



## wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 11:46 AM JST

PDB ID : 6KW4  
EMDB ID : EMD-0778  
Title : The ClassB RSC-Nucleosome Complex  
Authors : Ye, Y.P.; Wu, H.; Chen, K.J.; Verma, N.; Cairns, B.; Gao, N.; Chen, Z.C.  
Deposited on : 2019-09-06  
Resolution : 7.55 Å(reported)

This is a wwPDB EM Validation Summary 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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

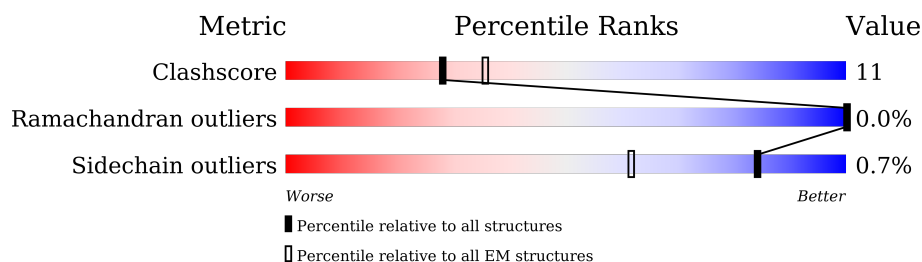
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






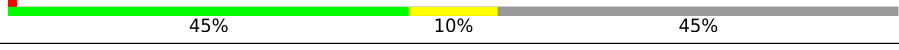


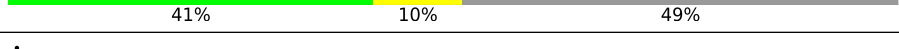
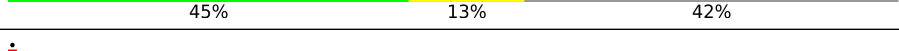
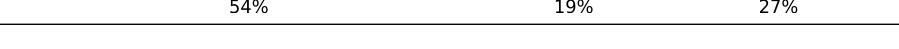
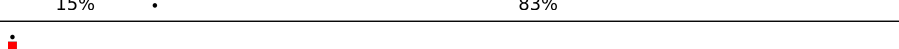
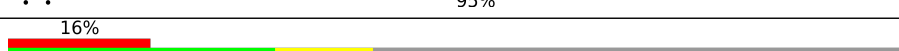


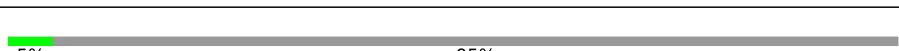






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	N	136	
1	Q	136	
2	B	103	
2	R	103	
3	O	130	
3	S	130	
4	U	167	
5	W	167	

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Mol	Chain	Length	Quality of chain
6	f	477	
7	h	157	
8	F	435	
9	D	557	
9	H	557	
10	M	581	
11	I	483	
12	G	426	
13	A	502	
14	J	1359	
14	V	1359	
14	Y	1359	
15	E	78	
16	C	883	
17	K	885	
18	X	625	
19	L	889	
20	P	126	
20	T	126	
21	g	467	

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 45924 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
1	N	98	Total	C	N	O	S	0	0
			810	511	157	139	3		
1	Q	95	Total	C	N	O	S	0	0
			784	494	151	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total	C	N	O	S	0	0
			657	416	128	112	1		
2	R	87	Total	C	N	O	S	0	0
			703	443	142	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	107	Total	C	N	O	0	0
			823	519	161	143		
3	S	107	Total	C	N	O	0	0
			823	519	161	143		

- Molecule 4 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	156	Total	C	N	O	P	0	0
			3183	1512	579	936	156		

- Molecule 5 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	156	Total	C	N	O	P	0	0
			3213	1522	599	936	156		

- Molecule 6 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	398	Total	C	N	O	S	3	0
			3219	2075	527	602	15		

- Molecule 7 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 8 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	118	Total	C	N	O	S	0	0
			964	601	164	197	2		

- Molecule 9 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	393	Total	C	N	O	S	0	0
			3215	2036	552	613	14		
9	D	305	Total	C	N	O	S	0	0
			2510	1613	416	471	10		

- Molecule 10 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	384	Total	C	N	O	S	0	0
			3058	1970	497	574	17		

- Molecule 11 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	244	Total	C	N	O	S	0	0
			1944	1234	328	377	5		

- Molecule 12 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	246	Total	C	N	O	S	0	0
			1996	1271	337	380	8		

- Molecule 13 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	365	Total	C	N	O	S	0	0
			3007	1942	509	547	9		

- Molecule 14 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	235	Total	C	N	O	S	0	0
			1814	1136	327	349	2		
14	V	69	Total	C	N	O	S	0	0
			592	364	121	105	2		
14	Y	548	Total	C	N	O	S	0	0
			4503	2873	780	832	18		

- Molecule 15 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	58	Total	C	N	O	S	0	0
			477	295	86	92	4		

- Molecule 16 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	33	Total	C	N	O	S	0	0
			269	177	39	52	1		

- Molecule 17 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	42	Total	C	N	O	S	0	0
			347	225	57	63	2		

- Molecule 18 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	147	Total	C	N	O	S	0	0
			1220	776	202	234	8		

- Molecule 19 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	85	Total	C	N	O	S	0	0
			669	428	120	119	2		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	93	Total	C	N	O	S	0	0
			717	450	128	137	2		
20	T	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 21 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	395	Total	C	N	O	S	1	0
			3191	2048	522	614	7		

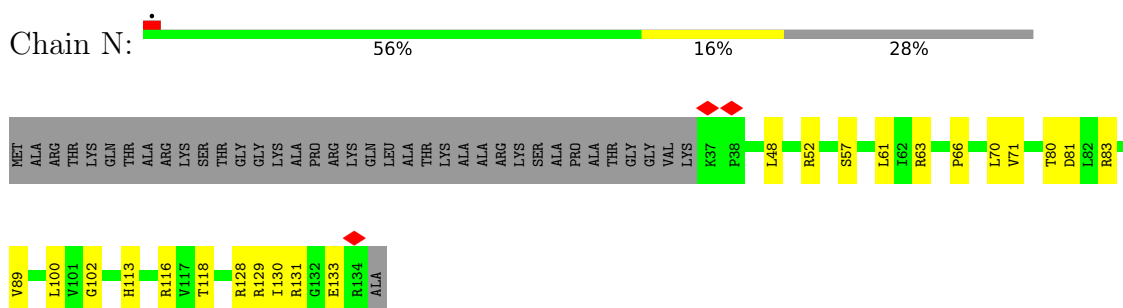
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total	Zn	0
			1	1	

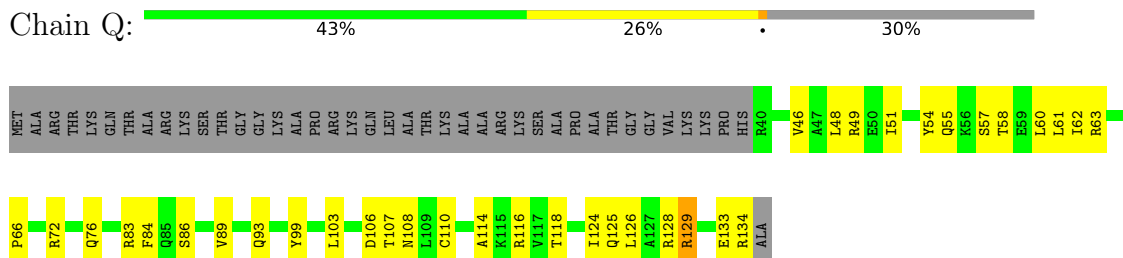
### 3 Residue-property plots [i](#)

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.

