



## Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 11:46 AM JST

PDB ID : 9J8O  
EMDB ID : EMD-61233  
Title : Cryo-EM structure of BAF-Lamin A/C IgF-H1-nucleosome complex  
Authors : Horikoshi, N.; Miyake, R.; Sogawa-Fujiwara, C.; Ogasawara, M.; Takizawa, Y.; Kurumizaka, H.  
Deposited on : 2024-08-21  
Resolution : 4.05 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.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

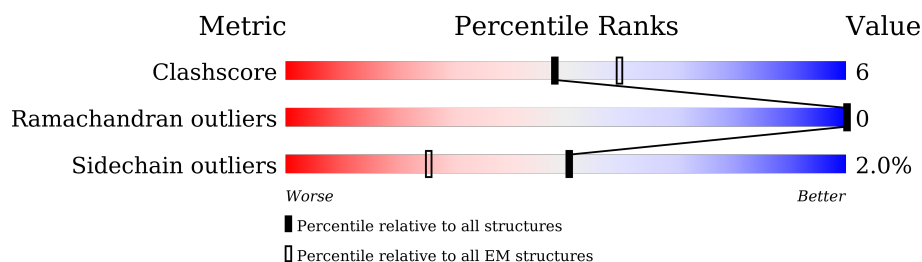
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.05 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.





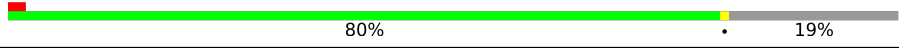



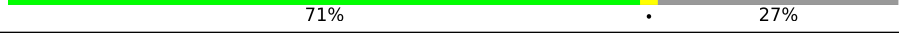
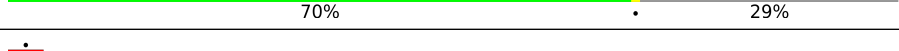
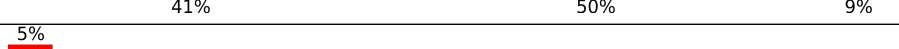
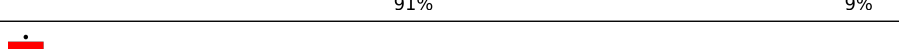
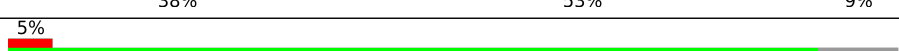
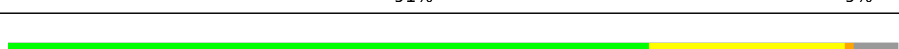

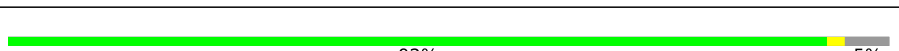
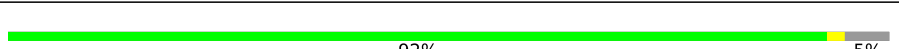





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	139	
1	E	139	
1	a	139	
1	e	139	
2	B	106	
2	F	106	
2	b	106	
2	f	106	

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Mol	Chain	Length	Quality of chain
3	C	133	
3	G	133	
3	c	133	
3	g	133	
4	D	129	
4	H	129	
4	d	129	
4	h	129	
5	I	193	
5	i	193	
6	J	193	
6	j	193	
7	K	93	
7	L	93	
7	k	93	
7	l	93	
8	M	158	
8	m	158	
9	N	221	
9	n	221	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 32116 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 H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	96	Total	C	N	O	S	0	0
			790	499	151	136	4		
1	E	98	Total	C	N	O	S	0	0
			810	511	157	138	4		
1	a	96	Total	C	N	O	S	0	0
			790	499	151	136	4		
1	e	98	Total	C	N	O	S	0	0
			810	511	157	138	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431
a	-3	GLY	-	expression tag	UNP P68431
a	-2	SER	-	expression tag	UNP P68431
a	-1	HIS	-	expression tag	UNP P68431
e	-3	GLY	-	expression tag	UNP P68431
e	-2	SER	-	expression tag	UNP P68431
e	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	78	Total	C	N	O	S	0	0
			619	391	120	107	1		
2	F	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	b	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

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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		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	108	Total	C	N	O	0	0
			835	526	165	144		
3	G	104	Total	C	N	O	0	0
			805	508	157	140		
3	c	108	Total	C	N	O	0	0
			835	526	165	144		
3	g	104	Total	C	N	O	0	0
			805	508	157	140		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			736	462	134	138	2		
4	H	91	Total	C	N	O	S	0	0
			708	447	125	134	2		
4	d	94	Total	C	N	O	S	0	0
			736	462	134	138	2		
4	h	91	Total	C	N	O	S	0	0
			708	447	125	134	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899
d	-3	GLY	-	expression tag	UNP P06899
d	-2	SER	-	expression tag	UNP P06899
d	-1	HIS	-	expression tag	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (193-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	176	Total	C	N	O	P	0	0
			3591	1704	654	1057	176		
5	i	176	Total	C	N	O	P	0	0
			3591	1704	654	1057	176		

- Molecule 6 is a DNA chain called DNA (193-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	176	Total	C	N	O	P	0	0
			3625	1715	679	1055	176		
6	j	176	Total	C	N	O	P	0	0
			3625	1715	679	1055	176		

- Molecule 7 is a protein called Barrier-to-autointegration factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	88	Total	C	N	O	S	0	0
			697	442	120	130	5		
7	L	88	Total	C	N	O	S	0	0
			697	442	120	130	5		
7	k	88	Total	C	N	O	S	0	0
			697	442	120	130	5		
7	l	88	Total	C	N	O	S	0	0
			697	442	120	130	5		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	GLY	-	expression tag	UNP O75531
K	-2	SER	-	expression tag	UNP O75531
K	-1	HIS	-	expression tag	UNP O75531
K	0	MET	-	expression tag	UNP O75531
L	-3	GLY	-	expression tag	UNP O75531
L	-2	SER	-	expression tag	UNP O75531
L	-1	HIS	-	expression tag	UNP O75531
L	0	MET	-	expression tag	UNP O75531
k	-3	GLY	-	expression tag	UNP O75531
k	-2	SER	-	expression tag	UNP O75531
k	-1	HIS	-	expression tag	UNP O75531
k	0	MET	-	expression tag	UNP O75531
l	-3	GLY	-	expression tag	UNP O75531
l	-2	SER	-	expression tag	UNP O75531
l	-1	HIS	-	expression tag	UNP O75531
l	0	MET	-	expression tag	UNP O75531

- Molecule 8 is a protein called Lamin-A/C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	119	Total	C	N	O	S	0	0
			928	575	174	176	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	119	Total	C	N	O	S	0	0
			928	575	174	176	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	409	SER	-	expression tag	UNP P02545
M	410	HIS	-	expression tag	UNP P02545
m	409	SER	-	expression tag	UNP P02545
m	410	HIS	-	expression tag	UNP P02545

- Molecule 9 is a protein called Histone H1.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	78	Total	C	N	O	0	0
			555	345	100	110		
9	n	78	Total	C	N	O	0	0
			555	345	100	110		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	216	LEU	-	expression tag	UNP Q02539
N	217	GLU	-	expression tag	UNP Q02539
N	218	VAL	-	expression tag	UNP Q02539
N	219	LEU	-	expression tag	UNP Q02539
N	220	PHE	-	expression tag	UNP Q02539
N	221	GLN	-	expression tag	UNP Q02539
n	216	LEU	-	expression tag	UNP Q02539
n	217	GLU	-	expression tag	UNP Q02539
n	218	VAL	-	expression tag	UNP Q02539
n	219	LEU	-	expression tag	UNP Q02539
n	220	PHE	-	expression tag	UNP Q02539
n	221	GLN	-	expression tag	UNP Q02539

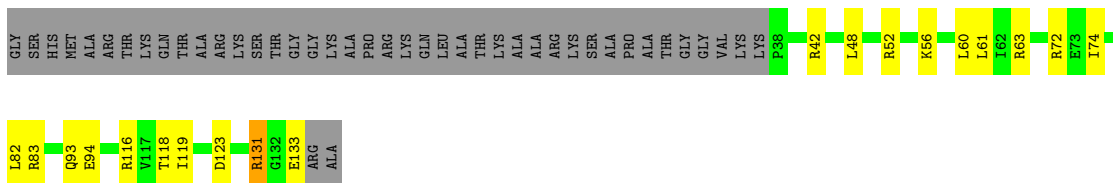


### 3 Residue-property plots [i](#)

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.

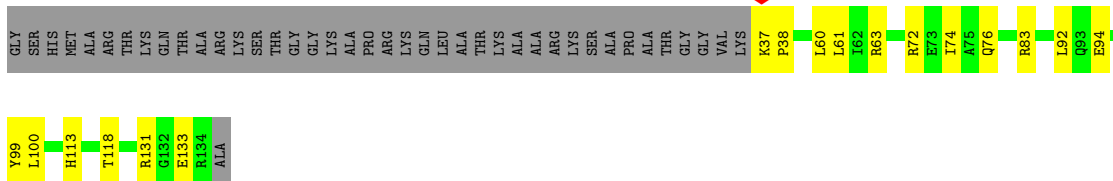
#### • Molecule 1: Histone H3.1

Chain A: 



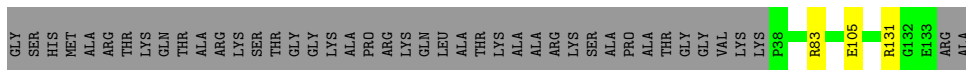
#### • Molecule 1: Histone H3.1

Chain E: 



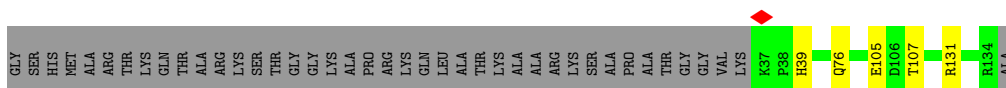
#### • Molecule 1: Histone H3.1

Chain a: 



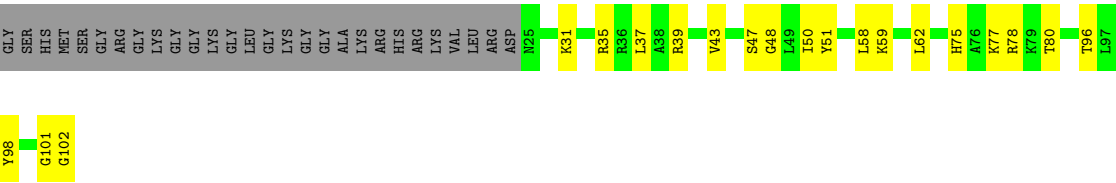
#### • Molecule 1: Histone H3.1

Chain e: 

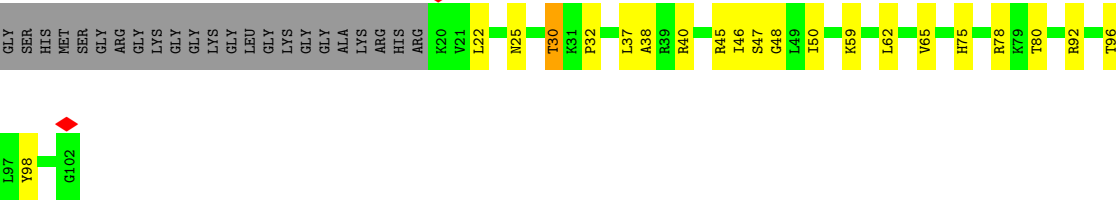


#### • Molecule 2: Histone H4

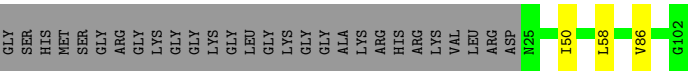
Chain B: 



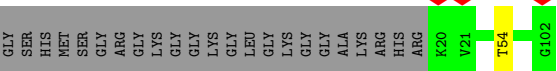
• Molecule 2: Histone H4



• Molecule 2: Histone H4



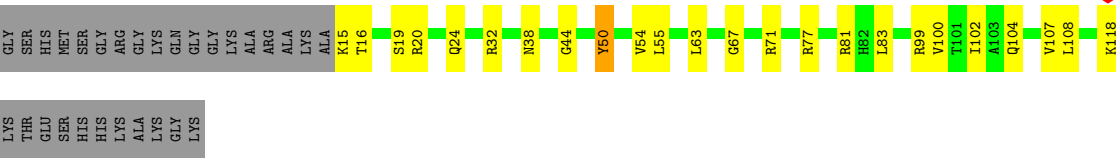
• Molecule 2: Histone H4



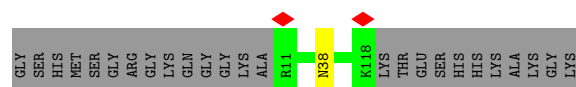
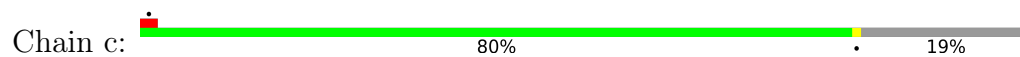
• Molecule 3: Histone H2A type 1-B/E



