



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:55 AM UTC

PDB ID : 6HQA / pdb_00006hqa
EMDB ID : EMD-0251
Title : Molecular structure of promoter-bound yeast TFIID
Authors : Kolesnikova, O.; Ben-Shem, A.; Luo, J.; Ranish, J.; Schultz, P.; Papai, G.
Deposited on : 2018-09-24
Resolution : 7.10 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.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

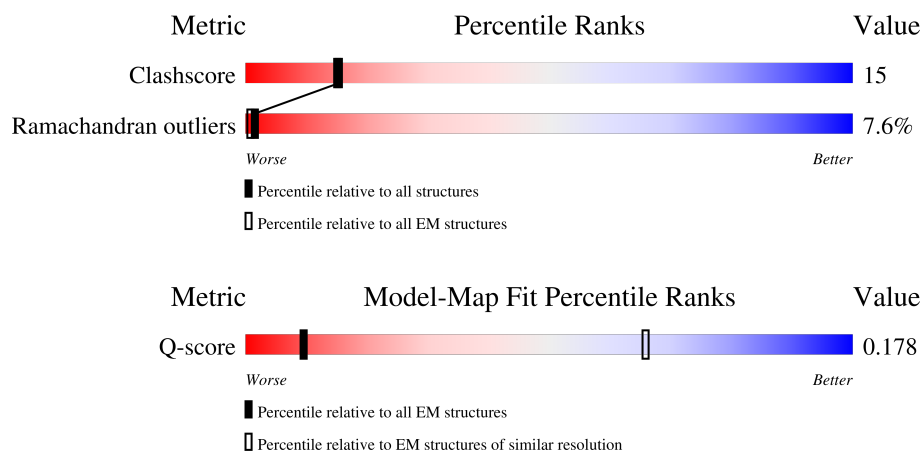
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.10 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	-
Q-score	-	25397	464 (6.60 - 7.60)

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	1756	13% 41% 9% 49%
2	B	722	42% 49% 20% 28%
2	C	722	11% 16% 81%
3	D	485	8% 43% 8% 48%
3	E	485	9% 56% 9% 34%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	153	28% 51% 16% 33%
5	G	75	95% 5%
6	I	64	52% 89% 11%
7	H	68	41% 88% 12%
8	K	609	6% 10% 88%
9	J	553	5% 8% 91%



2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12700 atoms, of which 63 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 Taf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	887	Total	C	N	O	0	0
			4396	2622	887	887		

- Molecule 2 is a protein called Subunit (90 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	522	Total	C	N	O	0	0
			2578	1534	522	522		
2	C	136	Total	C	N	O	0	0
			672	400	136	136		

- Molecule 3 is a protein called Subunit (60 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	254	Total	C	N	O	0	0
			1257	749	254	254		
3	E	320	Total	C	N	O	0	0
			1585	945	320	320		

- Molecule 4 is a protein called Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	103	Total	C	N	O	0	0
			511	305	103	103		

- Molecule 5 is a protein called Taf8.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	75	Total	C	N	O	0	0
			375	225	75	75		

- Molecule 6 is a protein called Histone-fold.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	64	Total	C	H	N	O	0	0
			383	192	63	64	64		

- Molecule 7 is a protein called Histone-fold.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	68	Total	C	N	O	0	0
			340	204	68	68		

- Molecule 8 is a protein called Subunit (61/68 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	71	Total	C	N	O	0	0
			351	209	71	71		

- Molecule 9 is a protein called TFIID subunit (48 kDa).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	51	Total	C	N	O	0	0
			252	150	51	51		

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-141	MET	-	initiating methionine	UNP C4R420
J	-140	SER	-	expression tag	UNP C4R420
J	-139	ARG	-	expression tag	UNP C4R420
J	-138	LYS	-	expression tag	UNP C4R420
J	-137	PRO	-	expression tag	UNP C4R420
J	-136	GLU	-	expression tag	UNP C4R420
J	-135	ARG	-	expression tag	UNP C4R420
J	-134	ARG	-	expression tag	UNP C4R420
J	-133	ARG	-	expression tag	UNP C4R420
J	-132	GLN	-	expression tag	UNP C4R420
J	-131	PRO	-	expression tag	UNP C4R420
J	-130	ARG	-	expression tag	UNP C4R420
J	-129	LEU	-	expression tag	UNP C4R420
J	-128	PHE	-	expression tag	UNP C4R420
J	-127	SER	-	expression tag	UNP C4R420
J	-126	ASN	-	expression tag	UNP C4R420
J	-125	ASP	-	expression tag	UNP C4R420
J	-124	MET	-	expression tag	UNP C4R420
J	-123	ARG	-	expression tag	UNP C4R420

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-122	THR	-	expression tag	UNP C4R420
J	-121	LEU	-	expression tag	UNP C4R420
J	-120	LEU	-	expression tag	UNP C4R420
J	-119	PHE	-	expression tag	UNP C4R420
J	-118	ALA	-	expression tag	UNP C4R420
J	-117	TYR	-	expression tag	UNP C4R420
J	-116	GLY	-	expression tag	UNP C4R420
J	-115	ASP	-	expression tag	UNP C4R420
J	-114	VAL	-	expression tag	UNP C4R420
J	-113	GLN	-	expression tag	UNP C4R420
J	-112	GLN	-	expression tag	UNP C4R420
J	-111	PRO	-	expression tag	UNP C4R420
J	-110	GLN	-	expression tag	UNP C4R420
J	-109	LEU	-	expression tag	UNP C4R420
J	-108	GLU	-	expression tag	UNP C4R420
J	-107	THR	-	expression tag	UNP C4R420
J	-106	ILE	-	expression tag	UNP C4R420
J	-105	GLN	-	expression tag	UNP C4R420
J	-104	ALA	-	expression tag	UNP C4R420
J	-103	LEU	-	expression tag	UNP C4R420
J	-102	GLU	-	expression tag	UNP C4R420
J	-101	ASP	-	expression tag	UNP C4R420
J	-100	VAL	-	expression tag	UNP C4R420
J	-99	MET	-	expression tag	UNP C4R420
J	-98	ILE	-	expression tag	UNP C4R420
J	-97	VAL	-	expression tag	UNP C4R420
J	-96	PHE	-	expression tag	UNP C4R420
J	-95	MET	-	expression tag	UNP C4R420
J	-94	THR	-	expression tag	UNP C4R420
J	-93	ASP	-	expression tag	UNP C4R420
J	-92	LEU	-	expression tag	UNP C4R420
J	-91	CYS	-	expression tag	UNP C4R420
J	-90	HIS	-	expression tag	UNP C4R420
J	-89	GLU	-	expression tag	UNP C4R420
J	-88	ALA	-	expression tag	UNP C4R420
J	-87	MET	-	expression tag	UNP C4R420
J	-86	THR	-	expression tag	UNP C4R420
J	-85	TYR	-	expression tag	UNP C4R420
J	-84	ALA	-	expression tag	UNP C4R420
J	-83	THR	-	expression tag	UNP C4R420
J	-82	TYR	-	expression tag	UNP C4R420
J	-81	GLN	-	expression tag	UNP C4R420

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-80	GLY	-	expression tag	UNP C4R420
J	-79	ARG	-	expression tag	UNP C4R420
J	-78	LYS	-	expression tag	UNP C4R420
J	-77	HIS	-	expression tag	UNP C4R420
J	-76	LYS	-	expression tag	UNP C4R420
J	-75	LEU	-	expression tag	UNP C4R420
J	-74	LYS	-	expression tag	UNP C4R420
J	-73	MET	-	expression tag	UNP C4R420
J	-72	GLU	-	expression tag	UNP C4R420
J	-71	ASP	-	expression tag	UNP C4R420
J	-70	PHE	-	expression tag	UNP C4R420
J	-69	LYS	-	expression tag	UNP C4R420
J	-68	PHE	-	expression tag	UNP C4R420
J	-67	ALA	-	expression tag	UNP C4R420
J	-66	LEU	-	expression tag	UNP C4R420
J	-65	ARG	-	expression tag	UNP C4R420
J	-64	LYS	-	expression tag	UNP C4R420
J	-63	ASP	-	expression tag	UNP C4R420
J	-62	ARG	-	expression tag	UNP C4R420
J	-61	LEU	-	expression tag	UNP C4R420
J	-60	LYS	-	expression tag	UNP C4R420
J	-59	LEU	-	expression tag	UNP C4R420
J	-58	GLY	-	expression tag	UNP C4R420
J	-57	ARG	-	expression tag	UNP C4R420
J	-56	VAL	-	expression tag	UNP C4R420
J	-55	GLU	-	expression tag	UNP C4R420
J	-54	GLU	-	expression tag	UNP C4R420
J	-53	LEU	-	expression tag	UNP C4R420
J	-52	MET	-	expression tag	UNP C4R420
J	-51	ASN	-	expression tag	UNP C4R420
J	-50	LYS	-	expression tag	UNP C4R420
J	-49	GLN	-	expression tag	UNP C4R420
J	-48	LYS	-	expression tag	UNP C4R420
J	-47	GLU	-	expression tag	UNP C4R420
J	-46	ILE	-	expression tag	UNP C4R420
J	-45	GLN	-	expression tag	UNP C4R420
J	-44	GLU	-	expression tag	UNP C4R420
J	-43	ALA	-	expression tag	UNP C4R420
J	-42	ARG	-	expression tag	UNP C4R420
J	-41	LYS	-	expression tag	UNP C4R420
J	-40	LEU	-	expression tag	UNP C4R420
J	-39	PHE	-	expression tag	UNP C4R420

Continued on next page...

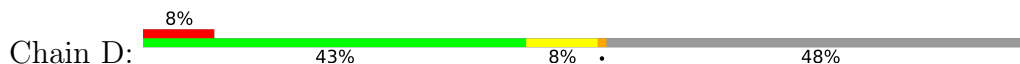
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-38	ASP	-	expression tag	UNP C4R420
J	-37	SER	-	expression tag	UNP C4R420
J	-36	ASN	-	expression tag	UNP C4R420
J	-35	GLU	-	expression tag	UNP C4R420
J	-34	LYS	-	expression tag	UNP C4R420
J	-33	GLU	-	expression tag	UNP C4R420
J	-32	THR	-	expression tag	UNP C4R420
J	-31	LYS	-	expression tag	UNP C4R420
J	-30	ASP	-	expression tag	UNP C4R420
J	-29	ASP	-	expression tag	UNP C4R420
J	-28	ASP	-	expression tag	UNP C4R420
J	-27	ILE	-	expression tag	UNP C4R420
J	-26	GLU	-	expression tag	UNP C4R420
J	-25	LYS	-	expression tag	UNP C4R420
J	-24	LYS	-	expression tag	UNP C4R420
J	-23	ARG	-	expression tag	UNP C4R420
J	-22	ARG	-	expression tag	UNP C4R420
J	-21	LYS	-	expression tag	UNP C4R420
J	-20	GLU	-	expression tag	UNP C4R420
J	-19	ALA	-	expression tag	UNP C4R420
J	-18	LYS	-	expression tag	UNP C4R420
J	-17	ARG	-	expression tag	UNP C4R420
J	-16	ALA	-	expression tag	UNP C4R420
J	-15	ILE	-	expression tag	UNP C4R420
J	-14	LYS	-	expression tag	UNP C4R420
J	-13	GLU	-	expression tag	UNP C4R420
J	-12	ALA	-	expression tag	UNP C4R420
J	-11	LYS	-	expression tag	UNP C4R420
J	-10	LYS	-	expression tag	UNP C4R420
J	-9	LEU	-	expression tag	UNP C4R420
J	-8	LYS	-	expression tag	UNP C4R420
J	-7	LEU	-	expression tag	UNP C4R420
J	-6	SER	-	expression tag	UNP C4R420
J	-5	LYS	-	expression tag	UNP C4R420
J	-4	GLY	-	expression tag	UNP C4R420
J	-3	ASP	-	expression tag	UNP C4R420
J	-2	THR	-	expression tag	UNP C4R420
J	-1	ALA	-	expression tag	UNP C4R420
J	0	PHE	-	expression tag	UNP C4R420



