



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 9RMC / pdb_00009rmc
EMDB ID : EMD-54056
Title : Structure of BAF in complex with OCT4-SOX2-bound nucleosome - SHL+6 class 1
Authors : Vecchia, L.; Weiss, J.; Cavadini, S.; Kempf, G.; Kater, L.; Pathare, G.; Thoma, N.H.
Deposited on : 2025-06-18
Resolution : 4.20 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.dev132
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

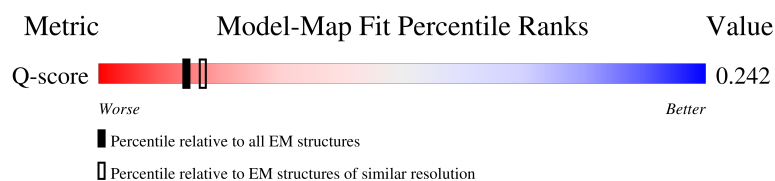
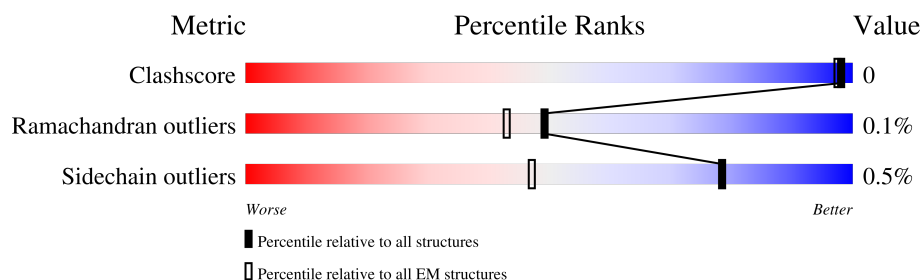
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



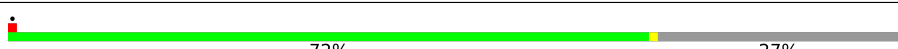
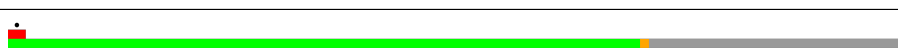
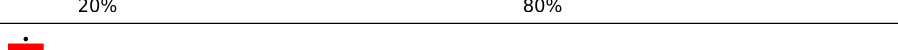
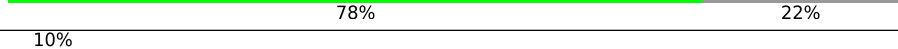
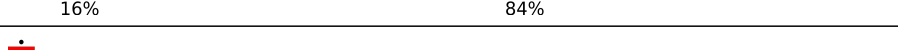
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	Q	411	
13	R	435	
14	V	645	
15	W	105	
16	X	227	
17	Y	227	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 27953 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	331	Total	C	N	O	S	0	0
			2021	1233	403	383	2		

- 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	466	Total	C	N	O	S	0	0
			3671	2341	620	689	21		

- 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	260	Total	C	N	O	S	0	0
			1622	1006	304	308	4		
10	O	315	Total	C	N	O		0	0
			1605	975	315	315			

- 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	235	Total	C	N	O	S	0	0
			1315	809	251	254	1		

- Molecule 12 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Q	105	Total	C	N	O	0	0
			529	319	105	105		

- Molecule 13 is a protein called Zinc finger protein ubi-d4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	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

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

- Molecule 14 is a protein called Green fluorescent protein,POU domain, class 5, transcription factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	68	Total	C	N	O	0	0
			338	202	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 15 is a protein called Transcription factor SOX-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	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
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 16 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	131	Total	C	N	O	P	0	0
			2662	1267	473	791	131		

- Molecule 17 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	131	Total	C	N	O	P	0	0
			2706	1281	516	779	130		

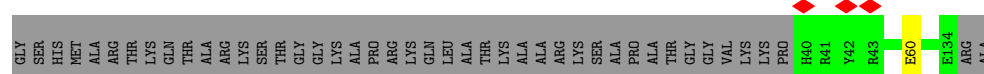
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	L	1	Total	Zn	0
			1	1	

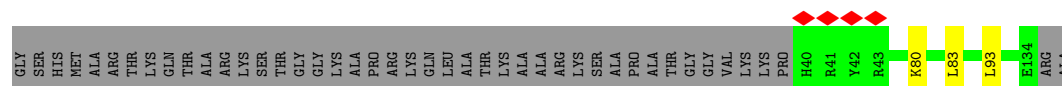
3 Residue-property plots [i](#)

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.

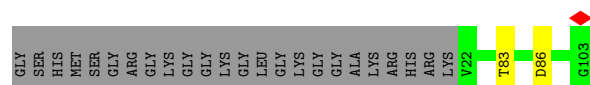
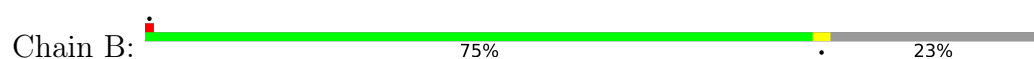
• Molecule 1: Histone H3.1



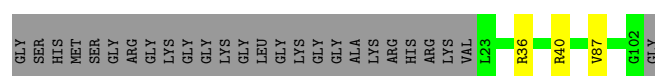
• Molecule 1: Histone H3.1



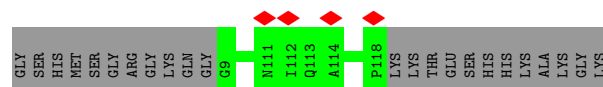
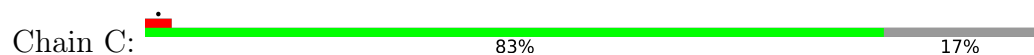
• Molecule 2: Histone H4