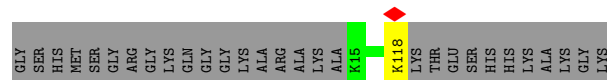
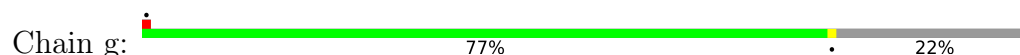
• Molecule 3: Histone H2A type 1-B/E



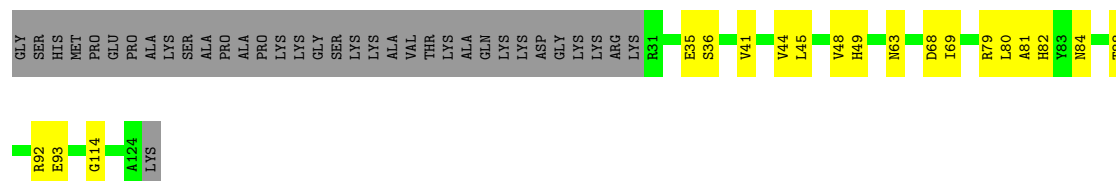
• Molecule 3: Histone H2A type 1-B/E



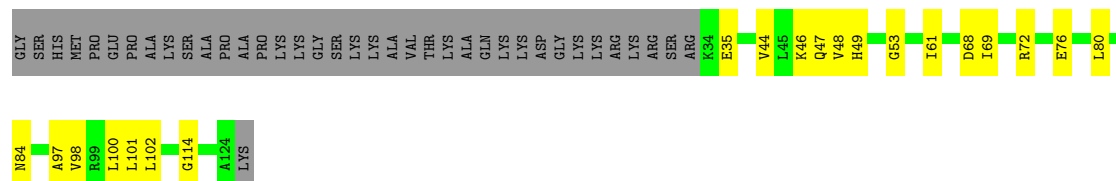
- Molecule 3: Histone H2A type 1-B/E



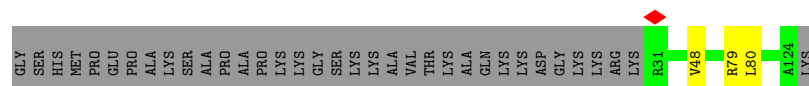
- Molecule 4: Histone H2B type 1-J



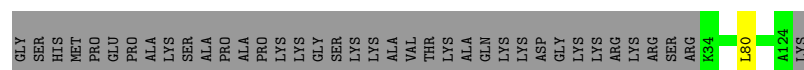
- Molecule 4: Histone H2B type 1-J



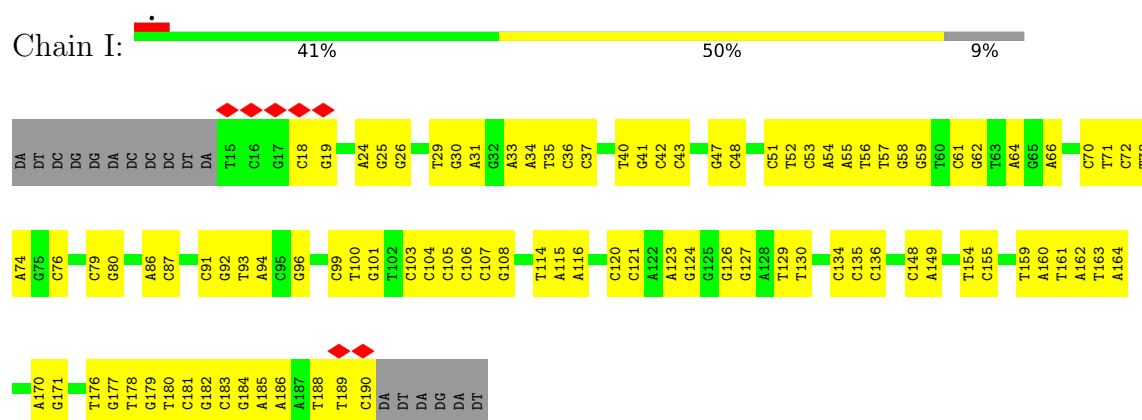
- Molecule 4: Histone H2B type 1-J



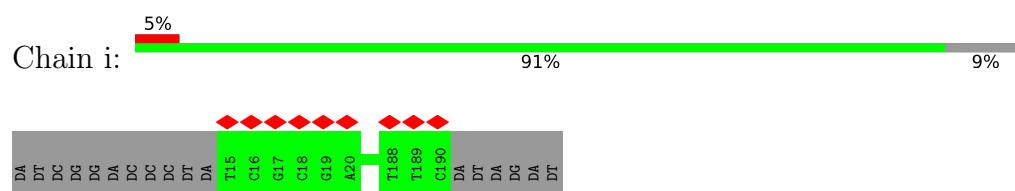
- Molecule 4: Histone H2B type 1-J



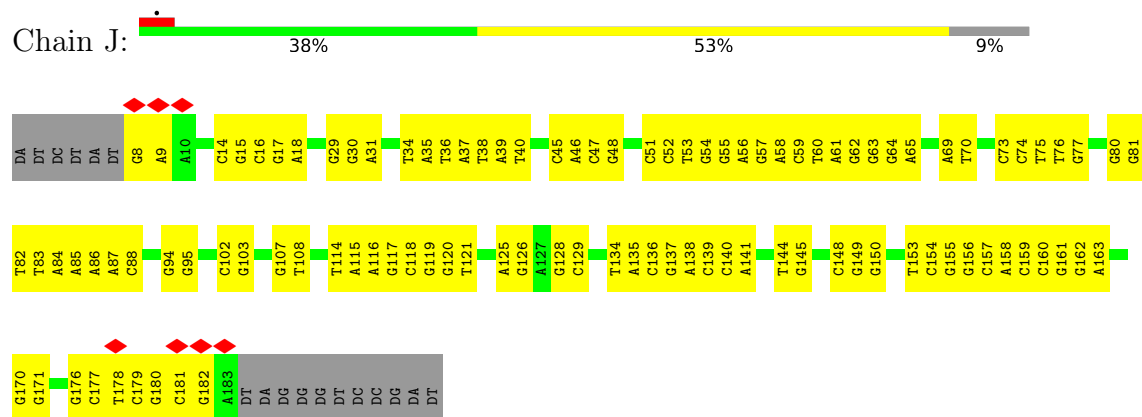
- Molecule 5: DNA (193-MER)



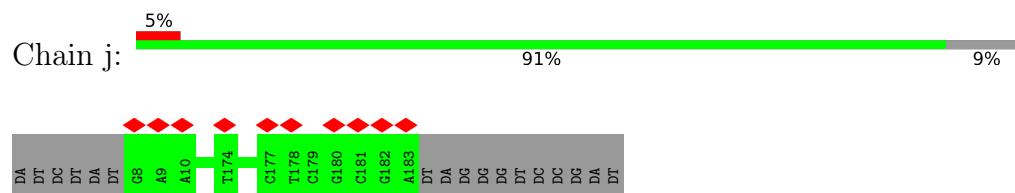
- Molecule 5: DNA (193-MER)



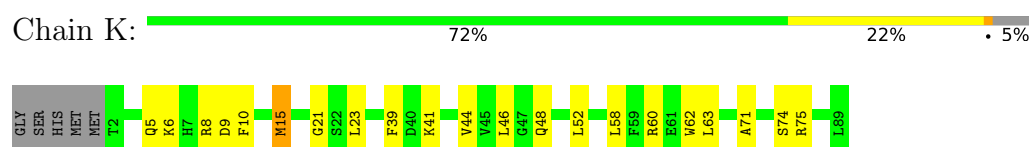
- Molecule 6: DNA (193-MER)



- Molecule 6: DNA (193-MER)



- Molecule 7: Barrier-to-autointegration factor



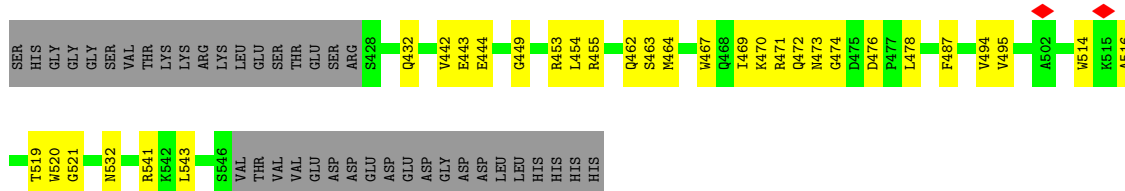
- Molecule 7: Barrier-to-autointegration factor

GLY	SER	HIS	MET	MET	T2	T3	S4	Q5	K6	H7	R8	D9	M15	V20	L23	L30	G31	K32	E35	E36	R37	F49	K54	F59	L63	T66	C67	S74	C77	C80	L81	L89
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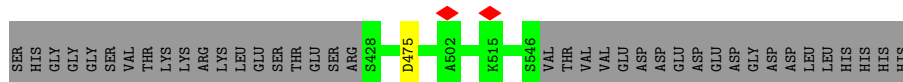
- GLY  
SER  
HIS  
MET  
MET  
T2  
R75  
C80  
L89

- GLY  
SER  
HIS  
MET  
MET  
T2  
M15  
C80  
L89

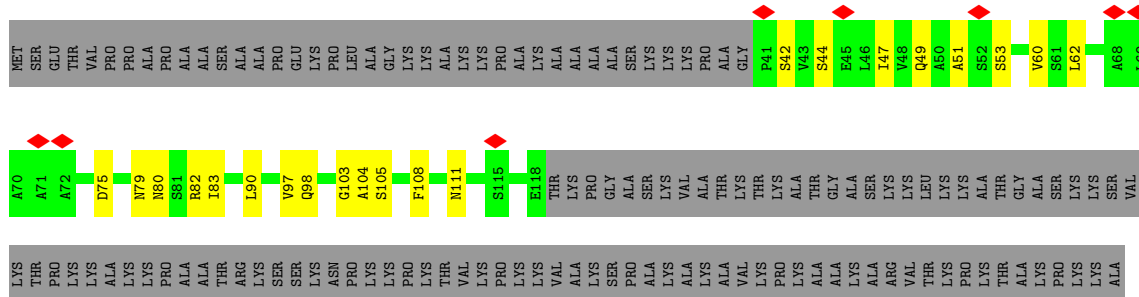
- Chain M:  56% 20% 25%



- Chain m: 



- Chain N:  26% 10% 65%



ALA  
PRO  
LYS  
LYS  
LYS  
LEU  
GLU  
VAL  
LEU  
PHE  
GLN

● Molecule 9: Histone H1.1



MET  
SER  
GLU  
THR  
VAL  
PRO  
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ALA  
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ALA  
GLY  
P41  
S42  
E45  
Q49  
S62  
S63  
S64  
K55  
E56  
R57  
A64  
A68  
L69  
A70  
A71

A72  
V76  
E77  
K78  
L110  
N111  
K112  
K113  
A114  
S115  
S116  
V117  
E118  
THR  
LYS  
PRO  
GLY  
ALA  
SER  
LYS  
VAL  
ALA  
THR  
LYS  
THR  
LYS  
ALA  
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LEU  
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THR  
GLY  
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SER  
VAL  
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THR  
PRO  
LYS  
LYS  
ALA  
ALA  
THR  
ARG

LYS  
SER  
SER  
LYS  
ASN  
PRO  
LYS  
LYS  
PRO  
LYS  
LYS  
THR  
VAL  
LYS  
PRO  
LYS  
LYS  
VAL  
ALA  
LYS  
SER  
PRO  
GLN

