE2	2.30	0.64
4:E:1398:MET:O	4:E:1398:MET:HG3	1.99	0.62
4:E:664:HIS:O	4:E:752:ARG:NH1	2.36	0.58
4:E:1228:ASP:N	4:E:1228:ASP:OD1	2.37	0.57
4:E:1225:ARG:HH11	4:E:1225:ARG:HG2	1.69	0.56
4:E:1017:GLU:N	4:E:1017:GLU:OE1	2.38	0.56
3:D:223:VAL:HG22	3:D:223:VAL:O	2.06	0.55
4:E:352:ARG:NH1	4:E:361:ASN:OD1	2.39	0.55
4:E:1204:ILE:HG21	4:E:1243:THR:HG23	1.89	0.54
4:E:1170:VAL:O	4:E:1174:THR:HG23	2.09	0.53
4:E:1336:VAL:HG12	4:E:1429:TYR:CD2	2.42	0.53
4:E:1235:LEU:O	4:E:1238:THR:OG1	2.21	0.52
4:E:844:GLN:NE2	4:E:848:ASN:OD1	2.42	0.52
4:E:392:THR:O	4:E:394:VAL:HG13	2.09	0.52
4:E:1154:ARG:NH2	4:E:1194:GLN:OE1	2.41	0.52
4:E:1535:GLU:N	4:E:1535:GLU:OE1	2.41	0.52
4:E:1077:GLU:N	4:E:1077:GLU:OE1	2.43	0.50
4:E:1257:PRO:CB	4:E:1260:LEU:HD22	2.42	0.50
4:E:472:VAL:HG23	4:E:512:LEU:HD21	1.94	0.50
4:E:839:VAL:HG22	4:E:921:VAL:HG22	1.93	0.50
4:E:1040:HIS:O	4:E:1042:ASP:N	2.45	0.49
4:E:1257:PRO:HB2	4:E:1260:LEU:HD22	1.94	0.49
4:E:19:LEU:HD21	4:E:1519:GLU:CG	2.43	0.49
4:E:656:GLU:OE1	4:E:656:GLU:N	2.46	0.49
4:E:418:HIS:ND1	4:E:467:MET:SD	2.86	0.48
4:E:970:ASN:OD1	4:E:972:GLU:N	2.46	0.48
4:E:1174:THR:HG22	4:E:1264:LEU:HD11	1.95	0.48
4:E:662:ALA:O	4:E:752:ARG:NH2	2.46	0.48
4:E:1081:THR:O	4:E:1084:THR:OG1	2.27	0.47
4:E:1097:ASP:OD1	4:E:1098:LEU:N	2.48	0.47
4:E:970:ASN:OD1	4:E:973:LEU:N	2.40	0.47
4:E:517:TRP:O	4:E:569:ARG:NH1	2.47	0.47
4:E:1354:GLU:N	4:E:1354:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1225:ARG:NE	4:E:1225:ARG:HA	2.31	0.46
4:E:167:GLU:OE1	4:E:167:GLU:N	2.49	0.46
3:D:212:MET:SD	3:D:214:LYS:N	2.89	0.46
4:E:840:ARG:NE	4:E:865:ALA:O	2.48	0.46
4:E:1388:TYR:HD1	4:E:1388:TYR:O	1.99	0.45
4:E:541:LEU:HD22	4:E:547:VAL:CG2	2.47	0.45
4:E:880:SER:N	4:E:883:ASN:OD1	2.48	0.45
4:E:1329:THR:HG23	4:E:1372:TRP:CZ2	2.51	0.45
4:E:1521:LEU:O	4:E:1525:VAL:HG22	2.17	0.44
4:E:1345:GLU:OE1	4:E:1349:ARG:NE	2.46	0.44
4:E:113:GLU:OE1	4:E:113:GLU:N	2.50	0.44
4:E:1225:ARG:HG2	4:E:1225:ARG:NH1	2.33	0.43
4:E:1007:PHE:O	4:E:1010:VAL:HG23	2.20	0.42
4:E:15:GLY:O	4:E:21:ARG:NH1	2.53	0.42
4:E:517:TRP:CD2	4:E:566:LEU:HD21	2.55	0.42
4:E:1465:ILE:HD12	4:E:1468:ASN:O	2.19	0.42
4:E:459:ASP:OD1	4:E:460:LEU:N	2.52	0.42
4:E:1204:ILE:HG21	4:E:1243:THR:CG2	2.50	0.42
4:E:1209:ASP:OD1	4:E:1209:ASP:N	2.53	0.42
4:E:386:THR:HG21	4:E:388:TYR:CZ	2.54	0.41
4:E:1226:MET:O	4:E:1226:MET:SD	2.79	0.41
4:E:1227:SER:OG	4:E:1315:HIS:CG	2.74	0.41
4:E:792:ALA:O	4:E:796:VAL:HG23	2.20	0.41
4:E:858:GLN:OE1	4:E:859:GLY:N	2.52	0.41
4:E:553:VAL:O	4:E:557:GLN:NE2	2.49	0.41
4:E:1316:LEU:O	4:E:1317:HIS:ND1	2.54	0.41
4:E:1017:GLU:HB2	4:E:1020:ILE:HD12	2.04	0.40
4:E:1319:ILE:HG23	4:E:1459:ILE:O	2.21	0.40
4:E:481:ASP:OD1	4:E:482:ILE:N	2.54	0.40
4:E:1296:GLU:OE1	4:E:1296:GLU:N	2.49	0.40
4:E:1135:VAL:O	4:E:1139:VAL:HG23	2.21	0.40
3:D:194:HIS:O	3:D:198:SER:N	2.55	0.40
4:E:1118:SER:HA	4:E:1121:ARG:HG2	2.04	0.40
4:E:1209:ASP:HA	4:E:1247:LEU:HD22	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	
3	D	176/276 (64%)	170 (97%)	6 (3%)	0	100	100
4	E	1296/1897 (68%)	1243 (96%)	53 (4%)	0	100	100
All	All	1472/2173 (68%)	1413 (96%)	59 (4%)	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	
3	D	154/219 (70%)	153 (99%)	1 (1%)	86	91
4	E	1114/1620 (69%)	1104 (99%)	10 (1%)	78	87
All	All	1268/1839 (69%)	1257 (99%)	11 (1%)	79	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	204	LEU
4	E	463	GLN
4	E	528	SER
4	E	530	SER
4	E	1067	LEU
4	E	1082	LEU
4	E	1209	ASP
4	E	1226	MET

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Mol	Chain	Res	Type
4	E	1228	ASP
4	E	1363	ILE
4	E	1389	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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.

