



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:11 PM UTC

PDB ID : 9EGY / pdb_00009egy
EMDB ID : EMD-48040
Title : RNA polymerase II-DSIF-SPT6-PAF1c-TFIIS-IWS1-nucleosome, bp +27
Authors : Markert, J.; Farnung, L.
Deposited on : 2024-11-21
Resolution : 2.90 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

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:

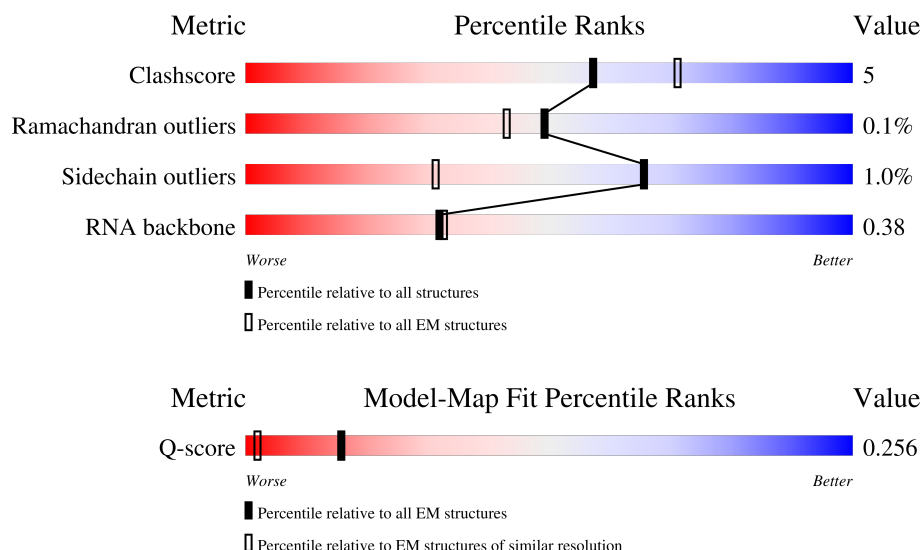
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.90 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	1984	
2	B	1251	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	206	
15	O	821	
16	P	21	
17	Q	1179	
18	R	713	
19	S	304	
20	T	215	
21	U	666	
22	V	531	
23	W	305	
24	X	531	
25	Y	121	
26	Z	1087	
27	a	136	
27	e	136	

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Mol	Chain	Length	Quality of chain
28	b	103	
28	f	103	
29	c	130	
29	g	130	
30	d	123	
30	h	123	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 66649 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1426	Total	C	N	O	P	S	0	0
			11210	7040	2013	2086	2	69		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1122	Total	C	N	O	S	0	0
			8980	5684	1576	1656	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 4 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			1004	630	170	200	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			626	401	106	114	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1197	759	195	238	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			942	582	168	181	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 11 is a protein called RNA polymerase II subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	47	Total	C	N	O	S	0	0
			397	246	77	68	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	1002	Total	C	N	O	0	0
			4309	2295	1003	1011		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	149	Total	C	N	O	P	0	0
			3070	1456	560	905	149		

- Molecule 15 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	132	Total	C	N	O	0	0
			656	392	132	132		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	SER	-	expression tag	UNP Q96ST2
O	0	ASN	-	expression tag	UNP Q96ST2
O	1	ALA	-	expression tag	UNP Q96ST2

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	21	Total	C	N	O	P	0	0
			432	193	59	159	21		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	N	O	S	0	0
			6427	4026	1164	1218	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	244	Total	C	N	O	S	0	0
			1428	866	281	280	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	161	Total	C	N	O	0	0
			657	334	161	162		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP P23193
S	-1	ASN	-	expression tag	UNP P23193
S	0	ALA	-	expression tag	UNP P23193

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	160	Total	C	N	O	P	0	0
			3264	1549	611	945	159		

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	125	Total	C	N	O	0	0
			617	367	125	125		

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	244	Total	C	N	O	S	0	0
			1378	842	267	267	2		

- Molecule 23 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	300	Total	C	N	O	S	0	0
			2333	1483	392	454	4		

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	43	Total	C	N	O	0	0
			353	220	69	64		

- Molecule 25 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	510	Total	C	N	O	P	S	0	0
			4025	2552	709	745	1	18		

- Molecule 27 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	92	Total	C	N	O	S	0	0
			751	474	142	132	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	97	Total	C	N	O	S	0	0
			801	504	155	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	36	MET	LYS	engineered mutation	UNP A0A310TTQ1
e	36	MET	LYS	engineered mutation	UNP A0A310TTQ1

- Molecule 28 is a protein called Histone H4.

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

- Molecule 29 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	103	Total	C	N	O		0	0
			795	501	155	139			
29	g	98	Total	C	N	O		0	0
			755	474	149	132			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	99	ARG	GLY	conflict	UNP P06897
c	123	SER	ALA	conflict	UNP P06897
g	99	ARG	GLY	conflict	UNP P06897
g	123	SER	ALA	conflict	UNP P06897

- Molecule 30 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	95	Total	C	N	O	S	0	0
			745	469	134	140	2		
30	h	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total 2	Zn 2	0
31	B	1	Total 1	Zn 1	0
31	C	1	Total 1	Zn 1	0
31	I	2	Total 2	Zn 2	0
31	J	1	Total 1	Zn 1	0
31	L	1	Total 1	Zn 1	0
31	Y	1	Total 1	Zn 1	0

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

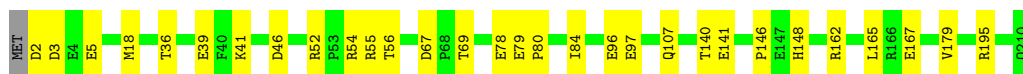
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total 1	Mg 1	0

Chain D:  84% 5% 11%



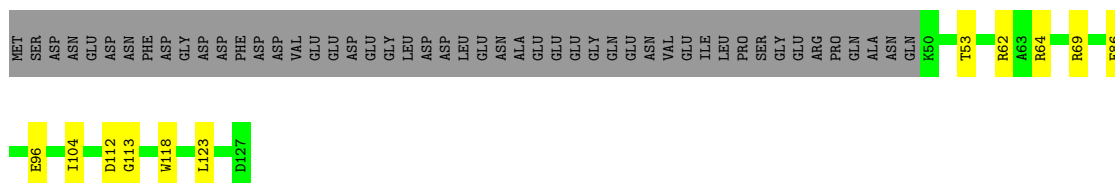
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:  85% 14%



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  53% 9% 39%



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:  88% 11%



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  82% 17%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  76% 17% 7%



