WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Dec 26, 2023 – 10:28 AM JST

PDB ID	:	8WAZ
EMDB ID	:	EMD-37410
Title	:	De novo transcribing complex 16 (TC16), the early elongation complex with Pol II positioned 16nt downstream of TSS
Authors	:	Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on	:	2023-09-08
Resolution	:	2.76 Å(reported)

1   Overall quality at a glance   ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 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		10
Ramachandran outliers		0.2%
Sidechain outliers		0.6%
RNA backbone		0.36

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
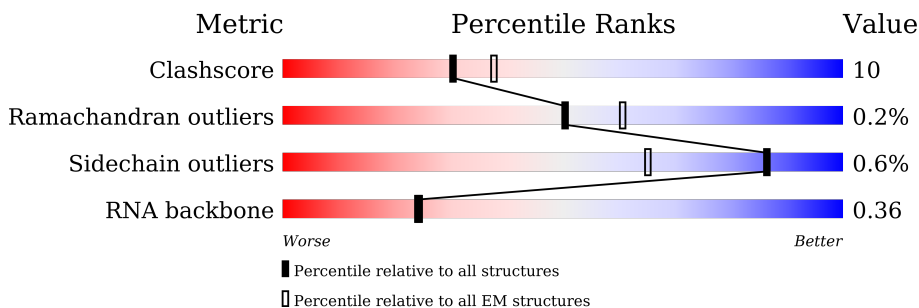
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	N	8	38% 50% 12%
2	S	517	27% 23% • 73%
3	T	249	41% 36% 5% 59%
4	X	99	27% 13% 30% 57%
5	Y	99	29% 30% 22% • 45%
6	Z	13	23% 46% 31% 15% 8%
7	o	1970	5% 73% • 26%

Continued on next page...

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

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	p	1174	8% ▬▬▬ 97% ▬▬▬▬▬▬ ··
9	q	275	· ▬▬▬▬▬ 92% ▬▬▬▬ · 7%
10	r	142	78% ▬▬▬▬▬ 90% ▬▬▬ 10%
11	s	210	· ▬▬▬▬▬ 100%
12	t	127	5% ▬▬▬ 65% ▬▬▬ 35%
13	u	172	60% ▬▬▬▬ 99% ▬▬▬▬ ·
14	v	150	· ▬▬▬▬▬ 97% ▬▬▬ ··
15	w	125	15% ▬▬▬ 91% ▬▬▬ 9%
16	x	67	· ▬▬▬▬▬ 97% ·
17	y	117	▬▬▬▬▬ 98% ·
18	z	58	· ▬▬▬▬▬ 76% ▬▬▬ 24%

2 Entry composition ⓘ

There are 21 unique types of molecules in this entry. The entry contains 35760 atoms, of which 30 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 Alpha-amanitin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	8	Total	C	H	N	O	S	0	0
			94	39	30	10	14	1		

- Molecule 2 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 3 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	103	Total	C	N	O	S	0	0
			789	492	142	154	1		

- Molecule 4 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	43	Total	C	N	O	P	0	0
			873	415	158	257	43		

- Molecule 5 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	54	Total	C	N	O	P	0	0
			1118	529	212	323	54		

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	13	Total	C	N	O	P	0	0
			272	123	45	91	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	1146	Total	C	N	O	S	0	0
			9149	5782	1610	1693	64		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	r	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 18 is a protein called RPB12.

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

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	o	2	Total 2	Zn 2	0
19	p	1	Total 1	Zn 1	0
19	q	1	Total 1	Zn 1	0
19	w	2	Total 2	Zn 2	0
19	x	1	Total 1	Zn 1	0
19	z	1	Total 1	Zn 1	0

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	o	1	Total 1	Mg 1	0

- Molecule 21 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: W0F) (formula: $C_{11}H_{18}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					AltConf
21	p	1	Total 33	C 11	N 5	O 14	P 3	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: Alpha-amanitin

Chain N: 38%   50%   12%

I1 W2 C6 N7 P8

- Molecule 2: General transcription factor IIF subunit 1

Chain S: 27%   23%   73%

MET ALA ALA LEU G5 P6 S7 S8 Q9 N10 V11 T12 E13 Y14 V15 V16 R17 V18 P19 K20 N21 T22 T23 K24 K25 Y26 N27 I28 M29 A30 F31 N32 A33 A34 D35 K36 V37 N38 F39 A40 T41 W42 N43 Q44 A45 R46 L47 E48 R49 D50 L51 S52 N53 K54 LYS ILE TYR GLN GLU GLU

GLU MET PRO GLU SER GLY ALA GLY SER GLU PHE ASN ARG LYS LEU ARG GLU GLU ALA ARG ARG LYS LYS TYR GLY ILE VAL LEU LYS GLU PHE ARG P93 E94 D95 Q96 P97 W98 L99 L100 R101 V102 N103 G104 K105 S106 G107 R108 K109 F110 K111 G112 I113 K114 K115 G116 G117 V118 T119 E120

N121 T122 S123 Y124 Y125 I126 F127 T128 Q129 C130 P131 D132 G133 A134 F135 E136 A137 F138 P139 V140 H141 N142 W143 Y144 N145 F146 T147 P148 L149 A150 R151 H152 R153 T154 L155 T156 A157 E158 E159 A160 E161 E162 E163 W164 E165 R166 R167 N168 K169 V170 L171 N172 H173 F174 S175 I176 M177 Q178 Q179 R180

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

ALA LYS GLY GLY ARG LYS LYS LYS LYS LYS LYS GLY SER ASP ASP GLU ALA PHE GLU ASP ASP ASP GLY ASP PHE GLU GLY GLN GLU VAL ASP TYR MET SER ASP GLY SER SER SER GLN GLU GLU GLU PRO GLU SER LYS ALA LYS PRO GLN GLN GLU GLU GLY GLY PRO LYS GLY

VAL ASP GLU GLN SER ASP SER GLU GLU SER GLU GLU GLU LYS PRO PRO GLU GLU ASP LYS GLU GLU LYS LYS ALA PRO THR PRO SER ALA GLU GLY GLY SER ASP SER GLU GLU GLY SER GLU GLU ASP ILE ASP SER GLU ALA SER SER ALA

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

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

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

- Molecule 3: General transcription factor IIF subunit 2

Chain T:

41%

36%   5%   59%

MET A2 E3 R4 G5 E6 L7 D8 L9 T10 G11 A12 K13 Q14 N15 T16 G17 V18 W19 L20 V21 K22 V23 P24 K25 Y26 L27 S28 Q29 Q30 W31 A32 K33 A34 S35 G36 R37 G38 E39 V40 G41 K42 L43 R44 I45 A46 K47 T48 Q49 G50 R51 T52 E53 V54 S55 F56 T57 L58 N59 E60

D61 L62 A63 N64 ILE HIS ASP ILE GLY LYS GLY LYS GLN ILE GLU GLU SER SER VAL SER ALA PRO ARG E80 H81 P82 F83 V84 L85 Q86 S87 V88 G89 G90 Q91 T92 L93 T94 V95 F96 T97 E98 S99 S100 S101 D102 K103 L104 S105 L106 E107 G108 I109 V110 V111 Q112 R113 A114 E115 C116 R117 P118 A119 ALA

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

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

HIS TYR GLN GLY GLU GLU LYS SER ASP

• Molecule 4: non-template DNA

Chain X:

27%

13%   30%   57%

DA DA DG DG DC DG DC DT DA DT DA DA DA DG DG DG DG DT DG DG DT DT DG DT DG DA DT T-8 C-7 T-6 T-5 C-4 T-3 T-2 C-1 A0 T1 C2 A3 A4 C5 DT DC DA DT DC DT DA DC DG DG C17 G18 A19

G20 C21 C22 G23 A24 G25 C26 A27 G28 A29 C30 G31 T32 G33 C34 C35 T36 A37 C38 G39 G40 A41 C42 C43 A44 T45 DG DT DC DC DG DA DA DC DT DG DA DC

• Molecule 5: template DNA

Chain Y:

29%

30%   22%   •   45%

DG DT DC DA DG DT DT DC DG DA DC A-45 T-44 G-43 G-42 T-41 C-40 C-39 G-38 T-37 A-36 G-35 G-34 C-33 A-32 C-31 G-30 T-29 C-28 T-27 G-26 C-25 T-24 C-23 G-22 G-17 C-16 C-15 G-14 T-13 A-12 G-11 A-10 T-9 G-8 A-7 A-6 G-5 T-4 T-3 G-2 A-1 T0 G1 A2 A3 G4

A5 A6 G7 A8 DA DT DC DC DA DC DC DC DC DA DC DC DC DC DT DT DT DT DA DT DG DG DC DC DC DT DT

• Molecule 6: RNA

Chain Z:

23%

46%   31%   15%   8%

A4 A5 C6 U7 U8 C9 A10 U11 C12 G16

• Molecule 7: DNA-directed RNA polymerase subunit

Chain o:

5%

73%   •   26%

MET HIS GLY GLY PRO SER GLY ASP S11 T46 T47 E48 G49 G50 R51 D120 S121 N122 N123 P124 K125 I126 K127 D128 A131 K132 S133 K134 G135 G150 E155 GLY GLU GLU MET ASP ASN LYS PHE GLY VAL GLU GLN PRO GLU ASP GLU ASP LEU THR LYS

GLU LYS GLY H181 C184 R190 K203 H204 V205 N206 E207 D208 S209 Q210 E211 K212 M266 Q267 G268 S269 A270 R271 N272 R292 N293 E294 Q295 N296 G297 A298 A299 A300 H301 V302 I303 E321 L322 P323 G324 L325 Q330 K331 S332 G333 H432 P433 K434 D437 F458