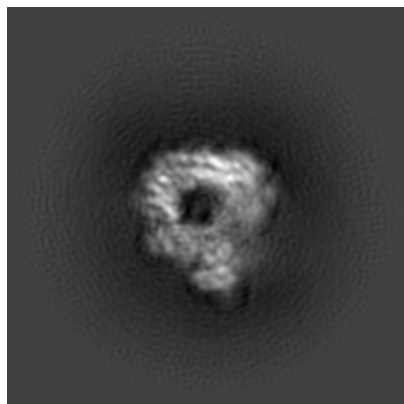
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14534. These allow visual inspection of the internal detail of the map and identification of artifacts.

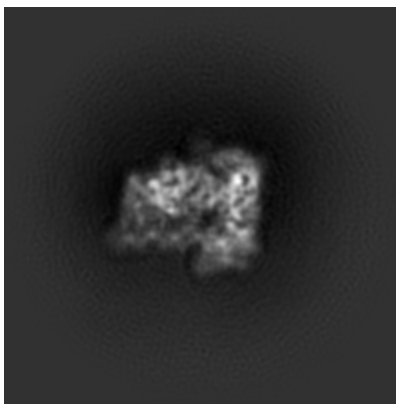
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

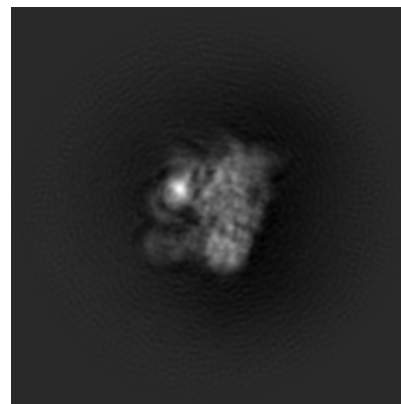
#### 6.1.1 Primary map



X

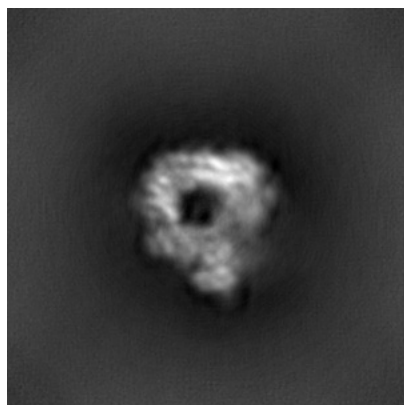


Y

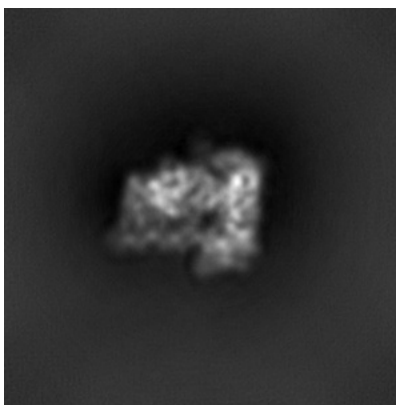


Z

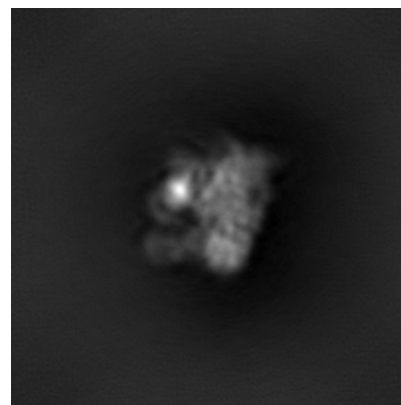
#### 6.1.2 Raw map



X



Y

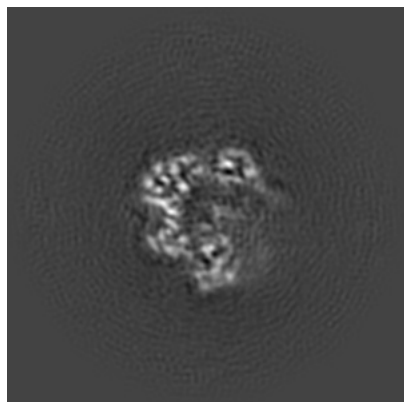


Z

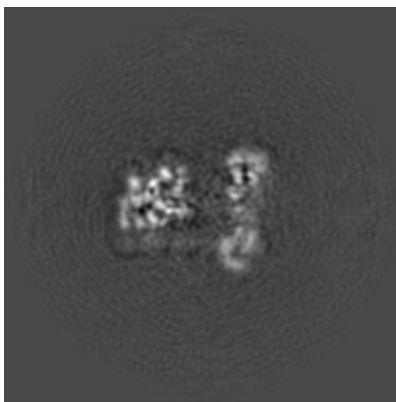
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

