W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 09:58 pm GMT

PDB ID	:	6EXV
EMDB ID	:	EMD-3981
Title	:	Structure of mammalian RNA polymerase II elongation complex inhibited by Alpha-amanitin
Authors	:	Liu, X.; Farnung, L.; Wigge, C.; Cramer, P.
Deposited on	:	2017-11-09
Resolution	:	3.60 Å(reported)

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

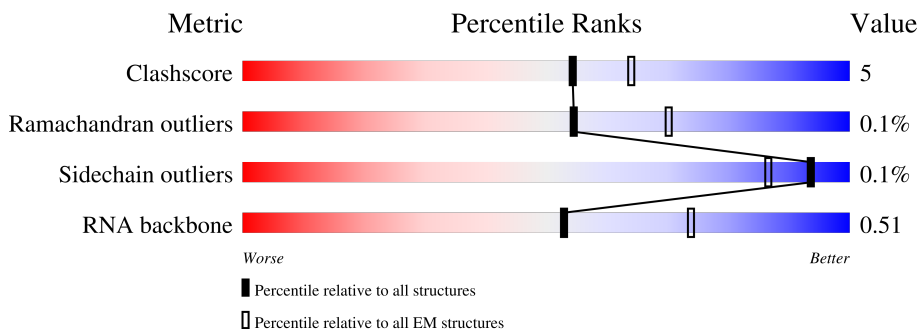|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.60 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		0.1%
Sidechain outliers		0.1%
RNA backbone		0.51

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
RNA backbone	4643	859

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	1970	9% — 61% / 11% / 28%
2	B	1167	13% — 83% / 14% / •
3	C	275	6% — 84% / 9% / 7%
4	D	142	90% — 65% / 25% / 10%
5	E	210	9% — 90% / 9%
6	F	127	14% — 57% / 8% / 35%
7	G	172	87% — 79% / 20% / •

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Mol	Chain	Length	Quality of chain
8	H	150	14% 87% 11%
9	I	125	32% 78% 14% 9%
10	J	67	84% 16%
11	K	117	6% 84% 15%
12	L	58	10% 55% 21% 24%
13	M	8	38% 25% 38%
14	N	43	33% 53% 5% 42%
15	P	20	25% 50% 10% 10% 30%
16	T	43	44% 81% 16%

2   Entry composition ⓘ

There are 18 unique types of molecules in this entry. The entry contains 32717 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1428	Total 11317	C 7120	N 2025	O 2100	S 72	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	526	VAL	-	insertion	UNP I3LJR4
A	527	THR	-	insertion	UNP I3LJR4
A	528	PRO	-	insertion	UNP I3LJR4
A	529	GLN	-	insertion	UNP I3LJR4
A	1299	GLN	-	insertion	UNP I3LJR4
A	1300	GLY	-	insertion	UNP I3LJR4
A	1301	ILE	-	insertion	UNP I3LJR4
A	1302	GLU	-	insertion	UNP I3LJR4
A	1303	GLN	-	insertion	UNP I3LJR4
A	1304	ILE	-	insertion	UNP I3LJR4
A	1305	SER	-	insertion	UNP I3LJR4
A	1308	TYR	SER	conflict	UNP I3LJR4
A	1309	MET	ARG	conflict	UNP I3LJR4
A	1310	HIS	SER	conflict	UNP I3LJR4
A	1313	GLN	ALA	conflict	UNP I3LJR4

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1134	Total 9062	C 5732	N 1595	O 1671	S 64	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total 2059	C 1294	N 351	O 408	S 6	0	0

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

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

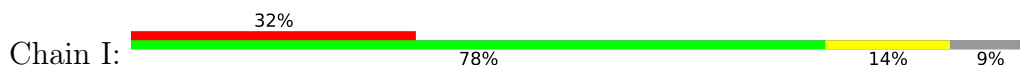- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a protein called AMATOXIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	8	Total	C	N	O	S	0	0
			64	39	10	14	1		

- Molecule 14 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	25	Total	C	N	O	P	0	0
			516	247	95	149	25		

- Molecule 15 is a RNA chain called RNA (5'-R(P*CP*AP*UP*AP*AP*AP*GP*AP*CP*C P*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	14	Total	C	N	O	P	0	0
			301	135	59	93	14		

