wwPDB EM Validation Summary Report ⓘ

Feb 19, 2024 – 10:31 AM EST

PDB ID	:	8H40
EMDB ID	:	EMD-34476
Title	:	Cryo-EM structure of the transcription activation complex NtcA-TAC
Authors	:	Han, S.J.; Jiang, Y.L.; You, L.L.; Shen, L.Q.; Wu, X.X.; Yang, F.; Kong, W.W.; Chen, Z.P.; Zhang, Y.; Zhou, C.Z.
Deposited on	:	2022-10-09
Resolution	:	3.60 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:

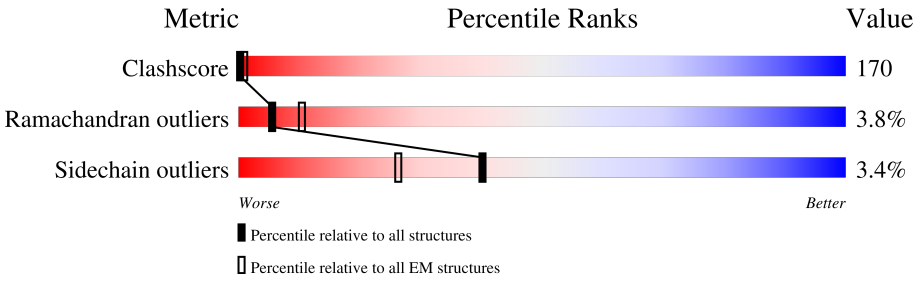
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	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	1	125	48% · 47%
2	2	125	7% 35% · 57%
3	A	1132	· 10% 41% 42% · 5%
4	B	1350	24% 8% 54% 26% · 10%
5	C	236	5% 7% 49% 37% · ·
5	D	236	9% 5% 49% 39% · ·
6	E	625	· 11% 46% 40% · ·
7	F	78	6% 21% 36% 17% · 26%

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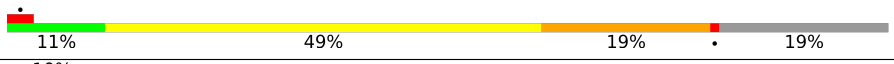
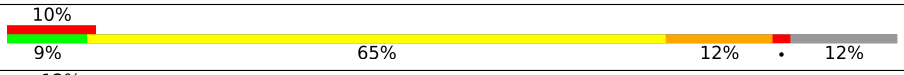
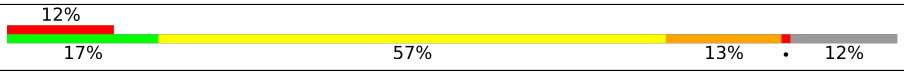
Mol	Chain	Length	Quality of chain
8	G	390	
9	X	223	
9	Y	223	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 34833 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 DNA chain called DNA (125-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	66	1358	651	243	398	66	0	0

- Molecule 2 is a DNA chain called DNA (125-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	54	1109	532	203	320	54	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1077	8473	5326	1505	1618	24	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P22703
A	1	VAL	-	expression tag	UNP P22703

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	1217	9292	5802	1639	1823	28	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	226	1762	1106	305	346	5	0	0

Continued on next page...

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	226	Total	C	N	O	S	0	0
			1762	1106	305	346	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q8YPK3
C	1	VAL	-	expression tag	UNP Q8YPK3
D	0	MET	-	initiating methionine	UNP Q8YPK3
D	1	VAL	-	expression tag	UNP Q8YPK3

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	620	Total	C	N	O	S	0	0
			4923	3107	885	910	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	58	Total	C	N	O	S	0	0
			474	290	90	90	4		

- Molecule 8 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	314	Total	C	N	O	S	0	0
			2600	1628	482	484	6		

- Molecule 9 is a protein called NtcA.

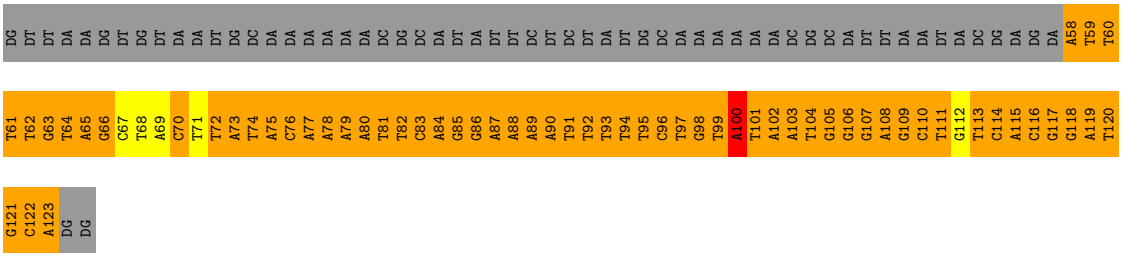
Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	196	Total	C	N	O	S	0	0
			1540	984	268	280	8		
9	Y	196	Total	C	N	O	S	0	0
			1540	984	268	280	8		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

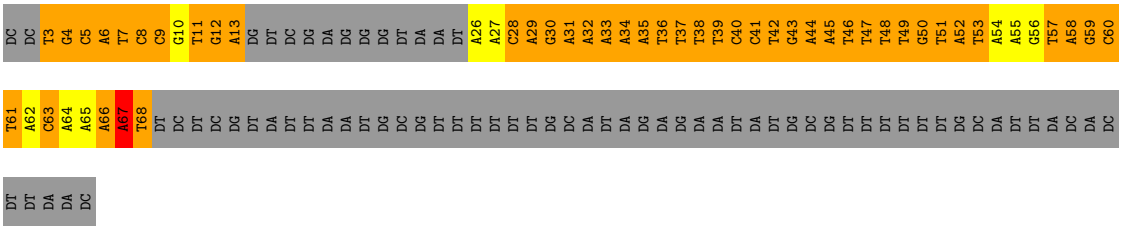
• Molecule 1: DNA (125-MER)

Chain 1:



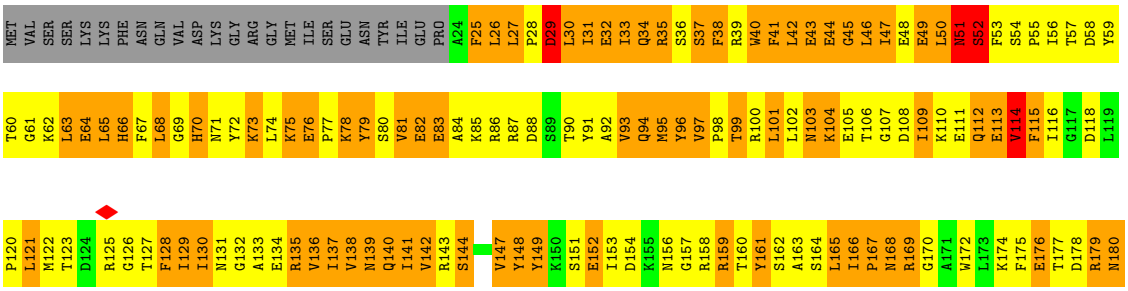
• Molecule 2: DNA (125-MER)

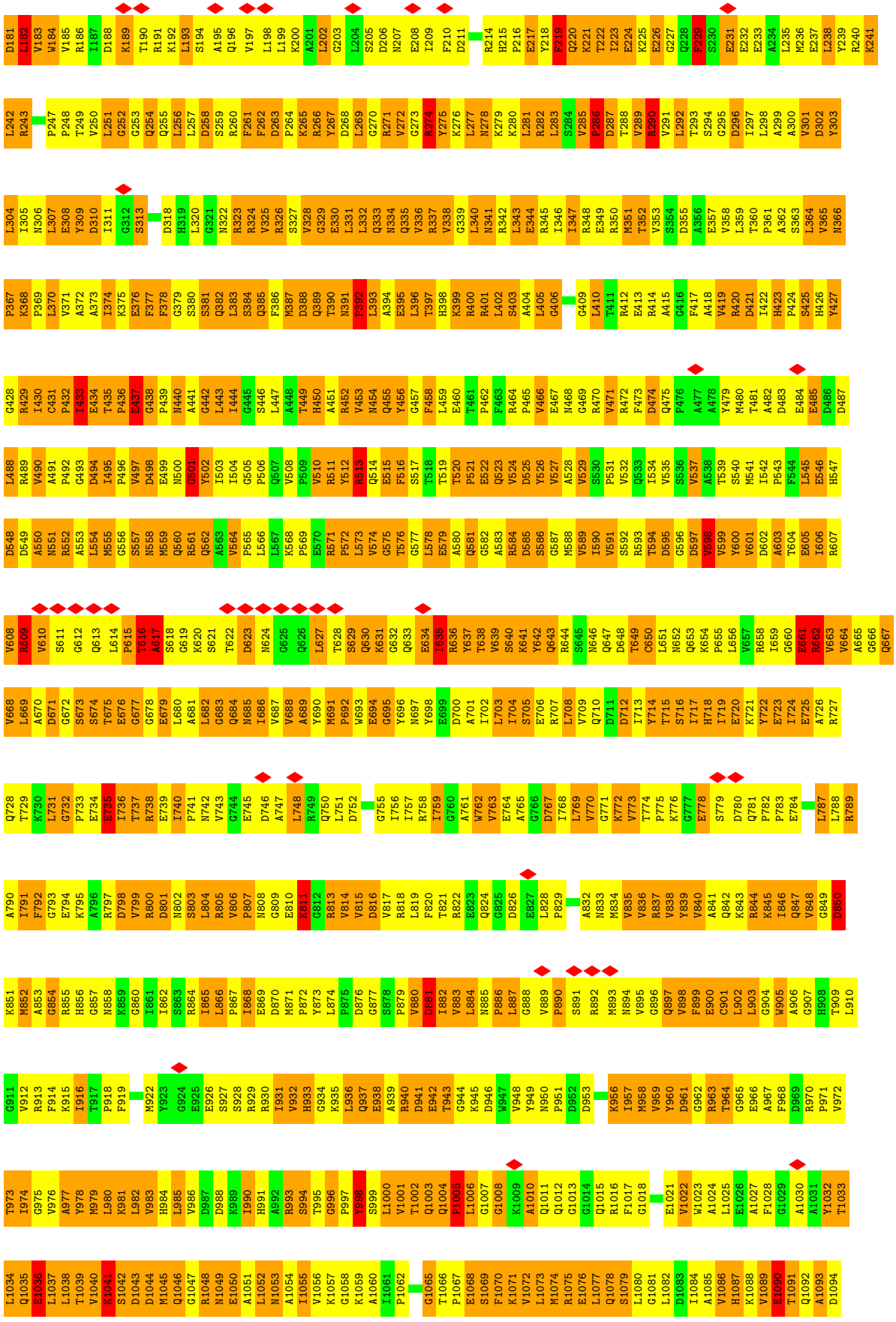
Chain 2:



• Molecule 3: DNA-directed RNA polymerase subunit beta

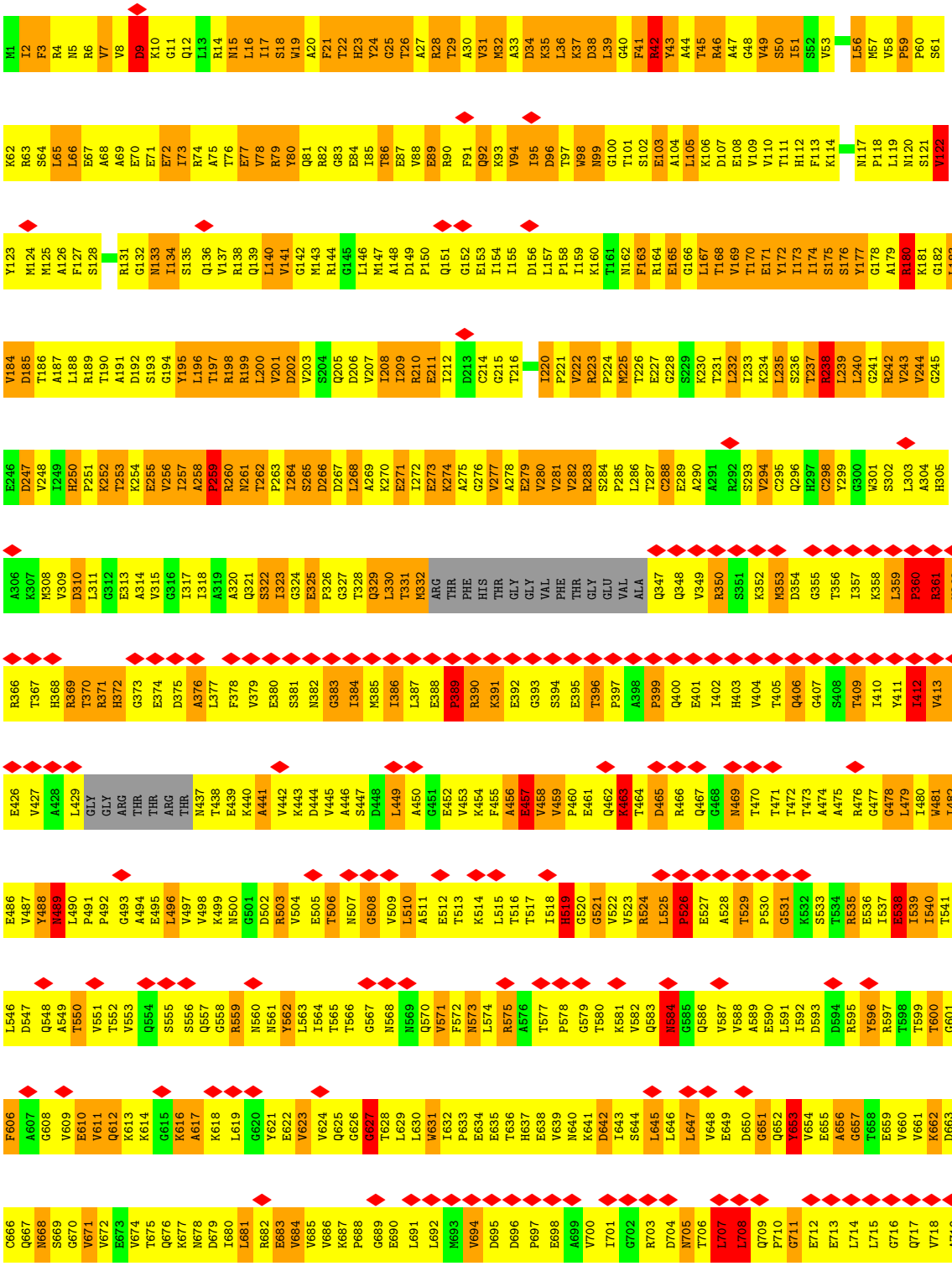
Chain A:

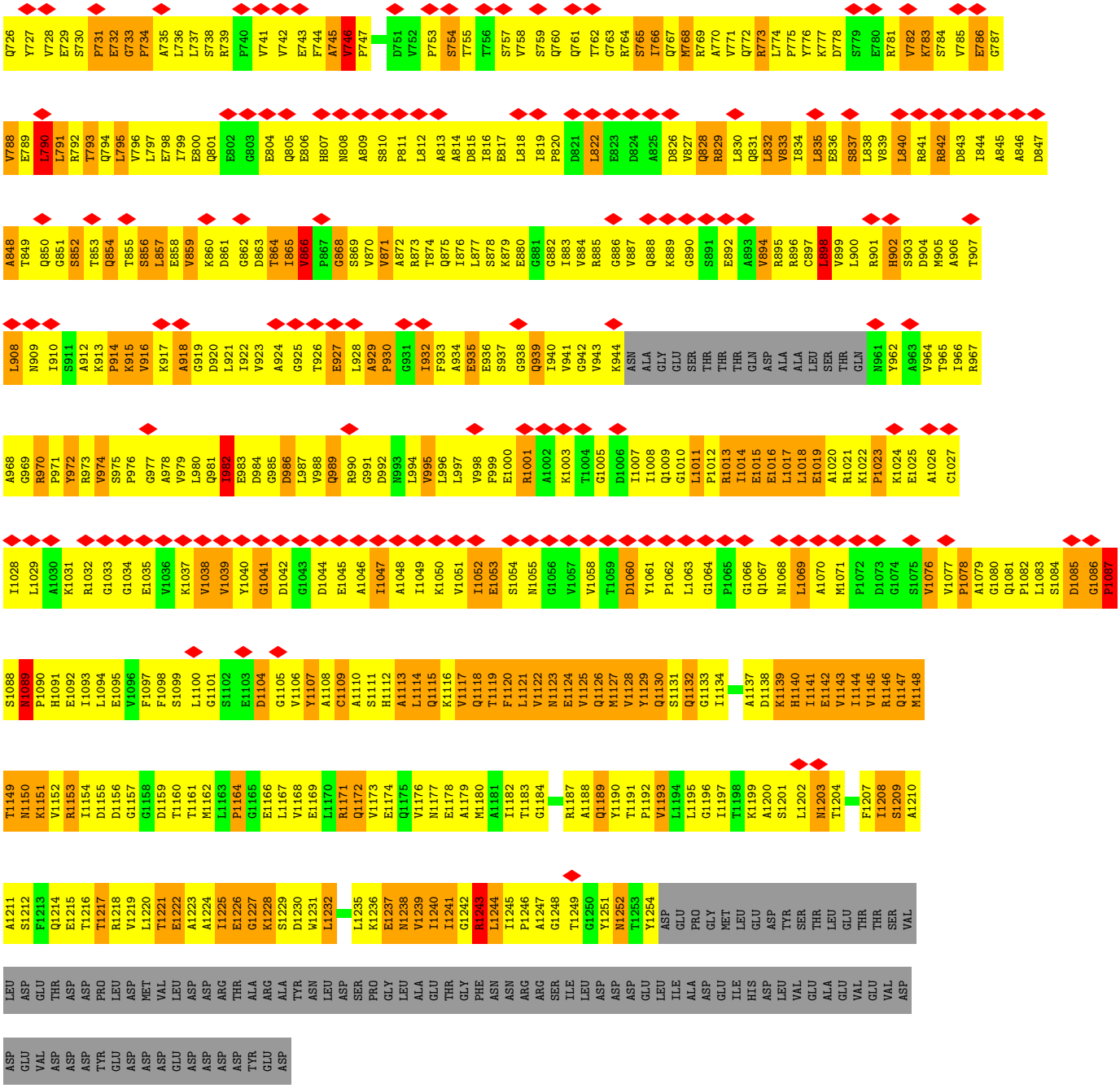



D181 L182 V183 W184 V185 R186 I187 D188 K189 T190 R191 K192 L193 S194 A195 Q196 V197 L198 L199 K200 A201 L202 G203 L204 S205 D206 N207 E208 I209 F210 D211 R214 H215 P216 E217 Y218 F219 Q220 K221 T222 I223 E224 K225 E226 G227 Q228 E229 S230 E231 E232 E233 A234 L235 M236 E237 L238 Y239 R240 K241
L242 R243 P247 P248 T249 V250 L251 G252 G253 Q254 Q255 L256 L257 D258 S259 R260 F261 F262 D263 P264 K265 R266 Y267 D268 L269 G270 R271 V272 G273 R274 Y275 K276 L277 N278 K279 K280 L281 R282 L283 S284 V285 P286 D287 T288 V289 R290 V291 L292 T293 S294 G295 D296 I297 L298 A299 A300 V301 D302 Y303
L304 I305 N306 L307 E308 Y309 D310 I311 G312 S313 D318 H319 L320 G321 N322 R323 R324 V325 R326 S327 V328 G329 Q330 L331 L332 Q333 N334 Q335 V336 R337 V338 G339 L340 N341 R342 L343 E344 R345 I346 I347 R348 E349 R350 M351 T352 V353 S354 D355 A356 E357 V358 L359 T360 P361 A362 S363 L364 V365 N366
P367 K368 P369 L370 V371 A372 A373 I374 K375 E376 F377 F378 G379 S380 S381 Q382 L383 S384 Q385 F386 M387 D388 Q389 T390 N391 P392 L393 A394 E395 L396 T397 H398 K399 R400 N401 L402 S403 A404 L405 G406 G409 L410 T411 R412 E413 R414 A415 G416 F417 A418 V419 R420 D421 I422 H423 P424 S425 H426 Y427
G428 R429 I430 C431 P432 I433 E434 T435 P436 E437 G438 P439 N440 A441 G442 L443 I444 G445 S446 L447 A448 T449 H450 A451 R452 V453 N454 Q455 Y456 G457 F458 L459 E460 T461 P462 F463 R464 P465 V466 E467 N468 G469 R470 V471 R472 F473 D474 Q475 P476 A477 A478 Y479 M480 T481 A482 D483 E484 E485 D486 D487
L488 R489 V490 A491 P492 G493 D494 I495 P496 V497 D498 E499 N500 G501 Y502 I503 I504 G505 P506 Q507 V508 P509 V510 R511 Y512 R513 Q514 E515 P516 S517 T518 T519 T520 P521 E522 Q523 V524 D525 Y526 V527 A528 V529 S530 P531 V532 Q533 I534 V535 S536 V537 A538 T539 S540 M541 I542 P543 F544 L545 E546 H547
D548 D549 A550 N551 R552 A553 L554 M555 G556 S557 N558 M559 Q560 R561 Q562 A563 V564 P565 L566 L567 K568 P569 E570 R571 P572 L573 V574 G575 T576 G577 L578 E579 A580 Q581 G582 A583 R584 D585 S586 G587 M588 V589 I590 V591 S592 R593 T594 D595 G596 D597 V598 V599 Y600 V601 D602 A603 T604 E605 I606 R607
V608 R609 V610 S611 G612 Q613 L614 P615 T616 A617 S618 G619 K620 S621 T622 D623 N624 G625 Q626 L627 T628 S629 Q630 K631 G632 Q633 E634 I635 R636 Y637 T638 V639 S640 K641 Y642 Q643 R644 S645 N646 Q647 D648 T649 C650 L651 N652 Q653 K654 P655 L656 V657 R658 I659 G660 E661 R662 V663 V664 A665 G666 Q667
V668 L669 A670 D671 G672 S673 S674 T675 E676 G677 G678 E679 L680 A681 L682 G683 Q684 N685 I686 V687 V688 A689 Y690 M691 P692 W693 E694 G695 Y696 N697 Y698 E699 D700 A701 I702 L703 I704 S705 E706 R707 L708 V709 Q710 D711 D712 I713 Y714 T715 S716 I717 H718 I719 E720 K721 Y722 E723 I724 E725 A726 R727
Q728 T729 K730 L731 G732 P733 E734 E735 I736 T737 R738 E739 I740 P741 N742 V743 G744 E745 D746 A747 L748 R749 Q750 L751 D752 G755 I756 I757 R758 I759 G760 A761 W762 V763 E764 A765 G766 D767 I768 L769 V770 G771 K772 V773 T774 P775 K776 G777 E778 S779 D780 Q781 P782 P783 E784 L787 L788 R789
A790 I791 F792 G793 E794 K795 A796 R797 D798 V799 R800 D801 N802 S803 L804 R805 V806 P807 N808 G809 E810 R811 G812 R813 V814 V815 D816 V817 R818 L819 F820 T821 R822 E823 Q824 G825 D826 E827 L828 P829 A832 N833 M834 V835 V836 R837 V838 Y839 V840 A841 Q842 K843 R844 K845 I846 Q847 V848 G849 D850
K851 M852 A853 G854 R855 H856 G857 N858 K859 G860 I861 I862 S863 R864 I865 L866 P867 I868 E869 D870 M871 P872 Y873 L874 P875 D876 G877 S878 P879 V880 D881 I882 V883 L884 N885 P886 L887 G888 V889 P890 S891 R892 M893 N894 V895 G896 Q897 V898 F899 E900 C901 L902 L903 G904 W905 A906 G907 H908 T909 L910
G911 V912 R913 F914 K915 I916 T917 P918 F919 M922 Y923 G924 E925 E926 S927 S928 R929 R930 I931 V932 H933 G934 K935 L936 Q937 E938 A939 R940 D941 E942 T943 G944 K945 D946 W947 V948 Y949 N950 P951 D952 D953 K956 I957 M958 V959 Y960 D961 G962 R963 T964 G965 E966 A967 F968 D969 R970 P971 V972
T973 I974 G975 V976 A977 Y978 M979 L980 K981 L982 V983 H984 L985 V986 D987 D988 K989 I990 H991 A992 R993 S994 T995 G996 P997 Y998 S999 L1000 V1001 T1002 Q1003 Q1004 P1005 L1006 G1007 G1008 K1009 A1010 Q1011 Q1012 G1013 G1014 Q1015 R1016 F1017 G1018 E1021 V1022 W1023 A1024 L1025 E1026 A1027 F1028 G1029 A1030 A1031 Y1032 T1033
L1034 Q1035 E1036 L1037 L1038 T1039 V1040 K1041 S1042 D1043 D1044 M1045 Q1046 G1047 R1048 N1049 E1050 A1051 L1052 N1053 A1054 I1055 V1056 K1057 G1058 K1059 A1060 I1061 P1062 G1065 T1066 P1067 E1068 S1069 F1070 K1071 V1072 L1073 M1074 R1075 E1076 L1077 Q1078 S1079 L1080 G1081 L1082 D1083 I1084 A1085 V1086 H1087 K1088 V1089 E1090 T1091 Q1092 A1093 D1094

• Molecule 4: DNA-directed RNA polymerase subunit beta'

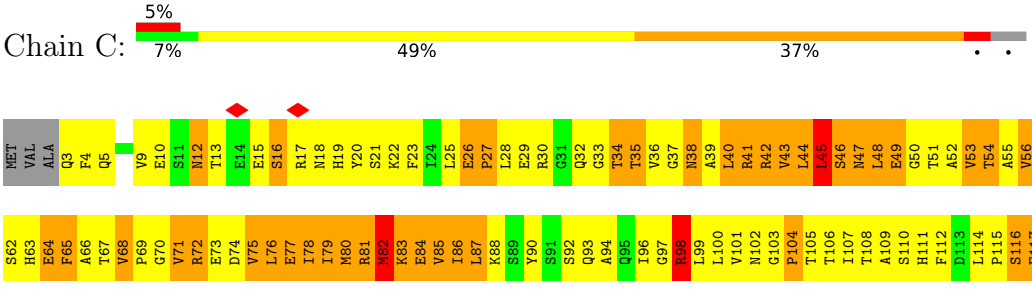
Chain B:

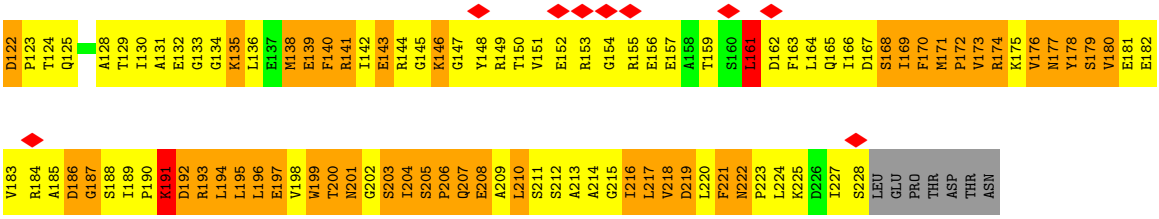




• Molecule 5: DNA-directed RNA polymerase subunit alpha

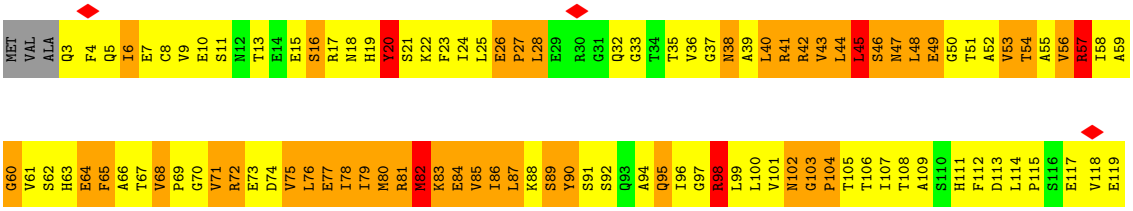
Chain C:

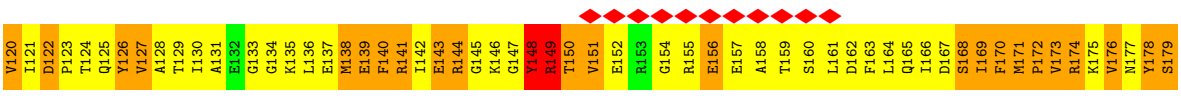


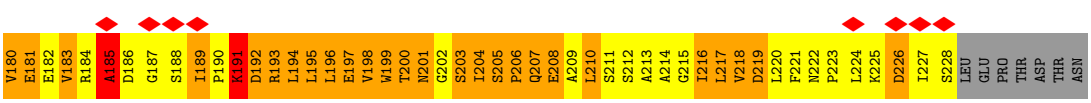


• Molecule 5: DNA-directed RNA polymerase subunit alpha

Chain D:

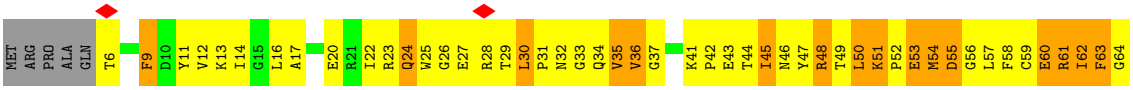


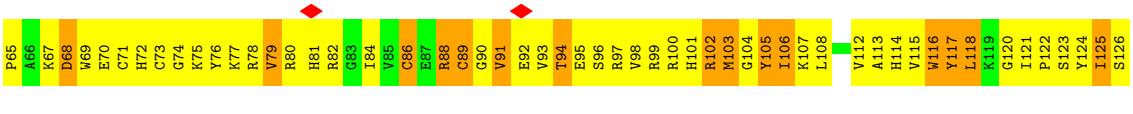


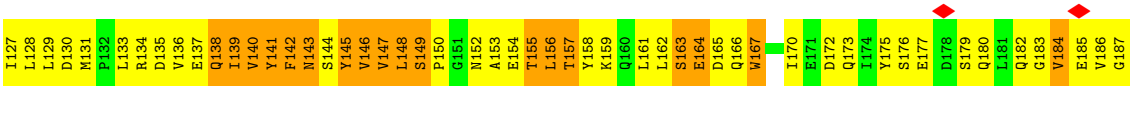


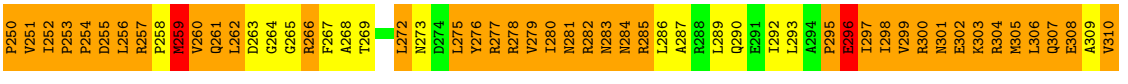
• Molecule 6: DNA-directed RNA polymerase subunit gamma

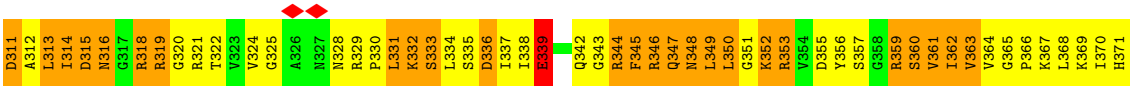
Chain E:

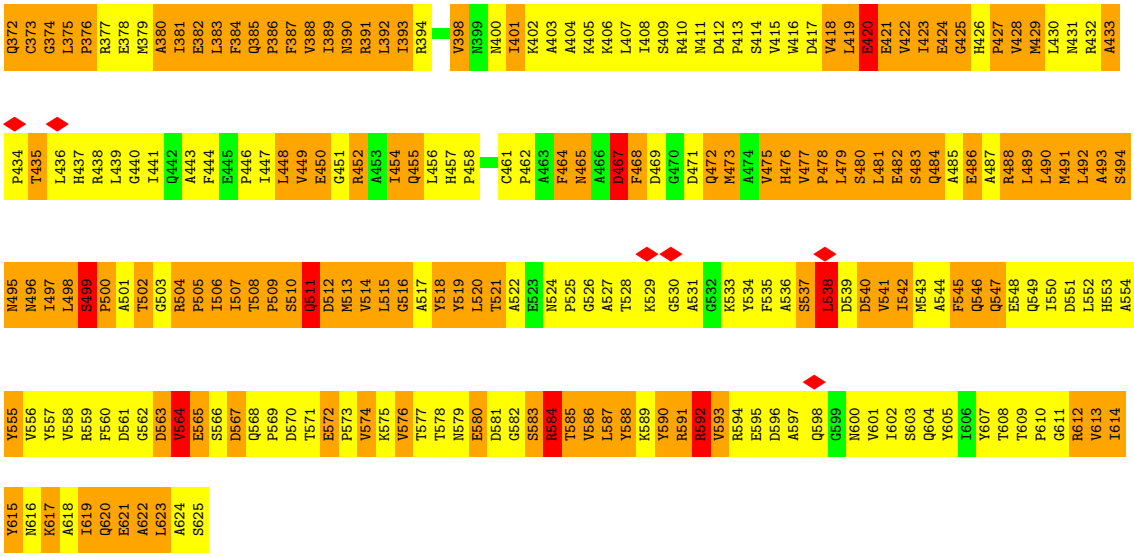






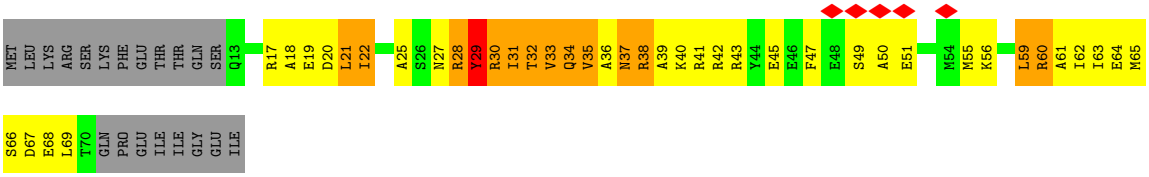






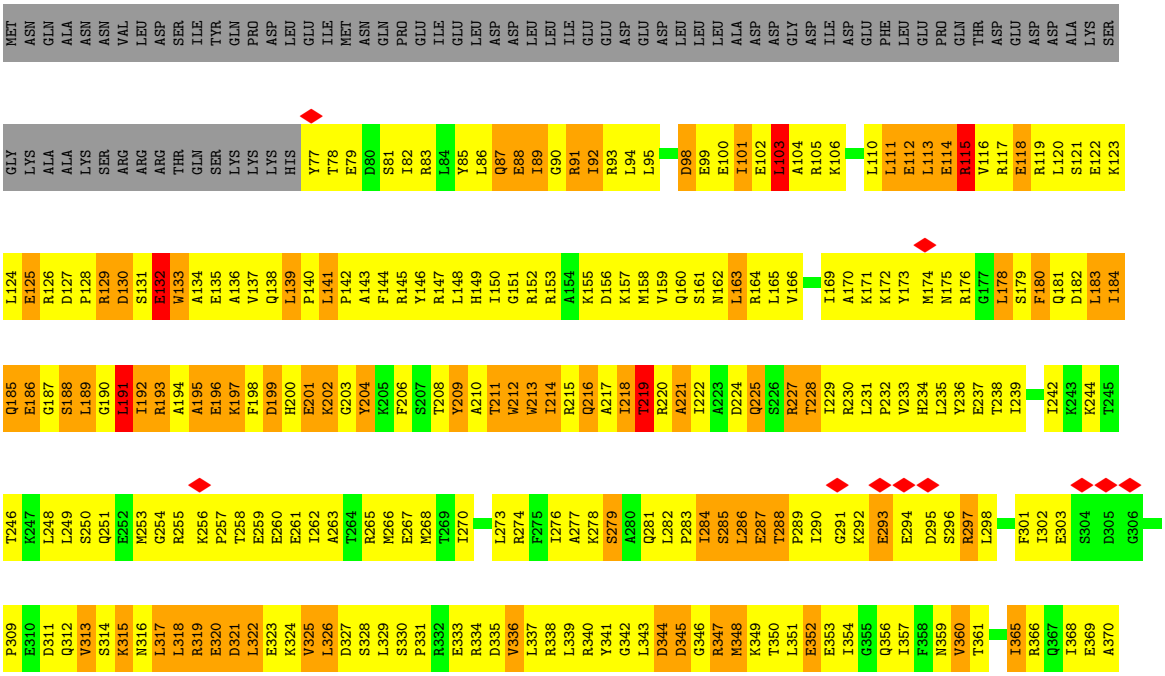
• Molecule 7: DNA-directed RNA polymerase subunit omega

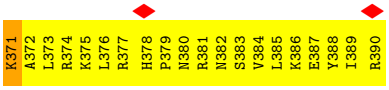
Chain F:



• Molecule 8: RNA polymerase sigma factor SigA

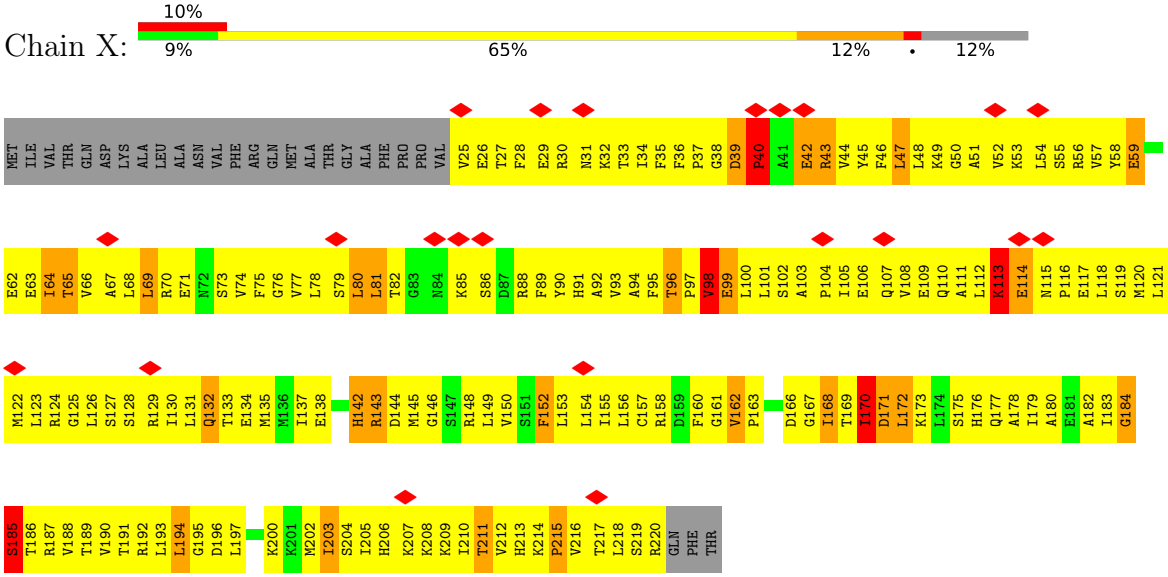
Chain G:





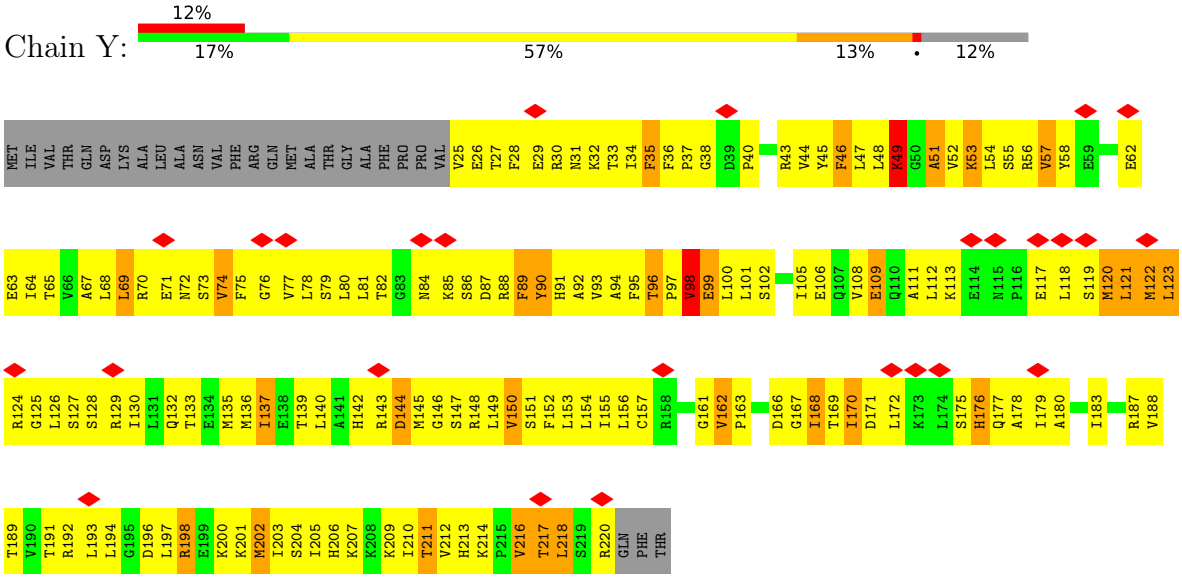
• Molecule 9: NtcA

Chain X:



• Molecule 9: NtcA

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45239	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	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

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	1	6.62	598/1523 (39.3%)	2.59	159/2350 (6.8%)
2	2	6.00	432/1244 (34.7%)	2.54	114/1915 (6.0%)
3	A	3.14	815/8632 (9.4%)	1.90	342/11688 (2.9%)
4	B	2.10	345/9414 (3.7%)	1.57	200/12760 (1.6%)
5	C	2.79	124/1788 (6.9%)	1.89	69/2420 (2.9%)
5	D	2.95	144/1788 (8.1%)	1.95	73/2420 (3.0%)
6	E	3.21	485/5014 (9.7%)	1.80	189/6789 (2.8%)
7	F	2.32	22/478 (4.6%)	1.46	12/639 (1.9%)
8	G	1.87	81/2635 (3.1%)	1.39	45/3533 (1.3%)
9	X	0.99	8/1563 (0.5%)	1.27	15/2107 (0.7%)
9	Y	0.94	6/1563 (0.4%)	1.27	20/2107 (0.9%)
All	All	3.06	3060/35642 (8.6%)	1.79	1238/48728 (2.5%)

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	1	0	1
2	2	0	1
3	A	0	48
4	B	0	87
5	C	0	10
5	D	0	13
6	E	0	17
7	F	0	1
8	G	0	6
9	X	0	5
9	Y	0	6
All	All	0	195

The worst 5 of 3060 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	62	DT	C1'-N1	-26.91	1.09	1.47
2	2	33	DA	N9-C4	-25.87	1.22	1.37
1	1	77	DA	N9-C4	-25.79	1.22	1.37
2	2	66	DA	N9-C4	-25.75	1.22	1.37
2	2	67	DA	O3'-P	24.28	1.90	1.61

The worst 5 of 1238 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Y	120	MET	CA-CB-CG	-20.38	78.66	113.30
9	X	113	LYS	CD-CE-NZ	-20.09	65.49	111.70
4	B	1018	LEU	CA-CB-CG	-19.77	69.82	115.30
4	B	239	LEU	CA-CB-CG	-19.46	70.55	115.30
9	X	172	LEU	CB-CG-CD1	18.29	142.09	111.00

There are no chirality outliers.

5 of 195 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	100	DA	Sidechain
2	2	67	DA	Sidechain
3	A	51	ASN	Peptide
3	A	52	SER	Mainchain
3	A	75	LYS	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	1	1358	0	694	737	0
2	2	1109	0	574	622	0
3	A	8473	0	8480	2770	0
4	B	9292	0	9457	3586	0
5	C	1762	0	1772	621	0
5	D	1762	0	1772	616	0
6	E	4923	0	4987	1470	0
7	F	474	0	477	96	0
8	G	2600	0	2685	873	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	X	1540	0	1613	549	0
9	Y	1540	0	1616	480	0
All	All	34833	0	34127	11682	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 170.

The worst 5 of 11682 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:B:125:MET:HG2	6:E:515:LEU:CD2	1.24	1.65
9:X:42:GLU:CB	9:X:78:LEU:HB3	1.25	1.64
9:Y:78:LEU:CD2	9:Y:88:ARG:HG2	1.15	1.62
3:A:74:LEU:HD21	3:A:95:MET:CG	1.14	1.60
6:E:28:ARG:NH2	6:E:102:ARG:CD	1.67	1.57

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
3	A	1075/1132 (95%)	634 (59%)	407 (38%)	34 (3%)	4 31
4	B	1209/1350 (90%)	684 (57%)	466 (38%)	59 (5%)	2 21
5	C	224/236 (95%)	131 (58%)	84 (38%)	9 (4%)	3 26
5	D	224/236 (95%)	144 (64%)	72 (32%)	8 (4%)	3 29
6	E	618/625 (99%)	405 (66%)	195 (32%)	18 (3%)	4 33
7	F	56/78 (72%)	36 (64%)	19 (34%)	1 (2%)	8 43
8	G	312/390 (80%)	201 (64%)	100 (32%)	11 (4%)	3 30
9	X	194/223 (87%)	122 (63%)	61 (31%)	11 (6%)	1 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Y	194/223 (87%)	124 (64%)	64 (33%)	6 (3%)	4	32
All	All	4106/4493 (91%)	2481 (60%)	1468 (36%)	157 (4%)	5	27

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	615	PRO
3	A	616	THR
3	A	636	ARG
3	A	778	GLU
3	A	890	PRO

5.3.2 Protein sidechains (i)

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	
3	A	918/969 (95%)	889 (97%)	29 (3%)	39	70
4	B	1017/1132 (90%)	983 (97%)	34 (3%)	38	69
5	C	196/205 (96%)	189 (96%)	7 (4%)	35	67
5	D	196/205 (96%)	189 (96%)	7 (4%)	35	67
6	E	534/538 (99%)	510 (96%)	24 (4%)	27	62
7	F	50/69 (72%)	50 (100%)	0	100	100
8	G	282/351 (80%)	272 (96%)	10 (4%)	36	68
9	X	172/194 (89%)	167 (97%)	5 (3%)	42	72
9	Y	172/194 (89%)	167 (97%)	5 (3%)	42	72
All	All	3537/3857 (92%)	3416 (97%)	121 (3%)	40	69

