WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Mar 5, 2024 – 11:07 AM EST

PDB ID	:	6MZM
EMDB ID	:	EMD-9306
Title	:	Human TFIID bound to promoter DNA and TFIIA
Authors	:	Patel, A.B.; Louder, R.K.; Greber, B.J.; Grunberg, S.; Luo, J.; Fang, J.; Liu, Y.; Ranish, J.; Hahn, S.; Nogales, E.
Deposited on	:	2018-11-05
Resolution	:	7.50 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:

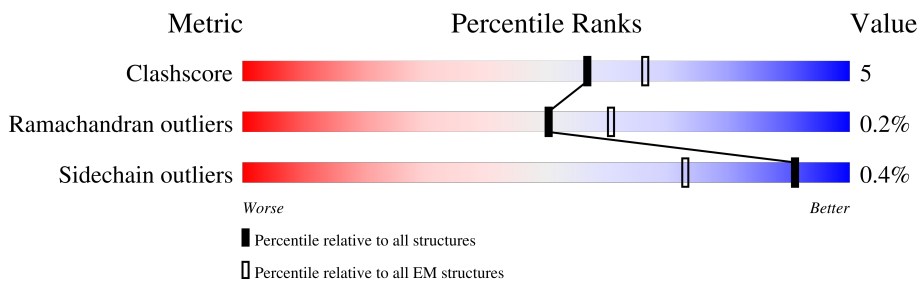|		
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 7.50 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.
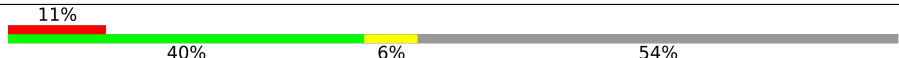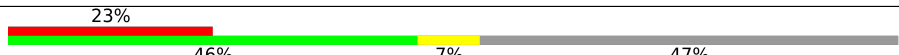
Metric	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		0.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
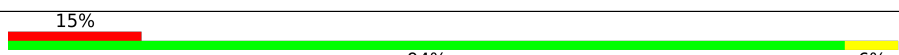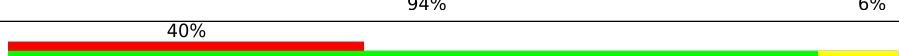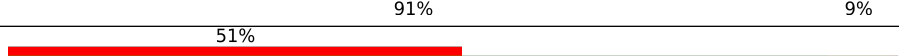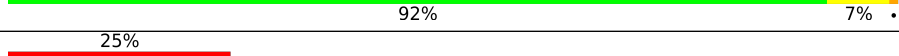
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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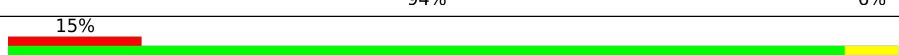segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion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

Mol	Chain	Length	Quality of chain
1	A	496	22% / 79% 10% 10%
2	B	1199	9% / 64% 16% 19%
3	D	1025	· / 12% · 88%
4	G	800	14% / 48% 11% 41%
5	H	677	· / 31% 7% 62%
6	I	677	6% / 43% 6% 50%
7	J	349	10% / 30% 5% 65%
8	K	310	12% / 56% 9% 35%

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Mol	Chain	Length	Quality of chain
9	L	264	37% · 61%
10	O	218	7% 30% 8% 62%
11	R	161	11% 40% 6% 54%
12	T	339	23% 46% 7% 47%
13	U	80	15% 94% 6%
14	V	80	15% 94% 6%
15	W	90	40% 91% 9%
16	X	97	51% 92% 7% ·
17	Z	238	25% 98% ·

2   Entry composition ⓘ

There are 17 unique types of molecules in this entry. The entry contains 32243 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 Transcription initiation factor TFIID subunit 1, TAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	445	Total 3610	C 2300	N 642	O 645	S 23	0	0

- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 2, TAF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	968	Total 7832	C 5031	N 1322	O 1421	S 58	0	0

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4, TAF4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	128	Total 816	C 501	N 156	O 159	0	0

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5,TAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	473	Total 3646	C 2314	N 638	O 679	S 15	0	0

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	257	Total 1943	C 1230	N 347	O 355	S 11	0	0

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	339	Total 2520	C 1585	N 445	O 474	S 16	0	0

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	123	Total	C	N	O	S	0	0
			998	638	184	172	4		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 8, TAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	202	Total	C	N	O	S	0	0
			1449	906	260	278	5		

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 9, TAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	104	Total	C	N	O	S	0	0
			732	456	129	142	5		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	82	Total	C	N	O	S	0	0
			645	413	102	126	4		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	74	Total	C	N	O	S	0	0
			611	381	107	120	3		

- Molecule 12 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	180	Total	C	N	O	S	0	0
			1429	927	252	243	7		

- Molecule 13 is a DNA chain called SCP DNA (80-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	80	Total	C	N	O	P	0	0
			1626	770	292	484	80		

- Molecule 14 is a DNA chain called SCP DNA (80-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	80	Total 1654	C 778	N 320	O 476	P 80	0	0

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	90	Total 749	C 478	N 126	O 141	S 4	0	0

- Molecule 16 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	97	Total 793	C 502	N 140	O 149	S 2	0	0

- Molecule 17 is a protein called Unk.

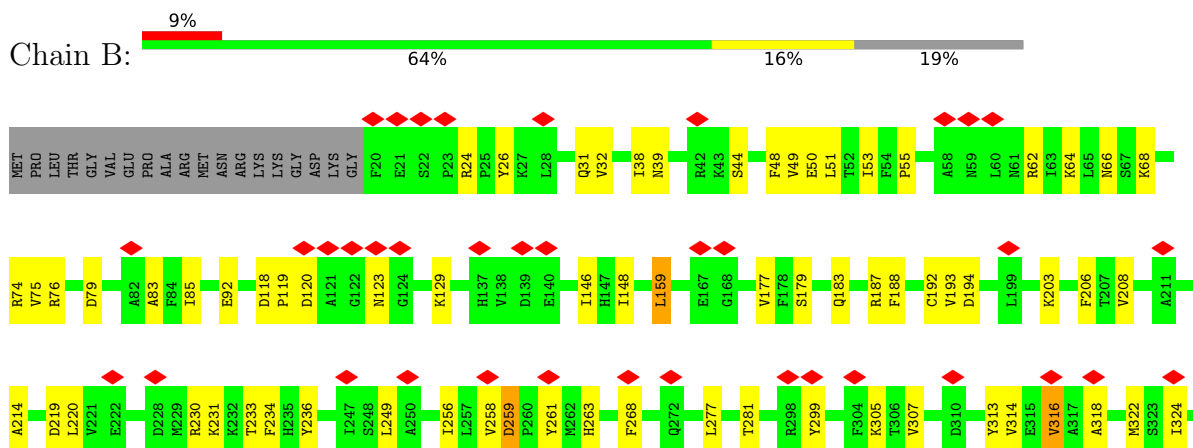| Mol	Chain	Residues	Atoms				AltConf	Trace
17	Z	238	Total 1190	C 714	N 238	O 238	0	0

3 Residue-property plots ⓘ

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.