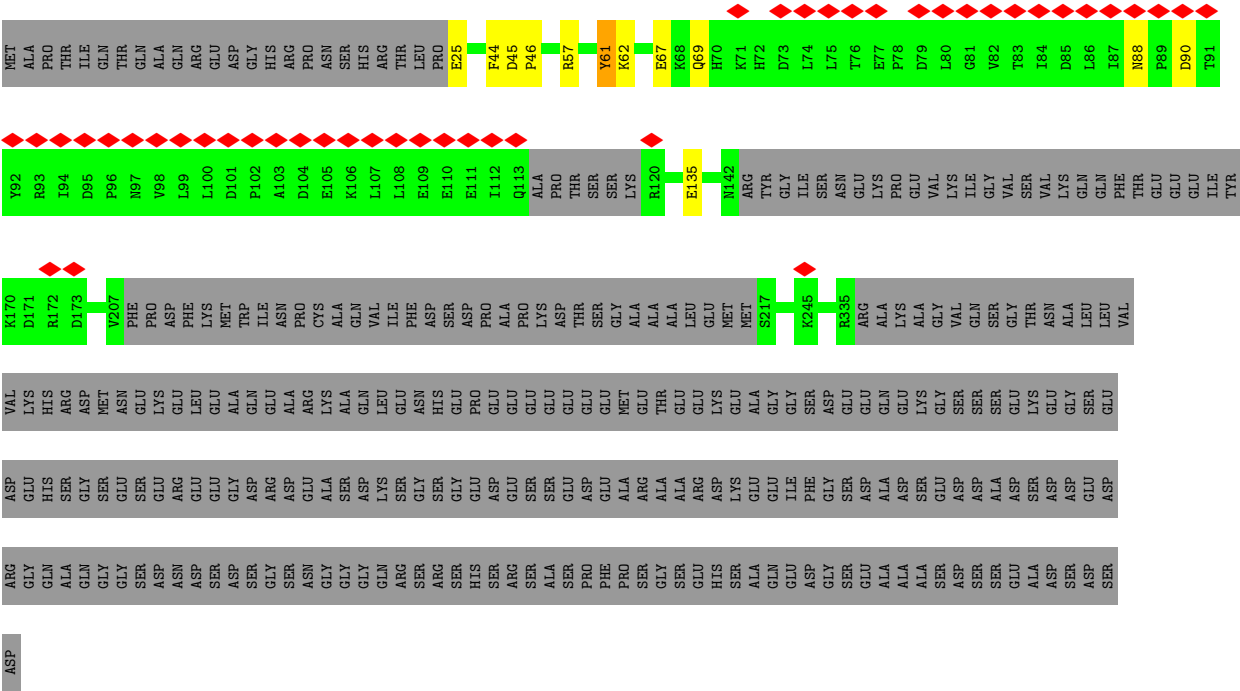
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  82% 16%









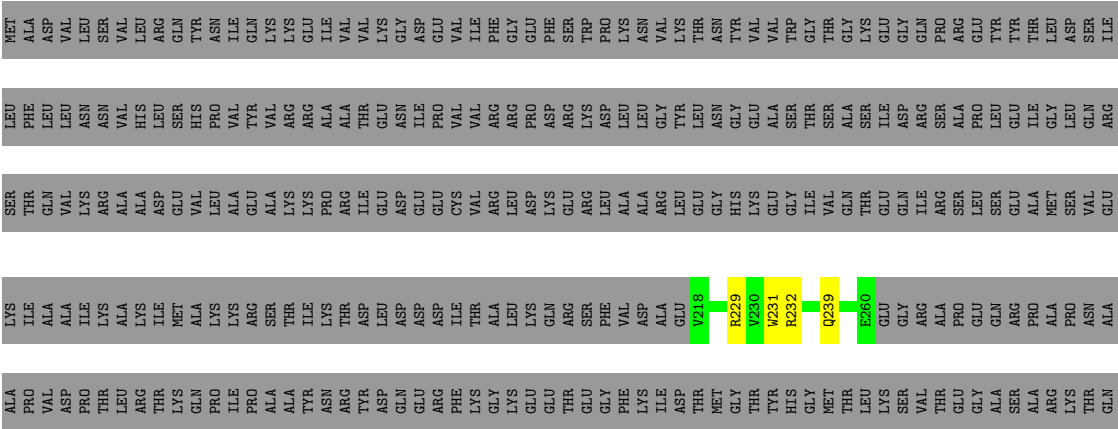
• Molecule 23: WDR61

Chain W: 77% 21% ..



• Molecule 24: Parafibromin

Chain X: 7% 92%



[illegible]

- Molecule 25: Transcription elongation factor SPT4

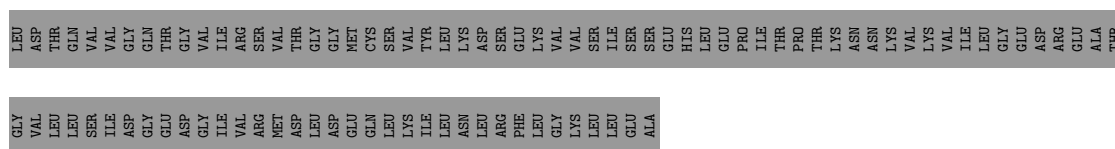
Chain Y: 83% 13% .

GLY
PRO
GLY
SER
MET
A2
L18
D26 Q27
A38
Q41
E47
M48 V49
C52 T53
Q75
K81
Y85 A86
R111 D112
K116 T117

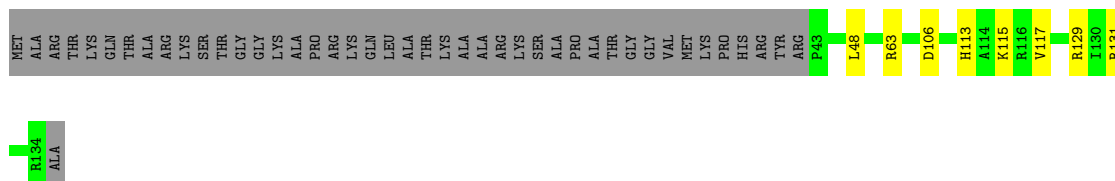
- Molecule 26: Transcription elongation factor SPT5