V488 T489 T490 D495 T626 V675 K910 R967 A1110 G1111 V1112 S1113 E1198 M1199 P1200 D1201 F1202 D1203 V1204 A1205 R1206 D1241 D1242 L1243 N1248 D1249 D1250 N1251 A1252 E1253 M1262 N1263 S1264 D1265 E1266 N1267 K1268 M1269 Q1270 E1271 E1272 E1273 E1274 V1275 V1276 D1277 K1278 M1279 Q1313

T1314 D1315 N1316 V1374 D1472 M1484 E1485 I1486 P1487 THR ASN ILE PRO GLY LEU GLY ALA ALA GLY PRO THR GLY MET PHE PHE GLY SER ALA PRO SER PRO MET GLY GLY ILE SER PRO ALA MET THR PRO TRP ASN GLN GLY ALA THR PRO ALA TYR GLY ALA TRP SER PRO SER VAL

GLY SER GLY MET THR PRO GLY GLY ALA ALA GLY PHE SER PRO SER ALA ALA SER ASP ALA SER GLY PHE SER PRO GLY TYR SER PRO ALA TRP SER PRO THR PRO GLY SER GLY SER PRO SER ALA SER PRO THR TYR ILE SER PRO GLY GLY ALA MET SER PRO SER TYR SER PRO

THR SER PRO ALA TYR GLU PRO ARG SER PRO GLY GLY TYR THR PRO GLN SER PRO SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO ASN TYR SER PRO ALA SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO

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SER PRO LYS TYR PRO THR PRO THR SER PRO SER TYR SER PRO SER PRO GLU TYR THR PRO THR SER PRO LYS TYR SER PRO THR SER PRO LYS TYR SER PRO THR SER PRO THR TYR SER PRO THR THR PRO LYS TYR SER PRO THR SER PRO THR TYR

SER PRO THR SER PRO VAL TYR THR PRO THR SER PRO SER PRO LYS TYR PRO THR PRO THR SER PRO SER TYR SER PRO SER PRO LYS TYR SER PRO THR SER PRO SER TYR GLY SER PRO THR SER PRO GLY TYR SER PRO THR SER PRO THR TYR SER

LEU THR SER PRO ALA ILE SER ASP SER ASP GLU GLU ASN

• Molecule 8: DNA-directed RNA polymerase subunit beta

8%

Chain p: 97%

MET TYR ASP ALA ASP GLU ASP MET GLN TYR ASP GLU ASP ASP E16 I17 T18 Q42 D61 D66 L67 Q68 A69 E70 A71 Q72 H73 A74 S75 G76 E77 V78 E79 E80 P81 P82 E100 R101 D102 I133 K134 E135 G136 E137 E138 Q139 K210 K211 D212 N227 R230

P231 R242 G243 G244 Q245 G246 A247 K248 K249 S250 A251 I252 G253 K264 E313 A326 K327 P328 G329 E341 K345 F356 D424 R425 G426 K427 D428 A434 R438 S447 D455 Q456 K457 K458 A459 H460 Q461 A462 R491 D492 G493 K494 L495 H518 S549

A559 A560 I561 A564 N570 D595 I614 D680 D681 K820 K821 G822 F823 D824 R834 H842 D849 L873 P874 GLU ASN GLU ASP GLU LEU GLU GLU GLY THR ASN ARG ARG TYR T888 I1067 R1106 V1174

• Molecule 9: DNA-directed RNA polymerase II subunit RPB3

Chain q:

92% 7%

MET P2 E13 I44 C90 C94 S132 ARG ASN ARG ASP ASN ASP PRO SER ASP TYR VAL GLU GLN D146 D214 D270 V271 LEU THR ILE ASN

• Molecule 10: DNA-directed RNA polymerase II subunit RPB4

Chain r:

78%

90% 10%

MET ALA ALA GLY GLY SER ASP PRO ARG ALA GLY ASP VAL E14 E15 D16 A17 S18 Q19 L20 I21 F22 P23 K24 E25 F26 E27 T28 A29 E30 T31 L32 L33 N34 S35 E36 V37 H38 E42 H43 R44 K45 Q46 Q47 N48 E49 S50 A51 E52 D53 E54 Q55 E56 L57 S58 E59 N66

A69 R70 F71 S72 R73 F74 K75 N76 R77 E78 T79 I80 A81 S82 V83 R84 S85 L86 L87 L88 Q89 K90 K91 L92 H93 K94 F95 E96 L97 A98 C99 L100 A101 N102 L103 C104 P105 E106 T107 A108 E109 E110 S111 K112 A113 L114 I115 P116 S117 L118 E119 G120 R121 F122 E123 D124 E125 E126 L127 Q128

Q129 I130 L131 D132 D133 I134 Q135 T136 K137 R138 S139 F140 Q141 TYR

• Molecule 11: DNA-directed RNA polymerase II subunit E

Chain s:

100%

MET D2 R52 Q116 D120 Q210

• Molecule 12: DNA-directed RNA polymerase II subunit F

Chain t:

5% 65% 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 GLU LEU GLU ASN ALA GLU GLU GLY GLY GLN GLU ASN VAL GLU ILE LEU PRO SER GLY GLU ARG PRO Q46 A47 N48 Q49 S126 D127

• Molecule 13: DNA-directed RNA polymerase II subunit RPB7

Chain u:

60% 99%

M1 F2 Y3 E8 E35 C38 T39 G40 K41 Y42 F77 R78 P79 F80 K81 G82 R83 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 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v:

97%

• Molecule 15: DNA-directed RNA polymerase II subunit RPB9

15%

Chain w:

91%   9%

• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain x:

97%

• Molecule 17: DNA-directed RNA polymerase II subunit RPB11-a

Chain y:

98%

• Molecule 18: RPB12

Chain z:

76%   24%

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	268921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.589	Depositor
Minimum map value	-4.750	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CSX, ZN, HYP, G2L, MG, TRX, ILX, W0F

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	N	0.45	0/22	1.01	0/26
2	S	0.24	0/1167	0.48	0/1576
3	T	0.24	0/799	0.50	0/1077
4	X	0.69	0/976	1.06	0/1499
5	Y	0.72	0/1256	1.00	2/1939 (0.1%)
6	Z	0.58	0/275	1.32	3/424 (0.7%)
7	o	0.35	1/11723 (0.0%)	0.53	0/15830
8	p	0.39	0/9332	0.54	0/12598
9	q	0.40	0/2102	0.53	0/2857
10	r	0.25	0/1064	0.42	0/1428
11	s	0.35	0/1751	0.51	0/2366
12	t	0.38	0/667	0.51	0/901
13	u	0.29	0/1382	0.48	0/1874
14	v	0.41	0/1207	0.53	0/1628
15	w	0.36	0/948	0.51	0/1284
16	x	0.41	0/542	0.50	0/730
17	y	0.36	0/939	0.49	0/1271
18	z	0.39	0/377	0.61	0/500
All	All	0.39	1/36529 (0.0%)	0.58	5/49808 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	1374	VAL	CB-CG2	-5.00	1.42	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	-6	DA	O5'-P-OP1	7.20	119.34	110.70
6	Z	6	C	N1-C2-O2	5.79	122.38	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	6	C	N3-C2-O2	-5.33	118.17	121.90
5	Y	-29	DT	C5-C4-O4	-5.22	121.24	124.90
6	Z	9	C	C5-C6-N1	5.12	123.56	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2　Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	64	30	51	1	0
2	S	1138	0	1103	10	0
3	T	789	0	795	7	0
4	X	873	0	484	26	0
5	Y	1118	0	607	26	0
6	Z	272	0	139	5	0
7	o	11510	0	11616	0	0
8	p	9149	0	9178	0	0
9	q	2059	0	2007	0	0
10	r	1050	0	1033	0	0
11	s	1720	0	1737	0	0
12	t	657	0	684	0	0
13	u	1351	0	1358	0	0
14	v	1186	0	1147	0	0
15	w	927	0	859	0	0
16	x	533	0	553	0	0
17	y	920	0	942	0	0
18	z	372	0	378	0	0
19	o	2	0	0	0	0
19	p	1	0	0	0	0
19	q	1	0	0	0	0
19	w	2	0	0	0	0
19	x	1	0	0	0	0
19	z	1	0	0	0	0
20	o	1	0	0	0	0
21	p	33	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35730	30	34671	67	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 10.