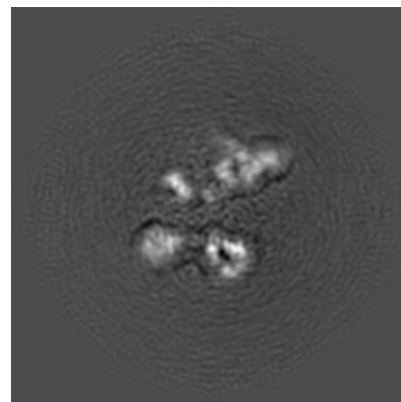
### 6.2.1 Primary map



X Index: 140

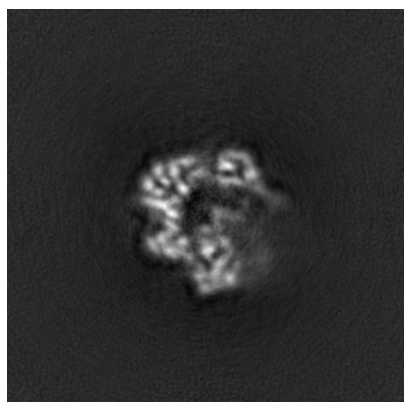


Y Index: 140

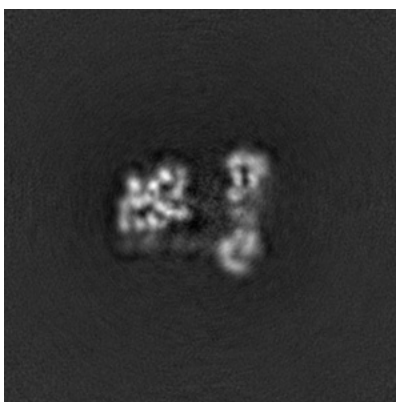


Z Index: 140

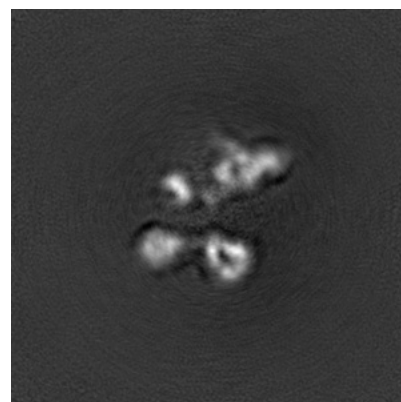
### 6.2.2 Raw map



X Index: 140



Y Index: 140

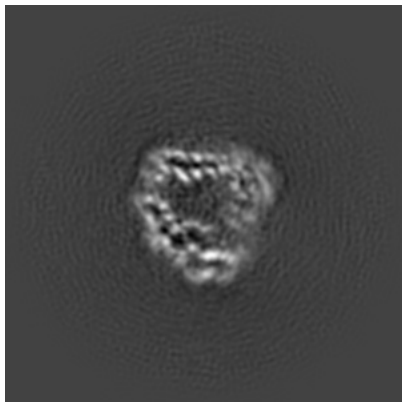


Z Index: 140

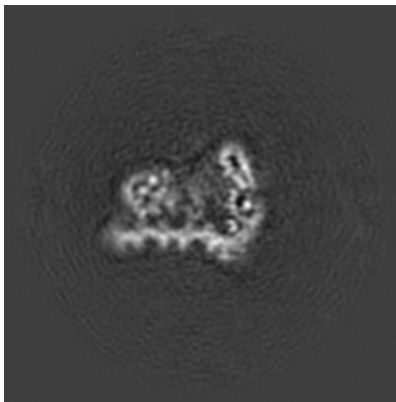
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

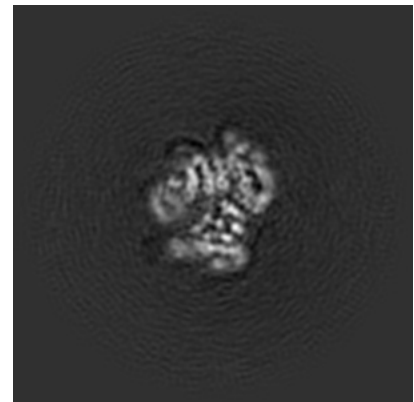
### 6.3.1 Primary map



X Index: 156

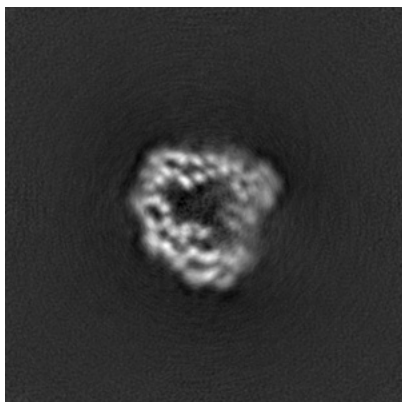


Y Index: 153

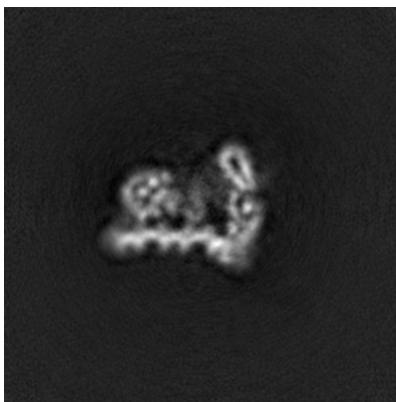


Z Index: 160

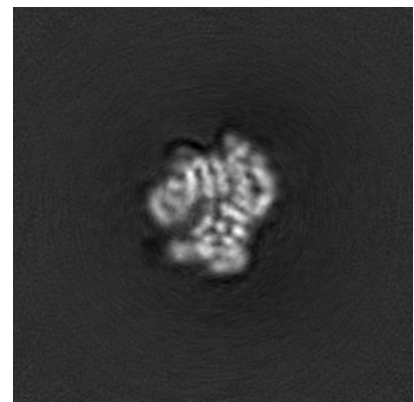
### 6.3.2 Raw map



X Index: 154



Y Index: 152

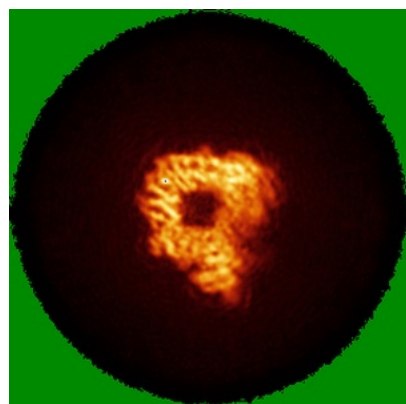


Z Index: 161

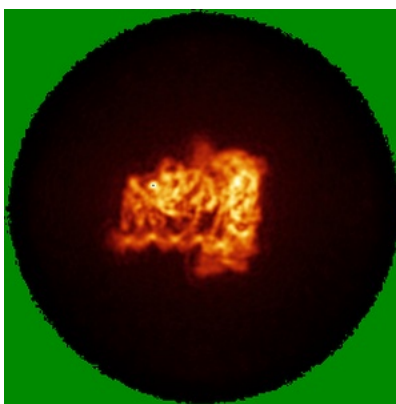
The images above show the largest variance slices of the map in three orthogonal directions.