- Molecule 16 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	36	Total	C	N	O	P	0	0
			735	352	131	216	36		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
17	B	1	Total 1	Zn 1	0
17	C	1	Total 1	Zn 1	0
17	I	2	Total 2	Zn 2	0
17	J	1	Total 1	Zn 1	0
17	L	1	Total 1	Zn 1	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total 1	Mg 1	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: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1
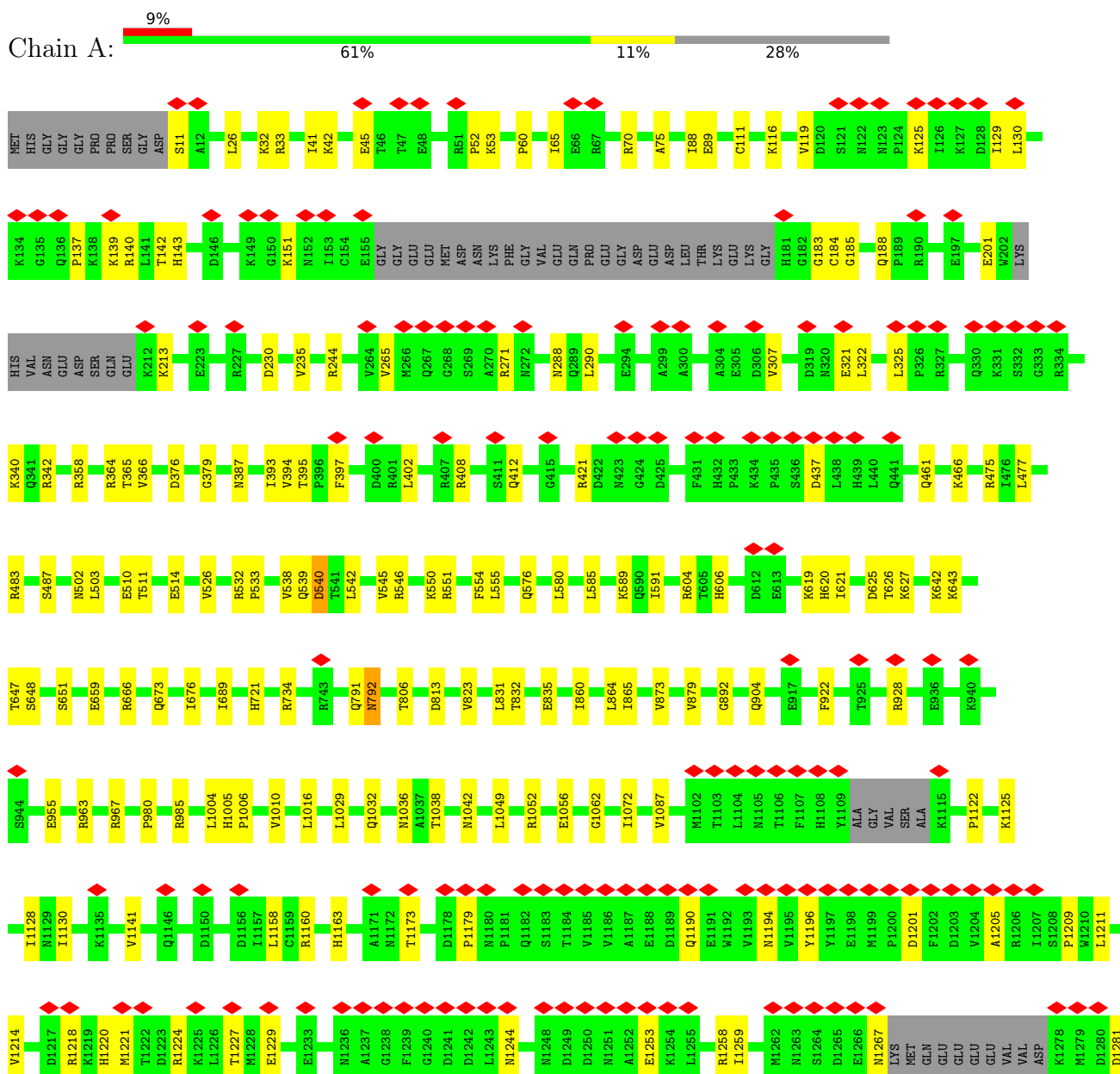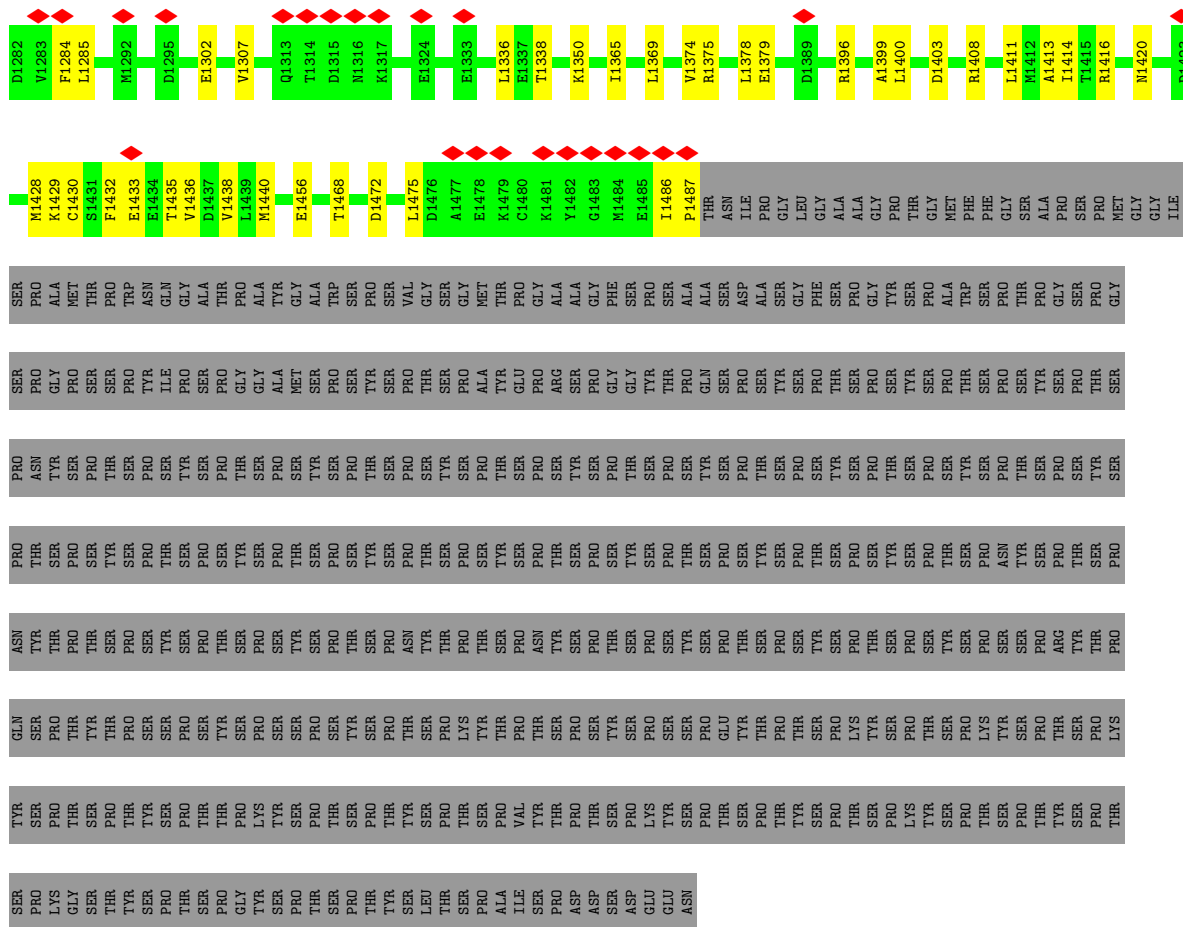
● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2
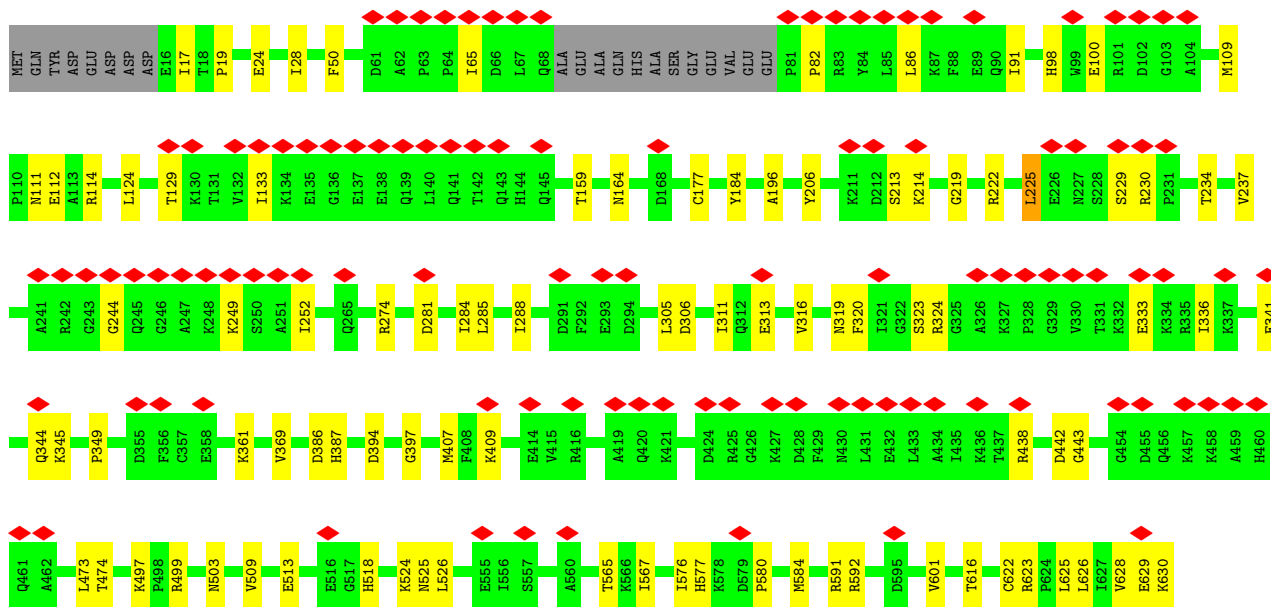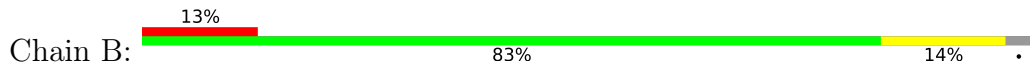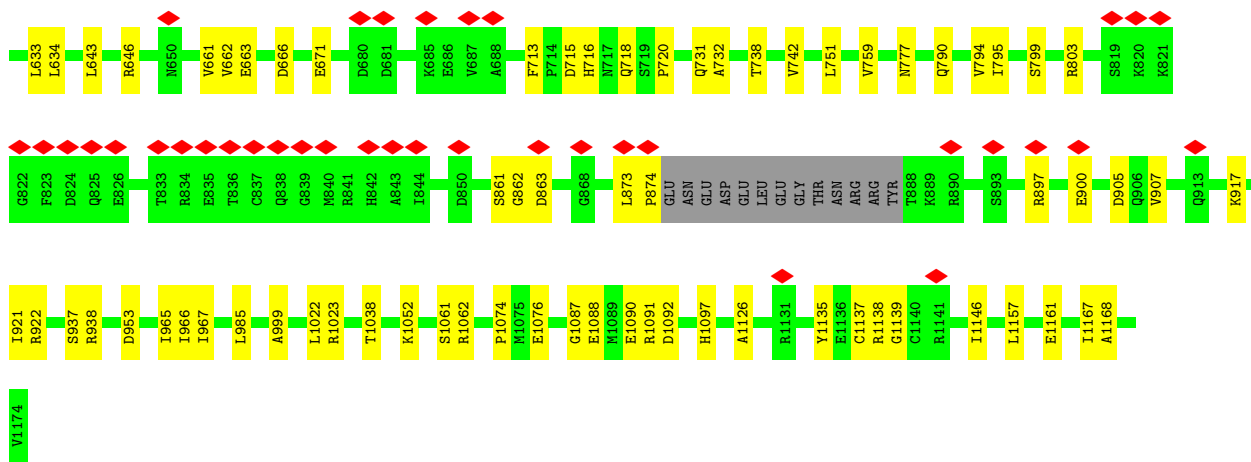
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:

6%
84% 9% 7%
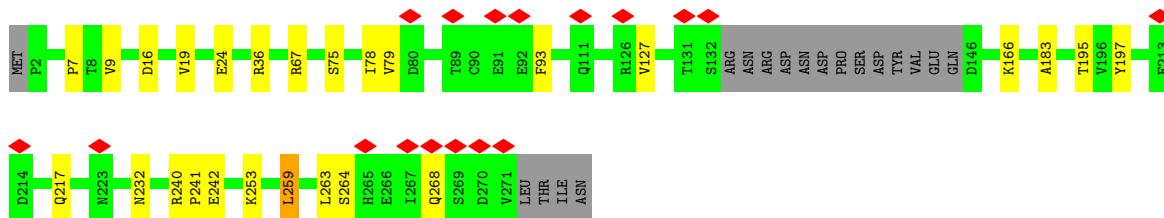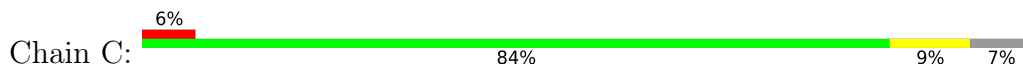
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain D:

90%
65% 25% 10%
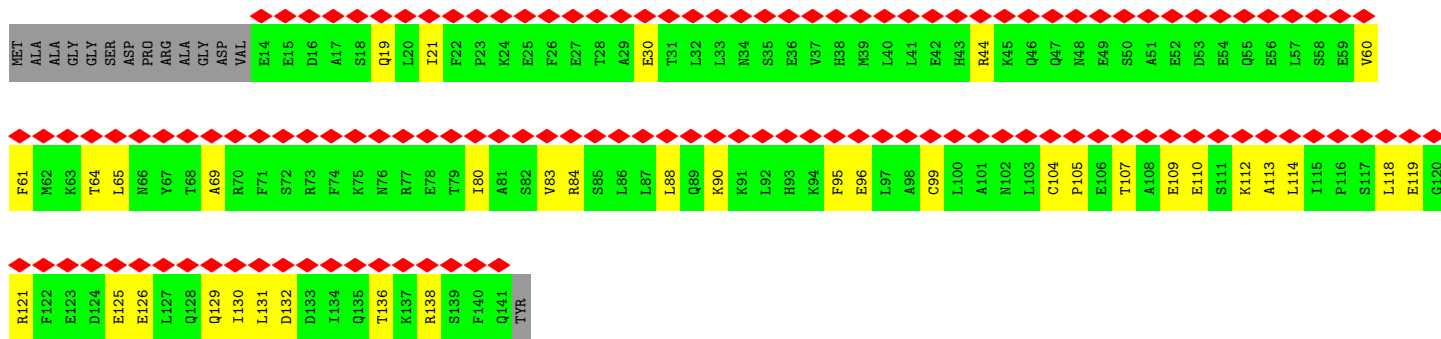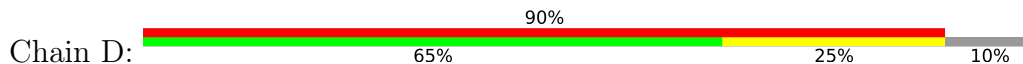
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E:

9%
90% 9%
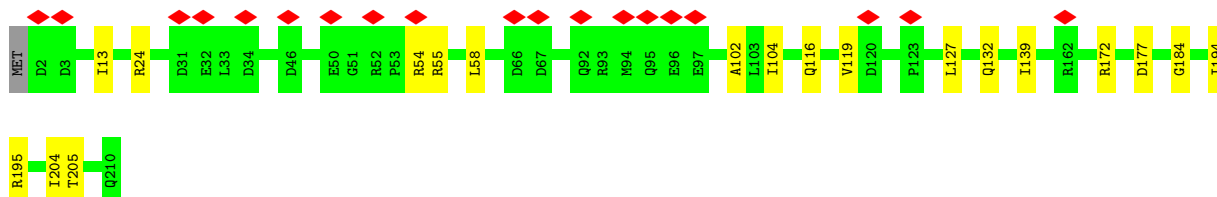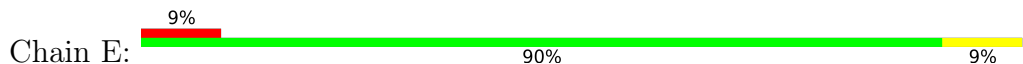
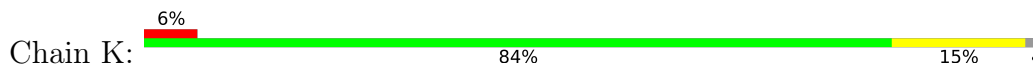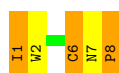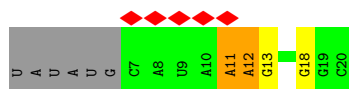• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain F:

14%
57%   8%   35%

MET SER ASP ASN GLU ASP ASN PHE ASP GLY ASP ASP PHE ASP ASP VAL GLU GLU ASP GLU GLY LEU ASP ASP LEU GLU ASN ALA GLU GLU GLY GLN GLU ASN VAL GLU ILE LEU PRO SER GLY GLU ARG PRO Q46 A47 N48 Q49 K50 R51 I52 E61 R64 L71 A74

M75 C76 A77 P78 V79 M80 V81 E82 L83 E84 G85 E86 K98 A99 R100 R108 S114 Y115 I125 S126 D127

• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:

87%
79%   20%   •

M1 F2 Y3 H4 I5 S6 L7 E8 H9 E10 I11 L12 G19 P20 N21 L22 L23 N24 K27 Q28 K29 L30 F31 T32 E33 V34 E35 G36 T37 C38 T39 G40 K41 Y42 G43 F44 V45 I46 A47 V48 T49 T50 I51 D52 N53 I54 G55 A56 I59 Q60 P61 G62 R63 G64 F65 V66 L67

K71 Y72 K73 A74 I75 V76 F77 R78 P79 F80 K81 G82 E83 V84 V85 D86 A87 V88 V89 T90 Q91 V92 N93 K94 V95 G96 L97 F98 T99 E100 I101 G102 P103 M104 S105 C106 F107 I108 S109 R110 H111 S112 I113 P114 S115 E116 M117 E118 F119 D120 P121 N122 S123 N124 P125 P126 C127 Y128 K129

T130 M131 D132 E133 D134 I135 V136 I137 Q138 Q139 D140 D141 E142 I143 R144 L145 K146 I147 V148 G149 T150 R151 V152 D153 K154 N155 D156 I157 F158 A159 I160 G161 S162 L163 M164 D165 D166 Y167 L168 G169 L170 V171 SER

• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

Chain H:

14%
87%   11%   ••

MET A2 D16 G19 K20 R27 C30 E31 S32 E33 S34 M37 D38 L39 I45 Q46 I47 D51 E66 D67 G68 T69 L70 D71 D72 G73 E74 D79 D80 R81 R84 R98 D102 E103 T104 S105 T106 E107 A108 Y115 R124 D128 N131 L132

H133 Y142 A149 PHE
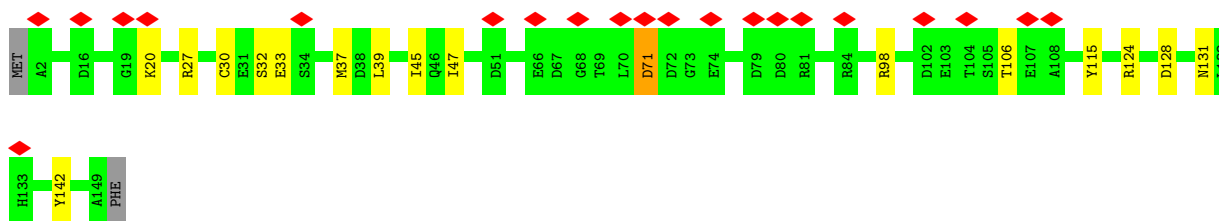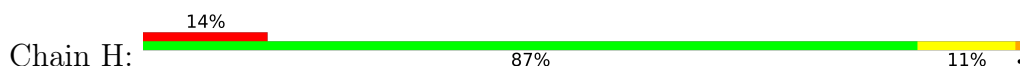
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:

32%
78%   14%   9%

MET GLU PRO ASP GLY THR TYR GLU PRO GLY PHE V12 G13 I14 R15 Q18 E19 M23 L24 Y25 E28 D29 K30 E31 N32 R33 I34 L35 L36 Y37 D43 Y44 Q45 Q46 E47 A48 D49 N50 I58 T59 H60 E61 V62 D63 E64 I68 I69 A70 D71 R80 T81 E82 D83

C86 Q87 K92 E93 F96 S99 H100 S101 A102 R103 A104 E105 D106 A107 M108 R109 L110 H118 R122 E125
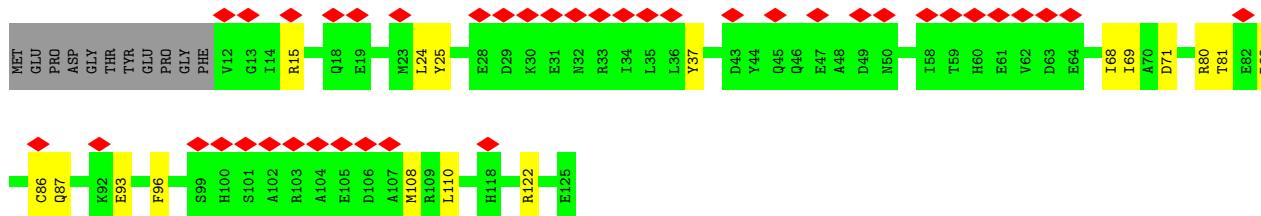
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