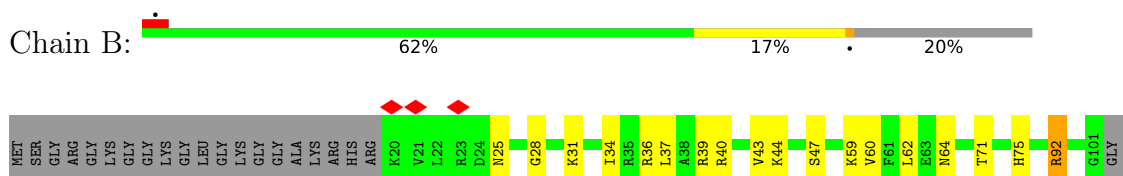
- Molecule 1: Histone H3.2



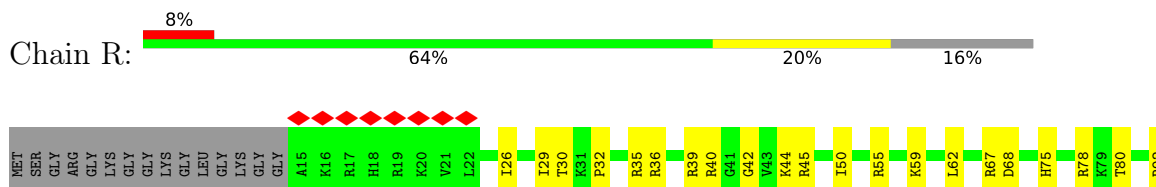
- Molecule 1: Histone H3.2



- Molecule 2: Histone H4



- Molecule 2: Histone H4

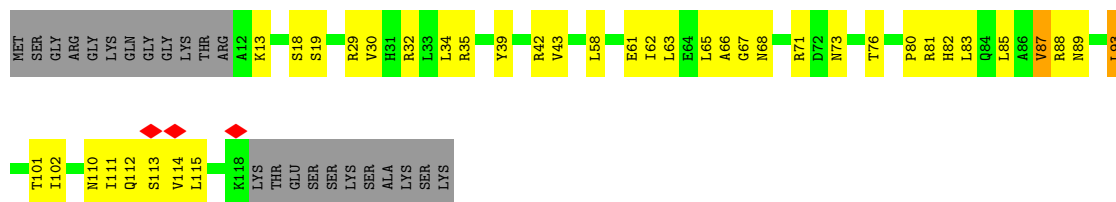






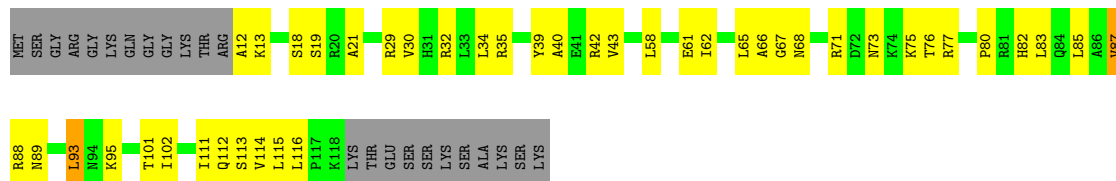
- Molecule 3: Histone H2A

Chain O: 52% 28% 18%



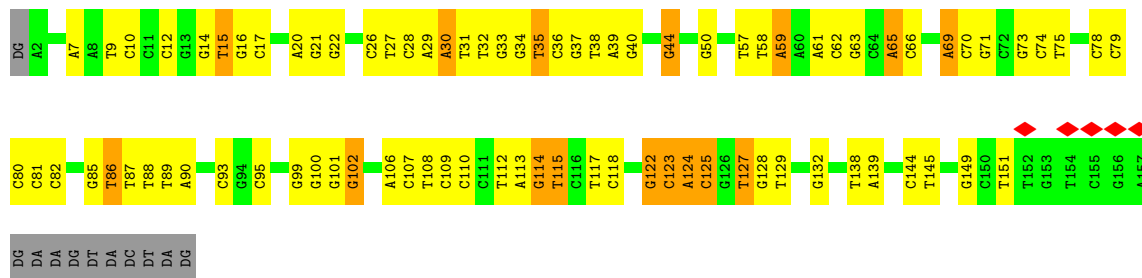
- Molecule 3: Histone H2A

Chain S: 49% 32% 18%



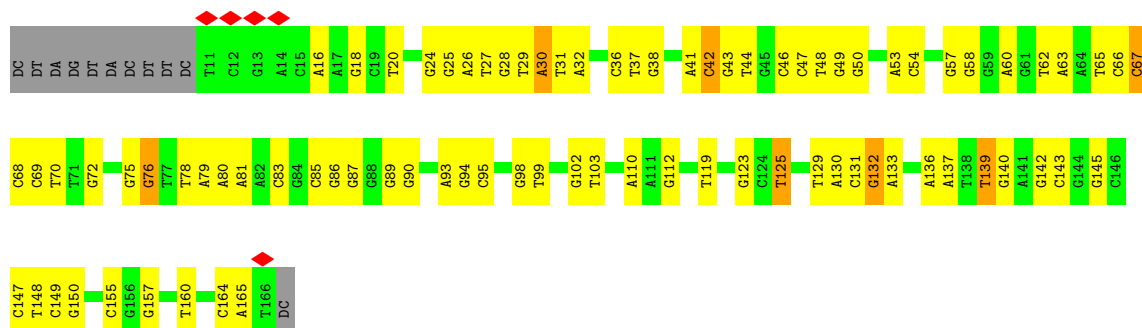
- Molecule 4: DNA 167


Chain U: 43% 41% 10% 7%

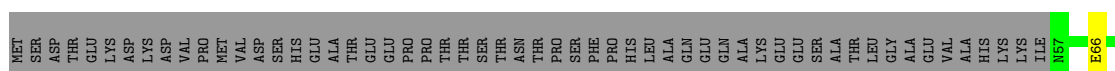


- Molecule 5: DNA 167

Chain W: 44% 46% 7%

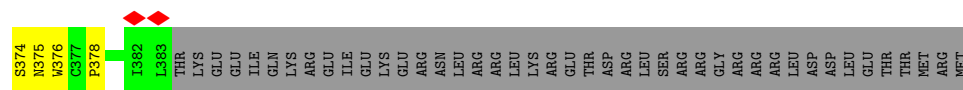


- Chain f:  83% 17%

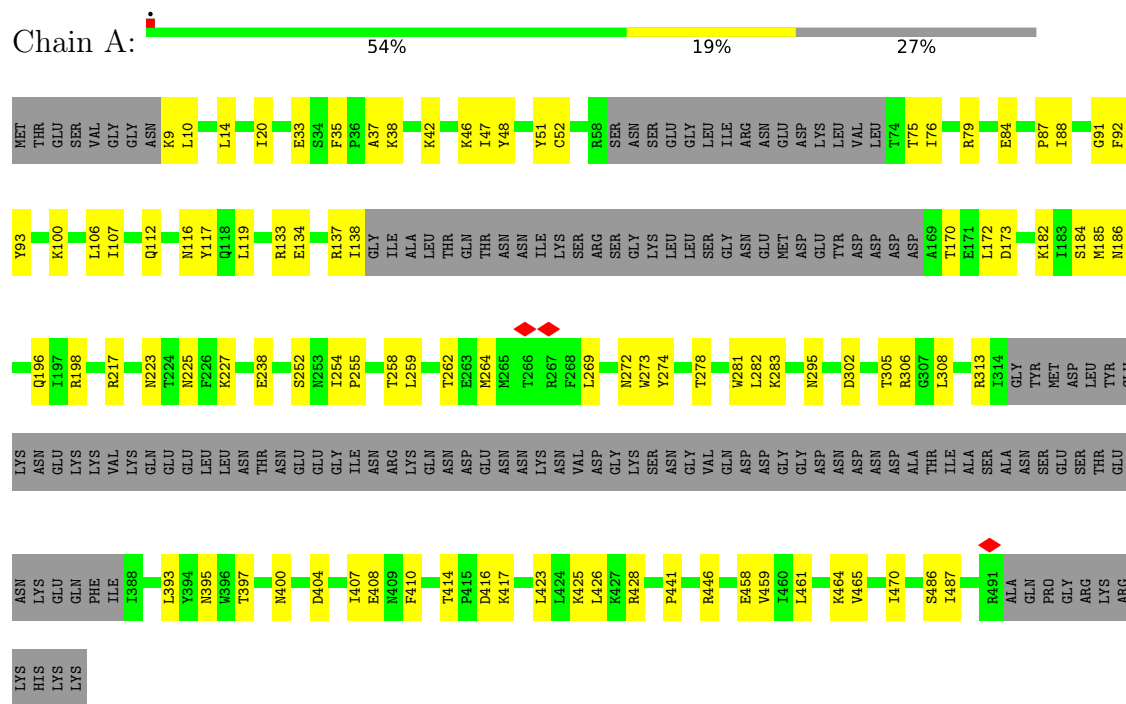




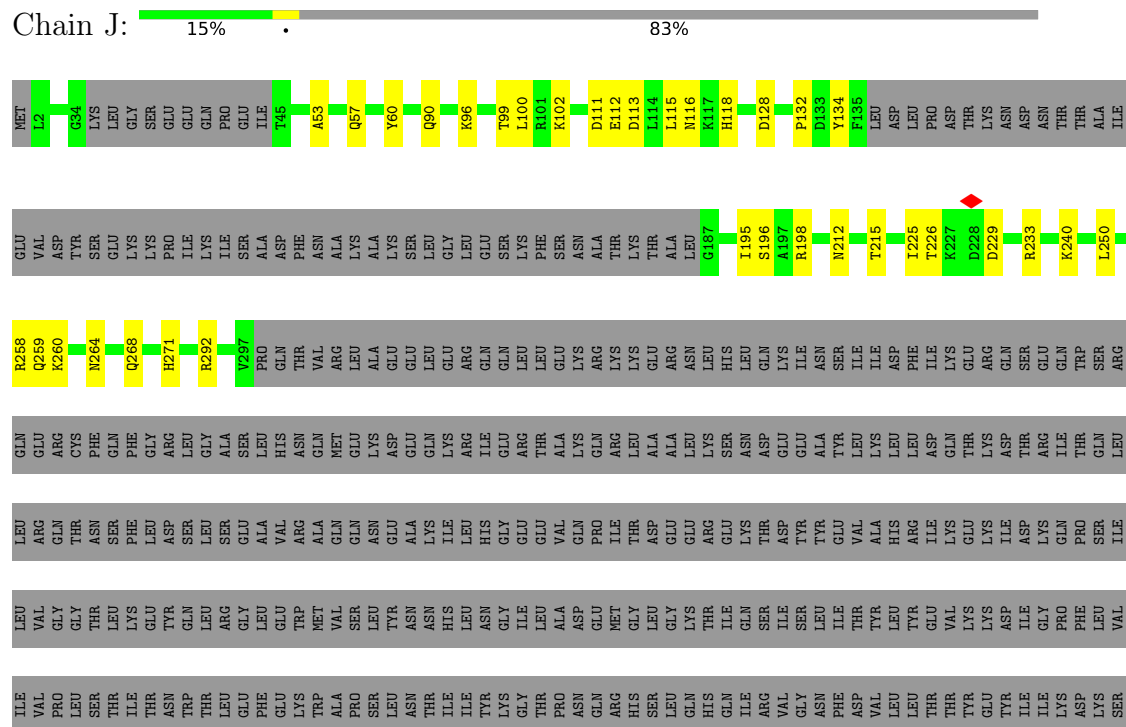




• Molecule 13: Chromatin structure-remodeling complex protein RSC58



• Molecule 14: Nuclear protein STH1/NPS1



- Molecule 14: Nuclear protein STH1/NPS1

VAL	ARG	LEU	ALA	GLU	GLU	LEU	GLU	ARG	GLN	GLN	LEU	LEU	E314	I334	R337	Q338	E339	E340	Q350	F351	L354	N360	E363	K364	Q367	K368	R369	E371	R372	T373	A374	K375	Q376	R377	L378	A379	A380	L381	K382	SER	ASN	ASP	GLU	GLU	ALA	THR	LEU	LYS	LEU	ASP	
GLN	THR	LYS	ASP	THR	LYS	GLN	THR	GLN	LEU	ARG	GLN	THR	ASN	SER	PHE	LEU	SER	LEU	GLU	VAL	ALA	ARG	GLN	ASN	LYS	ILE	LEU	LEU	VAL	GLU	PRO	ILE	THR	ASP	GLY	ARG	LYS	THR	THR	ASP	TYR	VAL	GLU	THR	VAL	ALA	HIS	GLU	ALA	THR	ILE
LYS	GLY	LYS	ILE	ASP	THR	LYS	ASP	PRO	LYS	VAL	VAL	GLY	THR	LEU	LYS	TYR	GLN	LEU	GLY	TRP	MET	ALA	VAL	ASN	HIS	ILE	GLY	GLY	PRO	ALA	ASN	GLM	GLM	THR	GLY	HIS	GLN	ARG	GLY	VAL	GLY	LYS	GLU	THR	THR	TYR	LEU	THR	GLU		
VAL	LYS	LYS	ASP	ILE	GLY	PRO	PHE	LEU	VAL	VAL	ILE	SER	THR	ILE	THR	ASN	TRP	THR	GLU	PHE	LYS	ALA	THR	THR	ILE	LEU	LEU	GLY	THR	PRO	ASN	ASN	GLN	SER	LEU	GLN	ARG	HIS	GLN	ILE	ARG	VAL	GLY	THR	ASP	VAL	GLU	THR	THR		
THR	TYR	GLU	TYR	TRP	TRP	ALA	ILE	ASN	PHE	VAL	SER	GLY	ASN	THR	TRP	ALA	ASP	ILE	ASP	GLU	THR	MET	PRO	GLY	THR	THR	GLY	LEU	LEU	GLY	THR	HIS	THR	ARG	THR	THR	THR	THR	THR	THR	GLY	VAL	THR	THR	PRO	GLN	ASN	LEU	THR		
PRO	GLU	LEU	TRP	ALA	LEU	ASN	PHE	VAL	VAL	LEU	PRO	LYS	ILE	PHE	ASN	LYS	VAL	GLY	GLY	THR	PHE	PRO	GLY	THR	THR	GLY	LEU	GLY	LEU	THR	THR	HIS	THR	ILE	GLY	ALA	ARG	ARG	THR	THR	GLY	THR	VAL	ARG	PRO	PHE	LEU	LEU			