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152402	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 ( $e^-/\text{\AA}^2$ )	59.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00667	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.46	0/802	0.59	0/1076
1	E	0.44	0/822	0.59	0/1102
1	a	0.42	0/802	0.58	0/1076
1	e	0.42	0/822	0.58	0/1102
2	B	0.55	0/626	0.60	0/837
2	F	0.53	0/669	0.61	0/894
2	b	0.53	0/626	0.61	0/837
2	f	0.50	0/669	0.63	0/894
3	C	0.43	0/845	0.59	0/1139
3	G	0.42	0/815	0.59	0/1100
3	c	0.44	0/845	0.60	0/1139
3	g	0.39	0/815	0.59	0/1100
4	D	0.49	0/747	0.55	0/1004
4	H	0.48	0/719	0.52	0/968
4	d	0.50	0/747	0.54	0/1004
4	h	0.45	0/719	0.52	0/968
5	I	0.69	0/4024	0.93	0/6204
5	i	0.68	0/4024	0.92	0/6204
6	J	0.70	0/4070	0.91	0/6284
6	j	0.70	0/4070	0.91	0/6284
7	K	0.28	0/710	0.46	0/949
7	L	0.27	0/710	0.46	0/949
7	k	0.29	0/710	0.47	0/949
7	l	0.26	0/710	0.45	0/949
8	M	0.26	0/947	0.50	0/1281
8	m	0.25	0/947	0.51	0/1281
9	N	0.26	0/557	0.44	0/742
9	n	0.24	0/557	0.42	0/742
All	All	0.56	0/34126	0.76	0/49058

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Too-close contacts

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	790	0	826	15	0
1	E	810	0	851	15	0
1	a	790	0	826	0	0
1	e	810	0	851	0	0
2	B	619	0	659	18	0
2	F	662	0	709	20	0
2	b	619	0	659	0	0
2	f	662	0	709	0	0
3	C	835	0	897	19	0
3	G	805	0	861	21	0
3	c	835	0	897	0	0
3	g	805	0	861	0	0
4	D	736	0	758	18	0
4	H	708	0	727	18	0
4	d	736	0	758	0	0
4	h	708	0	727	0	0
5	I	3591	0	1975	84	0
5	i	3591	0	1975	0	0
6	J	3625	0	1974	98	0
6	j	3625	0	1974	0	0
7	K	697	0	688	15	0
7	L	697	0	688	12	0
7	k	697	0	688	0	0
7	l	697	0	688	0	0
8	M	928	0	911	18	0
8	m	928	0	911	0	0
9	N	555	0	600	14	0
9	n	555	0	600	0	0
All	All	32116	0	26248	330	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 6.