All (67) 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)
4:X:17:DC:O2	5:Y:-17:DG:N2	2.07	0.87
4:X:19:DA:H4'	4:X:20:DG:H5'	1.61	0.82
4:X:19:DA:H1'	4:X:20:DG:C8	2.25	0.71
2:S:115:LYS:NZ	2:S:117:GLY:O	2.27	0.68
5:Y:-15:DC:O2	6:Z:16:G2L:N2	2.25	0.68
5:Y:-6:DA:H8	5:Y:-6:DA:H5"	1.59	0.67
4:X:4:DA:H2"	4:X:5:DC:C5	2.29	0.66
5:Y:5:DA:H2"	5:Y:6:DA:C8	2.32	0.64
5:Y:-29:DT:H1'	5:Y:-28:DC:H5'	1.80	0.64
4:X:24:DA:N6	5:Y:-24:DT:C4	2.66	0.63
4:X:30:DC:H2"	4:X:31:DG:C8	2.33	0.63
3:T:94:THR:HG22	3:T:109:ILE:HG22	1.80	0.62
5:Y:-15:DC:H2'	5:Y:-14:DG:C8	2.36	0.60
5:Y:-7:DA:H2"	5:Y:-6:DA:H5"	1.83	0.60
4:X:18:DG:H2"	4:X:19:DA:H2'	1.84	0.59
4:X:41:DA:H2"	4:X:42:DC:C5	2.38	0.59
5:Y:-16:DC:H2'	5:Y:-15:DC:C6	2.38	0.59
4:X:24:DA:N6	5:Y:-24:DT:N3	2.53	0.56
4:X:18:DG:H2"	4:X:19:DA:C8	2.41	0.55
4:X:24:DA:N6	5:Y:-24:DT:H3	2.04	0.55
5:Y:-7:DA:H2"	5:Y:-6:DA:C5'	2.36	0.55
4:X:22:DC:H2"	4:X:23:DG:C8	2.41	0.55
5:Y:-12:DA:H2'	5:Y:-11:DG:H8	1.73	0.52
5:Y:-10:DA:C8	5:Y:-9:DT:H72	2.45	0.52
5:Y:-23:DC:H2"	5:Y:-22:DG:H5'	1.92	0.51
4:X:-1:DC:H2"	4:X:0:DA:C8	2.45	0.51
2:S:169:LYS:HD2	2:S:173:HIS:CD2	2.45	0.51
4:X:36:DT:H2"	4:X:37:DA:N7	2.27	0.50
2:S:164:TRP:CZ2	2:S:167:ARG:HD3	2.47	0.49
5:Y:2:DA:H2"	5:Y:3:DA:C8	2.47	0.49
3:T:31:TRP:HD1	3:T:62:LEU:HD21	1.78	0.48
4:X:-8:DT:H2"	4:X:-7:DC:C5	2.48	0.48
2:S:142:ASN:OD1	2:S:143:TRP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:-12:DA:H2'	5:Y:-11:DG:C8	2.48	0.48
2:S:161:GLU:O	2:S:165:GLU:HG2	2.14	0.47
4:X:29:DA:N6	5:Y:-30:DG:C6	2.82	0.47
3:T:32:ALA:HA	3:T:35:SER:HB2	1.95	0.47
3:T:80:GLU:OE1	3:T:81:HIS:N	2.47	0.47
4:X:28:DG:H4'	4:X:29:DA:H5'	1.98	0.46
5:Y:-39:DC:H2"	5:Y:-38:DG:C8	2.52	0.44
2:S:175:SER:O	2:S:179:GLN:HG2	2.18	0.44
4:X:-7:DC:H2"	4:X:-6:DT:H72	1.98	0.44
5:Y:-6:DA:H5"	5:Y:-6:DA:C8	2.46	0.44
6:Z:6:C:H5'	6:Z:7:U:OP2	2.18	0.44
4:X:39:DG:H2"	4:X:40:DG:C8	2.53	0.44
4:X:18:DG:C2'	4:X:19:DA:C8	3.00	0.43
5:Y:-14:DG:N1	6:Z:16:G2L:C6	2.81	0.43
5:Y:-38:DG:H8	5:Y:-38:DG:OP2	2.02	0.43
4:X:3:DA:H2"	4:X:4:DA:C8	2.53	0.43
4:X:26:DC:C2	4:X:27:DA:C8	3.06	0.42
2:S:43:ASN:OD1	2:S:44:GLN:N	2.52	0.42
2:S:111:LYS:O	2:S:146:PHE:HA	2.20	0.42
3:T:9:LEU:O	3:T:13:LYS:HG2	2.19	0.42
4:X:24:DA:H4'	4:X:25:DG:OP1	2.20	0.42
2:S:47:LEU:HD11	2:S:98:TRP:HB3	2.01	0.42
4:X:41:DA:H2"	4:X:42:DC:C6	2.54	0.42
5:Y:-27:DT:C2	5:Y:-26:DG:C8	3.07	0.41
4:X:21:DC:H2"	4:X:22:DC:C6	2.55	0.41
5:Y:-14:DG:N1	6:Z:16:G2L:N1	2.68	0.41
3:T:43:LEU:HD12	3:T:55:SER:O	2.21	0.41
5:Y:-30:DG:H2"	5:Y:-29:DT:C5'	2.51	0.41
6:Z:11:U:H2'	6:Z:12:C:O4'	2.20	0.41
4:X:2:DC:H2"	4:X:3:DA:C8	2.56	0.40
2:S:172:ASN:O	2:S:176:ILE:HG12	2.21	0.40
3:T:30:GLN:O	3:T:62:LEU:HD11	2.22	0.40
1:N:6:CSX:HB2	1:N:7:ASN:H	1.42	0.40
5:Y:-29:DT:H2"	5:Y:-28:DC:O5'	2.21	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	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
2	S	134/517 (26%)	134 (100%)	0	0	100	100
3	T	99/249 (40%)	95 (96%)	4 (4%)	0	100	100
7	o	1448/1970 (74%)	1393 (96%)	53 (4%)	2 (0%)	51	75
8	p	1142/1174 (97%)	1072 (94%)	67 (6%)	3 (0%)	41	60
9	q	253/275 (92%)	245 (97%)	8 (3%)	0	100	100
10	r	126/142 (89%)	126 (100%)	0	0	100	100
11	s	207/210 (99%)	197 (95%)	10 (5%)	0	100	100
12	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
13	u	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
14	v	146/150 (97%)	138 (94%)	7 (5%)	1 (1%)	22	39
15	w	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
16	x	65/67 (97%)	63 (97%)	0	2 (3%)	4	6
17	y	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
18	z	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
All	All	4140/5361 (77%)	3965 (96%)	167 (4%)	8 (0%)	50	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	o	910	LYS
16	x	28	GLU
8	p	549	SER
14	v	34	SER
16	x	6	ARG
7	o	184	CYS
8	p	570	ASN
8	p	614	ILE

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	N	2/2 (100%)	2 (100%)	0	100	100
2	S	121/448 (27%)	120 (99%)	1 (1%)	81	88
3	T	85/218 (39%)	85 (100%)	0	100	100
7	o	1280/1749 (73%)	1270 (99%)	10 (1%)	81	88
8	p	1001/1027 (98%)	995 (99%)	6 (1%)	86	90
9	q	234/252 (93%)	230 (98%)	4 (2%)	60	76
10	r	118/126 (94%)	118 (100%)	0	100	100
11	s	191/192 (100%)	191 (100%)	0	100	100
12	t	71/111 (64%)	71 (100%)	0	100	100
13	u	152/153 (99%)	152 (100%)	0	100	100
14	v	129/131 (98%)	128 (99%)	1 (1%)	81	88
15	w	103/112 (92%)	103 (100%)	0	100	100
16	x	56/56 (100%)	56 (100%)	0	100	100
17	y	104/106 (98%)	104 (100%)	0	100	100
18	z	41/55 (74%)	41 (100%)	0	100	100
All	All	3688/4738 (78%)	3666 (99%)	22 (1%)	86	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	44	GLN
7	o	46	THR
7	o	184	CYS
7	o	458	PHE
7	o	488	VAL
7	o	490	THR
7	o	495	ASP
7	o	626	THR
7	o	675	VAL
7	o	967	ARG

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Mol	Chain	Res	Type
7	o	1472	ASP
8	p	18	THR
8	p	42	GLN
8	p	447	SER
8	p	849	ASP
8	p	1067	ILE
8	p	1106	ARG
9	q	13	GLU
9	q	44	ILE
9	q	90	CYS
9	q	94	CYS
14	v	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	44	GLN
2	S	178	GLN
7	o	62	GLN
7	o	181	HIS
7	o	449	HIS
7	o	531	ASN
7	o	539	GLN
7	o	671	ASN
7	o	721	HIS
7	o	780	ASN
7	o	791	GLN
7	o	792	ASN
7	o	804	HIS
7	o	904	GLN
7	o	1044	HIS
7	o	1163	HIS
7	o	1410	HIS
7	o	1422	GLN
7	o	1445	HIS
7	o	1462	GLN
8	p	43	GLN
8	p	117	ASN
8	p	144	HIS
8	p	245	GLN
8	p	312	GLN
8	p	387	HIS

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Mol	Chain	Res	Type
8	p	481	HIS
8	p	639	HIS
8	p	699	HIS
8	p	725	GLN
8	p	755	GLN
8	p	838	GLN
8	p	941	GLN
8	p	1094	GLN
8	p	1142	ASN
9	q	18	ASN
9	q	217	GLN
9	q	232	ASN
10	r	66	ASN
10	r	129	GLN
11	s	64	HIS
12	t	46	GLN
13	u	14	HIS
13	u	53	ASN
15	w	41	ASN
15	w	118	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Z	11/13 (84%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Z	5	A
6	Z	6	C
6	Z	7	U

There are no RNA pucker outliers to report.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	CSX	N	6	1	3,6,7	1.00	0	1,6,8	2.18	1 (100%)
1	HYP	N	8	1	6,8,9	0.74	0	5,10,12	2.17	2 (40%)
6	G2L	Z	16	20,5,6	19,26,30	0.99	1 (5%)	18,38,44	1.33	3 (16%)
1	ILX	N	1	1	8,9,10	0.60	0	9,11,13	1.31	2 (22%)
1	TRX	N	2	1	14,16,17	1.01	0	15,22,24	1.98	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSX	N	6	1	-	1/1/5/7	-
1	HYP	N	8	1	-	0/0/11/13	0/1/1/1
6	G2L	Z	16	20,5,6	-	0/5/27/31	0/3/3/3
1	ILX	N	1	1	-	7/11/12/14	-
1	TRX	N	2	1	-	0/4/6/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	16	G2L	C6-N1	-2.28	1.34	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	2	TRX	CG-CB-CA	5.73	123.39	114.53
1	N	8	HYP	O-C-CA	-3.29	116.15	124.78
1	N	2	TRX	CB-CG-CD1	-3.02	124.23	127.97
1	N	8	HYP	CB-CG-CD	2.97	106.91	103.27
1	N	1	ILX	OD1-CD1-CG1	-2.90	104.76	111.07
6	Z	16	G2L	C3'-C2'-C1'	2.76	106.00	99.89
1	N	2	TRX	CH2-CZ2-CE2	-2.37	116.79	119.29
6	Z	16	G2L	C8-N7-C5	2.34	107.45	102.99
6	Z	16	G2L	C5-C6-N1	2.30	118.01	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	2	TRX	CB-CG-CD2	2.30	129.82	126.25
1	N	6	CSX	CA-CB-SG	2.18	118.11	113.36
1	N	1	ILX	CB-CA-C	-2.04	110.19	112.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	ILX	C-CA-CB-CG2
1	N	1	ILX	OD1-CD1-CG1-CB
1	N	1	ILX	OD1-CD1-CG1-OG1
1	N	6	CSX	N-CA-CB-SG
1	N	1	ILX	C-CA-CB-CG1
1	N	1	ILX	CG2-CB-CG1-CD1
1	N	1	ILX	O-C-CA-CB
1	N	1	ILX	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	6	CSX	1	0
6	Z	16	G2L	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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
21	W0F	p	1201	-	25,35,35	3.21	7 (28%)	31,55,55	2.54	12 (38%)