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

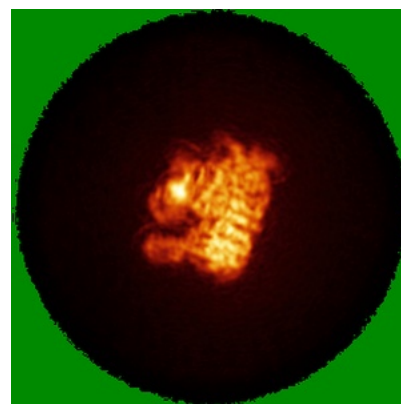
### 6.4.1 Primary map



X



Y

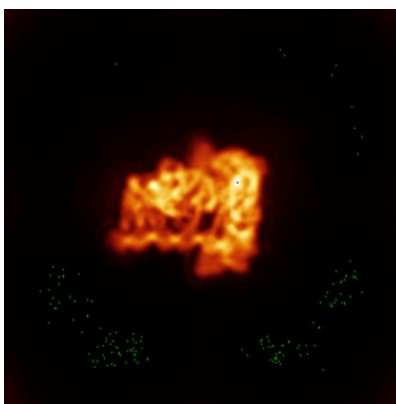


Z

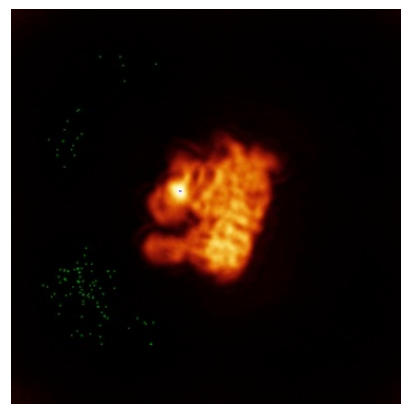
### 6.4.2 Raw map



X



Y

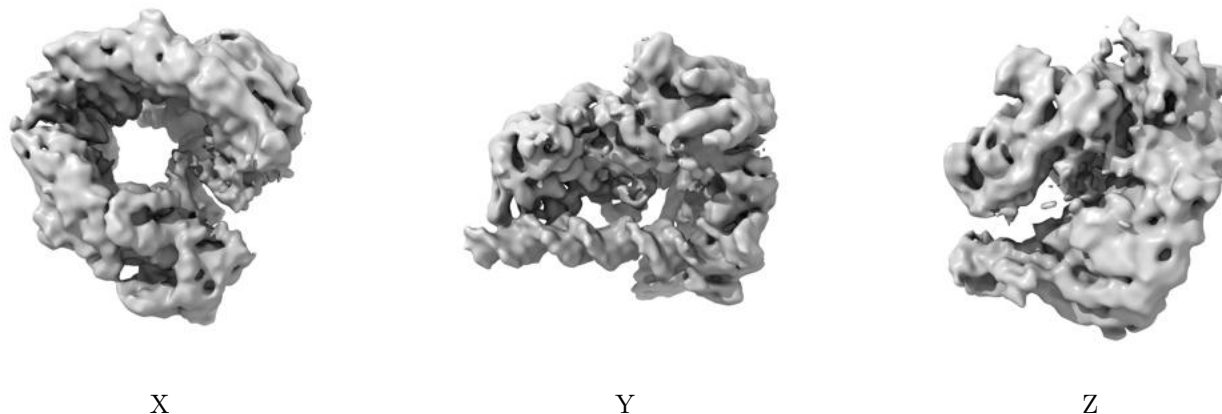


Z

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

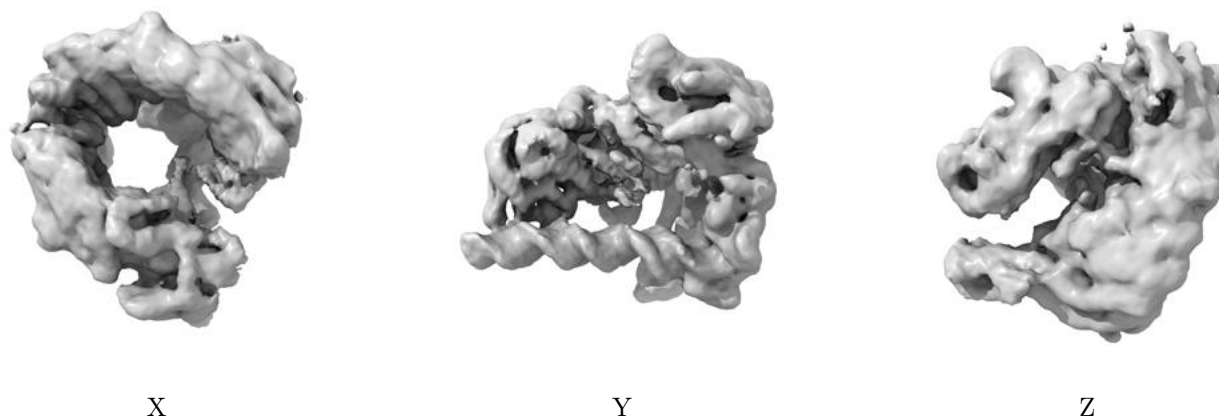
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.219. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

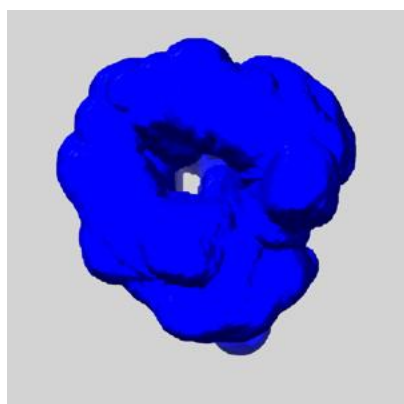
## 6.6 Mask visualisation [i](#)

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

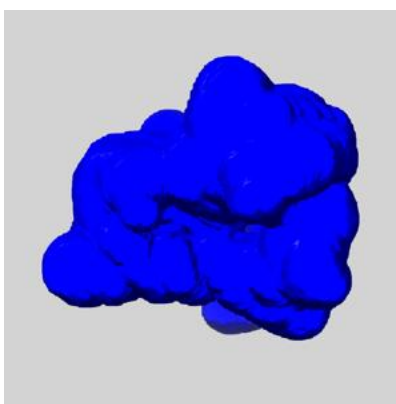
A mask typically either:

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

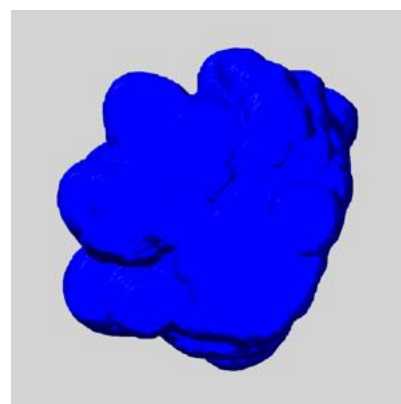
### 6.6.1 emd\_14534\_msk\_1.map [i](#)



X



Y



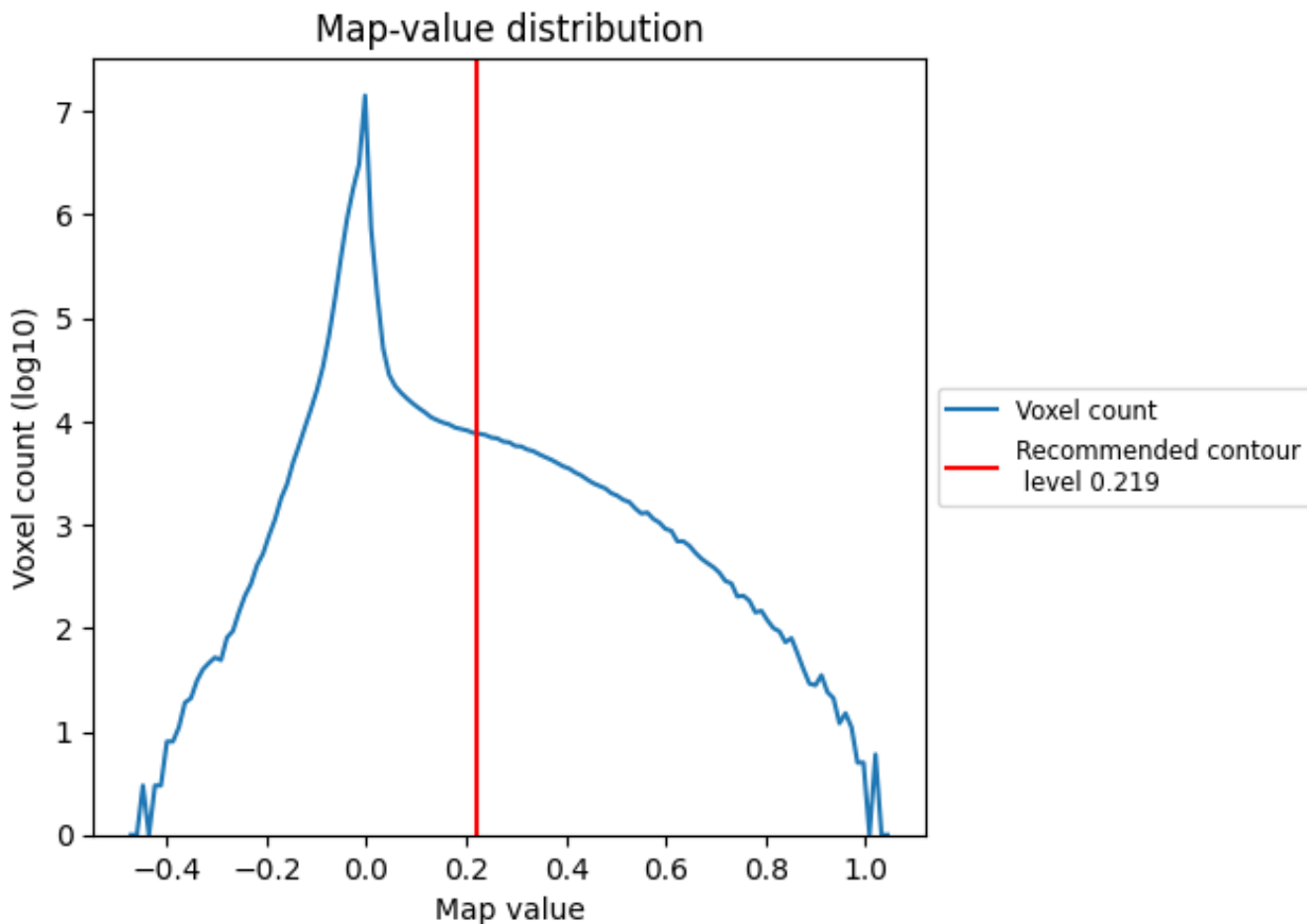
Z



## 7 Map analysis [i](#)

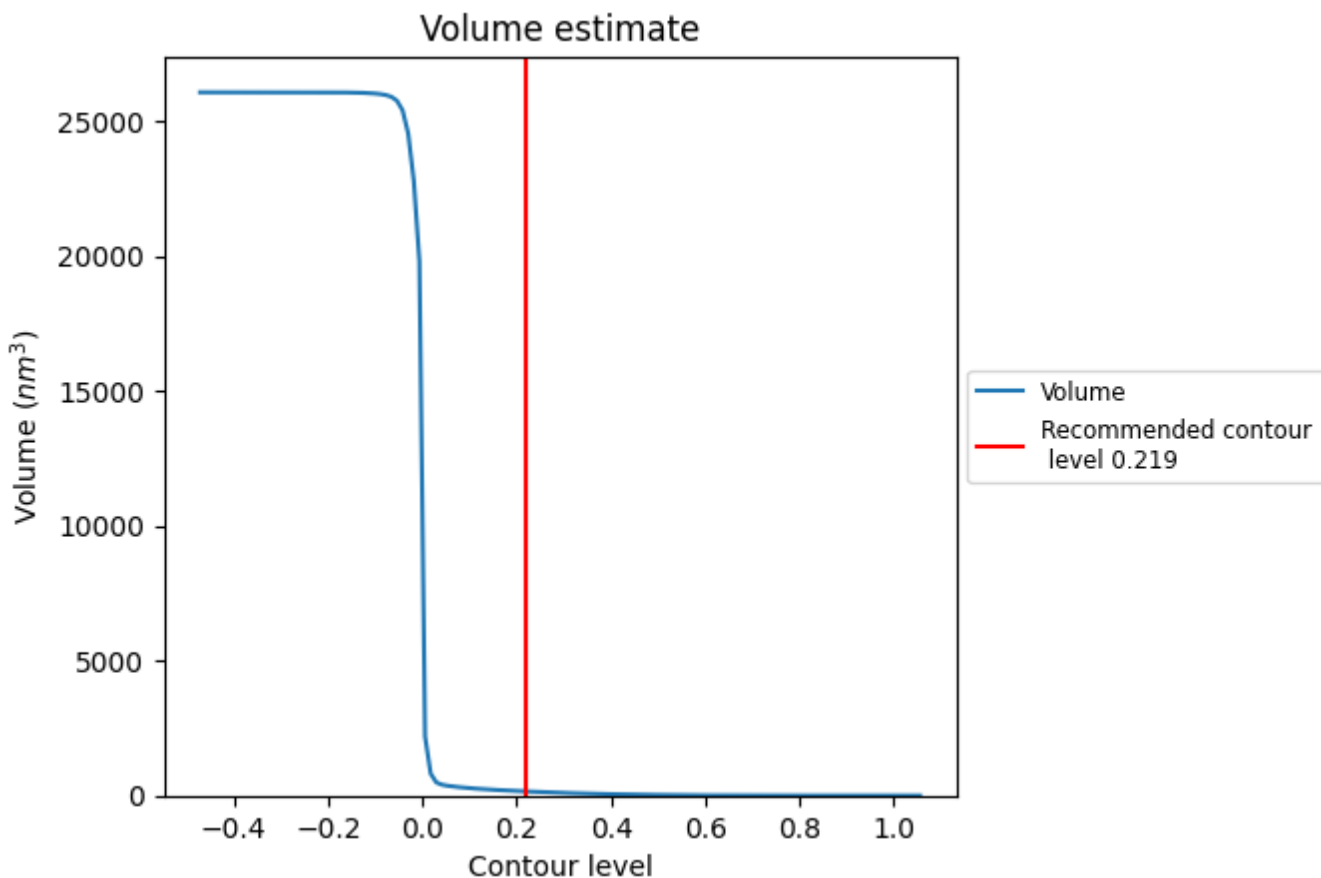
This section contains the results of statistical analysis of the map.