[illegible]

- Molecule 3: Subunit (60 kDa) of TFIID and SAGA complexes

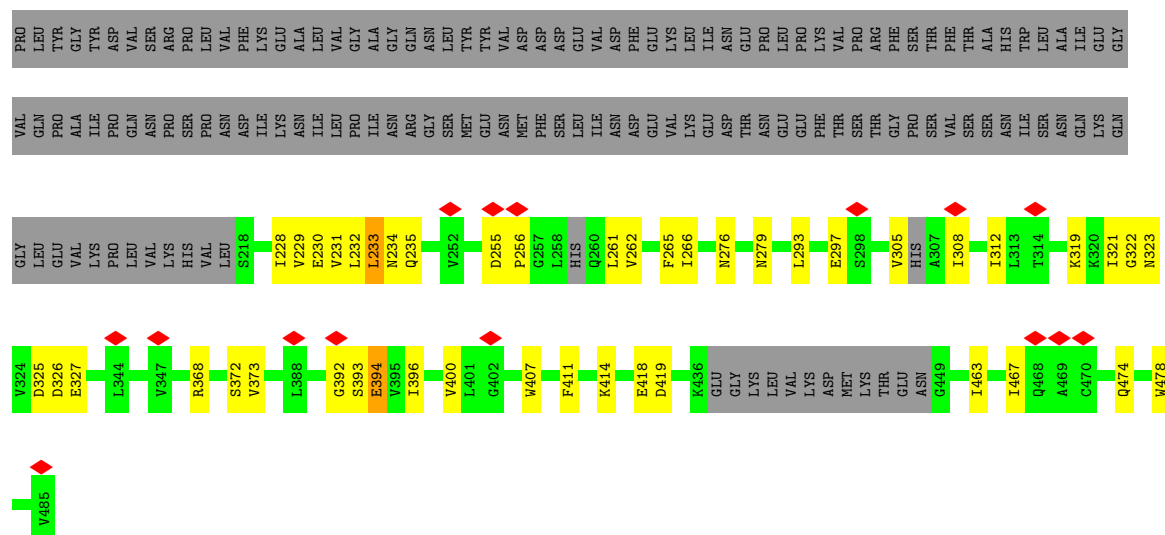


G387	L281	LYS	VAL	LYS	PHE	MET
L388	P262	ILE	GLU	ARG	ARG	LYS
R389	Y264	ASN	ASP	HIS	ASN	SER
G390		GLN	THR	GLY	LYS	SER
G392	T272	PRO	ASN	PRO	LYS	GLN
G393		LYS	GLU	ARG	ARG	ARG
E394	N276	LYS	PHE	THR	THR	SER
G396	T285	PRO	SER	PRO	HIS	ILE
	L289	THR	THR	ARG	THR	THR
G399		PHE	GLY	SER	SER	SER
	L293	PRO	PRO	ASP	ASP	HIS
M403		THR	VAL	PHE	ASP	THR
V404	E297	THR	SER	ALA	ALA	PRO
	F300	ASN	ASN	HIS	PRO	PRO
		ILE	ILE	LEU	LEU	SER
S409	V305	SER	SER	LEU	VAL	ASP
E413	HIS	ASN	ASN	ALA	VAL	VAL
K414	A307	GLN	GLN	ILE	ASN	THR
L415	I308	LYS	GLN	GLY	LEU	LYS
		GLY	GLY	VAL	PRO	ASP
K436	C311	LEU	LEU	GLN	LEU	ALA
	I312	GLU	GLU	PRO	GLY	ALA
		LYS	VAL	ALA	GLY	SER
	K319	LYS	LYS	ILE	TYR	LEU
	R320	PRO	PRO	PRO	ASP	GLY
L321	I321	LEU	LEU	GLN	VAL	ILE
ASP	G322	VAL	VAL	ASN	SER	PHE
MET	N323	LYS	LYS	PRO	ARG	ASN
	V324	HIS	HIS	SER	PRO	LEU
THR	D325	LYS	VAL	PRO	LEU	ASN
GLU	D326	ASN	ASN	ASN	VAL	GLU
ASN	E327	LEU	LEU	VAL	PHE	GLY
		S218		ILE	LYS	ALA
G449	A335	LYS	T228	GLY	GLY	LYS
V459	L336	ASN	V229	ALA	ALA	LYS
G460		ILE	E230	LYS	ASN	ASN
		LEU	V231	LEU	LEU	ALA
I463	E349	PRO	L232	VAL	GLY	ALA
A464		ILE	N234	GLY	ALA	MET
D465		ASN	D233	ASN	GLY	ASP
K466	G352	ARG	Q235	ARG	GLN	ILE
I467	S353	GLY		GLY	ASN	GLU
Q468		SER	T238	SER	TYR	TYR
A469	A369	MET	Q250	GLU	TYR	ARG
	F370	GLY		MET	ILE	ILE
Q474	V371	ASN	S251	ASN	VAL	GLU
	S372	PHE		MET	ASP	ILE
W478	V373	SER	A254	THR	ASP	LEU
		LEU	D255	GLY	ASP	GLY
	T377	ILE	P256	VAL	VAL	GLN
V485	P378	ALA	G257	ASP	ALA	ALA
	G379	SER	L258	PHE	GLY	LYS
		GLY				

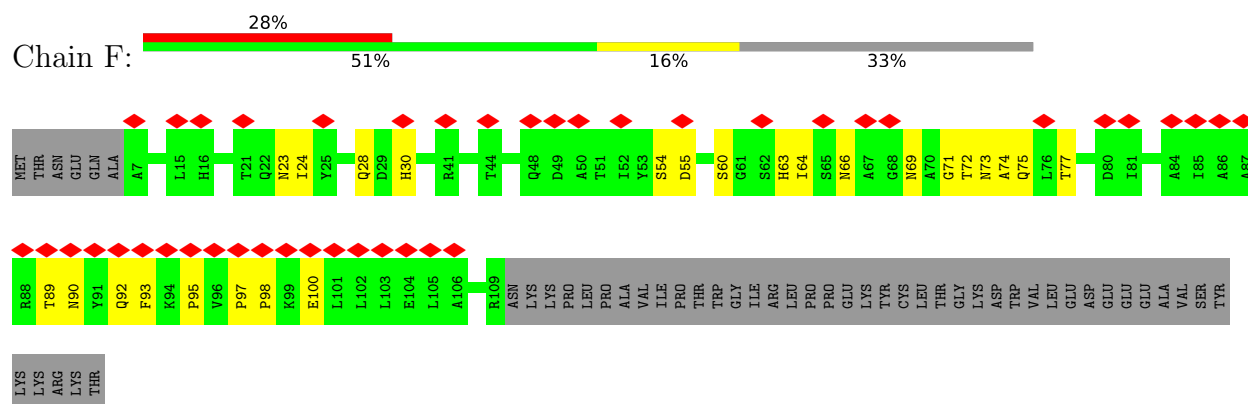
- Molecule 3: Subunit (60 kDa) of TFIID and SAGA complexes



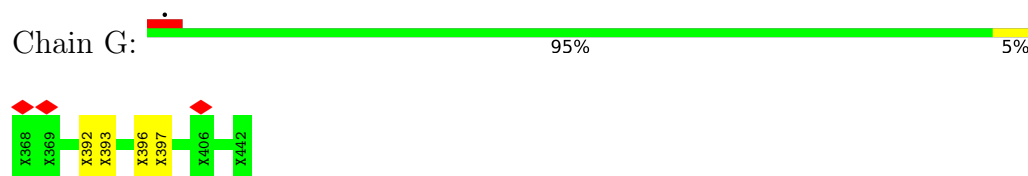
MET	SER	LYS	ASN	ASN	GLN	ARG	SER	SER	ILE	PRO	THR	SER	HIS	THR	LEU	TRP	SER	P19	V23	A26	S29	L30	G31	I32	F33	N34	N35	N36	A39	A40	L43	D46	I47	E48	V49	R50	I51	H52	E53	E53	I54	L55	D56	O57	A58	S59	T69	T72	S73	L84
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



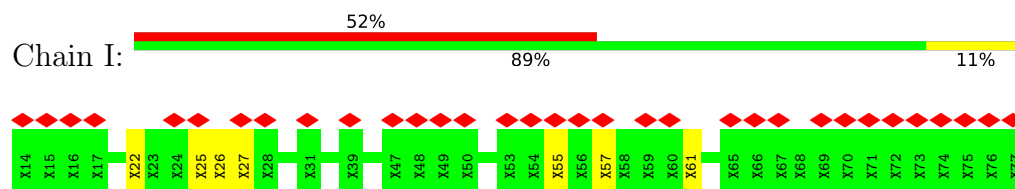
- Molecule 4: Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation