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
21	W0F	p	1201	-	-	3/20/40/40	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	p	1201	W0F	C03-C04	-9.40	1.27	1.52
21	p	1201	W0F	O05-C06	-9.24	1.28	1.41
21	p	1201	W0F	O05-C04	6.85	1.60	1.45
21	p	1201	W0F	C07-C03	-2.90	1.46	1.52
21	p	1201	W0F	C20-C04	2.46	1.59	1.51
21	p	1201	W0F	C17-N16	-2.15	1.34	1.39
21	p	1201	W0F	P22-O21	2.13	1.67	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	p	1201	W0F	O05-C06-C07	-6.28	97.75	106.93
21	p	1201	W0F	O05-C04-C03	-5.66	92.73	104.87
21	p	1201	W0F	O05-C04-C20	4.79	125.12	109.37
21	p	1201	W0F	O21-C20-C04	3.93	122.52	108.99
21	p	1201	W0F	O32-P30-O29	3.90	117.70	104.64
21	p	1201	W0F	O33-P30-O31	-3.30	97.75	110.68
21	p	1201	W0F	P26-O25-P22	-3.10	122.20	132.83
21	p	1201	W0F	P26-O29-P30	2.74	142.24	132.83
21	p	1201	W0F	O33-P30-O29	2.66	113.56	104.64
21	p	1201	W0F	O08-C07-C06	2.42	119.79	110.85
21	p	1201	W0F	C10-N11-C12	2.40	107.57	102.99
21	p	1201	W0F	O21-P22-O24	-2.36	99.84	109.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	p	1201	W0F	C20-O21-P22-O24
21	p	1201	W0F	C20-O21-P22-O25
21	p	1201	W0F	C03-C04-C20-O21

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand W0F p 1201

Bond lengths

Bond angles

Torsions

Rings
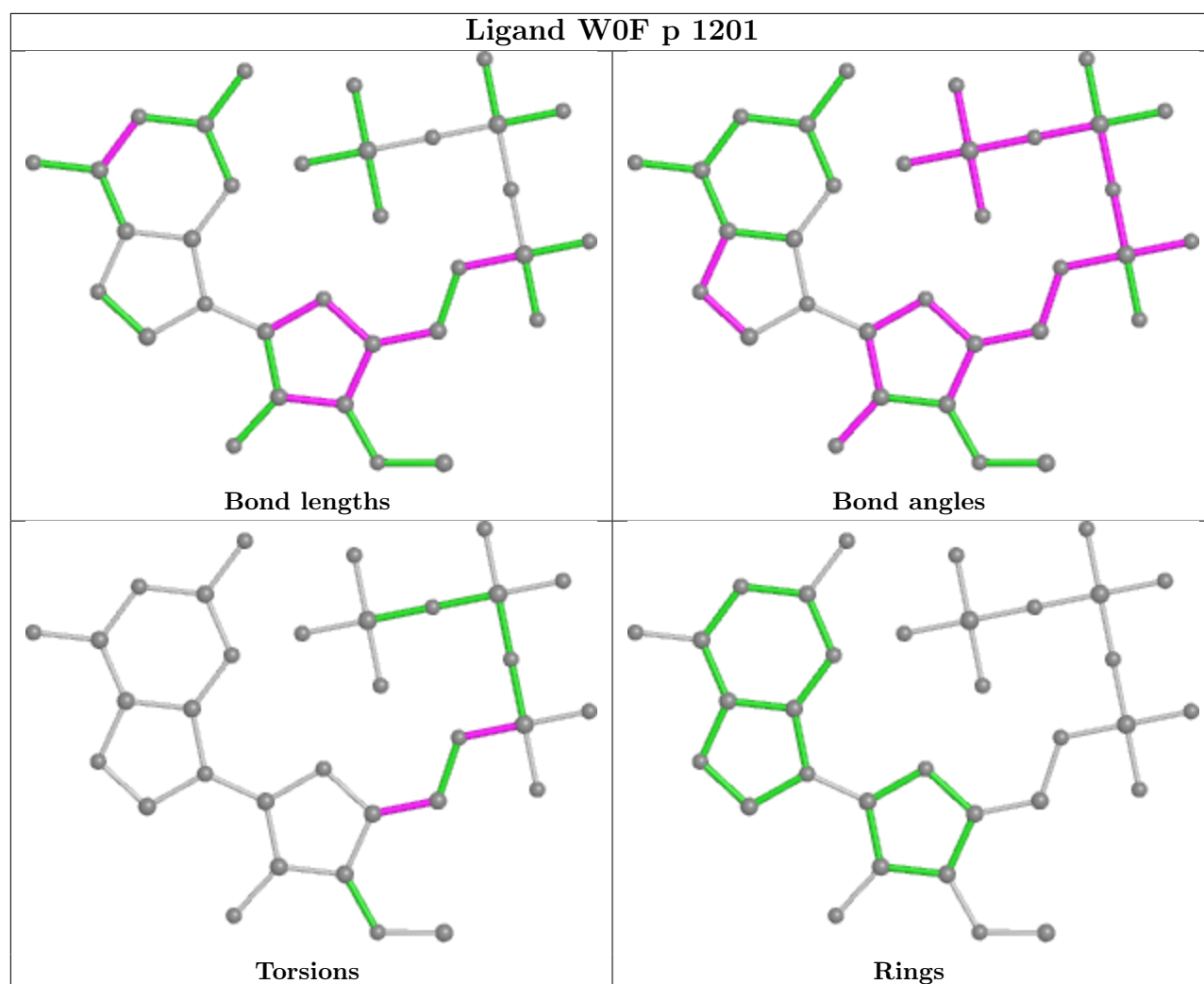
5.7 Other polymers ⓘ

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-37410. 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 ⓘ
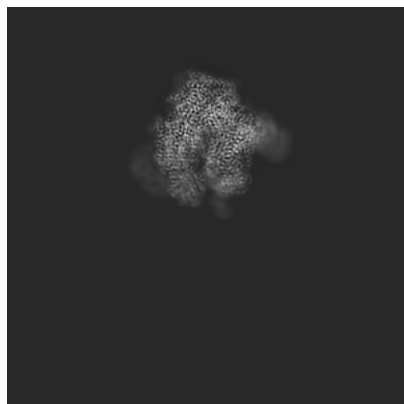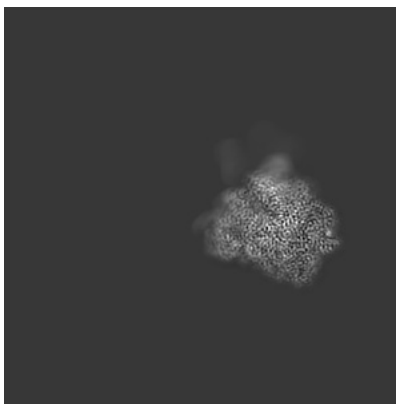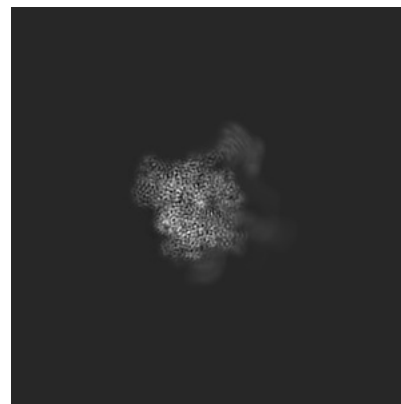
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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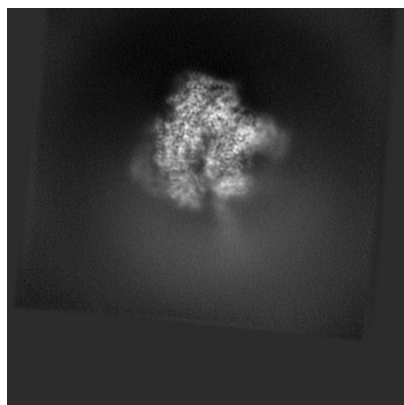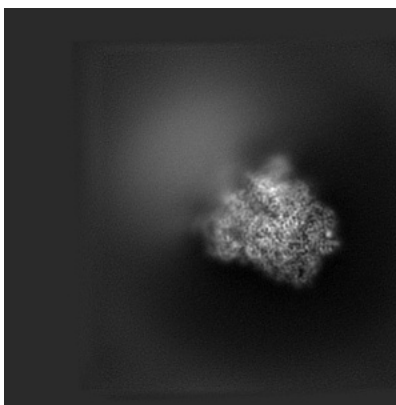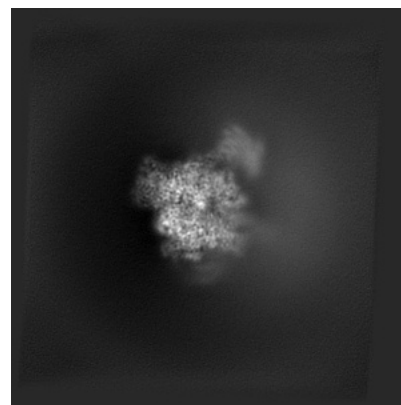
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
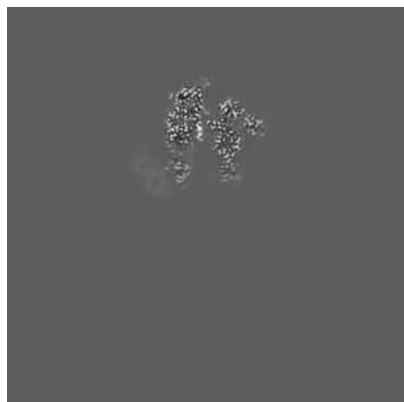
6.2.1 Primary map
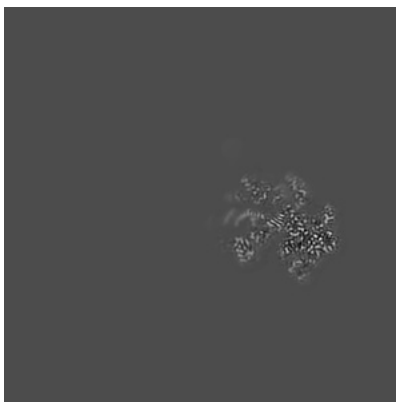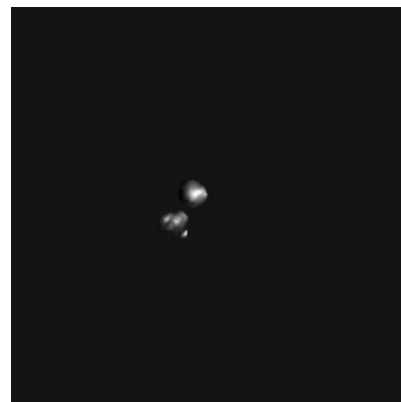
| X Index: 160 | Y Index: 160 | Z Index: 160 |