84%   16%

M1 I2 F8 V14 L40 R46 R47 M48 L49 L50 L55 L65 E66 K67
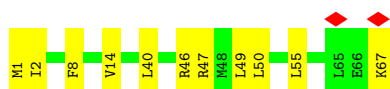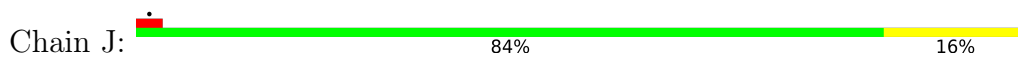
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

Chain K:

6%   84%   15%

M1 N2 A3 P4 P5 A6 F7 E8 S9 F10 L11 L12 F13 E14 G15 E16 I35 E38 D39 H40 T41 L42 Y61 I71 I72 D80 E97 E102 F105 R106 I109 G115 ILE GLU
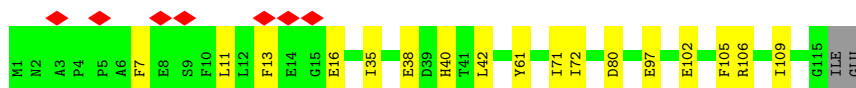
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

Chain L:

10%   55%   21%   24%

MET ASP THR GLN LYS ASP VAL GLN PRO PRO LYS GLN GLN PRO M15 I16 Y17 I18 C19 G20 H23 T24 E25 I28 K29 S30 R31 I34 R35 C36 R37 E38 M44 K47 R58

• Molecule 13: AMATOXIN

Chain M:

38%   25%   38%

I1 W2 C6 N7 P8

• Molecule 14: DNA (25-MER)

Chain N:

33%   53%   5%   42%

DG DG DC DA DG DT A7 C8 T9 A10 G11 T12 A13 DT DC DT DA DG DT DA DT DT DG A25 T32 T33 G34 A35 G36 A41 T42 DC
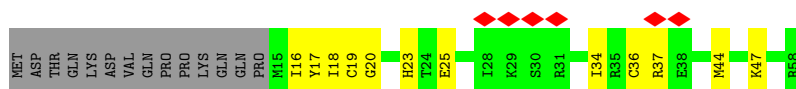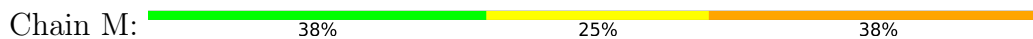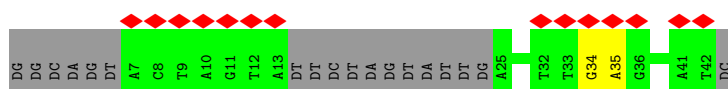
• Molecule 15: RNA (5'-R(P*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3')

Chain P:

25%   50%   10%   10%   30%

U A U A U G C7 A8 U9 A10 A11 A12 G13 G18 G19 C20

• Molecule 16: DNA (36-MER)

Chain T:

44%   81%   16%
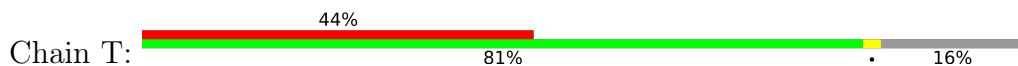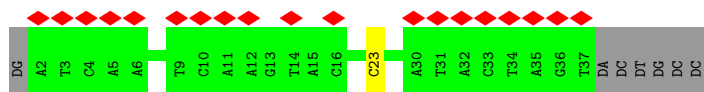
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134512	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 $(e^-/\text{Å}^2)$	35	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.309	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0577	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, HYP, CSX, ILX, TRX

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	0.40	0/11525	0.65	6/15559 (0.0%)
2	B	0.41	0/9243	0.63	6/12475 (0.0%)
3	C	0.44	0/2102	0.62	1/2857 (0.0%)
4	D	0.26	0/1019	0.52	0/1374
5	E	0.36	0/1751	0.59	0/2366
6	F	0.39	0/667	0.61	0/901
7	G	0.28	0/1365	0.61	0/1853
8	H	0.42	0/1207	0.65	0/1628
9	I	0.33	0/948	0.56	0/1284
10	J	0.53	0/542	0.70	0/730
11	K	0.41	0/939	0.67	1/1271 (0.1%)
12	L	0.36	0/377	0.58	0/500
13	M	0.44	0/22	1.00	0/26
14	N	0.59	0/578	1.01	0/888
15	P	0.58	0/337	0.92	1/523 (0.2%)
16	T	0.70	0/823	0.98	1/1267 (0.1%)
All	All	0.41	0/33445	0.66	16/45502 (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
5	E	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	80	ASP	CB-CG-OD1	8.88	126.29	118.30
1	A	503	LEU	CA-CB-CG	7.51	132.57	115.30
16	T	23	DC	O4'-C4'-C3'	-7.33	101.57	104.50
1	A	813	ASP	CB-CG-OD1	6.23	123.91	118.30
2	B	225	LEU	CA-CB-CG	5.76	128.55	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
5	E	54	ARG	Peptide

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	11317	0	11439	144	0
2	B	9062	0	9109	108	0
3	C	2059	0	2009	22	0
4	D	1005	0	964	24	0
5	E	1720	0	1737	12	0
6	F	657	0	684	7	0
7	G	1334	0	1333	23	0
8	H	1186	0	1147	14	0
9	I	927	0	862	13	0
10	J	533	0	555	8	0
11	K	920	0	942	12	0
12	L	372	0	378	7	0
13	M	64	0	51	3	0
14	N	516	0	285	2	0
15	P	301	0	153	1	0
16	T	735	0	408	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32717	0	32056	346	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 346 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:792:ASN:N	1:A:792:ASN:HD22	1.62	0.96
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.02	0.92
4:D:84:ARG:O	4:D:88:LEU:HB2	1.74	0.87
7:G:99:THR:O	7:G:106:CYS:HB3	1.74	0.86
4:D:104:CYS:SG	4:D:138:ARG:NH1	2.47	0.86

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	1418/1970 (72%)	1287 (91%)	129 (9%)	2 (0%)	51	83
2	B	1128/1167 (97%)	1027 (91%)	101 (9%)	0	100	100
3	C	253/275 (92%)	227 (90%)	26 (10%)	0	100	100
4	D	126/142 (89%)	114 (90%)	12 (10%)	0	100	100
5	E	207/210 (99%)	194 (94%)	13 (6%)	0	100	100
6	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100
7	G	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
8	H	146/150 (97%)	136 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	112/125 (90%)	93 (83%)	19 (17%)	0	100	100
10	J	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
11	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
12	L	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
13	M	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
All	All	3863/4588 (84%)	3518 (91%)	343 (9%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	539	GLN
1	A	540	ASP

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	1258/1749 (72%)	1257 (100%)	1 (0%)	93	98
2	B	993/1021 (97%)	993 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	106/126 (84%)	105 (99%)	1 (1%)	78	90
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	147/153 (96%)	147 (100%)	0	100	100
8	H	129/131 (98%)	128 (99%)	1 (1%)	81	91
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3435/4066 (84%)	3432 (100%)	3 (0%)	93 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	792	ASN
4	D	126	GLU
8	H	71	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	639	HIS
9	I	22	ASN
2	B	790	GLN
9	I	45	GLN
3	C	66	HIS

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	13/20 (65%)	3 (23%)	1 (7%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	11	A
15	P	13	G
15	P	18	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	12	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
13	CSX	M	6	13	3,6,7	1.00	0	1,6,8	2.24	1 (100%)
13	HYP	M	8	13	6,8,9	0.76	0	5,10,12	2.19	2 (40%)
13	TRX	M	2	13	14,16,17	1.01	0	15,22,24	1.99	4 (26%)
13	ILX	M	1	13	8,9,10	0.61	0	9,11,13	1.32	2 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CSX	M	6	13	-	1/1/5/7	-
13	HYP	M	8	13	-	0/0/11/13	0/1/1/1
13	TRX	M	2	13	-	0/4/6/8	0/2/2/2
13	ILX	M	1	13	-	7/11/12/14	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	2	TRX	CG-CB-CA	5.73	123.38	114.53
13	M	8	HYP	O-C-CA	-3.29	116.16	124.78
13	M	8	HYP	CB-CG-CD	3.12	107.08	103.27
13	M	2	TRX	CB-CG-CD1	-2.98	124.28	127.97
13	M	1	ILX	OD1-CD1-CG1	-2.90	104.75	111.07

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	1	ILX	C-CA-CB-CG2
13	M	1	ILX	OD1-CD1-CG1-CB

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Mol	Chain	Res	Type	Atoms
13	M	1	ILX	OD1-CD1-CG1-OG1
13	M	6	CSX	N-CA-CB-SG
13	M	1	ILX	C-CA-CB-CG1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	6	CSX	1	0
13	M	8	HYP	1	0
13	M	1	ILX	1	0

