



Full wwPDB EM Validation Report ⓘ

Jul 27, 2022 – 10:15 pm BST

PDB ID : 7PET
EMDB ID : EMD-13356
Title : The 4x177 nucleosome array containing H1
Authors : Dombrowski, M.; Cramer, P.
Deposited on : 2021-08-11
Resolution : 9.50 Å (reported)
Based on initial model : 7K5Y

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:

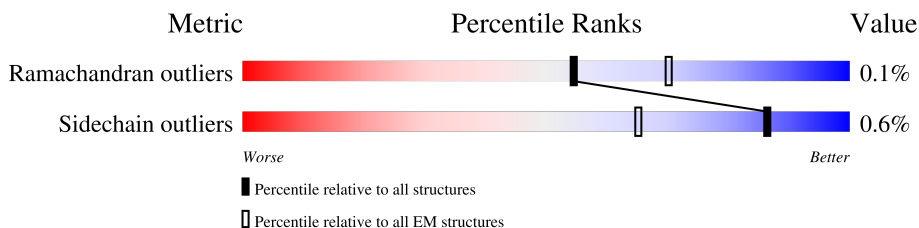
EMDB validation analysis : 0.0.1.dev8
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

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 9.50 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.









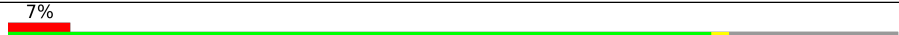
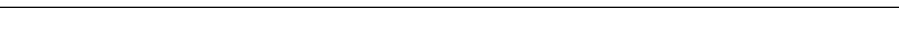
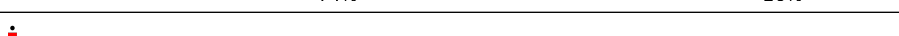
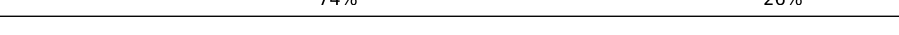
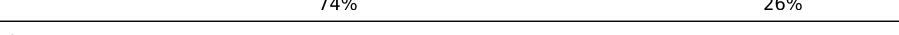
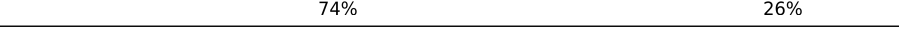













Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	136	68% 29%
1	E	136	71% 29%
1	K	136	71% 29%
1	O	136	71% 29%
1	a	136	71% 29%
1	e	136	71% 29%
1	k	136	5% 29%
1	o	136	5% 29%
2	B	103	79% 19%

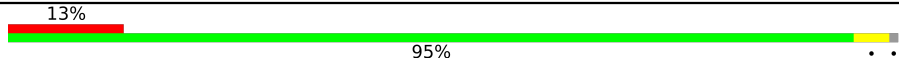
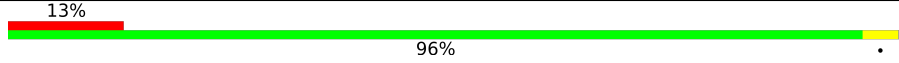
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Mol	Chain	Length	Quality of chain
2	F	103	 80% 19%
2	L	103	 79% 19%
2	P	103	 78% 19%
2	b	103	 80% 19%
2	f	103	 80% 19%
2	l	103	 79% 19%
2	p	103	 79% 19%
3	C	147	 74% 26%
3	G	147	 74% 26%
3	M	147	 74% 26%
3	Q	147	 74% 26%
3	c	147	 73% 26%
3	g	147	 74% 26%
3	m	147	 74% 26%
3	q	147	 74% 26%
4	D	126	 75% 25%
4	H	126	 75% 25%
4	N	126	 75% 25%
4	R	126	 75% 25%
4	d	126	 75% 25%
4	h	126	 75% 25%
4	n	126	 75% 25%
4	r	126	 74% 25%
5	s	218	 34% 66%
5	u	218	 34% 66%

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Mol	Chain	Length	Quality of chain
6	I	702	
7	J	702	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 54040 atoms, of which 0 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	97	798	505	153	138	2	0	0
1	E	97	798	505	153	138	2	0	0
1	a	97	798	505	153	138	2	0	0
1	e	97	798	505	153	138	2	0	0
1	K	97	798	505	153	138	2	0	0
1	O	97	798	505	153	138	2	0	0
1	k	97	798	505	153	138	2	0	0
1	o	97	798	505	153	138	2	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP Q71DI3
E	110	ALA	CYS	engineered mutation	UNP Q71DI3
a	110	ALA	CYS	engineered mutation	UNP Q71DI3
e	110	ALA	CYS	engineered mutation	UNP Q71DI3
K	110	ALA	CYS	engineered mutation	UNP Q71DI3
O	110	ALA	CYS	engineered mutation	UNP Q71DI3
k	110	ALA	CYS	engineered mutation	UNP Q71DI3
o	110	ALA	CYS	engineered mutation	UNP Q71DI3

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	83	662	418	129	114	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	b	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	f	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	L	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	P	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	l	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	p	83	Total	C	N	O	S	0	0
			662	418	129	114	1		

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total	C	N	O	0	0
			840	529	166	145		
3	G	109	Total	C	N	O	0	0
			840	529	166	145		
3	c	109	Total	C	N	O	0	0
			840	529	166	145		
3	g	109	Total	C	N	O	0	0
			840	529	166	145		
3	M	109	Total	C	N	O	0	0
			840	529	166	145		
3	Q	109	Total	C	N	O	0	0
			840	529	166	145		
3	m	109	Total	C	N	O	0	0
			840	529	166	145		
3	q	109	Total	C	N	O	0	0
			840	529	166	145		