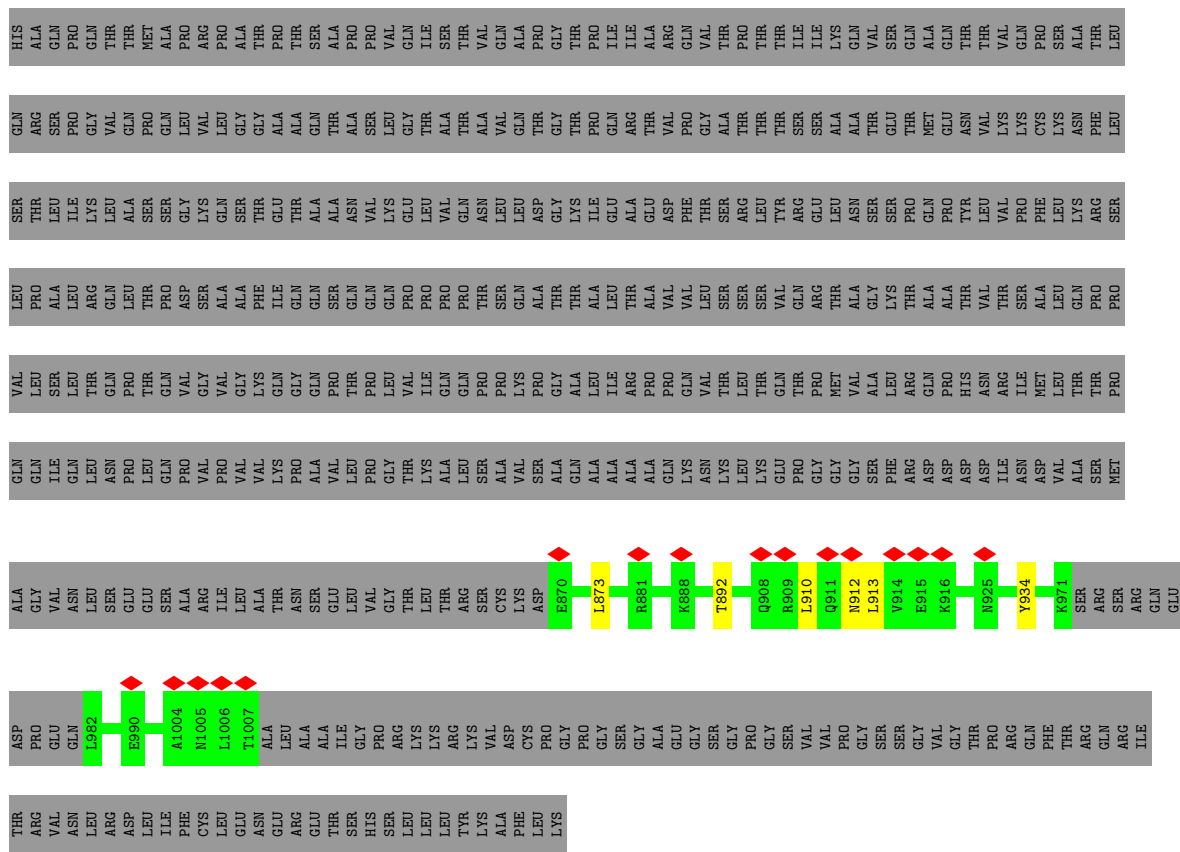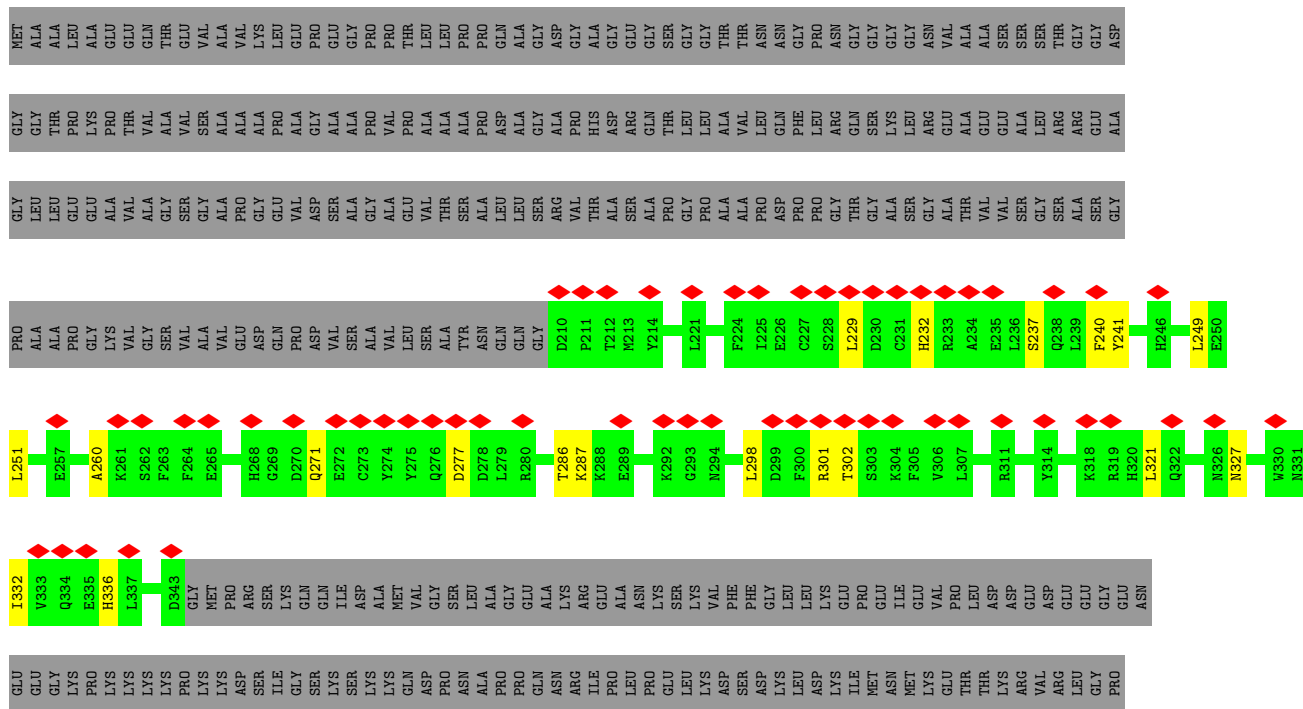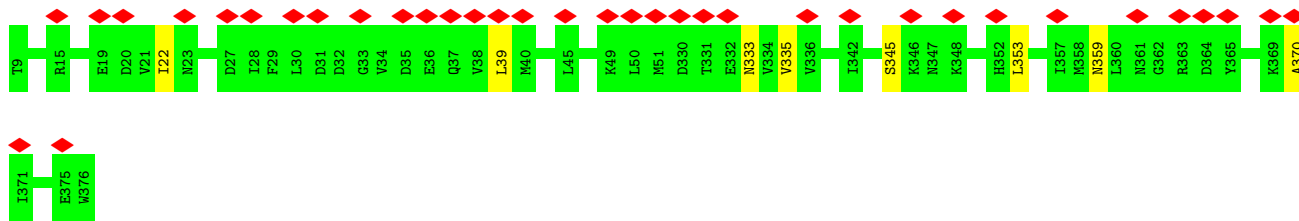• Molecule 1: Transcription initiation factor TFIID subunit 1, TAF1

Chain A:

22%
79%
10%
10%

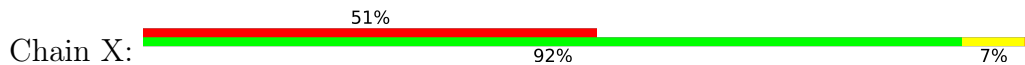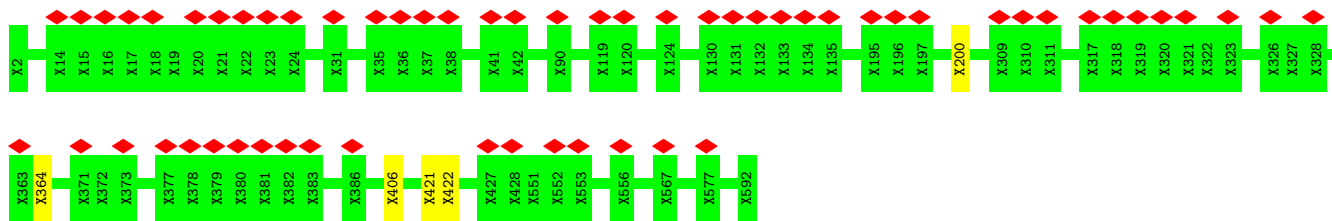• Molecule 2: Transcription initiation factor TFIID subunit 2, TAF2

Chain B:

9%
64%
16%
19%

N328 S332 I335 E338 L341 T342 R343 R344 Q348 S349 Q352 Q353 I359 S360 R361 M362 D366 E367 K371 M382 G387 V388 N389 E390 Y391 K396 I402 K408 H415 P416 I417 F418 G419 G420 G421 K422 E423 K424 D425 L431 H432 T440

W443 V446 C451 H454 L455 R458 N462 R463 Q471 S485 F488 H491 M492 V498 S499 D514 V528 V529 K530 N538 R539 K540 R541 N542 E545 L546 E547 I548 K549 Q550 D551 Y552 K559 L564 K565 V566 E570 H577 T578 L579 Q580

E583 N584 K587 P591 C592 H593 R597 R598 N599 K602 P605 N608 G609 E610 E611 V612 M619 D620 A621 I630 M634 R638 K639 L653 R657 D658 V659 V660 Q663 I666 L669 E670 R678 T682 F691 Y692 R693 V694 V710 S711

T714 M719 R725 C728 C729 K730 S731 I735 V736 K737 Q745 A756 D762 V763 H764 R785 L802 V806 T807 P808 A809 V810 S811 V812 N813 N814 E815 V816 R817 T818 L819 D820 N821 L822 I829 R835 F836 L837 N838 M839 E840 K841 L842 L843 P844 R847 H848

T849 I850 T851 R856 P871 F874 K875 D885 I886 R887 I888 L891 V894 T898 K899 L907 D917 R923 I926 M929 L930 T931 K932 P935 F936 N939 N946 K955 L956 M957 N958 S959 G960 T961 R966 F976 F979 G980 L981 P984

S985 C986 L987 PRO LEU PRO GLU LEU GLY LEU VAL LEU ASN LEU LYS GLU LYS LYS ALA VAL LEU ASN PRO THR ILE PRO GLU GLU SER VAL ALA GLY ASN GLN GLU ALA ALA ASN ASN PRO SER SER HIS PRO GLN LEU VAL GLY PHE GLN ASN PRO PHE SER SER GLN ASP GLU GLU

GLU ILE ASP MET ASP THR VAL HIS ASP SER GLN ALA PHE ILE SER HIS LEU ASN MET LEU GLU ARG PRO SER THR ILE PRO GLU GLY LEU SER LYS TYR ARG PRO ALA SER SER ARG SER ALA LEU ILE PRO GLN HIS SER ALA GLY HIS CYS ASP SER THR PRO THR THR LYS PRO GLN TRP SER

LEU GLU LEU ALA ARG LYS GLY THR GLY LYS GLU GLN ALA PRO LEU GLU MET SER MET HIS PRO ALA ALA SER ALA PRO LEU SER VAL PHE THR LYS GLU SER LYS TYR ARG PRO ALA SER ARG SER ALA LEU ILE PRO GLN HIS SER ALA GLY HIS HIS HIS HIS HIS GLU HIS LYS LYS LYS LYS LYS HIS LYS

HIS LYS HIS LYS HIS LYS HIS ASP SER LYS GLU LYS ASP ASP GLU PRO PHE THR PHE SER SER PRO ALA SER GLY ARG SER ILE ARG SER PRO SER LEU SER ASP

• **Molecule 3: Transcription initiation factor TFIID subunit 4, TAF4**

Chain D: 12% 88%

HIS VAL VAL SER GLY SER PRO ALA GLY ALA ALA GLY ALA GLY PRO ALA ALA PRO ALA GLU GLY ALA PRO GLY ALA ALA PRO GLU PRO PRO PRO ALA GLY ARG ALA ARG PRO GLY GLY GLY GLY PRO GLN ARG ARG PRO GLY PRO PRO SER PRO ARG ARG LEU VAL PRO ALA GLY PRO ALA

PRO PRO ALA ALA LYS LEU ARG PRO PRO GLU GLY GLY SER ALA GLY SER CYS ALA PRO VAL PRO ALA ALA ALA VAL ALA ALA GLY PRO GLU PRO ALA PRO ALA GLY PRO PRO LYS PRO ALA GLY PRO ALA ALA LEU ALA ALA ARG ALA GLY PRO GLY PRO GLY PRO GLY PRO