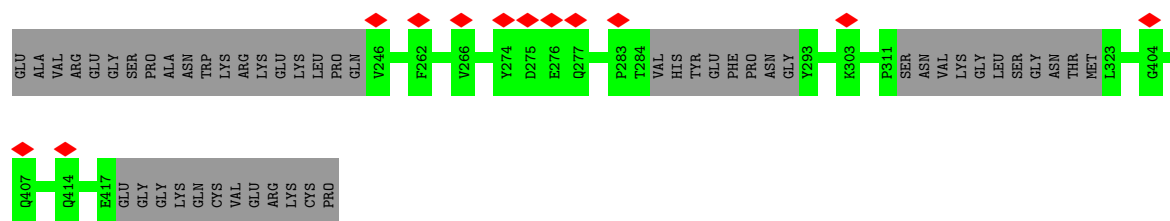
• Molecule 2: Histone H4



• Molecule 3: Histone H2A type 1-B/E

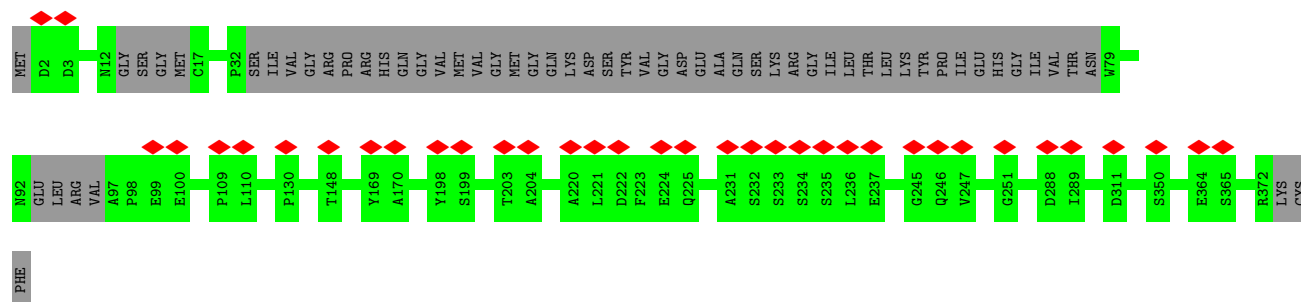


• Molecule 3: Histone H2A type 1-B/E



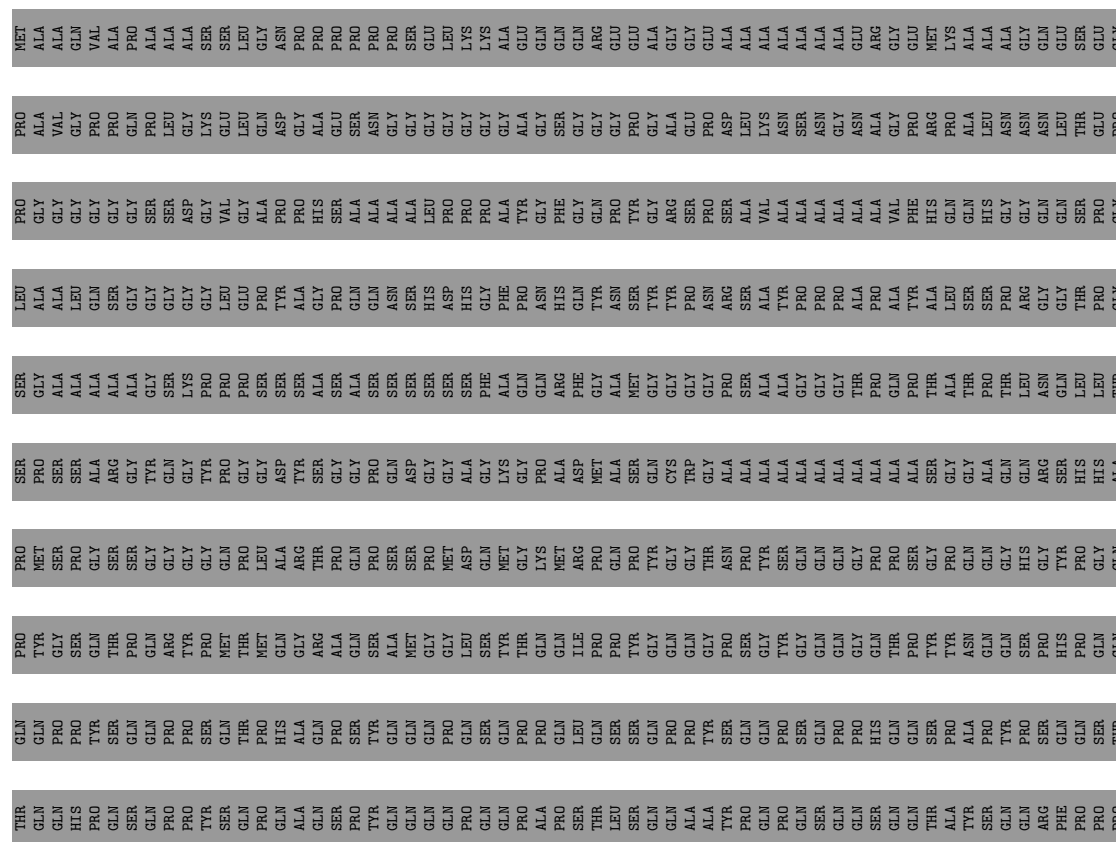
- Molecule 7: Actin, cytoplasmic 1, N-terminally processed

