



Full wwPDB EM Validation Report ⓘ

Sep 1, 2026 – 04:28 pm BST

PDB ID : 9RN2 / pdb_00009rn2
EMDB ID : EMD-54078
Title : Structure of BAF in complex with OCT4-SOX2-bound nucleosome - SHL+6 class 2
Authors : Vecchia, L.; Weiss, J.; Cavadini, S.; Kempf, G.; Kater, L.; Pathare, G.; Thoma, N.H.
Deposited on : 2025-06-19
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

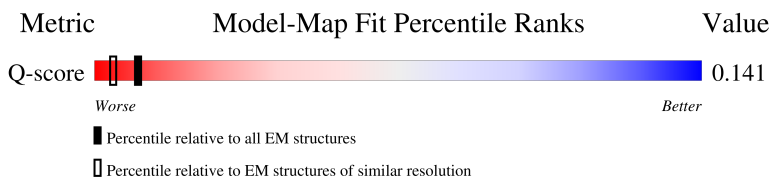
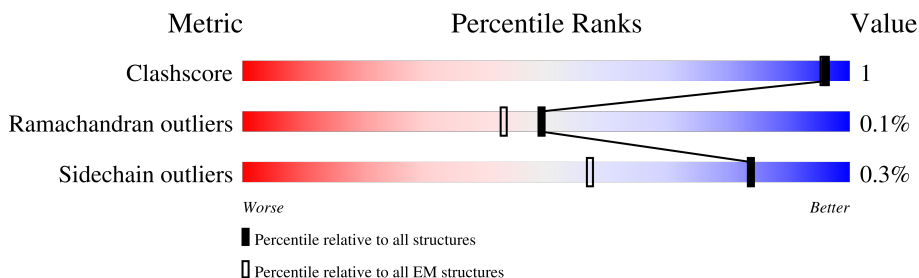
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	139	
1	E	139	
2	B	106	
2	F	106	

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Mol	Chain	Length	Quality of chain
3	C	133	
3	G	133	
4	D	128	
4	H	128	
5	I	1647	
6	J	429	
7	K	375	
8	L	2285	
9	M	385	
10	N	1214	
10	O	1214	
11	P	515	
12	R	435	
13	V	645	
14	W	105	
15	X	227	
16	Y	227	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 23353 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	95	Total	C	N	O	S	0	0
			783	494	150	135	4		
1	E	95	Total	C	N	O	S	0	0
			783	494	150	135	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P68431
A	-1	SER	-	expression tag	UNP P68431
A	0	HIS	-	expression tag	UNP P68431
E	-2	GLY	-	expression tag	UNP P68431
E	-1	SER	-	expression tag	UNP P68431
E	0	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
2	F	80	Total	C	N	O	S	0	0
			641	405	125	110	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62805
B	-1	SER	-	expression tag	UNP P62805
B	0	HIS	-	expression tag	UNP P62805
F	-2	GLY	-	expression tag	UNP P62805
F	-1	SER	-	expression tag	UNP P62805
F	0	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	110	Total	C	N	O	0	0
			844	531	167	146		
3	G	110	Total	C	N	O	0	0
			844	531	167	146		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P04908
C	-1	SER	-	expression tag	UNP P04908
C	0	HIS	-	expression tag	UNP P04908
G	-2	GLY	-	expression tag	UNP P04908
G	-1	SER	-	expression tag	UNP P04908
G	0	HIS	-	expression tag	UNP P04908

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			726	456	130	138	2		
4	H	92	Total	C	N	O	S	0	0
			720	453	129	136	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P06899
D	-1	SER	-	expression tag	UNP P06899
D	0	HIS	-	expression tag	UNP P06899
H	-2	GLY	-	expression tag	UNP P06899
H	-1	SER	-	expression tag	UNP P06899
H	0	HIS	-	expression tag	UNP P06899

- Molecule 5 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	469	Total	C	N	O	0	0
			2352	1414	469	469		

- Molecule 6 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	334	Total	C	N	O	0	0
			1677	1009	334	334		

- Molecule 7 is a protein called Actin, cytoplasmic 1, N-terminally processed.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	317	Total	C	N	O	0	0
			1600	966	317	317		

- Molecule 8 is a protein called AT-rich interactive domain-containing protein 1A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	396	Total	C	N	O	0	0
			1991	1199	396	396		

- Molecule 9 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	295	Total	C	N	O	0	0
			1488	898	295	295		

- Molecule 10 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	N	101	Total	C	N	O	0	0
			510	308	101	101		
10	O	175	Total	C	N	O	0	0
			895	545	175	175		

- Molecule 11 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	P	37	Total	C	N	O	0	0
			189	115	37	37		

- Molecule 12 is a protein called Zinc finger protein ubi-d4.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	R	70	Total	C	N	O	0	0
			351	211	70	70		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	392	GLY	-	expression tag	UNP Q92785
R	393	THR	-	expression tag	UNP Q92785
R	394	LEU	-	expression tag	UNP Q92785
R	395	GLU	-	expression tag	UNP Q92785
R	396	VAL	-	expression tag	UNP Q92785
R	397	LEU	-	expression tag	UNP Q92785
R	398	PHE	-	expression tag	UNP Q92785
R	399	GLN	-	expression tag	UNP Q92785
R	400	GLY	-	expression tag	UNP Q92785
R	401	PRO	-	expression tag	UNP Q92785
R	402	GLY	-	expression tag	UNP Q92785
R	403	GLY	-	expression tag	UNP Q92785
R	404	SER	-	expression tag	UNP Q92785
R	405	GLY	-	expression tag	UNP Q92785
R	406	SER	-	expression tag	UNP Q92785
R	407	ALA	-	expression tag	UNP Q92785
R	408	TRP	-	expression tag	UNP Q92785
R	409	SER	-	expression tag	UNP Q92785
R	410	HIS	-	expression tag	UNP Q92785
R	411	PRO	-	expression tag	UNP Q92785
R	412	GLN	-	expression tag	UNP Q92785
R	413	PHE	-	expression tag	UNP Q92785
R	414	GLU	-	expression tag	UNP Q92785
R	415	LYS	-	expression tag	UNP Q92785
R	416	GLY	-	expression tag	UNP Q92785
R	417	GLY	-	expression tag	UNP Q92785
R	418	GLY	-	expression tag	UNP Q92785
R	419	SER	-	expression tag	UNP Q92785
R	420	GLY	-	expression tag	UNP Q92785
R	421	GLY	-	expression tag	UNP Q92785
R	422	GLY	-	expression tag	UNP Q92785
R	423	SER	-	expression tag	UNP Q92785
R	424	GLY	-	expression tag	UNP Q92785
R	425	GLY	-	expression tag	UNP Q92785
R	426	SER	-	expression tag	UNP Q92785
R	427	ALA	-	expression tag	UNP Q92785
R	428	TRP	-	expression tag	UNP Q92785
R	429	SER	-	expression tag	UNP Q92785
R	430	HIS	-	expression tag	UNP Q92785
R	431	PRO	-	expression tag	UNP Q92785
R	432	GLN	-	expression tag	UNP Q92785
R	433	PHE	-	expression tag	UNP Q92785

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Chain	Residue	Modelled	Actual	Comment	Reference
R	434	GLU	-	expression tag	UNP Q92785
R	435	LYS	-	expression tag	UNP Q92785

- Molecule 13 is a protein called Green fluorescent protein,POU domain, class 5, transcription factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	V	68	Total	C	N	O	0	0
			275	139	68	68		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-272	MET	-	initiating methionine	UNP P42212
V	-271	ASP	-	expression tag	UNP P42212
V	-270	TRP	-	expression tag	UNP P42212
V	-269	SER	-	expression tag	UNP P42212
V	-268	HIS	-	expression tag	UNP P42212
V	-267	PRO	-	expression tag	UNP P42212
V	-266	GLN	-	expression tag	UNP P42212
V	-265	PHE	-	expression tag	UNP P42212
V	-264	GLU	-	expression tag	UNP P42212
V	-263	LYS	-	expression tag	UNP P42212
V	-262	SER	-	expression tag	UNP P42212
V	-261	ALA	-	expression tag	UNP P42212
V	-260	VAL	-	expression tag	UNP P42212
V	-259	ASP	-	expression tag	UNP P42212
V	-258	GLU	-	expression tag	UNP P42212
V	-257	ASN	-	expression tag	UNP P42212
V	-256	LEU	-	expression tag	UNP P42212
V	-255	TYR	-	expression tag	UNP P42212
V	-254	PHE	-	expression tag	UNP P42212
V	-253	GLN	-	expression tag	UNP P42212
V	-252	GLY	-	expression tag	UNP P42212
V	-251	GLY	-	expression tag	UNP P42212
V	-250	GLY	-	expression tag	UNP P42212
V	-249	ARG	-	expression tag	UNP P42212
V	-248	MET	-	expression tag	UNP P42212
V	-247	VAL	-	expression tag	UNP P42212
V	-184	LEU	PHE	conflict	UNP P42212
V	-183	THR	SER	conflict	UNP P42212
V	-42	LYS	ALA	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-17	LEU	HIS	conflict	UNP P42212
V	-9	GLU	-	linker	UNP P42212
V	-8	ALA	-	linker	UNP P42212
V	-7	ALA	-	linker	UNP P42212
V	-6	ALA	-	linker	UNP P42212
V	-5	LYS	-	linker	UNP P42212
V	-4	GLU	-	linker	UNP P42212
V	-3	ALA	-	linker	UNP P42212
V	-2	ALA	-	linker	UNP P42212
V	-1	ALA	-	linker	UNP P42212
V	0	LYS	-	linker	UNP P42212
V	361	LEU	-	expression tag	UNP Q01860
V	362	PRO	-	expression tag	UNP Q01860
V	363	GLU	-	expression tag	UNP Q01860
V	364	THR	-	expression tag	UNP Q01860
V	365	GLY	-	expression tag	UNP Q01860
V	366	GLY	-	expression tag	UNP Q01860
V	367	HIS	-	expression tag	UNP Q01860
V	368	HIS	-	expression tag	UNP Q01860
V	369	HIS	-	expression tag	UNP Q01860
V	370	HIS	-	expression tag	UNP Q01860
V	371	HIS	-	expression tag	UNP Q01860
V	372	HIS	-	expression tag	UNP Q01860