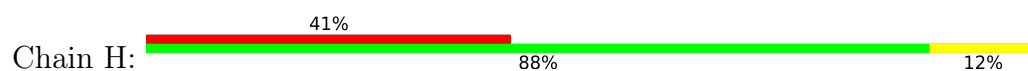
- Molecule 5: Taf8

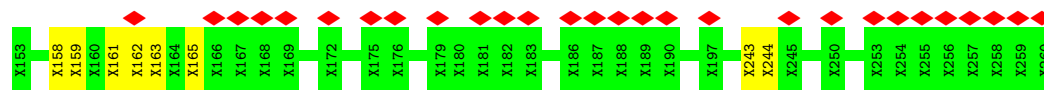


- Molecule 6: Histone-fold

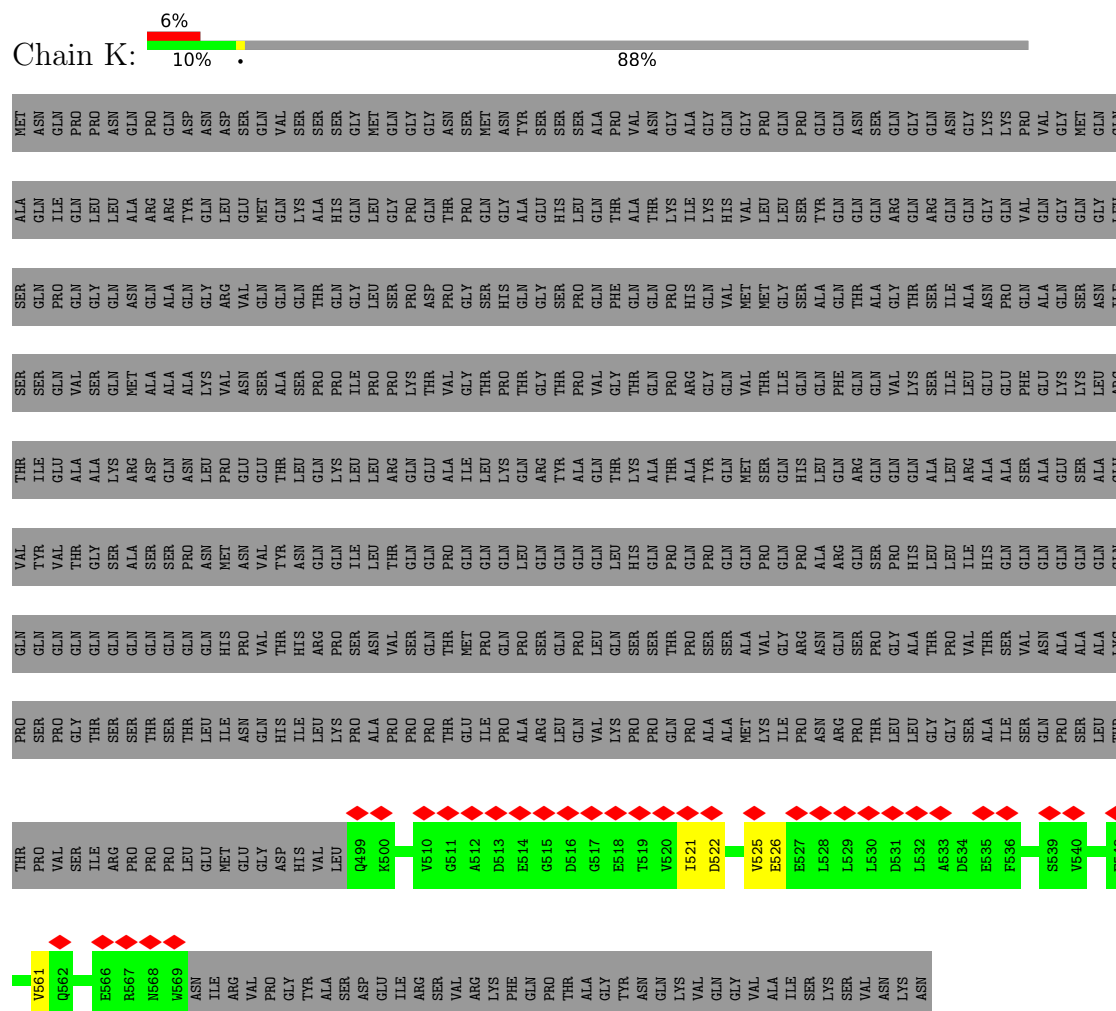


- Molecule 7: Histone-fold

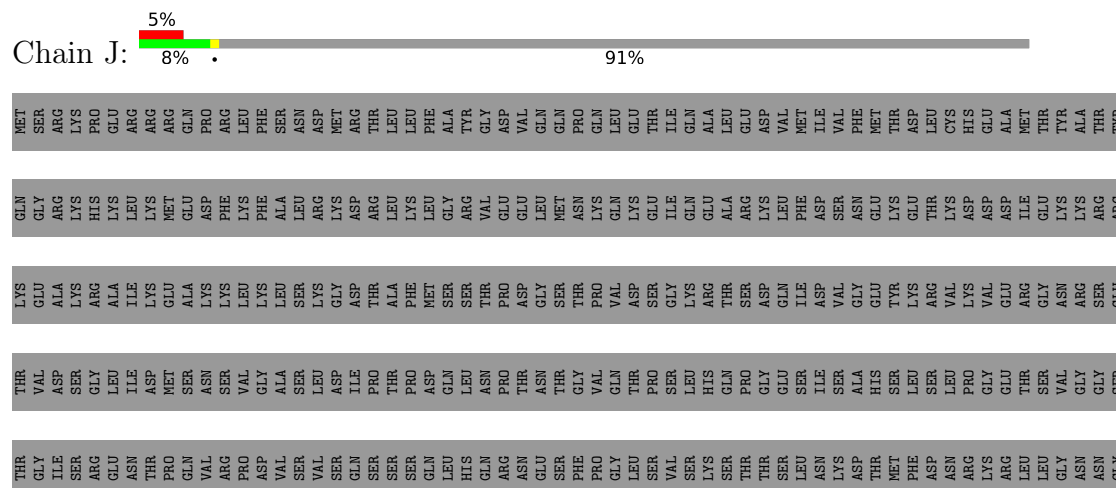




• Molecule 8: Subunit (61/68 kDa) of TFIID and SAGA complexes



• Molecule 9: TFIID subunit (48 kDa)



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	180823	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4900	Depositor
Magnification	45454	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.08	0/4156	0.24	0/5771
2	B	0.07	0/2572	0.21	0/3572
2	C	0.07	0/671	0.22	0/933
3	D	0.06	0/1254	0.19	0/1743
3	E	0.07	0/1582	0.21	0/2201
4	F	0.09	0/510	0.29	1/710 (0.1%)
8	K	0.05	0/349	0.15	0/483
9	J	0.06	0/251	0.12	0/348
All	All	0.07	0/11345	0.22	1/15761 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	93	PHE	CB-CA-C	-5.48	110.27	116.63

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	4396	0	1883	79	0
2	B	2578	0	1144	103	0
2	C	672	0	290	4	0
3	D	1257	0	548	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1585	0	703	29	0
4	F	511	0	246	10	0
5	G	375	0	84	2	0
6	I	320	63	67	4	0
7	H	340	0	72	4	0
8	K	351	0	156	3	0
9	J	252	0	116	2	0
All	All	12637	63	5309	265	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 15.