LEU	ARG	ARG	LEU	LYS	GLY	VAL	VAL	ASP	GLY	PRO	ASP	PRO	LYS	ILE	VAL	VAL	GLY	LYS	LEU	GLY	ASN	GLY	LEU	GLN	GLN	GLN	MET	LYS	ALA	ALA	PHE	THR	LEU	THR	THR	GLY	ALA	THR	LYS	THR	GLY	GLY	ILE	ILE	GLY	ASN	ASN	ASN			
LYS	ILE	MET	GLN	LEU	LYS	ILE	CYS	ASN	HIS	PRO	PHE	VAL	PHE	VAL	ASN	PRO	GLY	VAL	ASN	PRO	GLY	THR	GLY	THR	GLN	MET	VAL	ALA	GLY	LYS	PHE	LEU	LEU	GLY	VAL	VAL	ALA	SER	LEU	GLY	THR	GLY	HIS	VAL	LEU	MET	PHE				
GLN	MET	THR	GLN	VAL	ASP	MET	ASP	ILE	GLU	PHE	LEU	ARG	MET	MET	LYS	VAL	VAL	VAL	ASN	GLY	THR	SER	GLY	THR	THR	GLU	ASN	ALA	ALA	ALA	PRO	ASP	VAL	VAL	ALA	THR	LYS	GLY	THR	ARG	THR	GLY	GLY	LEU	GLY	LEU	GLY				
ASN	LEU	GLN	THR	ALA	ASP	THR	VAL	ASP	PHE	THR	ASP	THR	TRP	ASN	PRO	HIS	GLN	ASP	LEU	ARG	ALA	THR	GLN	LYS	ILE	LEU	ARG	GLU	VAL	ARG	ILE	THR	THR	ILE	ILE	VAL	ILE	THR	GLU	ARG	THR	ALA	GLU	ARG	GLN	LYS	LEU	ASP			
ILE	ASP	GLY	LYS	VAL	GLN	ALA	GLY	THR	ASN	LYS	ALA	GLY	THR	THR	ALA	GLU	LEU	ALA	PHE	LEU	ARG	ILE	THR	THR	ASP	ASP	ASP	ALA	GLU	LEU	ILE	GLU	GLY	THR	LEU	ALA	ARG	THR	LEU	ALA	THR	GLY	THR	ARG	THR	LYS	LEU				
PHE	ASP	LYS	ILE	ASP	GLY	GLY	ASP	ASN	GLU	ALA	ALA	ASP	ASP	ASP	LYS	GLN	GLY	LEU	PRO	PRO	ARG	LEU	THR	GLY	THR	GLU	PRO	VAL	VAL	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
LYS	ARG	VAL	TYR	TYR	ASP	GLY	ASP	GLY	THR	GLN	PHE	GLU	ASP	LEU	VAL	GLU	VAL	GLU	ASP	GLY	ASP	GLY	ASP	GLY	ARG	GLY	LEU	LEU	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
SER	GLU	THR	SER	LEU	ASN	ASN	PHE	THR	ALA	THR	ALA	VAL	VAL	VAL	GLU	GLU	THR	GLY	THR	THR	ALA	THR	THR	ARG	LYS	LYS	THR	THR	ILE	ILE	LYS	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
ASN	GLY	ALA	LYS	VAL	GLU	GLU	VAL	LYS	SER	SER	ILE	ILE	ASN	SER	GLY	ASN	GLY	SER	LYS	LYS	LYS	VAL	VAL	ILE	LYS	THR	THR	VAL	VAL	GLU	GLU	ASN	ASN	ASP	GLY	THR	GLU	GLU	LYS	GLU	PRO	GLU	GLU	PRO	GLU	SER	LYS	ALA			
LYS	LYS	THR	ALA	LYS	THR	LYS	THR	LYS	SER	SER	PHE	THR	THR	LEU	PRO	THR	VAL	ARG	GLU	VAL	GLU	LEU	LEU	ASN	PRO	HIS	ASN	THR	ARG	THR	THR	ILE	PHE	GLY	LYS	LYS	THR	LYS	TYR	THR	ASP	THR	VAL	ILE	THR	GLU	THR	GLU			
GLU	LYS	PRO	MET	ILE	ASP	ILE	LYS	LYS	LYS	LYS	ASN	CYS	LYS	ASN	THR	THR	THR	GLU	VAL	ARG	GLN	THR	THR	THR	ASN	ASN	GLU	GLY	GLY	SER	TRP	VAL	TYR	VAL	VAL	ASP	ALA	ASP	LYS	ARG	ASN	GLU	THR	VAL	PHE						
LYS	GLU	HIS	SER	SER																																															