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	HIS	-	expression tag	UNP P04908
C	-16	HIS	-	expression tag	UNP P04908
C	-15	HIS	-	expression tag	UNP P04908
C	-14	HIS	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP P04908
C	-12	HIS	-	expression tag	UNP P04908
C	-11	GLU	-	expression tag	UNP P04908
C	-10	ASN	-	expression tag	UNP P04908
C	-9	LEU	-	expression tag	UNP P04908
C	-8	TYR	-	expression tag	UNP P04908
C	-7	PHE	-	expression tag	UNP P04908
C	-6	GLN	-	expression tag	UNP P04908
C	-5	SER	-	expression tag	UNP P04908
C	-4	ASN	-	expression tag	UNP P04908
C	-3	ALA	-	expression tag	UNP P04908
C	-2	PRO	-	expression tag	UNP P04908
C	-1	TRP	-	expression tag	UNP P04908
G	-17	HIS	-	expression tag	UNP P04908
G	-16	HIS	-	expression tag	UNP P04908
G	-15	HIS	-	expression tag	UNP P04908
G	-14	HIS	-	expression tag	UNP P04908
G	-13	HIS	-	expression tag	UNP P04908
G	-12	HIS	-	expression tag	UNP P04908
G	-11	GLU	-	expression tag	UNP P04908
G	-10	ASN	-	expression tag	UNP P04908
G	-9	LEU	-	expression tag	UNP P04908
G	-8	TYR	-	expression tag	UNP P04908
G	-7	PHE	-	expression tag	UNP P04908
G	-6	GLN	-	expression tag	UNP P04908
G	-5	SER	-	expression tag	UNP P04908
G	-4	ASN	-	expression tag	UNP P04908
G	-3	ALA	-	expression tag	UNP P04908
G	-2	PRO	-	expression tag	UNP P04908
G	-1	TRP	-	expression tag	UNP P04908
c	-17	HIS	-	expression tag	UNP P04908
c	-16	HIS	-	expression tag	UNP P04908
c	-15	HIS	-	expression tag	UNP P04908
c	-14	HIS	-	expression tag	UNP P04908
c	-13	HIS	-	expression tag	UNP P04908
c	-12	HIS	-	expression tag	UNP P04908
c	-11	GLU	-	expression tag	UNP P04908
c	-10	ASN	-	expression tag	UNP P04908
c	-9	LEU	-	expression tag	UNP P04908
c	-8	TYR	-	expression tag	UNP P04908
c	-7	PHE	-	expression tag	UNP P04908
c	-6	GLN	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
c	-5	SER	-	expression tag	UNP P04908
c	-4	ASN	-	expression tag	UNP P04908
c	-3	ALA	-	expression tag	UNP P04908
c	-2	PRO	-	expression tag	UNP P04908
c	-1	TRP	-	expression tag	UNP P04908
g	-17	HIS	-	expression tag	UNP P04908
g	-16	HIS	-	expression tag	UNP P04908
g	-15	HIS	-	expression tag	UNP P04908
g	-14	HIS	-	expression tag	UNP P04908
g	-13	HIS	-	expression tag	UNP P04908
g	-12	HIS	-	expression tag	UNP P04908
g	-11	GLU	-	expression tag	UNP P04908
g	-10	ASN	-	expression tag	UNP P04908
g	-9	LEU	-	expression tag	UNP P04908
g	-8	TYR	-	expression tag	UNP P04908
g	-7	PHE	-	expression tag	UNP P04908
g	-6	GLN	-	expression tag	UNP P04908
g	-5	SER	-	expression tag	UNP P04908
g	-4	ASN	-	expression tag	UNP P04908
g	-3	ALA	-	expression tag	UNP P04908
g	-2	PRO	-	expression tag	UNP P04908
g	-1	TRP	-	expression tag	UNP P04908
M	-17	HIS	-	expression tag	UNP P04908
M	-16	HIS	-	expression tag	UNP P04908
M	-15	HIS	-	expression tag	UNP P04908
M	-14	HIS	-	expression tag	UNP P04908
M	-13	HIS	-	expression tag	UNP P04908
M	-12	HIS	-	expression tag	UNP P04908
M	-11	GLU	-	expression tag	UNP P04908
M	-10	ASN	-	expression tag	UNP P04908
M	-9	LEU	-	expression tag	UNP P04908
M	-8	TYR	-	expression tag	UNP P04908
M	-7	PHE	-	expression tag	UNP P04908
M	-6	GLN	-	expression tag	UNP P04908
M	-5	SER	-	expression tag	UNP P04908
M	-4	ASN	-	expression tag	UNP P04908
M	-3	ALA	-	expression tag	UNP P04908
M	-2	PRO	-	expression tag	UNP P04908
M	-1	TRP	-	expression tag	UNP P04908
Q	-17	HIS	-	expression tag	UNP P04908
Q	-16	HIS	-	expression tag	UNP P04908
Q	-15	HIS	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-14	HIS	-	expression tag	UNP P04908
Q	-13	HIS	-	expression tag	UNP P04908
Q	-12	HIS	-	expression tag	UNP P04908
Q	-11	GLU	-	expression tag	UNP P04908
Q	-10	ASN	-	expression tag	UNP P04908
Q	-9	LEU	-	expression tag	UNP P04908
Q	-8	TYR	-	expression tag	UNP P04908
Q	-7	PHE	-	expression tag	UNP P04908
Q	-6	GLN	-	expression tag	UNP P04908
Q	-5	SER	-	expression tag	UNP P04908
Q	-4	ASN	-	expression tag	UNP P04908
Q	-3	ALA	-	expression tag	UNP P04908
Q	-2	PRO	-	expression tag	UNP P04908
Q	-1	TRP	-	expression tag	UNP P04908
m	-17	HIS	-	expression tag	UNP P04908
m	-16	HIS	-	expression tag	UNP P04908
m	-15	HIS	-	expression tag	UNP P04908
m	-14	HIS	-	expression tag	UNP P04908
m	-13	HIS	-	expression tag	UNP P04908
m	-12	HIS	-	expression tag	UNP P04908
m	-11	GLU	-	expression tag	UNP P04908
m	-10	ASN	-	expression tag	UNP P04908
m	-9	LEU	-	expression tag	UNP P04908
m	-8	TYR	-	expression tag	UNP P04908
m	-7	PHE	-	expression tag	UNP P04908
m	-6	GLN	-	expression tag	UNP P04908
m	-5	SER	-	expression tag	UNP P04908
m	-4	ASN	-	expression tag	UNP P04908
m	-3	ALA	-	expression tag	UNP P04908
m	-2	PRO	-	expression tag	UNP P04908
m	-1	TRP	-	expression tag	UNP P04908
q	-17	HIS	-	expression tag	UNP P04908
q	-16	HIS	-	expression tag	UNP P04908
q	-15	HIS	-	expression tag	UNP P04908
q	-14	HIS	-	expression tag	UNP P04908
q	-13	HIS	-	expression tag	UNP P04908
q	-12	HIS	-	expression tag	UNP P04908
q	-11	GLU	-	expression tag	UNP P04908
q	-10	ASN	-	expression tag	UNP P04908
q	-9	LEU	-	expression tag	UNP P04908
q	-8	TYR	-	expression tag	UNP P04908
q	-7	PHE	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
q	-6	GLN	-	expression tag	UNP P04908
q	-5	SER	-	expression tag	UNP P04908
q	-4	ASN	-	expression tag	UNP P04908
q	-3	ALA	-	expression tag	UNP P04908
q	-2	PRO	-	expression tag	UNP P04908
q	-1	TRP	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
4	H	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
4	d	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
4	h	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
4	N	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
4	R	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
4	n	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
4	r	95	Total	C	N	O	S	0	0
			744	467	136	139	2		

- Molecule 5 is a protein called Histone H1.4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	u	75	Total	C	N	O	0	0
			535	336	97	102		
5	s	75	Total	C	N	O	0	0
			535	336	97	102		

- Molecule 6 is a DNA chain called DNA (702-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	698	Total	C	N	O	P	0	0
			14198	6739	2567	4194	698		

- Molecule 7 is a DNA chain called DNA (702-MER).

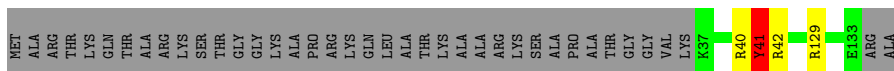
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	J	698	14420	6811	2729	4182	698	0	0

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.

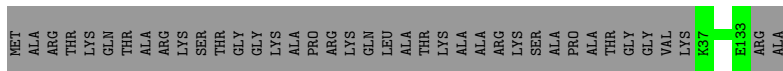
- Molecule 1: Histone H3.2

Chain A:  68% 29%



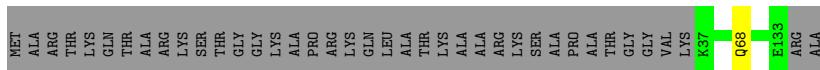
- Molecule 1: Histone H3.2

Chain E:  71% 29%



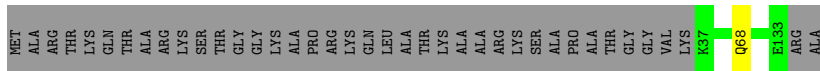
- Molecule 1: Histone H3.2

Chain a:  71% 29%



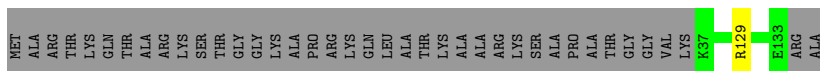
- Molecule 1: Histone H3.2

Chain e:  71% 29%



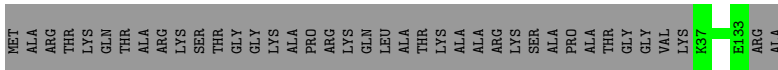
- Molecule 1: Histone H3.2

Chain K:  71% 29%

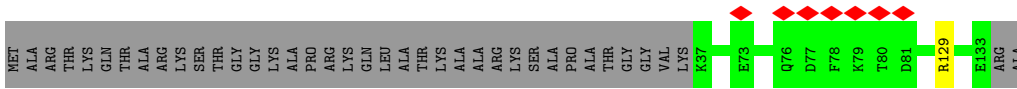


- Molecule 1: Histone H3.2

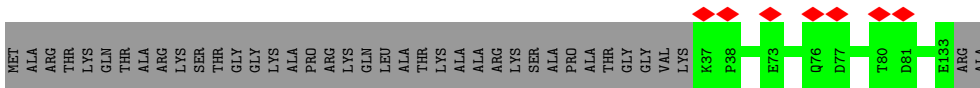
Chain O:  71% 29%



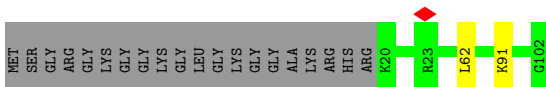
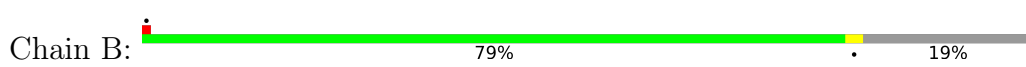
● Molecule 1: Histone H3.2