Chain K: 10% 85% 15%

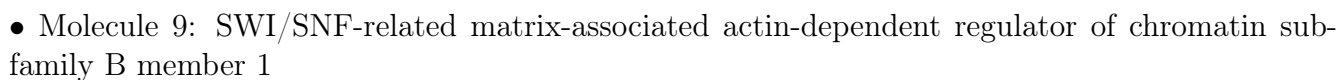


- Molecule 8: AT-rich interactive domain-containing protein 1A

Chain L: 20% 80%



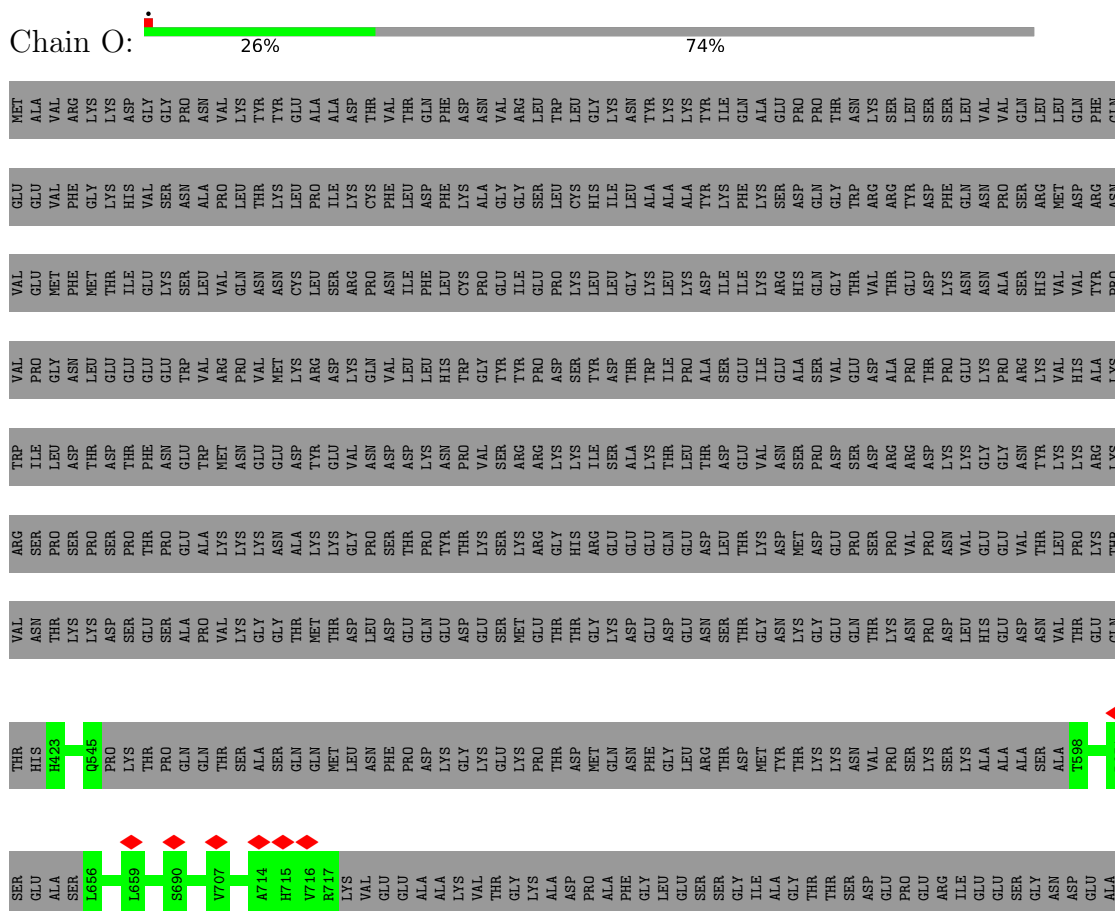


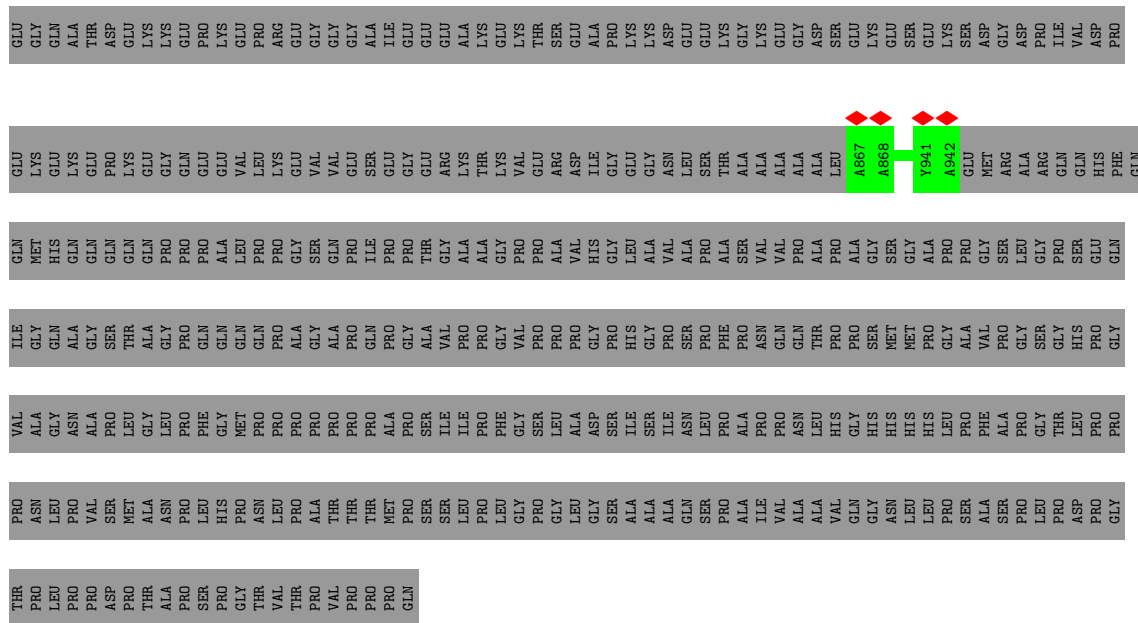


- Molecule 10: SWI/SNF complex subunit SMARCC2

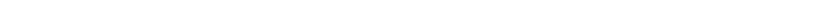
LEU	GLU	VAL	ARG	TRP	ARG	TRP	VAL	GLU	LEU	MET
THR	SER	ASN	PRO	ILE	SER	ILE	ASN	GLU	VAL	ALA
ASP	PRO	THR	SER	LEU	PRO	LEU	GLY	VAL	VAL	ARG
THR	PRO	LYS	SER	ASP	SER	THR	ASN	PHE	THR	LYS
THR	MET	ASP	SER	THR	PRO	THR	GLU	THR	ILE	ASP
LYS	GLY	GLU	THR	PHE	THR	THR	GLU	GLU	VAL	GLY
ASN	PRO	SER	PRO	ASN	GLU	ASN	TRP	SER	LYS	PRO
VAL	PRO	ALA	ALA	GLU	GLU	TRP	VAL	ALA	LEU	ASN
PRO	THR	VAL	LYS	MET	LYS	ARG	ARG	VAL	PRO	VAL
SER	SER	LYS	LYS	ASN	LYS	VAL	PRO	GLN	LEU	LYS
LYS	HIS	GLY	LYS	GLU	ASN	GLU	VAL	ASN	THR	THR
SER	PHE	GLY	ASN	GLU	GLU	MET	ASN	LYS	THR	TYR
LYS	HIS	THR	ALA	ASP	ALA	LYS	LYS	GLU	LEU	ALA
ALA	VAL	MET	LYS	TYR	LYS	ARG	ARG	PRO	PRO	ALA
ALA	LEU	THR	GLY	VAL	LYS	GLU	ASP	SER	ILE	ALA
ALA	ASP	ASP	GLY	VAL	GLY	VAL	LYS	ARG	LYS	ASP
SER	ASP	LEU	PRO	ASN	PRO	ASN	GLN	PRO	CYS	THR
THR	THR	ASP	SER	ASP	SER	THR	ASN	PHE	CYS	VAL
ALA	PRO	GLU	THR	THR	THR	THR	VAL	GLY	ALA	ASN
THR	GLY	GLU	GLN	PRO	LYS	VAL	GLY	PRO	GLY	VAL
ARG	SER	GLU	THR	ASN	THR	THR	THR	LEU	GLY	THR
GLU	GLY	ASP	GLU	PRO	THR	VAL	THR	PRO	ILE	ASP
THR	VAL	GLU	GLU	LYS	LYS	ARG	GLY	ALA	LYS	ASN
PRO	PRO	SER	LEU	ILE	ARG	ILE	THR	GLY	ILE	VAL
GLN	GLN	MET	GLU	SER	GLU	THR	TYR	LEU	LYS	ARG
PRO	GLN	ASP	GLU	ALA	GLU	ALA	THR	GLY	LEU	THR
GLU	THR	THR	ASP	THR	GLN	THR	ILE	LEU	ALA	LYS
SER	SER	SER	GLU	LEU	GLU	LEU	PRO	LYS	ALA	LYS
ASP	ALA	ASN	ASN	THR	ASP	THR	ALA	ASP	TYR	THR
PRO	ASN	GLY	ASP	PRO	ASP	ASP	SER	GLN	GLY	PRO
GLU	PHE	GLU	GLU	ASP	GLU	VAL	VAL	THR	THR	PRO
ALA	PRO	GLN	THR	SER	PRO	ASP	GLY	TRP	TRP	ASN
SER	ASP	THR	SER	ASP	PRO	VAL	ASN	ARG	ARG	LYS
LEU	GLY	ASN	VAL	ARG	VAL	ARG	GLU	GLU	TYR	LEU
PRO	LYS	PRO	PRO	ASP	ASN	ASP	THR	ASP	ASP	SER
LEU	GLU	ASP	ASN	LYS	ASN	LYS	PRO	LYS	PHE	SER
ALA	LYS	THR	VAL	GLY	VAL	GLY	GLN	GLN	GLN	LEU
THR	THR	HIS	HIS	THR	THR	THR	LYS	ASN	THR	VAL
GLN	THR	E414	E414	LYS	GLU	LYS	GLY	ASN	GLN	VAL
THR	THR	HIS	GLU	GLY	GLU	GLY	GLY	GLY	GLN	ASN
ASP	ASP	E414	GLU	LYS	VAL	THR	THR	THR	THR	GLN
MET	MET	D434	THR	TYR	THR	TYR	LYS	ARG	ARG	LEU
GLN	GLN	Y435	LEU	LYS	PRO	LYS	VAL	VAL	THR	LEU
PHE	PHE	D515	PRO	LYS	THR	LYS	HIS	VAL	ASP	GLN
ASN	PHE	ALA	LYS	ARG	THR	LYS	ALA	TYR	ASP	PHE
LEU	GLY	D619	THR	GLY	THR	ARG	LYS	PRO	ASN	GLN
THR	THR	K617	THR	THR	THR	THR	ALA	GLY	GLY	THR
GLU	THR	D619	THR	THR	THR	THR	GLY	THR	THR	THR
THR	THR	K641	THR	THR	THR	THR	GLY	THR	THR	THR
PRO	PRO	K617	THR	THR	THR	THR	GLY	THR	THR	THR
GLU	GLU	D618	THR	THR	THR	THR	GLY	THR	THR	THR
THR	THR	T602	THR	THR	THR	THR	GLY	THR	THR	THR
ASP	ASP	K617	THR	THR	THR	THR	GLY	THR	THR	THR
THR	THR	D618	THR	THR	THR	THR	GLY	THR	THR	THR
GLN	GLN	D619	THR	THR	THR	THR	GLY	THR	THR	THR
LEU	LEU	K641</								