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3981. 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 ⓘ
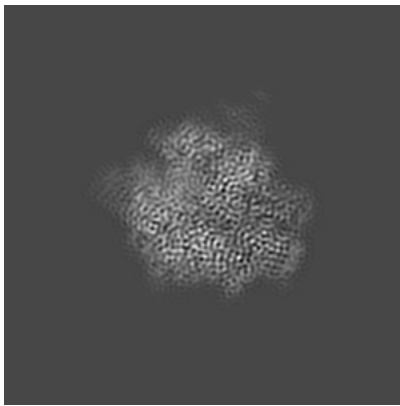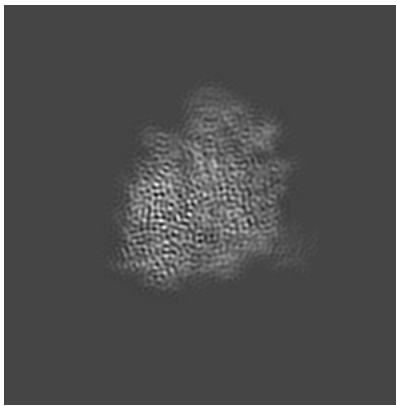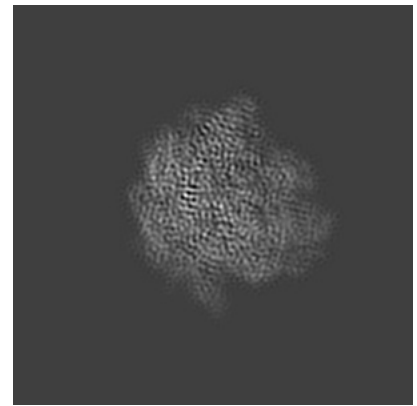
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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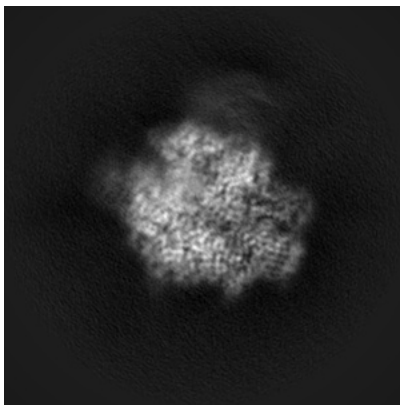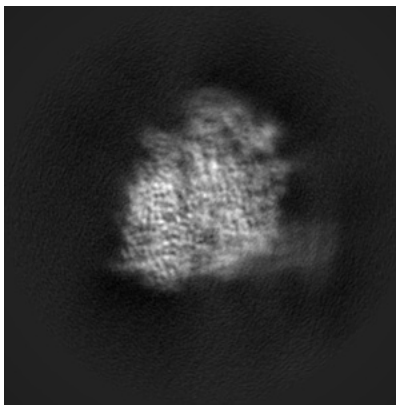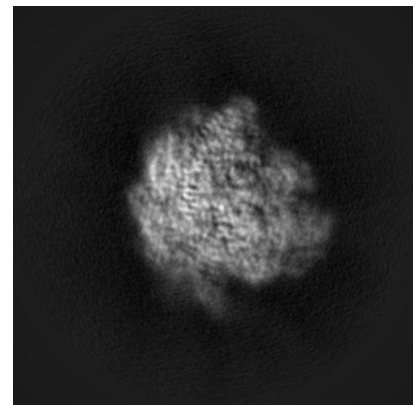
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
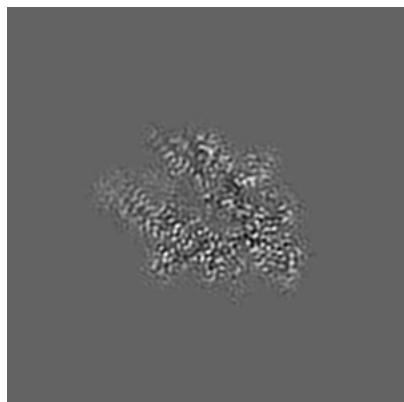
6.2.1   Primary map
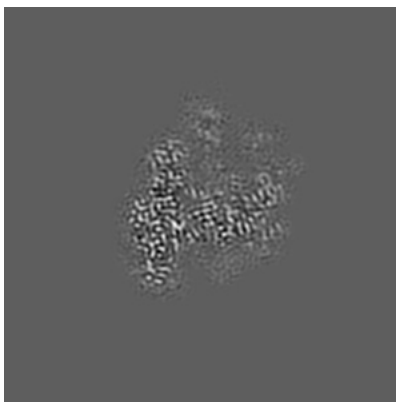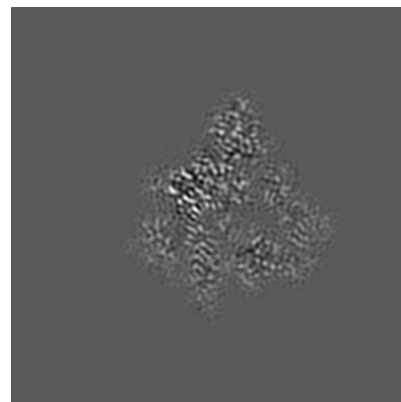
| X Index: 128 | Y Index: 128 | Z Index: 128 |

6.2.2   Raw map
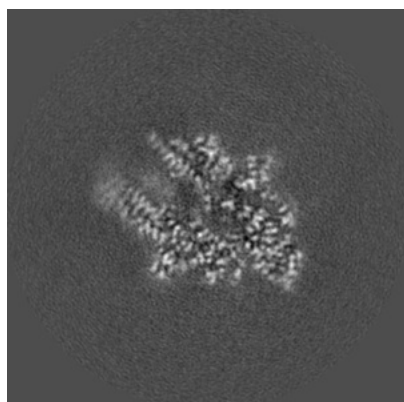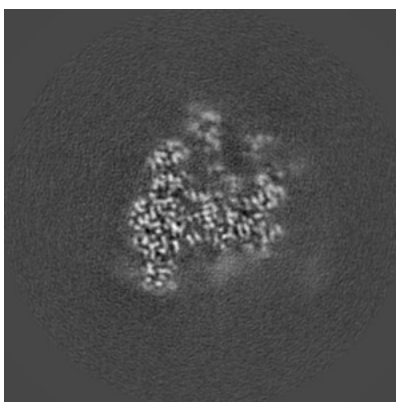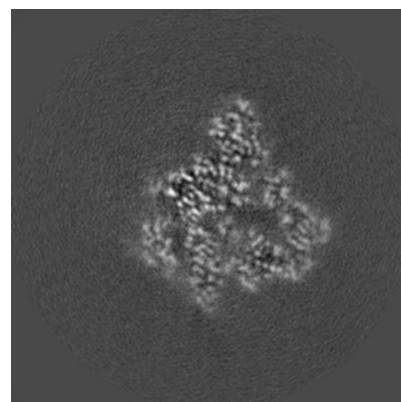
| X Index: 128 | Y Index: 128 | Z Index: 128 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
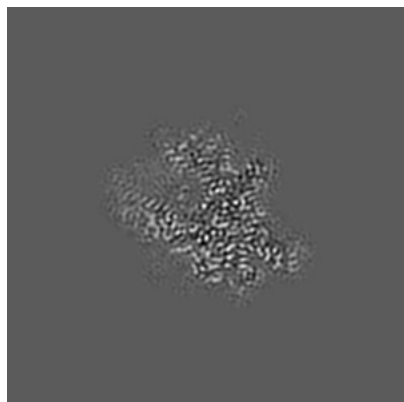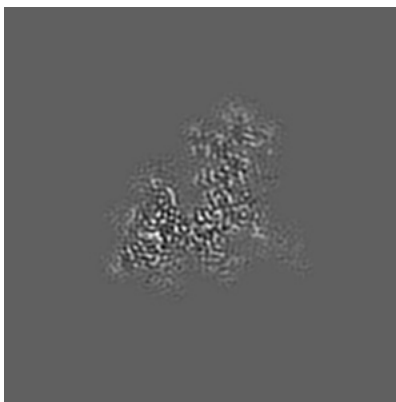
| X Index: 118 | Y Index: 142 | Z Index: 101 |
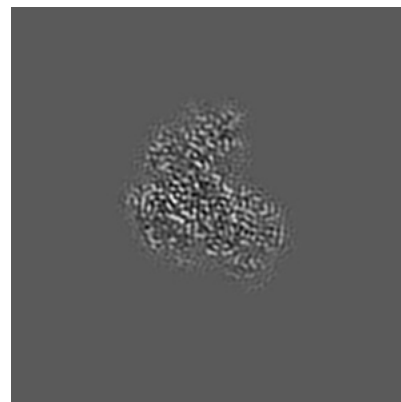
6.3.2 Raw map
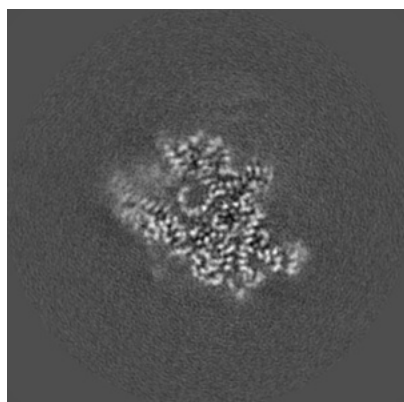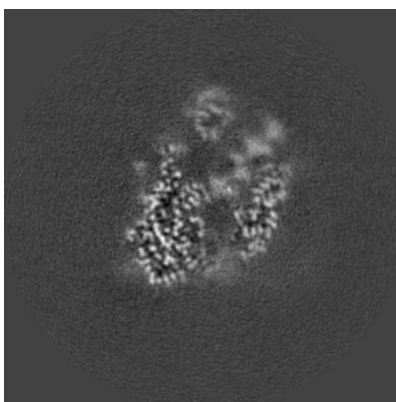
| X Index: 118 | Y Index: 119 | Z Index: 99 |
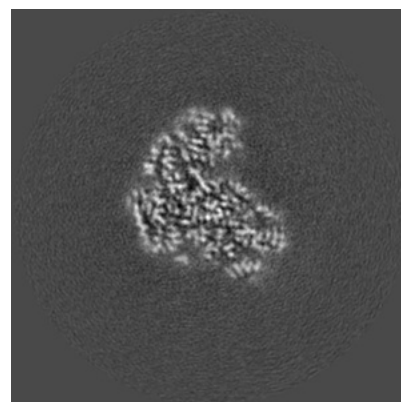
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.0577. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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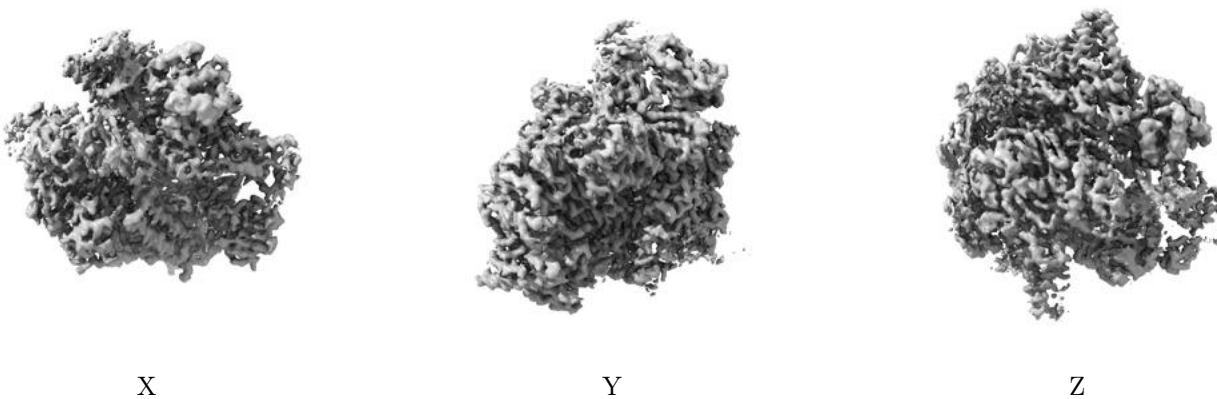
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5   Mask visualisation ⓘ