Chain Z: 42% 5% 53%

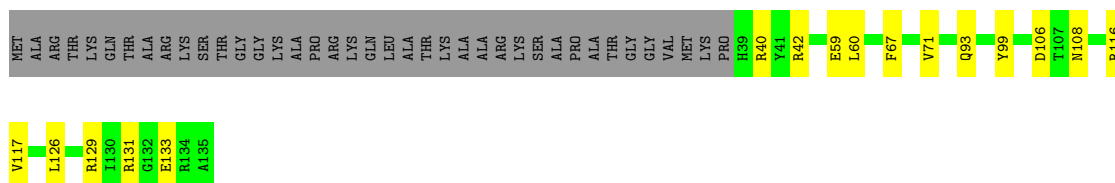
THR	GLN	ARG	MET	ASN	THR	GLN	ASP	GLY	THR	GLY	GLU	MET
PRO	TYR	THR	SER	ASN	PRO	D604	R416	T192	ALA	ASP	ASP	SER
PRO	ASN	PRO	ARG	PRO	G605	Q421	Q421	T206	ARG	ASP	ASP	ARG
PRO	GLN	ALA	GLY	GLN	E613	D424	D424	D207	ARG	ASP	ARG	GLU
ALA	THR	SER	GLY	THR	G625	N425	N425	V215	GLN	PRO	PRO	ASP
TYR	PRO	GLY	ARG	GLY	E427	E426	E426	V227	ASN	ASN	LYS	SER
GLN	GLY	ALA	ARG	ARG	C626	V428	V428	Y227	LEU	PRO	LYS	ASN
ALA	THR	TRP	ARG	THR	K627	C429	C429	N244	TRP	PRO	LYS	PHE
SER	PRO	ASP	N703	ASP	C428	C428	C428	N244	ARG	PRO	PRO	SER
PRO	ALA	PRO	+	PRO	V637	+	+	+	ASP	GLU	GLU	GLU
SER	MET	ASN	P716	ASN	A646	Q437	Q437	K268	GLN	HIS	HIS	GLU
PRO	TYR	ASN	G719	ASN	GLY	I440	I440	GLU	ARG	GLY	GLY	GLU
SER	ASN	PRO	E729	ASN	GLY	+	+	VAL	GLU	ASP	ASP	SER
VAL	ASP	THR	+	THR	LYS	E455	E455	A271	GLU	ILE	ILE	GLU
GLY	GLN	PRO	+	PRO	PRO	E462	E462	+	LEU	LEU	LEU	ARG
TYR	PHE	SER	D746	SER	ARG	+	+	+	GLY	ASP	ASP	SER
SER	SER	ARG	R747	ARG	ASP	Q466	Q466	A318	GLU	GLU	GLU	SER
PRO	PRO	ALA	+	THR	THR	E467	E467	+	TYR	ALA	ALA	ASP
THR	TYR	GLU	R767	THR	VAL	L468	L468	MET	MET	VAL	VAL	GLY
PRO	ALA	GLU	+	GLY	ASN	R469	R469	ARG	SER	LYS	ASP	GLU
GLY	PRO	TYR	MET	THR	PHE	+	+	LEU	LYS	ASP	ASP	GLU
ALA	SER	GLU	T771	GLY	THR	V478	V478	LYS	THR	GLU	GLU	GLU
PRO	PRO	TYR	+	THR	VAL	+	+	ASP	ALA	TYR	TYR	VAL
SER	GLN	ALA	T775	GLY	GLY	E486	E486	THR	LYS	GLY	GLY	ASP
PRO	GLY	PHE	+	GLY	GLY	+	+	PHE	SER	GLU	GLU	GLU
GLY	SER	ASP	G781	PHE	THR	E497	E497	ALA	VAL	ASP	ASP	ARG
GLY	THR	GLU	SER	ALA	ALA	+	+	LYS	VAL	ARG	ARG	GLN
TYR	GLN	GLU	ARG	PRO	PRO	S504	S504	ARG	GLY	GLN	GLN	ASP
ASN	PRO	PRO	THR	THR	MET	+	+	LYS	THR	TRP	TRP	SER
PRO	SER	THR	PRO	PRO	PRO	T507	T507	LYS	THR	GLU	GLU	ALA
HIS	PRO	PRO	MET	PRO	PRO	+	+	PHE	VAL	ASP	ASP	ALA
THR	SER	SER	TYR	THR	ARG	L518	L518	LYS	TYR	GLY	GLY	GLY
PRO	PRO	PRO	GLY	ILE	ILE	+	+	ARG	ALA	ALA	ALA	SER
GLY	GLN	GLN	SER	SER	SER	E523	E523	+	GLY	GLU	GLU	GLU
SER	SER	ALA	GLN	GLN	THR	+	+	ASP	ASP	ASP	ASP	LYS
GLY	TYR	TYR	THR	PRO	PRO	Q541	Q541	D341	ILE	ILE	ILE	GLU
ILE	HIS	GLY	PRO	THR	THR	L542	L542	A342	GLU	GLU	GLU	GLU
GLU	GLN	GLY	MET	HIS	MET	D543	D543	+	LEU	LEU	LEU	GLU
GLN	VAL	THR	PRO	GLN	PRO	+	+	F396	SER	SER	LYS	PRO
ASN	ALA	PRO	ASN	ASP	SER	I550	I550	GLU	ASP	GLU	GLU	GLU
SER	PRO	ASN	GLY	ALA	ALA	+	+	ASP	ASP	GLU	GLU	ASP
SER	SER	PRO	SER	GLY	GLY	E554	E554	GLN	ILE	ILE	ILE	GLU
TRP	PRO	GLN	ARG	GLY	GLY	R555	R555	PRO	THR	GLU	GLU	GLU
VAL	ALA	THR	THR	GLN	GLN	+	+	GLU	GLN	ALA	ALA	GLU
THR	GLY	PRO	PRO	ARG	ARG	F558	F558	GLY	GLN	SER	SER	GLU
THR	TYR	GLY	HIS	GLY	GLY	Q559	Q559	ILE	GLN	GLU	GLU	GLU
THR	GLN	TYR	TYR	PHE	PHE	V560	V560	LEU	LEU	ASN	ASN	GLU
ILE	THR	ASP	SER	GLY	GLY	N563	N563	VAL	PRO	VAL	VAL	GLU
VAL	HIS	PRO	GLN	SER	SER	+	+	VAL	GLY	VAL	VAL	TYR
LYS	PRO	SER	THR	PRO	PRO	D588	D588	THR	LYS	VAL	VAL	TYR
VAL	ALA	PRO	PRO	GLY	GLY	+	+	GLU	VAL	LEU	LEU	GLU
ARG	SER	GLN	HIS	GLY	GLY	N592	N592	THR	ASP	ASP	ASP	GLU
ASP	TYR	VAL	ASP	SER	SER	N593	N593	THR	+	GLU	GLU	GLU
THR	HIS	ASN	GLY	GLY	GLY	D598	D598	LYS	K185	ASP	ASP	GLU
THR	PRO	PRO	SER	THR	GLY	+	+	LYS	+	SER	SER	GLU



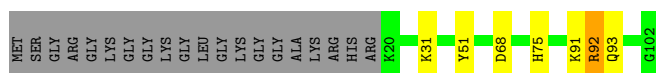
- Molecule 27: Histone H3



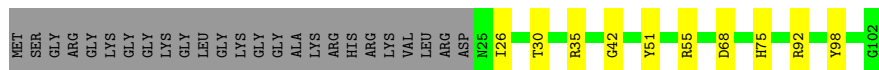
- Molecule 27: Histone H3



- Molecule 28: Histone H4



- Molecule 28: Histone H4



- Molecule 29: Histone H2A type 1

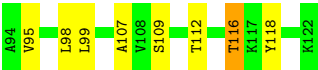
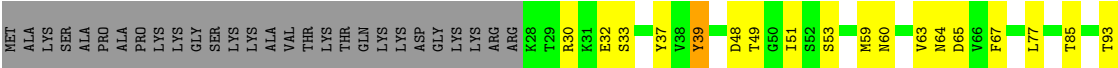


- Molecule 29: Histone H2A type 1

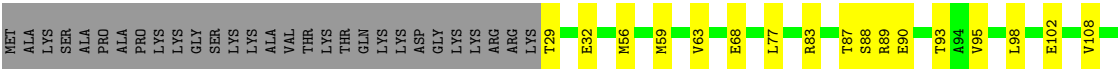




• Molecule 30: Histone H2B 1.1



• Molecule 30: Histone H2B 1.1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1139653	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)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.746	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	549.46, 549.46, 549.46	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09892, 1.09892, 1.09892	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.12	0/11384	0.30	0/15361
2	B	0.12	0/9158	0.29	0/12360
3	C	0.12	0/2115	0.27	0/2873
4	D	0.10	0/1017	0.28	0/1368
5	E	0.13	0/1751	0.30	0/2366
6	F	0.10	0/636	0.24	0/859
7	G	0.09	0/1364	0.26	0/1853
8	H	0.12	0/1219	0.30	0/1644
9	I	0.10	0/964	0.27	0/1305
10	J	0.13	0/533	0.30	0/719
11	K	0.11	0/939	0.26	0/1271
12	L	0.12	0/403	0.29	0/536
13	M	0.07	0/4330	0.20	0/5591
14	N	0.21	0/3442	0.44	0/5314
15	O	0.08	0/655	0.20	0/913
16	P	0.11	0/477	0.27	0/738
17	Q	0.12	0/6531	0.32	2/8861 (0.0%)
18	R	0.11	0/1437	0.26	0/1972
19	S	0.06	0/659	0.16	0/827
20	T	0.19	0/3663	0.40	0/5646
21	U	0.07	0/613	0.25	0/847
22	V	0.09	0/1386	0.32	2/1909 (0.1%)
23	W	0.09	0/2392	0.23	0/3257
24	X	0.09	0/356	0.28	0/478
25	Y	0.09	0/927	0.25	0/1250
26	Z	0.09	0/4084	0.24	0/5498
27	a	0.13	0/760	0.30	0/1019
27	e	0.11	0/812	0.29	0/1088
28	b	0.13	0/669	0.28	0/894
28	f	0.16	0/626	0.32	0/837
29	c	0.12	0/805	0.29	0/1088
29	g	0.11	0/764	0.29	0/1031