- Molecule 10: SWI/SNF complex subunit SMARCC2



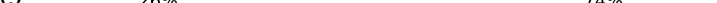


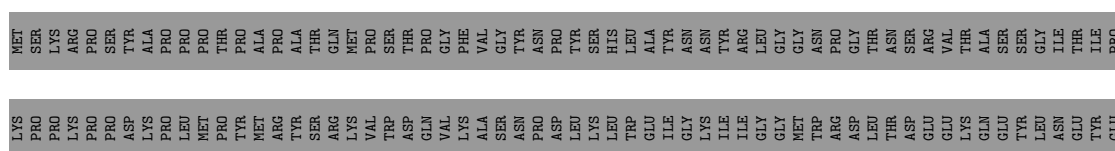
- Molecule 11: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1

Chain P:  45% 54%



- Molecule 12: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1

Chain Q:  26% 74%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30808	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	0.554	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.061	Depositor
Map size ($\text{\AA}$)	405.6, 405.6, 405.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.845, 0.845, 0.845	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	A	0.16	0/794	0.33	0/1065
1	E	0.17	0/794	0.33	0/1065
2	B	0.17	0/660	0.36	0/883
2	F	0.18	0/648	0.36	0/868
3	C	0.18	0/854	0.37	0/1151
3	G	0.17	0/854	0.34	0/1151
4	D	0.14	0/737	0.35	0/990
4	H	0.17	0/731	0.33	0/982
5	I	0.18	0/2030	0.47	0/2778
6	J	0.21	0/1687	0.39	0/2352
7	K	0.20	0/1613	0.38	0/2254
8	L	0.15	0/3740	0.35	0/5070
9	M	0.15	0/1498	0.35	0/2095
10	N	0.14	0/1643	0.32	0/2262
10	O	0.15	0/1620	0.36	0/2272
11	P	0.20	0/1333	0.42	0/1855
12	Q	0.20	0/531	0.41	0/743
13	R	0.23	0/353	0.45	0/492
14	V	0.24	0/338	0.35	0/470
15	W	0.23	0/377	0.38	0/529
16	X	0.37	0/2979	0.70	0/4590
17	Y	0.36	0/3042	0.69	0/4699
All	All	0.23	0/28856	0.47	0/40616

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	783	0	818	1	0
1	E	783	0	818	2	0
2	B	653	0	696	1	0
2	F	641	0	684	2	0
3	C	844	0	905	0	0
3	G	844	0	905	2	0
4	D	726	0	745	0	0
4	H	720	0	740	2	0
5	I	2021	0	1495	3	0
6	J	1677	0	833	0	0
7	K	1600	0	818	0	0
8	L	3671	0	3724	6	0
9	M	1488	0	716	0	0
10	N	1622	0	1182	1	0
10	O	1605	0	831	0	0
11	P	1315	0	740	0	0
12	Q	529	0	241	0	0
13	R	351	0	177	0	0
14	V	338	0	156	0	0
15	W	373	0	187	1	0
16	X	2662	0	1474	3	0
17	Y	2706	0	1470	0	0
18	L	1	0	0	0	0
All	All	27953	0	20355	20	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 0.

All (20) 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:454:GLU:N	5:I:454:GLU:OE1	2.26	0.69
3:G:11:ALA:O	4:H:121:LYS:NZ	2.38	0.56
10:N:434:ASP:OD1	10:N:435:TYR:N	2.45	0.50
8:L:1662:LYS:O	8:L:1663:ASP:CG	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:1810:ASP:OD1	8:L:1811:LYS:N	2.46	0.48
8:L:2157:ASP:OD1	8:L:2158:ARG:N	2.46	0.48
16:X:134:DC:H2''	16:X:135:DA:C8	2.50	0.47
1:E:80:LYS:HB3	1:E:83:LEU:HD11	1.98	0.46
16:X:134:DC:H2''	16:X:135:DA:N7	2.32	0.45
8:L:2138:THR:HG22	8:L:2140:PRO:HD2	2.00	0.43
3:G:11:ALA:O	4:H:121:LYS:CE	2.67	0.43
8:L:2051:ASP:OD1	8:L:2052:CYS:N	2.52	0.43
15:W:72:SER:CB	16:X:125:DT:H1'	2.49	0.41
5:I:806:PHE:N	5:I:878:MET:HA	2.35	0.41
1:E:93:LEU:HD12	2:F:87:VAL:HG13	2.03	0.41
2:F:36:ARG:O	2:F:40:ARG:HG2	2.21	0.40
2:B:83:THR:HG22	2:B:86:ASP:OD2	2.22	0.40
1:A:60:GLU:OE1	1:A:60:GLU:N	2.51	0.40
5:I:358:PRO:O	5:I:359:ARG:HB3	2.22	0.40
8:L:2245:ASP:HA	8:L:2248:HIS:CD2	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%)	93 (100%)	0	0	100	100
1	E	93/139 (67%)	93 (100%)	0	0	100	100
2	B	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	F	78/106 (74%)	76 (97%)	2 (3%)	0	100	100
3	C	108/133 (81%)	106 (98%)	2 (2%)	0	100	100
3	G	108/133 (81%)	105 (97%)	3 (3%)	0	100	100
4	D	91/128 (71%)	88 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	90/128 (70%)	90 (100%)	0	0	100	100
5	I	321/1647 (20%)	272 (85%)	47 (15%)	2 (1%)	21	58
6	J	324/429 (76%)	311 (96%)	13 (4%)	0	100	100
7	K	309/375 (82%)	298 (96%)	11 (4%)	0	100	100
8	L	456/2285 (20%)	440 (96%)	16 (4%)	0	100	100
9	M	289/385 (75%)	283 (98%)	6 (2%)	0	100	100
10	N	252/1214 (21%)	251 (100%)	1 (0%)	0	100	100
10	O	307/1214 (25%)	302 (98%)	5 (2%)	0	100	100
11	P	227/515 (44%)	220 (97%)	6 (3%)	1 (0%)	30	66
12	Q	103/411 (25%)	101 (98%)	2 (2%)	0	100	100
13	R	68/435 (16%)	66 (97%)	2 (3%)	0	100	100
14	V	66/645 (10%)	66 (100%)	0	0	100	100
15	W	71/105 (68%)	71 (100%)	0	0	100	100
All	All	3534/10672 (33%)	3410 (96%)	121 (3%)	3 (0%)	49	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	P	368	PRO
5	I	797	MET
5	I	874	ARG