GLY PRO GLY GLY PRO GLY LYS PRO ALA GLY PRO GLY ALA ALA GLN THR LEU ASN GLY SER ALA ALA LEU LEU ASN SER HIS HIS ALA ALA ALA PRO ALA VAL SER LEU LEU VAL ASN ASN GLY PRO ALA ALA LEU LEU PRO LEU LYS PRO ALA ALA PRO GLY THR VAL ILE GLN THR

PRO PRO PHE GLY ALA ALA PRO ALA PRO ALA PRO ALA ALA ALA PRO SER PRO ALA ALA ALA PRO ALA PRO PRO PRO ALA PRO ALA PRO THR LEU ALA ARG PRO GLY HIS PRO ALA GLY PRO PRO THR ALA ALA PRO ALA VAL PRO PRO PRO

ALA ALA ALA GLN ASN GLY SER ALA GLY ALA ALA PRO ALA PRO ALA ALA PRO ALA GLY PRO ALA ALA ALA ALA ALA PRO GLY PRO VAL LYS SER PRO LYS ARG VAL VAL GLN GLY ALA ALA PRO PRO ALA ALA GLN THR

LEU ALA ALA SER GLY PRO ALA SER THR ALA ALA MET VAL ILE GLY PRO THR MET GLN GLY ALA LEU PRO SER GLY PRO GLY PRO ALA ALA ALA ALA PRO GLY GLY MET VAL LEU VAL ARG SER GLU GLU ASN GLY GLN LEU LEU MET ILE PRO GLN GLN ALA LEU ALA GLN MET ALA GLN THR

SER GLY ILE ARG ALA THR LEU THR PRO THR VAL LEU ALA PRO ARG LEU PRO ARG PRO PRO GLN ALA ASN PRO THR ASN ILE GLN ASN PHE GLN LEU PRO LEU PRO GLY MET VAL LEU VAL ARG SER GLU GLU ASN GLY GLN LEU LEU MET ILE PRO GLN GLN ALA LEU ALA GLN MET ALA GLN ALA

• Molecule 4: Transcription initiation factor TFIID subunit 5,TAF5

Chain G:

14%

48% 11% 41%

• Molecule 5: Transcription initiation factor TFIID subunit 6

Chain H:

31%	7%	62%

• Molecule 6: Transcription initiation factor TFIID subunit 6

Chain I:

6%

43%	6%	50%

• Molecule 7: Transcription initiation factor TFIID subunit 7

Chain J:

10%

30%   5%   65%

• Molecule 8: Transcription initiation factor TFIID subunit 8, TAF8

Chain K:

12%

56%   9%   35%

MET ALA ASP ALA ALA THR ALA GLY ALA GLY GLY SER GLY THR ARG SER GLY SER LYS GLN SER THR ASN PRO ALA ASP N28 L31 R34 E51 L65 S70 G73 R74 S75 A76 K77 S78 Y79 T86 Q87 V98 E99 M100 G101 F102 N103 V104 D105 T106 L107

P108 A109 Y110 A111 K112 R113 S114 Q115 R116 T120 X121 X122 X123 X126 X129 X130 X131 X132 X133 X134 X135 X136 X144 X154 X167 X168 X169 X170 X171 Y172 Q173 R176 R184 R188 T191 A195 S202 K205 D206 D207 P212 R217 L227 L228

P229 SER GLU LEU GLU MET GLN GLN MET GLU GLU THR ASP SER SER GLU GLN ASP GLU GLN THR ASP THR GLU ASN LEU ALA LEU HIS ILE SER GLU MET GLU ASP SER GLY ALA GLU LYS GLU ASN THR SER VAL LEU GLN GLN ASN PRO SER LEU SER GLY SER ARG ASN GLY GLU GLU ASN

ILE ILE ASP ASN PRO TYR LEU ARG PRO VAL VAL LYS LYS PRO LYS ILE ARG LYS LYS SER LEU SER

• Molecule 9: Transcription initiation factor TFIID subunit 9, TAF9

Chain L: 37%   •   61%

MET GLU SER GLY LYS THR ALA SER PRO LYS SER MET P13 I28 N37 T49 Y57 K62 L73 C77 R78 A79 D80 Q81 S82 P86 P87 P105 L106 X116 PRO ASP ARG TYR CYS LEU THR ALA PRO ASN TYR ARG LEU LYS SER LEU GLN LYS LYS ALA

SER THR SER ALA GLY ARG ILE THR VAL PRO ARG LEU SER VAL GLY SER VAL LEU ILE ASN PRO SER LEU ILE GLY SER LYS ASN ILE LEU ILE THR ASN MET MET SER VAL SER THR LYS VAL GLY THR PRO MET LEU THR GLY GLN ARG PHE THR VAL GLN MET PRO THR SER GLN SER

PRO ALA VAL LYS ALA SER ILE PRO ALA THR SER ALA VAL GLN ASN VAL LEU ILE ASN PRO SER LEU ILE GLY SER LYS ASN ILE LEU ILE THR THR ASN MET MET SER SER GLN ASN THR ALA ASN GLU SER SER ASN ALA LEU LYS ARG LYS ARG GLU ASP ASP ASP ASP ASP ASP

ASP ASP ASP ASP TYR ASP ASN LEU

• Molecule 10: Transcription initiation factor TFIID subunit 10

Chain O: 7%   30%   8%   62%

MET SER CYS SER GLY SER ALA ASP PRO GLU ALA ALA PRO ALA SER ALA ALA SER ALA PRO GLY PRO ALA PRO PRO VAL SER ALA PRO ALA ALA LEU PRO SER SER THR ALA ALA GLU ASN LYS ALA SER PRO ALA GLY THR ALA GLY GLY PRO GLY ALA GLY ALA ALA ALA GLY GLY

THR GLY PRO LEU ALA ALA ARG ALA GLY GLU PRO ALA GLU ARG ALA GLY ALA ALA PRO VAL SER ALA GLY LEU ALA ALA PRO PRO GLU GLY ALA ILE SER ASN GLY VAL TYR VAL LEU PRO SER ALA ALA ASN ASP VAL LYS PRO VAL VAL SER S113 T114 P115 D118 F119 Q122

L123 E124 D125 Y126 T129 I130 P131 D132 L139 A142 G143 F144 E145 A146 S147 D148 P149 R150 R153 A159 Q160 I166 A170 C174 K177 GLY THR ALA SER GLY SER SER ARG SER LYS SER ASP ARG K192 L195 E206 Y207 G208 ILE ASN VAL LYS LYS

PRO HIS TYR PHE THR

• Molecule 11: Transcription initiation factor TFIID subunit 12

Chain R: 11%   40%   6%   54%

MET ASN GLN PHE GLY PRO SER ALA LEU ILE ASN LEU SER ASN PHE SER SER ILE LYS PRO GLU PRO ALA SER THR PRO PRO GLN GLY THR MET ALA ASN SER THR ALA VAL VAL LYS ILE PRO GLY THR PRO GLY GLY GLY ARG LEU SER PRO GLU ASN **N55** **L58** **R68** **E69**

V70 **D71** **P72** **N73** **E74** **D77** **E78** **M83** **I87** **D90** **S94** **R106** **S109** **E112** **L120** **E121** **R122** **Q123** **W124** **N125** **M126** **W127** **I128** PRO GLY PHE GLY SER GLU GLU ILE ARG PRO TYR LYS LYS ALA CYS THR THR GLU ALA HIS LYS GLN ARG MET ALA LEU ILE ARG

LYS THR THR LYS LYS

• Molecule 12: TATA-box-binding protein

23%

Chain T:

46%   7%   47%

MET ASP GLN ASN ASN SER LEU PRO PRO TYR ALA GLN GLY LEU ALA SER PRO GLN GLY ALA MET THR PRO GLY ILE PRO ILE PHE SER PRO MET MET PRO TYR GLY THR GLY LEU THR PRO GLN PRO ILE GLN ASN THR ASN SER LEU SER ILE LEU GLU GLU GLN GLN ARG GLN GLN

GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN ALA VAL ALA ALA ALA VAL GLN SER THR SER GLN GLN ALA THR GLN GLY THR SER GLY GLN ALA PRO GLN

LEU PHE HIS SER GLN THR LEU THR THR ALA PRO LEU PRO GLY THR THR PRO LEU TYR PRO SER PRO MET THR PRO MET THR PRO ILE THR PRO ALA THR PRO ALA SER GLU SER **S159** **G160** **I161** **V162** **N167** **I168** **V169** **S170** **T171** **L174** **G175** **L178** **D179** **L180** **K181** **T182** **R186** **A187**

R188 **E191** **Y192** **N193** **A198** **I201** **M202** **E206** **P207** **F214** **S215** **V220** **S226** **R231** **L232** **A233** **A234** **Y237** **L244** **G245** **F246** **P247** **A248** **K249** **F253** **K254** **N257** **M258** **V259** **D263** **V264** **K265** **F266** **P267** **I268** **R269** **L273** **V274** **L275** **T276** **H277** **Q278** **Q279** **F280** **S281** **S282**

Y283 **E284** **P285** **E286** **L287** **L291** **I292** **Y293** **R294** **M295** **I296** **K297** **P298** **R299** **I300** **V301** **L302** **L303** **I304** **F305** **V306** **S307** **G308** **K309** **V310** **V311** **K316** **V317** **E320** **A324** **F325** **E326** **P330** **I331** **L332** **K333** **G334** **F335** **R336** **K337** **T338** THR

• Molecule 13: SCP DNA (80-MER)

15%

Chain U:

94%   6%

C81 **C82** **G83** **T84** **T94** **A129** **A130** **C142** **T149** **A150** **T151** **A152** **G153** **G154** **C155** **G156** **C157** **C158** **C159** **T160**