All (330) 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)
6:J:120:DG:H2'	6:J:121:DT:H71	1.83	0.81
6:J:119:DG:H2'	6:J:120:DG:H8	1.53	0.76
5:I:72:DC:H2''	5:I:73:DT:H71	1.93	0.72
6:J:119:DG:H2'	6:J:120:DG:C8	2.36	0.70
8:M:473:ASN:ND2	8:M:520:TRP:O	2.55	0.70
3:C:20:ARG:NH2	6:J:57:DG:OP1	3.43	0.69
4:D:36:SER:HB2	4:D:63:ASN:HD21	1.57	0.69
7:K:5:GLN:OE1	7:K:8:ARG:NH1	2.25	0.68
3:C:16:THR:O	3:C:19:SER:OG	2.23	0.68
8:M:462:GLN:NE2	8:M:463:SER:O	2.28	0.67
3:C:32:ARG:NH2	4:D:35:GLU:OE1	2.50	0.66
8:M:472:GLN:NE2	8:M:474:GLY:O	2.56	0.65
7:K:6:LYS:NZ	7:K:23:LEU:O	2.45	0.65
4:D:68:ASP:OD2	2:F:98:TYR:OH	2.16	0.64
5:I:42:DC:H2''	5:I:43:DC:C5	2.48	0.63
5:I:100:DT:OP1	9:N:80:ASN:ND2	2.32	0.63
7:L:5:GLN:NE2	7:L:9:ASP:OD1	2.32	0.62
6:J:118:DC:H2''	6:J:119:DG:H8	1.80	0.62
2:B:98:TYR:OH	4:H:68:ASP:OD2	2.13	0.62
7:L:6:LYS:NZ	7:L:23:LEU:O	2.39	0.61
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.21	0.61
4:H:98:VAL:HG13	4:H:102:LEU:HD22	1.82	0.61
1:A:61:LEU:HD12	2:B:37:LEU:HD23	1.84	0.60
2:F:22:LEU:HB3	2:F:25:ASN:HD21	1.66	0.60
5:I:161:DT:H2'	5:I:162:DA:C8	2.36	0.60
3:C:100:VAL:HG22	2:F:96:THR:HB	2.28	0.60
6:J:102:DC:H2''	6:J:103:DG:C8	2.50	0.60
5:I:62:DG:O6	6:J:135:DA:N6	2.83	0.59
5:I:178:DT:H2''	5:I:179:DG:H8	1.82	0.59
9:N:79:ASN:OD1	9:N:82:ARG:NH1	2.34	0.59
9:N:62:LEU:HD12	9:N:105:SER:HA	1.84	0.59
1:A:116:ARG:NH1	1:A:118:THR:O	2.35	0.59
1:E:63:ARG:HD2	6:J:116:DA:H4'	1.85	0.58
5:I:73:DT:H2''	5:I:74:DA:C8	2.40	0.58
8:M:470:LYS:HB3	8:M:478:LEU:HD11	2.15	0.58
3:C:77:ARG:NH2	6:J:45:DC:H4'	2.18	0.58
4:D:81:ALA:HB2	4:D:93:GLU:HG2	2.52	0.58
6:J:179:DC:OP2	9:N:42:SER:OG	3.34	0.58
1:A:94:GLU:OE2	3:G:104:GLN:NE2	2.90	0.58
5:I:30:DG:H2''	5:I:31:DA:C8	2.53	0.58
8:M:449:GLY:HA2	8:M:520:TRP:HB2	2.05	0.58
6:J:170:DG:H2''	6:J:171:DG:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:47:ILE:HD11	9:N:83:ILE:HG23	2.83	0.57
3:G:16:THR:O	3:G:19:SER:OG	2.32	0.57
7:L:3:THR:O	7:L:8:ARG:NH2	2.64	0.57
1:A:42:ARG:NH2	6:J:94:DG:OP1	2.38	0.56
5:I:148:DC:H2''	5:I:149:DA:C8	2.40	0.56
2:F:75:HIS:CD2	4:H:84:ASN:HD21	2.23	0.56
5:I:180:DT:H2''	5:I:181:DC:C5	2.51	0.56
2:B:35:ARG:NH2	2:B:51:TYR:OH	2.39	0.56
8:M:472:GLN:NE2	8:M:476:ASP:O	2.31	0.55
6:J:81:DG:H5'	6:J:81:DG:C8	2.72	0.55
6:J:54:DG:H2''	6:J:55:DG:C8	2.42	0.55
5:I:134:DC:H2''	5:I:135:DC:C5	2.46	0.55
6:J:119:DG:H2''	6:J:120:DG:O5'	2.07	0.55
5:I:115:DA:H1'	5:I:116:DA:N7	2.24	0.55
2:F:47:SER:OG	2:F:48:GLY:N	2.44	0.55
6:J:39:DA:C8	6:J:40:DT:H72	4.19	0.55
1:A:48:LEU:HB3	1:A:52:ARG:HH12	3.00	0.54
5:I:33:DA:H2''	5:I:34:DA:C8	2.43	0.54
6:J:148:DC:H2''	6:J:149:DG:C8	2.59	0.54
5:I:129:DT:H2'	5:I:130:DT:H71	3.66	0.54
2:B:47:SER:OG	2:B:48:GLY:N	2.41	0.54
1:E:74:ILE:HD11	2:F:59:LYS:HD2	1.90	0.54
5:I:34:DA:H1'	5:I:35:DT:H5'	2.41	0.54
1:A:74:ILE:HD11	2:B:59:LYS:HD2	1.90	0.53
5:I:93:DT:H2''	5:I:94:DA:N7	2.23	0.53
6:J:16:DC:H2''	6:J:17:DG:C8	2.43	0.53
6:J:160:DC:H2''	6:J:161:DG:H8	1.74	0.53
5:I:170:DA:H2''	5:I:171:DG:H8	1.95	0.53
6:J:140:DC:N3	6:J:141:DA:N6	2.57	0.53
2:B:75:HIS:CD2	4:D:84:ASN:HD21	2.56	0.53
3:G:67:GLY:HA3	4:H:49:HIS:CD2	2.52	0.53
6:J:53:DT:H2''	6:J:54:DG:C8	2.57	0.53
7:K:10:PHE:HZ	7:K:15:MET:HE3	1.73	0.53
5:I:105:DC:H1'	5:I:106:DC:C5	2.47	0.52
8:M:449:GLY:O	8:M:519:THR:OG1	2.24	0.52
2:B:96:THR:HB	3:G:100:VAL:HG22	2.10	0.52
5:I:160:DA:H2'	5:I:161:DT:H71	3.62	0.52
6:J:136:DC:H2''	6:J:137:DG:C8	2.49	0.52
6:J:134:DT:H2''	6:J:135:DA:C8	2.45	0.52
7:K:52:LEU:HD13	7:K:58:LEU:HB3	1.92	0.52
4:D:36:SER:HB2	4:D:63:ASN:ND2	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:45:DC:H2''	6:J:46:DA:H8	1.90	0.52
5:I:86:DA:H1'	5:I:87:DC:H5'	1.92	0.52
1:A:119:ILE:HD13	2:B:43:VAL:HG11	1.97	0.51
6:J:83:DT:H2''	6:J:84:DA:C8	2.45	0.51
3:C:63:LEU:HD13	4:D:45:LEU:HB2	1.92	0.51
6:J:30:DG:H2''	6:J:31:DA:C8	2.46	0.51
5:I:99:DC:H2'	5:I:100:DT:H71	2.00	0.51
5:I:160:DA:C8	5:I:161:DT:H72	2.45	0.51
6:J:55:DG:H2''	6:J:56:DA:H8	1.95	0.51
6:J:114:DT:H2''	6:J:115:DA:C8	2.58	0.51
5:I:106:DC:H5''	5:I:106:DC:H6	1.79	0.51
5:I:107:DC:H2''	5:I:108:DG:C8	2.46	0.51
8:M:432:GLN:HG2	8:M:543:LEU:HD22	1.96	0.51
1:E:72:ARG:HH22	5:I:76:DC:P	2.57	0.50
5:I:91:DC:H2''	5:I:92:DG:C8	2.54	0.50
7:K:60:ARG:NH2	7:K:71:ALA:O	2.45	0.50
8:M:442:VAL:O	8:M:541:ARG:NE	2.41	0.50
9:N:51:ALA:HA	9:N:60:VAL:HG21	2.25	0.50
9:N:97:VAL:HG23	9:N:111:ASN:HB2	1.94	0.50
5:I:100:DT:H2''	5:I:101:DG:C8	3.13	0.50
5:I:123:DA:H2''	5:I:124:DG:C8	2.47	0.50
6:J:87:DA:H1'	6:J:88:DC:H5'	2.36	0.50
8:M:443:GLU:OE1	8:M:455:ARG:HD2	2.12	0.50
6:J:14:DC:H2''	6:J:15:DG:C8	2.60	0.50
6:J:35:DA:H1'	6:J:36:DT:H5'	2.43	0.50
8:M:471:ARG:NE	8:M:473:ASN:OD1	2.53	0.50
6:J:37:DA:H2'	6:J:38:DT:H71	1.93	0.49
9:N:49:GLN:O	9:N:53:SER:OG	2.18	0.49
4:H:76:GLU:HB3	4:H:97:ALA:HB1	2.38	0.49
2:F:92:ARG:CZ	2:F:92:ARG:HB3	2.46	0.49
6:J:69:DA:H1'	6:J:70:DT:H5'	1.93	0.49
5:I:36:DC:H1'	5:I:37:DC:H5'	3.33	0.49
6:J:56:DA:H2''	6:J:57:DG:H8	1.77	0.49
5:I:29:DT:H2''	5:I:30:DG:H8	1.78	0.49
6:J:162:DG:H2''	6:J:163:DA:C8	2.54	0.49
5:I:126:DG:H1'	5:I:127:DG:C8	2.48	0.49
4:D:82:HIS:O	4:D:82:HIS:ND1	2.90	0.48
6:J:45:DC:H2''	6:J:46:DA:C8	2.65	0.48
8:M:454:LEU:HD11	8:M:469:ILE:HD11	2.16	0.48
5:I:51:DC:H2''	5:I:52:DT:C6	2.52	0.48
7:K:39:PHE:HD2	7:K:44:VAL:HG12	2.06	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:96:DG:C2	6:J:103:DG:N2	2.82	0.48
2:F:38:ALA:HB3	2:F:46:ILE:HD11	2.19	0.48
5:I:185:DA:H2''	5:I:186:DA:C8	2.48	0.48
6:J:82:DT:H2''	6:J:83:DT:C6	2.83	0.48
7:K:5:GLN:NE2	7:K:9:ASP:OD1	2.47	0.48
2:F:78:ARG:NH1	2:F:80:THR:O	2.49	0.48
5:I:170:DA:H2''	5:I:171:DG:C8	2.57	0.48
5:I:178:DT:H2''	5:I:179:DG:C8	2.56	0.48
6:J:144:DT:H2''	6:J:145:DG:C8	2.49	0.48
6:J:160:DC:H2''	6:J:161:DG:C8	2.49	0.48
7:K:15:MET:SD	7:K:46:LEU:HD22	2.66	0.48
2:F:30:THR:HB	2:F:32:PRO:HD2	1.95	0.47
5:I:120:DC:H2''	5:I:121:DC:O4'	2.59	0.47
6:J:85:DA:H2''	6:J:86:DA:C8	2.59	0.47
6:J:29:DG:H2''	6:J:30:DG:C8	2.49	0.47
7:L:37:ARG:NE	7:L:66:THR:O	2.76	0.47
4:H:69:ILE:HD13	4:H:69:ILE:HA	1.86	0.47
1:A:63:ARG:HD2	5:I:116:DA:H4'	2.04	0.47
1:E:131:ARG:NH1	1:E:133:GLU:OE2	2.48	0.47
3:G:24:GLN:NE2	4:H:47:GLN:OE1	4.74	0.47
4:H:44:VAL:O	4:H:48:VAL:HG22	2.15	0.47
5:I:52:DT:H2''	5:I:53:DC:C5	2.49	0.47
6:J:177:DC:H2'	6:J:178:DT:H71	3.92	0.47
1:E:61:LEU:HD11	2:F:40:ARG:CZ	3.14	0.47
1:A:72:ARG:HH22	6:J:76:DT:P	2.38	0.47
5:I:66:DA:C8	5:I:66:DA:H5'	3.22	0.47
7:K:41:LYS:HB2	7:K:44:VAL:HG23	2.07	0.47
2:F:50:ILE:HD13	2:F:50:ILE:HA	1.71	0.47
4:H:72:ARG:HB3	4:H:101:LEU:HD13	2.23	0.47
6:J:148:DC:H2''	6:J:149:DG:H8	1.82	0.47
6:J:64:DG:H2''	6:J:65:DA:C8	2.59	0.46
7:K:48:GLN:HG2	7:K:62:TRP:CZ2	2.50	0.46
6:J:56:DA:H2''	6:J:57:DG:C8	2.61	0.46
3:G:44:GLY:HA2	6:J:137:DG:H5''	2.10	0.46
5:I:162:DA:H2'	5:I:163:DT:H71	2.52	0.46
6:J:39:DA:H2'	6:J:40:DT:H71	1.97	0.46
6:J:170:DG:H2''	6:J:171:DG:H8	1.81	0.46
5:I:79:DC:H2'	5:I:80:DG:C8	2.92	0.46
9:N:104:ALA:HA	9:N:108:PHE:HZ	2.30	0.46
3:G:63:LEU:HA	3:G:63:LEU:HD23	1.77	0.46
6:J:51:DC:H2''	6:J:52:DC:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:157:DC:H2''	6:J:158:DA:C8	2.51	0.46
2:B:101:GLY:HA2	2:B:102:GLY:HA3	1.90	0.46
4:D:44:VAL:O	4:D:48:VAL:HG22	2.33	0.46
3:G:77:ARG:HA	4:H:53:GLY:O	2.15	0.46
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.98	0.46
5:I:163:DT:H2''	5:I:164:DA:C8	2.51	0.46
6:J:46:DA:C4	6:J:47:DC:C5	3.11	0.46
5:I:24:DA:C8	5:I:24:DA:H5'	2.60	0.45
9:N:98:GLN:HE22	9:N:103:GLY:N	2.14	0.45
2:F:46:ILE:HG22	2:F:47:SER:O	2.28	0.45
8:M:514:TRP:HE1	8:M:516:ALA:HB3	1.82	0.45
5:I:189:DT:H2''	5:I:190:DC:C6	2.72	0.45
3:C:42:ARG:O	4:D:88:THR:HA	2.43	0.45
5:I:114:DT:H2''	5:I:115:DA:C8	2.66	0.45
6:J:14:DC:H2''	6:J:15:DG:H8	1.92	0.45
6:J:47:DC:H2''	6:J:48:DG:C8	2.75	0.45
3:G:32:ARG:NH2	4:H:35:GLU:OE1	2.66	0.45
5:I:37:DC:C2	6:J:162:DG:N2	2.84	0.45
3:C:85:LEU:HD23	3:C:85:LEU:HA	1.77	0.45
6:J:119:DG:H2''	6:J:120:DG:C5'	2.47	0.45
1:E:92:LEU:HD21	2:F:65:VAL:HG11	2.00	0.45
5:I:93:DT:H2''	5:I:94:DA:C8	2.51	0.45
4:D:80:LEU:HD23	4:D:80:LEU:HA	1.69	0.45
6:J:178:DT:C2	6:J:179:DC:C5	3.05	0.45
5:I:154:DT:H2''	5:I:155:DC:C5	2.79	0.45
1:A:83:ARG:O	2:B:80:THR:HA	2.24	0.45
5:I:181:DC:H2''	5:I:182:DG:C8	2.68	0.45
1:E:83:ARG:O	2:F:80:THR:HA	2.17	0.44
6:J:52:DC:H2''	6:J:53:DT:C5	2.51	0.44
8:M:467:TRP:CD2	8:M:532:ASN:HA	2.52	0.44
5:I:47:DG:H2''	5:I:48:DC:C6	2.69	0.44
5:I:124:DG:N2	6:J:75:DT:O2	2.50	0.44
8:M:464:MET:HB2	8:M:487:PHE:HD2	2.09	0.44
3:C:32:ARG:HH22	4:D:35:GLU:CD	2.56	0.44
5:I:70:DC:C6	5:I:71:DT:H72	2.95	0.44
1:E:100:LEU:HD23	1:E:100:LEU:HA	1.77	0.44
2:B:62:LEU:HD23	2:B:62:LEU:HA	1.69	0.44
3:G:55:LEU:HD23	3:G:55:LEU:HA	1.84	0.44
5:I:58:DG:H2''	5:I:59:DG:C8	2.74	0.44
6:J:181:DC:H2''	6:J:182:DG:C8	2.58	0.44
9:N:44:SER:HB3	9:N:90:LEU:HD21	2.09	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:LYS:HB3	1:E:38:PRO:HD3	2.07	0.44
5:I:100:DT:H2''	5:I:101:DG:H8	2.70	0.44
5:I:159:DT:C2	5:I:160:DA:C8	3.05	0.44
6:J:140:DC:C4	6:J:141:DA:N6	2.85	0.44
8:M:455:ARG:HG3	8:M:494:VAL:HG22	2.48	0.44
3:C:63:LEU:HD11	4:D:41:VAL:HG13	1.99	0.44
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.64	0.44
2:F:75:HIS:CD2	4:H:80:LEU:HD22	2.81	0.44
1:A:60:LEU:HD13	1:A:93:GLN:NE2	2.54	0.44
2:B:50:ILE:HD13	2:B:50:ILE:HA	1.82	0.44
5:I:179:DG:H2'	5:I:180:DT:H71	2.11	0.44
6:J:47:DC:C2	6:J:48:DG:N7	2.86	0.44
6:J:149:DG:H2''	6:J:150:DG:H8	1.83	0.44
7:K:6:LYS:NZ	7:K:21:GLY:O	2.29	0.44
5:I:184:DG:H2''	5:I:185:DA:C8	2.53	0.43
6:J:149:DG:H2''	6:J:150:DG:C8	2.53	0.43
3:G:102:ILE:HG23	4:H:61:ILE:HD13	2.00	0.43
5:I:72:DC:H2''	5:I:73:DT:C7	2.48	0.43
5:I:188:DT:C6	5:I:189:DT:H72	2.53	0.43
6:J:34:DT:H2''	6:J:35:DA:H8	1.97	0.43
6:J:153:DT:H2''	6:J:154:DC:C6	2.76	0.43
6:J:155:DG:H2''	6:J:156:DG:N7	2.33	0.43
7:K:15:MET:H	7:K:15:MET:HG2	1.62	0.43
7:L:63:LEU:HD23	7:L:74:SER:HA	2.00	0.43
5:I:181:DC:H2''	5:I:182:DG:N7	2.39	0.43
6:J:47:DC:H2''	6:J:48:DG:H8	1.96	0.43
5:I:29:DT:H2''	5:I:30:DG:C8	2.54	0.43
6:J:153:DT:H4'	6:J:154:DC:OP1	2.18	0.43
7:L:49:PHE:CE1	7:L:54:LYS:HA	2.71	0.43
1:A:131:ARG:NH1	1:A:133:GLU:OE2	2.52	0.43
2:B:31:LYS:HE3	2:B:35:ARG:HH21	1.87	0.43
1:E:60:LEU:HD21	1:E:94:GLU:OE2	2.19	0.43
7:L:15:MET:H	7:L:15:MET:HG2	1.52	0.43
3:G:99:ARG:HA	3:G:99:ARG:HD3	1.78	0.43
1:A:123:ASP:OD1	1:E:113:HIS:NE2	3.07	0.43
6:J:55:DG:C2	6:J:56:DA:C5	3.07	0.43
5:I:106:DC:H5''	5:I:106:DC:C6	2.60	0.43
6:J:80:DG:H1'	6:J:81:DG:H5''	2.01	0.43
6:J:83:DT:H2''	6:J:84:DA:N7	2.34	0.43
3:G:81:ARG:NH2	3:G:107:VAL:O	3.12	0.43
7:K:63:LEU:HD23	7:K:74:SER:HA	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:15:LYS:HB3	3:G:15:LYS:HE2	1.87	0.42
5:I:18:DC:H2''	5:I:19:DG:C8	2.54	0.42
7:K:39:PHE:CZ	7:K:62:TRP:HZ2	2.41	0.42
7:L:80:CYS:SG	7:L:81:LEU:N	2.91	0.42
4:H:46:LYS:HA	4:H:46:LYS:HD3	1.74	0.42
5:I:64:DA:H5'	5:I:64:DA:C8	2.81	0.42
7:L:30:LEU:HD22	7:L:67:CYS:SG	2.60	0.42
2:B:78:ARG:NH1	2:B:80:THR:O	2.52	0.42
5:I:55:DA:H1'	5:I:56:DT:H5'	2.75	0.42
5:I:61:DC:H2''	5:I:62:DG:C8	2.62	0.42
1:E:118:THR:HA	2:F:45:ARG:O	2.19	0.42
3:G:50:TYR:CE1	4:H:114:GLY:HA3	2.55	0.42
6:J:116:DA:C6	6:J:117:DG:C6	3.19	0.42
8:M:444:GLU:HB3	8:M:453:ARG:HB3	2.08	0.42
6:J:159:DC:C2	6:J:160:DC:C5	3.14	0.42
4:D:69:ILE:HD13	4:D:69:ILE:HA	1.98	0.42
5:I:25:DG:H2''	5:I:26:DG:C8	2.55	0.42
5:I:104:DC:H2''	5:I:105:DC:C5	2.57	0.42
5:I:161:DT:H2''	5:I:162:DA:O4'	2.20	0.42
6:J:17:DG:H2''	6:J:18:DA:C8	2.58	0.42
3:C:67:GLY:HA3	4:D:49:HIS:CE1	2.54	0.42
4:H:100:LEU:HD23	4:H:100:LEU:HA	1.91	0.42
3:C:33:LEU:HA	3:C:33:LEU:HD23	1.80	0.42
3:C:55:LEU:HA	3:C:55:LEU:HD23	1.90	0.42
3:C:77:ARG:CZ	6:J:45:DC:H4'	2.49	0.42
2:F:62:LEU:HA	2:F:62:LEU:HD23	1.77	0.42
5:I:71:DT:H2''	5:I:72:DC:C6	2.97	0.42
5:I:115:DA:H1'	5:I:116:DA:C8	2.55	0.42
6:J:107:DG:H2'	6:J:108:DT:H71	2.01	0.42
1:A:82:LEU:HD23	1:A:82:LEU:HA	2.05	0.41
3:C:37:GLY:HA3	3:C:39:TYR:CE2	2.58	0.41
3:C:88:ARG:HA	3:C:88:ARG:HD3	1.95	0.41
6:J:51:DC:H2''	6:J:52:DC:C5	2.55	0.41
6:J:58:DA:H1'	6:J:59:DC:H5'	2.14	0.41
6:J:85:DA:H2''	6:J:86:DA:H8	1.88	0.41
6:J:153:DT:H2''	6:J:154:DC:O5'	2.19	0.41
6:J:94:DG:H2''	6:J:95:DG:C8	2.63	0.41
3:G:108:LEU:HD23	3:G:108:LEU:HA	1.76	0.41
6:J:60:DT:H2''	6:J:61:DA:C8	2.78	0.41
5:I:25:DG:H2''	5:I:26:DG:H8	1.85	0.41
6:J:54:DG:H2''	6:J:55:DG:H8	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:473:ASN:ND2	8:M:521:GLY:HA3	2.35	0.41
2:B:58:LEU:HD23	2:B:58:LEU:HA	2.61	0.41
2:B:77:LYS:HE3	4:D:92:ARG:NH1	2.35	0.41
3:C:34:LEU:HD23	3:C:34:LEU:HA	1.88	0.41
3:G:54:VAL:HG21	4:H:98:VAL:HG21	2.02	0.41
5:I:40:DT:H2''	5:I:41:DG:C8	2.55	0.41
5:I:92:DG:H2''	5:I:93:DT:C6	2.56	0.41
6:J:178:DT:OP1	9:N:82:ARG:NH1	2.53	0.41
2:B:35:ARG:O	2:B:39:ARG:HG2	2.20	0.41
3:C:50:TYR:CE1	4:D:114:GLY:HA3	2.65	0.41
3:G:83:LEU:HD23	3:G:83:LEU:HA	1.90	0.41
6:J:128:DG:C4	6:J:129:DC:C5	3.09	0.41
3:G:24:GLN:HE21	4:H:47:GLN:HE22	1.67	0.41
6:J:118:DC:H2''	6:J:119:DG:C8	2.69	0.41
7:L:59:PHE:HZ	7:L:77:CYS:HG	1.67	0.41
1:A:56:LYS:HE3	1:A:56:LYS:HB2	1.91	0.41
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.64	0.41
5:I:53:DC:H1'	5:I:54:DA:C8	2.55	0.41
5:I:100:DT:H5''	9:N:80:ASN:ND2	3.92	0.41
5:I:176:DT:H2''	5:I:177:DG:H8	1.86	0.41
6:J:8:DG:H2''	6:J:9:DA:C8	2.56	0.41
6:J:62:DG:H2''	6:J:63:DG:C8	2.66	0.41
6:J:76:DT:H2''	6:J:77:DG:H5'	2.15	0.41
6:J:119:DG:C2	6:J:120:DG:C5	3.16	0.41
6:J:180:DG:C5	6:J:181:DC:N4	2.94	0.41
7:K:60:ARG:NH2	7:K:75:ARG:HB2	2.46	0.41
7:L:2:THR:OG1	7:L:3:THR:N	2.72	0.41
7:L:20:VAL:HG11	7:L:35:GLU:HG3	2.02	0.41
5:I:55:DA:H2''	5:I:56:DT:H71	2.03	0.41
5:I:103:DC:H2''	5:I:104:DC:C5	2.55	0.41
5:I:183:DC:H2''	5:I:184:DG:C8	2.56	0.41
6:J:125:DA:H2''	6:J:126:DG:C8	2.56	0.41
4:D:80:LEU:O	4:D:84:ASN:ND2	2.54	0.40
5:I:136:DC:H6	5:I:136:DC:H2'	1.69	0.40
6:J:176:DG:H2''	6:J:177:DC:H6	2.19	0.40
9:N:75:ASP:HB3	9:N:79:ASN:ND2	2.36	0.40
3:G:20:ARG:NH2	5:I:57:DT:OP1	3.95	0.40
6:J:73:DC:H2''	6:J:74:DC:C5	2.56	0.40
6:J:137:DG:C2	6:J:138:DA:C6	3.17	0.40
5:I:93:DT:C2	5:I:94:DA:C6	3.17	0.40
6:J:138:DA:H1'	6:J:139:DC:H5'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.71	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	94/139 (68%)	91 (97%)	3 (3%)	0	100	100
1	E	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	a	94/139 (68%)	92 (98%)	2 (2%)	0	100	100
1	e	96/139 (69%)	92 (96%)	4 (4%)	0	100	100
2	B	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
2	F	81/106 (76%)	78 (96%)	3 (4%)	0	100	100
2	b	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
2	f	81/106 (76%)	79 (98%)	2 (2%)	0	100	100
3	C	106/133 (80%)	103 (97%)	3 (3%)	0	100	100
3	G	102/133 (77%)	98 (96%)	4 (4%)	0	100	100
3	c	106/133 (80%)	102 (96%)	4 (4%)	0	100	100
3	g	102/133 (77%)	100 (98%)	2 (2%)	0	100	100
4	D	92/129 (71%)	90 (98%)	2 (2%)	0	100	100
4	H	89/129 (69%)	85 (96%)	4 (4%)	0	100	100
4	d	92/129 (71%)	88 (96%)	4 (4%)	0	100	100
4	h	89/129 (69%)	85 (96%)	4 (4%)	0	100	100
7	K	86/93 (92%)	84 (98%)	2 (2%)	0	100	100
7	L	86/93 (92%)	84 (98%)	2 (2%)	0	100	100
7	k	86/93 (92%)	81 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	l	86/93 (92%)	85 (99%)	1 (1%)	0	100	100
8	M	117/158 (74%)	114 (97%)	3 (3%)	0	100	100
8	m	117/158 (74%)	117 (100%)	0	0	100	100
9	N	76/221 (34%)	75 (99%)	1 (1%)	0	100	100
9	n	76/221 (34%)	76 (100%)	0	0	100	100
All	All	2202/3158 (70%)	2137 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/113 (74%)	83 (99%)	1 (1%)	67	79
1	E	86/113 (76%)	85 (99%)	1 (1%)	67	79
1	a	84/113 (74%)	81 (96%)	3 (4%)	30	53
1	e	86/113 (76%)	81 (94%)	5 (6%)	17	40
2	B	63/81 (78%)	63 (100%)	0	100	100
2	F	68/81 (84%)	67 (98%)	1 (2%)	60	75
2	b	63/81 (78%)	60 (95%)	3 (5%)	21	45
2	f	68/81 (84%)	67 (98%)	1 (2%)	60	75
3	C	85/102 (83%)	83 (98%)	2 (2%)	44	63
3	G	83/102 (81%)	79 (95%)	4 (5%)	21	45
3	c	85/102 (83%)	84 (99%)	1 (1%)	67	79
3	g	83/102 (81%)	82 (99%)	1 (1%)	67	79
4	D	80/107 (75%)	79 (99%)	1 (1%)	65	77
4	H	77/107 (72%)	77 (100%)	0	100	100
4	d	80/107 (75%)	77 (96%)	3 (4%)	28	51
4	h	77/107 (72%)	76 (99%)	1 (1%)	65	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	K	73/77 (95%)	72 (99%)	1 (1%)	62	76
7	L	73/77 (95%)	71 (97%)	2 (3%)	40	61
7	k	73/77 (95%)	71 (97%)	2 (3%)	40	61
7	l	73/77 (95%)	71 (97%)	2 (3%)	40	61
8	M	99/134 (74%)	98 (99%)	1 (1%)	73	82
8	m	99/134 (74%)	98 (99%)	1 (1%)	73	82
9	N	60/166 (36%)	60 (100%)	0	100	100
9	n	60/166 (36%)	60 (100%)	0	100	100
All	All	1862/2520 (74%)	1825 (98%)	37 (2%)	50	68