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	d	0.12	0/756	0.31	0/1015
30	h	0.11	0/737	0.28	0/993
All	All	0.12	0/68364	0.30	4/93581 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	772	GLU	CA-C-N	7.01	134.33	121.70
17	Q	772	GLU	C-N-CA	7.01	134.33	121.70
22	V	61	TYR	CA-C-N	5.64	131.85	121.70
22	V	61	TYR	C-N-CA	5.64	131.85	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11210	0	11292	119	0
2	B	8980	0	9019	97	0
3	C	2072	0	2020	27	0
4	D	1004	0	980	5	0
5	E	1720	0	1737	21	0
6	F	626	0	657	8	0
7	G	1333	0	1321	12	0
8	H	1197	0	1156	15	0
9	I	942	0	872	19	0
10	J	524	0	541	10	0
11	K	920	0	942	11	0
12	L	397	0	405	9	0
13	M	4309	0	1506	4	0
14	N	3070	0	1680	28	0
15	O	656	0	290	0	0
16	P	432	0	219	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	6427	0	5646	87	0
18	R	1428	0	922	10	0
19	S	657	0	199	2	0
20	T	3264	0	1791	24	0
21	U	617	0	263	0	0
22	V	1378	0	806	11	0
23	W	2333	0	2246	38	0
24	X	353	0	371	4	0
25	Y	911	0	907	9	0
26	Z	4025	0	4041	36	0
27	a	751	0	792	2	0
27	e	801	0	838	10	0
28	b	662	0	709	7	0
28	f	619	0	659	6	0
29	c	795	0	846	12	0
29	g	755	0	800	5	0
30	d	745	0	773	15	0
30	h	726	0	747	8	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	Y	1	0	0	0	0
32	A	1	0	0	0	0
All	All	66649	0	57993	595	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 5.

The worst 5 of 595 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)
17:Q:371:TYR:OH	22:V:69:GLN:NE2	2.07	0.88
17:Q:276:ALA:HB1	17:Q:288:VAL:HG23	1.61	0.82
2:B:790:GLN:O	2:B:968:ASN:ND2	2.15	0.79
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.65	0.78
17:Q:605:LEU:O	17:Q:609:ASN:ND2	2.18	0.76

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	1408/1984 (71%)	1286 (91%)	121 (9%)	1 (0%)	48	77
2	B	1112/1251 (89%)	1009 (91%)	102 (9%)	1 (0%)	48	77
3	C	254/275 (92%)	229 (90%)	25 (10%)	0	100	100
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	194 (94%)	13 (6%)	0	100	100
6	F	76/127 (60%)	72 (95%)	4 (5%)	0	100	100
7	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
8	H	147/150 (98%)	133 (90%)	14 (10%)	0	100	100
9	I	114/125 (91%)	103 (90%)	11 (10%)	0	100	100
10	J	64/67 (96%)	57 (89%)	7 (11%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	45/58 (78%)	41 (91%)	3 (7%)	1 (2%)	5	20
13	M	976/1729 (56%)	910 (93%)	65 (7%)	1 (0%)	48	77
15	O	130/821 (16%)	125 (96%)	4 (3%)	1 (1%)	16	44
17	Q	888/1179 (75%)	851 (96%)	37 (4%)	0	100	100
18	R	240/713 (34%)	228 (95%)	12 (5%)	0	100	100
19	S	157/304 (52%)	153 (98%)	4 (2%)	0	100	100
21	U	117/666 (18%)	101 (86%)	15 (13%)	1 (1%)	14	41
22	V	234/531 (44%)	214 (92%)	20 (8%)	0	100	100
23	W	298/305 (98%)	284 (95%)	14 (5%)	0	100	100
24	X	41/531 (8%)	40 (98%)	1 (2%)	0	100	100
25	Y	114/121 (94%)	106 (93%)	8 (7%)	0	100	100
26	Z	497/1087 (46%)	451 (91%)	46 (9%)	0	100	100
27	a	90/136 (66%)	88 (98%)	2 (2%)	0	100	100
27	e	95/136 (70%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
28	f	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
29	c	101/130 (78%)	99 (98%)	2 (2%)	0	100	100
29	g	96/130 (74%)	92 (96%)	4 (4%)	0	100	100
30	d	93/123 (76%)	90 (97%)	3 (3%)	0	100	100
30	h	91/123 (74%)	89 (98%)	2 (2%)	0	100	100
All	All	8248/13649 (60%)	7680 (93%)	562 (7%)	6 (0%)	49	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	39	CYS
13	M	700	HIS
1	A	1343	LEU
21	U	510	LYS
2	B	684	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	A	1229/1761 (70%)	1227 (100%)	2 (0%)	87	96
2	B	986/1084 (91%)	984 (100%)	2 (0%)	87	96
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/126 (86%)	109 (100%)	0	100	100
5	E	191/192 (100%)	190 (100%)	1 (0%)	81	93
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	146/153 (95%)	146 (100%)	0	100	100
8	H	130/131 (99%)	130 (100%)	0	100	100
9	I	104/112 (93%)	103 (99%)	1 (1%)	68	89
10	J	55/56 (98%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	44/55 (80%)	44 (100%)	0	100	100
13	M	41/1524 (3%)	41 (100%)	0	100	100
17	Q	533/1011 (53%)	525 (98%)	8 (2%)	57	84
18	R	57/625 (9%)	56 (98%)	1 (2%)	51	80
19	S	4/268 (2%)	4 (100%)	0	100	100
22	V	46/462 (10%)	46 (100%)	0	100	100
23	W	255/260 (98%)	251 (98%)	4 (2%)	55	83
24	X	40/467 (9%)	40 (100%)	0	100	100
25	Y	102/105 (97%)	102 (100%)	0	100	100
26	Z	435/939 (46%)	434 (100%)	1 (0%)	87	96
27	a	80/111 (72%)	75 (94%)	5 (6%)	16	45
27	e	84/111 (76%)	81 (96%)	3 (4%)	31	65
28	b	68/79 (86%)	66 (97%)	2 (3%)	37	71
28	f	63/79 (80%)	61 (97%)	2 (3%)	34	68
29	c	82/102 (80%)	77 (94%)	5 (6%)	17	46
29	g	76/102 (74%)	73 (96%)	3 (4%)	28	63
30	d	81/103 (79%)	73 (90%)	8 (10%)	7	24
30	h	79/103 (77%)	71 (90%)	8 (10%)	7	24
All	All	5527/10590 (52%)	5471 (99%)	56 (1%)	65	89

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	c	81	ARG
30	h	112	THR
30	d	77	LEU
30	h	102	GLU
30	h	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	57	GLN

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Mol	Chain	Res	Type
29	g	38	ASN
23	W	268	HIS
26	Z	519	GLN
30	h	64	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	20/21 (95%)	7 (35%)	3 (15%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	8	U
16	P	9	U
16	P	10	U
16	P	11	U
16	P	16	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	8	U
16	P	16	U
16	P	18	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	1547	1	8,9,10	1.62	1 (12%)	7,12,14	1.44	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	A	1525	1	8,10,11	1.11	0	10,14,16	2.08	1 (10%)
26	TPO	Z	775	26	8,10,11	1.14	0	10,14,16	1.77	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	1547	1	-	0/6/8/10	-
1	TPO	A	1525	1	-	0/9/11/13	-
26	TPO	Z	775	26	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.54	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	P-OG1-CB	-5.92	107.23	123.33
26	Z	775	TPO	P-OG1-CB	-4.89	110.03	123.33
1	A	1547	SEP	OG-CB-CA	3.21	111.27	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	Z	775	TPO	C-CA-CB-CG2
26	Z	775	TPO	CB-OG1-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1525	TPO	1	0
26	Z	775	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	1
22	V	1
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	27.14
1	V	299:GLU	C	310:ASN	N	12.59
1	M	1334:ASN	C	1338:ILE	N	5.53

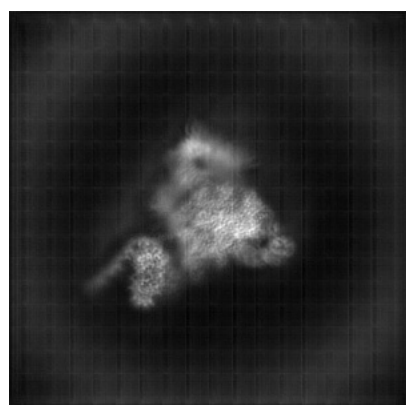
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48040. These allow visual inspection of the internal detail of the map and identification of artifacts.