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%)	83 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	78 (99%)	1 (1%)	61	71
4	H	78/106 (74%)	77 (99%)	1 (1%)	61	71
5	I	104/1422 (7%)	101 (97%)	3 (3%)	37	58
6	J	15/364 (4%)	15 (100%)	0	100	100
7	K	17/318 (5%)	17 (100%)	0	100	100
8	L	418/1845 (23%)	416 (100%)	2 (0%)	81	81
9	M	13/346 (4%)	13 (100%)	0	100	100
10	N	87/1030 (8%)	87 (100%)	0	100	100
10	O	19/1030 (2%)	19 (100%)	0	100	100
11	P	39/442 (9%)	39 (100%)	0	100	100
12	Q	3/361 (1%)	3 (100%)	0	100	100
13	R	3/373 (1%)	3 (100%)	0	100	100
14	V	1/537 (0%)	1 (100%)	0	100	100
15	W	5/95 (5%)	5 (100%)	0	100	100
All	All	1350/8967 (15%)	1343 (100%)	7 (0%)	78	81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	106	GLU
4	H	121	LYS
5	I	416	LEU
5	I	418	GLN
5	I	454	GLU
8	L	1692	ASN
8	L	2007	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	96	GLN
3	G	83	HIS
8	L	1692	ASN

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Mol	Chain	Res	Type
8	L	1843	HIS
8	L	2210	GLN
11	P	484	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

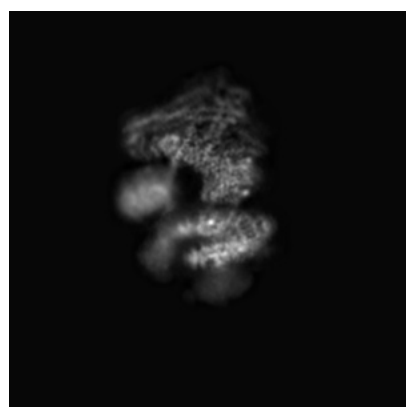
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54056. These allow visual inspection of the internal detail of the map and identification of artifacts.

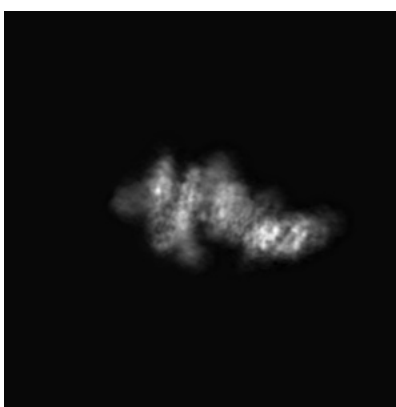
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

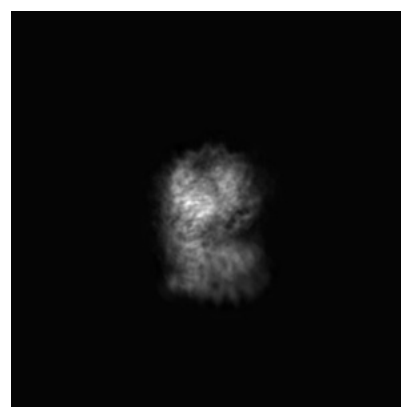
6.1.1 Primary map



X



Y

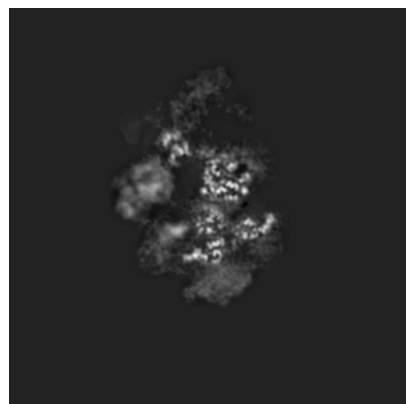


Z

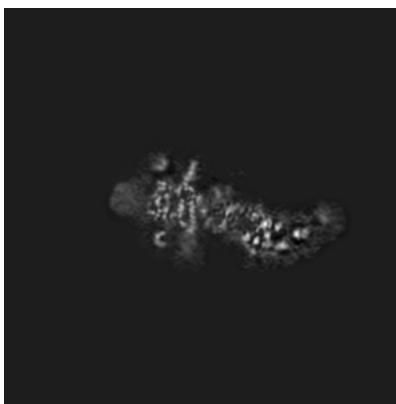
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

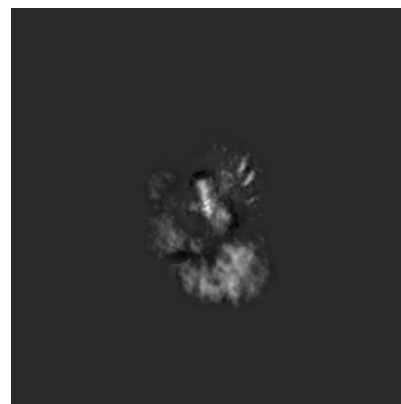
6.2.1 Primary map



X Index: 240



Y Index: 240

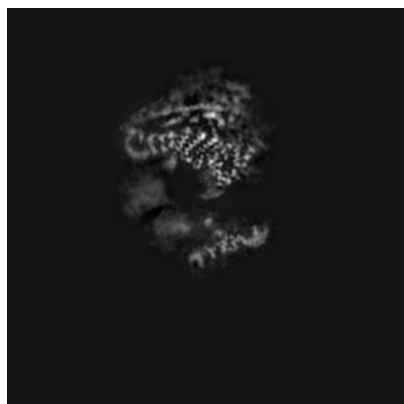


Z Index: 240

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

6.3 Largest variance slices [i](#)

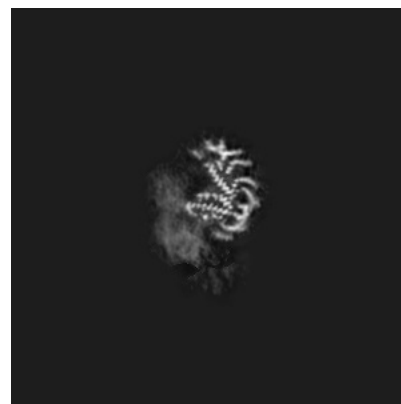
6.3.1 Primary map



X Index: 211



Y Index: 249



Z Index: 223

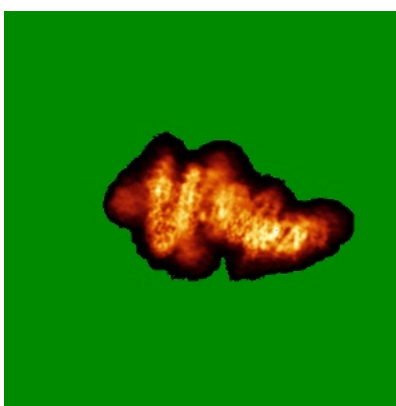
The images above show the largest variance slices of the map in three orthogonal directions.