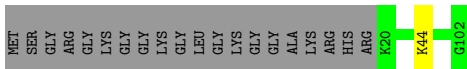
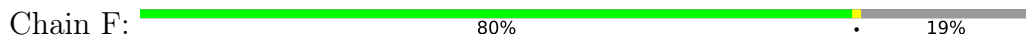
● Molecule 1: Histone H3.2



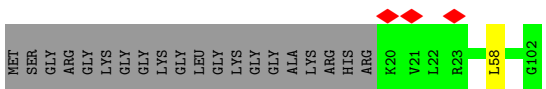
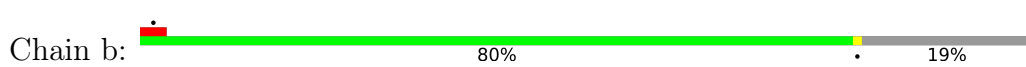
● Molecule 2: Histone H4



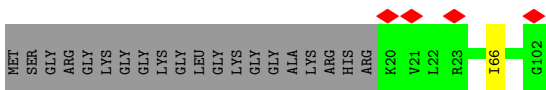
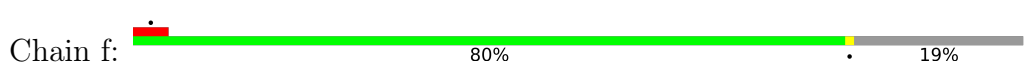
● Molecule 2: Histone H4



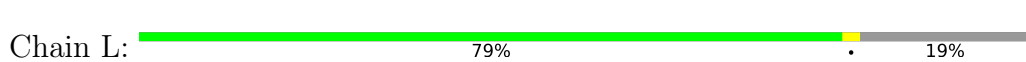
● Molecule 2: Histone H4



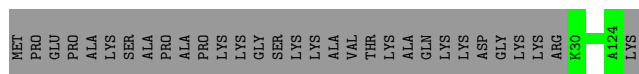
● Molecule 2: Histone H4



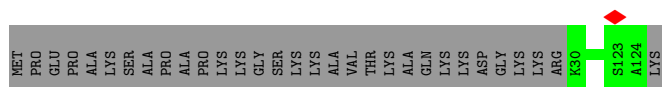
● Molecule 2: Histone H4



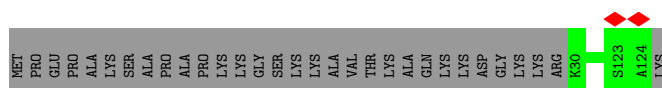
• Molecule 4: Histone H2B type 1-K



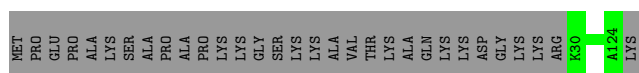
• Molecule 4: Histone H2B type 1-K



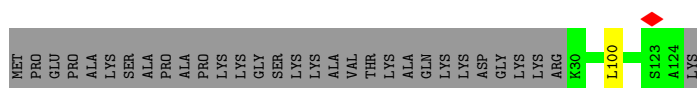
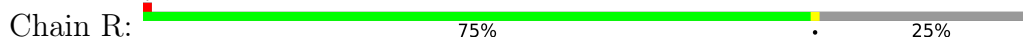
• Molecule 4: Histone H2B type 1-K



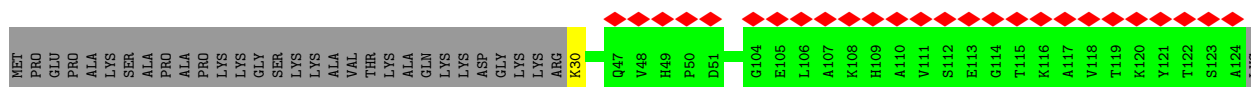
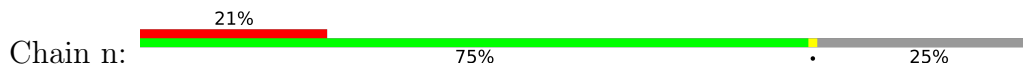
• Molecule 4: Histone H2B type 1-K



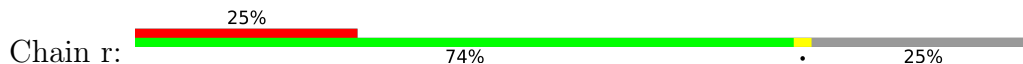
• Molecule 4: Histone H2B type 1-K

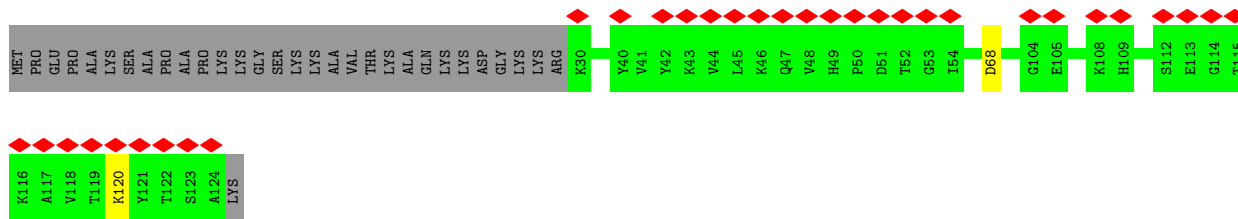


• Molecule 4: Histone H2B type 1-K

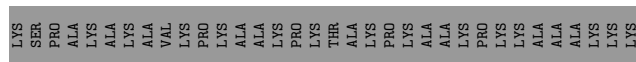
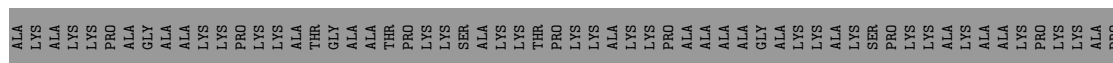
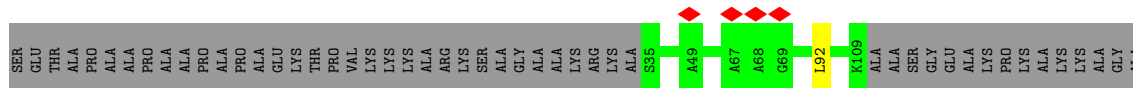


• Molecule 4: Histone H2B type 1-K

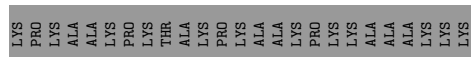
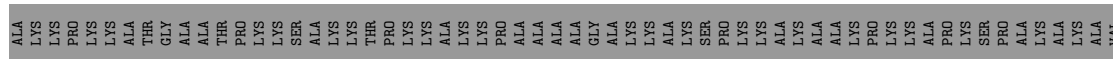
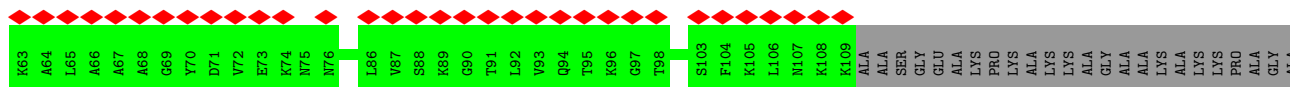
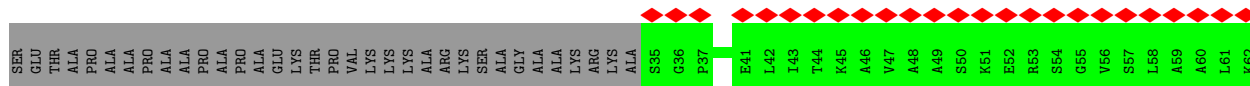




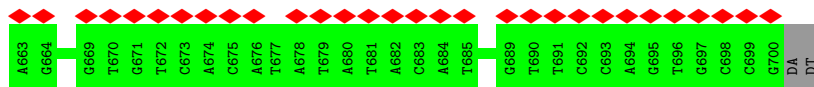
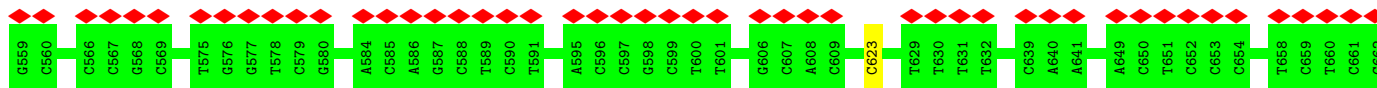
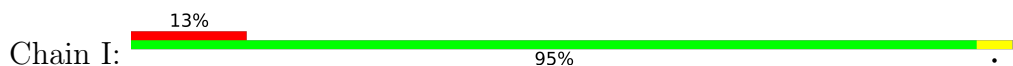
• Molecule 5: Histone H1.4