6.2.2 Raw map
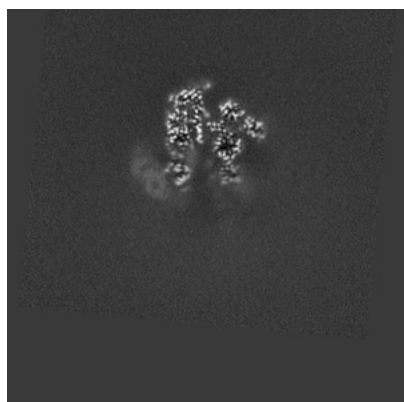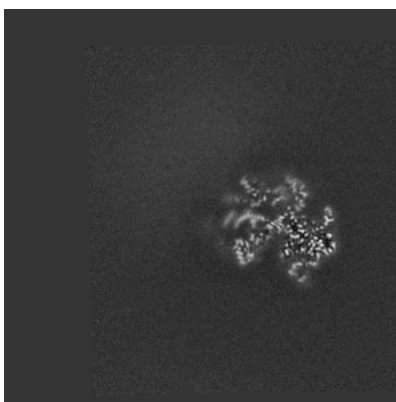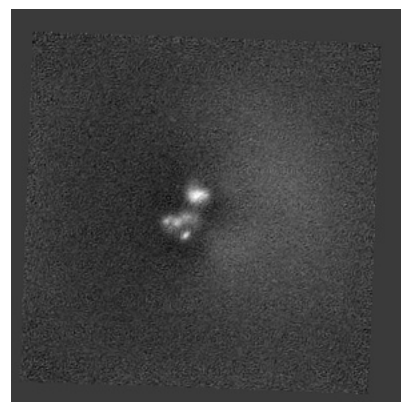
| X Index: 160 | Y Index: 160 | Z Index: 160 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
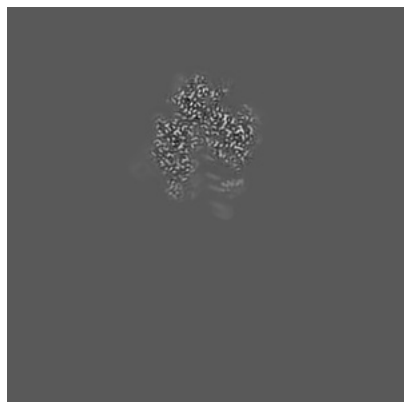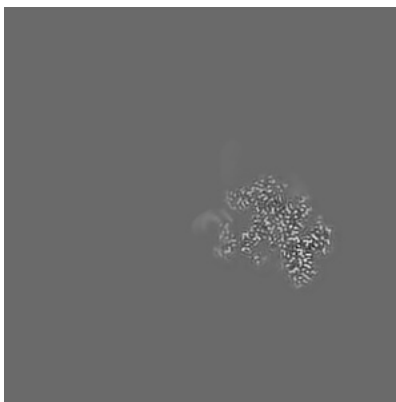
| X Index: 145 | Y Index: 172 | Z Index: 224 |
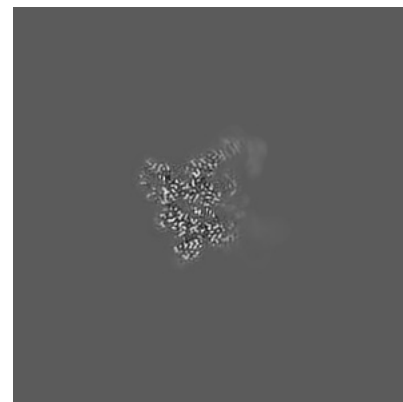
6.3.2 Raw map
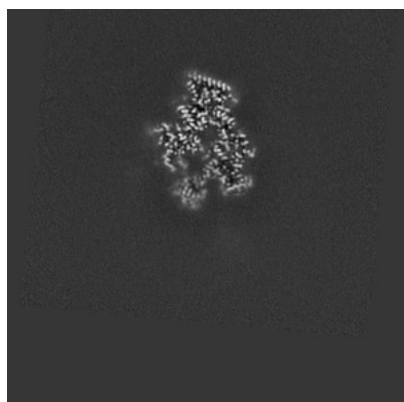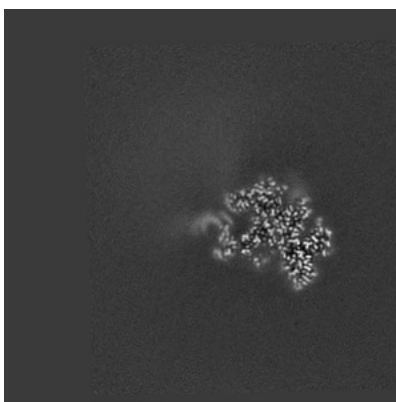
| X Index: 133 | Y Index: 172 | Z Index: 224 |
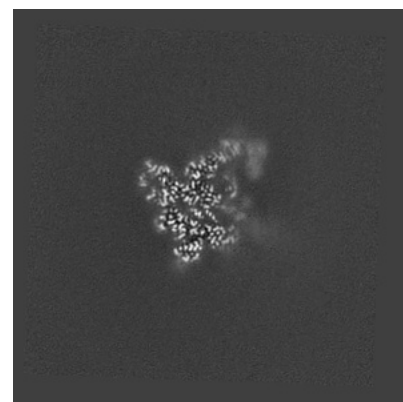
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
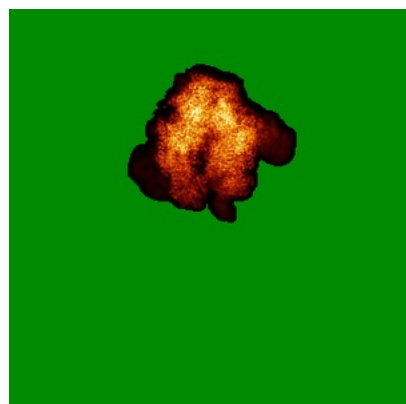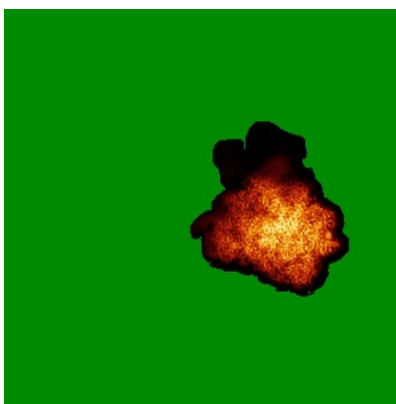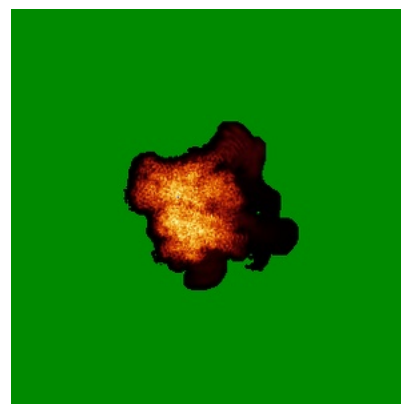
X   Y   Z