All (265) 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)
1:A:67:SER:HA	1:A:167:LEU:O	1.27	1.30
1:A:45:ASP:CA	1:A:50:THR:O	1.85	1.24
2:B:592:ARG:HA	2:B:608:ILE:O	1.32	1.23
2:B:550:THR:HA	2:B:566:ILE:O	1.29	1.23
2:B:466:ARG:HA	2:B:482:LEU:O	1.40	1.18
1:A:45:ASP:HA	1:A:50:THR:O	0.98	1.13
2:B:572:VAL:O	2:B:573:ARG:O	1.69	1.10
2:B:508:HIS:HA	2:B:524:CYS:O	1.47	1.09
2:B:480:TRP:HA	2:B:487:CYS:HA	1.39	1.04
2:B:545:PHE:HA	2:B:552:LEU:HA	1.42	1.01
1:A:400:ARG:O	1:A:438:SER:HA	1.59	1.00
2:B:461:PHE:HA	2:B:468:LEU:HA	1.45	0.98
2:B:550:THR:CA	2:B:566:ILE:O	2.10	0.98
1:A:399:ALA:HA	1:A:437:TYR:O	1.64	0.97
1:A:224:ILE:O	1:A:242:THR:HA	1.62	0.97
2:B:629:ALA:HB1	2:B:670:ALA:HB2	1.47	0.96
2:B:606:TRP:HA	2:B:613:ARG:HA	1.46	0.95
2:B:676:LYS:HA	2:B:682:ARG:HA	1.51	0.92
1:A:41:GLN:O	1:A:53:GLY:HA3	1.68	0.91
2:B:592:ARG:CA	2:B:608:ILE:O	2.18	0.89
3:E:36:ASN:HA	4:F:66:ASN:HA	1.54	0.89
2:B:564:TRP:HA	2:B:571:CYS:HA	1.55	0.89
4:F:63:HIS:HA	4:F:73:ASN:HA	1.55	0.89
2:B:604:CYS:HA	2:B:616:ALA:HA	1.54	0.88
3:E:229:VAL:O	3:E:232:LEU:O	1.90	0.88
1:A:270:GLN:HA	1:A:343:VAL:O	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:VAL:HA	2:B:512:THR:HA	1.54	0.88
3:D:229:VAL:O	3:D:232:LEU:O	1.91	0.88
3:D:464:ALA:O	3:D:467:ILE:O	1.92	0.88
2:B:470:SER:O	2:B:477:VAL:HA	1.75	0.86
3:E:232:LEU:O	3:E:234:ASN:N	2.09	0.86
2:B:508:HIS:HA	2:B:524:CYS:C	2.01	0.85
3:D:467:ILE:O	3:D:469:ALA:N	2.09	0.85
3:D:232:LEU:O	3:D:234:ASN:N	2.09	0.85
2:B:562:ARG:HA	2:B:574:VAL:HA	1.59	0.85
1:A:402:TYR:O	1:A:440:VAL:HA	1.77	0.84
2:B:587:VAL:HA	2:B:594:LEU:HA	1.59	0.83
2:B:466:ARG:CA	2:B:482:LEU:O	2.24	0.83
3:D:465:ASP:O	3:D:469:ALA:HB3	1.79	0.81
2:B:149:TYR:O	2:B:153:ALA:HB3	1.81	0.80
1:A:67:SER:CA	1:A:167:LEU:O	2.21	0.80
1:A:1170:UNK:HA	1:A:1172:UNK:N	1.97	0.80
1:A:1172:UNK:O	1:A:1176:UNK:CB	2.30	0.79
2:B:129:LEU:O	2:B:133:LEU:CB	2.33	0.77
1:A:68:LYS:HA	1:A:166:TYR:HA	1.65	0.77
1:A:1170:UNK:O	1:A:1174:UNK:CB	2.33	0.77
2:B:508:HIS:CA	2:B:524:CYS:O	2.32	0.76
3:E:231:VAL:O	3:E:235:GLN:CB	2.34	0.76
1:A:1171:UNK:O	1:A:1175:UNK:CB	2.33	0.76
2:B:650:ASP:H	2:B:654:ASN:HA	1.49	0.76
2:B:502:LYS:O	2:B:511:ALA:HB3	1.86	0.75
2:B:552:LEU:CB	2:B:564:TRP:O	2.34	0.75
2:B:555:GLY:HA2	2:B:561:ALA:HA	1.66	0.75
3:D:231:VAL:O	3:D:235:GLN:CB	2.35	0.75
3:E:321:ILE:O	3:E:325:ASP:CB	2.34	0.74
3:D:230:GLU:O	3:D:234:ASN:CB	2.35	0.74
1:A:711:ILE:HA	1:A:799:ILE:HA	1.69	0.74
1:A:45:ASP:HA	1:A:50:THR:C	2.08	0.74
2:B:603:VAL:CB	2:B:617:MET:O	2.36	0.74
1:A:399:ALA:CA	1:A:437:TYR:O	2.36	0.74
2:B:546:HIS:O	2:B:551:TYR:CB	2.36	0.74
3:E:230:GLU:O	3:E:234:ASN:CB	2.36	0.73
1:A:70:ARG:HA	1:A:163:LEU:O	1.88	0.73
7:H:161:UNK:O	7:H:165:UNK:CB	2.37	0.73
2:C:129:LEU:O	2:C:133:LEU:CB	2.37	0.73
1:A:401:VAL:HA	1:A:439:MET:H	1.53	0.72
1:A:1182:UNK:O	1:A:1186:UNK:CB	2.37	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:222:VAL:O	9:J:226:ASN:CB	2.38	0.72
3:D:321:ILE:O	3:D:325:ASP:CB	2.37	0.72
2:B:592:ARG:HA	2:B:608:ILE:C	2.15	0.71
2:B:693:MET:O	2:B:694:SER:O	2.08	0.71
1:A:629:PHE:O	1:A:633:TRP:CB	2.39	0.71
2:B:685:GLU:HA	2:B:691:ASP:O	1.90	0.70
2:B:408:GLY:HA2	2:B:414:ILE:HA	1.74	0.70
2:B:466:ARG:HA	2:B:482:LEU:C	2.16	0.70
7:H:159:UNK:O	7:H:163:UNK:CB	2.40	0.70
1:A:991:THR:O	1:A:995:ALA:HB3	1.91	0.70
2:B:191:LYS:O	2:B:195:SER:CB	2.39	0.70
1:A:401:VAL:HA	1:A:439:MET:N	2.07	0.70
2:B:149:TYR:O	2:B:153:ALA:CB	2.39	0.69
1:A:194:SER:O	1:A:198:LEU:CB	2.41	0.69
1:A:628:SER:O	1:A:632:ASN:CB	2.40	0.69
1:A:645:THR:O	1:A:657:MET:HA	1.94	0.68
2:B:186:GLU:N	2:B:190:ALA:HB2	2.09	0.68
3:E:261:LEU:O	3:E:265:PHE:CB	2.42	0.68
1:A:711:ILE:O	1:A:719:TYR:CB	2.42	0.67
2:B:638:VAL:HA	2:B:648:VAL:HA	1.76	0.67
5:G:393:UNK:O	5:G:397:UNK:CB	2.42	0.67
8:K:521:ILE:O	8:K:525:VAL:CB	2.43	0.67
1:A:1122:PHE:O	1:A:1126:LEU:CB	2.43	0.66
3:E:262:VAL:O	3:E:266:ILE:CB	2.42	0.66
2:B:504:SER:O	2:B:509:TYR:CB	2.44	0.66
2:B:462:SER:O	2:B:467:TYR:CB	2.43	0.65
2:B:466:ARG:O	2:B:481:SER:HA	1.96	0.65
3:E:308:ILE:O	3:E:312:ILE:CB	2.45	0.65
1:A:1186:UNK:O	1:A:1190:UNK:CB	2.43	0.65
3:D:229:VAL:O	3:D:232:LEU:C	2.40	0.65
5:G:392:UNK:O	5:G:396:UNK:CB	2.45	0.65
2:B:682:ARG:O	2:B:696:TYR:CB	2.45	0.64
1:A:654:PHE:HA	1:A:735:GLN:HA	1.79	0.64
2:B:592:ARG:C	2:B:608:ILE:H	2.05	0.64
4:F:89:THR:CB	4:F:90:ASN:HA	2.25	0.64
3:E:229:VAL:O	3:E:232:LEU:C	2.40	0.64
2:B:650:ASP:N	2:B:654:ASN:HA	2.13	0.64
1:A:484:ALA:HB1	1:A:507:ALA:HA	1.78	0.64
2:B:647:ARG:CB	2:B:657:SER:HA	2.28	0.63
1:A:71:LEU:O	1:A:163:LEU:CB	2.47	0.63
1:A:269:LEU:O	1:A:345:VAL:CB	2.47	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:GLY:O	1:A:1129:HIS:CB	2.47	0.62
3:D:308:ILE:O	3:D:312:ILE:CB	2.47	0.62
3:E:463:ILE:O	3:E:467:ILE:CB	2.48	0.62
2:B:466:ARG:C	2:B:482:LEU:H	2.07	0.62
2:B:572:VAL:C	2:B:573:ARG:O	2.43	0.62
1:A:707:MET:O	1:A:723:VAL:CB	2.48	0.62
2:B:550:THR:HA	2:B:566:ILE:C	2.20	0.61
2:B:503:PHE:CB	2:B:510:PHE:HA	2.31	0.61
3:E:293:LEU:O	3:E:297:GLU:CB	2.49	0.61
3:D:464:ALA:O	3:D:467:ILE:C	2.43	0.61
2:B:125:TYR:O	2:B:129:LEU:CB	2.49	0.61
3:D:323:ASN:HA	3:D:327:GLU:HA	1.83	0.60
1:A:368:PRO:HA	1:A:399:ALA:O	2.02	0.60
2:B:508:HIS:C	2:B:524:CYS:H	2.09	0.60
1:A:41:GLN:O	1:A:53:GLY:CA	2.48	0.60
1:A:942:ALA:O	1:A:946:ILE:CB	2.49	0.60
1:A:644:VAL:HA	1:A:658:GLY:O	2.02	0.59
2:B:471:CYS:HA	2:B:477:VAL:HA	1.83	0.59
3:E:407:TRP:O	3:E:411:PHE:CB	2.50	0.59
4:F:66:ASN:H	4:F:71:GLY:HA2	1.67	0.59
2:B:564:TRP:HA	2:B:571:CYS:CA	2.30	0.59
2:B:550:THR:CB	2:B:566:ILE:O	2.51	0.59
3:D:463:ILE:O	3:D:467:ILE:CB	2.50	0.58
2:B:601:SER:H	2:B:624:SER:HA	1.68	0.58
2:B:581:ALA:O	2:B:599:GLU:N	2.29	0.58
3:D:464:ALA:O	3:D:468:GLN:CB	2.52	0.58
2:B:136:VAL:O	2:B:140:CYS:CB	2.51	0.58
3:E:396:ILE:O	3:E:400:VAL:CB	2.53	0.57
1:A:45:ASP:CB	1:A:50:THR:O	2.51	0.57
2:B:171:GLU:O	2:B:175:LEU:CB	2.53	0.57
3:E:323:ASN:HA	3:E:327:GLU:HA	1.86	0.57
1:A:270:GLN:CA	1:A:343:VAL:O	2.52	0.57
3:E:39:ALA:HB2	4:F:77:THR:H	1.68	0.56
1:A:55:THR:O	1:A:211:LYS:HA	2.04	0.56
2:B:508:HIS:C	2:B:524:CYS:N	2.63	0.56
2:B:508:HIS:O	2:B:523:SER:HA	2.05	0.56
2:B:587:VAL:CA	2:B:594:LEU:HA	2.33	0.56
2:B:592:ARG:O	2:B:607:ASP:HA	2.05	0.56
1:A:224:ILE:O	1:A:242:THR:CA	2.47	0.56
2:B:706:VAL:HA	2:B:716:ALA:O	2.06	0.56
2:C:125:TYR:O	2:C:129:LEU:CB	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:229:VAL:O	3:D:233:LEU:CB	2.55	0.55
7:H:158:UNK:O	7:H:162:UNK:CB	2.54	0.55
1:A:709:ILE:O	1:A:721:HIS:CB	2.55	0.55
3:D:322:GLY:O	3:D:325:ASP:C	2.49	0.55
3:E:322:GLY:O	3:E:325:ASP:C	2.50	0.55
3:D:293:LEU:O	3:D:297:GLU:CB	2.55	0.55
3:E:229:VAL:O	3:E:233:LEU:CB	2.55	0.55
1:A:399:ALA:C	1:A:437:TYR:O	2.51	0.54
1:A:655:ILE:H	1:A:735:GLN:HA	1.71	0.54
1:A:54:GLU:HA	1:A:213:ASN:HA	1.89	0.53
2:B:565:ASP:CB	2:B:570:GLU:O	2.56	0.53
2:B:221:GLY:O	2:B:225:VAL:CB	2.57	0.53
2:B:665:ILE:HA	2:B:677:THR:HA	1.90	0.53
2:B:650:ASP:O	2:B:654:ASN:HA	2.08	0.53
3:D:272:THR:O	3:D:276:ASN:CB	2.57	0.53
3:E:414:LYS:O	3:E:418:GLU:CB	2.56	0.53
2:B:470:SER:O	2:B:477:VAL:CA	2.52	0.53
2:B:186:GLU:H	2:B:190:ALA:HB2	1.75	0.52
1:A:959:ARG:O	1:A:963:ARG:CB	2.58	0.52
1:A:656:GLU:HA	1:A:734:ILE:H	1.73	0.52
1:A:47:ALA:O	1:A:227:GLY:HA3	2.11	0.51
1:A:1126:LEU:O	1:A:1130:PHE:CB	2.59	0.51
2:B:358:ASP:O	2:B:359:ILE:N	2.44	0.51
1:A:367:LEU:H	1:A:402:TYR:HA	1.76	0.50
3:D:322:GLY:O	3:D:326:ASP:C	2.53	0.50
2:B:410:GLN:O	2:B:455:ALA:HA	2.12	0.50
3:E:322:GLY:O	3:E:326:ASP:C	2.54	0.50
2:B:630:PHE:HA	2:B:637:LEU:CB	2.42	0.50
2:B:650:ASP:H	2:B:654:ASN:CA	2.19	0.50
2:B:554:THR:O	2:B:561:ALA:HA	2.11	0.50
3:E:323:ASN:HA	3:E:327:GLU:CB	2.42	0.50
2:B:508:HIS:HA	2:B:524:CYS:CA	2.42	0.49
3:D:322:GLY:O	3:D:325:ASP:O	2.30	0.49
2:B:562:ARG:CA	2:B:574:VAL:HA	2.37	0.49
3:D:323:ASN:HA	3:D:327:GLU:CB	2.42	0.49
6:I:57:UNK:O	6:I:61:UNK:CB	2.61	0.49
2:B:545:PHE:CA	2:B:552:LEU:HA	2.30	0.49
2:C:186:GLU:CB	2:C:190:ALA:HB2	2.43	0.49
2:B:649:TRP:HA	2:B:655:THR:CB	2.43	0.48
2:B:135:PRO:O	2:B:139:HIS:CB	2.61	0.48
2:B:606:TRP:CA	2:B:613:ARG:HA	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:ARG:O	1:A:962:LEU:CB	2.61	0.48
3:D:474:GLN:O	3:D:478:TRP:CB	2.62	0.47
1:A:557:ALA:O	1:A:561:LYS:CB	2.62	0.47
3:E:322:GLY:O	3:E:325:ASP:O	2.33	0.47
6:I:22:UNK:HA	6:I:26:UNK:CB	2.45	0.47
1:A:68:LYS:CA	1:A:166:TYR:HA	2.41	0.47
1:A:259:ASP:HA	1:A:354:ALA:HB1	1.96	0.47
1:A:641:VAL:CB	1:A:662:VAL:O	2.62	0.47
3:E:474:GLN:O	3:E:478:TRP:CB	2.63	0.47
3:D:323:ASN:HA	3:D:327:GLU:CA	2.43	0.46
8:K:522:ASP:O	8:K:526:GLU:CB	2.64	0.46
1:A:399:ALA:HA	1:A:437:TYR:C	2.38	0.46
4:F:64:ILE:N	4:F:72:THR:O	2.41	0.46
1:A:1170:UNK:HA	1:A:1171:UNK:C	2.45	0.46
1:A:244:ASN:H	1:A:360:PHE:HA	1.81	0.46
2:B:421:GLY:HA2	2:B:442:ALA:O	2.16	0.46
2:B:704:TYR:N	2:B:718:GLY:O	2.42	0.46
1:A:1170:UNK:CA	1:A:1171:UNK:CB	2.94	0.45
3:E:323:ASN:HA	3:E:327:GLU:CA	2.45	0.45
1:A:1039:GLN:O	1:A:1043:ALA:CB	2.64	0.45
2:B:703:VAL:HA	2:B:719:VAL:HA	1.98	0.45
4:F:28:GLN:O	4:F:30:HIS:N	2.48	0.45
9:J:227:GLY:O	9:J:229:ARG:N	2.49	0.45
3:E:392:GLY:O	3:E:394:GLU:N	2.50	0.45
2:B:342:LYS:O	2:B:344:THR:N	2.49	0.45
2:B:588:SER:O	2:B:593:TRP:CB	2.65	0.45
1:A:366:GLN:HA	1:A:402:TYR:CB	2.47	0.44
2:B:587:VAL:CB	2:B:594:LEU:HA	2.48	0.44
3:D:250:GLN:O	3:D:254:ALA:CB	2.66	0.44
1:A:371:THR:HA	1:A:419:TYR:CB	2.47	0.44
4:F:55:ASP:HA	4:F:74:ALA:HB1	2.00	0.44
1:A:1101:LEU:O	1:A:1103:ASN:N	2.51	0.44
2:B:514:SER:H	2:B:519:ALA:HA	1.81	0.44
2:B:451:GLY:HA2	6:I:55:UNK:CB	2.48	0.43
2:B:550:THR:CB	2:B:567:ALA:HB2	2.48	0.43
2:B:594:LEU:O	2:B:606:TRP:CB	2.66	0.43
3:E:368:ARG:O	3:E:372:SER:CB	2.67	0.43
6:I:25:UNK:O	6:I:27:UNK:N	2.51	0.43
2:B:564:TRP:HA	2:B:571:CYS:CB	2.47	0.43
1:A:1039:GLN:O	1:A:1043:ALA:HB3	2.19	0.43
3:D:377:THR:HA	3:D:378:PRO:HA	1.73	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ALA:HB2	1:A:1057:ASN:CB	2.49	0.43
1:A:46:LEU:O	1:A:48:THR:N	2.52	0.43
2:B:418:SER:O	2:B:420:ASP:N	2.52	0.43
2:B:668:VAL:HA	2:B:675:LYS:HA	2.00	0.43
1:A:227:GLY:HA2	1:A:240:CYS:CB	2.49	0.43
1:A:494:PRO:HA	1:A:609:LEU:CB	2.48	0.43
2:B:513:ALA:HB2	2:B:543:VAL:CB	2.49	0.43
2:B:600:ASP:HA	2:B:623:SER:O	2.18	0.43
1:A:963:ARG:O	1:A:967:TYR:CB	2.67	0.42
2:B:478:ARG:HA	2:B:490:SER:HA	2.00	0.42
1:A:73:ALA:HA	1:A:252:SER:O	2.19	0.42
3:D:228:ILE:O	3:D:232:LEU:CB	2.67	0.42
1:A:954:PHE:O	1:A:958:ARG:CB	2.67	0.42
3:E:39:ALA:HB2	4:F:77:THR:N	2.35	0.42
3:D:465:ASP:O	3:D:467:ILE:O	2.38	0.42
3:D:230:GLU:O	3:D:232:LEU:O	2.38	0.42
1:A:69:VAL:O	1:A:164:THR:HA	2.20	0.41
1:A:597:ALA:O	1:A:605:ASN:N	2.53	0.41
1:A:950:ASP:O	1:A:952:ASP:N	2.53	0.41
2:B:185:GLN:HA	2:B:190:ALA:CB	2.50	0.41
3:E:228:ILE:O	3:E:232:LEU:CB	2.68	0.41
1:A:949:LYS:O	1:A:951:SER:N	2.54	0.41
2:B:685:GLU:CB	2:B:692:HIS:HA	2.50	0.41
3:D:409:SER:O	3:D:413:GLU:CB	2.68	0.41
1:A:654:PHE:HA	1:A:735:GLN:CA	2.49	0.41
2:B:678:GLU:O	2:B:702:PRO:HA	2.21	0.41
4:F:54:SER:C	4:F:74:ALA:HB1	2.46	0.41
2:B:604:CYS:CA	2:B:616:ALA:HA	2.39	0.41
3:E:230:GLU:O	3:E:232:LEU:O	2.38	0.41
8:K:548:ALA:HB1	8:K:553:VAL:O	2.21	0.41
2:C:198:PHE:O	2:C:200:VAL:N	2.54	0.40
2:B:550:THR:O	2:B:565:ASP:HA	2.21	0.40
2:B:464:ASP:C	2:B:466:ARG:H	2.30	0.40
7:H:243:UNK:HA	7:H:244:UNK:HA	1.70	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	813/1756 (46%)	623 (77%)	131 (16%)	59 (7%)	1	10
2	B	511/722 (71%)	352 (69%)	99 (19%)	60 (12%)	0	4
2	C	134/722 (19%)	109 (81%)	14 (10%)	11 (8%)	0	9
3	D	248/485 (51%)	201 (81%)	32 (13%)	15 (6%)	1	13
3	E	314/485 (65%)	268 (85%)	35 (11%)	11 (4%)	3	20
4	F	101/153 (66%)	71 (70%)	20 (20%)	10 (10%)	0	7
8	K	67/609 (11%)	59 (88%)	6 (9%)	2 (3%)	3	22
9	J	49/553 (9%)	43 (88%)	5 (10%)	1 (2%)	6	31
All	All	2237/5485 (41%)	1726 (77%)	342 (15%)	169 (8%)	1	10