• Molecule 5: Histone H1.4

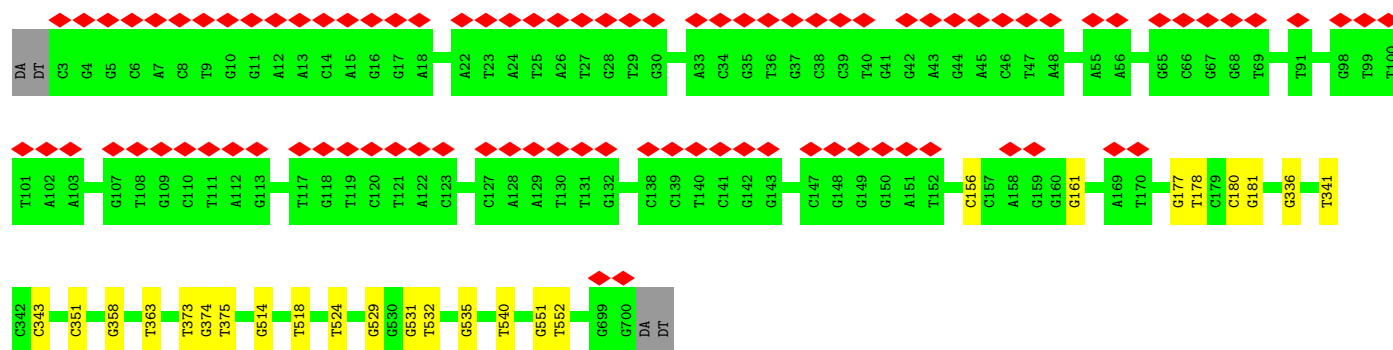


• Molecule 6: DNA (702-MER)



- Molecule 7: DNA (702-MER)

Chain J:  13% 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20621	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0635	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.1, 2.1, 2.1	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	A	0.57	3/810 (0.4%)	0.88	7/1087 (0.6%)
1	E	0.33	0/810	0.69	0/1087
1	K	0.35	0/810	0.65	0/1087
1	O	0.34	0/810	0.65	0/1087
1	a	0.32	0/810	0.70	0/1087
1	e	0.42	0/810	0.77	0/1087
1	k	0.32	0/810	0.60	0/1087
1	o	0.34	0/810	0.63	0/1087
2	B	0.35	0/669	0.73	1/894 (0.1%)
2	F	0.32	0/669	0.66	0/894
2	L	0.34	0/669	0.72	1/894 (0.1%)
2	P	0.34	0/669	0.74	0/894
2	b	0.33	0/669	0.74	1/894 (0.1%)
2	f	0.33	0/669	0.73	1/894 (0.1%)
2	l	0.32	0/669	0.72	1/894 (0.1%)
2	p	0.34	0/669	0.72	0/894
3	C	0.30	0/850	0.62	0/1146
3	G	0.34	0/850	0.64	0/1146
3	M	0.34	0/850	0.67	0/1146
3	Q	0.32	0/850	0.62	0/1146
3	c	0.33	0/850	0.71	1/1146 (0.1%)
3	g	0.35	0/850	0.70	0/1146
3	m	0.30	0/850	0.61	0/1146
3	q	0.33	0/850	0.67	0/1146
4	D	0.41	0/755	0.77	0/1014
4	H	0.34	0/755	0.69	0/1014
4	N	0.39	0/755	0.75	0/1014
4	R	0.34	0/755	0.66	1/1014 (0.1%)
4	d	0.30	0/755	0.67	0/1014
4	h	0.36	0/755	0.67	0/1014
4	n	0.32	0/755	0.67	0/1014
4	r	0.31	0/755	0.65	1/1014 (0.1%)
5	s	0.27	0/538	0.64	0/718
5	u	0.30	0/538	0.70	1/718 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	I	0.91	5/15903 (0.0%)	1.36	36/24514 (0.1%)
7	J	0.89	6/16203 (0.0%)	1.38	33/25036 (0.1%)
All	All	0.71	14/57854 (0.0%)	1.14	85/84114 (0.1%)

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	1
2	l	0	1
3	c	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	373	DT	O3'-P	11.37	1.74	1.61
6	I	546	DG	O3'-P	-9.73	1.49	1.61
7	J	531	DG	O3'-P	9.49	1.72	1.61
6	I	343	DG	O3'-P	8.55	1.71	1.61
7	J	156	DC	O3'-P	7.76	1.70	1.61
1	A	40	ARG	C-N	7.64	1.51	1.34
7	J	177	DG	O3'-P	6.15	1.68	1.61
6	I	161	DC	C3'-O3'	-6.13	1.35	1.44
1	A	41	TYR	N-CA	6.03	1.58	1.46
7	J	532	DT	O3'-P	5.91	1.68	1.61
6	I	157	DT	C3'-O3'	5.78	1.51	1.44
7	J	552	DT	O3'-P	5.73	1.68	1.61
1	A	41	TYR	C-N	5.53	1.46	1.34
6	I	343	DG	C4'-O4'	-5.12	1.40	1.45