- Molecule 14 is a protein called Transcription factor SOX-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	W	73	Total	C	N	O	0	0
			373	227	73	73		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	14	MET	-	initiating methionine	UNP P48431
W	15	ASP	-	expression tag	UNP P48431
W	16	TRP	-	expression tag	UNP P48431
W	17	SER	-	expression tag	UNP P48431
W	18	HIS	-	expression tag	UNP P48431
W	19	PRO	-	expression tag	UNP P48431
W	20	GLN	-	expression tag	UNP P48431
W	21	PHE	-	expression tag	UNP P48431
W	22	GLU	-	expression tag	UNP P48431

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Chain	Residue	Modelled	Actual	Comment	Reference
W	23	LYS	-	expression tag	UNP P48431
W	24	SER	-	expression tag	UNP P48431
W	25	ALA	-	expression tag	UNP P48431
W	26	VAL	-	expression tag	UNP P48431
W	27	ASP	-	expression tag	UNP P48431
W	28	GLU	-	expression tag	UNP P48431
W	29	ASN	-	expression tag	UNP P48431
W	30	LEU	-	expression tag	UNP P48431
W	31	TYR	-	expression tag	UNP P48431
W	32	PHE	-	expression tag	UNP P48431
W	33	GLN	-	expression tag	UNP P48431
W	34	GLY	-	expression tag	UNP P48431
W	35	GLY	-	expression tag	UNP P48431
W	36	MET	-	expression tag	UNP P48431

- Molecule 15 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	138	Total	C	N	O	P	0	0
			2803	1334	496	835	138		

- Molecule 16 is a DNA chain called DNA (147-MER).

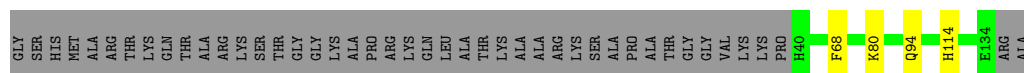
Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	138	Total	C	N	O	P	0	0
			2855	1349	547	821	138		

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.

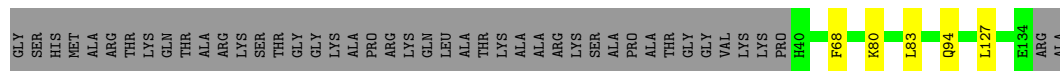
- Molecule 1: Histone H3.1

Chain A:  65% 32%



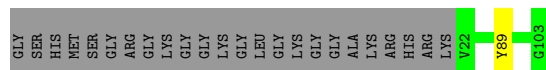
- Molecule 1: Histone H3.1

Chain E:  65% 32%



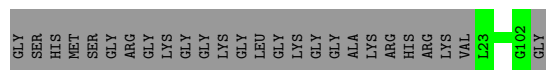
- Molecule 2: Histone H4

Chain B:  76% 23%



- Molecule 2: Histone H4

Chain F:  75% 25%



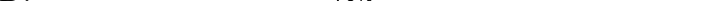
- Molecule 3: Histone H2A type 1-B/E

Chain C:  80% 17%

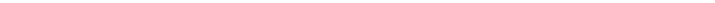


- Molecule 3: Histone H2A type 1-B/E

GLY	SER	HIS	MET	SER	GLY	ARG	GLY	LYS	GLN	GLY	G9	T17	E65	E93	Q113	P118	LYS	LYS	THR	GLU	SER	HIS	HIS	LYS	ALA	LYS	GLY	LYS
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- Chain D:  70% . 27%

GLY	SER	HIS	MET	PRO	GLU	ALA	LYS	SER	ALA	PRO	PRO	LYS	LYS	GLY	SER	LYS	ALA	VAL	THR	LYS	ALA	GLN	LYS	LYS	ASP	GLY	LYS	LYS	ARG	LYS	ARG	S33	Y84	G105	K121	Y122	A125
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- Chain H:  69% . 28%

GLY	HIS	PRO	GLU	PRO	ALA	LYS	SSR	ALA	PRO	PRO	LYS	LYS	GLY	SSR	LYS	LYS	ALA	GLN	LYS	LYS	ASP	GLY	LYS	LYS	ARG	LYS	ARG	SSR	R34	V49	F71	L107	K121	A125
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- Chain I: 11% 27% 72%

MET	SER	THR	PRO	ASP	PRO	PRO	LEU	GLY	GLY	THR	PRO	ARG	PRO	GLY	PRO	SER	SER	GLY	GLY	ALA	MET	LEU	PRO	PRO	SER	GLY	PRO	SER	GLY	GLY	HIS	MET	MET	GLY	PRO	PRO	SER	SER	PRO	ALA	ALA	GLY	HIS	ILE	PRO	THR	THR	GLN	GLY
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PRO	GLY	GLY	TYR	PRO	GLN	ASP	ASN	MET	HIS	GLN	MET	HIS	LYS	PRO	MET	GLU	SER	HIS	GLU	LYS	GLY	MET	SER	ASP	ASP	PRO	PRO	ARG	ARG	TYR	ASN	GLN	MET	LYS	GLY	MET	MET	GLY	GLY	GLY	HIS	ALA	GLY	MET	GLY	GLY	PRO	PRO	PRO	SER	SER	PRO	MET	ASP	GLN	HIS	HIS	SER	SER	GLN	GLN	GLY	TYR
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PRO	SER	PRO	PRO	GLY	GLY	SER	GLU	HIS	ALA	SER	SER	PRO	VAL	PRO	PRO	ALA	ALA	GLY	PRO	SER	SER	SER	PRO	GLN	MET	SER	SER	GLY	GLY	GLY	ALA	ALA	LEU	ASP	GLY	ALA	ASP	PRO	PRO	GLN	ASN	ARG	GLY	PRO	THR	PRO	PHE	ASN	GLN	GLN	LEU	HIS	GLN	LEU
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[illegible]