6.4.2 Raw map

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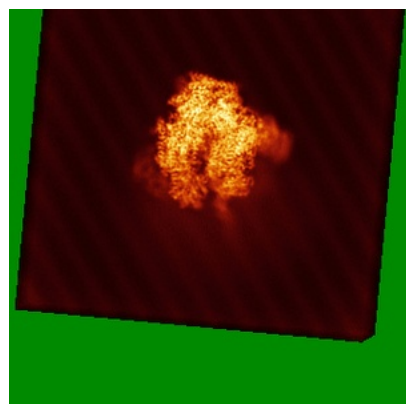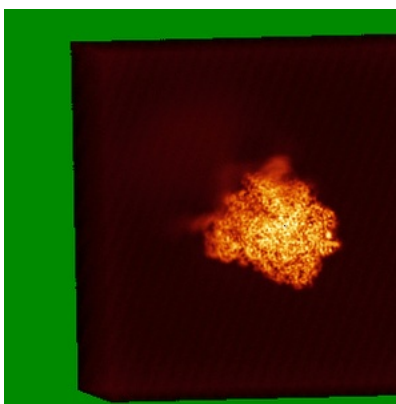
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
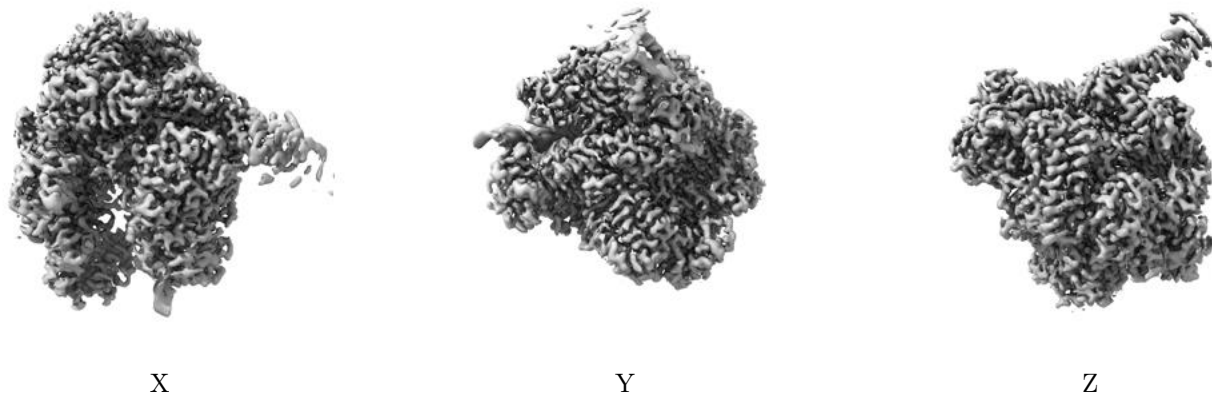
The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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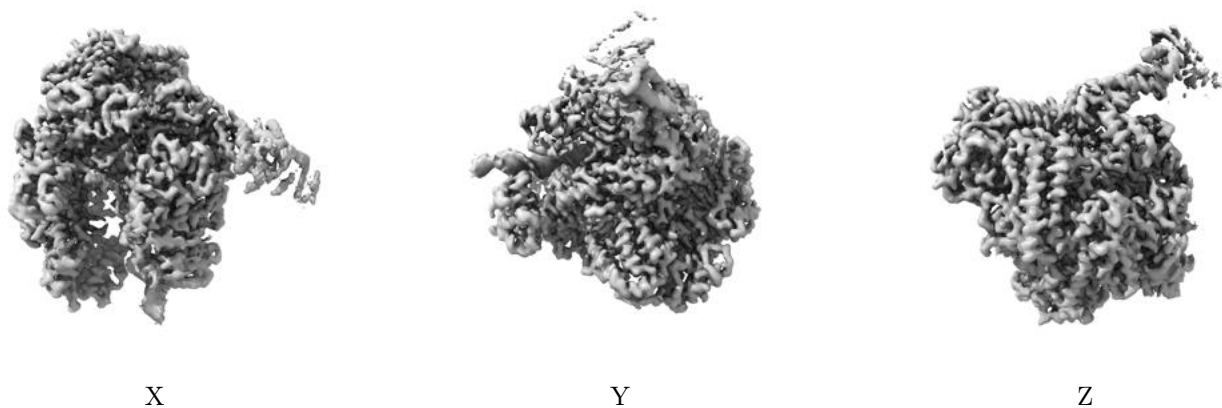
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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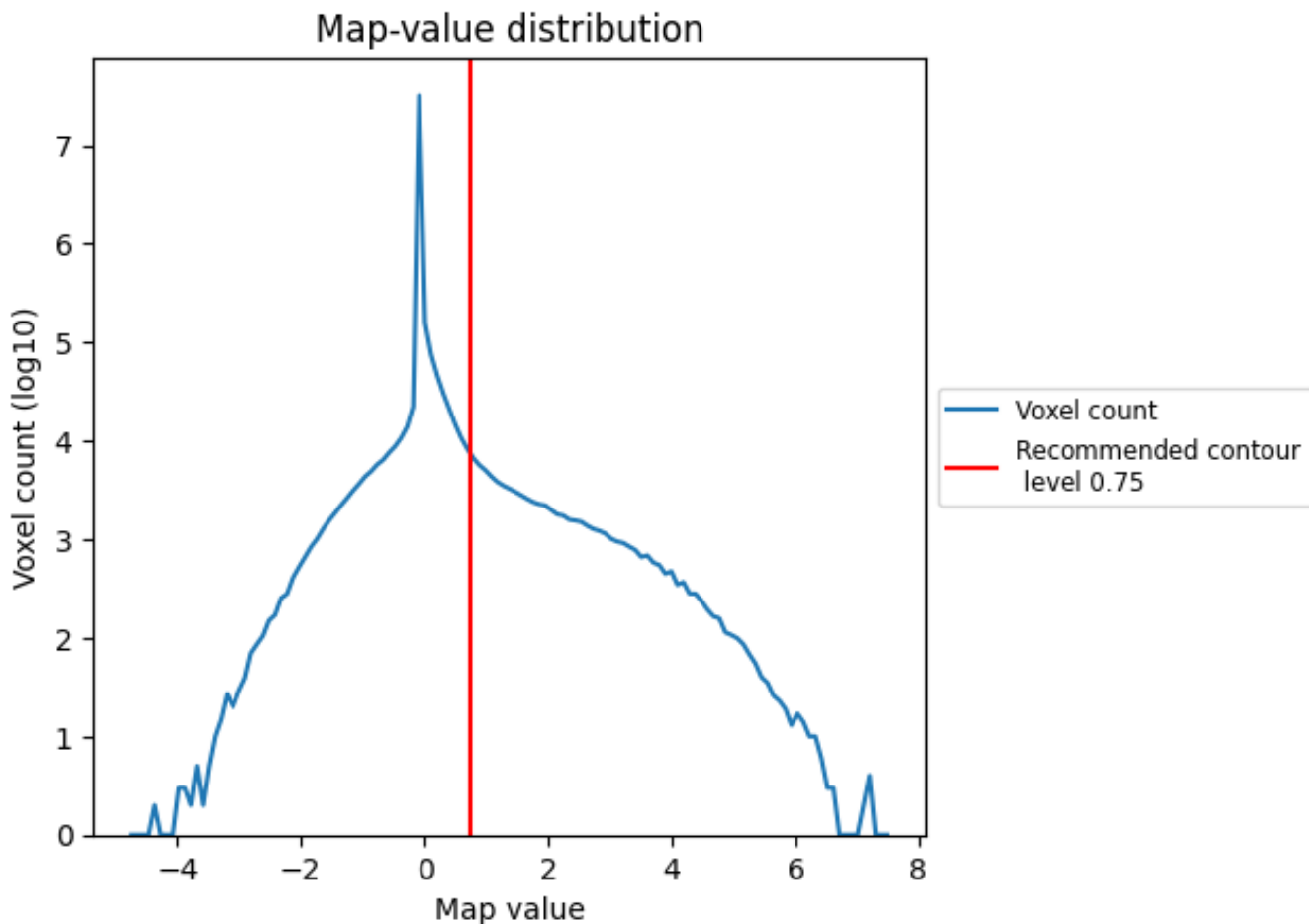
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
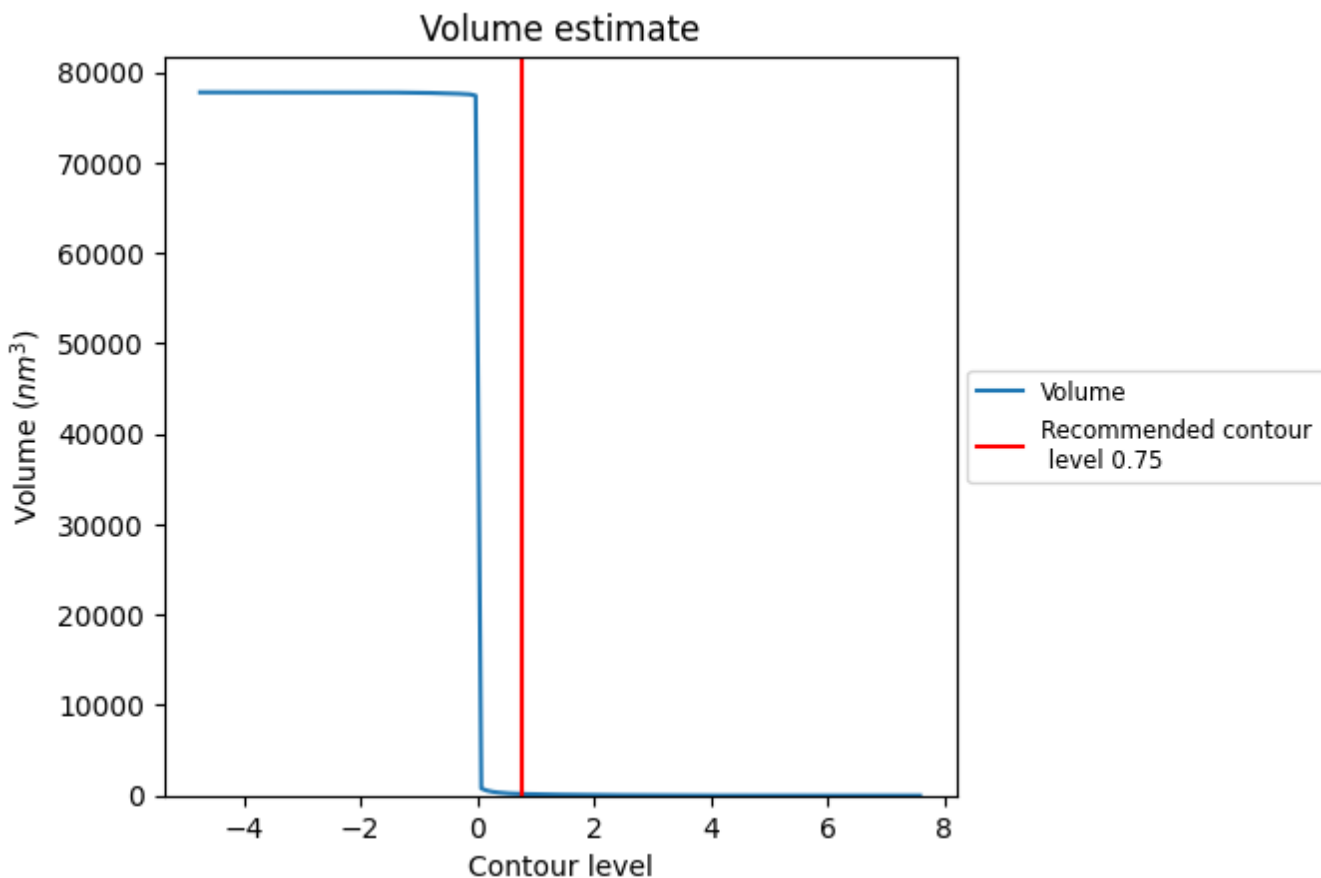
The volume at the recommended contour level is 183 nm^3; this corresponds to an approximate mass of 165 kDa.