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	532	DT	O5'-P-OP2	-18.09	88.99	110.70
7	J	532	DT	O5'-P-OP1	-14.03	93.07	105.70
7	J	535	DG	O4'-C1'-N9	8.52	113.97	108.00
7	J	374	DG	N9-C1'-C2'	8.44	128.63	112.60
6	I	623	DC	O4'-C4'-C3'	-7.94	101.23	106.00
7	J	341	DT	O4'-C1'-N1	7.88	113.51	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	r	68	ASP	CB-CG-OD2	7.73	125.26	118.30
1	A	41	TYR	CB-CG-CD2	7.69	125.62	121.00
6	I	217	DC	O4'-C4'-C3'	-7.53	101.48	106.00
1	A	41	TYR	CA-CB-CG	7.53	127.70	113.40
3	c	72	ASP	CB-CG-OD1	7.46	125.01	118.30
6	I	175	DG	O4'-C1'-N9	7.42	113.20	108.00
6	I	328	DA	C4'-C3'-O3'	7.31	127.97	109.70
6	I	157	DT	O4'-C1'-N1	7.30	113.11	108.00
7	J	529	DG	O4'-C1'-N9	7.29	113.11	108.00
7	J	531	DG	C4'-C3'-O3'	6.96	127.10	109.70
6	I	160	DT	C4'-C3'-O3'	-6.94	92.35	109.70
6	I	343	DG	C1'-O4'-C4'	-6.88	103.22	110.10
7	J	514	DG	O4'-C1'-N9	6.84	112.79	108.00
6	I	343	DG	C4'-C3'-C2'	-6.77	97.01	103.10
6	I	159	DT	C1'-O4'-C4'	-6.76	103.34	110.10
6	I	526	DC	O4'-C1'-N1	6.75	112.72	108.00
6	I	351	DC	O4'-C1'-N1	6.59	112.61	108.00
7	J	161	DG	O4'-C1'-N9	6.58	112.61	108.00
7	J	336	DG	O4'-C1'-N9	6.56	112.59	108.00
7	J	531	DG	C5'-C4'-O4'	-6.53	96.89	109.30
6	I	328	DA	P-O3'-C3'	6.45	127.44	119.70
7	J	178	DT	C1'-O4'-C4'	-6.41	103.69	110.10
7	J	358	DG	O4'-C1'-N9	6.34	112.44	108.00
6	I	160	DT	P-O3'-C3'	6.34	127.30	119.70
7	J	177	DG	O4'-C1'-C2'	-6.31	100.85	105.90
7	J	351	DC	O4'-C1'-N1	6.30	112.41	108.00
7	J	374	DG	C3'-C2'-C1'	-6.18	95.08	102.50
7	J	518	DT	P-O3'-C3'	6.14	127.07	119.70
6	I	161	DC	O4'-C1'-N1	6.13	112.29	108.00
6	I	158	DG	O5'-P-OP1	6.13	118.06	110.70
6	I	175	DG	C1'-O4'-C4'	-6.09	104.01	110.10
1	A	41	TYR	CA-C-O	-6.07	107.35	120.10
7	J	177	DG	N9-C1'-C2'	-6.02	101.16	112.60
7	J	540	DT	O4'-C1'-N1	6.01	112.21	108.00
6	I	112	DG	O4'-C4'-C3'	-5.94	102.12	104.50
6	I	180	DT	O4'-C1'-N1	5.84	112.09	108.00
7	J	518	DT	OP2-P-O3'	5.73	117.80	105.20
7	J	531	DG	N9-C1'-C2'	-5.72	101.74	112.60
6	I	155	DC	O4'-C1'-N1	5.71	112.00	108.00
2	b	58	LEU	CA-CB-CG	5.67	128.33	115.30
6	I	92	DC	O4'-C4'-C3'	-5.66	102.23	104.50
6	I	344	DC	O4'-C1'-N1	5.66	111.96	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	551	DG	C2'-C3'-O3'	-5.64	93.99	112.60
6	I	345	DC	O4'-C1'-N1	5.63	111.94	108.00
7	J	177	DG	C4'-C3'-O3'	5.50	123.44	109.70
7	J	181	DG	O4'-C1'-N9	5.49	111.84	108.00
2	L	62	LEU	CA-CB-CG	5.44	127.81	115.30
2	l	62	LEU	CA-CB-CG	5.43	127.78	115.30
4	R	100	LEU	CA-CB-CG	5.42	127.75	115.30
7	J	374	DG	C1'-O4'-C4'	-5.41	104.69	110.10
6	I	366	DC	O4'-C1'-N1	5.36	111.75	108.00
7	J	343	DC	C1'-O4'-C4'	-5.32	104.78	110.10
6	I	349	DC	O4'-C1'-N1	5.31	111.72	108.00
6	I	157	DT	C1'-O4'-C4'	-5.30	104.80	110.10
6	I	523	DG	O4'-C1'-N9	5.28	111.69	108.00
7	J	375	DT	P-O5'-C5'	5.27	129.33	120.90
5	u	92	LEU	CA-CB-CG	5.25	127.37	115.30
6	I	237	DT	O4'-C4'-C3'	-5.23	102.41	104.50
2	f	66	ILE	CG1-CB-CG2	-5.22	99.91	111.40
6	I	157	DT	C3'-C2'-C1'	-5.22	96.24	102.50
6	I	525	DA	OP2-P-O3'	5.20	116.65	105.20
7	J	531	DG	OP2-P-O3'	5.17	116.57	105.20
7	J	532	DT	OP1-P-OP2	5.17	127.35	119.60
2	B	62	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	41	TYR	CD1-CG-CD2	-5.12	112.27	117.90
7	J	524	DT	O4'-C1'-N1	5.11	111.58	108.00
7	J	177	DG	C1'-O4'-C4'	-5.11	104.99	110.10
6	I	161	DC	O4'-C1'-C2'	-5.10	101.82	105.90
7	J	363	DT	O4'-C1'-N1	5.10	111.57	108.00
6	I	540	DT	O4'-C1'-N1	5.09	111.56	108.00
1	A	40	ARG	C-N-CA	5.08	134.39	121.70
6	I	336	DT	C3'-C2'-C1'	-5.07	96.42	102.50
6	I	183	DG	O4'-C1'-N9	5.04	111.53	108.00
1	A	41	TYR	CG-CD1-CE1	5.02	125.32	121.30
6	I	162	DC	C3'-C2'-C1'	-5.02	96.48	102.50
6	I	343	DG	P-O3'-C3'	5.01	125.72	119.70
7	J	180	DC	O4'-C1'-N1	5.01	111.51	108.00
1	A	41	TYR	CA-C-N	5.01	128.23	117.20
6	I	328	DA	C2'-C3'-O3'	-5.01	96.07	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	TYR	Mainchain
3	c	42	ARG	Sidechain
2	l	92	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	95/136 (70%)	92 (97%)	1 (1%)	2 (2%)	7	36
1	E	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
1	K	95/136 (70%)	95 (100%)	0	0	100	100
1	O	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
1	a	95/136 (70%)	95 (100%)	0	0	100	100
1	e	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
1	k	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
1	o	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
2	B	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
2	F	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
2	L	81/103 (79%)	78 (96%)	3 (4%)	0	100	100
2	P	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
2	b	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
2	f	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
2	l	81/103 (79%)	78 (96%)	3 (4%)	0	100	100
2	p	81/103 (79%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	107/147 (73%)	105 (98%)	2 (2%)	0	100	100
3	G	107/147 (73%)	106 (99%)	1 (1%)	0	100	100
3	M	107/147 (73%)	104 (97%)	3 (3%)	0	100	100
3	Q	107/147 (73%)	105 (98%)	2 (2%)	0	100	100
3	c	107/147 (73%)	103 (96%)	4 (4%)	0	100	100
3	g	107/147 (73%)	103 (96%)	4 (4%)	0	100	100
3	m	107/147 (73%)	106 (99%)	1 (1%)	0	100	100
3	q	107/147 (73%)	104 (97%)	3 (3%)	0	100	100
4	D	93/126 (74%)	93 (100%)	0	0	100	100
4	H	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
4	N	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
4	R	93/126 (74%)	93 (100%)	0	0	100	100
4	d	93/126 (74%)	93 (100%)	0	0	100	100
4	h	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
4	n	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
4	r	93/126 (74%)	93 (100%)	0	0	100	100
5	s	73/218 (34%)	71 (97%)	2 (3%)	0	100	100
5	u	73/218 (34%)	72 (99%)	1 (1%)	0	100	100
All	All	3154/4532 (70%)	3103 (98%)	49 (2%)	2 (0%)	54	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	TYR
1	A	42	ARG

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	84/110 (76%)	83 (99%)	1 (1%)	71	83
1	E	84/110 (76%)	84 (100%)	0	100	100
1	K	84/110 (76%)	83 (99%)	1 (1%)	71	83
1	O	84/110 (76%)	84 (100%)	0	100	100
1	a	84/110 (76%)	83 (99%)	1 (1%)	71	83
1	e	84/110 (76%)	83 (99%)	1 (1%)	71	83
1	k	84/110 (76%)	83 (99%)	1 (1%)	71	83
1	o	84/110 (76%)	84 (100%)	0	100	100
2	B	68/79 (86%)	67 (98%)	1 (2%)	65	80
2	F	68/79 (86%)	67 (98%)	1 (2%)	65	80
2	L	68/79 (86%)	67 (98%)	1 (2%)	65	80
2	P	68/79 (86%)	65 (96%)	3 (4%)	28	53
2	b	68/79 (86%)	68 (100%)	0	100	100
2	f	68/79 (86%)	68 (100%)	0	100	100
2	l	68/79 (86%)	67 (98%)	1 (2%)	65	80
2	p	68/79 (86%)	66 (97%)	2 (3%)	42	64
3	C	85/116 (73%)	85 (100%)	0	100	100
3	G	85/116 (73%)	85 (100%)	0	100	100
3	M	85/116 (73%)	85 (100%)	0	100	100
3	Q	85/116 (73%)	85 (100%)	0	100	100
3	c	85/116 (73%)	85 (100%)	0	100	100
3	g	85/116 (73%)	85 (100%)	0	100	100
3	m	85/116 (73%)	85 (100%)	0	100	100
3	q	85/116 (73%)	85 (100%)	0	100	100
4	D	81/105 (77%)	81 (100%)	0	100	100
4	H	81/105 (77%)	81 (100%)	0	100	100
4	N	81/105 (77%)	81 (100%)	0	100	100
4	R	81/105 (77%)	81 (100%)	0	100	100
4	d	81/105 (77%)	81 (100%)	0	100	100
4	h	81/105 (77%)	81 (100%)	0	100	100
4	n	81/105 (77%)	80 (99%)	1 (1%)	71	83
4	r	81/105 (77%)	80 (99%)	1 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	s	57/145 (39%)	57 (100%)	0	100	100
5	u	57/145 (39%)	57 (100%)	0	100	100
All	All	2658/3570 (74%)	2642 (99%)	16 (1%)	86	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
2	B	91	LYS
2	F	44	LYS
1	a	68	GLN
1	e	68	GLN
1	K	129	ARG
2	L	44	LYS
2	P	23	ARG
2	P	67	ARG
2	P	91	LYS
1	k	129	ARG
2	l	92	ARG
4	n	30	LYS
2	p	23	ARG
2	p	92	ARG
4	r	120	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	93	GLN
1	a	55	GLN
1	a	93	GLN
1	e	39	HIS
1	e	93	GLN
4	h	84	ASN
1	O	55	GLN
3	m	84	GLN
1	o	108	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13356. These allow visual inspection of the internal detail of the map and identification of artifacts.