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

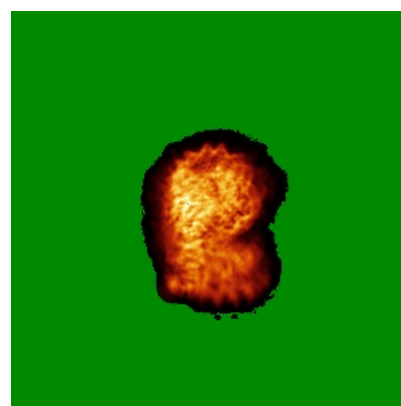
6.4.1 Primary map



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

This section was not generated.

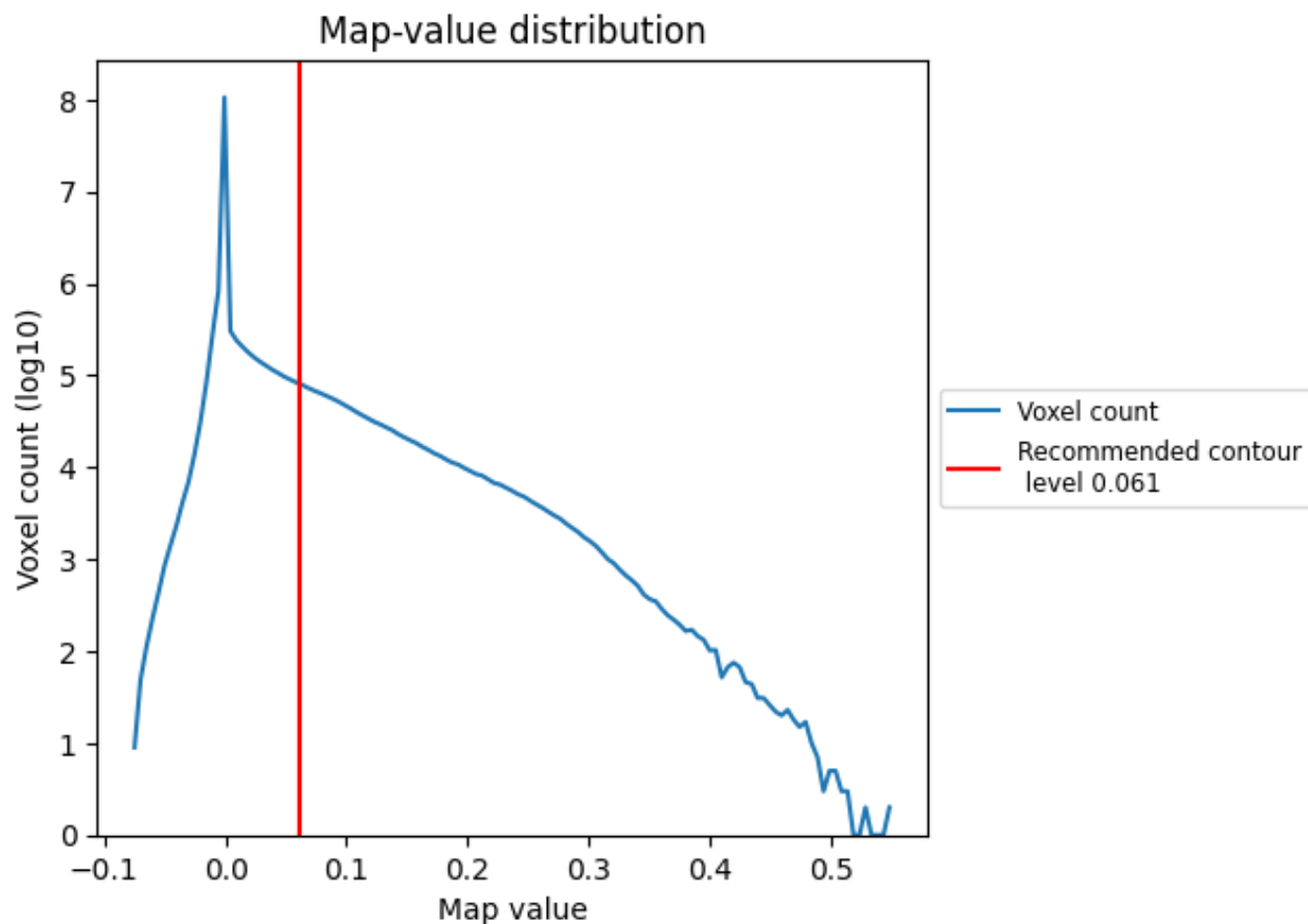
6.6 Mask visualisation

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

7 Map analysis [i](#)

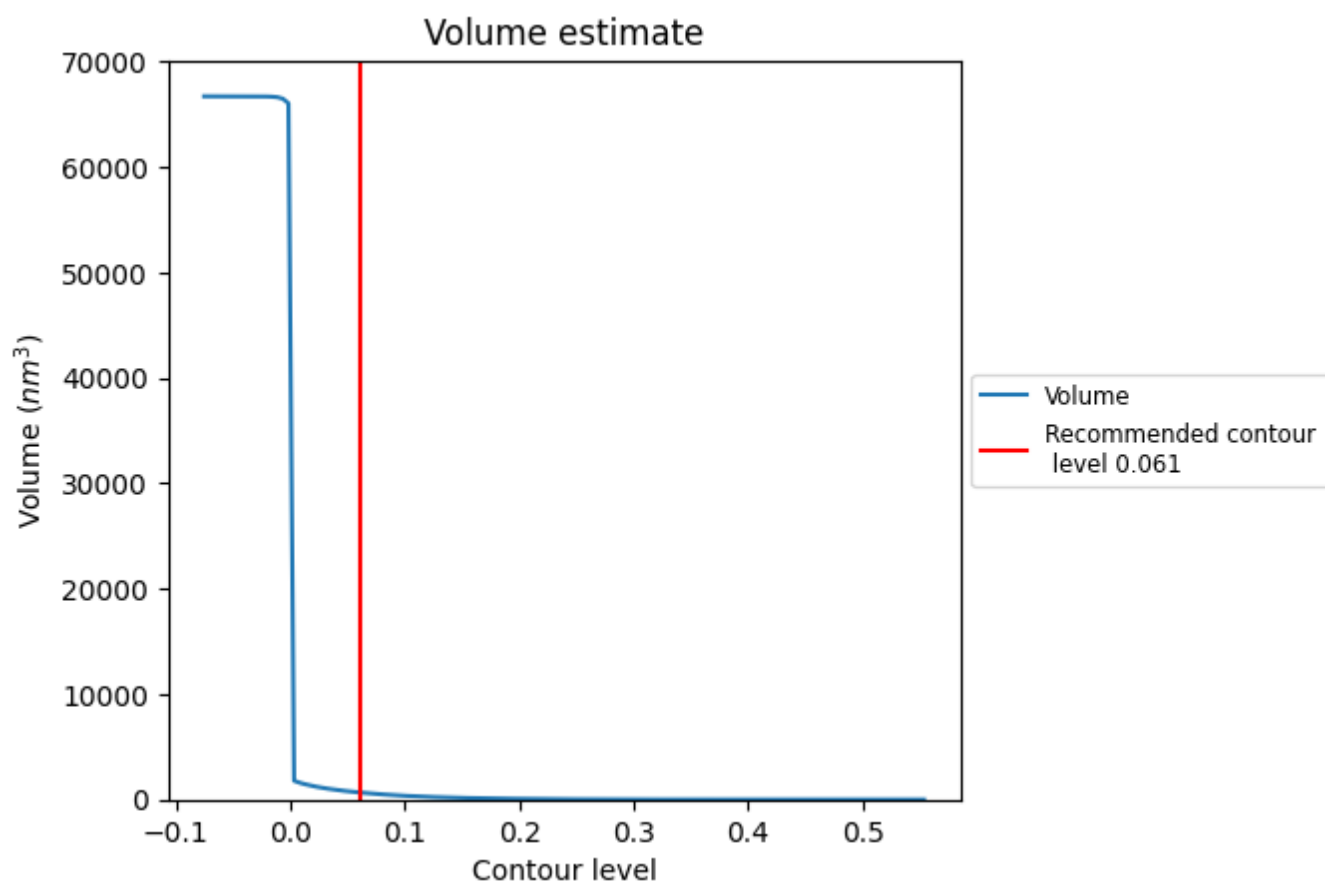
This section contains the results of statistical analysis of the map.

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.