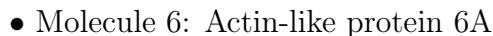
GLY	PRO	GLY	PRO	ALA	PRO	PRO	ASN	TYR	SER	ARG	PRO	HIS	GLY	GLY	GLY	PRO	ASN	MET	PRO	PRO	PRO	PRO	GLY	GLY	PRO	PRO	SER	GLY	VAL	PRO	PRO	PRO	GLY	GLY	GLN	PRO	PRO	GLY	GLY	PRO	PRO	PRO	PRO	LYS	PRO	TRP	TRP	GLU	GLY	GLY	PRO	PRO	MET	ALA	ASN	ALA	ALA	ALA	ALA	ALA	THR	THR	SER	THR	THR	PRO	GLN
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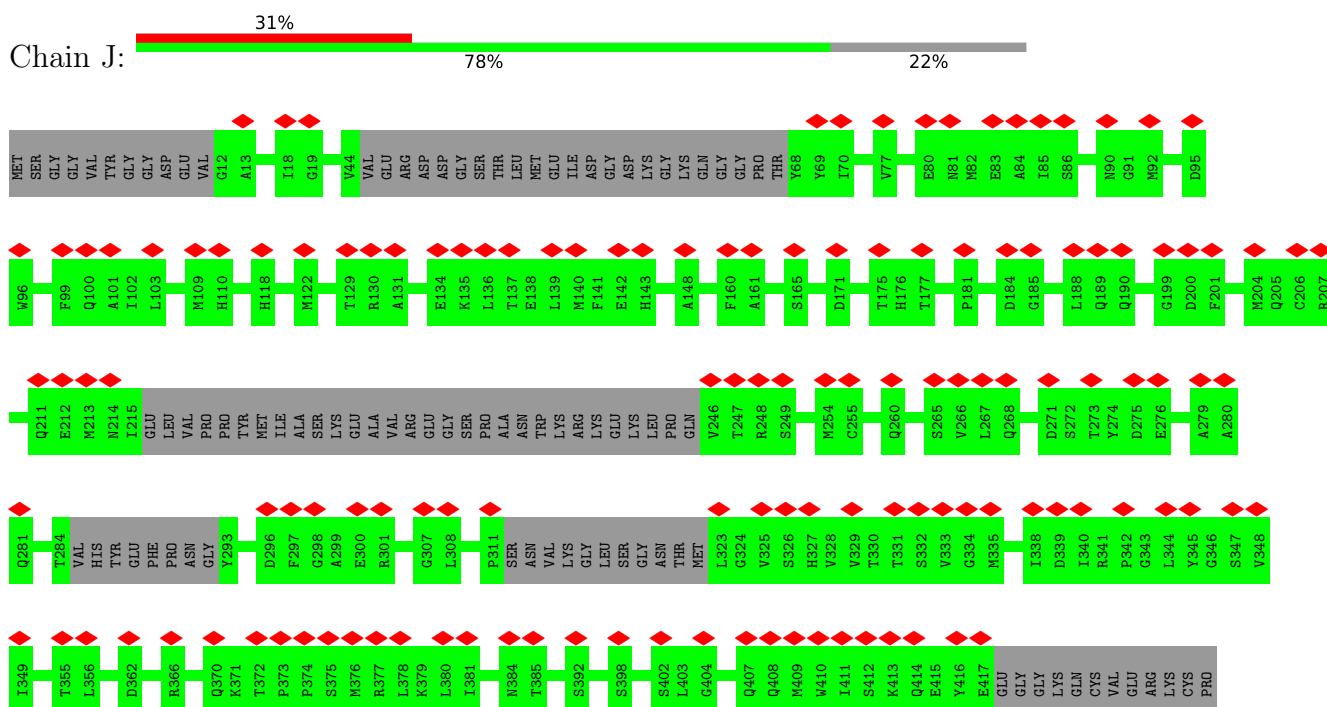
LYS	LEU	ILE	PRO	PRO	GLN	THR	GLY	ARG	PRO	SER	PRO	ALA	VAL	PRO	ALA	ALA	ALA	SER	SER	PRO	VAL	MET	PRO	PRO	PRO	GLN	THR	GLN	SER	PRO	GLY	GLN	PRO	ALA	ALA	PRO	MET	VAL	PRO	PRO	LEU	HIS	LYS	GLN	GLN	SER	ARG	ILE	THR	PRO	PRO	ILE	GLN	LYS	PRO	PRO	ARG	GLY
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LEU	ASP	PRO	VAL	GLU	ILE	LEU	GLN	GLU	ARG	GLU	TYR	ARG	LEU	GLN	ALA	ARG	ILE	ALA	HIS	ARG	ILE	GLN	GLU	LEU	GLU	ASN	LEU	PRO	GLY	SER	LEU	ALA	GLY	ASP	LEU	R397	T398	R399	A400	T401	L402	E403	L404	K405	A406	L407	L410	Q413	R414	Q415	L416	R417	C423	R426	D427
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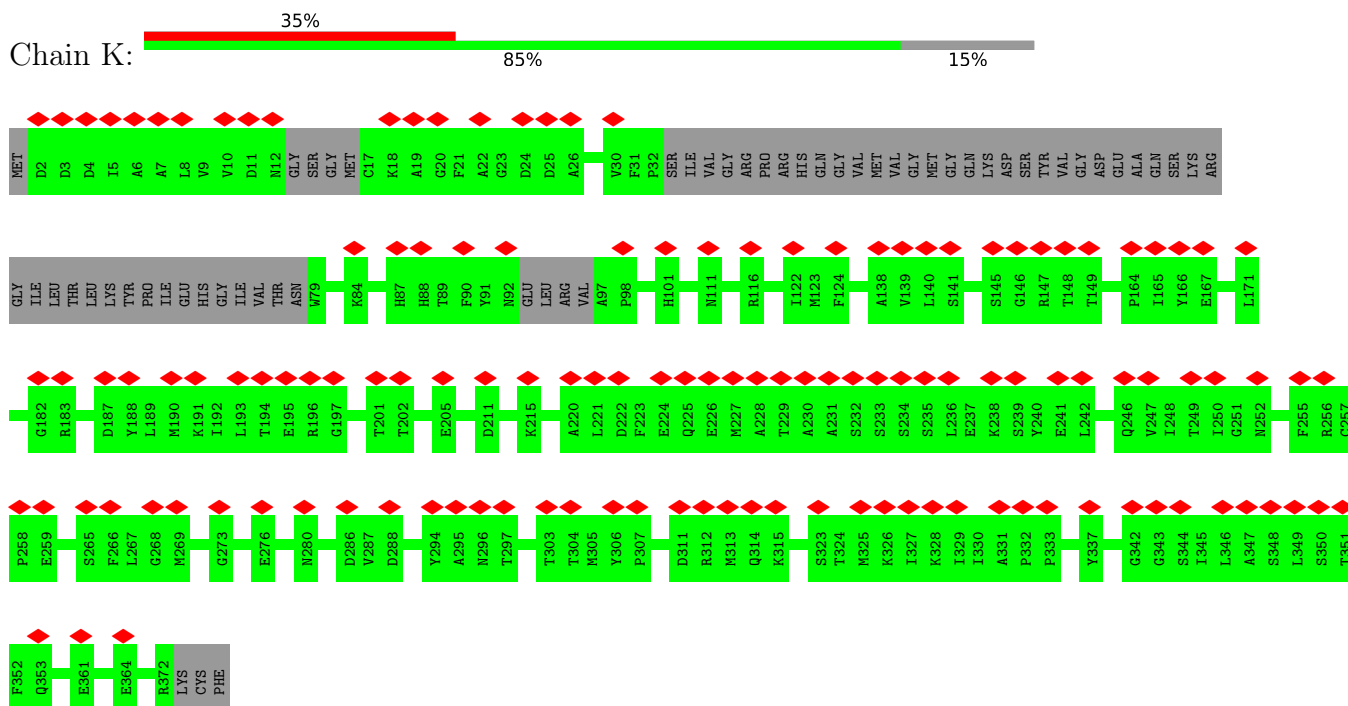
T428	A429	L430	F431	T432	A433	L434	A435	A436	K437		R444	Q445	S446	LEU	ARG	GLU	ALA	ARG	ILE	THR	GLU	LYS	LEU	GLU	LYS	GLN	GLN	LYS	ILE	GLU	GLN	GLU	ARG	K467	R468	R469	Q470	K471	H472	Q473	E474	Y475	Y476	L477	M478	S478	L479	L480	Q481	H482	A483	K484	D485		E488	Y489	H490	R491	S492	V493
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T494	G495	G496	I497	G498	K499	L500	T501	K502	A503	F504	A505	T506	F507	H508	A509	N510	T511	E512	R513	E514	Q515	K516	K517	GLU	ASN	GLU	ARG	ILE	GLU	LYS	GLU	ARG	MET	ARG	ARG	ARG	LEU	MET	ALA	GLU	ASP	GLU	GLU	GLY	TYR	ARG	LYS	LEU	ILE	ASP	GLN	LYS	LYS	ASP	LYS	ARG	LEU	ALA	TYR	LEU
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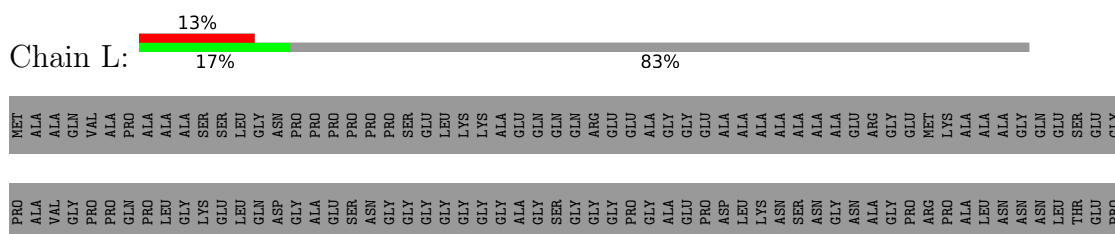




- Molecule 7: Actin, cytoplasmic 1, N-terminally processed



- Molecule 8: AT-rich interactive domain-containing protein 1A

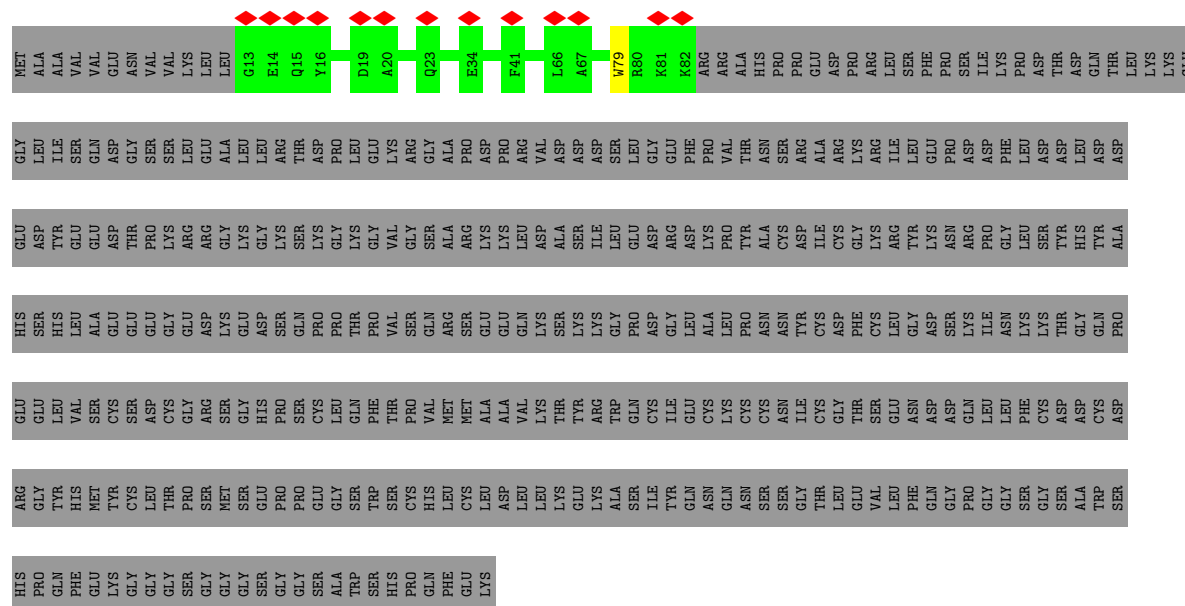








Chain R: 16% 84%



Chain V: 6% 11% 89%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27074	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.792	Depositor
Minimum map value	-1.798	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	405.6, 405.6, 405.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.69, 1.69, 1.69	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	0.30	0/794	0.47	0/1065
1	E	0.29	0/794	0.50	0/1065
2	B	0.26	0/660	0.49	0/883
2	F	0.26	0/648	0.46	0/868
3	C	0.29	0/854	0.48	0/1151
3	G	0.27	0/854	0.47	0/1151
4	D	0.32	0/737	0.58	0/990
4	H	0.28	0/731	0.53	0/982
5	I	0.40	0/2352	0.68	1/3275 (0.0%)
6	J	0.44	0/1687	0.54	0/2352
7	K	0.42	0/1613	0.50	0/2254
8	L	0.37	0/2001	0.50	1/2790 (0.0%)
9	M	0.39	0/1498	0.47	0/2095
10	N	0.40	0/513	0.68	1/718 (0.1%)
10	O	0.36	0/906	0.48	0/1272
11	P	0.36	0/190	0.54	0/265
12	R	0.38	0/353	0.53	0/492
13	V	0.28	0/275	0.42	0/344
14	W	0.41	0/377	0.51	0/529
15	X	0.60	0/3136	1.07	4/4832 (0.1%)
16	Y	0.59	0/3210	1.05	3/4958 (0.1%)
All	All	0.44	0/24183	0.72	10/34331 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	X	129	DT	O5'-C5'-C4'	5.93	119.69	110.80
10	N	415	ASP	N-CA-C	5.80	117.95	108.55
16	Y	91	DA	O3'-P-O5'	-5.71	95.43	104.00
16	Y	60	DA	C4'-C3'-O3'	-5.45	101.82	110.00
5	I	770	ASN	N-CA-C	5.30	119.23	112.87
15	X	68	DT	O3'-P-O5'	-5.30	96.05	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	69	DG	C4'-C3'-O3'	-5.29	102.06	110.00
8	L	1662	LYS	N-CA-C	-5.22	103.59	110.33
15	X	68	DT	C4'-C3'-O3'	-5.11	102.33	110.00
15	X	38	DT	C4'-C3'-O3'	-5.04	102.44	110.00

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	783	0	818	2	0
1	E	783	0	818	3	0
2	B	653	0	696	1	0
2	F	641	0	684	0	0
3	C	844	0	905	3	0
3	G	844	0	905	5	0
4	D	726	0	745	3	0
4	H	720	0	740	4	0
5	I	2352	0	1087	11	0
6	J	1677	0	833	0	0
7	K	1600	0	818	0	0
8	L	1991	0	952	0	0
9	M	1488	0	716	0	0
10	N	510	0	251	1	0
10	O	895	0	455	0	0
11	P	189	0	96	1	0
12	R	351	0	177	1	0
13	V	275	0	81	0	0
14	W	373	0	187	1	0
15	X	2803	0	1553	4	0
16	Y	2855	0	1546	7	0
All	All	23353	0	15063	35	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 1.