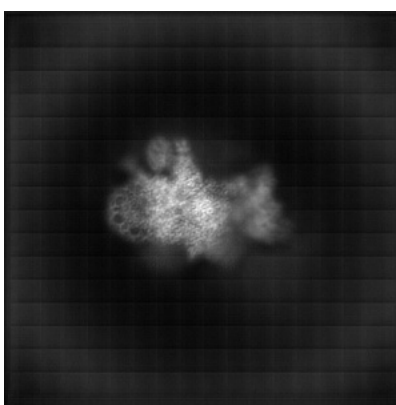
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

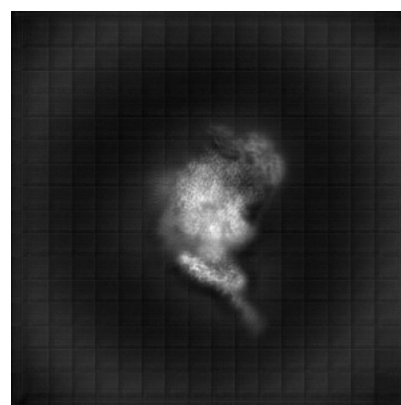
6.1.1 Primary map



X



Y

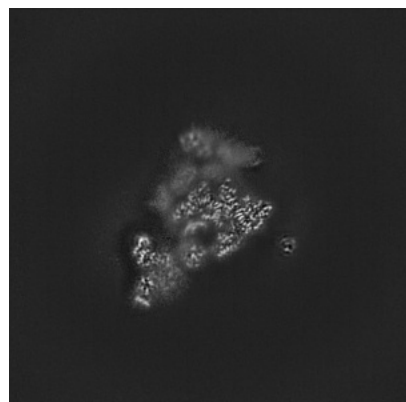


Z

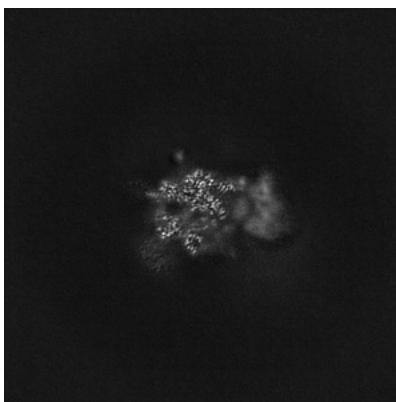
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

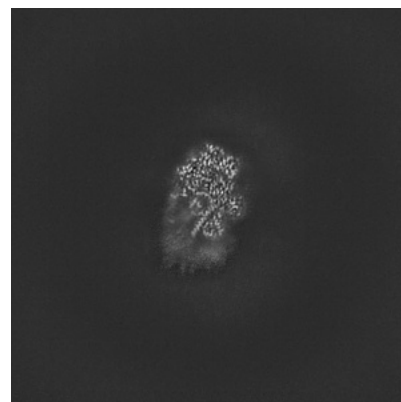
6.2.1 Primary map



X Index: 250



Y Index: 250

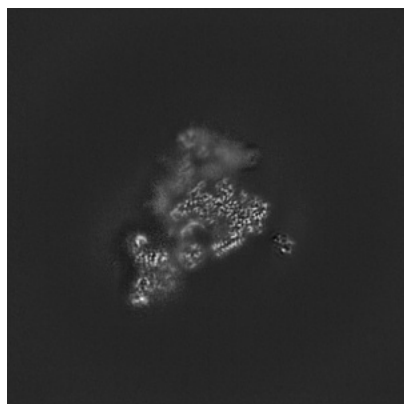


Z Index: 250

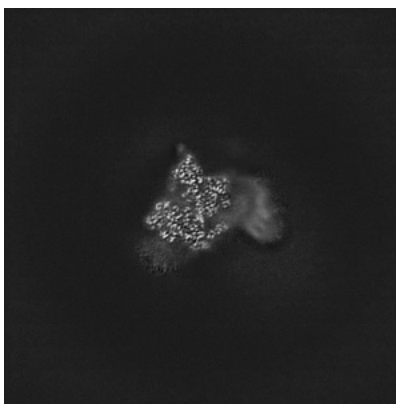
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

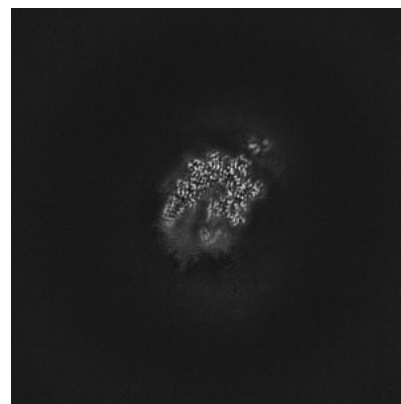
6.3.1 Primary map



X Index: 253



Y Index: 264

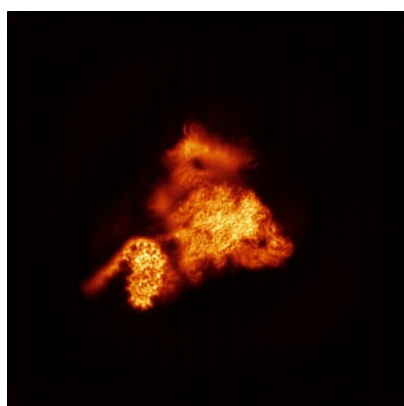


Z Index: 236

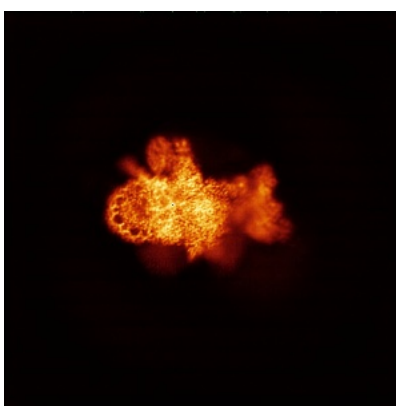
The images above show the largest variance slices of the map in three orthogonal directions.