### 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.

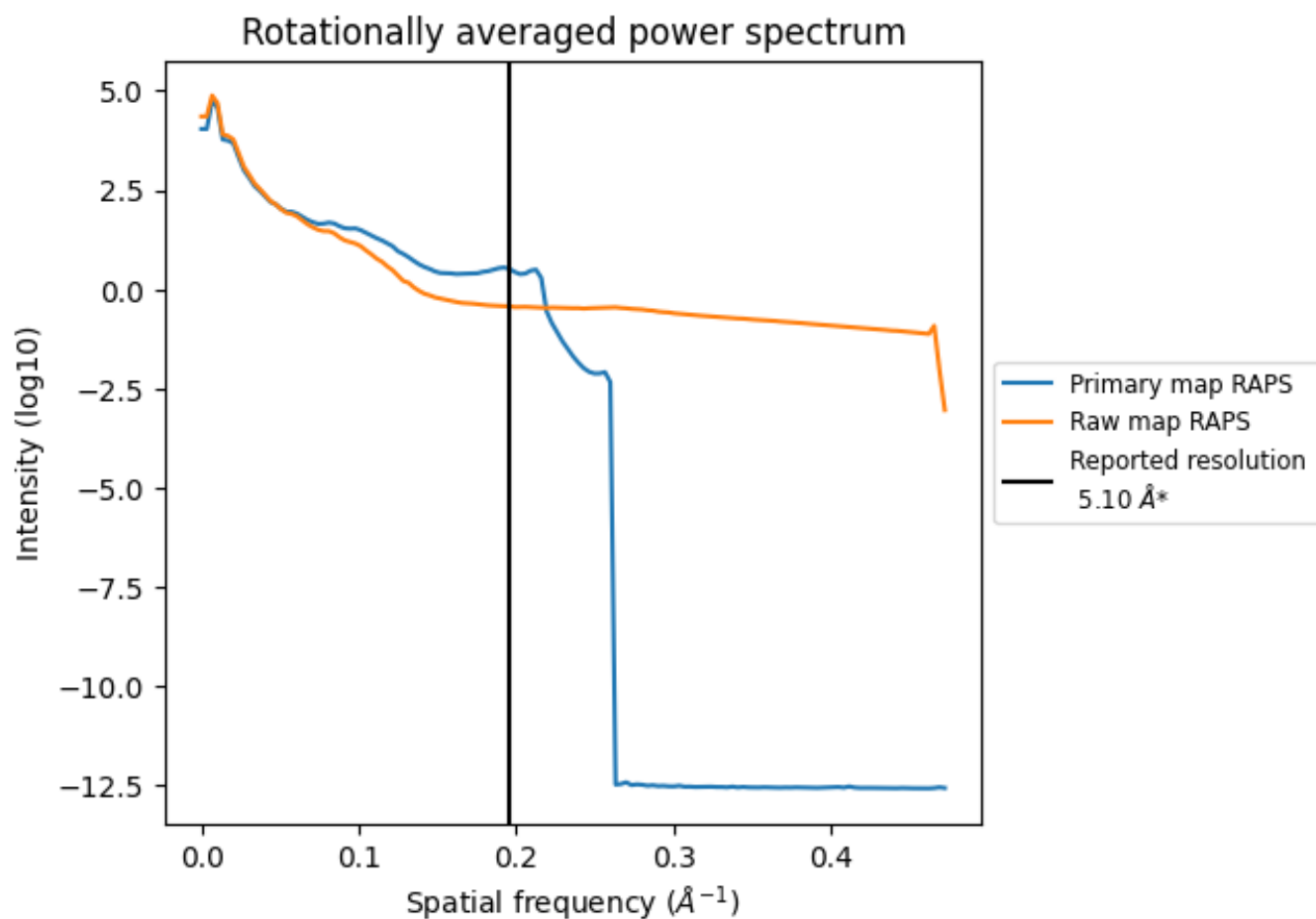
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm<sup>3</sup>; this corresponds to an approximate mass of 140 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](#)