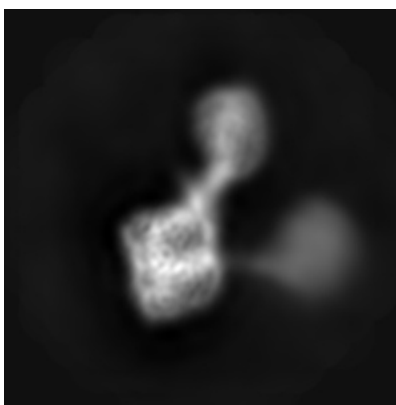
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

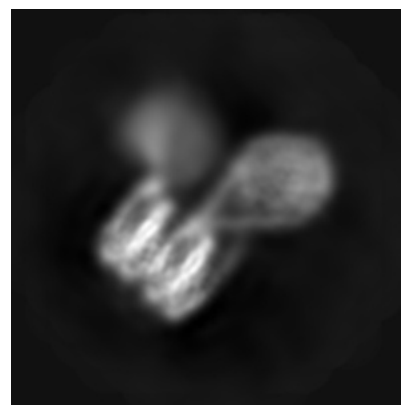
6.1.1 Primary map



X



Y

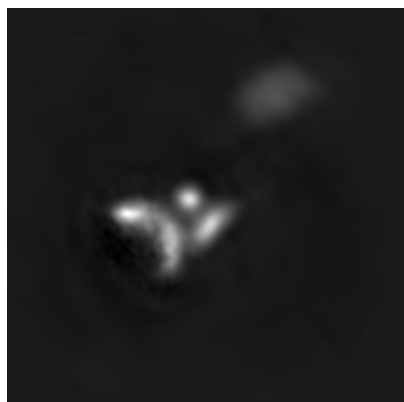


Z

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

6.2 Central slices [i](#)

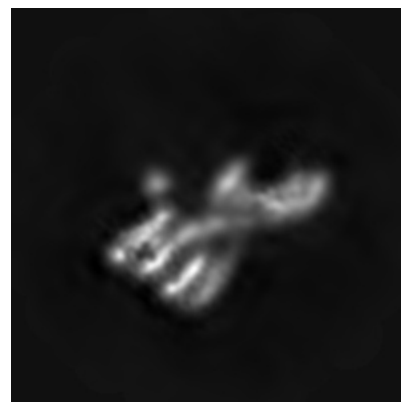
6.2.1 Primary map



X Index: 100



Y Index: 100

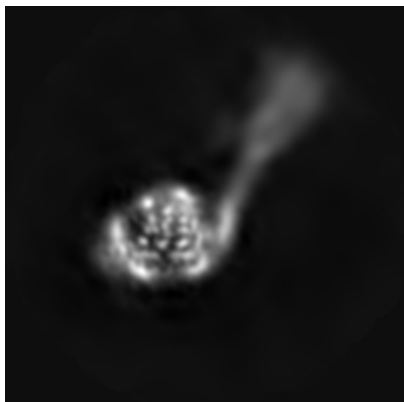


Z Index: 100

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: 71



Y Index: 92



Z Index: 102

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

6.4 Orthogonal surface views [i](#)

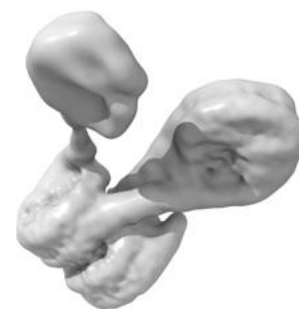
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0635. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