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ARG
3	C	42	ARG
3	C	50	TYR
4	D	79	ARG
1	E	76	GLN
2	F	30	THR
3	G	38	ASN
3	G	50	TYR
3	G	71	ARG
3	G	118	LYS
7	K	15	MET
7	L	15	MET
7	L	32	LYS
8	M	495	VAL
1	a	83	ARG
1	a	105	GLU
1	a	131	ARG
2	b	50	ILE
2	b	58	LEU
2	b	86	VAL
3	c	38	ASN
4	d	48	VAL
4	d	79	ARG
4	d	80	LEU
1	e	39	HIS
1	e	76	GLN

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Mol	Chain	Res	Type
1	e	105	GLU
1	e	107	THR
1	e	131	ARG
2	f	54	THR
3	g	118	LYS
4	h	80	LEU
7	k	75	ARG
7	k	80	CYS
7	l	15	MET
7	l	80	CYS
8	m	475	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
2	B	25	ASN
2	B	93	GLN
3	C	31	HIS
4	D	84	ASN
1	E	39	HIS
1	E	113	HIS
2	F	25	ASN
2	F	93	GLN
3	G	112	GLN
4	H	47	GLN
4	H	49	HIS
4	H	84	ASN
7	K	48	GLN
9	N	98	GLN
2	b	93	GLN
3	c	24	GLN
3	c	38	ASN
4	d	84	ASN
1	e	68	GLN
1	e	76	GLN
2	f	75	HIS
2	f	93	GLN
3	g	104	GLN
3	g	112	GLN
4	h	95	GLN
8	m	433	HIS

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Mol	Chain	Res	Type
9	n	80	ASN
9	n	98	GLN

### 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 oligosaccharides 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.

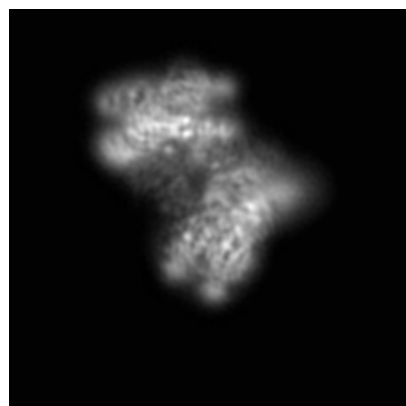
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61233. These allow visual inspection of the internal detail of the map and identification of artifacts.

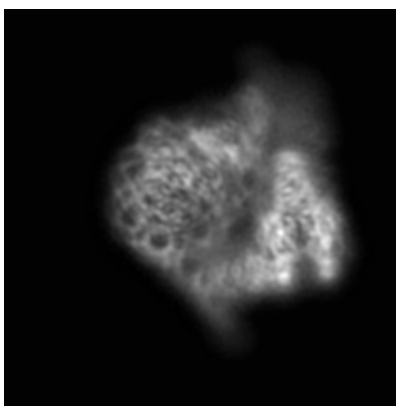
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

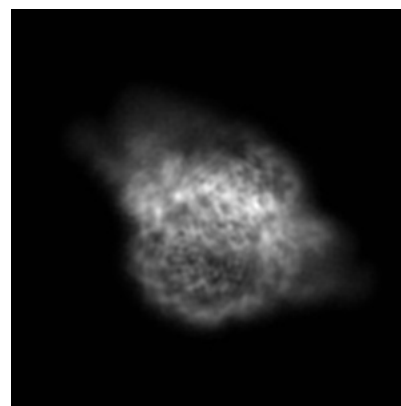
#### 6.1.1 Primary map



X

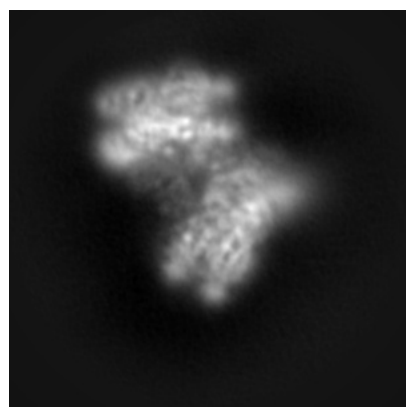


Y

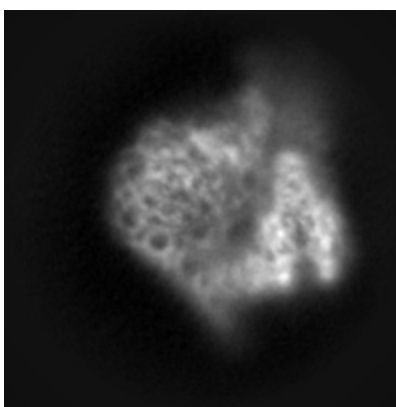


Z

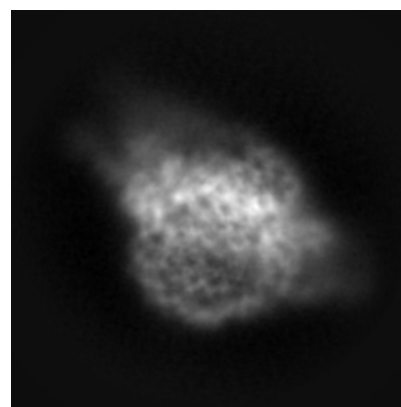
#### 6.1.2 Raw map



X



Y

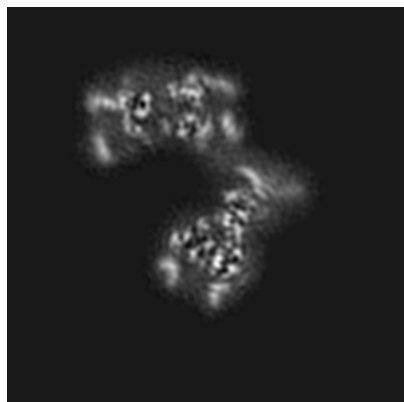


Z

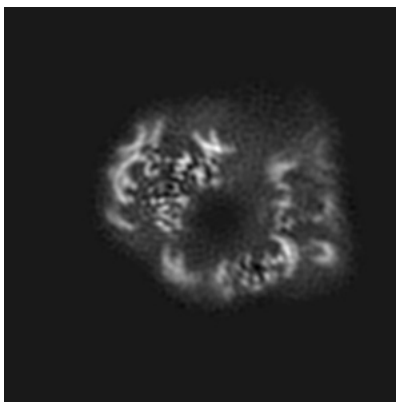
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 128