● Molecule 14: Nuclear protein STH1/NPS1









[illegible]

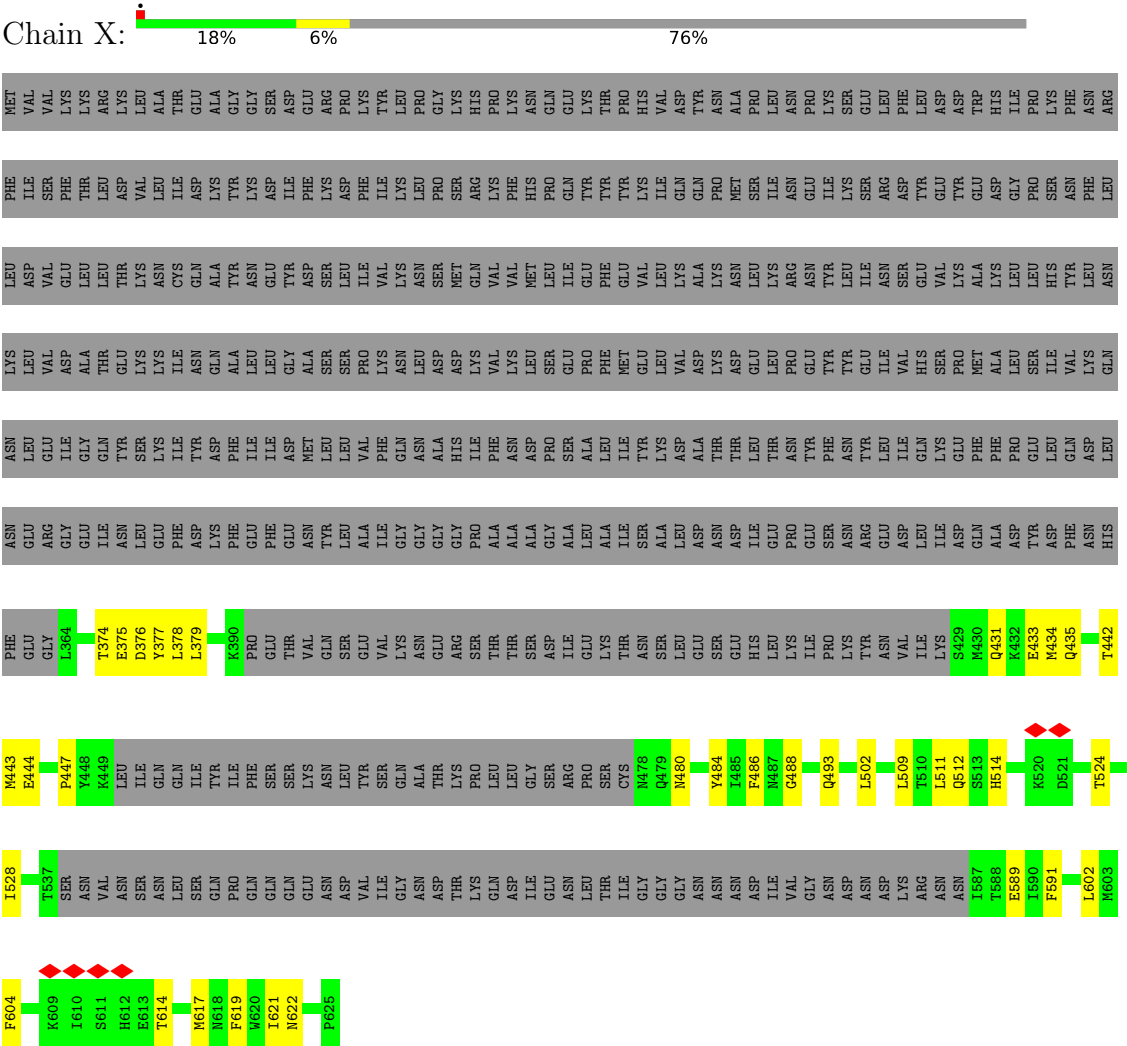
- Molecule 17: Chromatin structure-remodeling complex protein RSC3

Chain K:  5%  95%

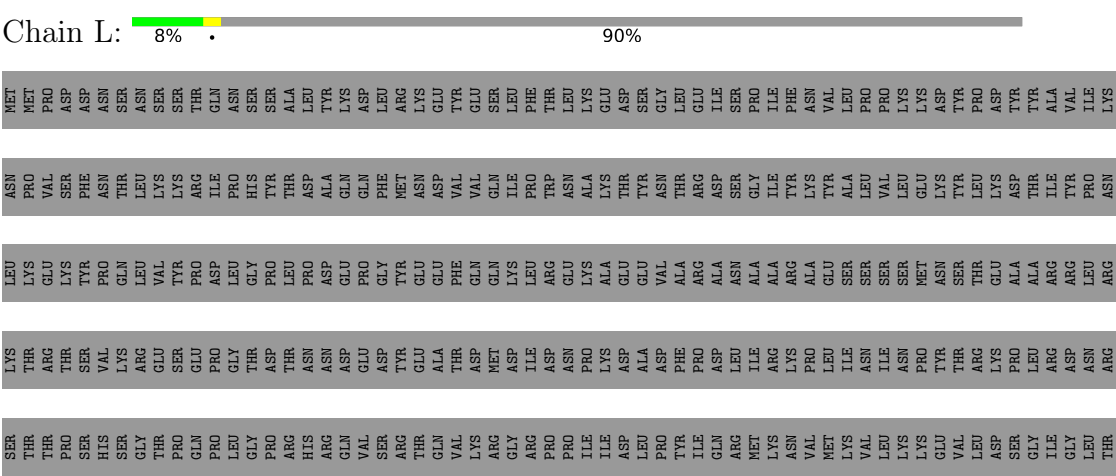
[illegible]

THR  
LYS  
GLU  
ASN  
PHE  
ASN  
GLU  
VAL  
PHE  
GLU  
ALA  
ILE  
ARG  
SER

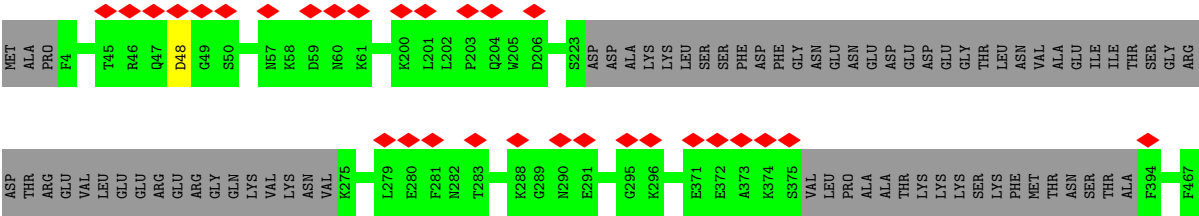
● Molecule 18: Chromatin structure-remodeling complex subunit RSC4



● Molecule 19: Chromatin structure-remodeling complex subunit RSC2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45256	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 ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.14, 2.14, 2.14	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	N	0.30	0/822	0.53	0/1102
1	Q	0.29	0/794	0.49	0/1064
2	B	0.31	0/664	0.55	0/889
2	R	0.30	0/711	0.52	0/950
3	O	0.29	0/833	0.56	0/1124
3	S	0.29	0/833	0.56	0/1124
4	U	1.07	9/3567 (0.3%)	1.20	18/5499 (0.3%)
5	W	1.13	4/3607 (0.1%)	1.18	12/5569 (0.2%)
6	f	0.28	0/3295	0.49	0/4454
7	h	0.26	0/501	0.49	0/669
8	F	0.27	0/983	0.53	0/1337
9	D	0.26	0/2557	0.46	0/3442
9	H	0.27	0/3275	0.46	0/4409
10	M	0.29	0/3113	0.53	2/4215 (0.0%)
11	I	0.25	0/1976	0.48	0/2685
12	G	0.27	0/2039	0.53	1/2769 (0.0%)
13	A	0.28	0/3077	0.48	0/4169
14	J	0.25	0/1836	0.46	0/2480
14	V	0.24	0/598	0.37	0/789
14	Y	0.28	0/4580	0.54	0/6167
15	E	0.26	0/480	0.50	0/643
16	C	0.25	0/272	0.41	0/366
17	K	0.27	0/356	0.50	0/483
18	X	0.28	0/1243	0.55	0/1672
19	L	0.27	0/681	0.51	0/921
20	P	0.30	0/728	0.46	0/983
20	T	0.29	0/736	0.45	0/991
21	g	0.28	0/3261	0.50	0/4421
All	All	0.50	13/47418 (0.0%)	0.67	33/65386 (0.1%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	53	DA	N9-C4	-8.46	1.32	1.37
4	U	65	DA	N9-C4	-6.03	1.34	1.37
4	U	99	DG	N9-C4	-5.90	1.33	1.38
5	W	32	DA	N9-C4	-5.74	1.34	1.37
4	U	124	DA	N9-C4	-5.65	1.34	1.37