All (169) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PRO
1	A	81	VAL
1	A	168	PRO
1	A	184	PRO
1	A	333	PRO
1	A	367	LEU
1	A	380	PRO
1	A	404	LEU
1	A	405	PRO
1	A	471	PRO
1	A	543	ALA
1	A	640	PRO
1	A	717	THR
1	A	718	PRO
1	A	845	ARG
1	A	1045	VAL
2	B	431	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	432	PRO
2	B	466	ARG
2	B	477	VAL
2	B	550	THR
2	B	567	ALA
2	B	568	ARG
2	B	573	ARG
2	B	615	LYS
2	B	636	VAL
2	B	654	ASN
2	B	655	THR
2	B	658	PRO
2	B	673	ILE
2	B	694	SER
2	B	701	THR
3	D	233	LEU
3	D	255	ASP
3	D	256	PRO
3	D	373	VAL
3	D	378	PRO
3	D	468	GLN
3	E	233	LEU
3	E	255	ASP
3	E	256	PRO
4	F	95	PRO
4	F	97	PRO
4	F	98	PRO
1	A	63	ASP
1	A	86	ILE
1	A	256	PRO
1	A	346	GLN
1	A	702	ILE
1	A	882	GLU
1	A	948	ILE
1	A	1087	VAL
1	A	1119	SER
2	B	121	SER
2	B	179	SER
2	B	202	ILE
2	B	234	GLU
2	B	237	ILE
2	B	238	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	414	ILE
2	B	421	GLY
2	B	429	LYS
2	B	441	VAL
2	B	483	ASP
2	B	508	HIS
2	B	525	ASP
2	B	592	ARG
2	B	609	SER
2	B	668	VAL
2	B	672	GLY
2	B	706	VAL
2	C	179	SER
2	C	233	ILE
3	D	404	VAL
3	E	373	VAL
3	E	393	SER
3	E	419	ASP
4	F	92	GLN
1	A	47	ALA
1	A	84	ASN
1	A	207	PRO
1	A	334	HIS
1	A	351	PRO
1	A	374	PHE
1	A	430	GLY
1	A	453	ALA
1	A	544	PRO
1	A	725	LEU
1	A	726	LYS
1	A	735	GLN
1	A	950	ASP
2	B	150	PRO
2	B	167	LEU
2	B	180	LEU
2	B	371	LEU
2	B	379	PRO
2	B	439	ASP
2	B	594	LEU
2	B	626	TYR
2	C	146	ALA
2	C	199	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	238	THR
3	D	415	LEU
3	E	394	GLU
4	F	69	ASN
4	F	75	GLN
4	F	100	GLU
1	A	199	MET
1	A	233	ILE
1	A	399	ALA
1	A	450	SER
1	A	458	ILE
1	A	523	ASN
1	A	796	ALA
1	A	951	SER
1	A	1048	HIS
2	B	218	ASP
2	B	383	MET
2	B	501	VAL
2	B	659	SER
2	C	185	GLN
3	D	300	PHE
3	D	460	GLY
3	E	276	ASN
3	E	279	ASN
3	E	319	LYS
4	F	60	SER
8	K	556	ILE
8	K	561	VAL
1	A	189	ASN
1	A	398	ALA
1	A	1050	CYS
1	A	1102	LYS
2	B	343	ASP
2	B	442	ALA
2	B	702	PRO
2	C	147	ARG
3	D	319	LYS
1	A	338	HIS
1	A	691	VAL
1	A	1084	SER
2	B	168	HIS
2	B	440	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	450	VAL
2	B	489	VAL
2	B	561	ALA
2	B	651	VAL
2	B	689	THR
2	C	180	LEU
2	C	232	TYR
3	D	305	VAL
3	D	467	ILE
3	E	305	VAL
4	F	23	ASN
4	F	24	ILE
9	J	228	LEU
1	A	223	ILE
1	A	401	VAL
1	A	51	VAL
1	A	716	GLY
2	B	419	ILE
2	C	148	GLY
2	B	381	VAL
1	A	641	VAL
2	B	572	VAL
2	C	234	GLU
3	D	459	VAL
2	B	574	VAL
2	C	150	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6
2	B	4
3	D	1
5	G	1
8	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	357:ASN	C	358:ASP	N	14.12
1	B	372:SER	C	373:ALA	N	6.29
1	D	394:GLU	C	395:VAL	N	5.84
1	A	930:PHE	C	931:GLN	N	5.73
1	A	802:ASP	C	803:ALA	N	5.20
1	A	60:PHE	C	61:ALA	N	5.02
1	A	808:ILE	C	809:CYS	N	4.88
1	G	403:UNK	C	404:UNK	N	4.69
1	A	551:ARG	C	552:PHE	N	4.42
1	K	513:ASP	C	514:GLU	N	4.39
1	B	369:ILE	C	370:LYS	N	3.92
1	A	549:HIS	C	550:PHE	N	3.66
1	B	358:ASP	C	359:ILE	N	3.63

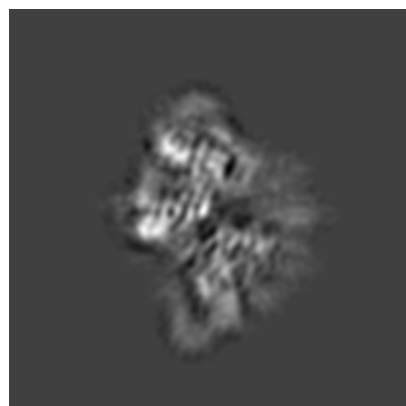
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0251. 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](#)

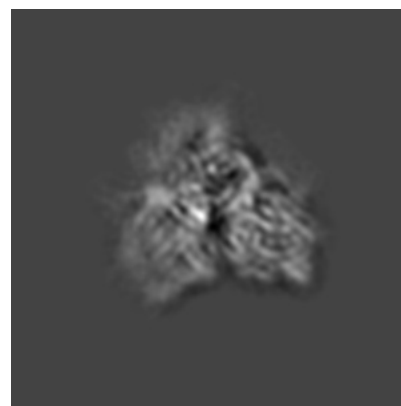
6.1.1 Primary map



X

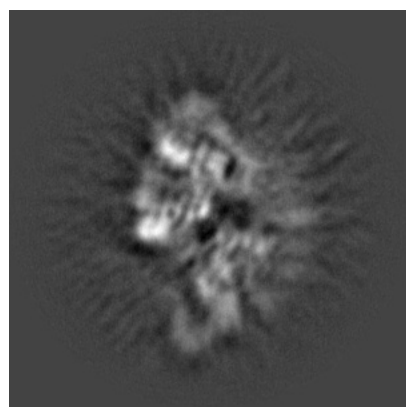


Y

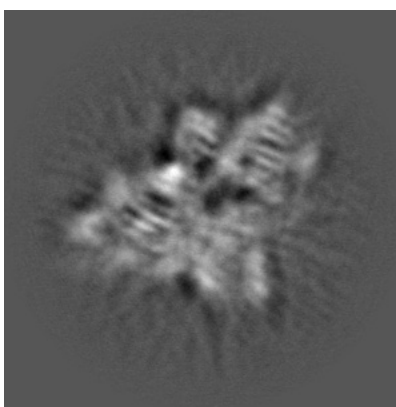


Z

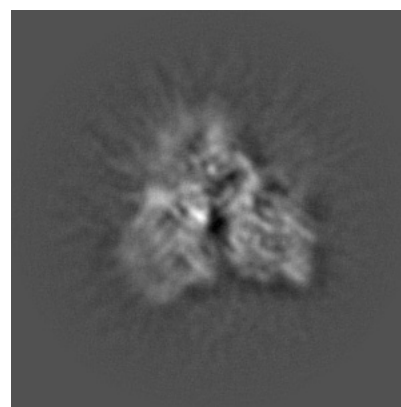
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