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

6.5.1   emd_3981_msk_1.map ⓘ

X   Y   Z
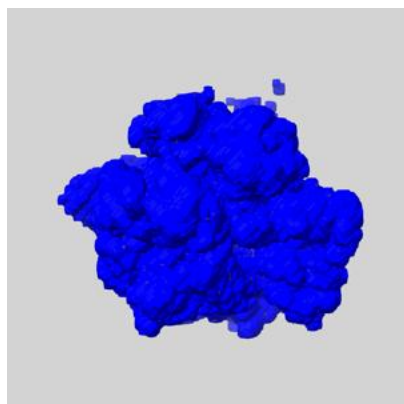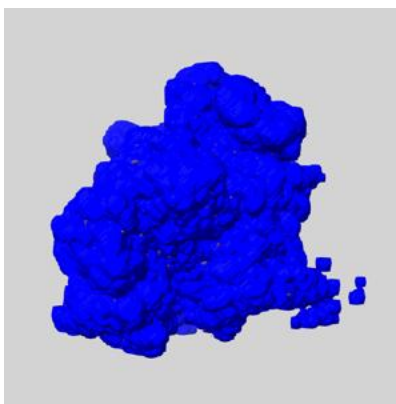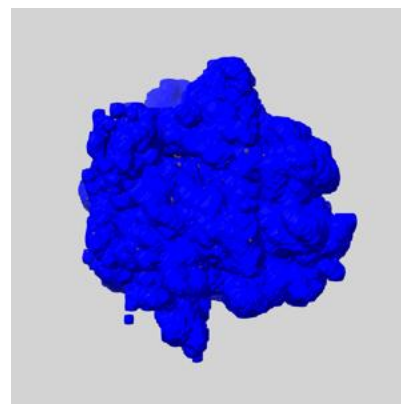
7 Map analysis ⓘ

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 ⓘ
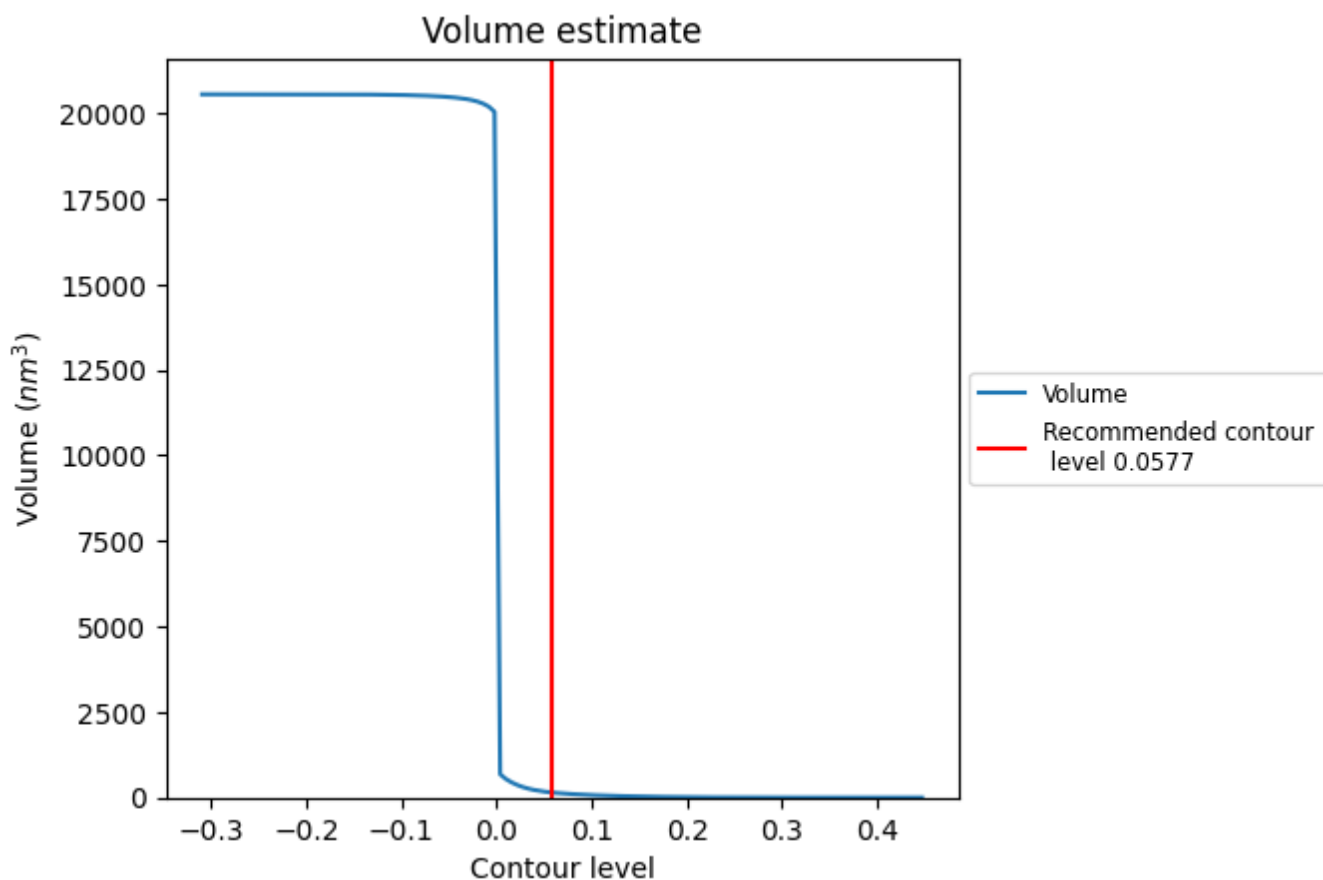
The volume at the recommended contour level is 149 nm^3; this corresponds to an approximate mass of 134 kDa.