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

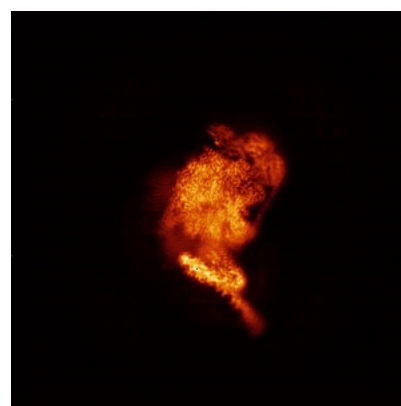
6.4.1 Primary map



X



Y

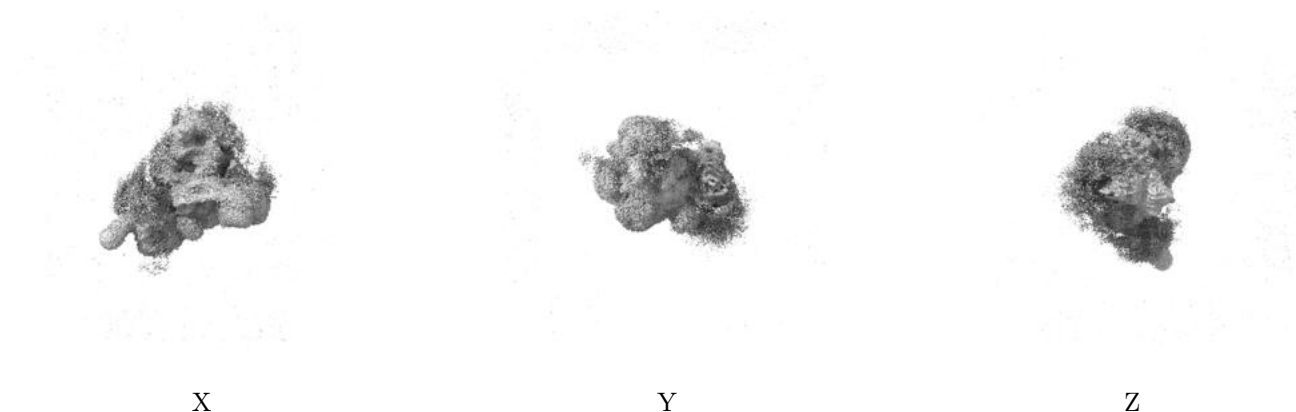


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

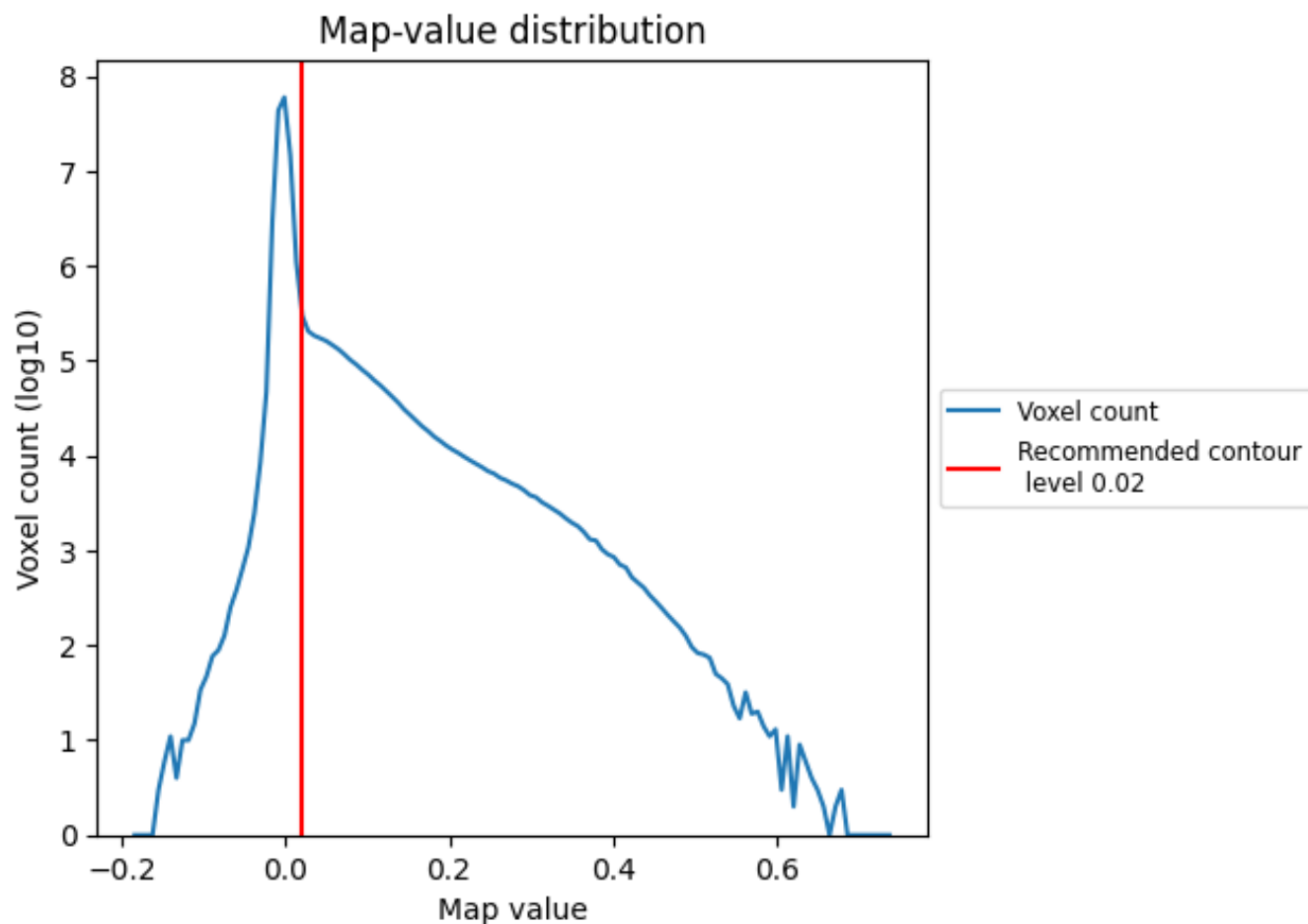
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

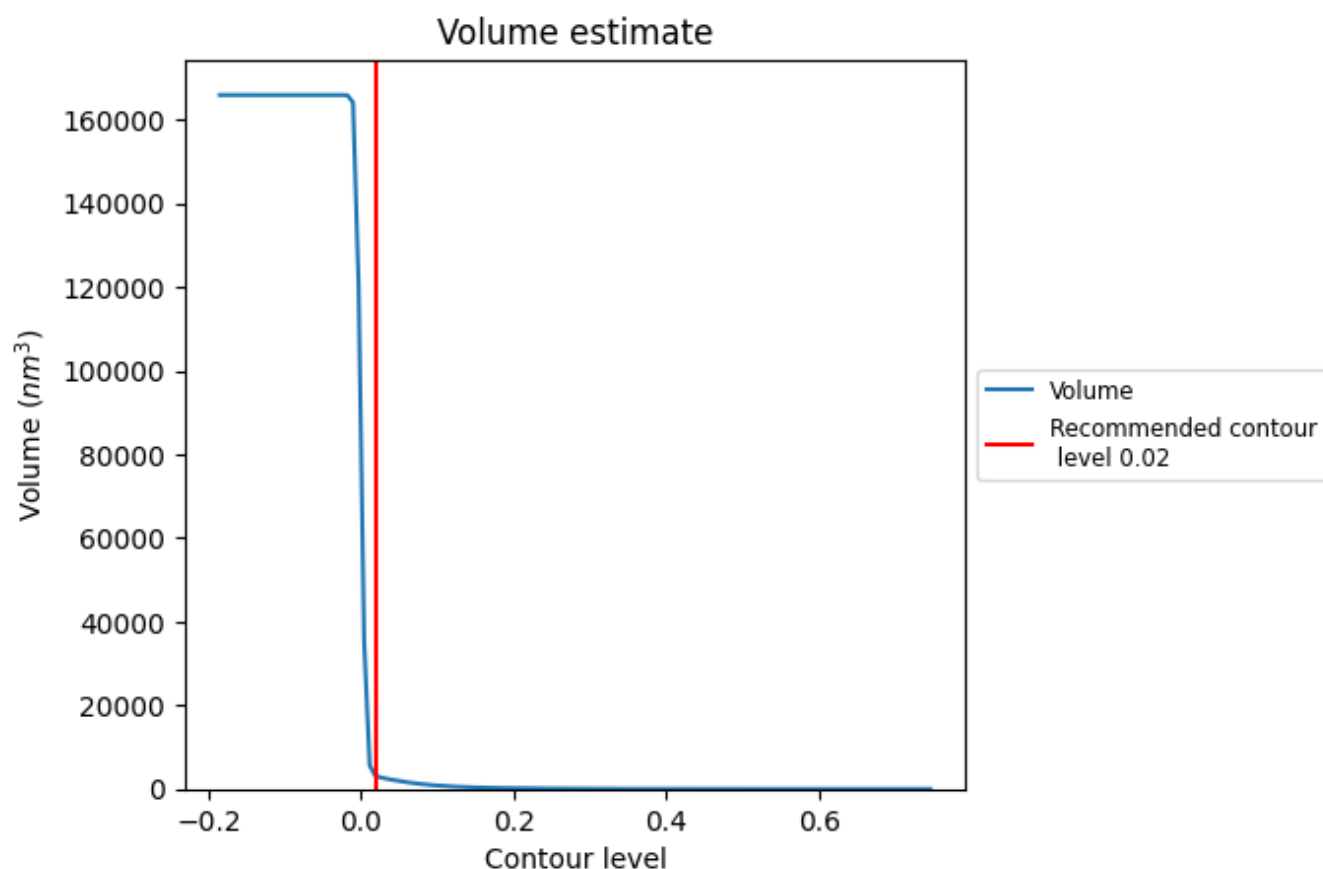
This section contains the results of statistical analysis of the map.