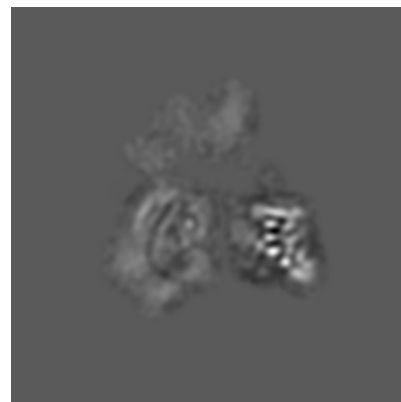
6.2.1 Primary map



X Index: 160

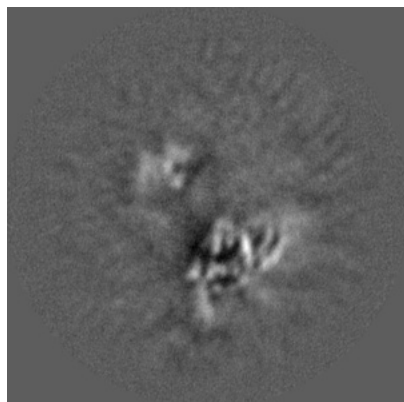


Y Index: 160

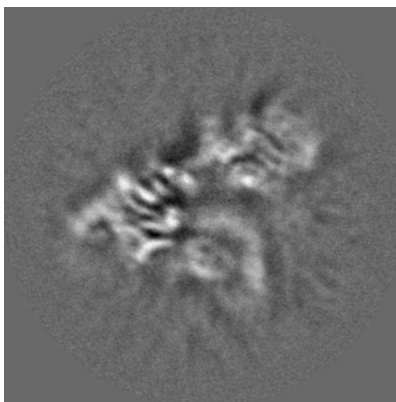


Z Index: 160

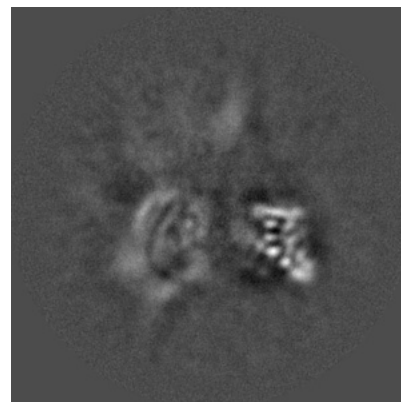
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 183

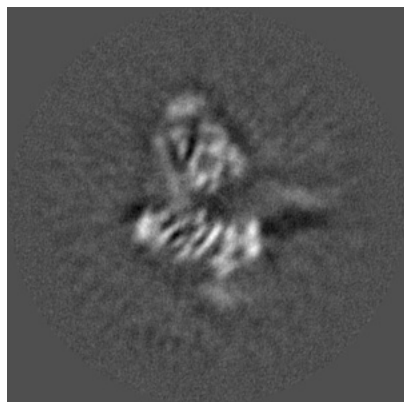


Y Index: 156

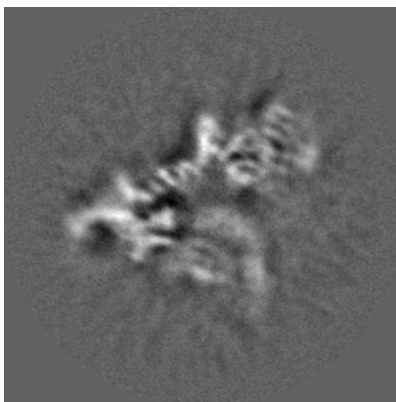


Z Index: 137

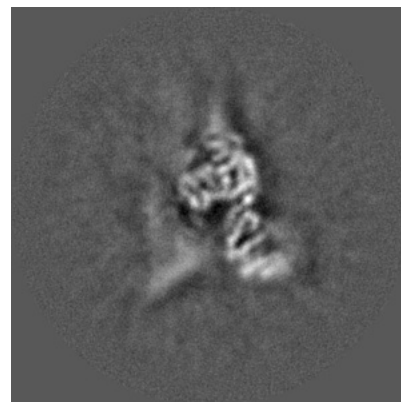
6.3.2 Raw map



X Index: 188



Y Index: 156

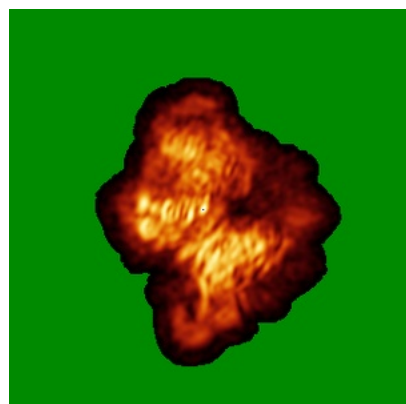


Z Index: 138

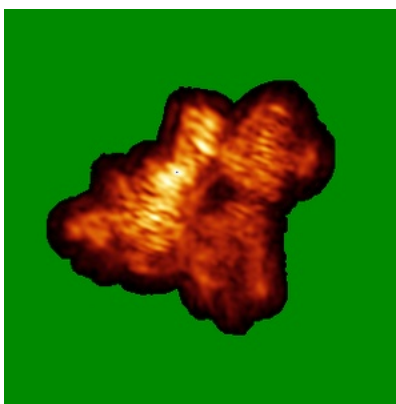
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

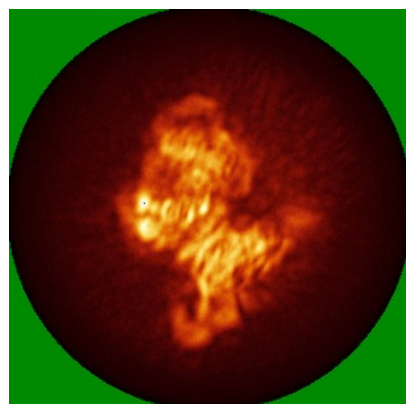


Y

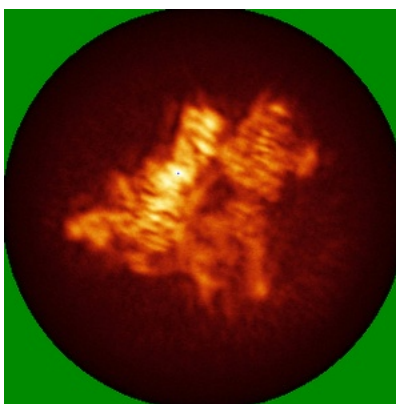


Z

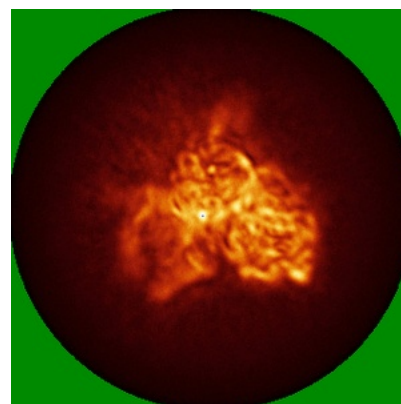
6.4.2 Raw map



X



Y

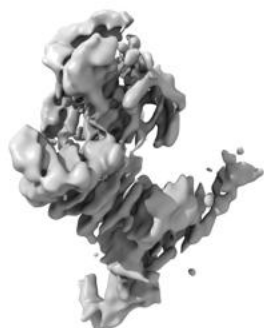


Z

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

6.5 Orthogonal surface views [i](#)

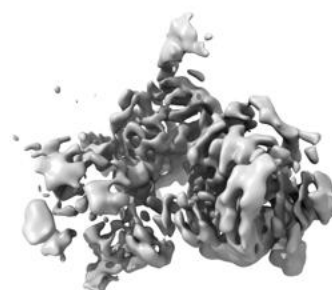
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

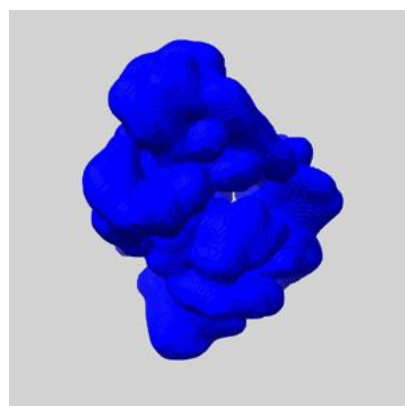
6.6 Mask visualisation [i](#)

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

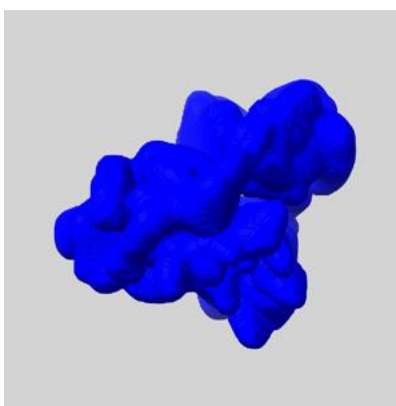
A mask typically either:

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

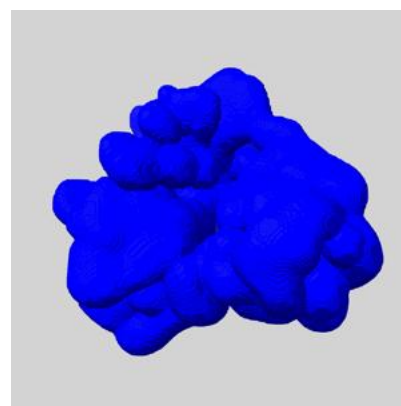
6.6.1 emd_0251_msk_1.map [i](#)