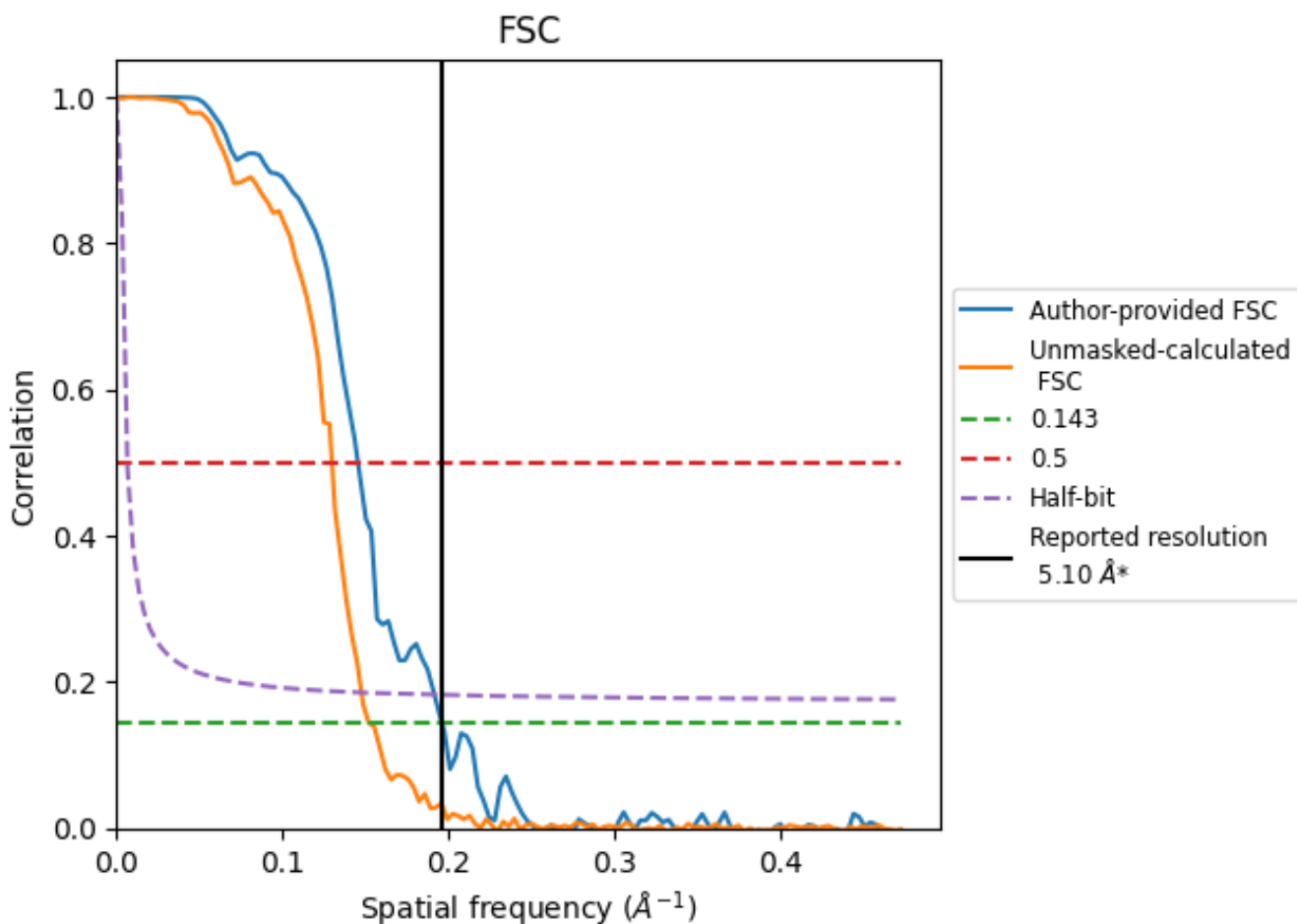


\*Reported resolution corresponds to spatial frequency of 0.196 Å<sup>-1</sup>

## 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  $0.196 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

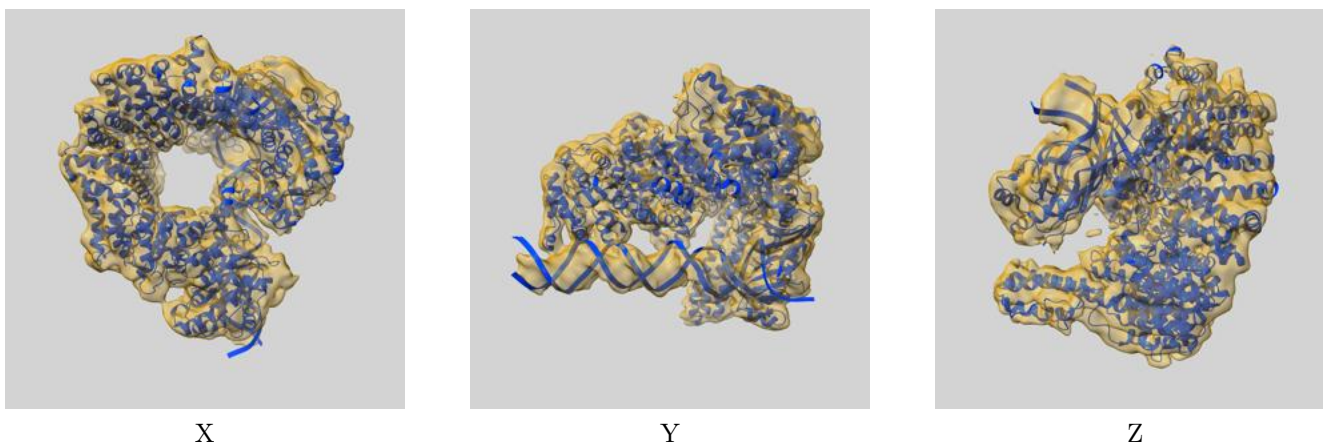
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.10	-	-
Author-provided FSC curve	5.10	6.88	5.22
Unmasked-calculated*	6.57	7.71	6.78