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	1189	GLN
8	G	387	GLU

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Mol	Chain	Res	Type
5	D	95	GLN
8	G	371	LYS
9	Y	137	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
5	C	93	GLN
5	D	125	GLN
8	G	378	HIS
5	C	125	GLN
5	D	18	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	18
6	E	16
4	B	7
5	C	5
5	D	5
8	G	2
2	2	1

The worst 5 of 54 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	67:DA	O3'	68:DT	P	1.90
1	A	144:SER	C	145:PRO	N	1.20
1	E	256:LEU	C	257:ARG	N	1.20
1	E	374:GLY	C	375:LEU	N	1.20
1	A	247:PRO	C	248:PRO	N	1.19

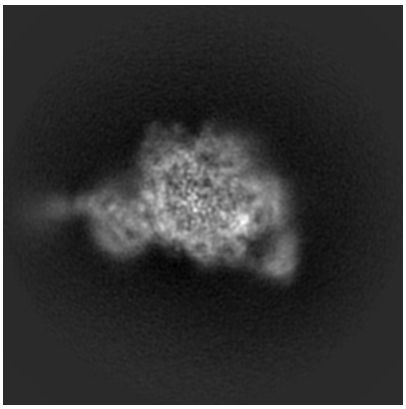
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34476. These allow visual inspection of the internal detail of the map and identification of artifacts.

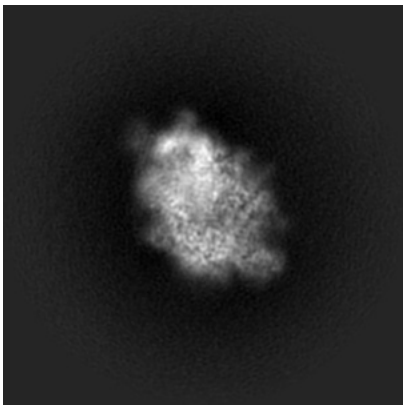
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

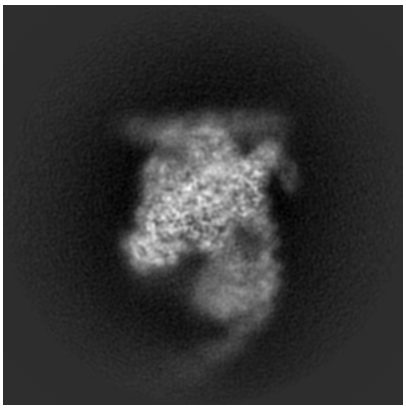
6.1.1 Primary map



X

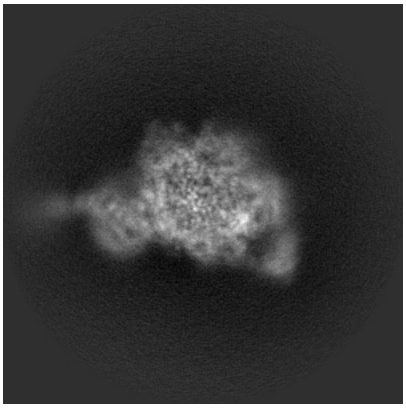


Y

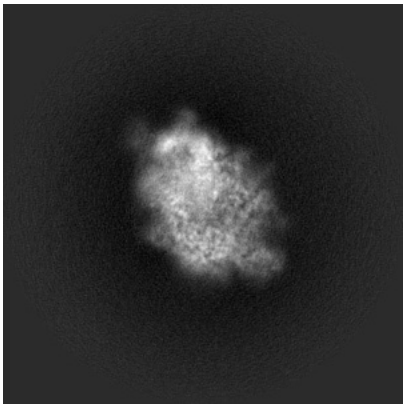


Z

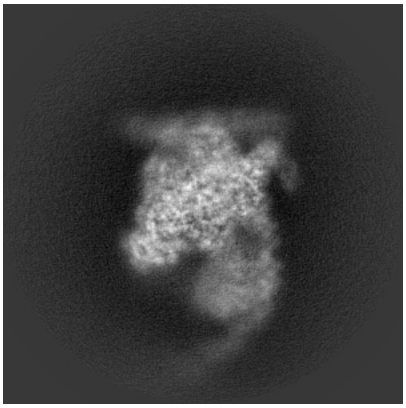
6.1.2 Raw map



X



Y

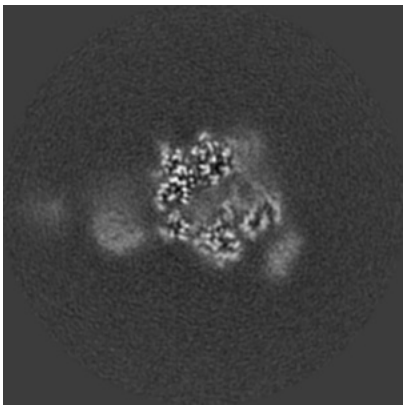


Z

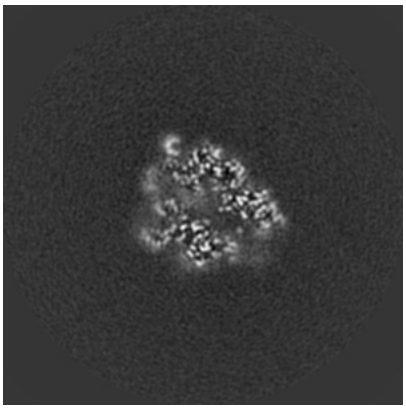
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

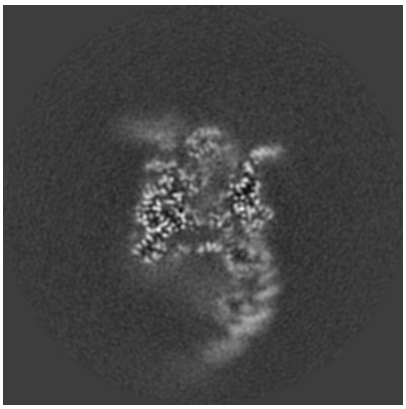
6.2.1 Primary map



X Index: 150

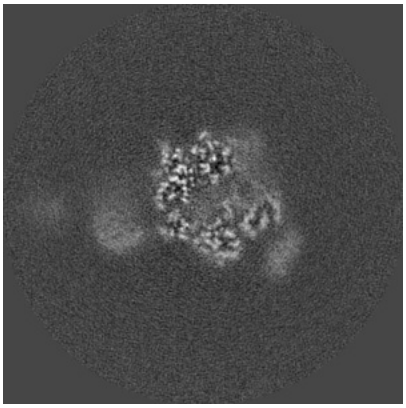


Y Index: 150

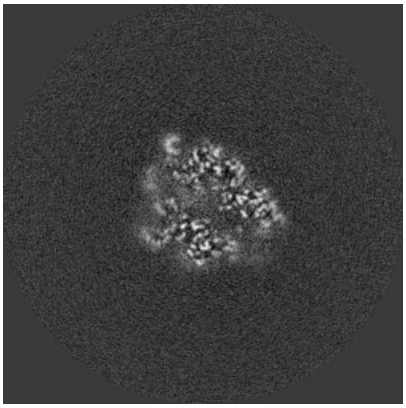


Z Index: 150

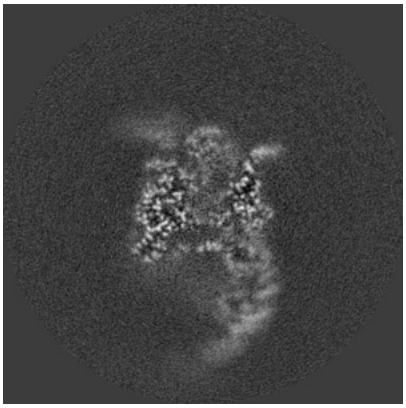
6.2.2 Raw map



X Index: 150



Y Index: 150

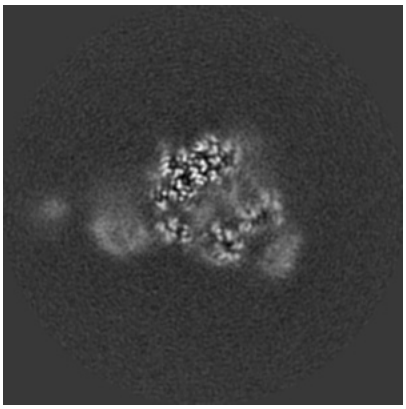


Z Index: 150

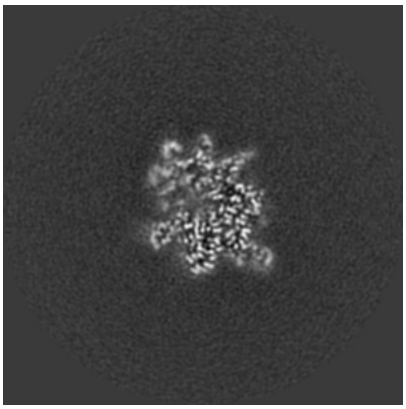
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