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	127	DT	O4'-C1'-N1	7.24	113.07	108.00
5	W	67	DC	O4'-C1'-N1	6.60	112.62	108.00
5	W	30	DA	O4'-C4'-C3'	-6.43	101.93	104.50
5	W	27	DT	O4'-C1'-N1	6.43	112.50	108.00
12	G	300	LEU	CA-CB-CG	6.16	129.47	115.30

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	N	810	0	851	18	0
1	Q	784	0	824	30	0
2	B	657	0	706	16	0
2	R	703	0	757	23	0
3	O	823	0	882	33	0
3	S	823	0	882	32	0
4	U	3183	0	1752	74	0
5	W	3213	0	1752	67	0
6	f	3219	0	3240	0	0
7	h	490	0	467	0	0
8	F	964	0	919	24	0
9	D	2510	0	2542	48	0
9	H	3215	0	3196	73	0
10	M	3058	0	3127	53	0
11	I	1944	0	1964	42	0
12	G	1996	0	1948	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	3007	0	3045	70	0
14	J	1814	0	1777	26	0
14	V	592	0	610	4	0
14	Y	4503	0	4573	97	0
15	E	477	0	491	14	0
16	C	269	0	279	3	0
17	K	347	0	342	3	0
18	X	1220	0	1192	22	0
19	L	669	0	693	12	0
20	P	717	0	723	26	0
20	T	725	0	745	21	0
21	g	3191	0	3179	0	0
22	H	1	0	0	0	0
All	All	45924	0	43458	661	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 11.

The worst 5 of 661 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)
14:Y:710:VAL:CG2	14:Y:912:ILE:H	1.60	1.15
14:Y:710:VAL:HG21	14:Y:912:ILE:H	1.17	1.05
14:Y:710:VAL:HG21	14:Y:912:ILE:N	1.74	1.02
14:Y:710:VAL:O	14:Y:712:LYS:HG2	1.77	0.85
14:Y:710:VAL:O	14:Y:712:LYS:N	2.10	0.85

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	Q	93/136 (68%)	90 (97%)	3 (3%)	0	100	100
2	B	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
2	R	85/103 (82%)	81 (95%)	4 (5%)	0	100	100
3	O	105/130 (81%)	98 (93%)	7 (7%)	0	100	100
3	S	105/130 (81%)	98 (93%)	7 (7%)	0	100	100
6	f	391/477 (82%)	382 (98%)	9 (2%)	0	100	100
7	h	46/157 (29%)	44 (96%)	2 (4%)	0	100	100
8	F	116/435 (27%)	104 (90%)	12 (10%)	0	100	100
9	D	295/557 (53%)	282 (96%)	13 (4%)	0	100	100
9	H	387/557 (70%)	360 (93%)	27 (7%)	0	100	100
10	M	378/581 (65%)	349 (92%)	29 (8%)	0	100	100
11	I	236/483 (49%)	220 (93%)	16 (7%)	0	100	100
12	G	238/426 (56%)	221 (93%)	17 (7%)	0	100	100
13	A	357/502 (71%)	332 (93%)	25 (7%)	0	100	100
14	J	229/1359 (17%)	203 (89%)	26 (11%)	0	100	100
14	V	67/1359 (5%)	67 (100%)	0	0	100	100
14	Y	536/1359 (39%)	483 (90%)	52 (10%)	1 (0%)	47	81
15	E	56/78 (72%)	54 (96%)	2 (4%)	0	100	100
16	C	31/883 (4%)	31 (100%)	0	0	100	100
17	K	40/885 (4%)	37 (92%)	3 (8%)	0	100	100
18	X	139/625 (22%)	124 (89%)	15 (11%)	0	100	100
19	L	79/889 (9%)	68 (86%)	11 (14%)	0	100	100
20	P	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
20	T	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
21	g	390/467 (84%)	377 (97%)	13 (3%)	0	100	100
All	All	4757/13069 (36%)	4458 (94%)	298 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	Y	711	GLU

### 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	N	86/111 (78%)	85 (99%)	1 (1%)	71	83
1	Q	83/111 (75%)	82 (99%)	1 (1%)	71	83
2	B	68/79 (86%)	67 (98%)	1 (2%)	65	80
2	R	72/79 (91%)	72 (100%)	0	100	100
3	O	84/102 (82%)	77 (92%)	7 (8%)	11	34
3	S	84/102 (82%)	77 (92%)	7 (8%)	11	34
6	f	356/420 (85%)	356 (100%)	0	100	100
7	h	53/140 (38%)	53 (100%)	0	100	100
8	F	111/388 (29%)	110 (99%)	1 (1%)	78	87
9	D	285/500 (57%)	283 (99%)	2 (1%)	84	90
9	H	363/500 (73%)	362 (100%)	1 (0%)	92	95
10	M	349/521 (67%)	349 (100%)	0	100	100
11	I	223/435 (51%)	222 (100%)	1 (0%)	91	94
12	G	226/384 (59%)	225 (100%)	1 (0%)	91	94
13	A	343/462 (74%)	343 (100%)	0	100	100
14	J	187/1228 (15%)	185 (99%)	2 (1%)	73	84
14	V	63/1228 (5%)	62 (98%)	1 (2%)	62	79
14	Y	502/1228 (41%)	500 (100%)	2 (0%)	91	94
15	E	56/75 (75%)	55 (98%)	1 (2%)	59	77
16	C	32/824 (4%)	32 (100%)	0	100	100
17	K	39/832 (5%)	39 (100%)	0	100	100
18	X	141/578 (24%)	141 (100%)	0	100	100
19	L	77/810 (10%)	77 (100%)	0	100	100
20	P	77/105 (73%)	77 (100%)	0	100	100
20	T	79/105 (75%)	79 (100%)	0	100	100
21	g	362/423 (86%)	361 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4401/11770 (37%)	4371 (99%)	30 (1%)	84	90

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	93	LEU
14	V	368	LYS
8	F	390	ILE
14	Y	947	ASN
14	J	226	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
11	I	29	ASN
14	Y	488	HIS
13	A	223	ASN
14	Y	487	ASN
14	Y	854	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

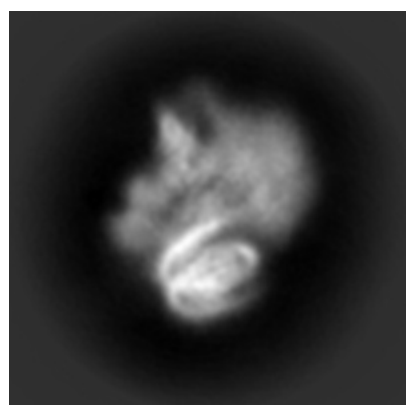
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0778. These allow visual inspection of the internal detail of the map and identification of artifacts.

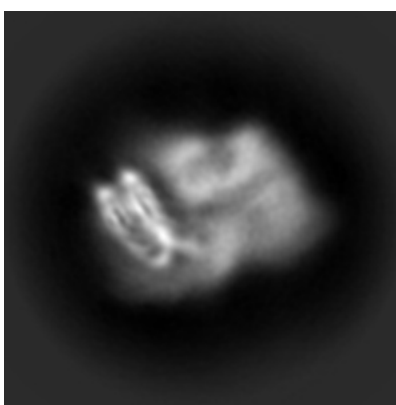
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