All (35) 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)
5:I:892:LYS:O	5:I:896:VAL:N	2.31	0.63
3:C:17:THR:OG1	3:C:20:SER:OG	2.21	0.58
5:I:1307:ALA:HB1	5:I:1312:GLU:HA	1.88	0.55
2:B:89:TYR:CE2	4:D:84:TYR:CD2	2.96	0.53
11:P:508:GLN:O	11:P:509:ALA:C	2.54	0.50
15:X:139:DA:C2	16:Y:11:DA:C2	3.00	0.48
3:G:17:THR:HA	16:Y:32:DA:OP1	2.15	0.47
5:I:778:ALA:HA	5:I:910:THR:O	2.15	0.47
3:C:11:ALA:O	4:D:121:LYS:HE2	2.15	0.47
1:E:80:LYS:HB3	1:E:83:LEU:HD11	1.97	0.46
3:G:65:GLU:CB	4:H:49:VAL:HG11	2.47	0.45
3:G:93:GLU:CD	4:H:107:LEU:HD13	2.42	0.44
16:Y:125:DG:C6	16:Y:126:DG:C6	3.05	0.44
3:C:17:THR:HG1	3:C:20:SER:CB	2.30	0.44
3:G:65:GLU:HB2	4:H:49:VAL:HG11	2.00	0.44
1:A:68:PHE:CZ	1:A:94:GLN:HA	2.53	0.43
5:I:973:ARG:N	5:I:974:PRO:HD2	2.33	0.43
5:I:776:ILE:O	5:I:976:LEU:HA	2.18	0.43
5:I:1307:ALA:CB	5:I:1312:GLU:HA	2.49	0.43
5:I:929:LEU:O	5:I:931:THR:N	2.52	0.42
1:A:114:HIS:CG	1:E:127:LEU:HD22	2.54	0.42
14:W:72:SER:CB	15:X:125:DT:H1'	2.49	0.42
4:H:71:PHE:CD1	4:H:71:PHE:C	2.97	0.42
5:I:929:LEU:C	5:I:931:THR:N	2.77	0.42
5:I:831:LYS:HA	5:I:855:VAL:H	1.84	0.42
3:G:113:GLN:N	3:G:113:GLN:OE1	2.51	0.42
16:Y:126:DG:C5	16:Y:127:DC:C4	3.08	0.42
5:I:778:ALA:N	5:I:977:LEU:O	2.53	0.41
5:I:779:ASP:HA	5:I:979:ARG:H	1.85	0.41
10:N:414:GLU:O	12:R:79:TRP:HA	2.20	0.41
16:Y:104:DG:C5	16:Y:105:DC:C4	3.07	0.41
15:X:120:DA:N6	16:Y:28:DC:N4	2.69	0.41
15:X:59:DA:C2	16:Y:91:DA:C2	3.10	0.40
4:D:122:TYR:CD2	4:D:122:TYR:C	2.98	0.40
1:E:68:PHE:CZ	1:E:94:GLN:HA	2.56	0.40

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	A	93/139 (67%)	92 (99%)	1 (1%)	0	100	100
1	E	93/139 (67%)	93 (100%)	0	0	100	100
2	B	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	F	78/106 (74%)	77 (99%)	1 (1%)	0	100	100
3	C	108/133 (81%)	104 (96%)	4 (4%)	0	100	100
3	G	108/133 (81%)	105 (97%)	3 (3%)	0	100	100
4	D	91/128 (71%)	90 (99%)	0	1 (1%)	11	44
4	H	90/128 (70%)	90 (100%)	0	0	100	100
5	I	447/1647 (27%)	410 (92%)	34 (8%)	3 (1%)	18	55
6	J	324/429 (76%)	310 (96%)	14 (4%)	0	100	100
7	K	309/375 (82%)	298 (96%)	11 (4%)	0	100	100
8	L	384/2285 (17%)	373 (97%)	11 (3%)	0	100	100
9	M	289/385 (75%)	283 (98%)	6 (2%)	0	100	100
10	N	99/1214 (8%)	98 (99%)	1 (1%)	0	100	100
10	O	171/1214 (14%)	167 (98%)	4 (2%)	0	100	100
11	P	35/515 (7%)	35 (100%)	0	0	100	100
12	R	68/435 (16%)	66 (97%)	2 (3%)	0	100	100
13	V	66/645 (10%)	66 (100%)	0	0	100	100
14	W	71/105 (68%)	71 (100%)	0	0	100	100
All	All	3004/10261 (29%)	2907 (97%)	93 (3%)	4 (0%)	49	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	105	GLY
5	I	811	PRO

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Mol	Chain	Res	Type
5	I	812	LEU
5	I	930	PRO

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	83/113 (74%)	82 (99%)	1 (1%)	63	73
1	E	83/113 (74%)	83 (100%)	0	100	100
2	B	67/81 (83%)	67 (100%)	0	100	100
2	F	66/81 (82%)	66 (100%)	0	100	100
3	C	85/102 (83%)	85 (100%)	0	100	100
3	G	85/102 (83%)	85 (100%)	0	100	100
4	D	79/106 (74%)	79 (100%)	0	100	100
4	H	78/106 (74%)	77 (99%)	1 (1%)	61	72
5	I	11/1422 (1%)	11 (100%)	0	100	100
6	J	15/364 (4%)	15 (100%)	0	100	100
7	K	17/318 (5%)	17 (100%)	0	100	100
8	L	16/1845 (1%)	16 (100%)	0	100	100
9	M	13/346 (4%)	13 (100%)	0	100	100
10	N	4/1030 (0%)	4 (100%)	0	100	100
10	O	13/1030 (1%)	13 (100%)	0	100	100
11	P	2/442 (0%)	2 (100%)	0	100	100
12	R	3/373 (1%)	3 (100%)	0	100	100
13	V	1/537 (0%)	1 (100%)	0	100	100
14	W	5/95 (5%)	5 (100%)	0	100	100
All	All	726/8606 (8%)	724 (100%)	2 (0%)	84	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
4	H	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	25	GLN
4	D	48	GLN
4	D	96	GLN
1	E	77	GLN
4	H	110	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

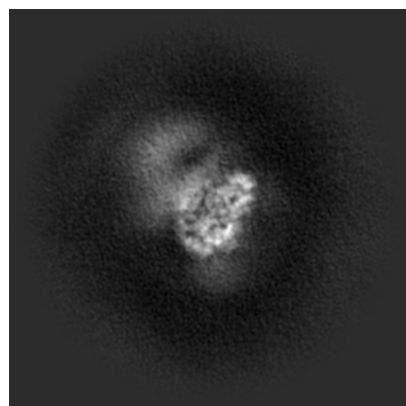
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54078. These allow visual inspection of the internal detail of the map and identification of artifacts.

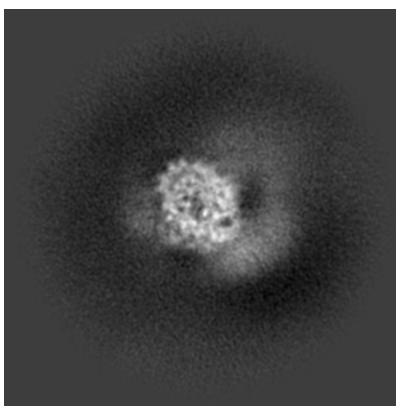
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