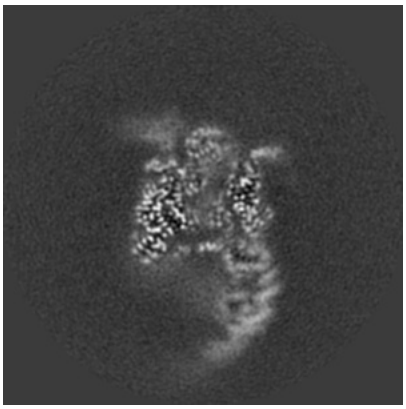
6.3.1 Primary map



X Index: 154

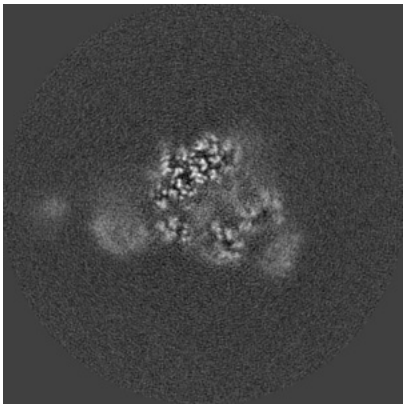


Y Index: 143

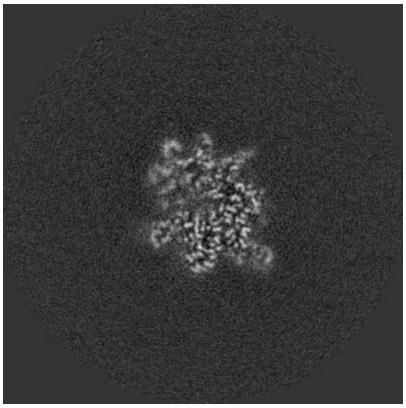


Z Index: 149

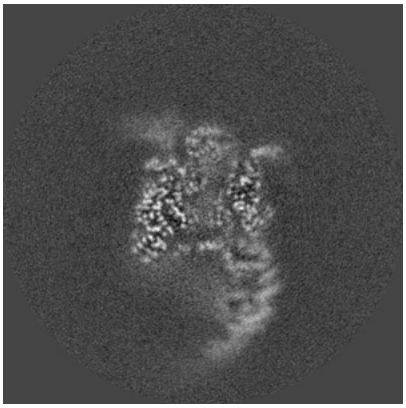
6.3.2 Raw map



X Index: 154



Y Index: 143

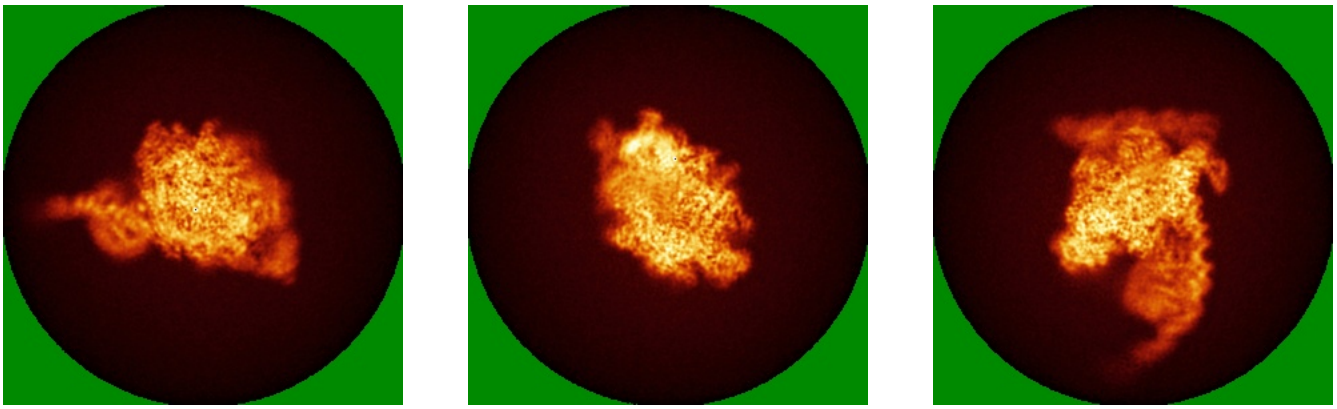


Z Index: 149

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

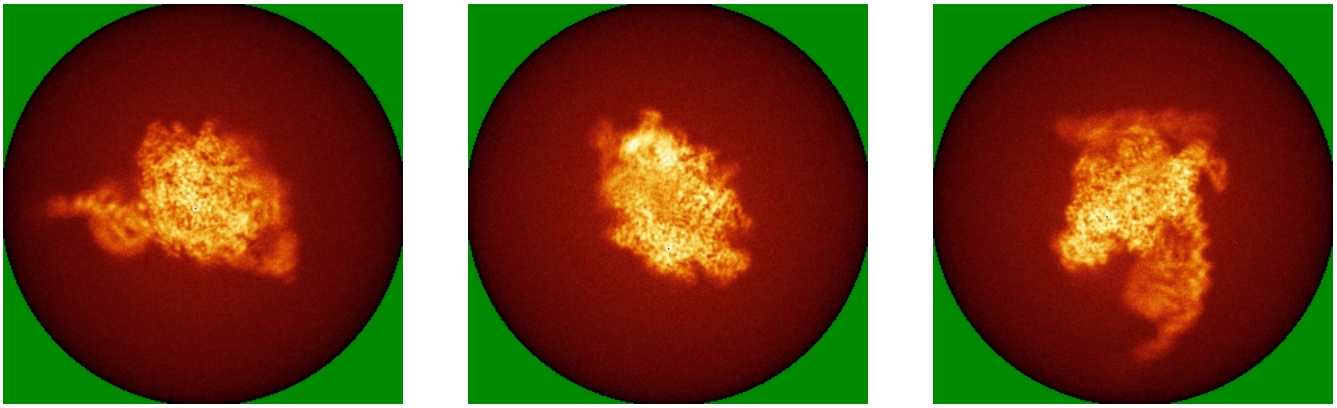
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

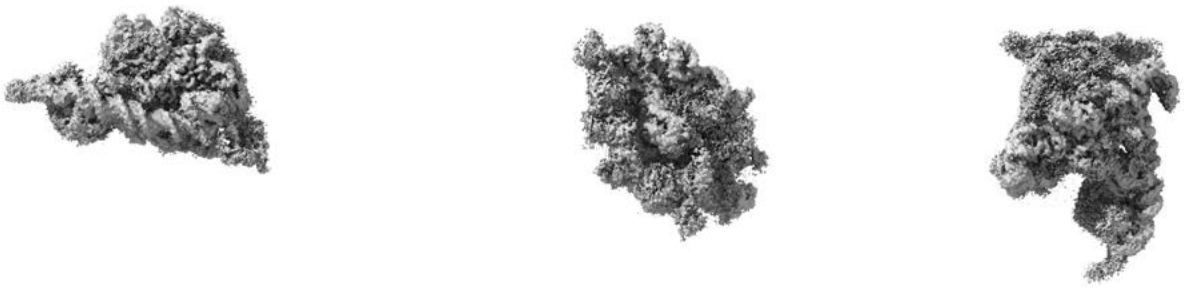
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

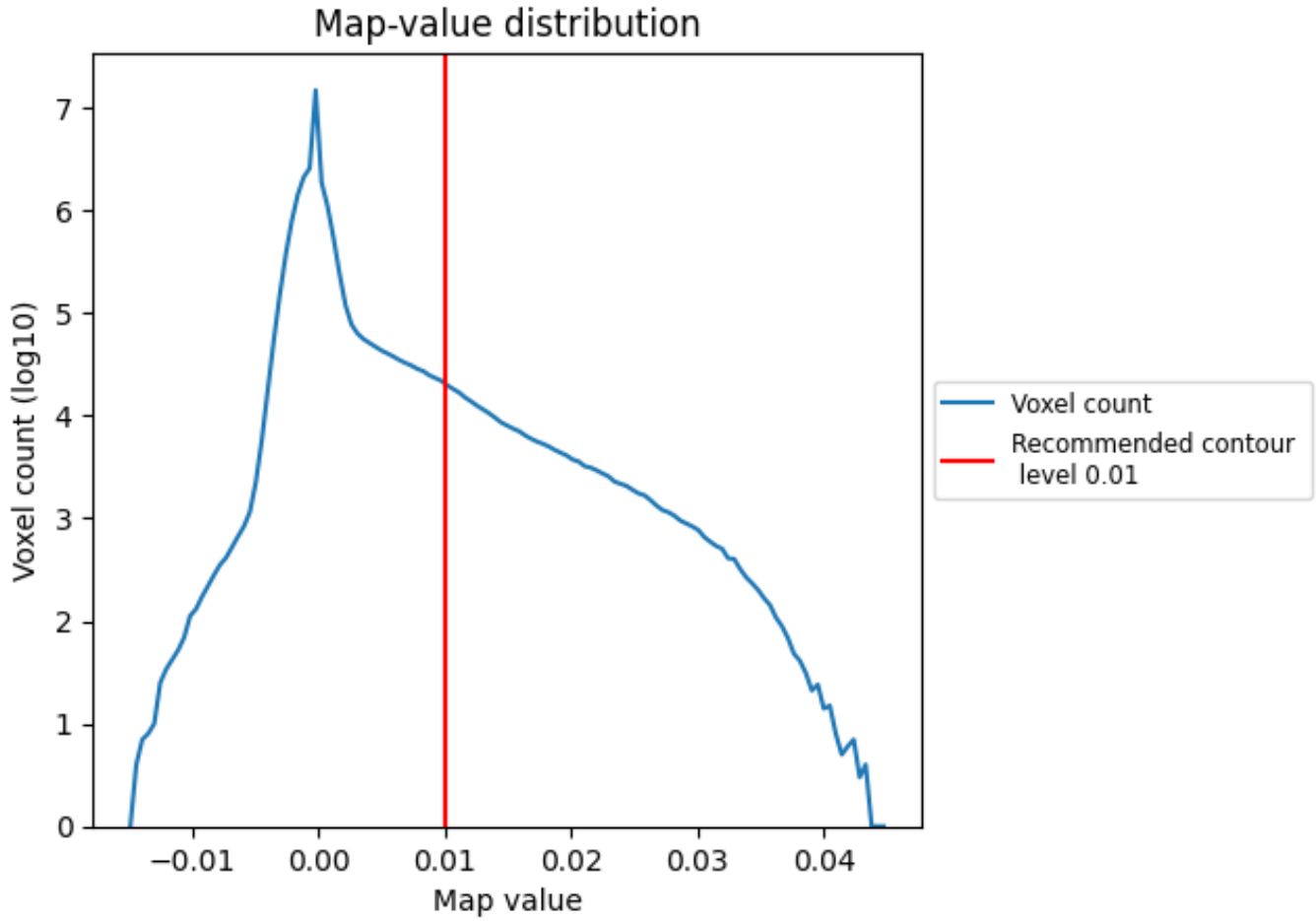
6.6 Mask visualisation (i)