• Molecule 14: SCP DNA (80-MER)

15%

Chain V:

94%   6%

A1 **G2** **G3** **C7** **C8** **T11** **A12** **G18** **C37** **T38** **T48** **G68** **A69** **G79** **G80**

• Molecule 15: Transcription initiation factor IIA subunit 1

40%

Chain W:

91%   9%

T9 R15 E19 D20 V21 I22 N23 D27 I28 F29 L30 D31 D32 G33 V34 D35 E36 Q37 V38 L39 M40 L45 K49 L50 M51 D330 T331 E332 N333 V334 V335 V336 I342 S345 K346 N347 K348 H352 L353 I357 M358 N359 L360 N361 G362 R363 D364 Y365 K369 A370

I371 E375 W376

• Molecule 16: Transcription initiation factor IIA subunit 2

Chain X:

51%

92%

7% •

Y3 Q4 L5 Y6 L11 S14 L15 Q16 E17 S18 E21 L22 I23 Q24 S25 Q26 Q27 I28 T29 P30 Q31 L32 Q35 V36 L37 F40 D41 K42 A46 A47 L48 A49 Q50 R51 V52 R53 N54 R55 V56 L62 N63 T64 D69 T73 F74 V75 L76 E80 F81 R82

E83 V84 T85 E86 L87 I88 K89 I95 D99

• Molecule 17: Unk

Chain Z:

25%

98%

X2 X14 X15 X16 X17 X18 X19 X20 X21 X22 X23 X24 X31 X35 X36 X37 X38 X41 X42 X90 X119 X120 X124 X130 X131 X132 X133 X134 X135 X195 X196 X197 X200 X309 X310 X311 X317 X318 X319 X320 X321 X322 X323 X326 X327 X328

X363 X364 X371 X372 X373 X377 X378 X379 X380 X381 X382 X383 X386 X406 X421 X422 X427 X428 X551 X552 X553 X556 X567 X577 X592

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5   Model quality   ⓘ

5.1   Standard geometry   ⓘ

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	0.27	0/3694	0.51	1/4967 (0.0%)
2	B	0.30	0/8029	0.60	1/10882 (0.0%)
3	D	0.25	0/821	0.44	0/1124
4	G	0.28	0/3537	0.59	0/4802
5	H	0.30	0/1978	0.58	1/2693 (0.0%)
6	I	0.26	0/2506	0.50	0/3402
7	J	0.26	0/1017	0.53	0/1370
8	K	0.26	0/1212	0.50	1/1640 (0.1%)
9	L	0.25	0/705	0.49	0/955
10	O	0.26	0/657	0.46	0/891
11	R	0.26	0/618	0.50	0/835
12	T	0.28	0/1455	0.52	0/1958
13	U	0.69	0/1819	0.99	6/2802 (0.2%)
14	V	0.67	0/1859	0.93	1/2870 (0.0%)
15	W	0.29	0/762	0.56	0/1026
16	X	0.29	0/803	0.63	1/1088 (0.1%)
All	All	0.35	0/31472	0.62	12/43305 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	8
4	G	0	3
5	H	0	4
6	I	0	1
8	K	0	3
15	W	0	1
16	X	0	1
17	Z	0	1

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	23

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	U	151	DT	O4'-C1'-N1	7.93	113.55	108.00
13	U	149	DT	O4'-C1'-N1	7.02	112.92	108.00
16	X	76	LEU	CA-CB-CG	6.36	129.94	115.30
8	K	227	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	1020	LEU	CA-CB-CG	5.74	128.51	115.30

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	949	GLU	Peptide
2	B	193	VAL	Peptide
2	B	259	ASP	Peptide
2	B	316	VAL	Peptide
2	B	415	HIS	Peptide

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	3610	0	3640	31	0
2	B	7832	0	7789	121	0
3	D	816	0	632	5	0
4	G	3646	0	3312	51	0
5	H	1943	0	1922	23	0
6	I	2520	0	2422	26	0
7	J	998	0	1055	13	0
8	K	1449	0	1281	20	0
9	L	732	0	624	5	0
10	O	645	0	640	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	611	0	610	9	0
12	T	1429	0	1521	15	0
13	U	1626	0	897	1	0
14	V	1654	0	893	6	0
15	W	749	0	740	4	0
16	X	793	0	801	4	0
17	Z	1190	0	276	4	0
All	All	32243	0	29055	313	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 313 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)
2:B:31:GLN:HA	2:B:50:GLU:O	1.41	1.17
2:B:835:ARG:HH21	8:K:188:ARG:HD2	1.58	0.68
2:B:564:LEU:H	2:B:580:GLN:HB2	1.59	0.68
4:G:718:ARG:HG2	4:G:771:GLY:H	1.59	0.67
4:G:321:LEU:HD22	4:G:327:ASN:HD21	1.60	0.66

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	437/496 (88%)	431 (99%)	4 (1%)	2 (0%)	29	69
2	B	966/1199 (81%)	823 (85%)	143 (15%)	0	100	100
3	D	124/1025 (12%)	118 (95%)	6 (5%)	0	100	100
4	G	429/800 (54%)	382 (89%)	47 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	255/677 (38%)	237 (93%)	17 (7%)	1 (0%)	34	72
6	I	326/677 (48%)	303 (93%)	21 (6%)	2 (1%)	25	66
7	J	119/349 (34%)	117 (98%)	2 (2%)	0	100	100
8	K	149/310 (48%)	140 (94%)	9 (6%)	0	100	100
9	L	96/264 (36%)	93 (97%)	3 (3%)	0	100	100
10	O	78/218 (36%)	74 (95%)	4 (5%)	0	100	100
11	R	72/161 (45%)	70 (97%)	2 (3%)	0	100	100
12	T	178/339 (52%)	175 (98%)	3 (2%)	0	100	100
15	W	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
16	X	95/97 (98%)	91 (96%)	3 (3%)	1 (1%)	14	52
All	All	3410/6702 (51%)	3139 (92%)	265 (8%)	6 (0%)	50	81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	LEU
1	A	950	VAL
16	X	86	GLU
6	I	256	LEU
6	I	257	PRO

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/437 (90%)	389 (99%)	4 (1%)	76	86
2	B	879/1083 (81%)	876 (100%)	3 (0%)	92	95
3	D	52/771 (7%)	52 (100%)	0	100	100
4	G	367/619 (59%)	365 (100%)	2 (0%)	88	93
5	H	200/574 (35%)	200 (100%)	0	100	100
6	I	252/564 (45%)	252 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	J	113/322 (35%)	113 (100%)	0	100	100
8	K	132/223 (59%)	132 (100%)	0	100	100
9	L	61/229 (27%)	60 (98%)	1 (2%)	62	79
10	O	71/154 (46%)	71 (100%)	0	100	100
11	R	70/141 (50%)	69 (99%)	1 (1%)	67	80
12	T	155/293 (53%)	154 (99%)	1 (1%)	86	92
15	W	84/84 (100%)	84 (100%)	0	100	100
16	X	89/89 (100%)	89 (100%)	0	100	100
All	All	2918/5583 (52%)	2906 (100%)	12 (0%)	91	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	558	LEU
4	G	607	ARG
12	T	193	ASN
9	L	73	LEU
1	A	1022	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
7	J	48	HIS
8	K	173	GLN
12	T	193	ASN
2	B	848	HIS
2	B	838	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry ⓘ

There are no ligands in this entry.

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	Z	8
15	W	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	95:UNK	C	119:UNK	N	129.92
1	Z	52:UNK	C	81:UNK	N	114.22
1	Z	143:UNK	C	195:UNK	N	96.41
1	Z	223:UNK	C	309:UNK	N	55.85
1	Z	386:UNK	C	401:UNK	N	34.49

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9306. 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
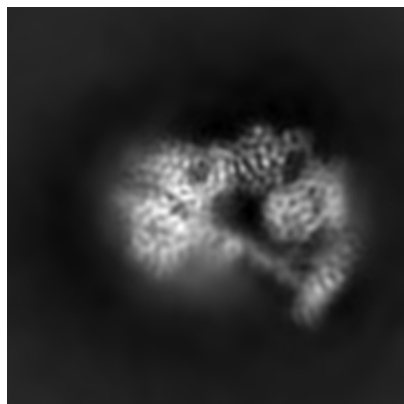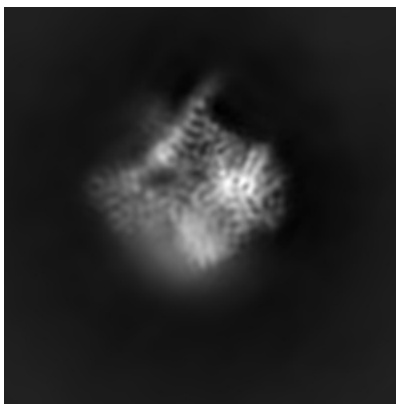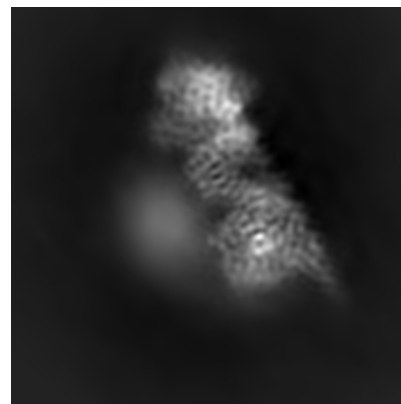
X　　　　　　　　　　　Y　　　　　　　　　　　Z