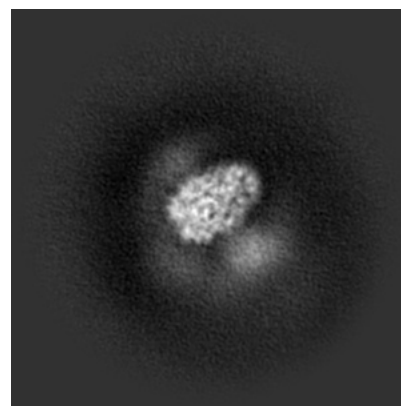
6.1.1 Primary map



X

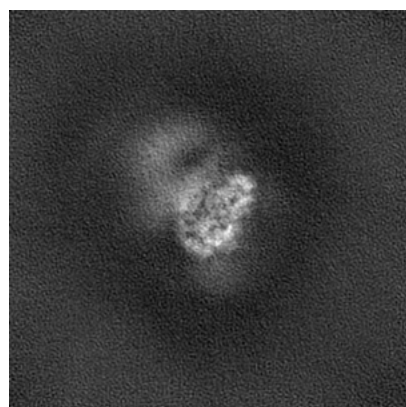


Y

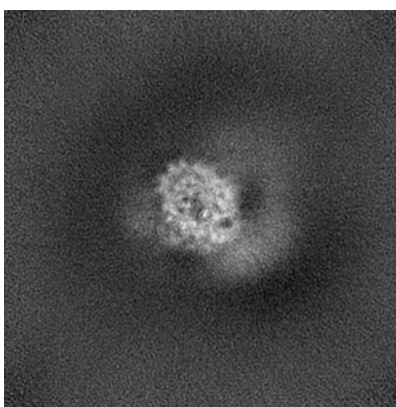


Z

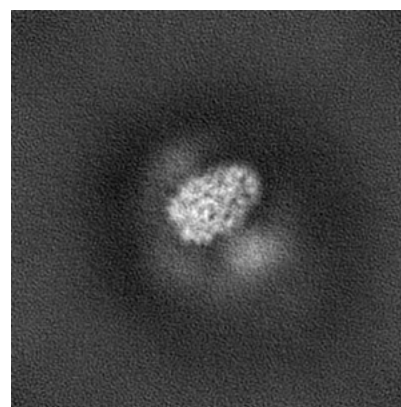
6.1.2 Raw map



X



Y

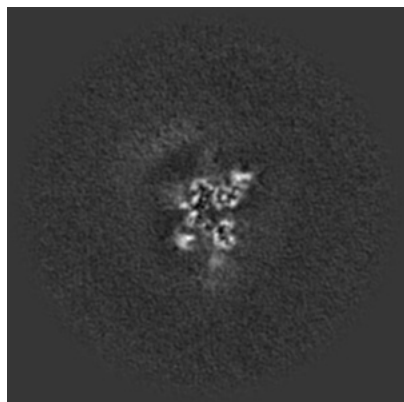


Z

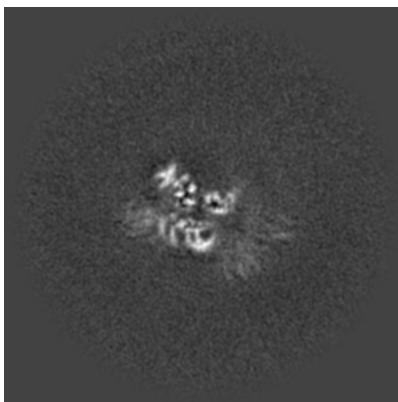
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

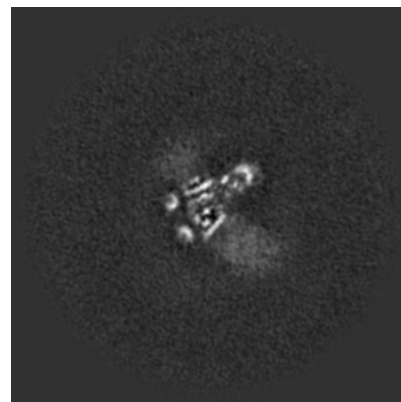
6.2.1 Primary map



X Index: 120

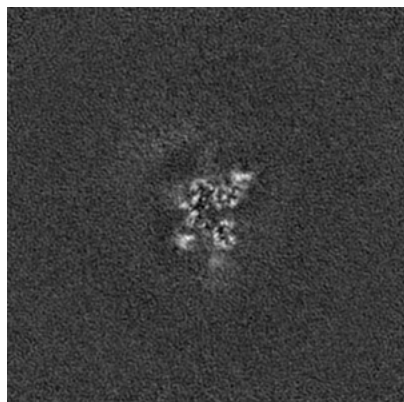


Y Index: 120

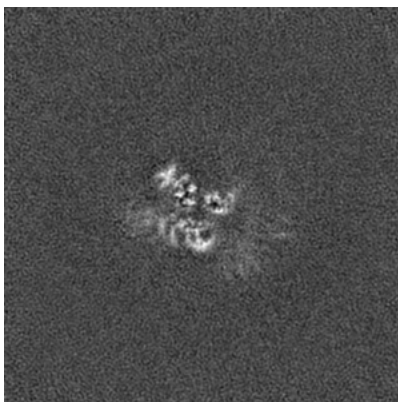


Z Index: 120

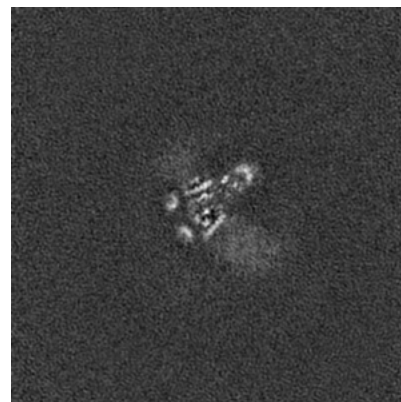
6.2.2 Raw map



X Index: 120



Y Index: 120

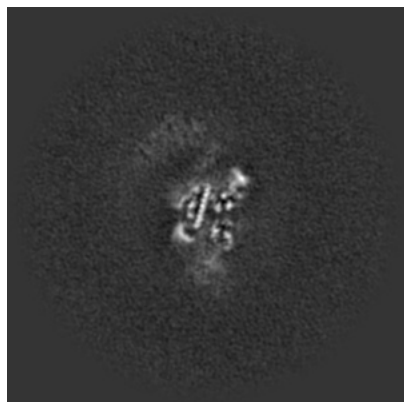


Z Index: 120

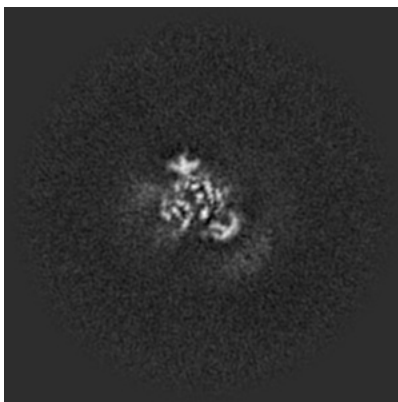
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

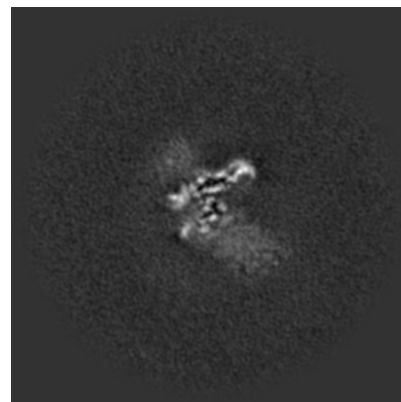
6.3.1 Primary map



X Index: 117

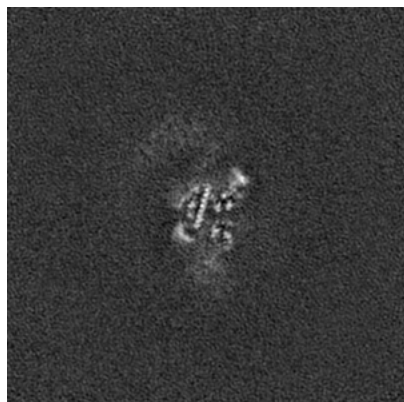


Y Index: 132

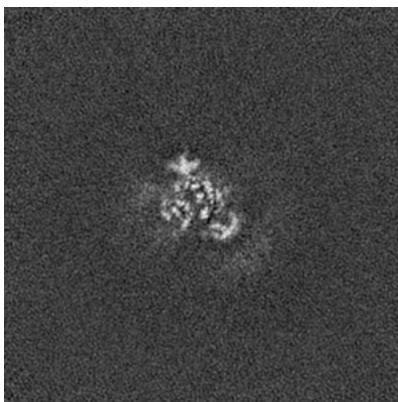


Z Index: 125

6.3.2 Raw map



X Index: 117



Y Index: 132

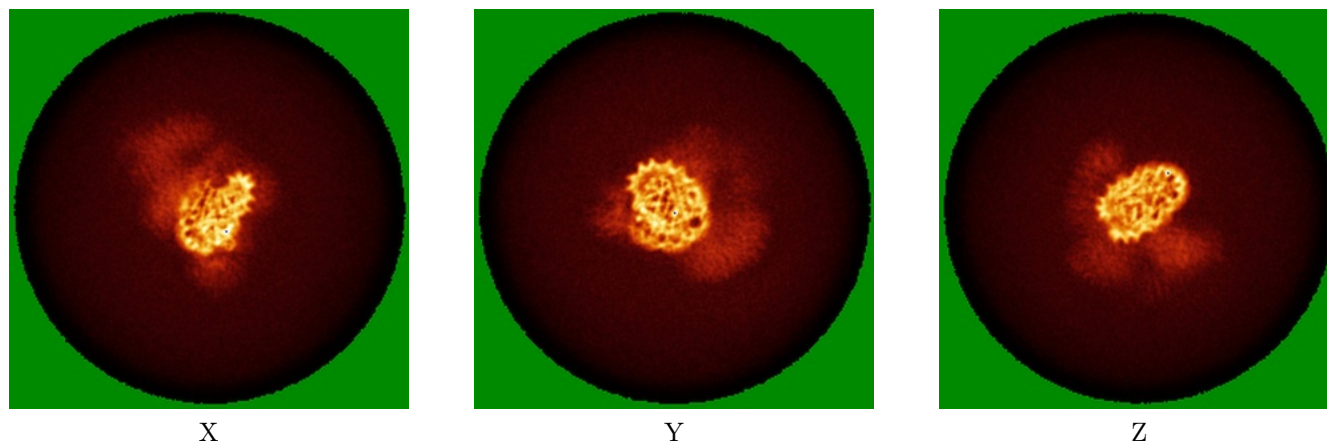


Z Index: 125

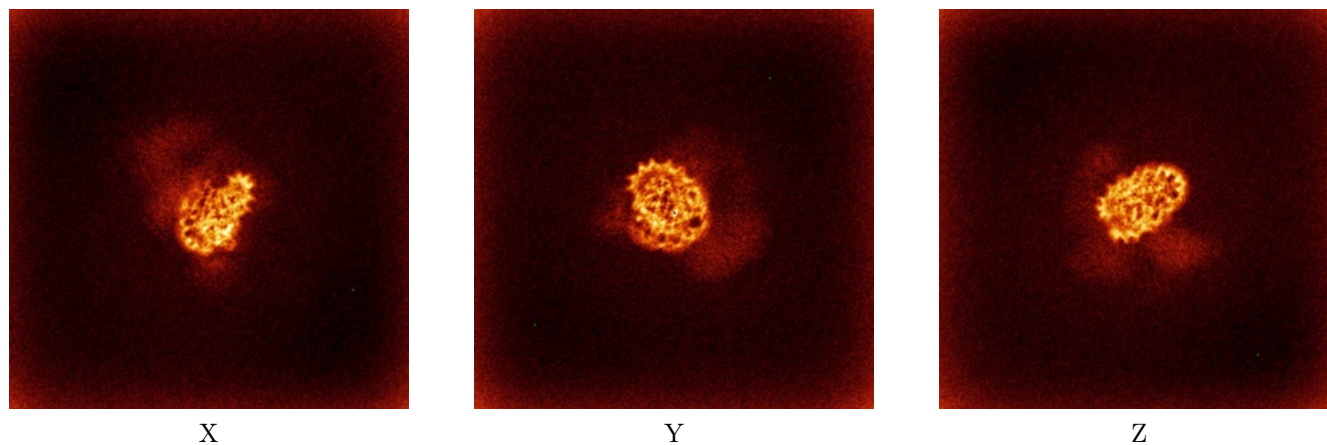
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