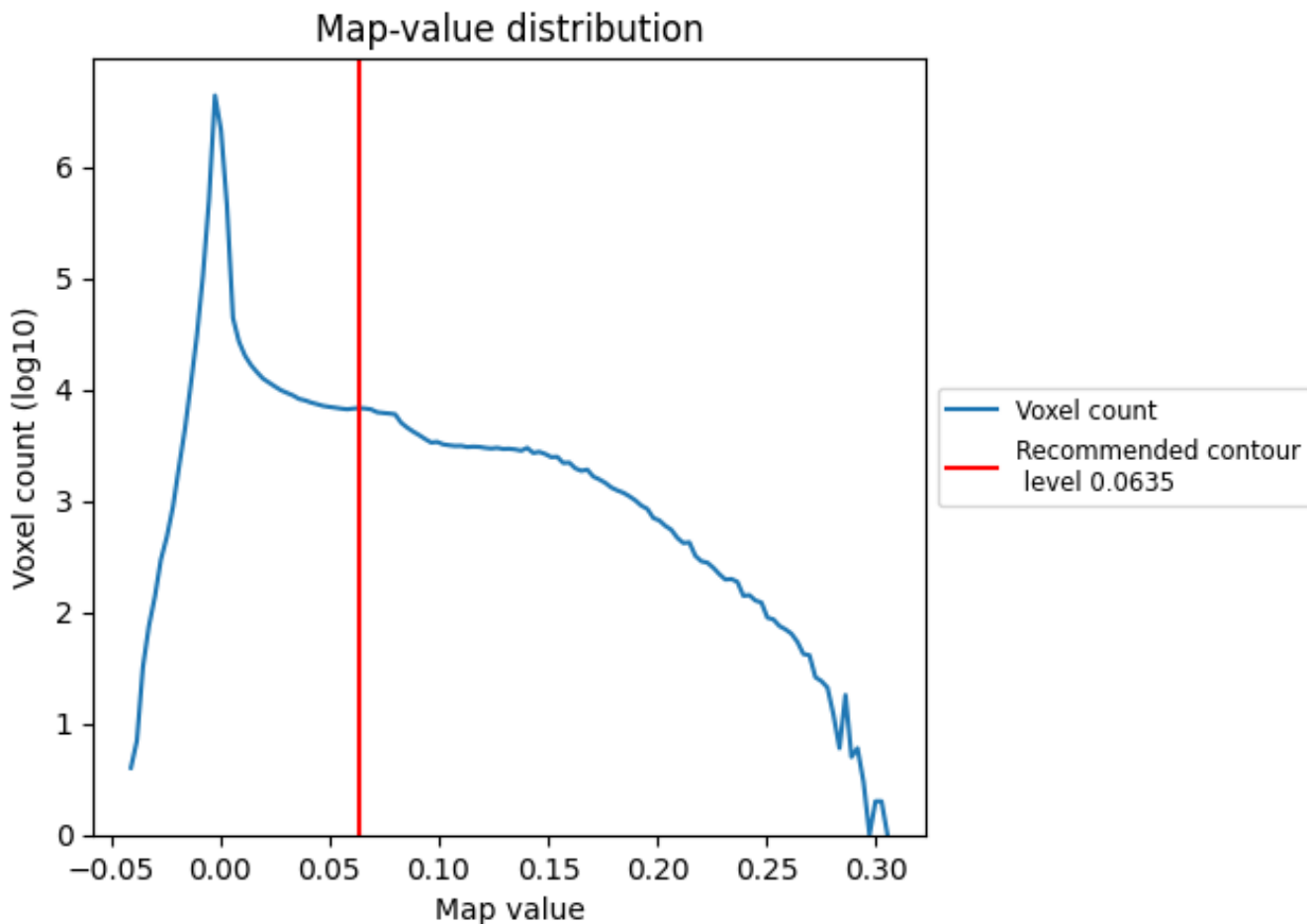
6.5 Mask visualisation

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

7 Map analysis [i](#)

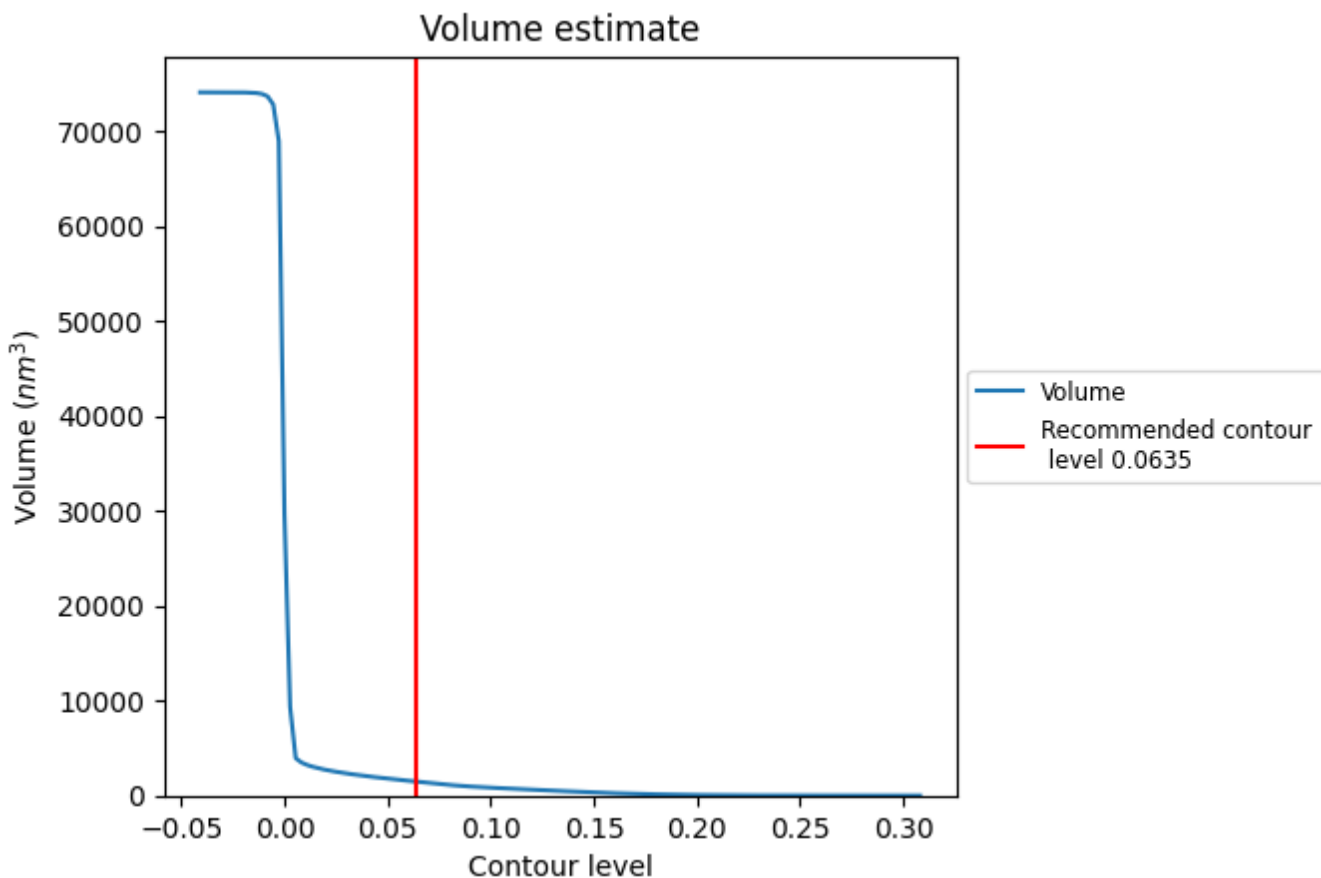
This section contains the results of statistical analysis of the map.

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.

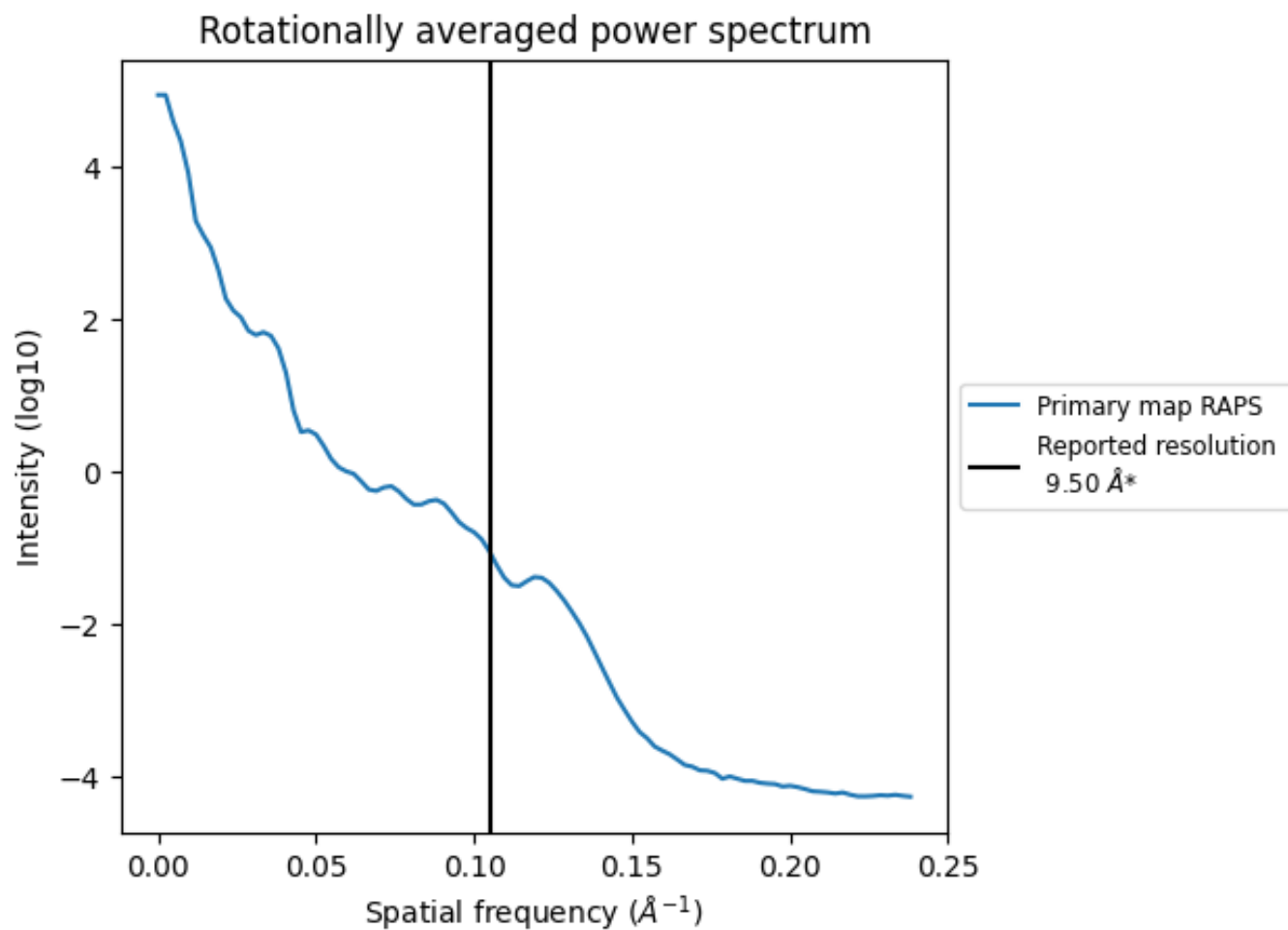
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1482 nm^3 ; this corresponds to an approximate mass of 1339 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](#)