6.1.2 Raw map

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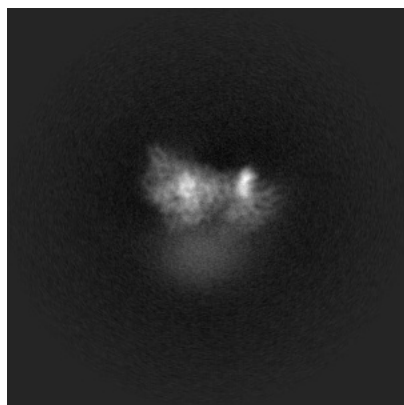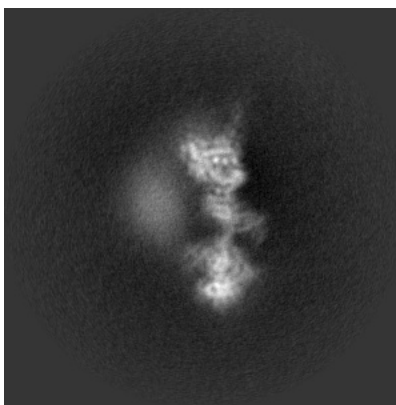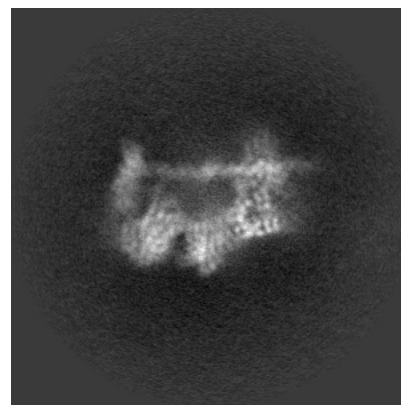
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
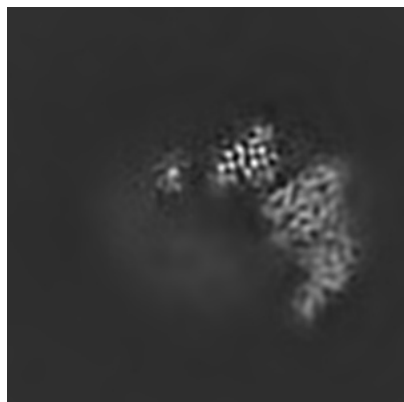
6.2.1   Primary map
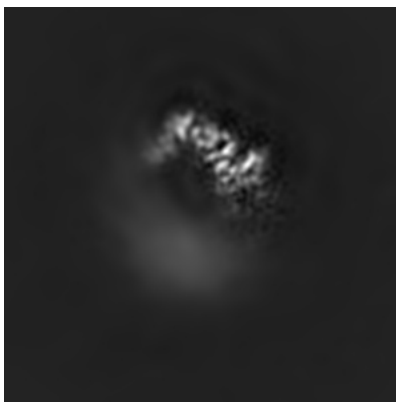
| X Index: 144 | Y Index: 144 | Z Index: 144 |

6.2.2   Raw map
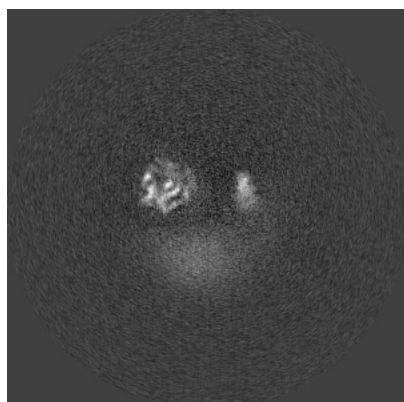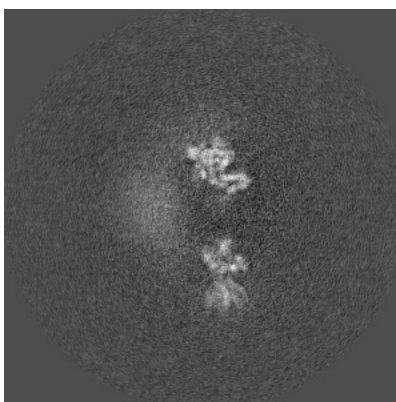
| X Index: 192 | Y Index: 192 | Z Index: 192 |
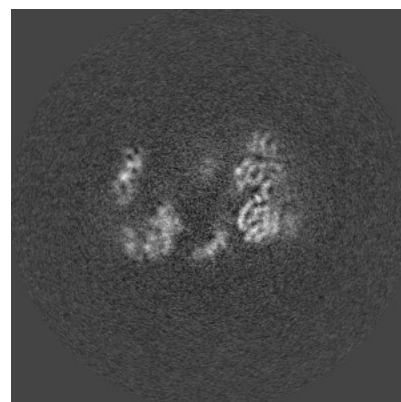
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
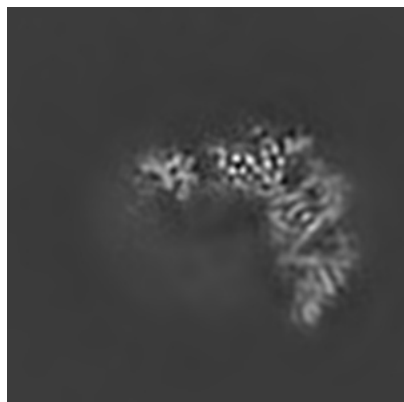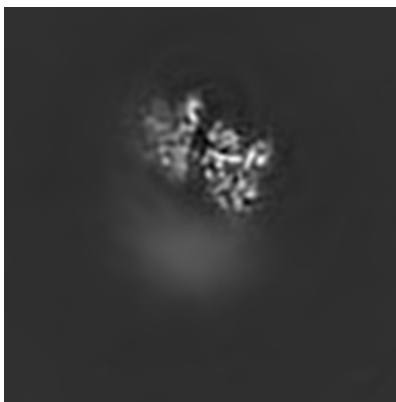
X Index: 153   Y Index: 122   Z Index: 158
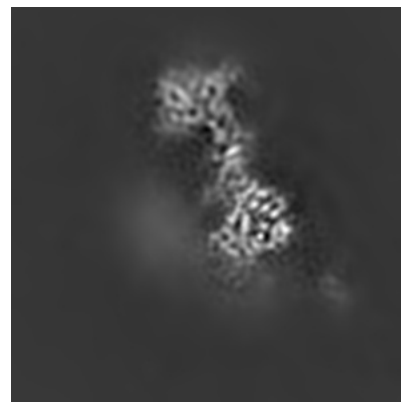
6.3.2 Raw map
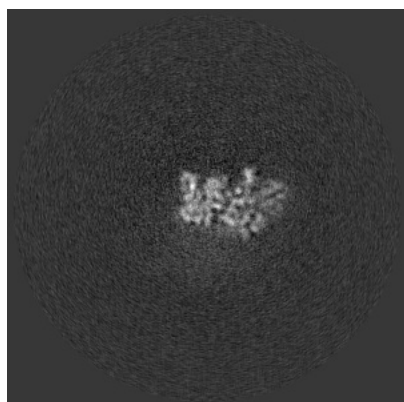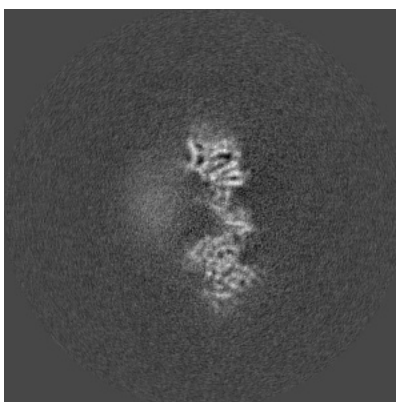
X Index: 245   Y Index: 172   Z Index: 213
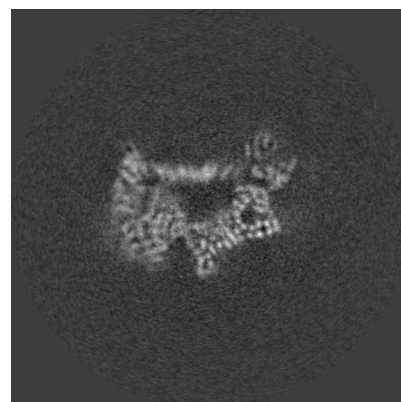
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
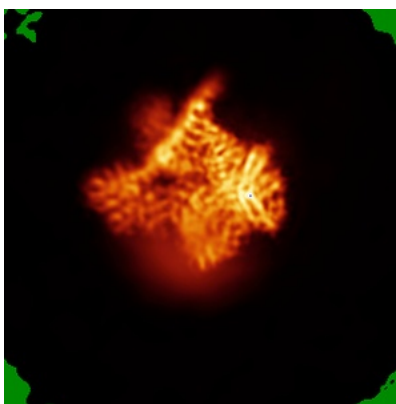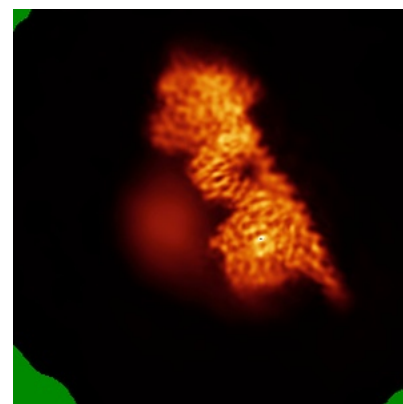
X	Y	Z