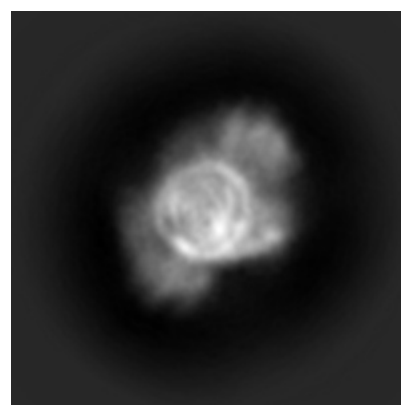
#### 6.1.1 Primary map



X



Y

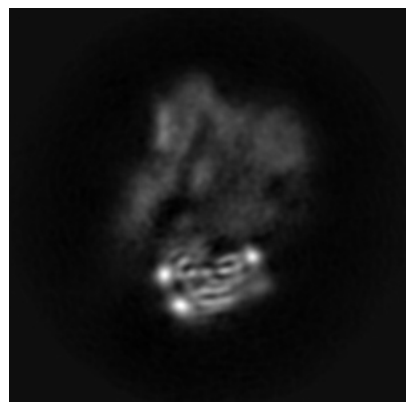


Z

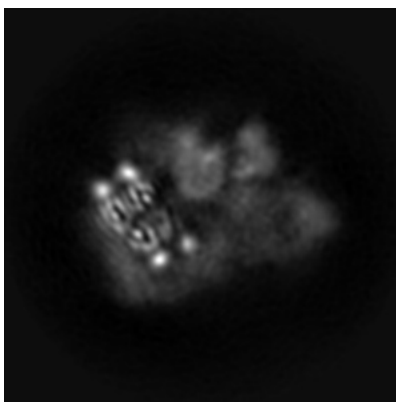
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

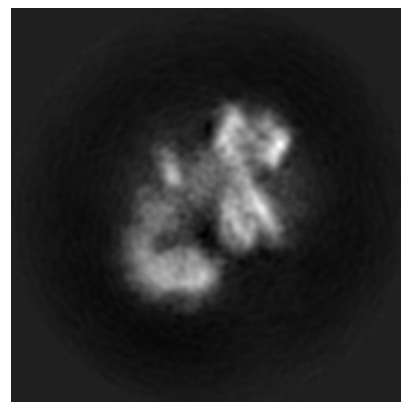
#### 6.2.1 Primary map



X Index: 90



Y Index: 90

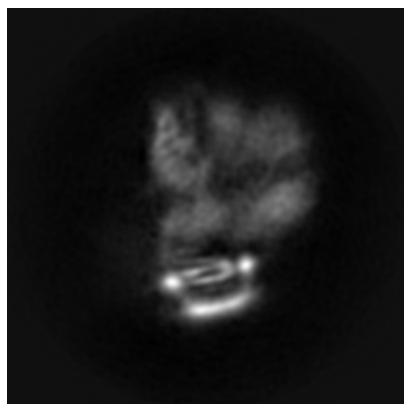


Z Index: 90

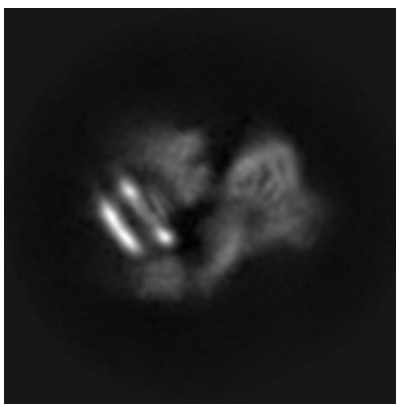
The images above show central slices of the map in three orthogonal directions.

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

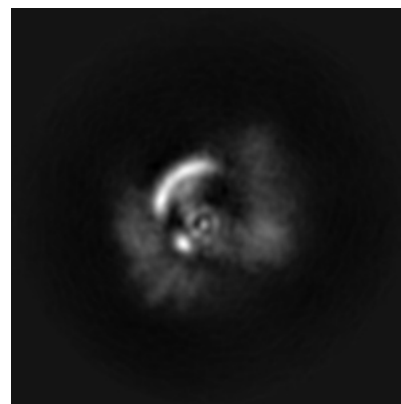
### 6.3.1 Primary map



X Index: 97



Y Index: 74

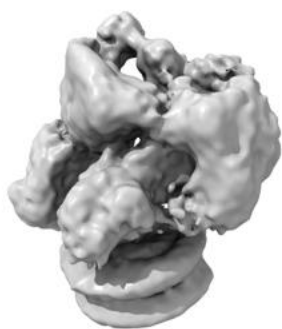


Z Index: 71

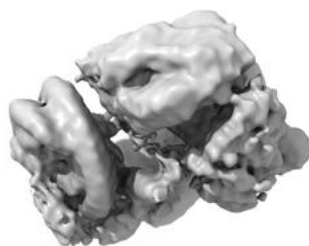
The images above show the largest variance slices of the map in three orthogonal directions.

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

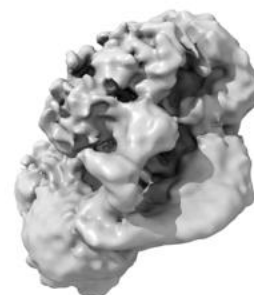
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

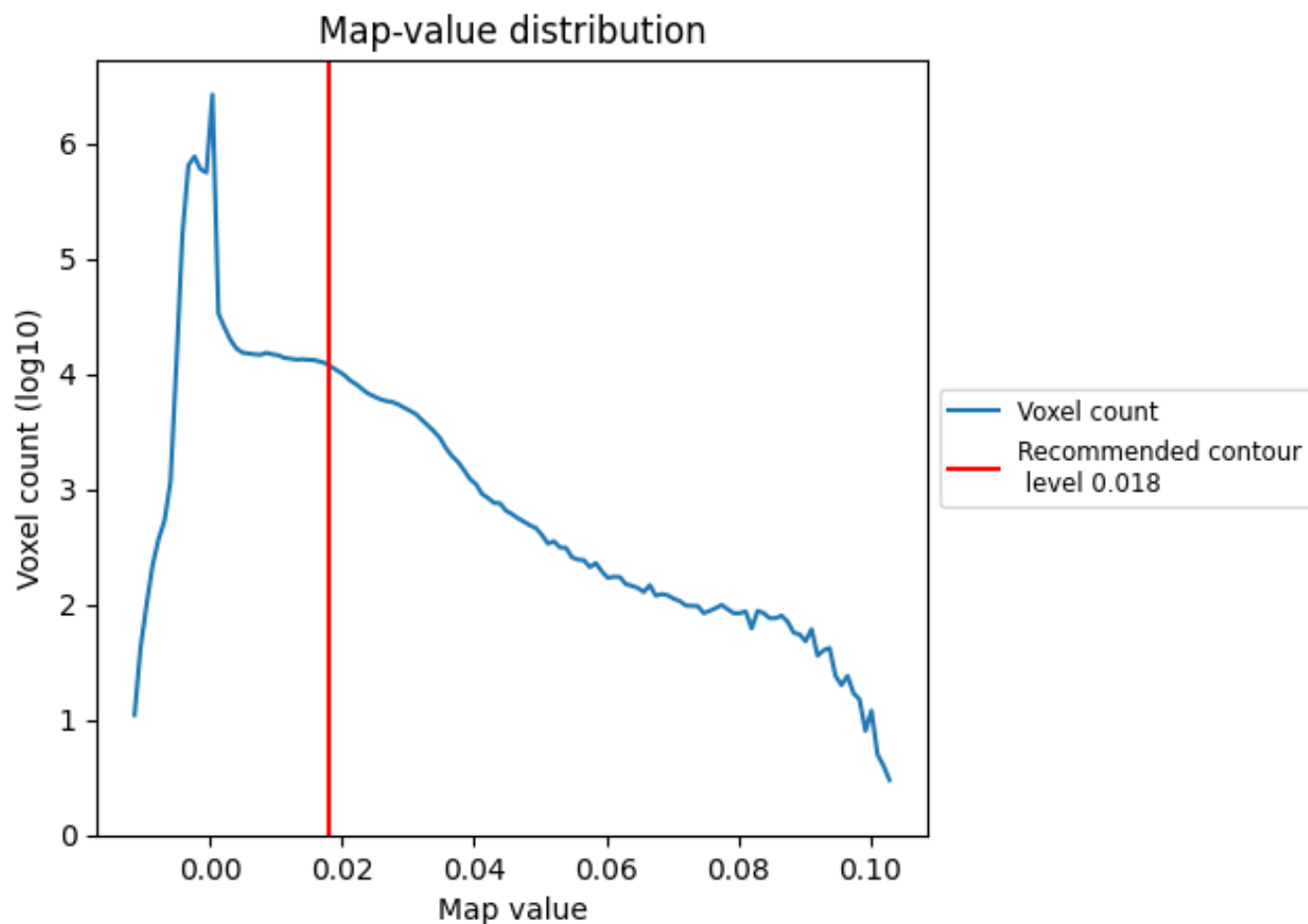
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