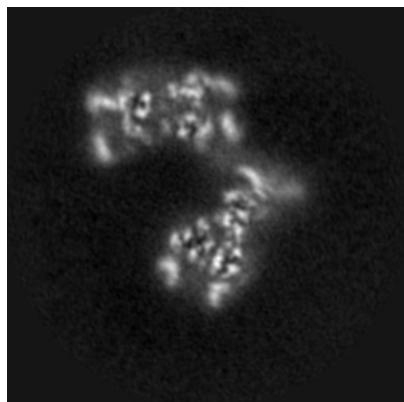


Y Index: 128

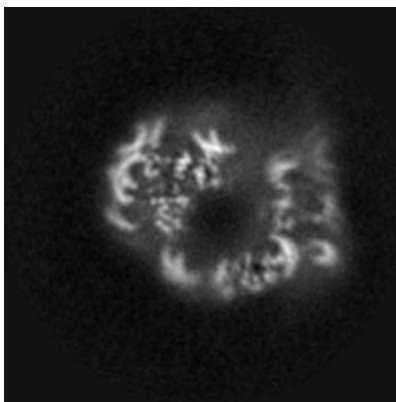


Z Index: 128

### 6.2.2 Raw map



X Index: 128



Y Index: 128



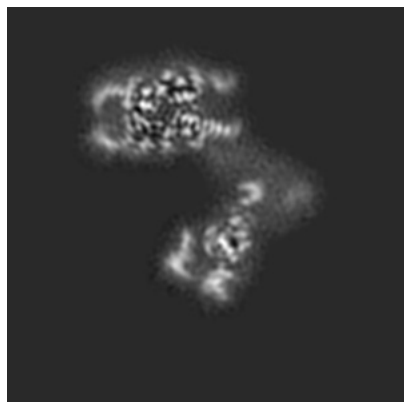
Z Index: 128

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

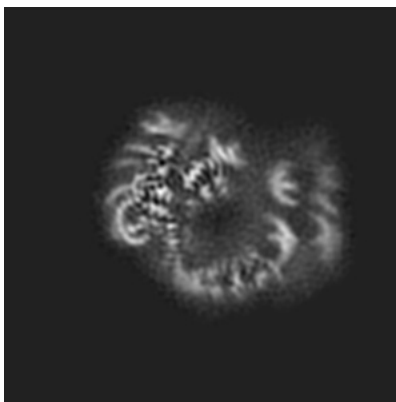


## 6.3 Largest variance slices [i](#)

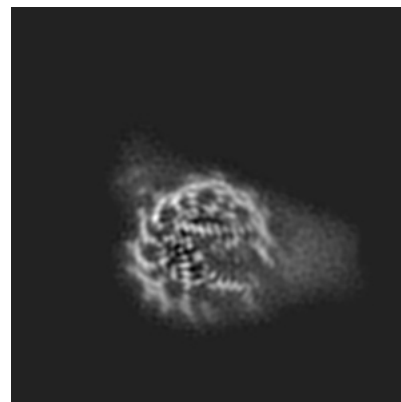
### 6.3.1 Primary map



X Index: 115

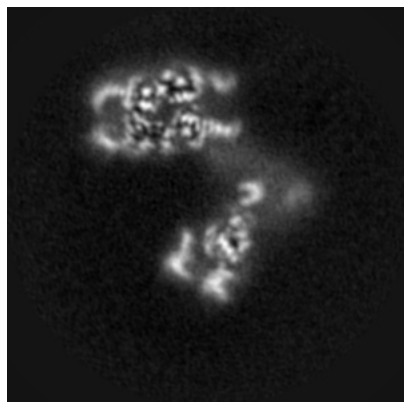


Y Index: 136

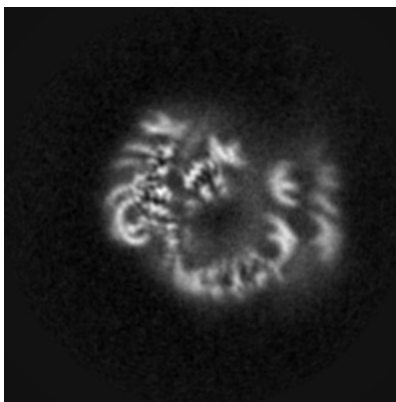


Z Index: 177

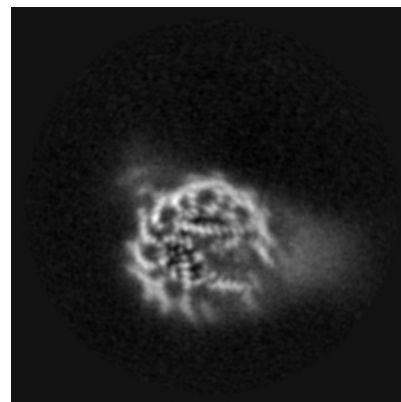
### 6.3.2 Raw map



X Index: 115



Y Index: 136

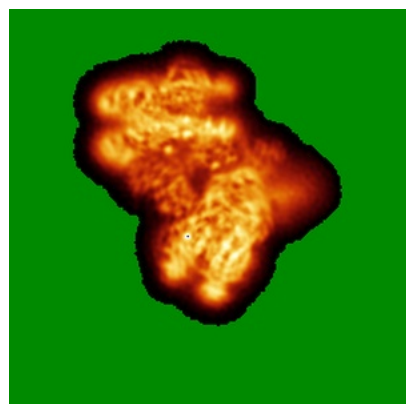


Z Index: 177

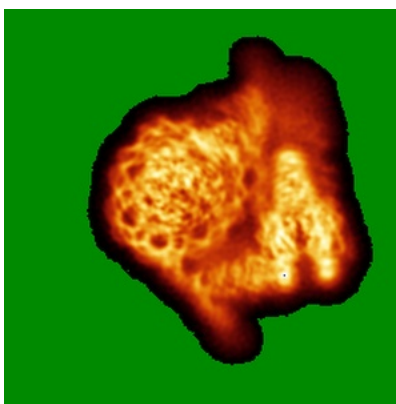
The images above show the largest variance slices of the map in three orthogonal directions.

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

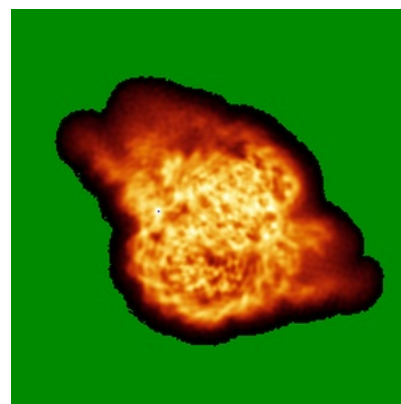
### 6.4.1 Primary map



X

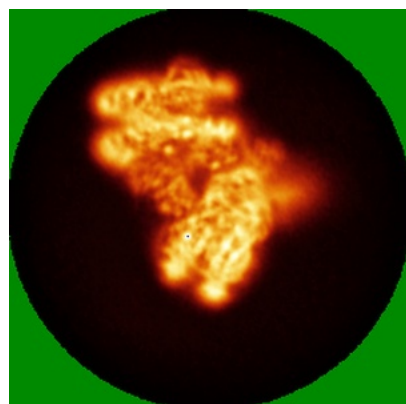


Y

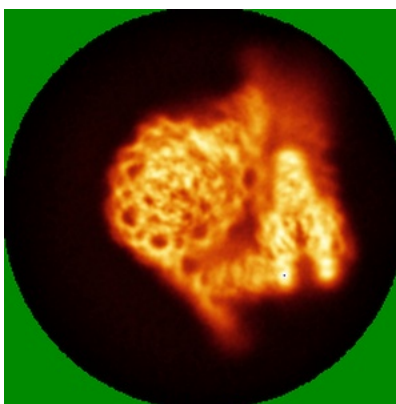


Z

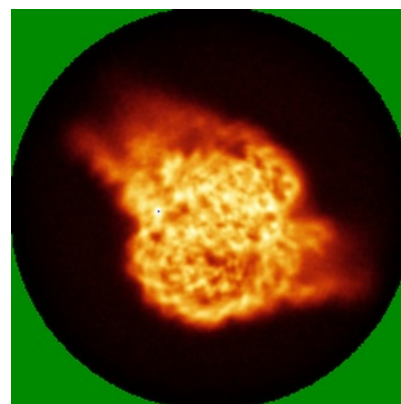
### 6.4.2 Raw map



X



Y



Z

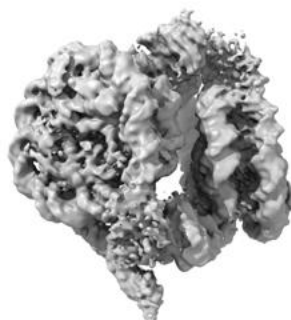
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

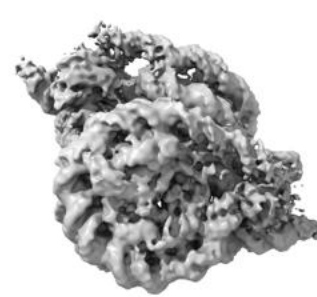
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00667. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

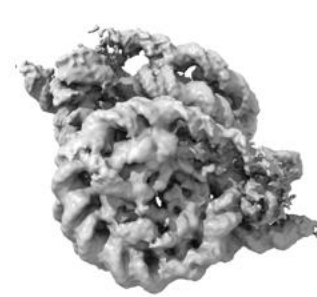
### 6.5.2 Raw map



X



Y



Z

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.

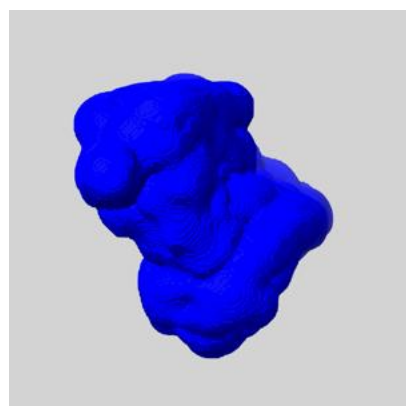
## 6.6 Mask visualisation [i](#)

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

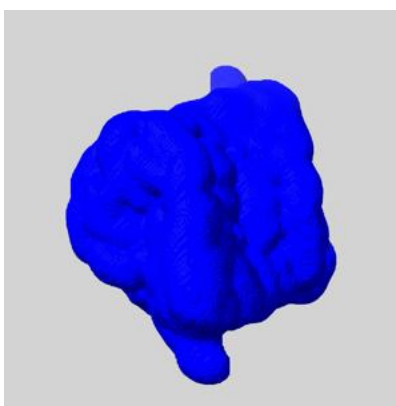
A mask typically either:

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

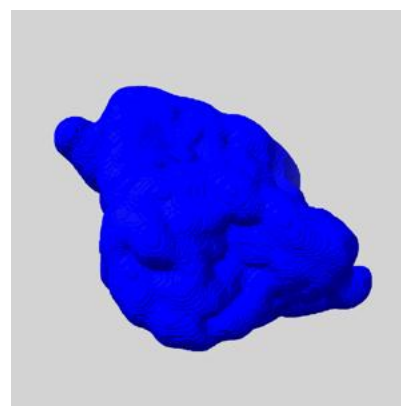
### 6.6.1 emd\_61233\_msk\_1.map [i](#)