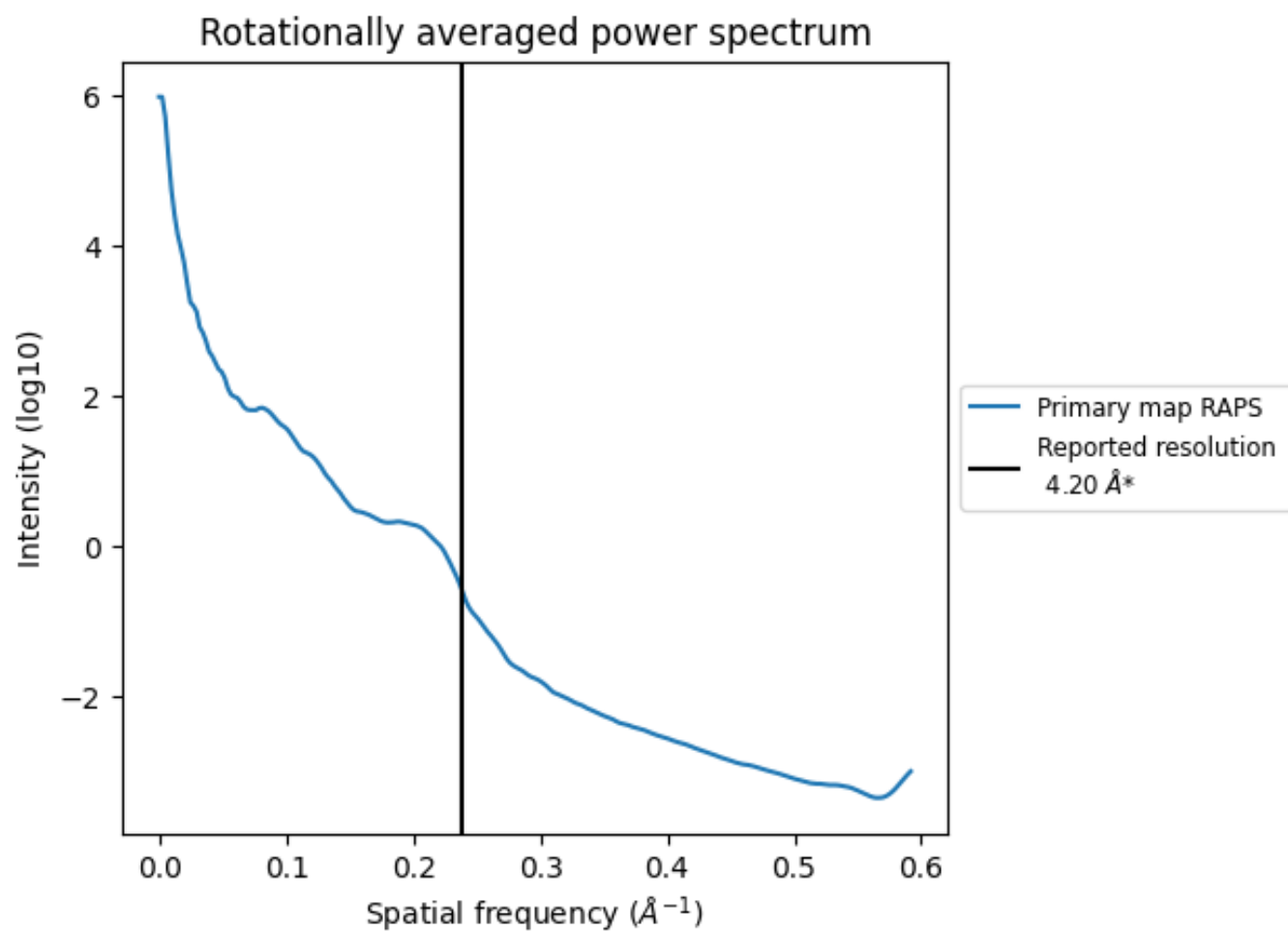
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 668 nm³; this corresponds to an approximate mass of 604 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 0.238 Å⁻¹

8 Fourier-Shell correlation

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

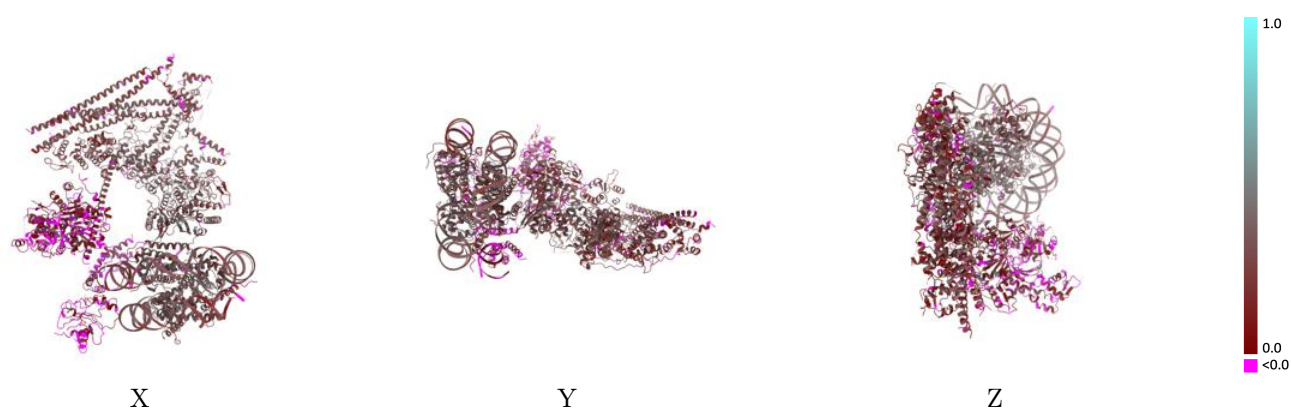
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54056 and PDB model 9RMC. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