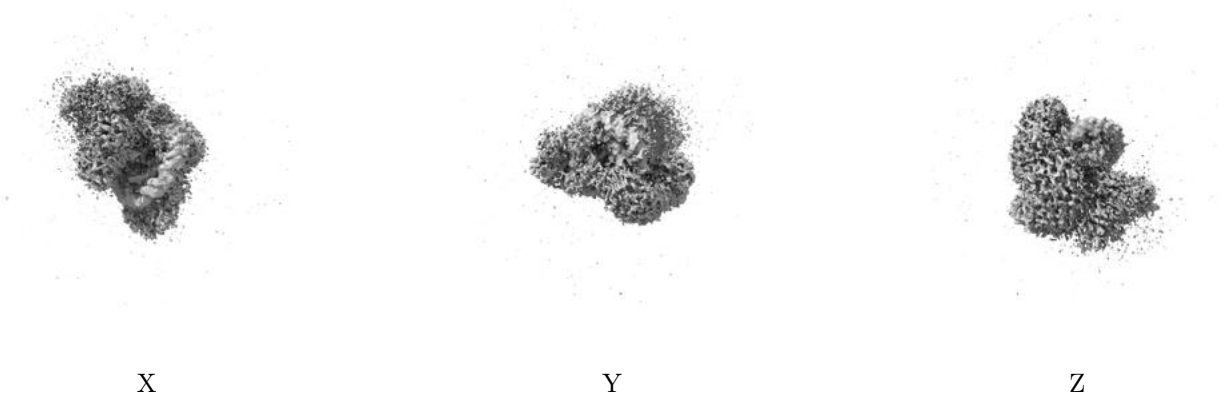
6.4.2 Raw map



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

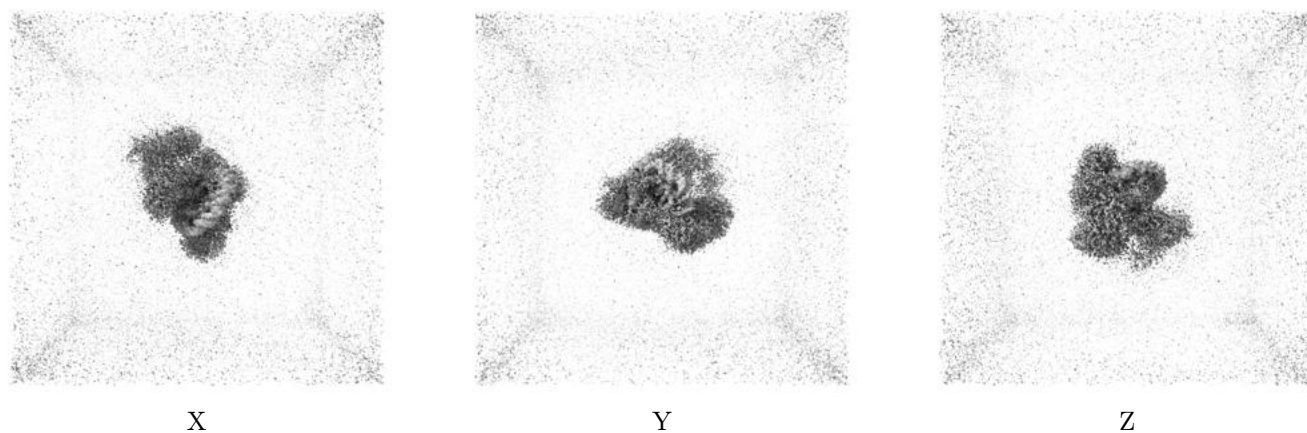
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

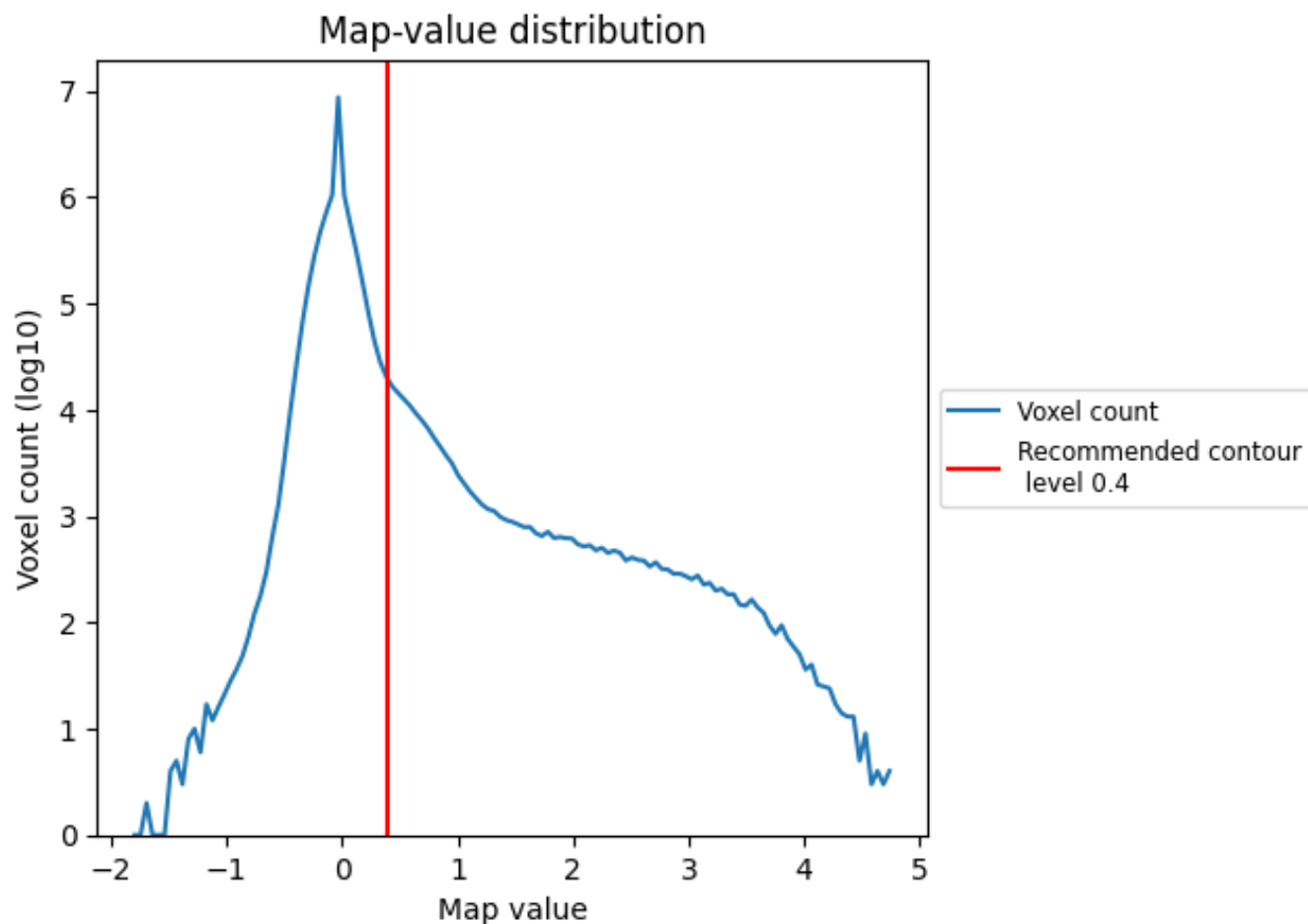
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