X



Y

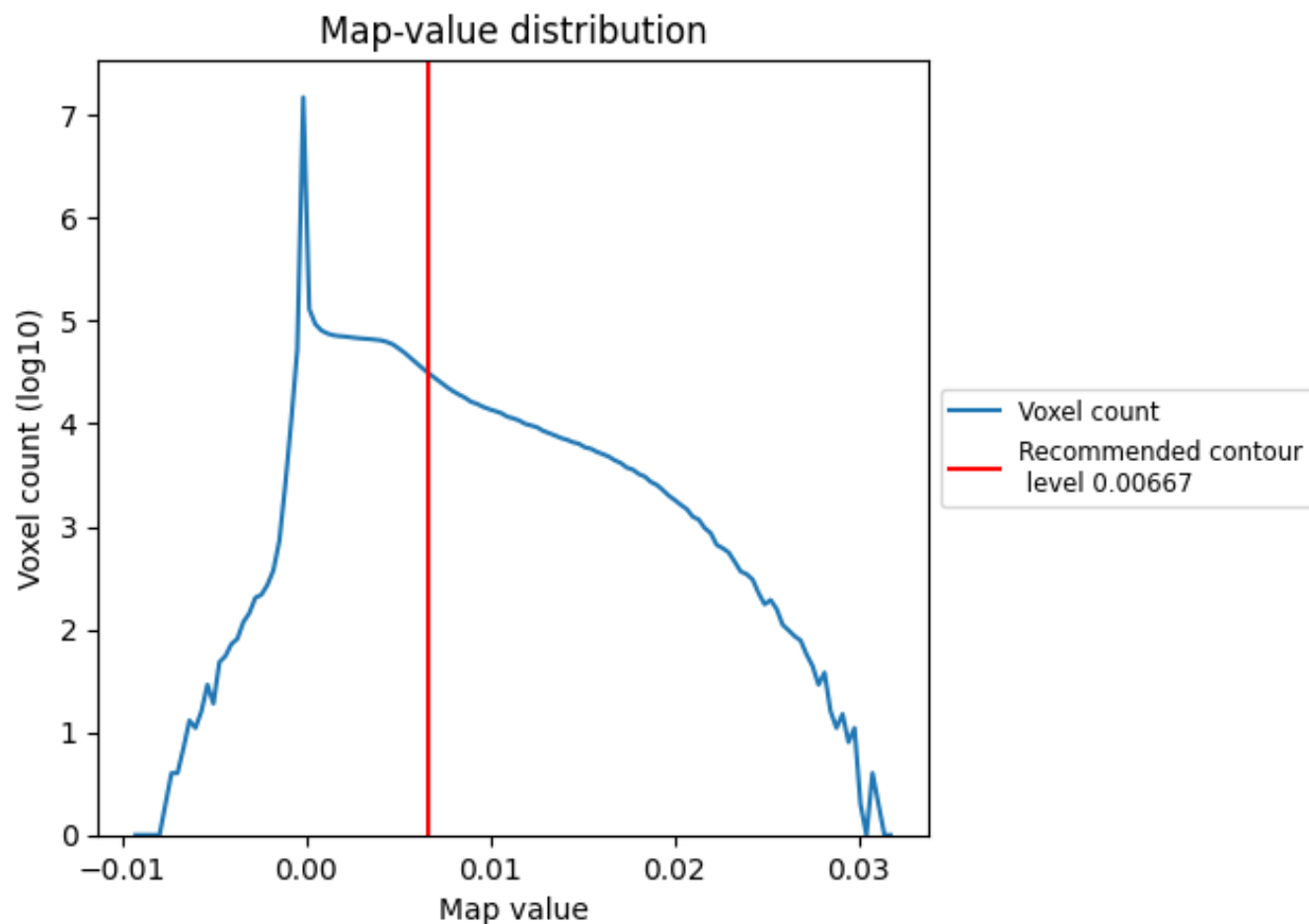


Z

## 7 Map analysis [i](#)

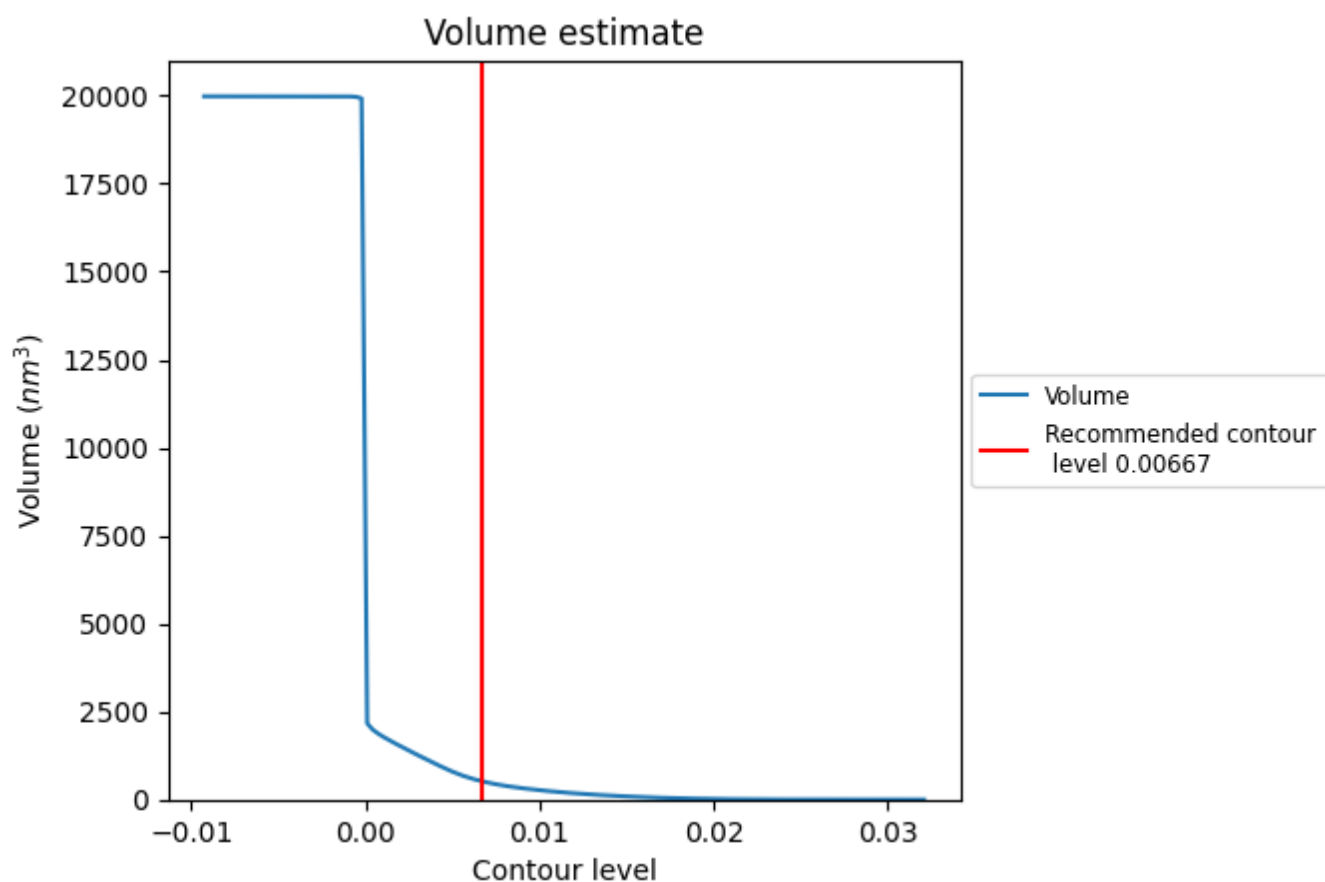
This section contains the results of statistical analysis of the map.

### 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.

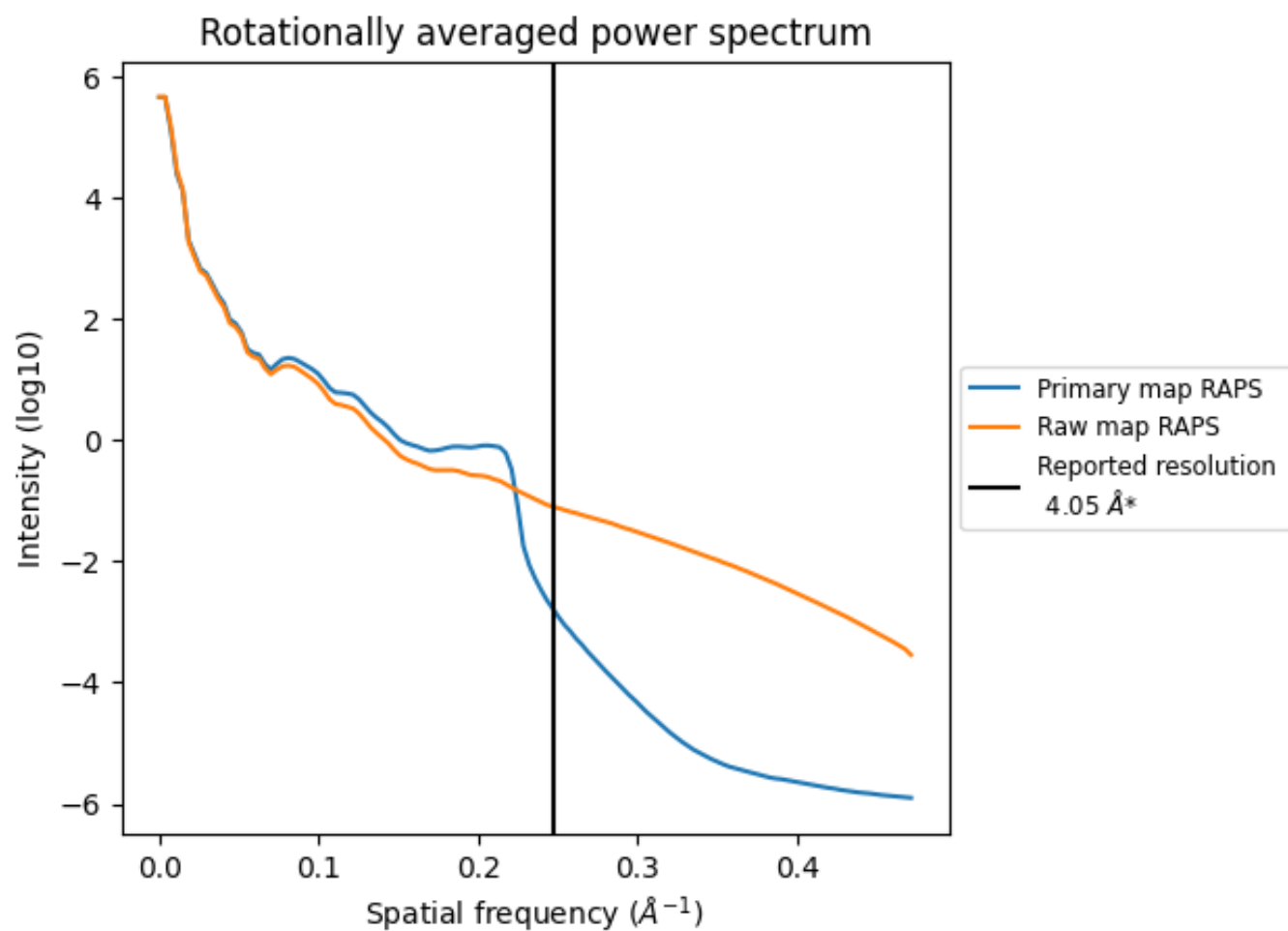
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 522 nm<sup>3</sup>; this corresponds to an approximate mass of 472 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