X



Y

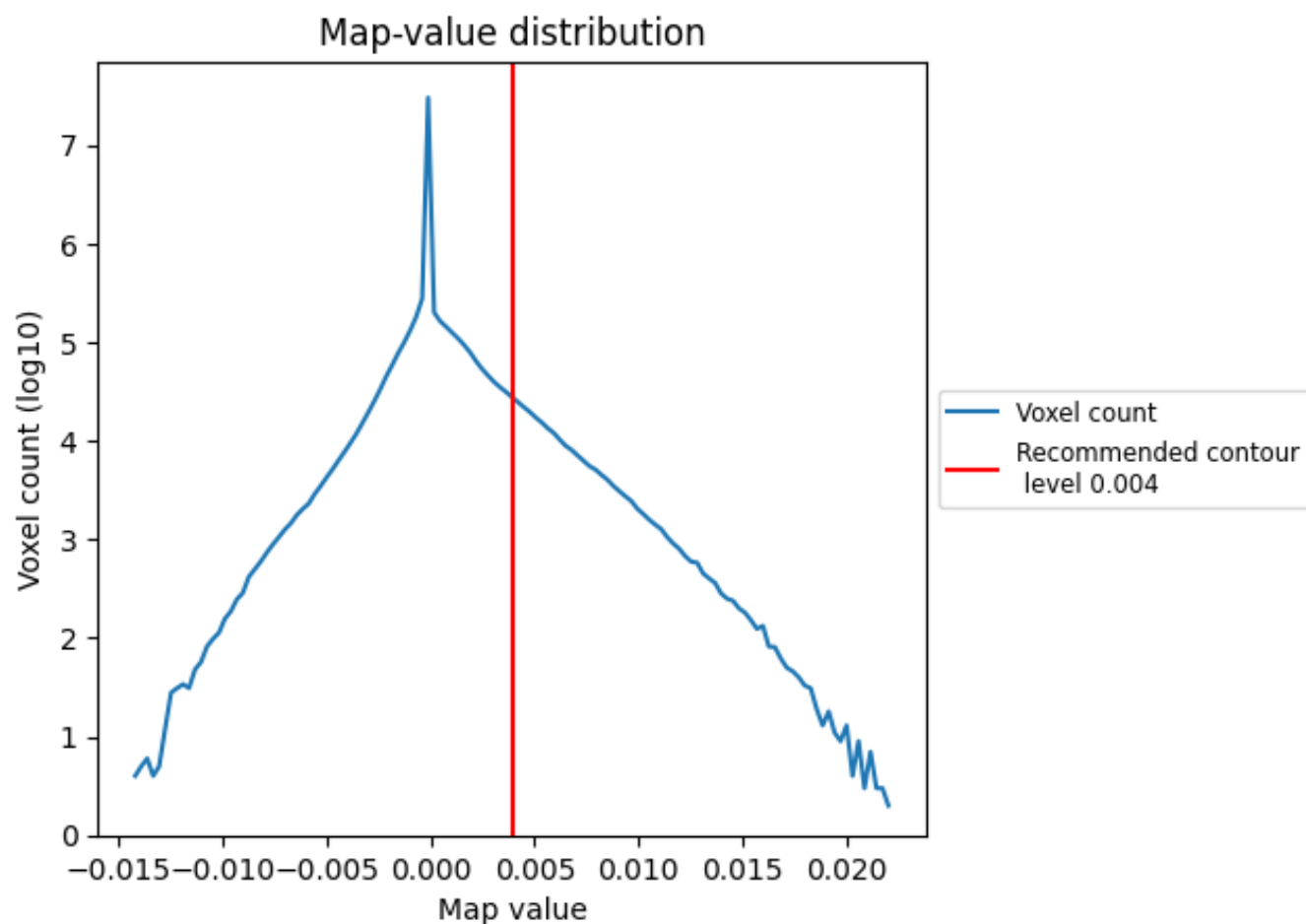


Z

7 Map analysis [i](#)

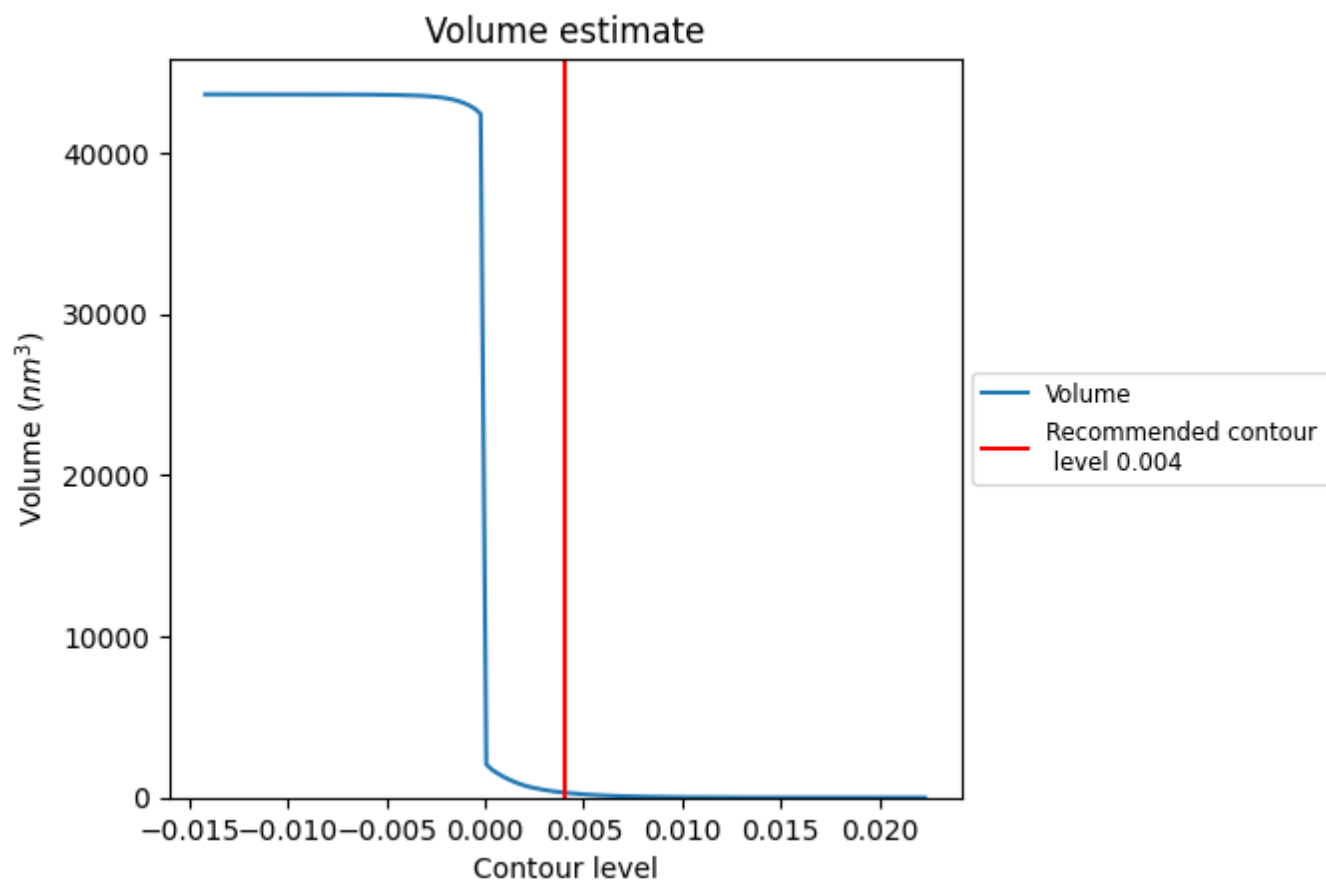
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

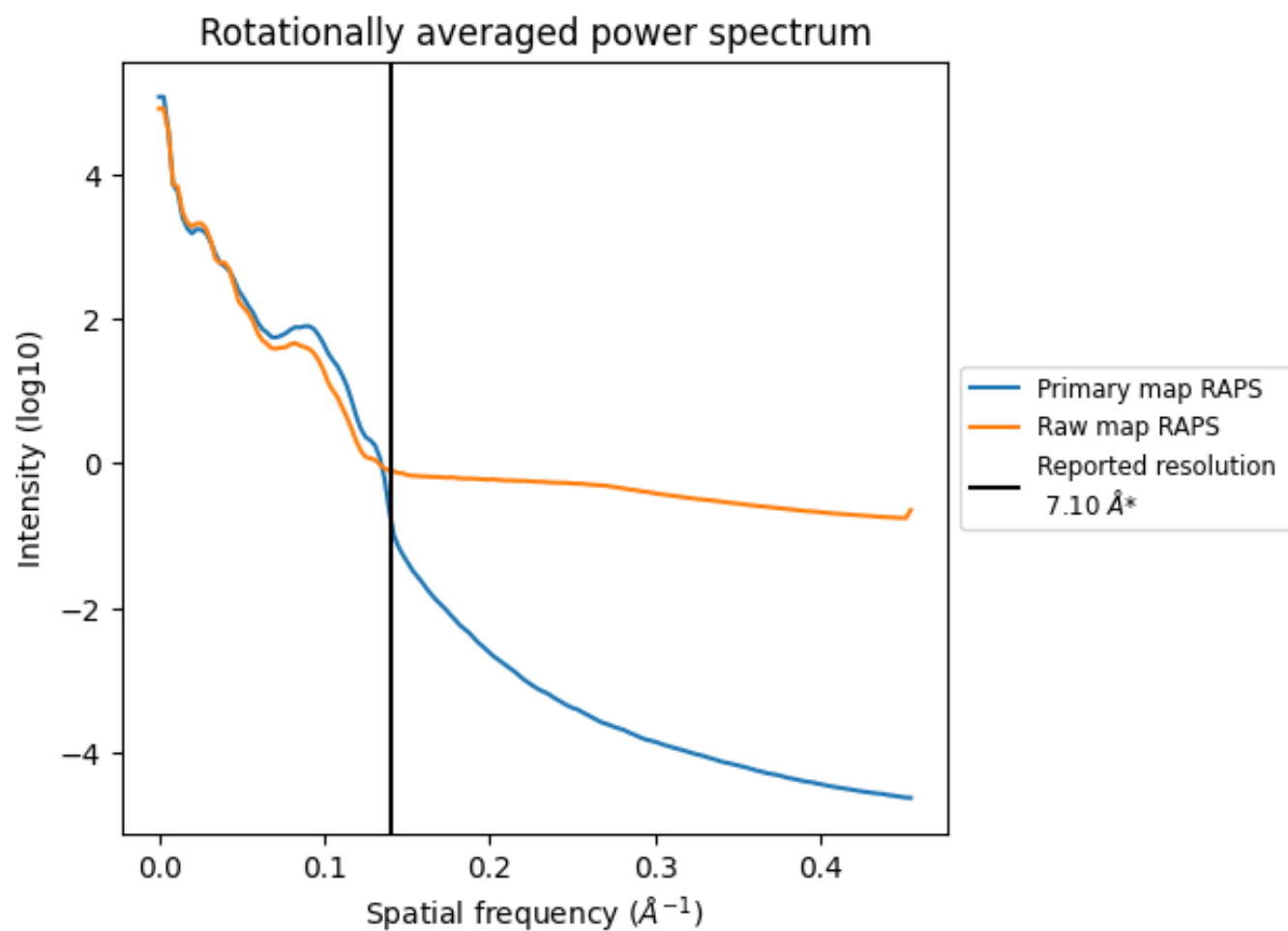
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm³; this corresponds to an approximate mass of 278 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 ⓘ