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.

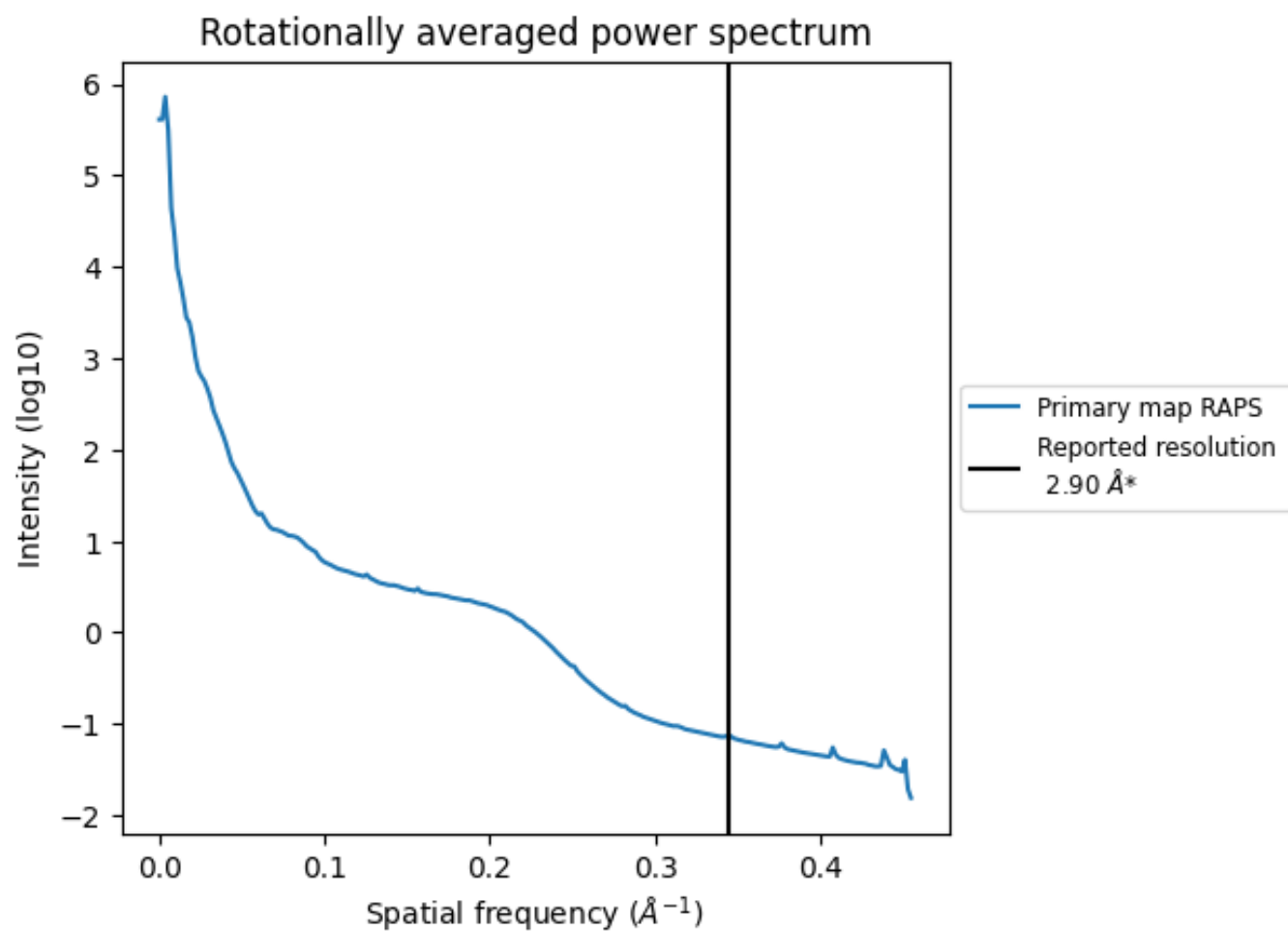
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3120 nm³; this corresponds to an approximate mass of 2818 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 0.345 Å⁻¹

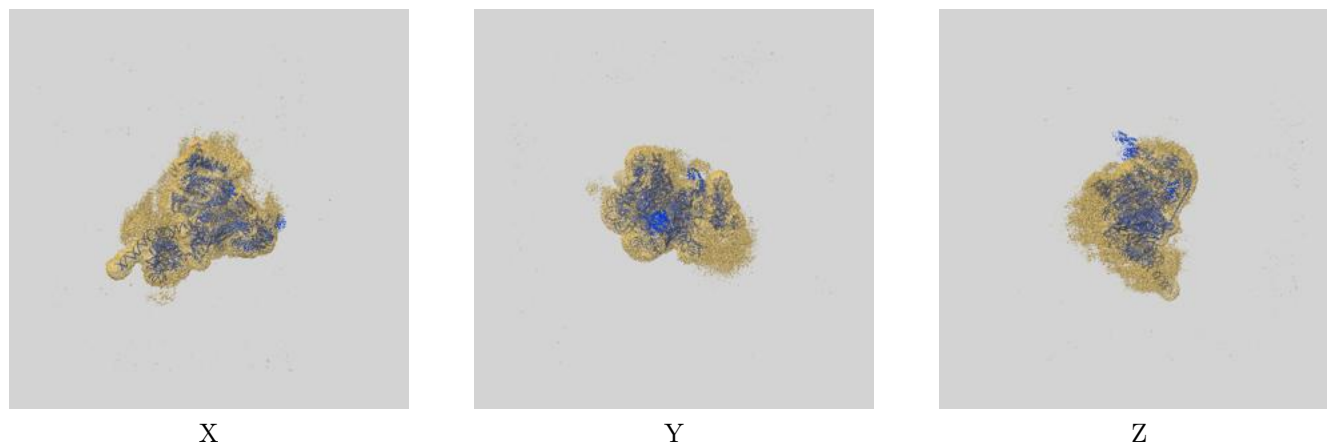
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