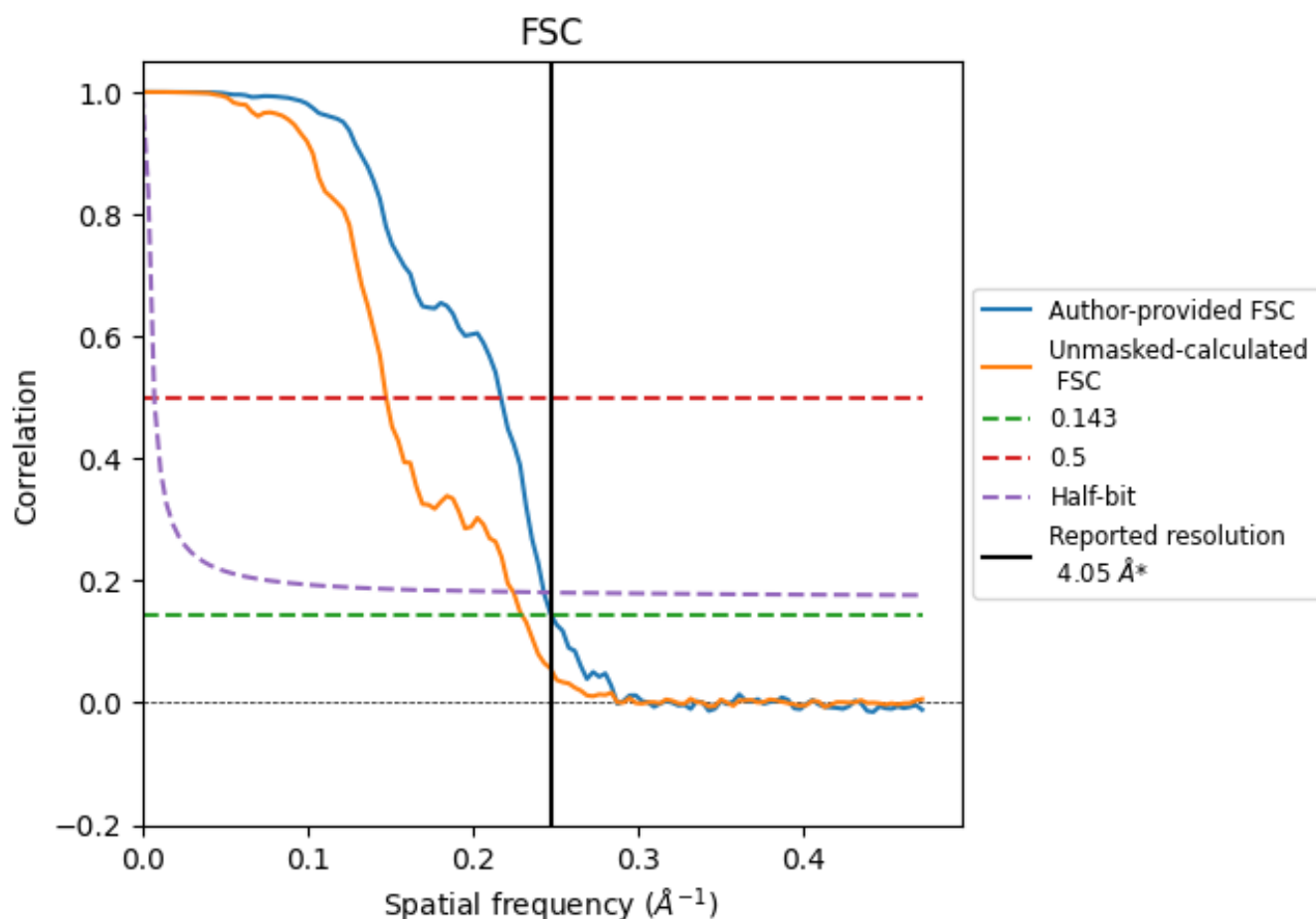


\*Reported resolution corresponds to spatial frequency of  $0.247 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.247 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

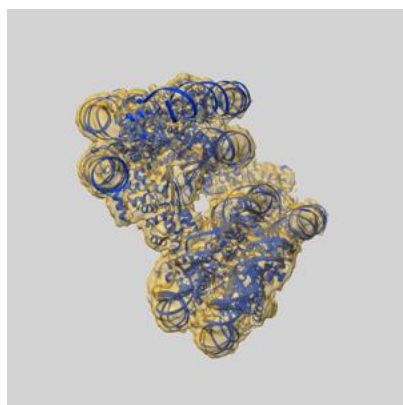
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.04	4.61	4.12
Unmasked-calculated*	4.35	6.78	4.46

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

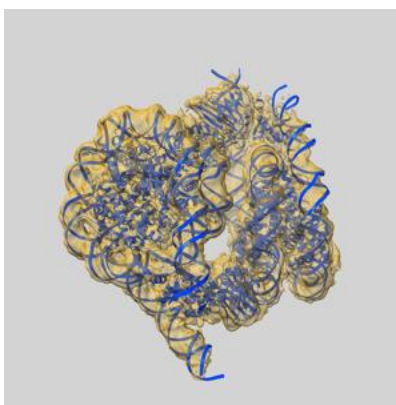
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61233 and PDB model 9J8O. Per-residue inclusion information can be found in section [3](#) on page [9](#).

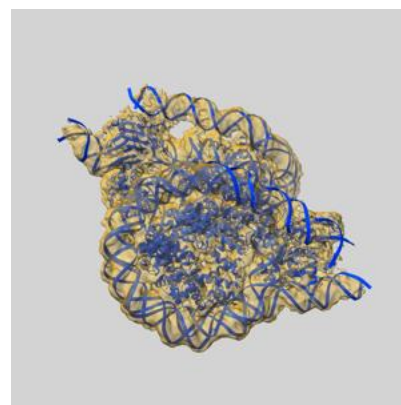
### 9.1 Map-model overlay [i](#)



X



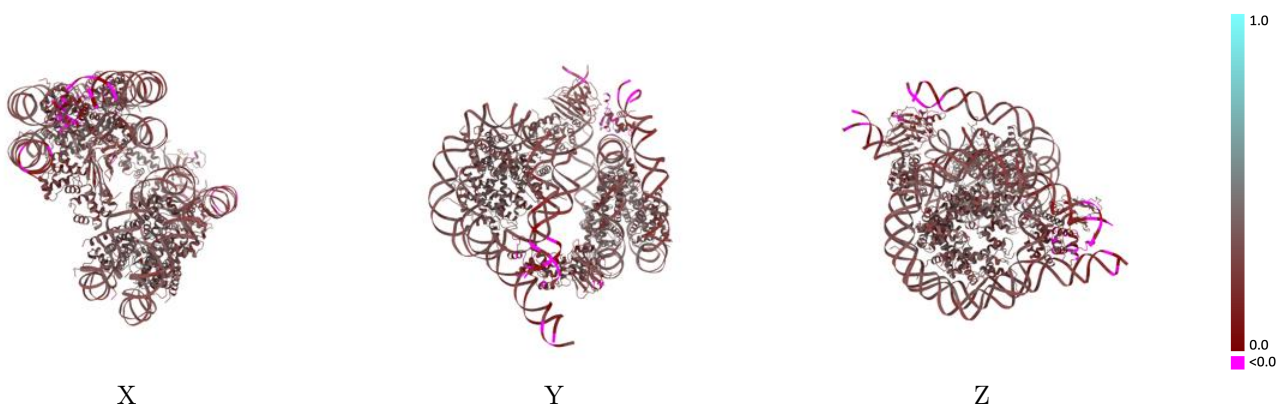
Y



Z

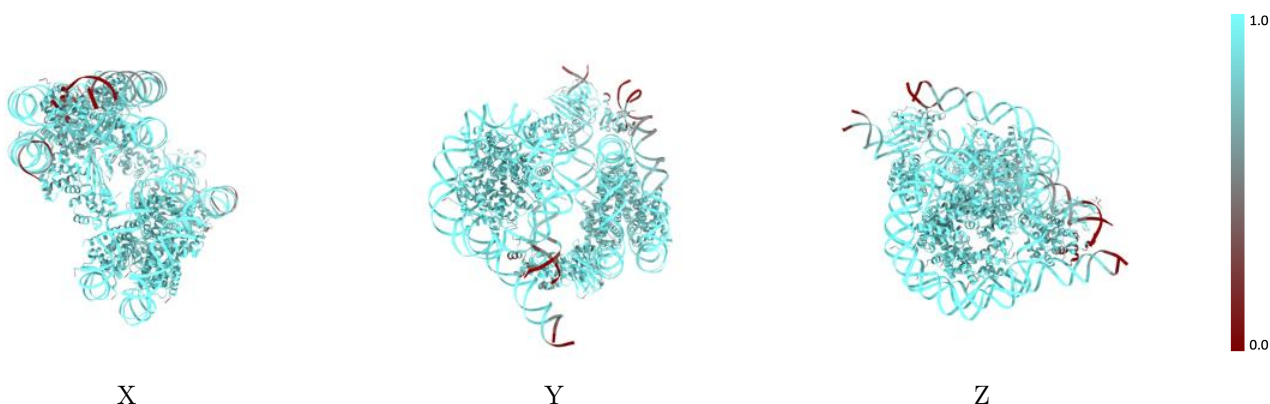
The images above show the 3D surface view of the map at the recommended contour level 0.00667 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



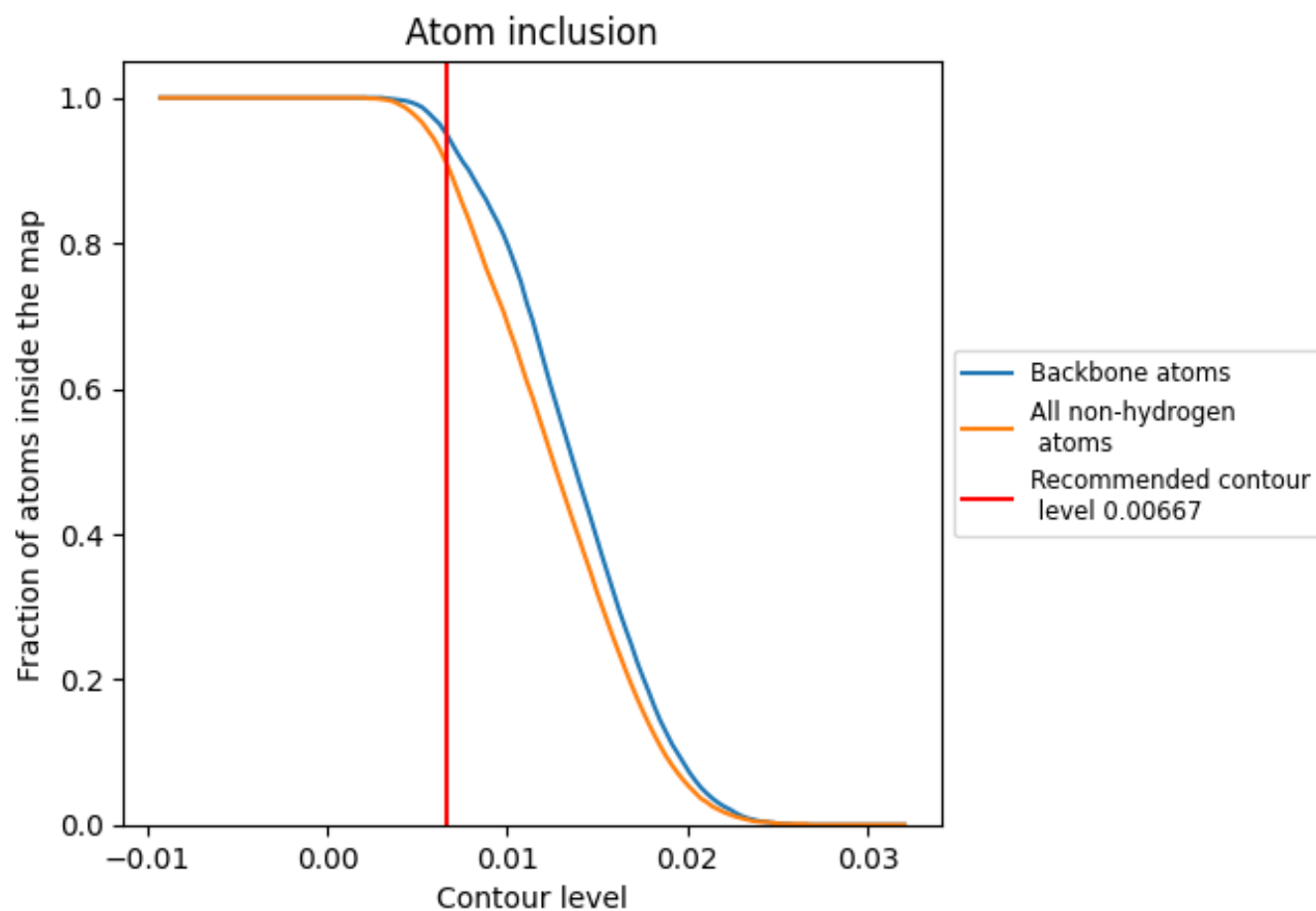
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00667).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00667) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.2920
A	 0.9290	 0.3310
B	 0.9280	 0.3470
C	 0.9010	 0.3410
D	 0.9290	 0.3360
E	 0.9370	 0.3430
F	 0.9260	 0.3560
G	 0.9040	 0.3380
H	 0.9450	 0.3370
I	 0.9290	 0.2730
J	 0.9250	 0.2790
K	 0.9240	 0.3250
L	 0.9270	 0.2780
M	 0.9030	 0.2690
N	 0.7710	 0.1630
a	 0.9120	 0.3080
b	 0.9210	 0.3400
c	 0.8810	 0.3390
d	 0.9080	 0.3310
e	 0.9200	 0.3230
f	 0.9210	 0.3370
g	 0.9000	 0.3180
h	 0.9350	 0.3200
i	 0.8960	 0.2710
j	 0.8990	 0.2700
k	 0.9240	 0.3220
l	 0.9180	 0.2740
m	 0.8810	 0.2630
n	 0.6420	 0.0910