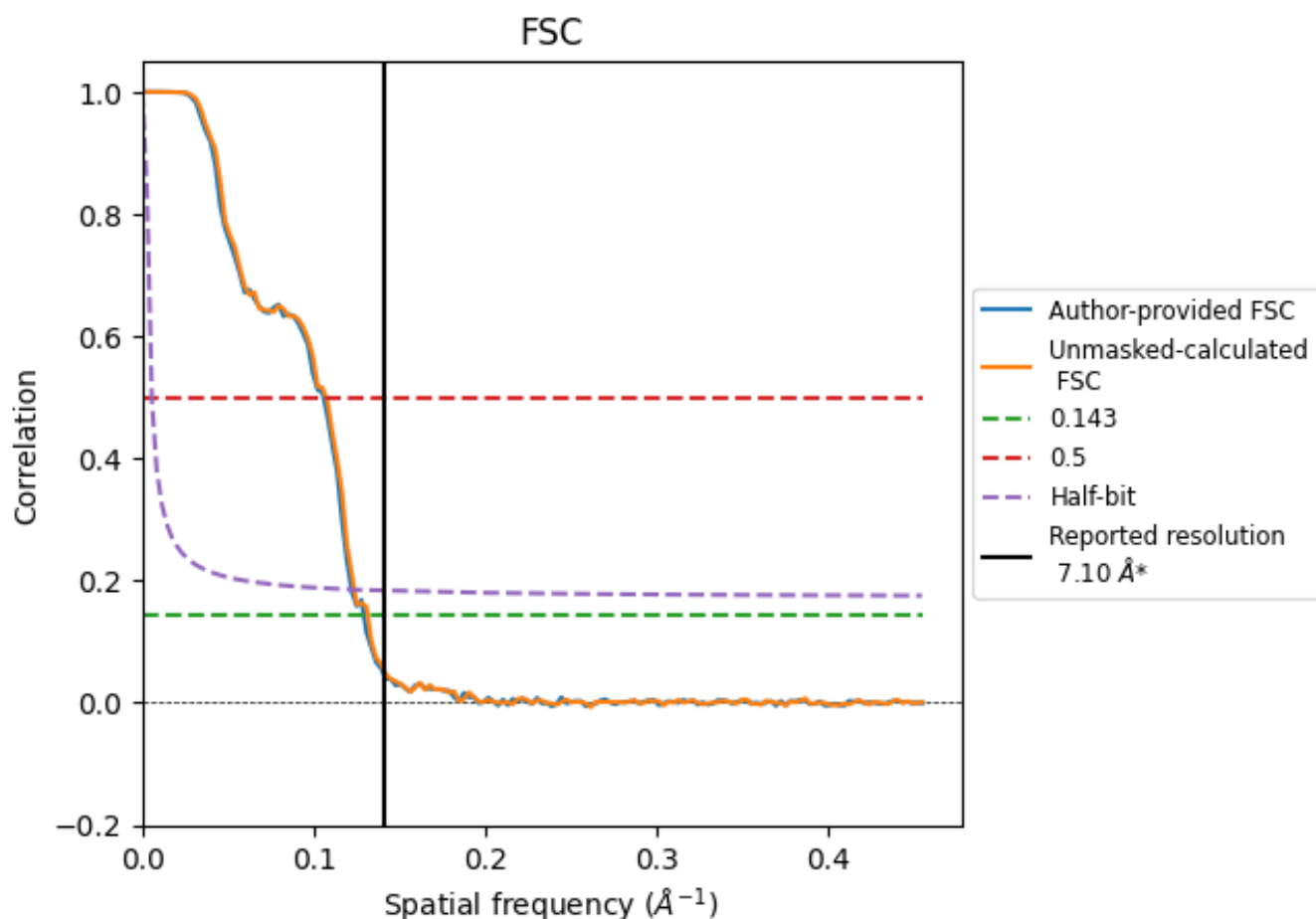


*Reported resolution corresponds to spatial frequency of 0.141 Å⁻¹

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 0.141 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

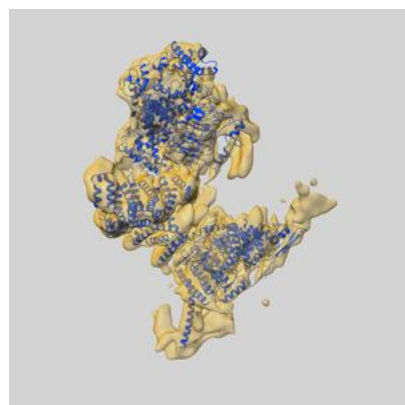
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.10	-	-
Author-provided FSC curve	7.74	9.46	8.20
Unmasked-calculated*	7.61	9.35	8.09

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

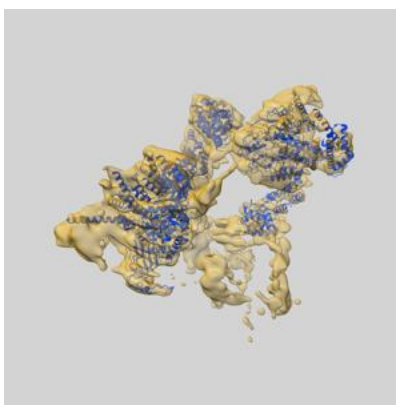
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0251 and PDB model 6HQA. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

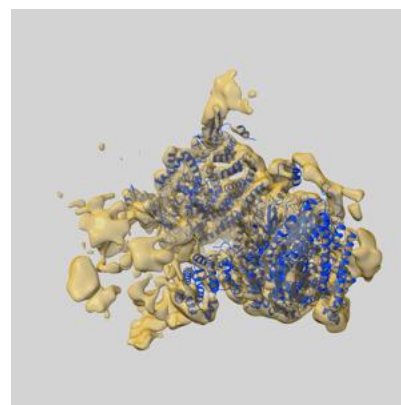
9.1 Map-model overlay [i](#)



X



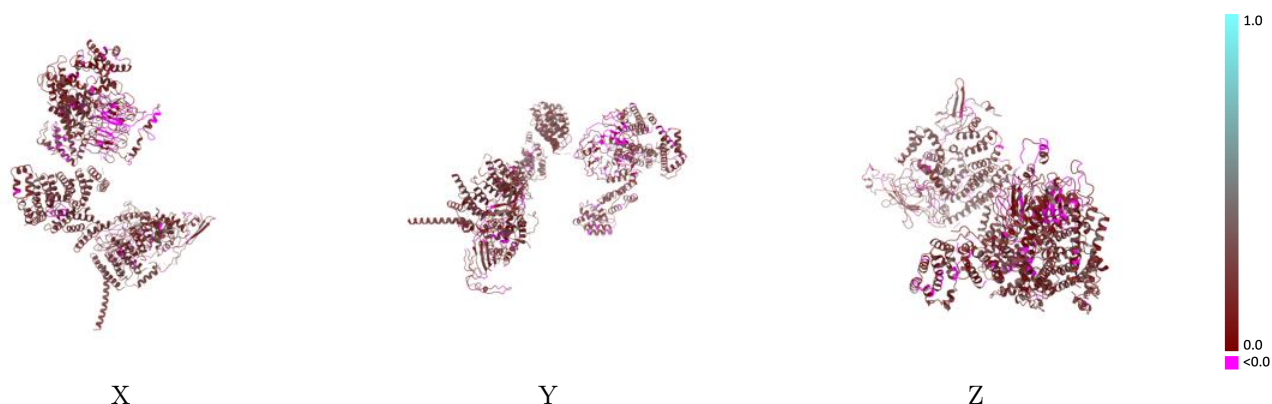
Y



Z

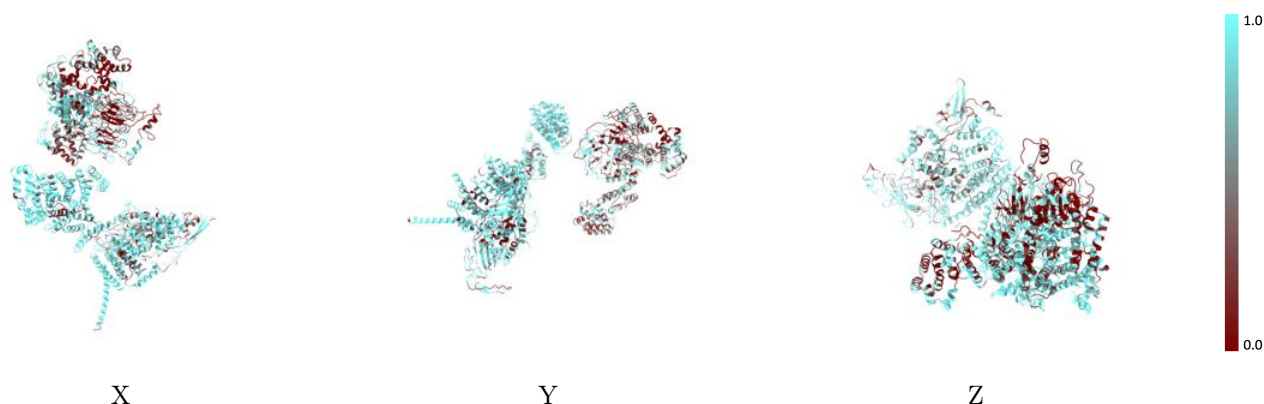
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



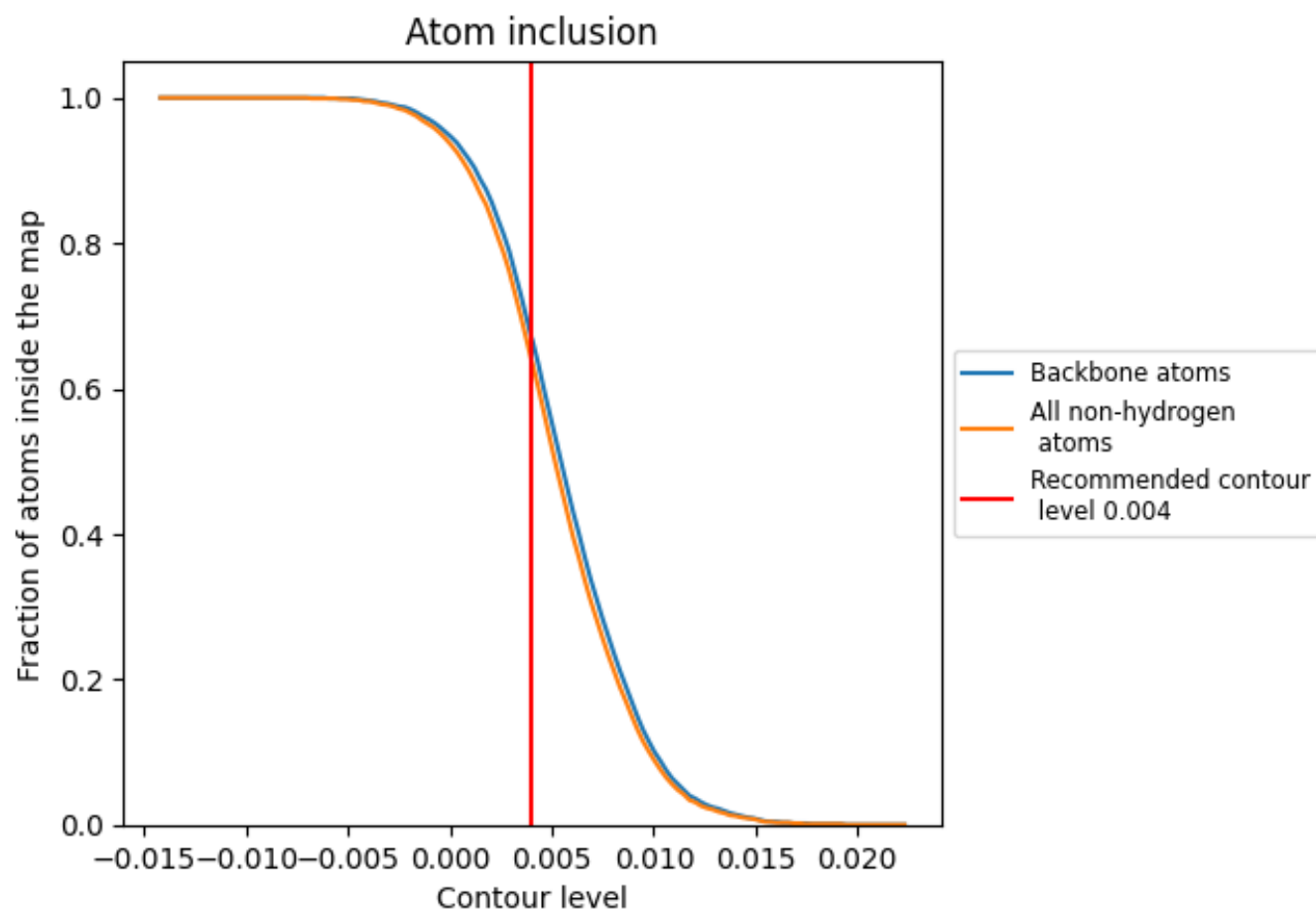
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 64% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6390	 0.1780
A	 0.7010	 0.1920
B	 0.4280	 0.0980
C	 0.4720	 0.1600
D	 0.8090	 0.2040
E	 0.8290	 0.2250
F	 0.5460	 0.2020
G	 0.9520	 0.2540
H	 0.5530	 0.2110
I	 0.4870	 0.2040
J	 0.4440	 0.1520
K	 0.4160	 0.1590