6.4.2 Raw map

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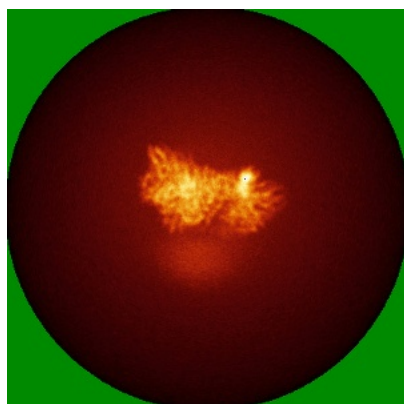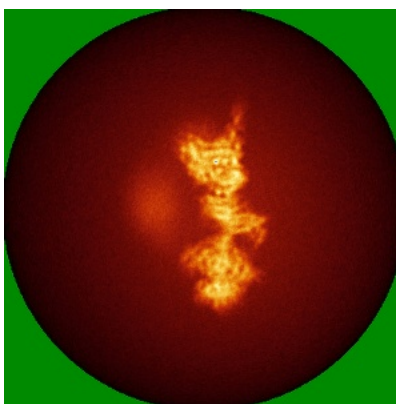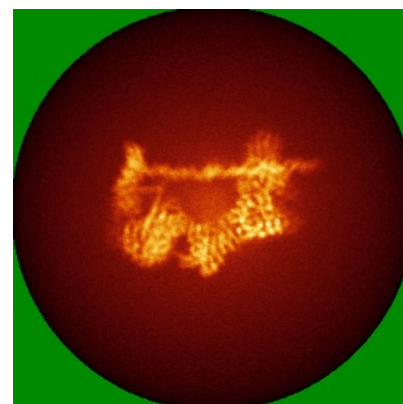
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
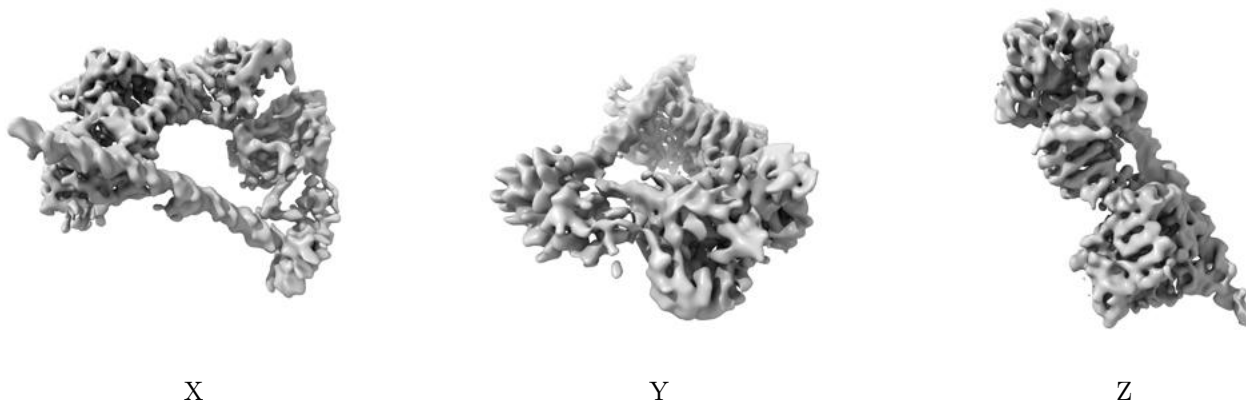
The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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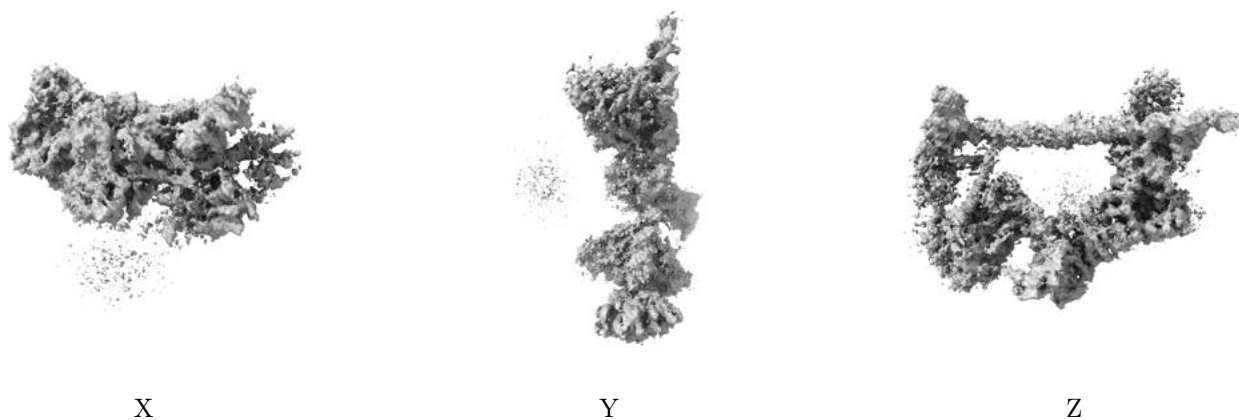
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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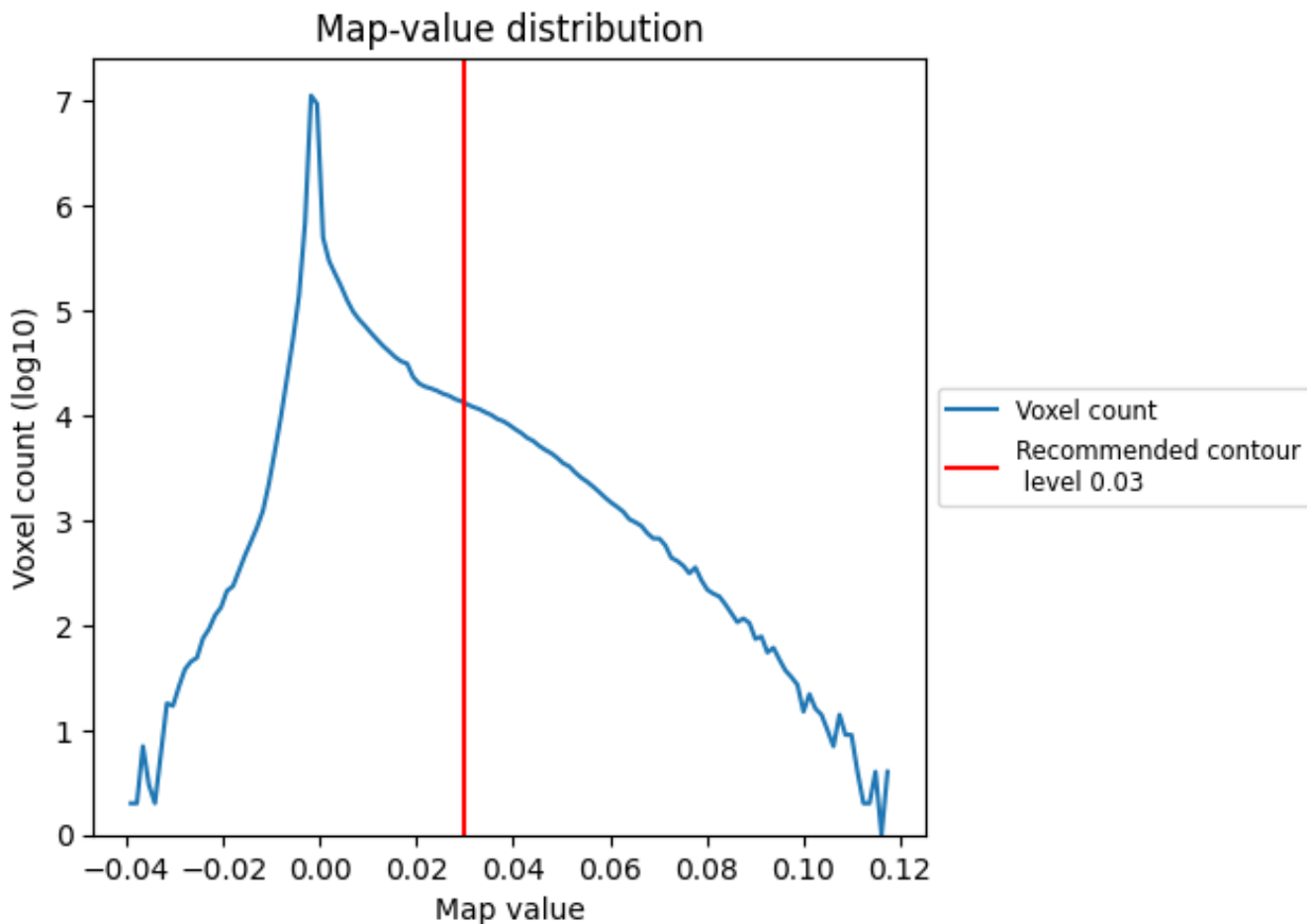
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
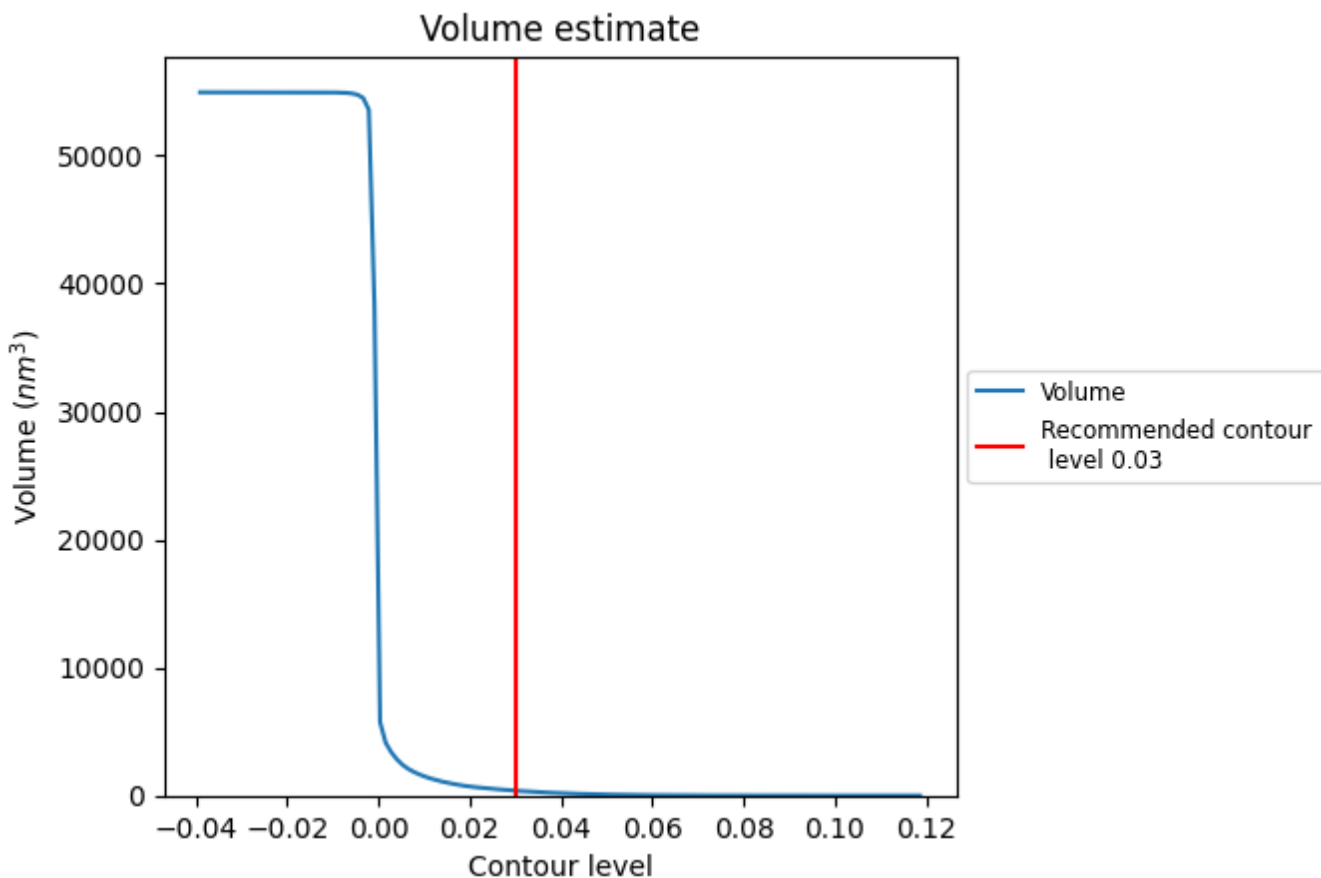
The volume at the recommended contour level is 384 nm^3; this corresponds to an approximate mass of 347 kDa.