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 ⓘ
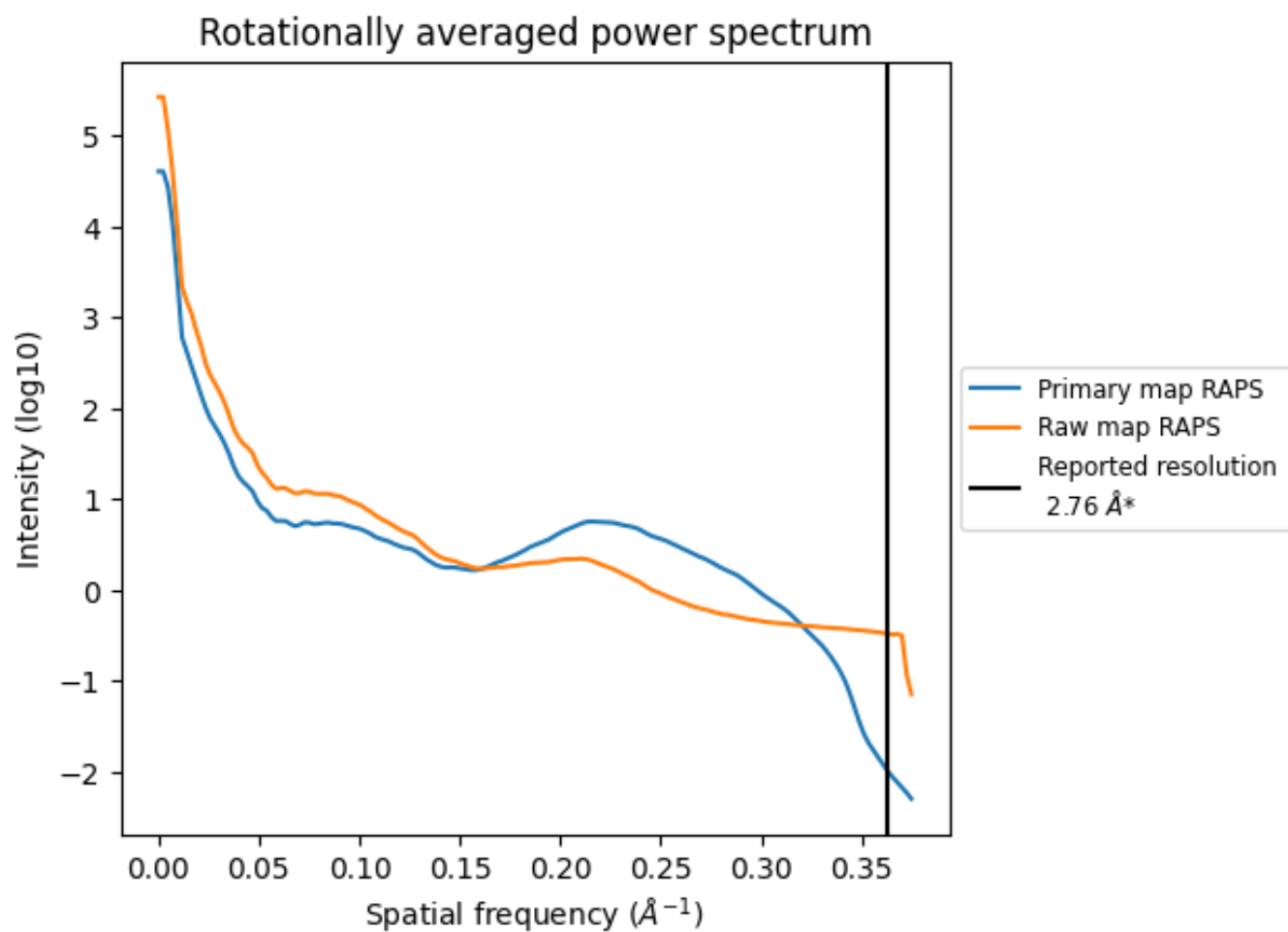
*Reported resolution corresponds to spatial frequency of 0.362 Å^{-1}

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 ⓘ
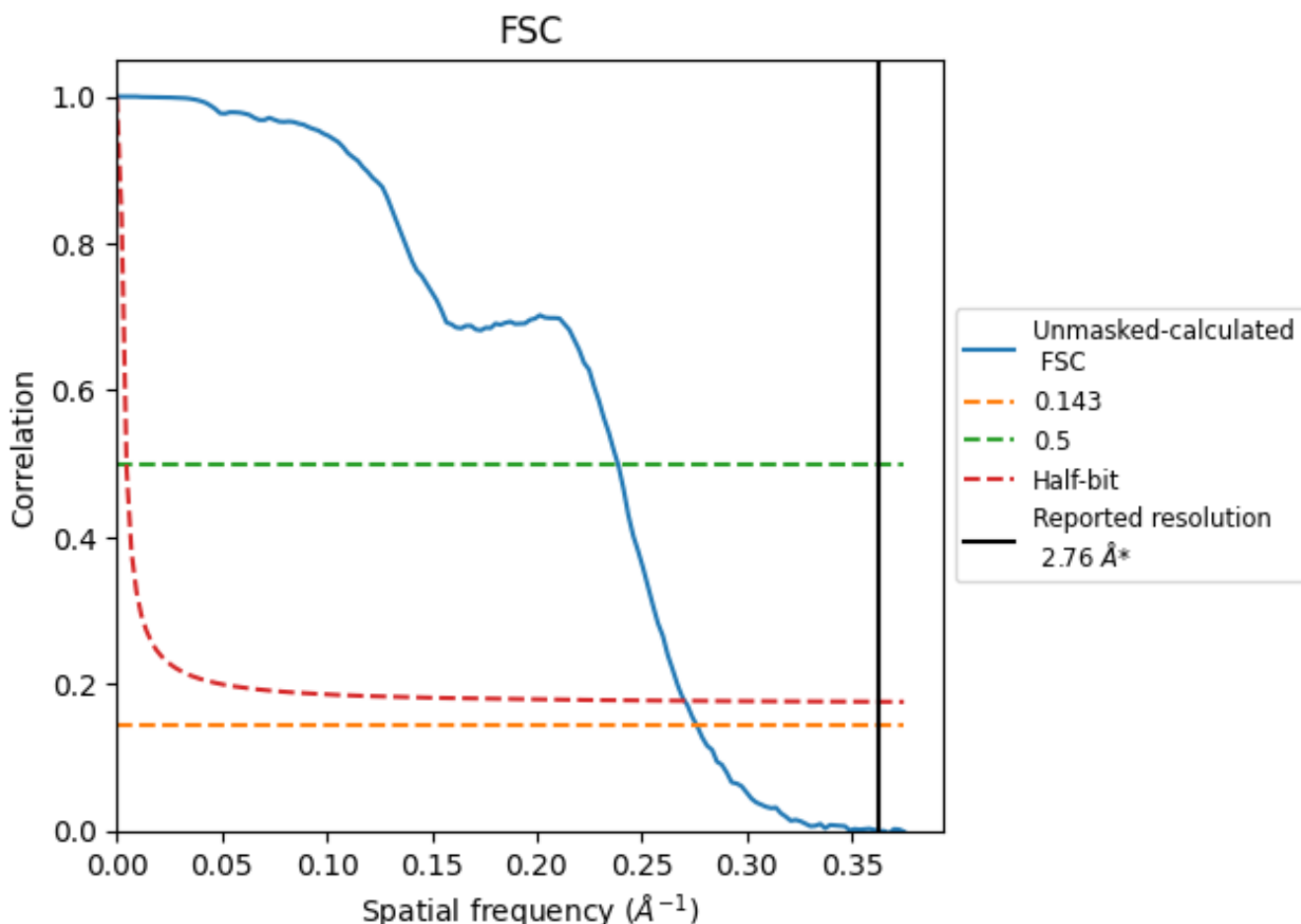
*Reported resolution corresponds to spatial frequency of 0.362 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.62	4.19	3.70

*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 3.62 differs from the reported value 2.76 by more than 10 %