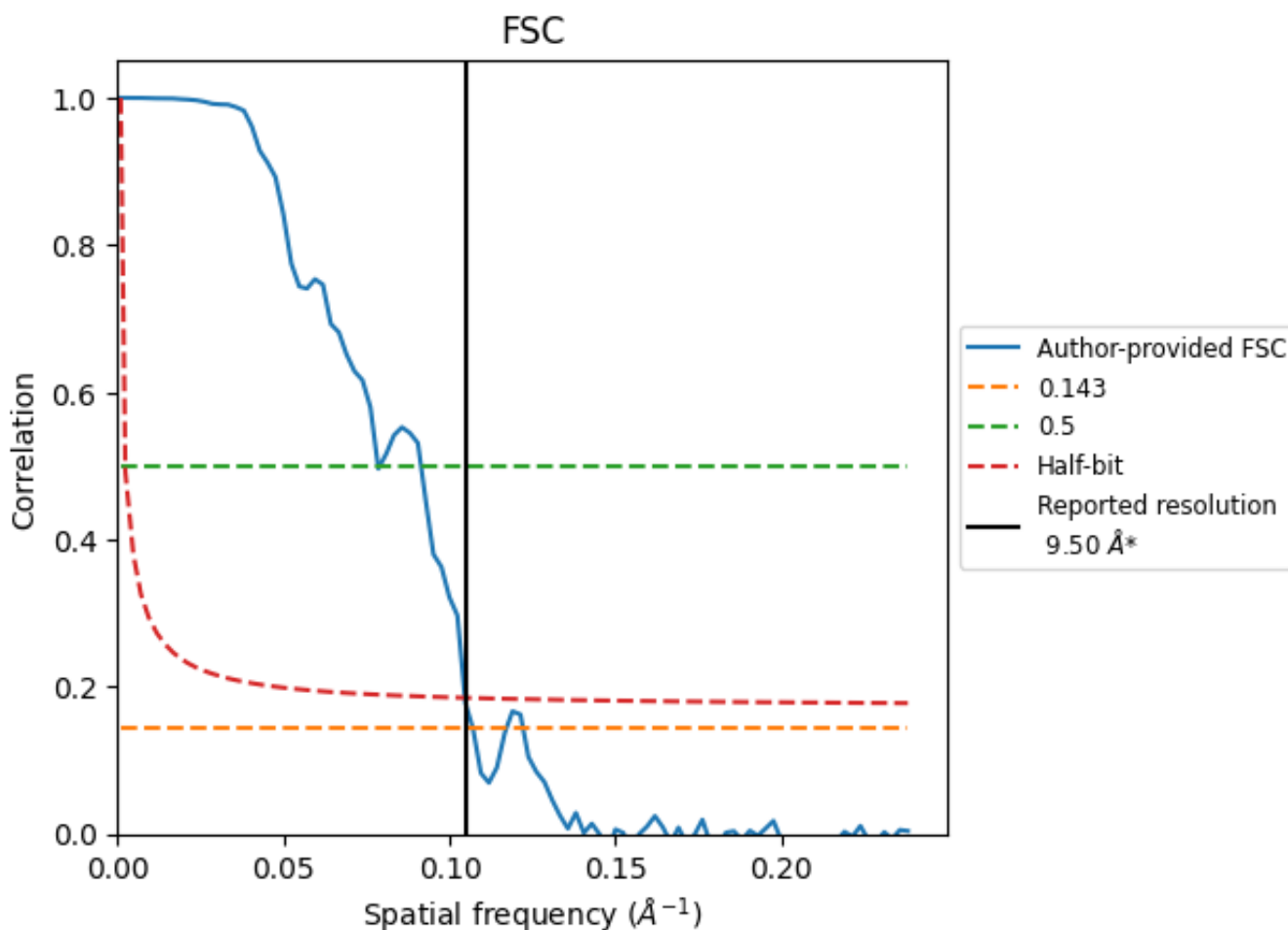


*Reported resolution corresponds to spatial frequency of 0.105 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.105 Å⁻¹

8.2 Resolution estimates [i](#)

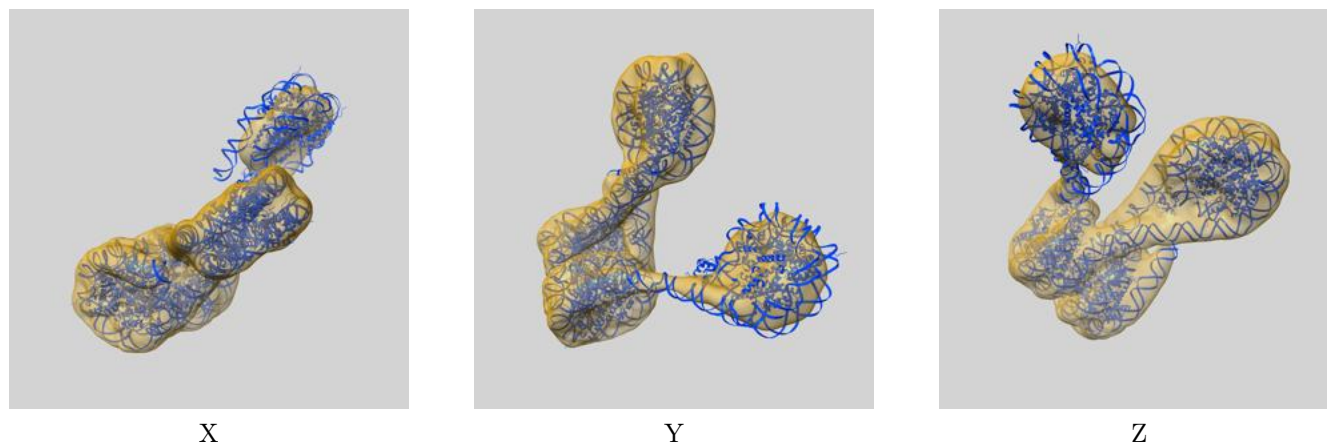
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.50	-	-
Author-provided FSC curve	9.34	12.74	9.56
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

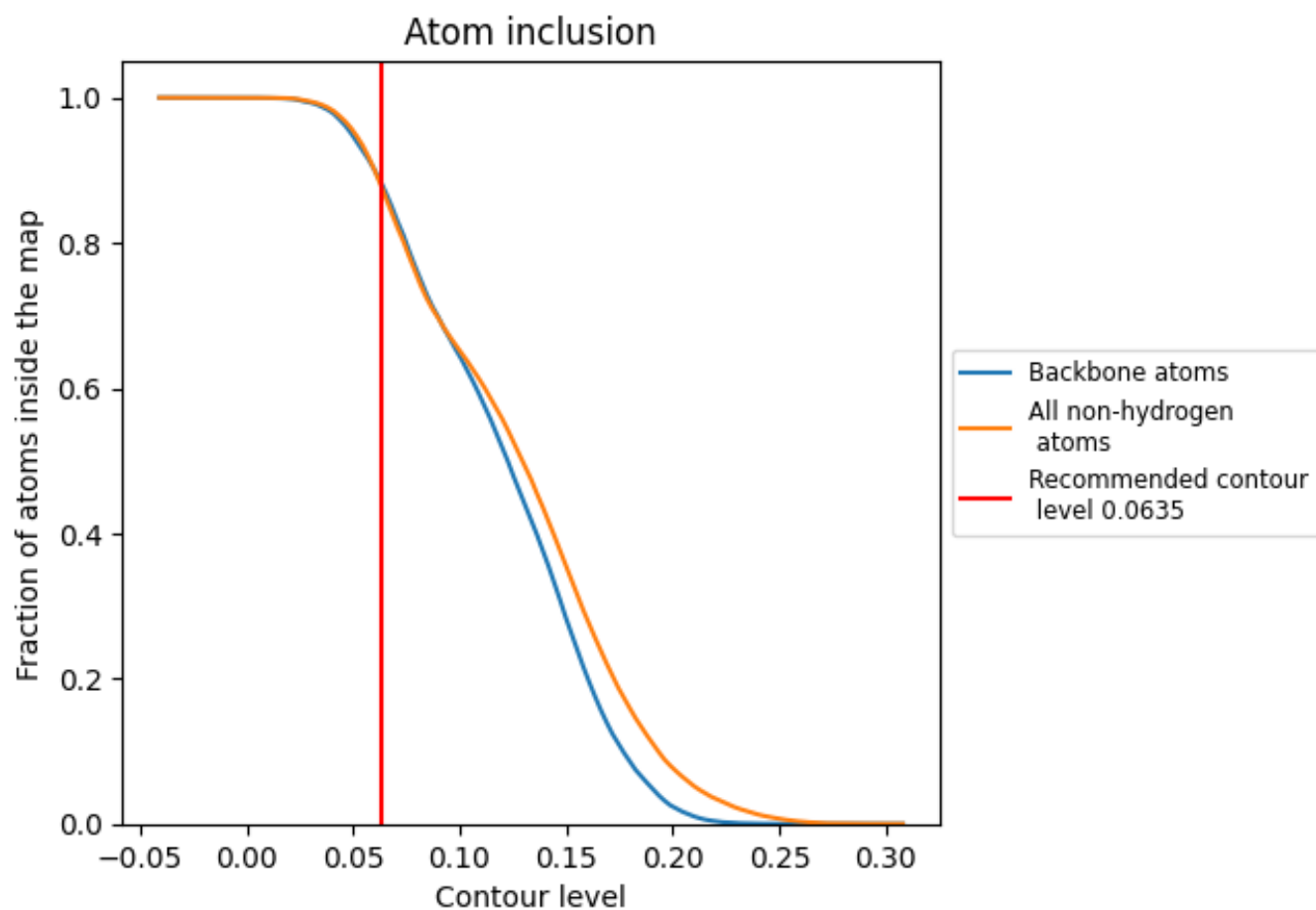
This section contains information regarding the fit between EMDB map EMD-13356 and PDB model 7PET. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0635 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 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.