\*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 6.57 differs from the reported value 5.1 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14534 and PDB model 7Z7N. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



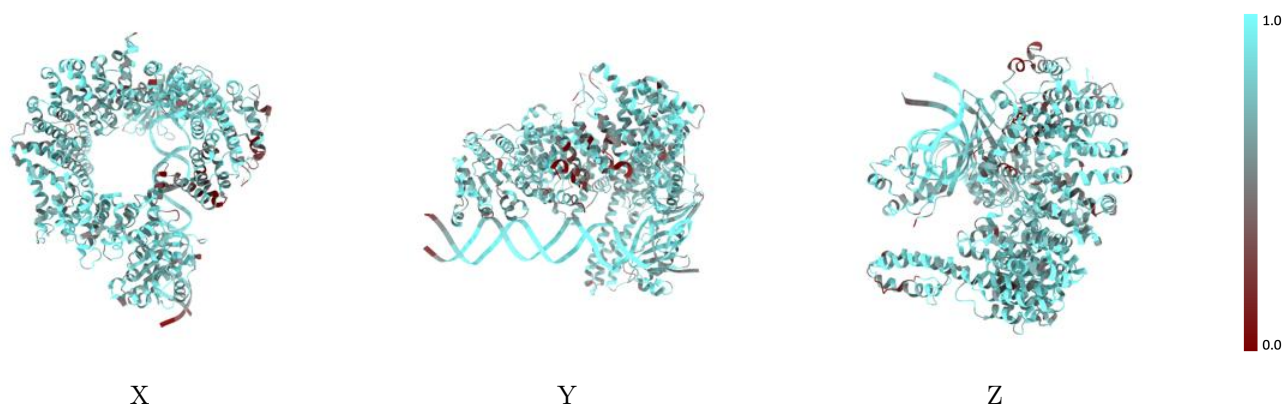
The images above show the 3D surface view of the map at the recommended contour level 0.219 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



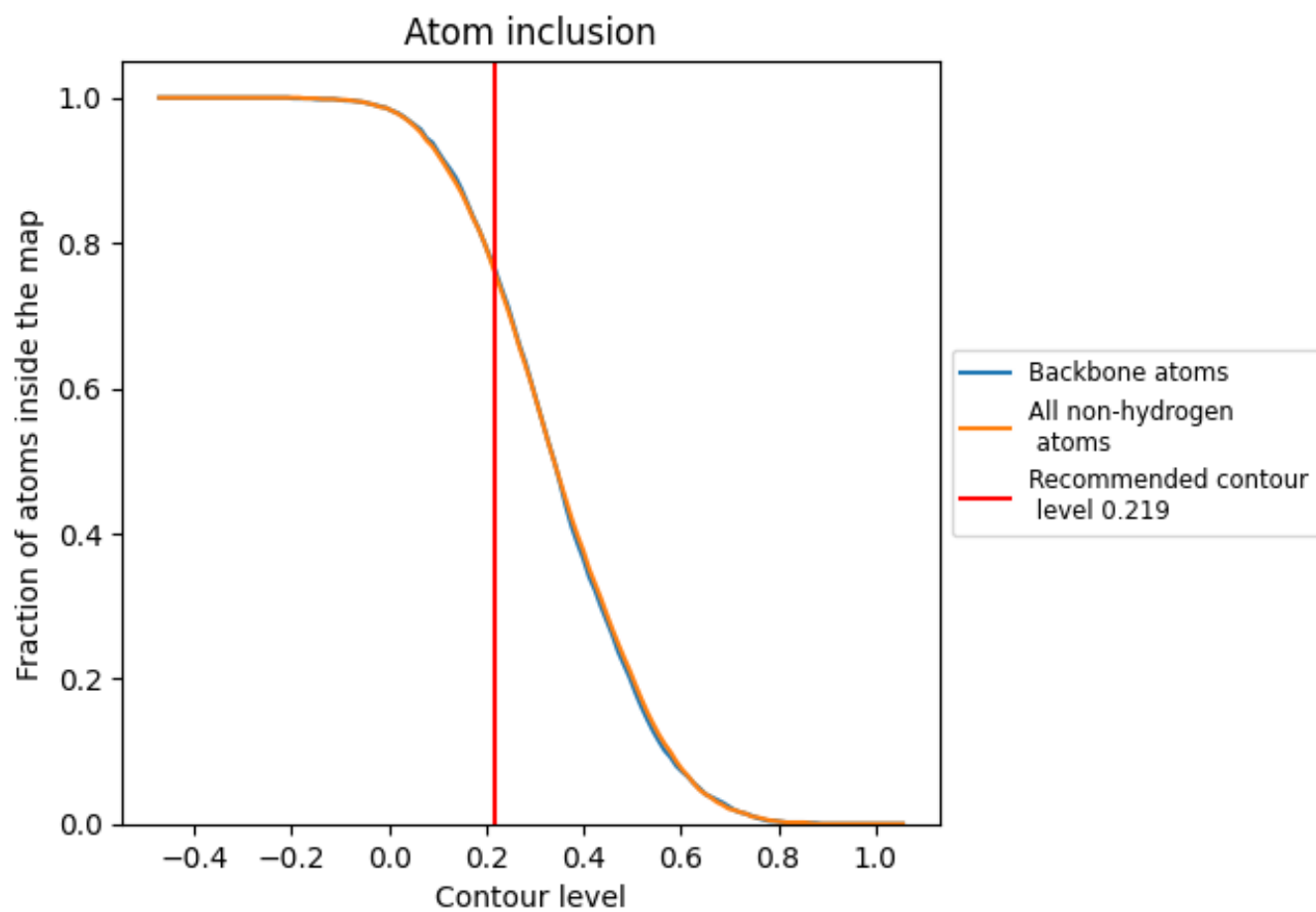
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.219).

## 9.4 Atom inclusion [i](#)













At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.219) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.2420
A	 0.8660	 0.2710
B	 0.8180	 0.2560
D	 0.7630	 0.2440
E	 0.7570	 0.2380