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 ⓘ
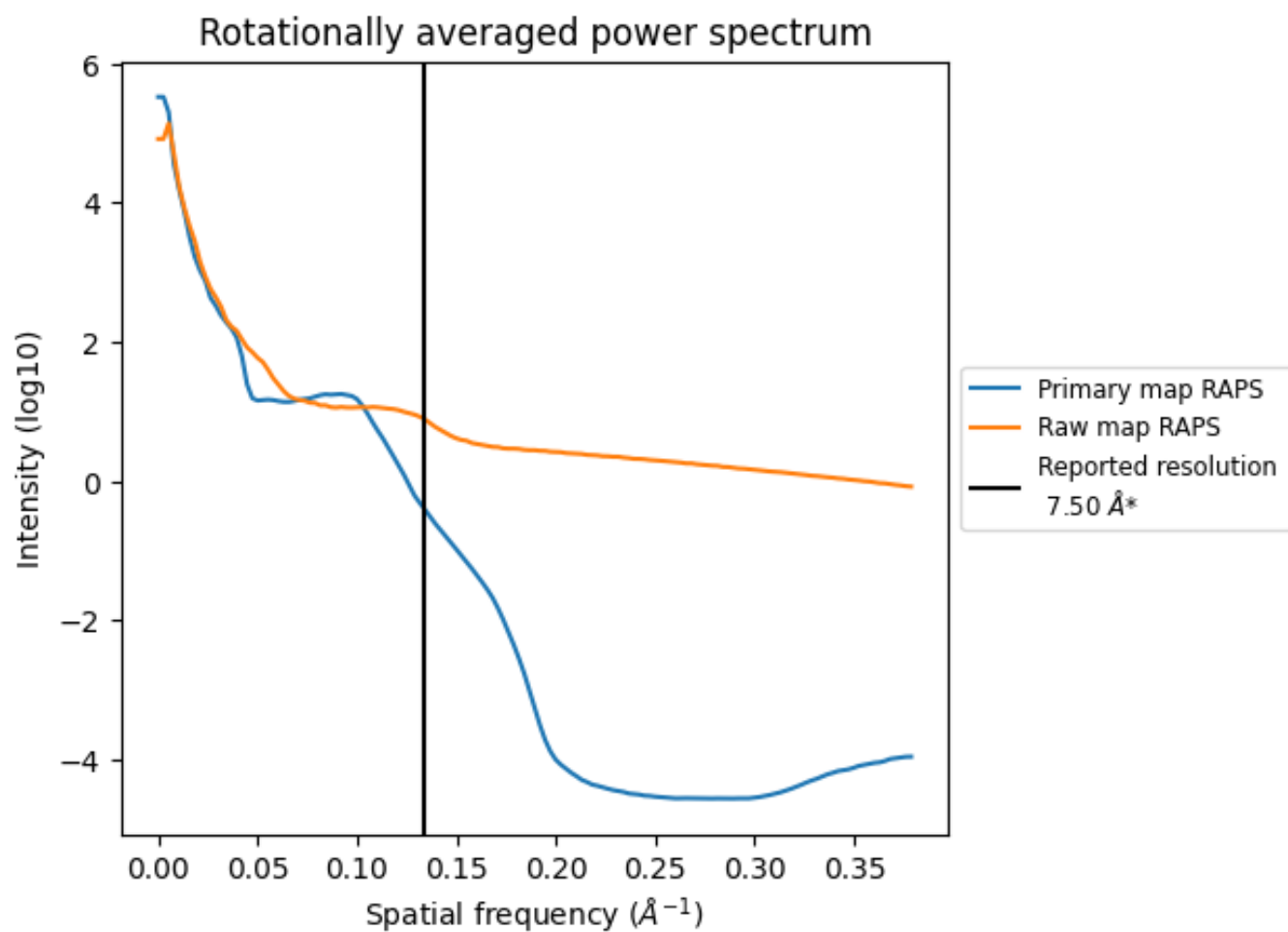
*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

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)
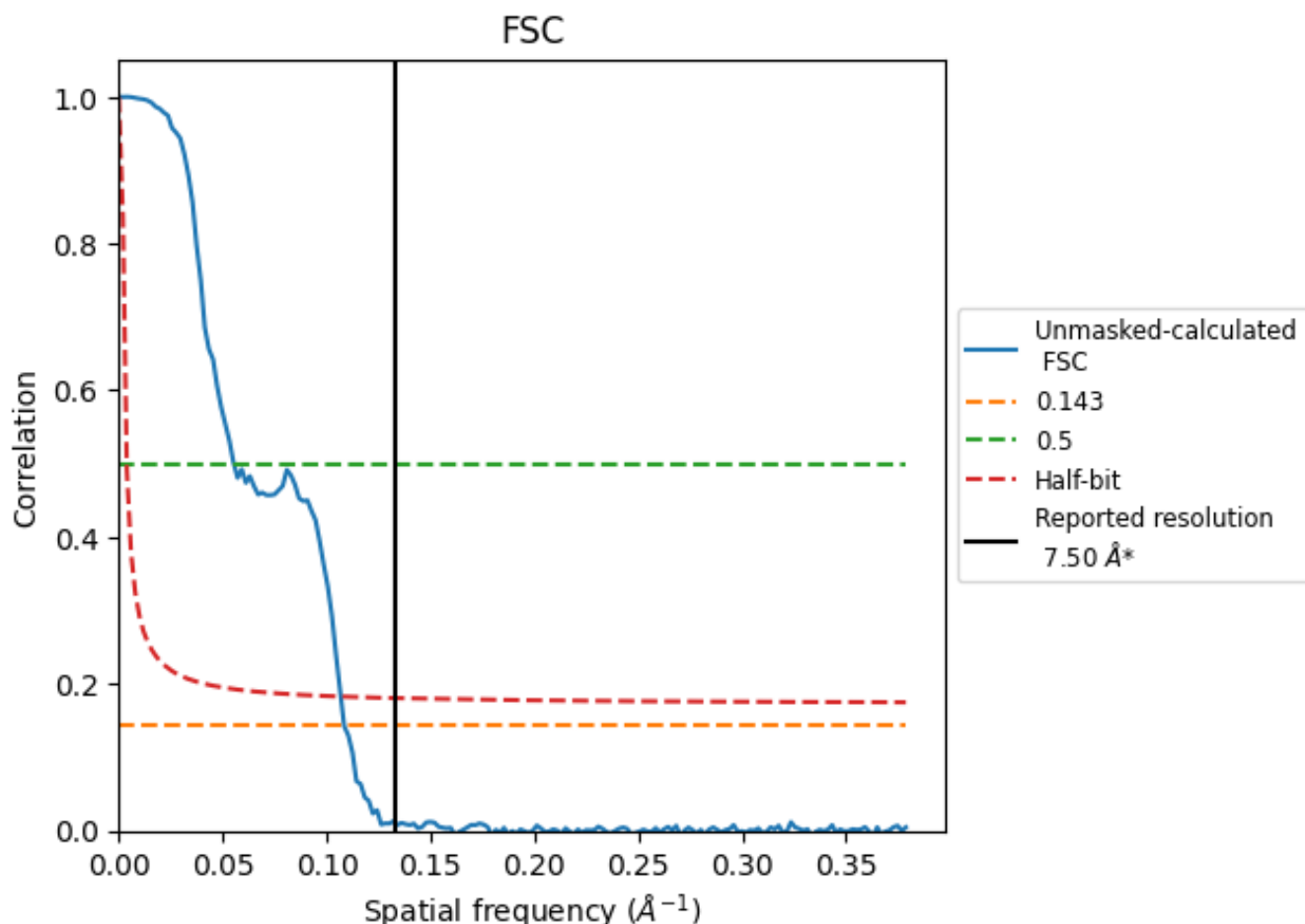
*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.22	18.05	9.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.22 differs from the reported value 7.5 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9306 and PDB model 6MZM. Per-residue inclusion information can be found in section 3 on page 7.