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 ⓘ
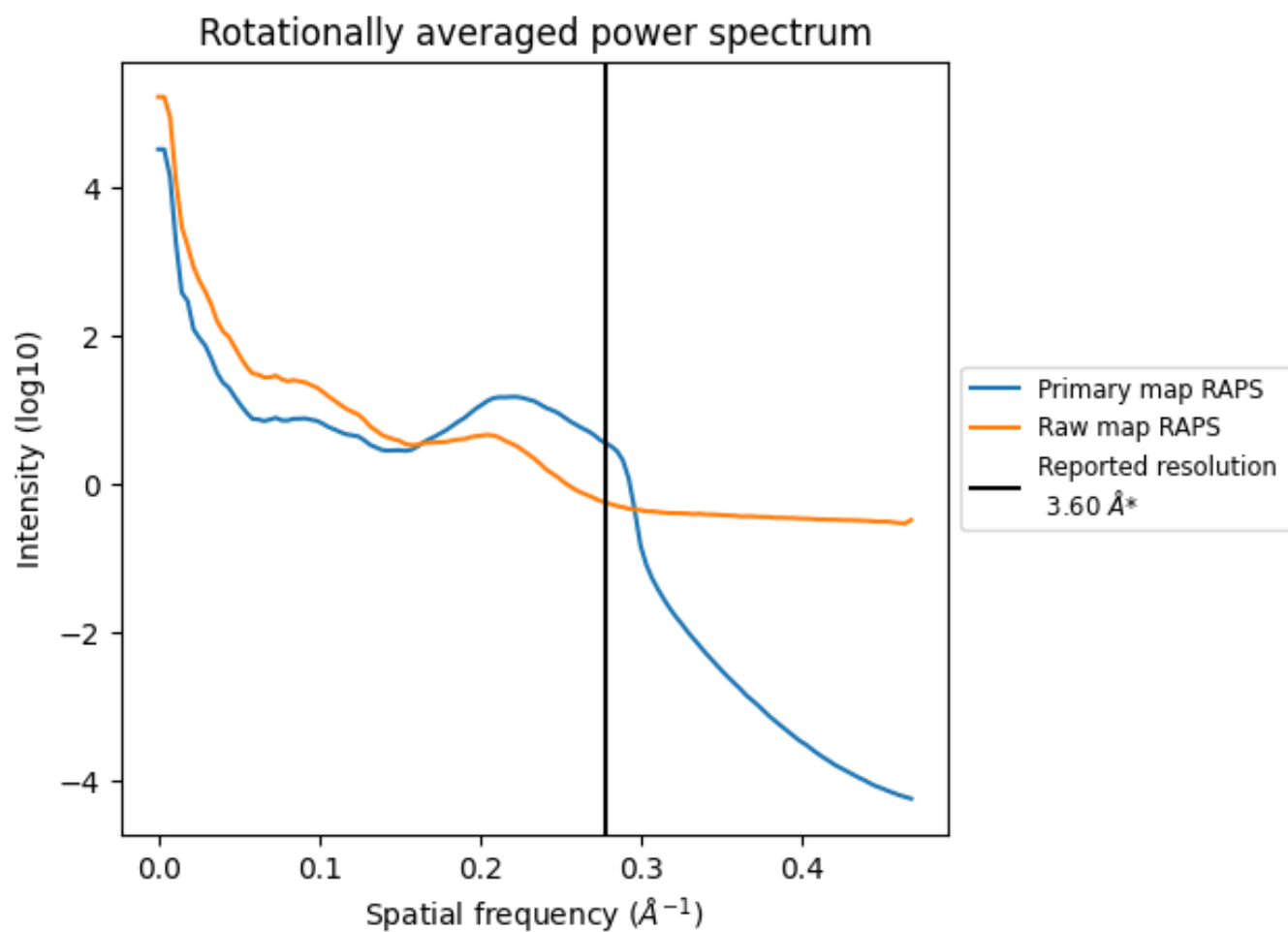
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
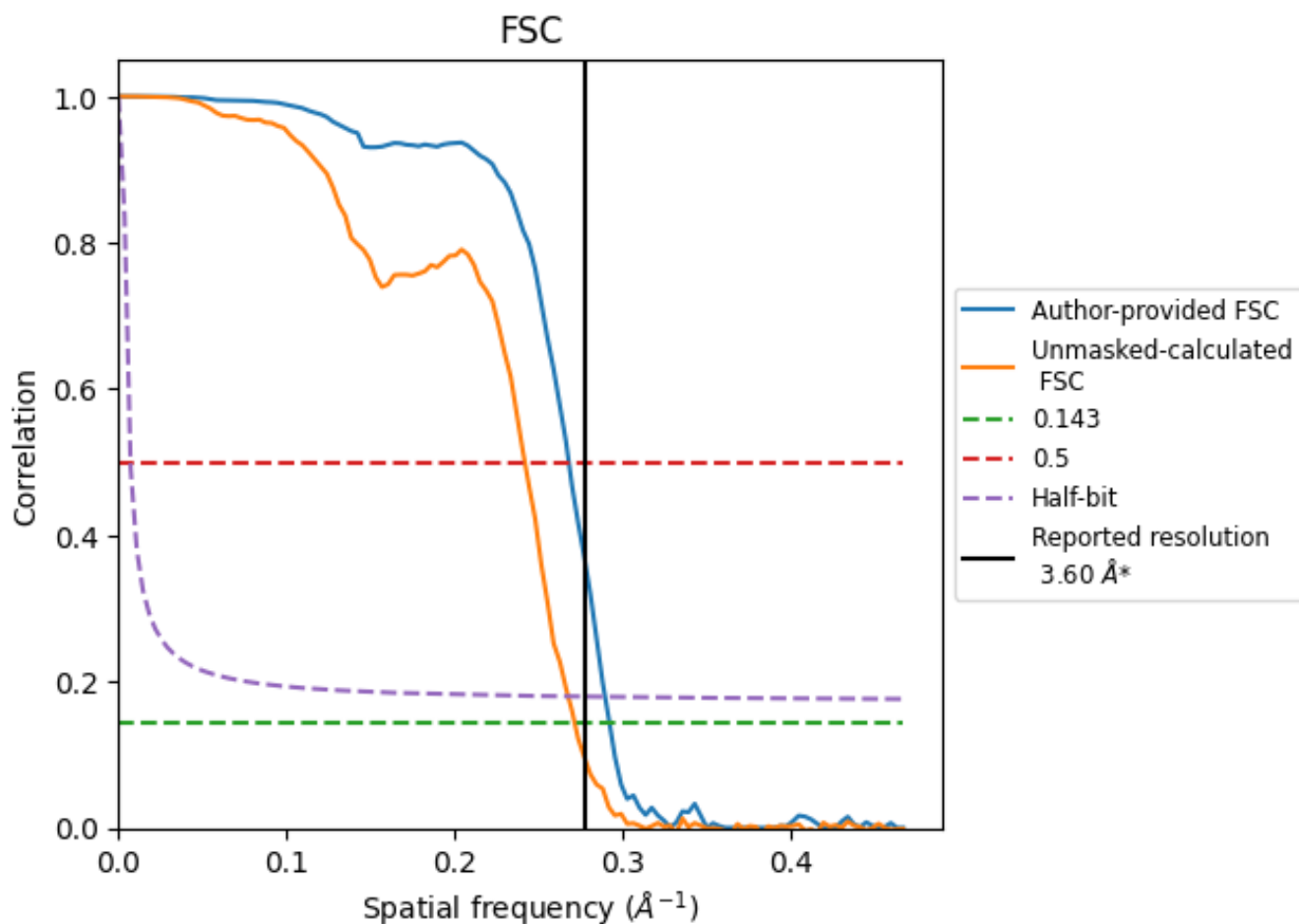
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.42	3.73	3.45
Unmasked-calculated*	3.68	4.13	3.73