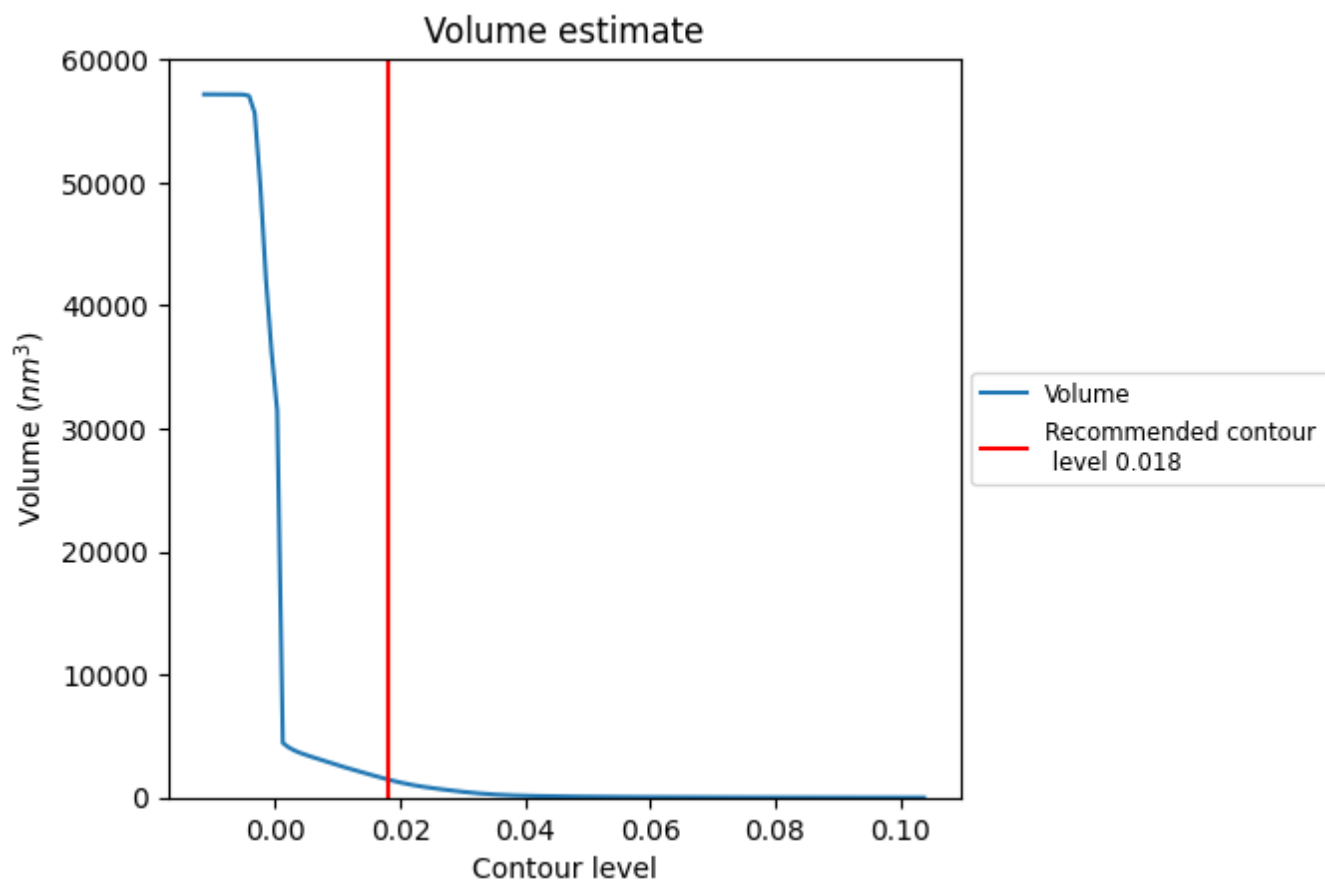
This section contains the results of statistical analysis of the map.

### 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.

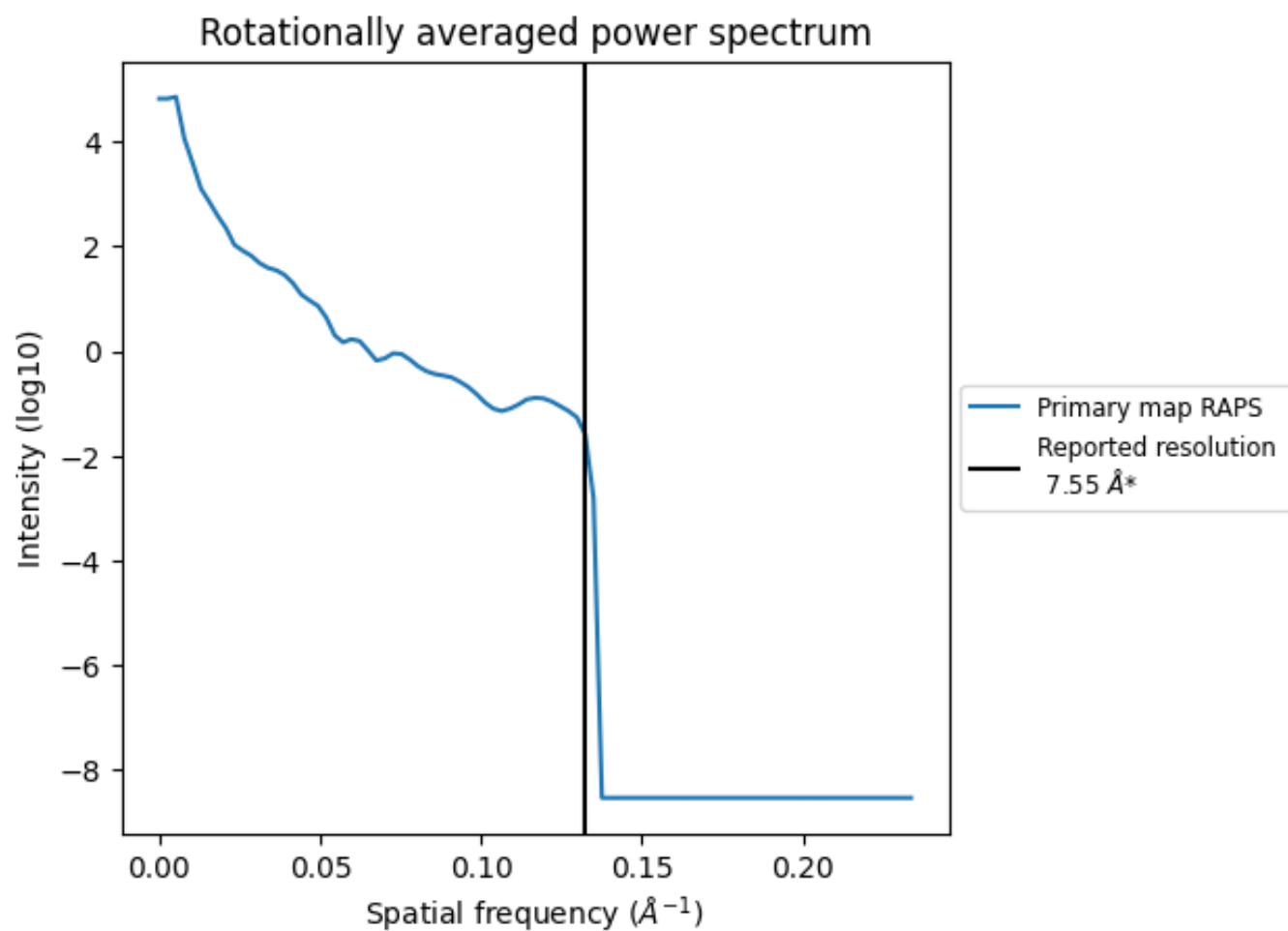
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1474 nm<sup>3</sup>; this corresponds to an approximate mass of 1331 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 0.132 Å<sup>-1</sup>

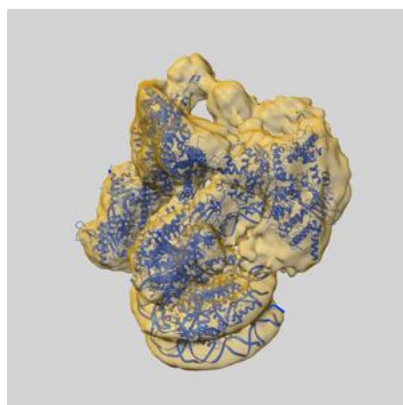
## 8 Fourier-Shell correlation

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

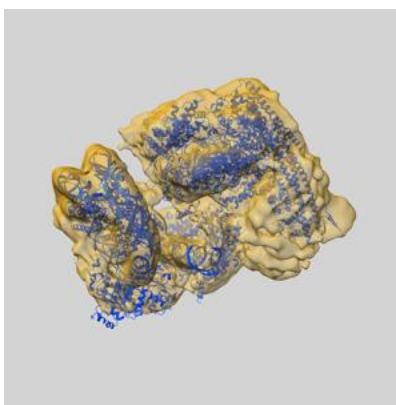
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0778 and PDB model 6KW4. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