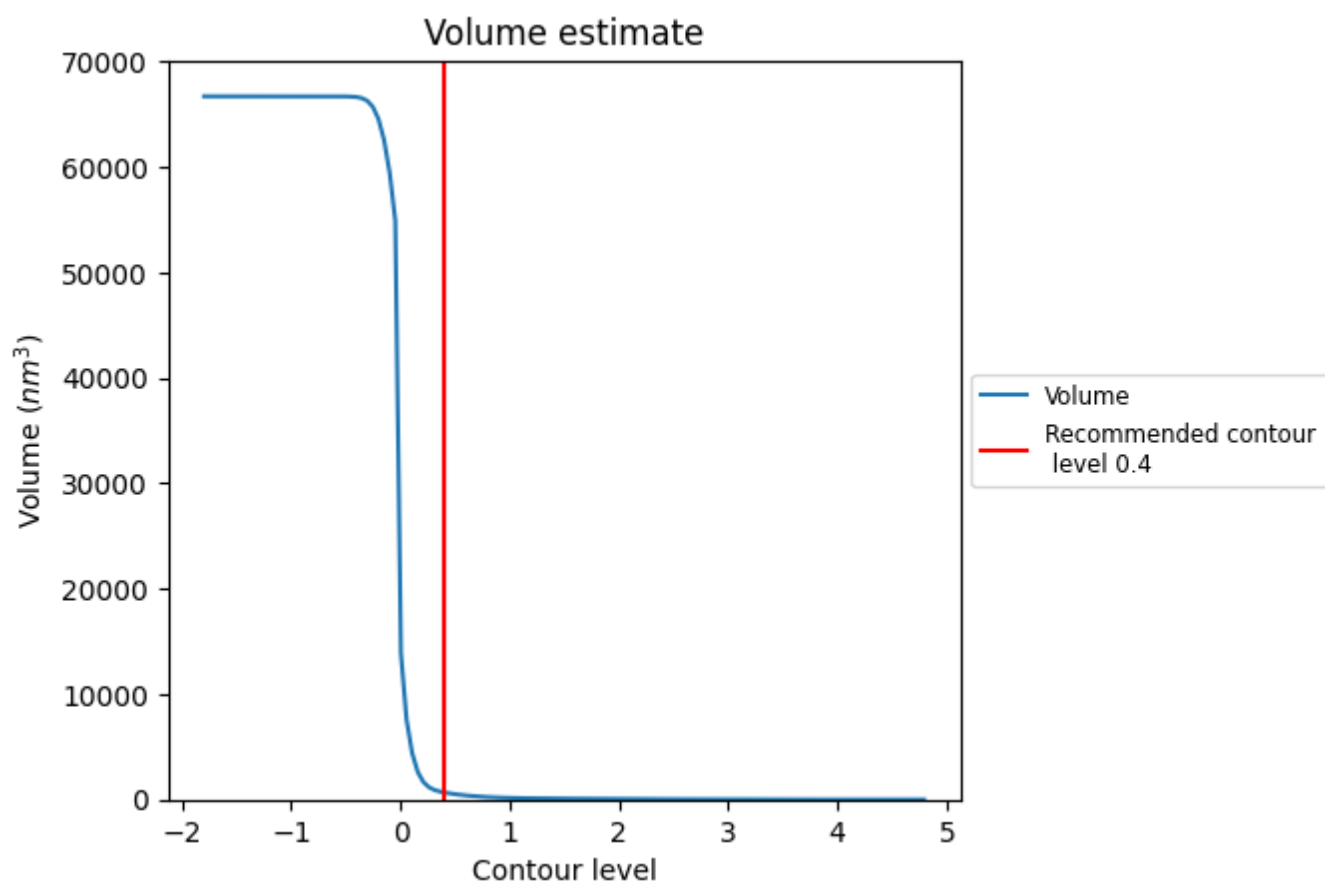
This section contains the results of statistical analysis of the map.

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.

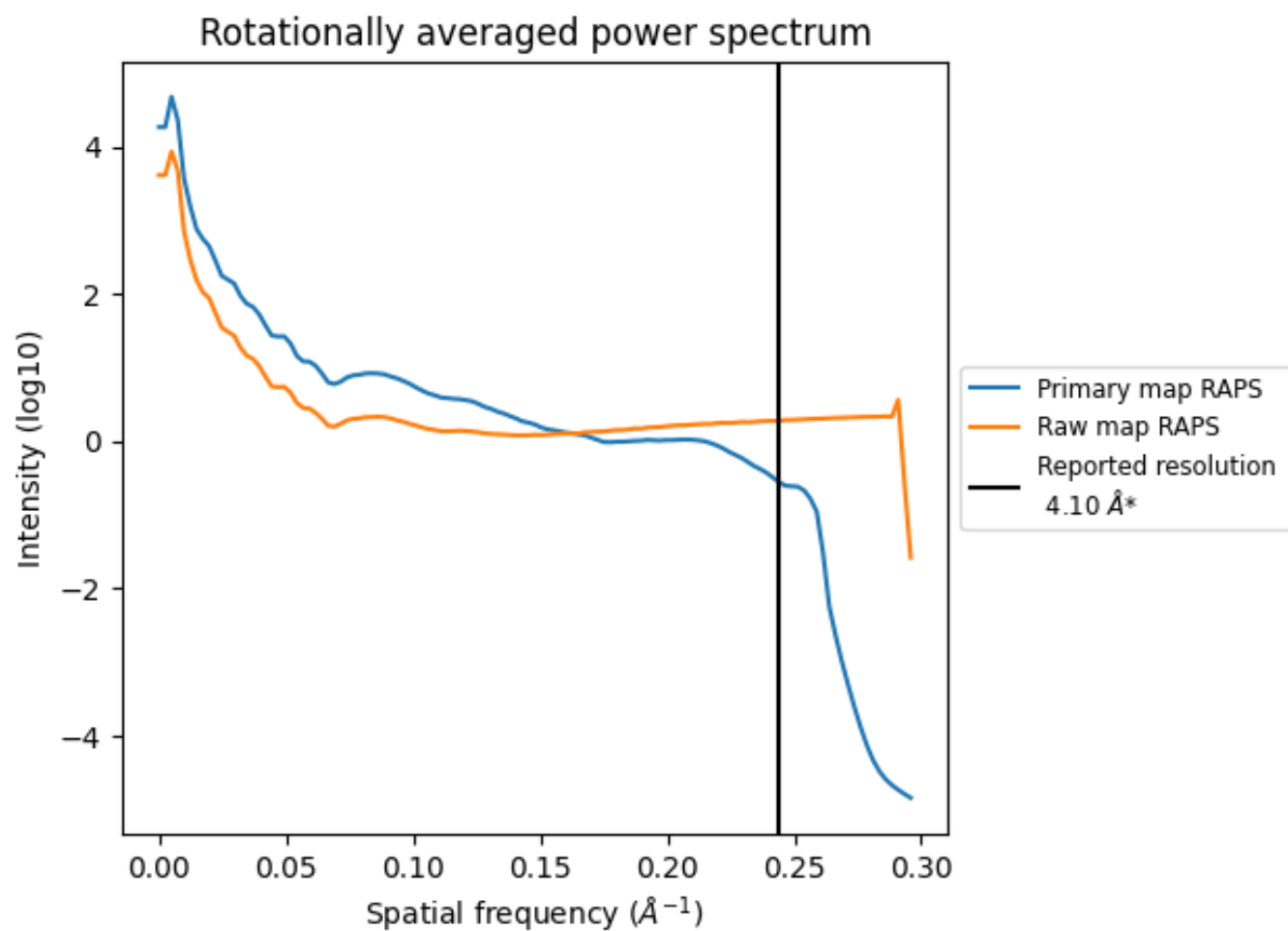
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 674 nm³; this corresponds to an approximate mass of 609 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 ⓘ