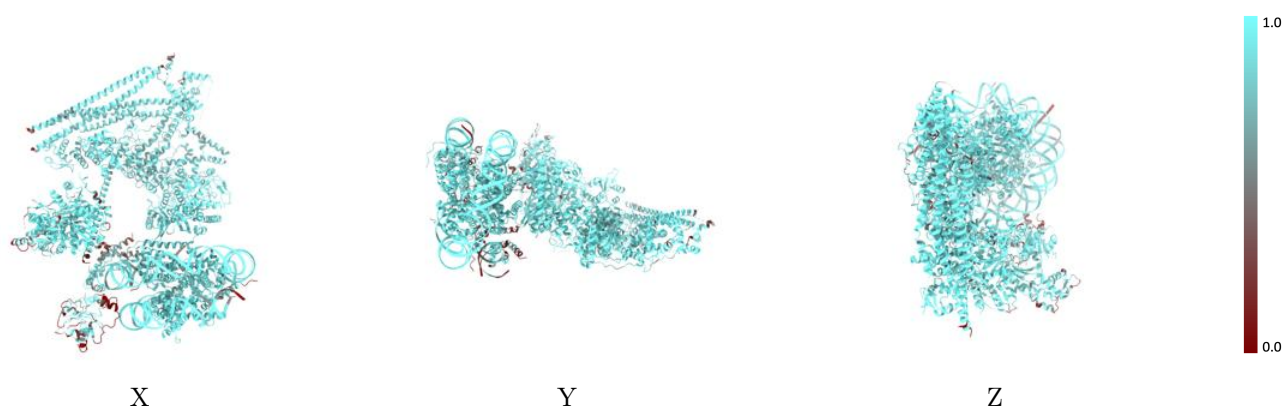
This section was not generated.

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



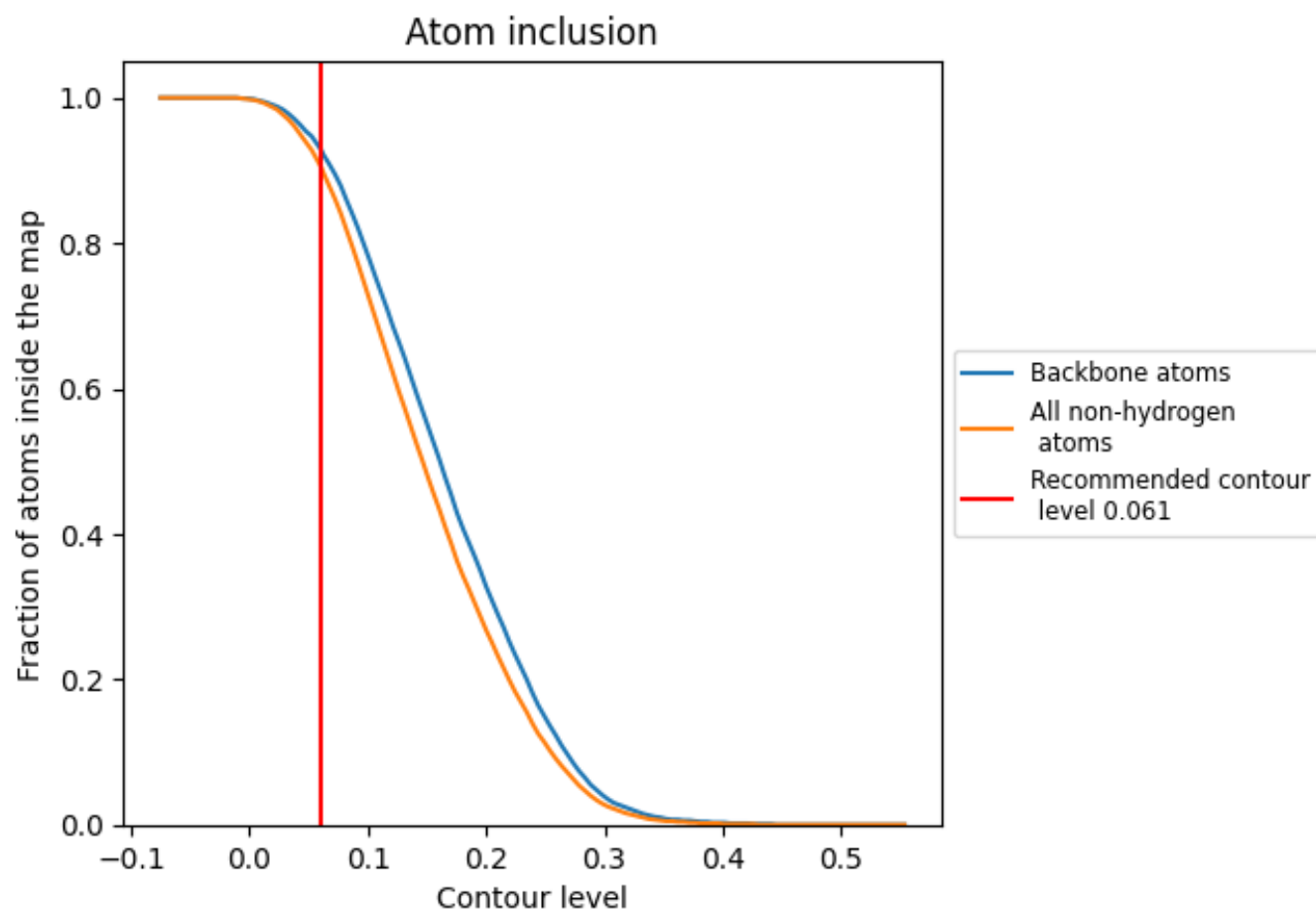
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.061).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.061) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.2420
A	 0.9220	 0.3450
B	 0.9600	 0.3900
C	 0.9180	 0.3240
D	 0.9700	 0.3420
E	 0.8970	 0.3090
F	 0.9460	 0.3440
G	 0.8760	 0.3160
H	 0.9430	 0.3400
I	 0.7150	 0.1120
J	 0.9310	 0.0980
K	 0.8680	 0.0520
L	 0.8920	 0.2540
M	 0.9810	 0.3030
N	 0.9420	 0.2710
O	 0.9490	 0.2660
P	 0.9550	 0.2490
Q	 0.9130	 0.2180
R	 0.9860	 0.3500
V	 0.7040	 0.0430
W	 0.7080	 0.0470
X	 0.9000	 0.2620
Y	 0.9300	 0.2670