*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-3981 and PDB model 6EXV. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)
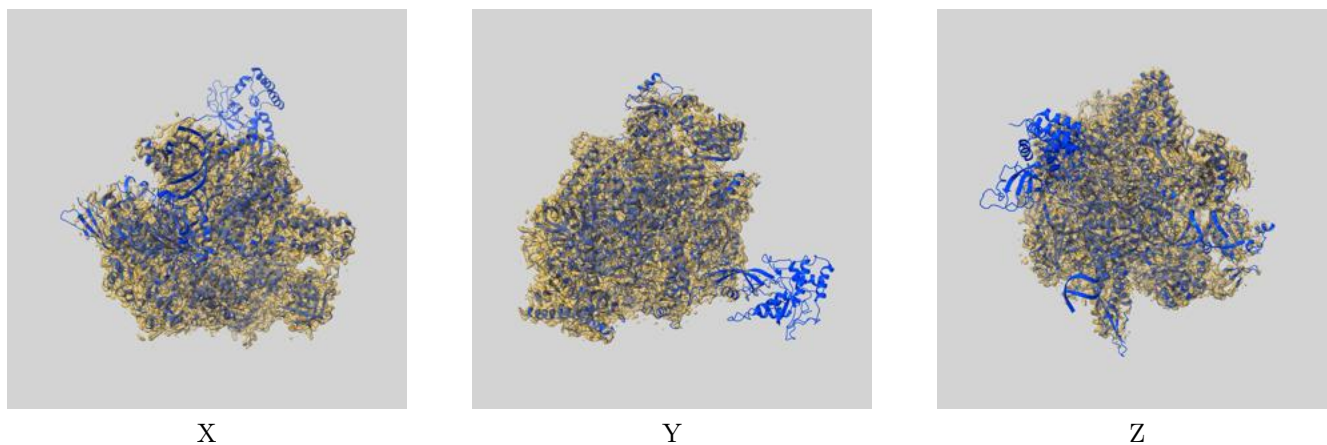
X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0577 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
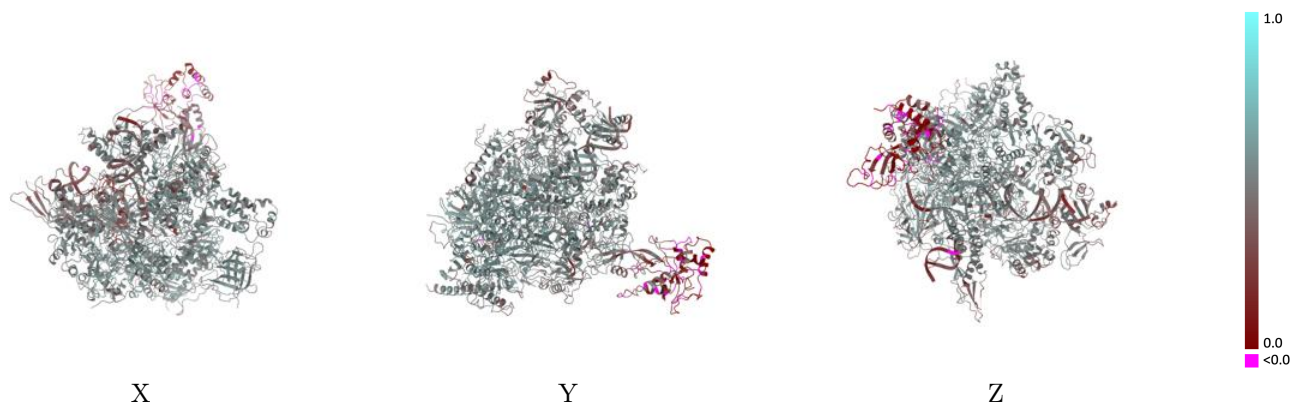
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
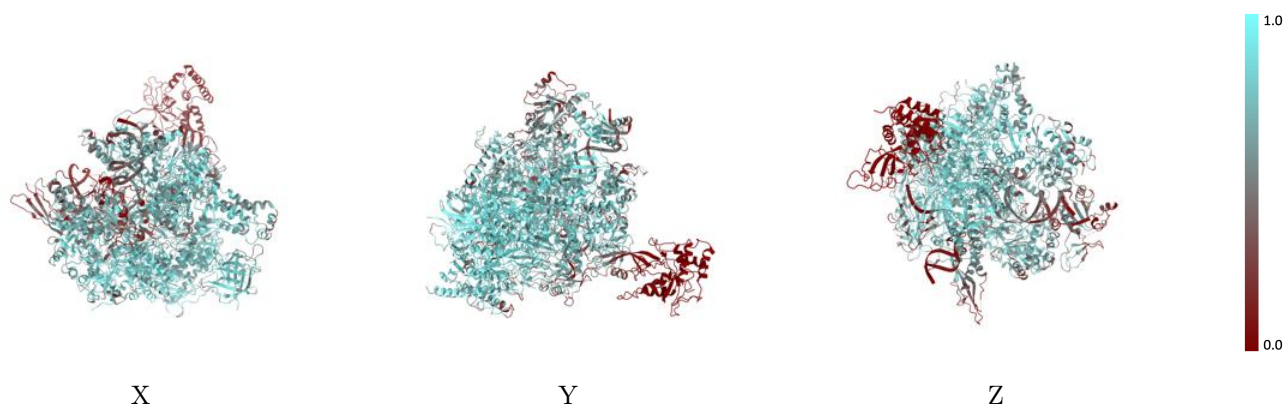
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0577).

9.4   Atom inclusion ⓘ
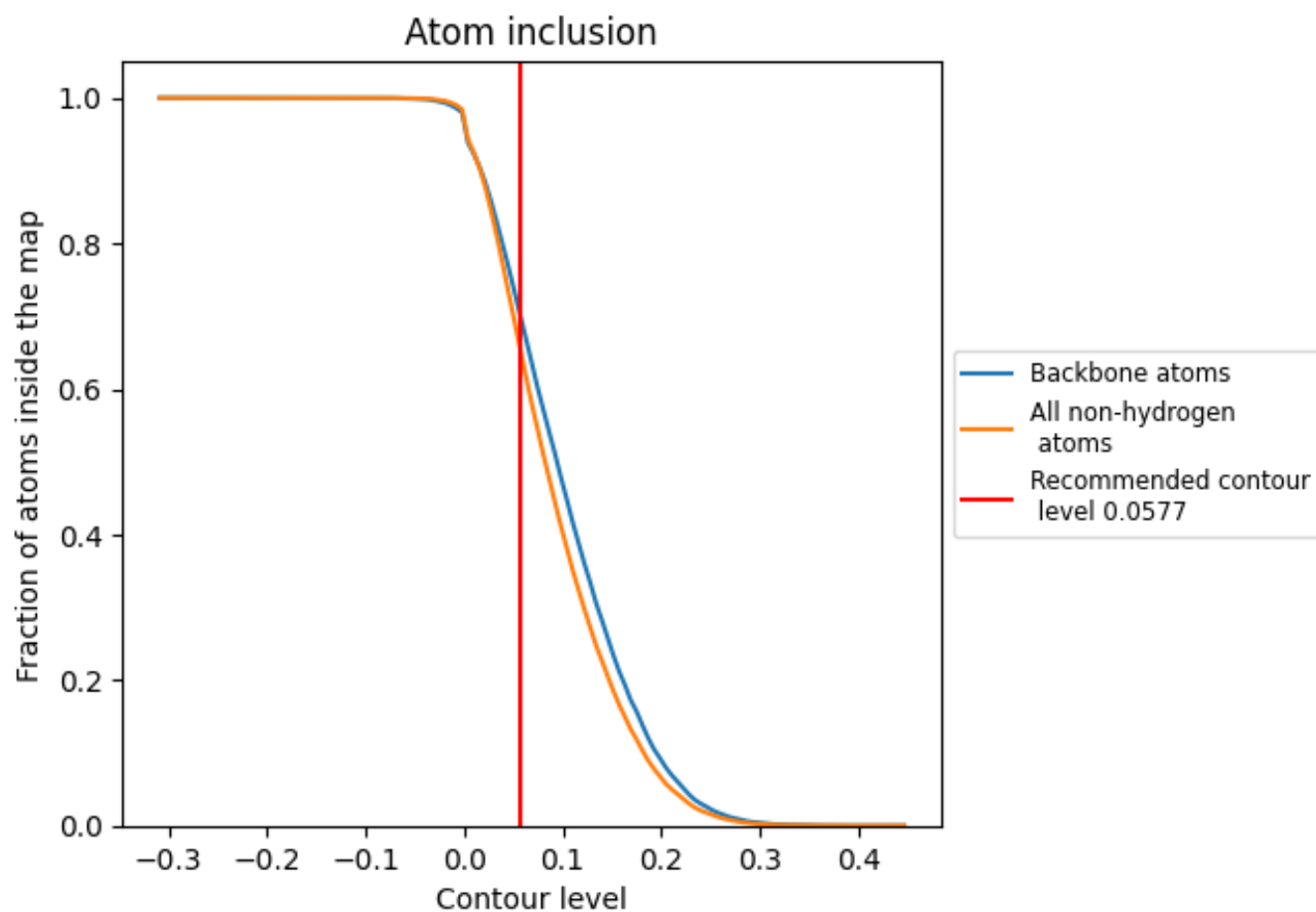
At the recommended contour level, 70% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0577) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6487	0.4820
A	0.6969	0.5100
B	0.7256	0.5150
C	0.7671	0.5280
D	0.0020	0.1280
E	0.6933	0.4950
F	0.6520	0.5010
G	0.0989	0.2170
H	0.7144	0.5060
I	0.5286	0.4660
J	0.8273	0.5500
K	0.7555	0.5230
L	0.6517	0.4980
M	0.9194	0.5860
N	0.3004	0.3230
P	0.6113	0.4400
T	0.4435	0.4140

1.0

0.0
<0.0