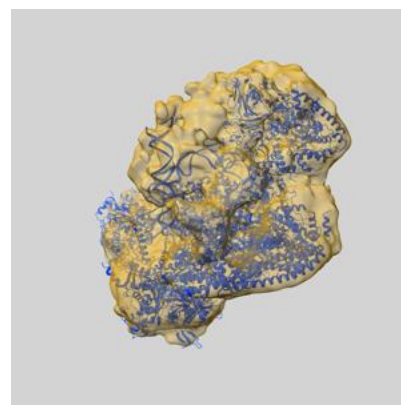
### 9.1 Map-model overlay [i](#)



X



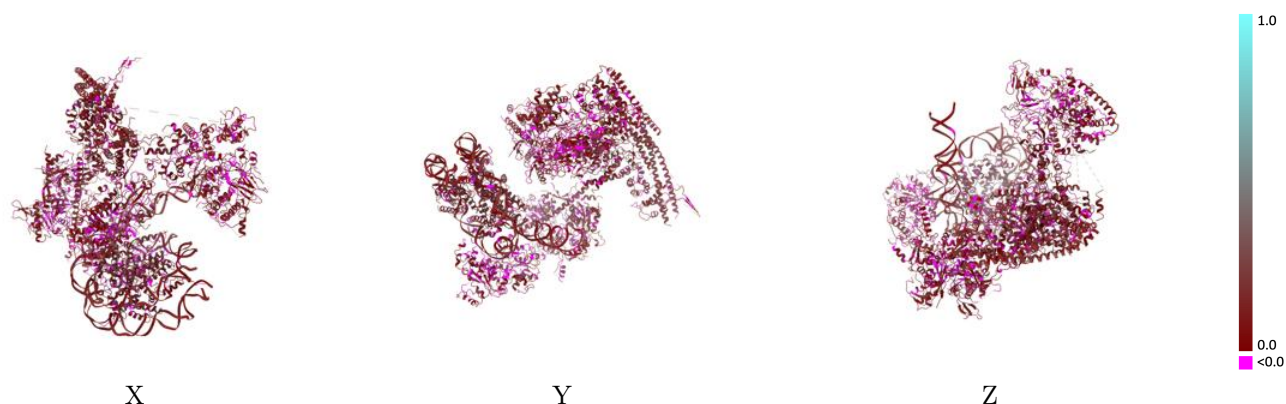
Y



Z

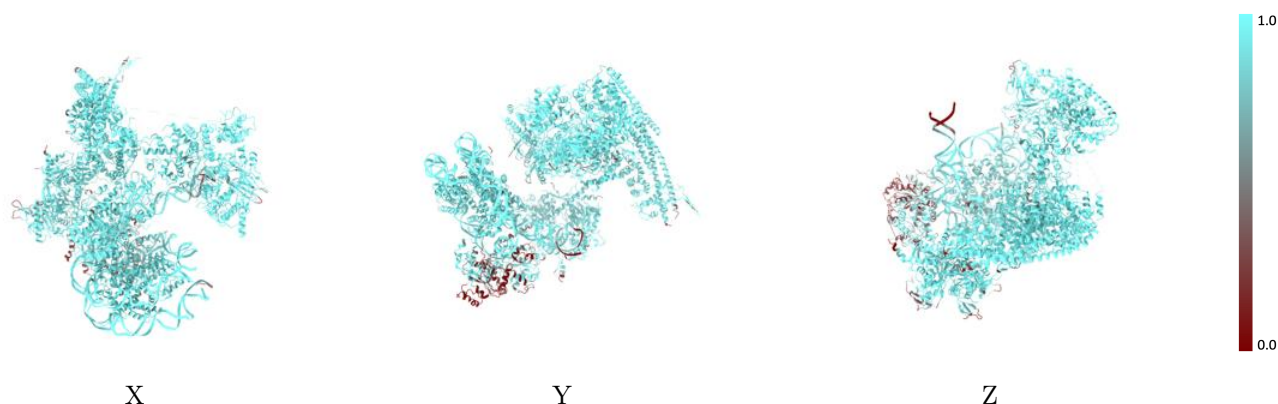
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



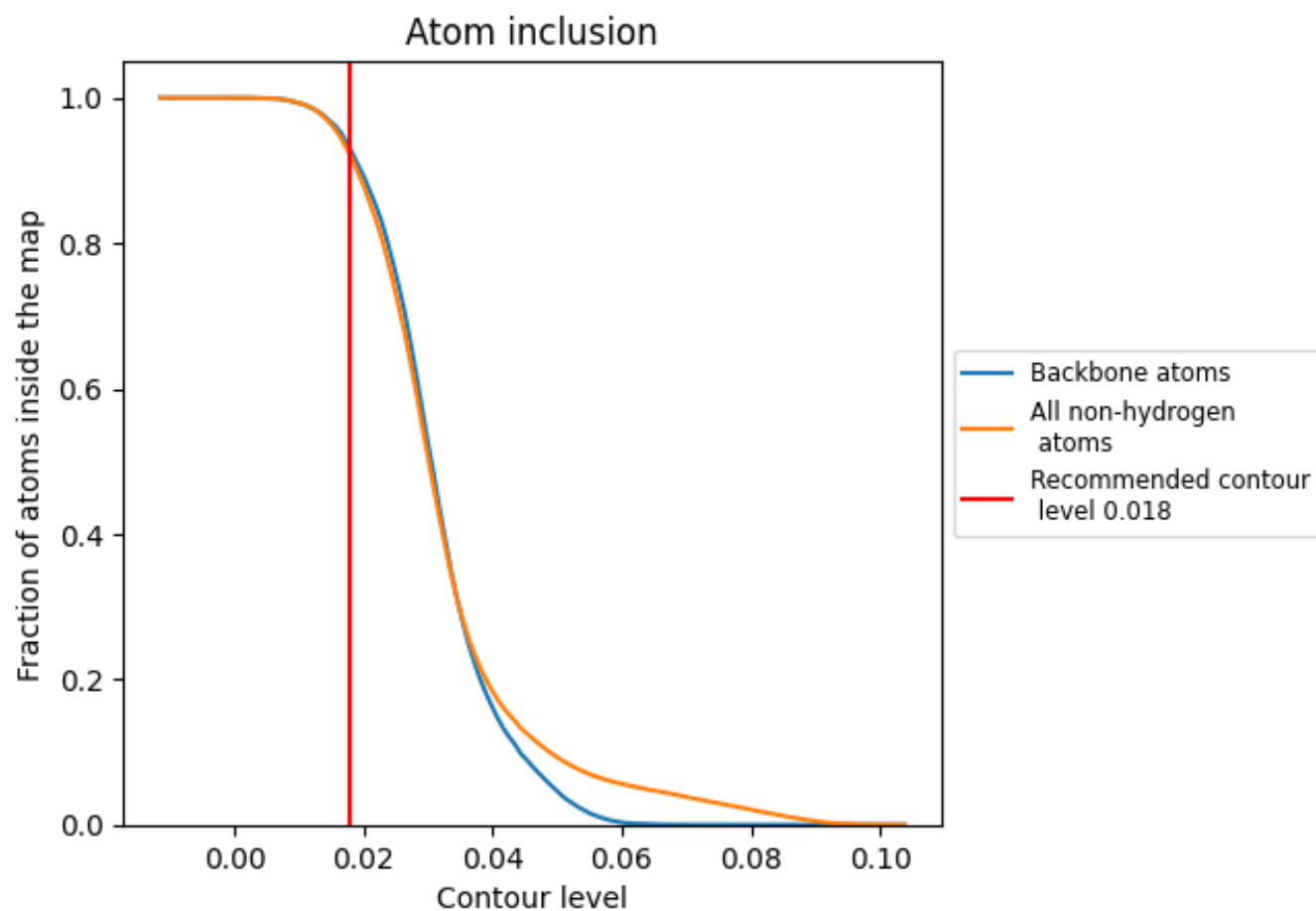
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).



























































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9205	 0.0990
A	 0.9844	 0.0990
B	 0.9588	 0.1370
C	 0.9703	 0.1140
D	 0.9773	 0.1080
E	 0.9957	 0.1150
F	 0.9725	 0.0990
G	 0.9512	 0.0870
H	 0.9779	 0.1040
I	 0.9727	 0.1180
J	 0.9747	 0.0830
K	 0.9067	 0.1210
L	 0.9465	 0.0440
M	 0.9794	 0.1170
N	 0.9653	 0.1300
O	 0.9361	 0.1150
P	 0.9929	 0.1580
Q	 0.9907	 0.1440
R	 0.9138	 0.1290
S	 0.9962	 0.1360
T	 0.9661	 0.1490
U	 0.9566	 0.1270
V	 0.7435	 0.0870
W	 0.9452	 0.1230
X	 0.9320	 0.0820
Y	 0.5682	 0.0540
f	 0.9768	 0.0780
g	 0.9040	 0.0540
h	 0.9366	 0.0660