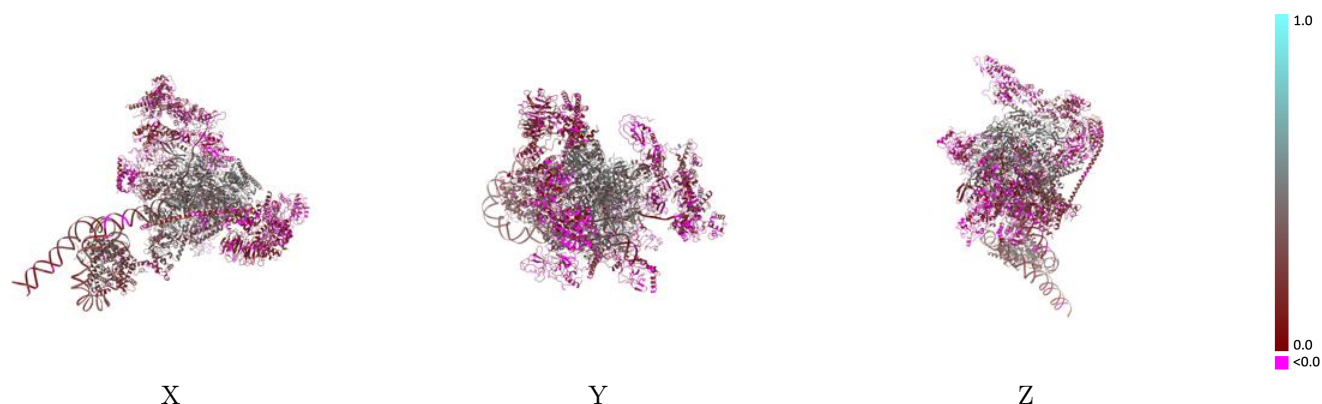
This section contains information regarding the fit between EMDB map EMD-48040 and PDB model 9EGY. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



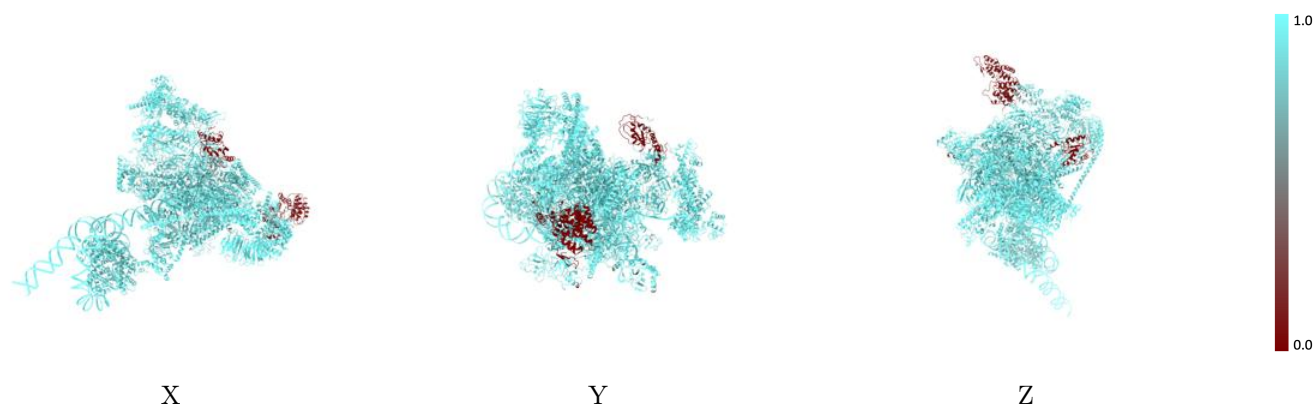
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



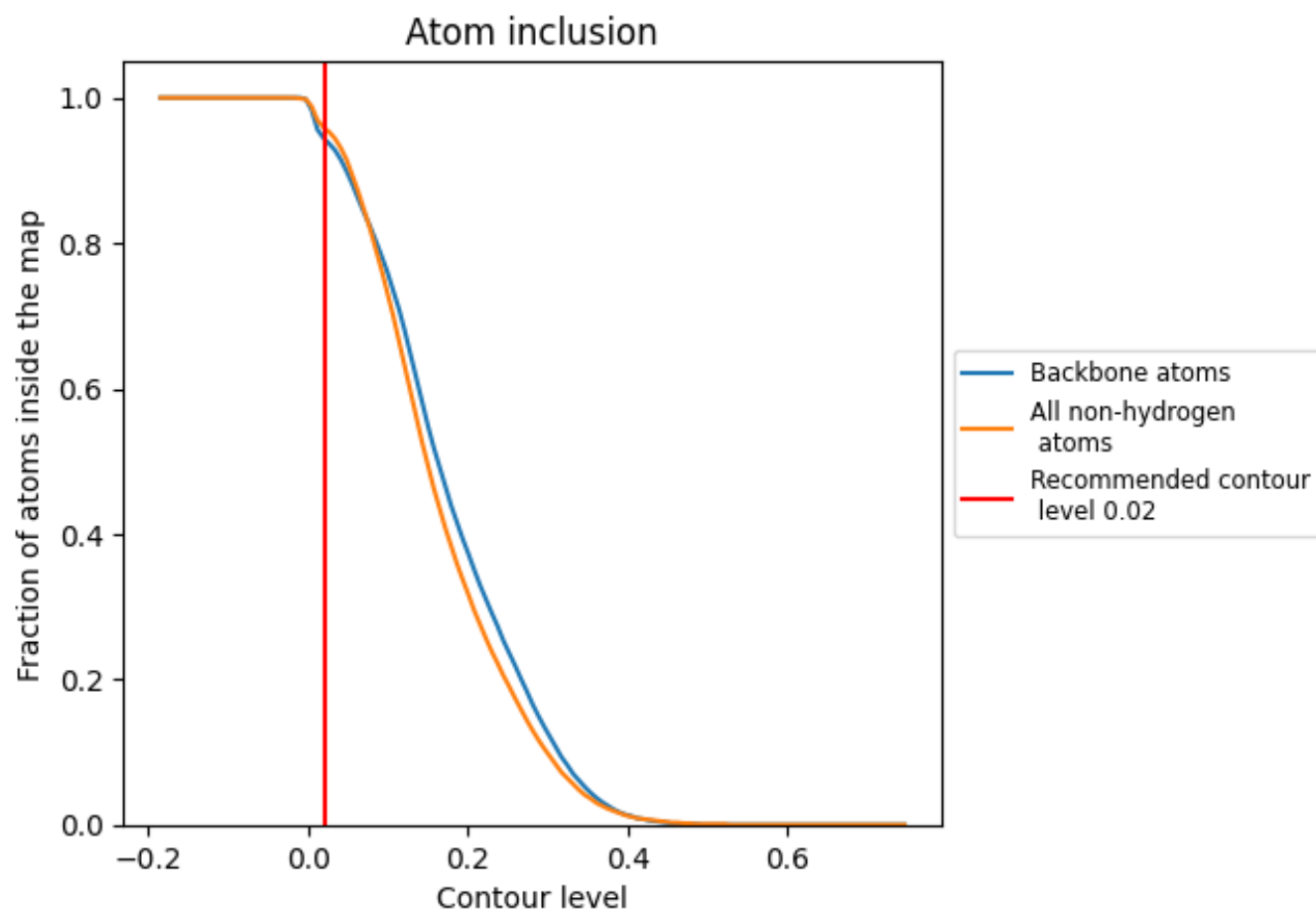
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 96% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.2560
A	 0.9920	 0.3920
B	 1.0000	 0.4070
C	 1.0000	 0.4310
D	 1.0000	 0.1860
E	 1.0000	 0.3790
F	 1.0000	 0.4340
G	 1.0000	 0.2110
H	 0.9980	 0.4220
I	 1.0000	 0.3590
J	 0.9980	 0.4150
K	 1.0000	 0.4340
L	 1.0000	 0.3690
M	 0.8460	 0.0910
N	 0.9960	 0.2020
O	 1.0000	 -0.0010
P	 1.0000	 0.1900
Q	 0.7640	 0.0890
R	 0.9040	 0.0540
S	 1.0000	 0.2010
T	 0.9950	 0.2100
U	 0.9820	 0.0890
V	 0.8080	 0.0670
W	 1.0000	 0.1380
X	 1.0000	 0.1470
Y	 1.0000	 0.0270
Z	 0.9930	 0.0810
a	 0.9930	 0.2890
b	 0.9980	 0.3080
c	 0.9970	 0.3350
d	 0.9990	 0.3120
e	 0.9950	 0.3300
f	 0.9970	 0.3340
g	 0.9950	 0.1950
h	 1.0000	 0.1990