9.1   Map-model overlay ⓘ
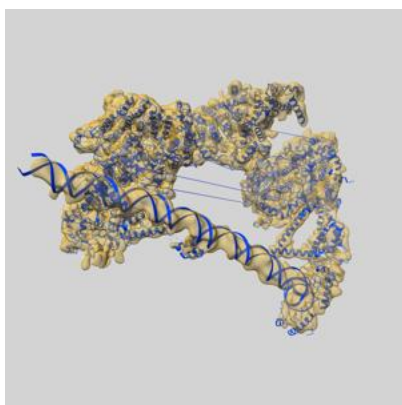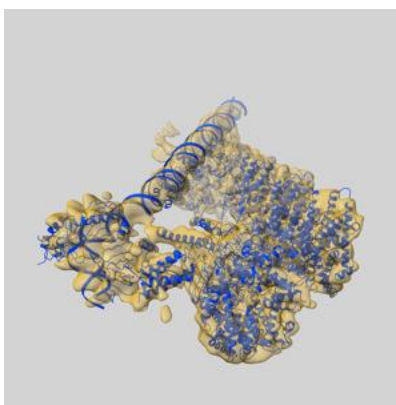
| X | Y | Z |
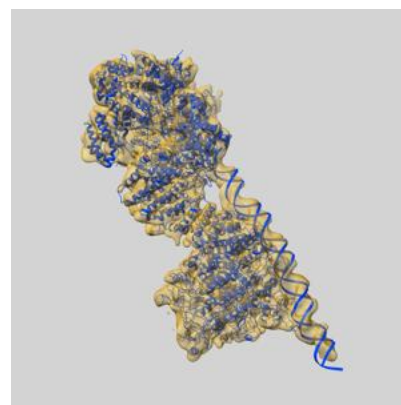
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

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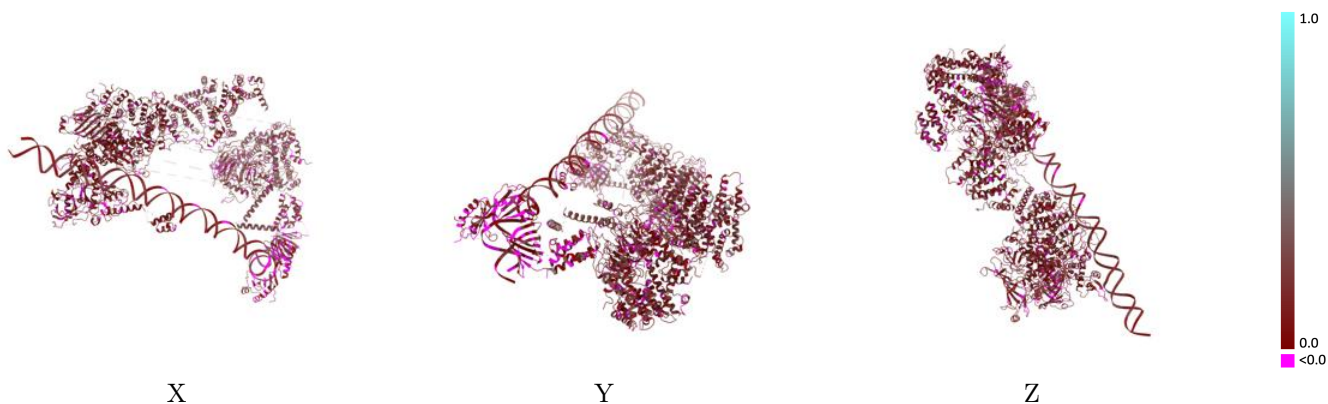
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X　　　　　　　　　Y　　　　　　　　　Z
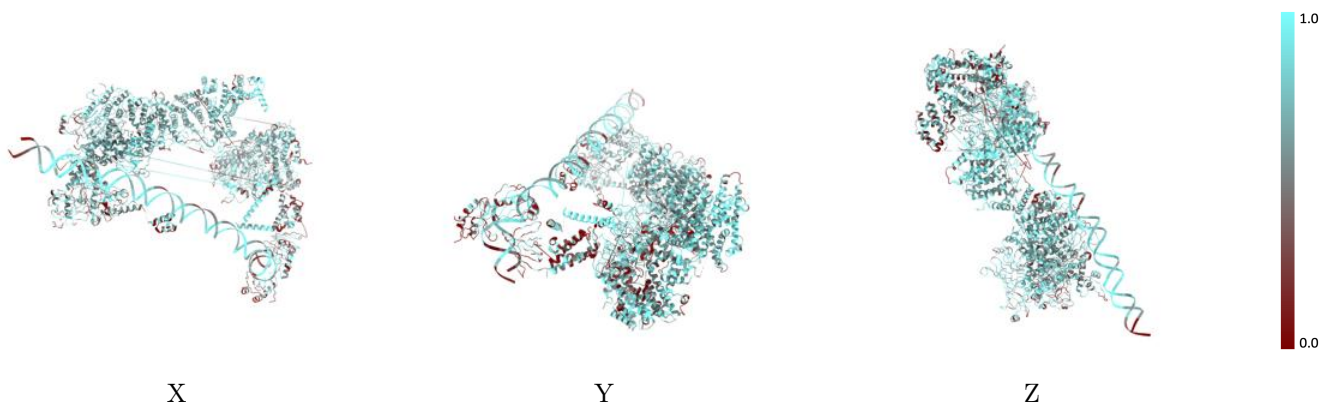
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4   Atom inclusion ⓘ
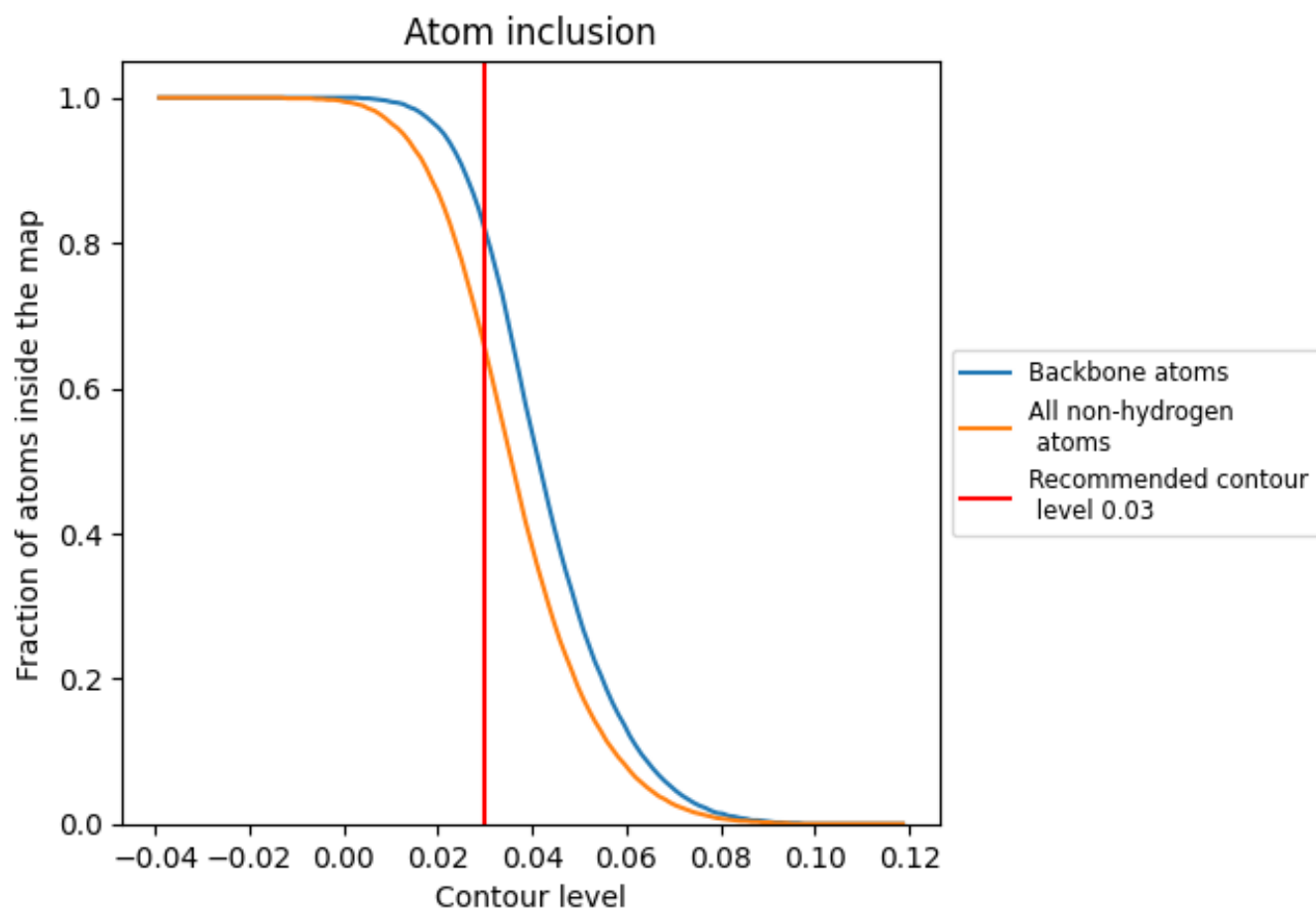
At the recommended contour level, 82% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6540	0.1350
A	0.5890	0.1280
B	0.6840	0.1460
D	0.7430	0.1970
G	0.6550	0.1160
H	0.7130	0.1520
I	0.7050	0.1420
J	0.5950	0.1050
K	0.6580	0.1590
L	0.7170	0.1700
O	0.6510	0.1420
R	0.5760	0.1460
T	0.4820	0.0480
U	0.7070	0.1370
V	0.7070	0.1340
W	0.5140	0.0710
X	0.4370	0.0390
Z	0.7250	0.2280

1.0

0.0
<0.0