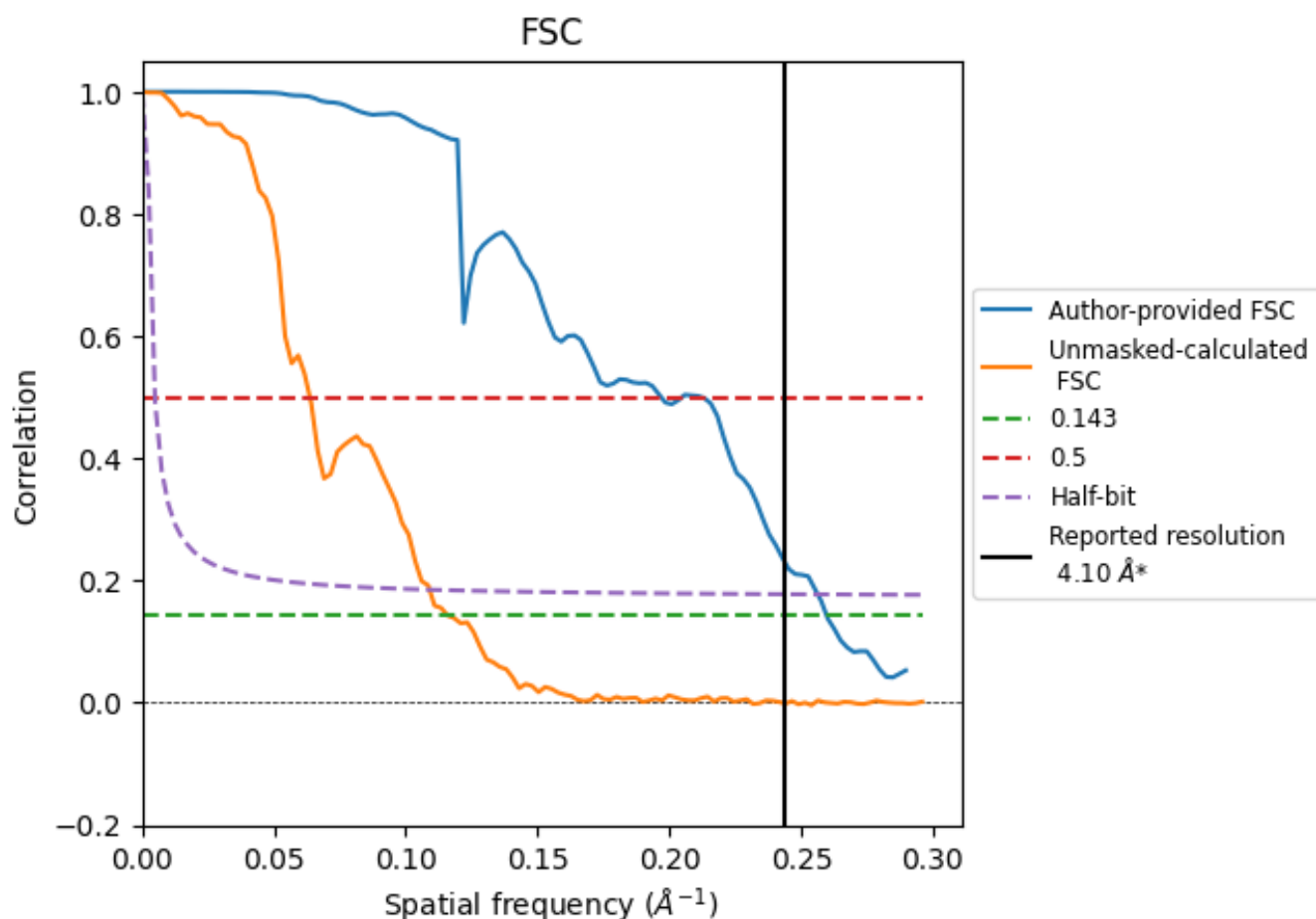


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

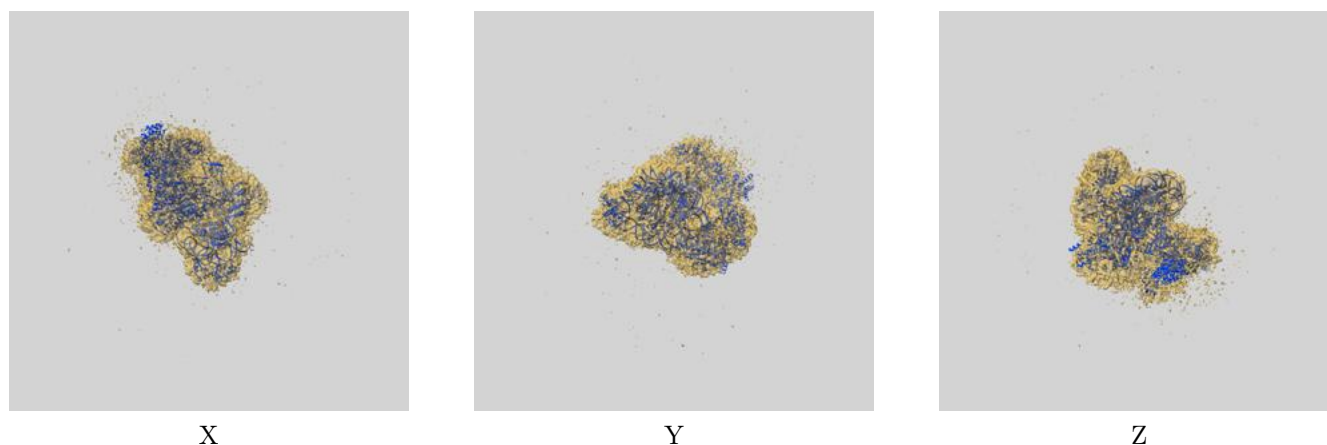
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	3.85	5.08	3.90
Unmasked-calculated*	8.64	15.72	9.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.64 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

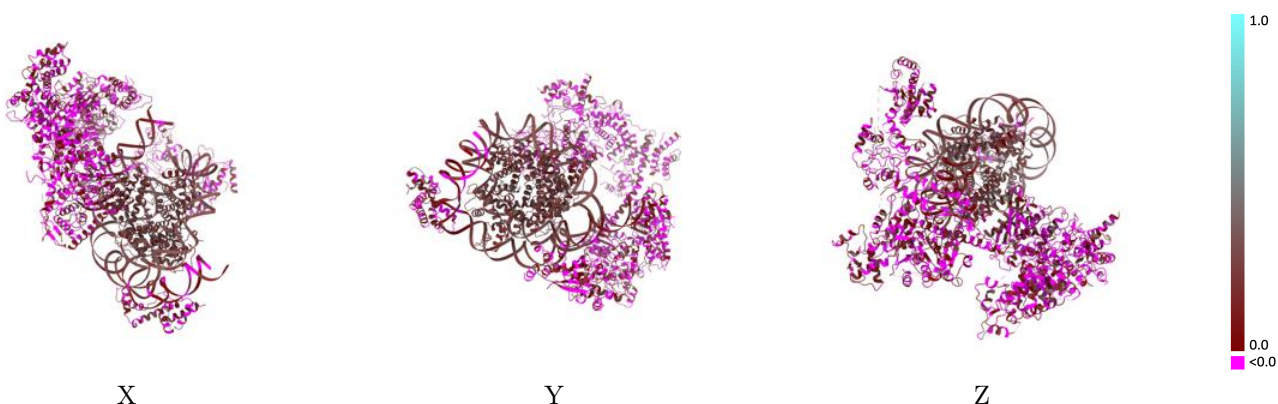
This section contains information regarding the fit between EMDB map EMD-54078 and PDB model 9RN2. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



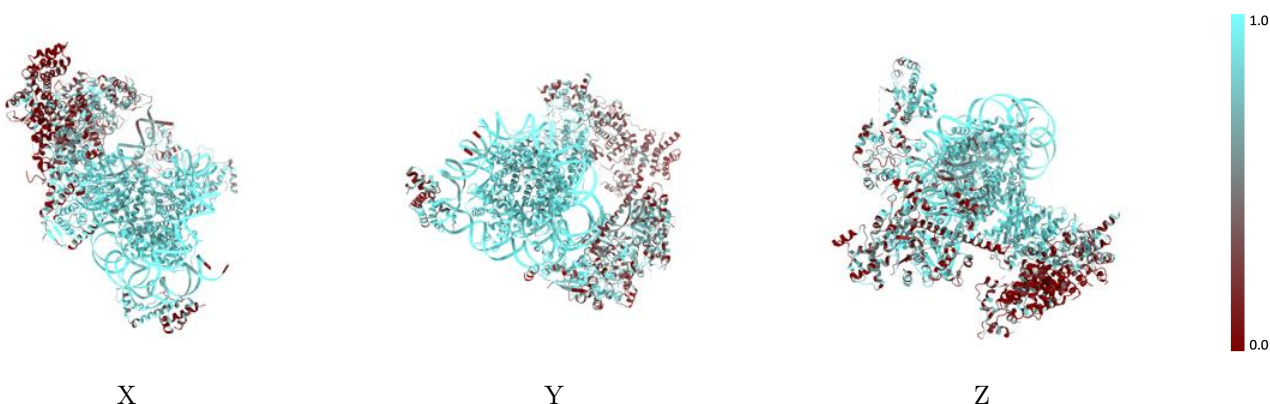
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



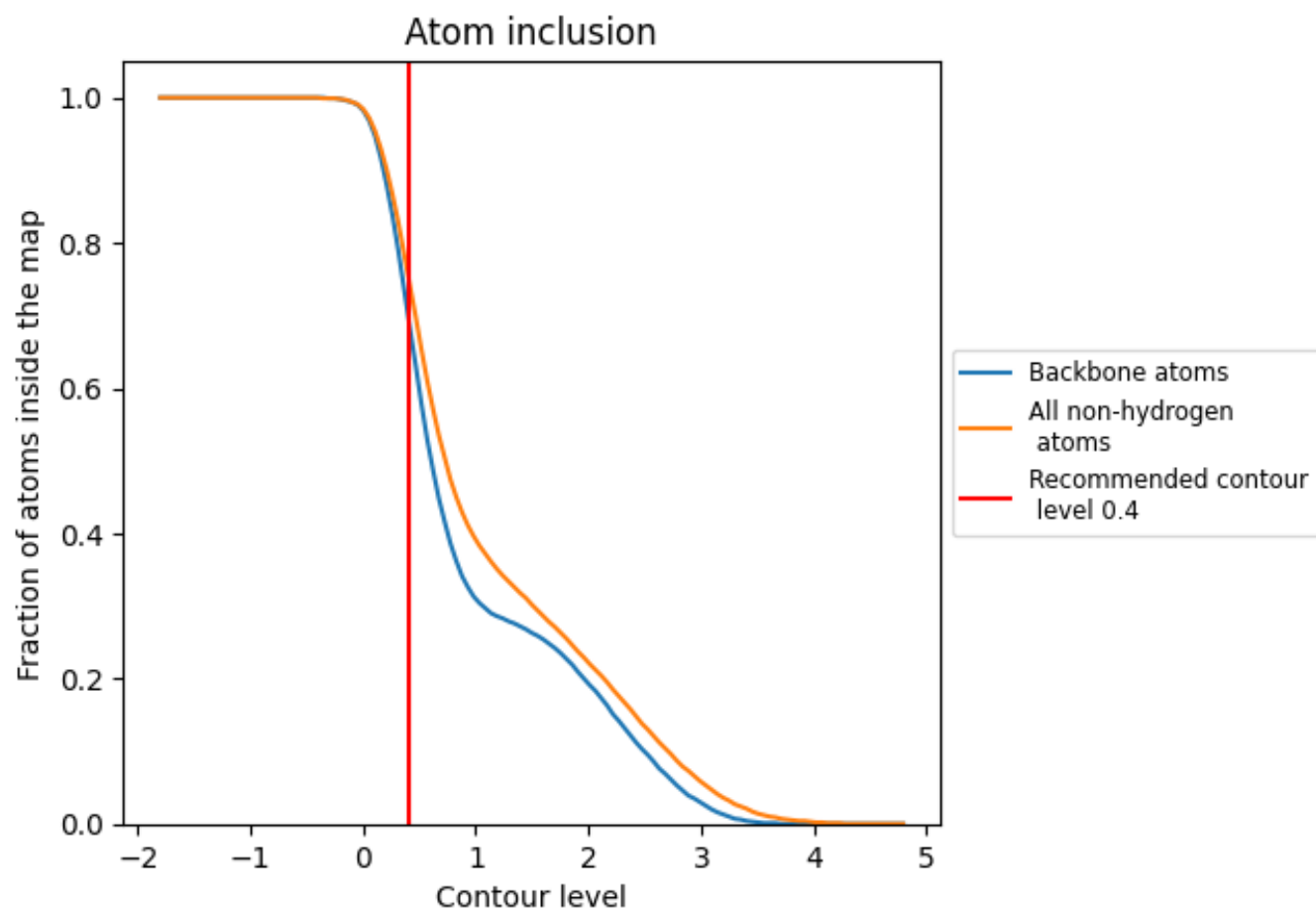
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 75% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7540	 0.1410
A	 0.9660	 0.2540
B	 0.9490	 0.2840
C	 0.9510	 0.2650
D	 0.9690	 0.2810
E	 0.9430	 0.2410
F	 0.9460	 0.2740
G	 0.9630	 0.2720
H	 0.9760	 0.2750
I	 0.5660	 0.0310
J	 0.5680	 0.0270
K	 0.5420	 0.0350
L	 0.2830	 0.0080
M	 0.6910	 0.0710
N	 0.9250	 0.0270
O	 0.7550	 0.0240
P	 0.3970	 -0.0010
R	 0.7610	 0.0580
V	 0.3890	 0.0760
W	 0.7400	 0.0580
X	 0.9240	 0.2260
Y	 0.9490	 0.2290