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-37410 and PDB model 8WAZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1　Map-model overlay ⓘ

| X | Y | Z |
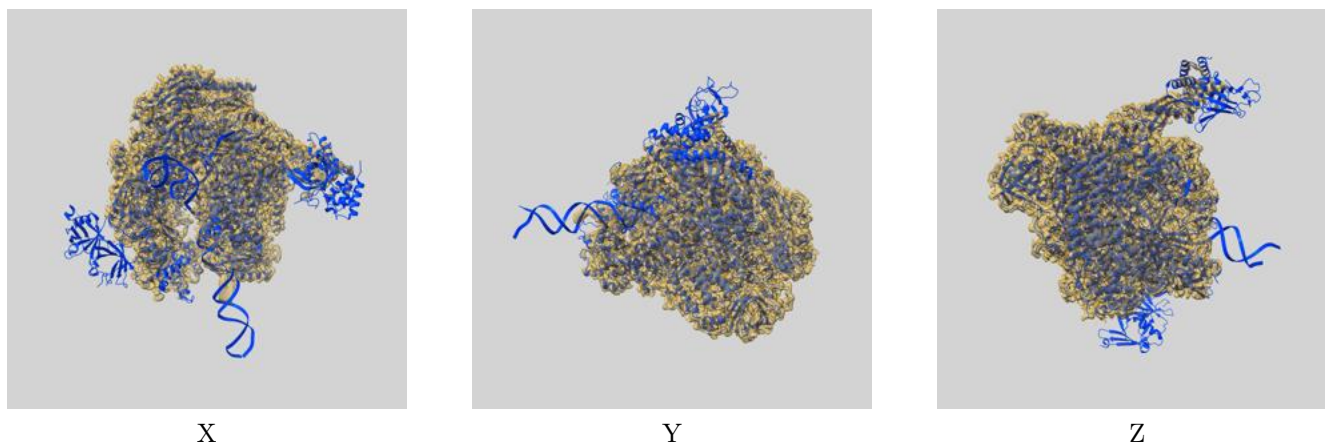
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　　　Y　　　　　　　　　　　Z
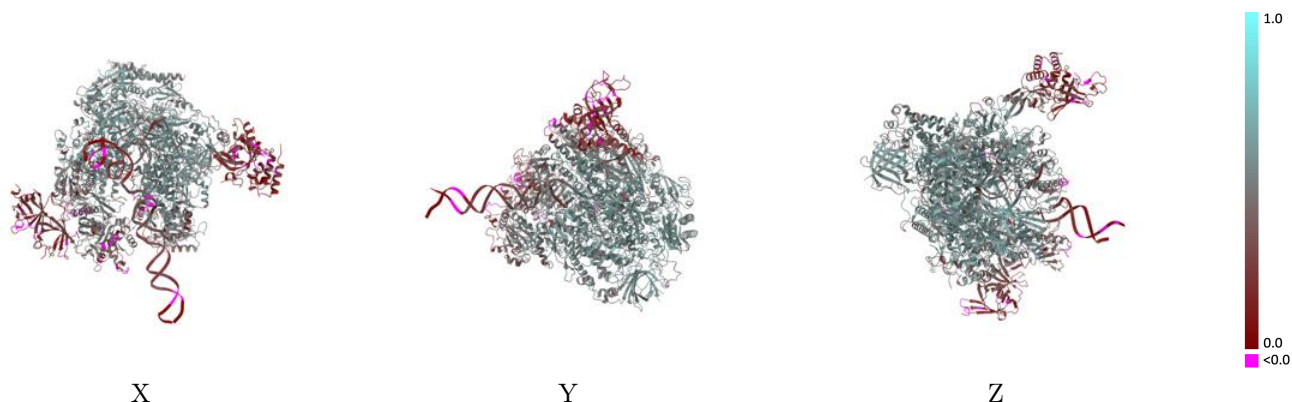
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
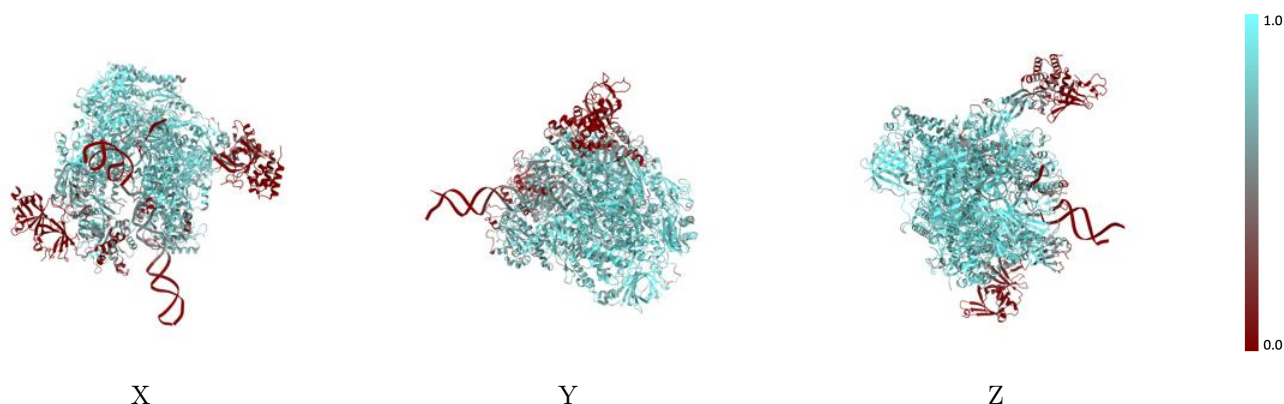
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.75).

9.4 Atom inclusion ⓘ
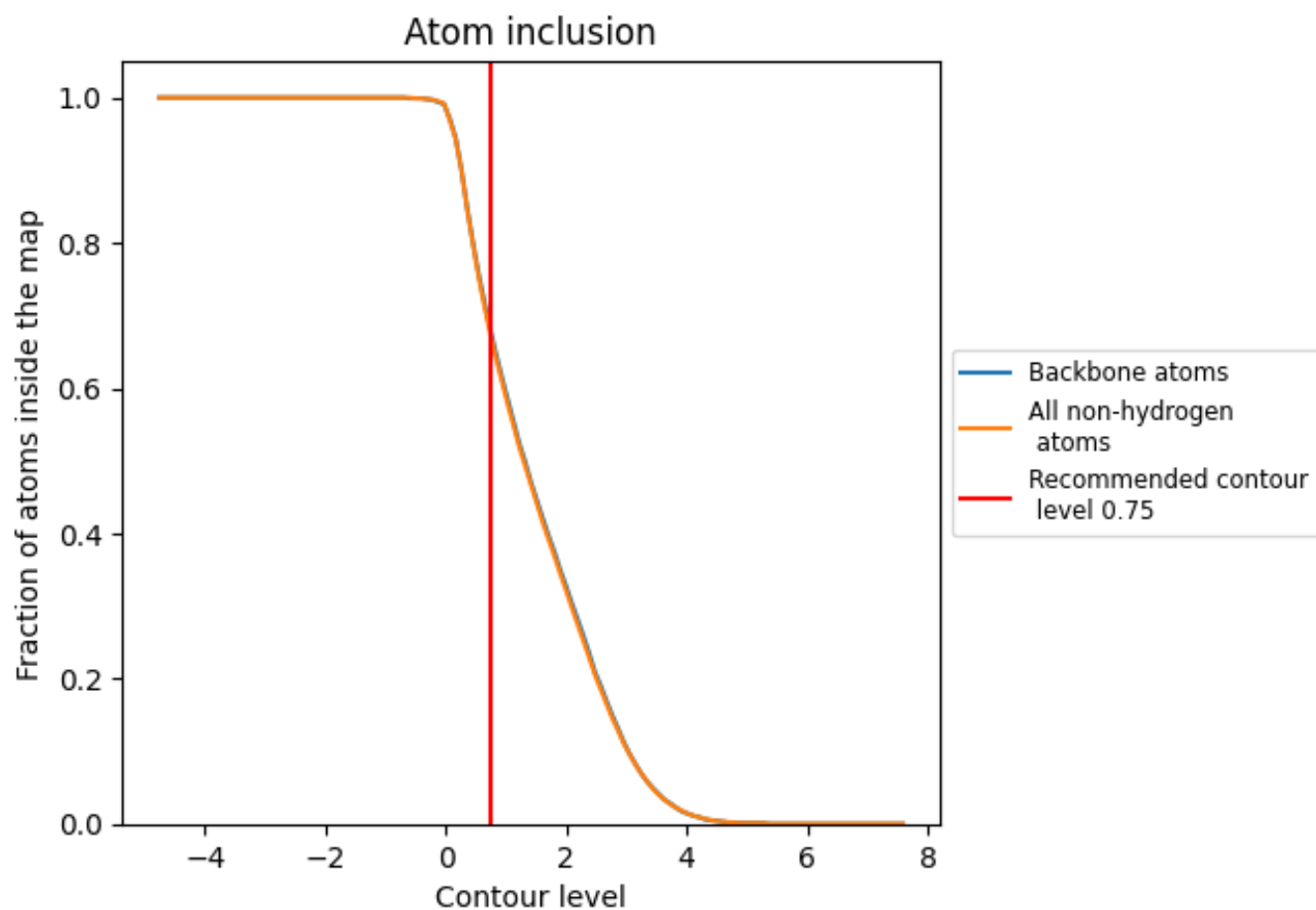
At the recommended contour level, 68% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6720	0.4590
N	0.8710	0.5780
S	0.0000	0.1780
T	0.0000	0.1650
X	0.2140	0.1860
Y	0.3820	0.2850
Z	0.7020	0.4710
o	0.7720	0.5080
p	0.7810	0.5110
q	0.8590	0.5400
r	0.1170	0.1870
s	0.7810	0.4910
t	0.8090	0.5270
u	0.3090	0.2750
v	0.8150	0.5120
w	0.7020	0.4530
x	0.8580	0.5620
y	0.8660	0.5550
z	0.7720	0.4740

1.0

0.0
<0.0