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

7 Map analysis

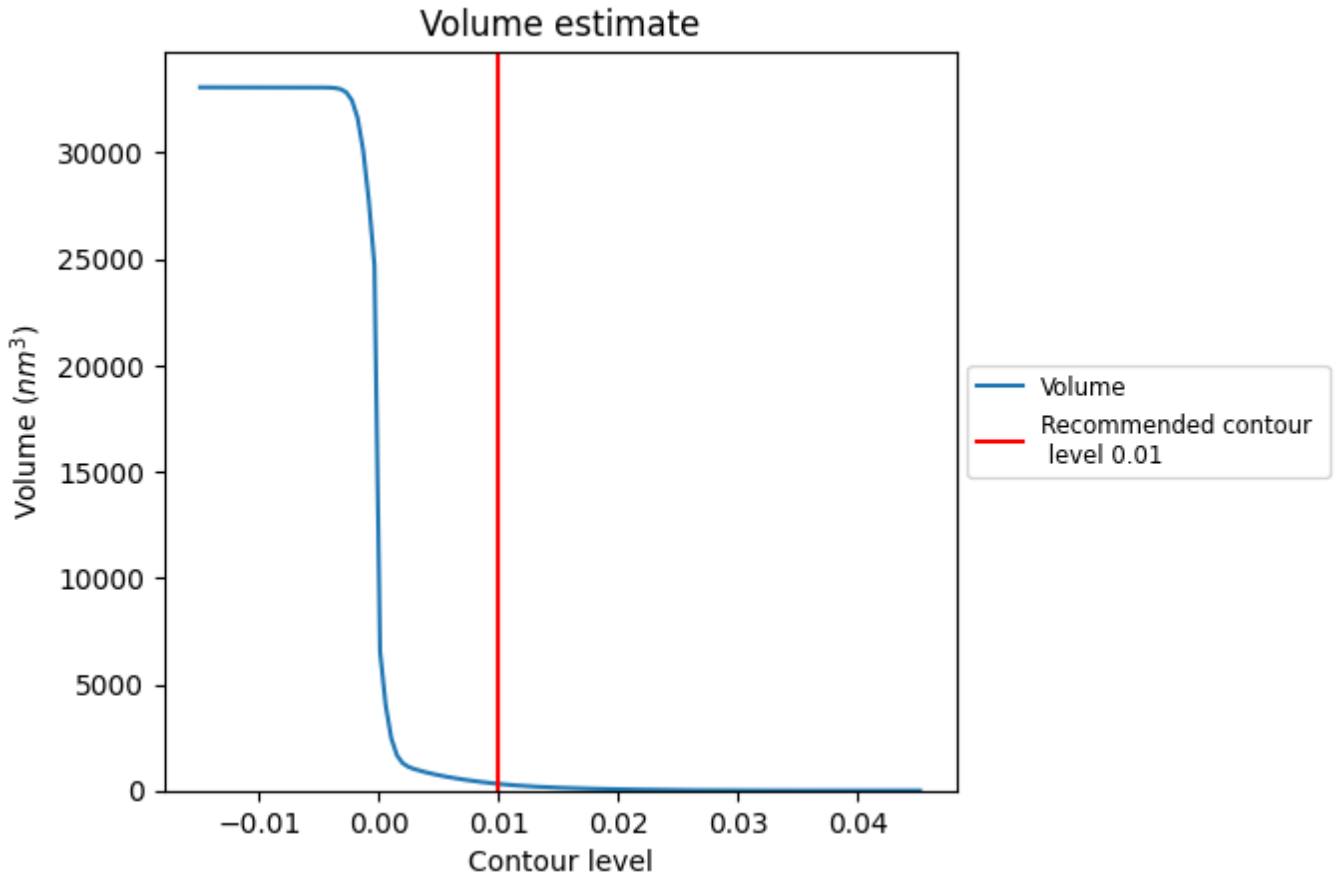
This section contains the results of statistical analysis of the map.

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.

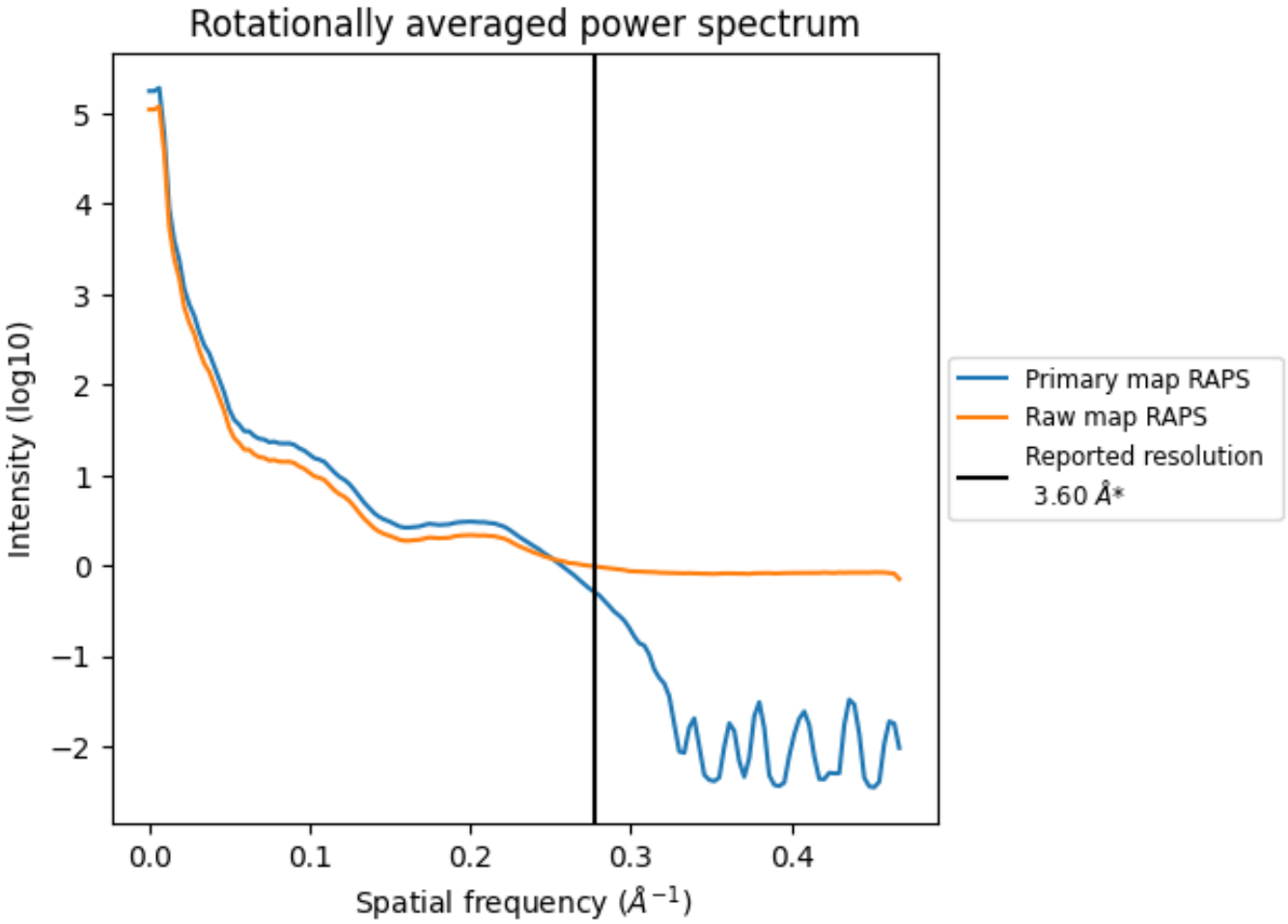
7.2 Volume estimate (i)



The volume at the recommended contour level is 315 nm^3; this corresponds to an approximate mass of 284 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 (i)

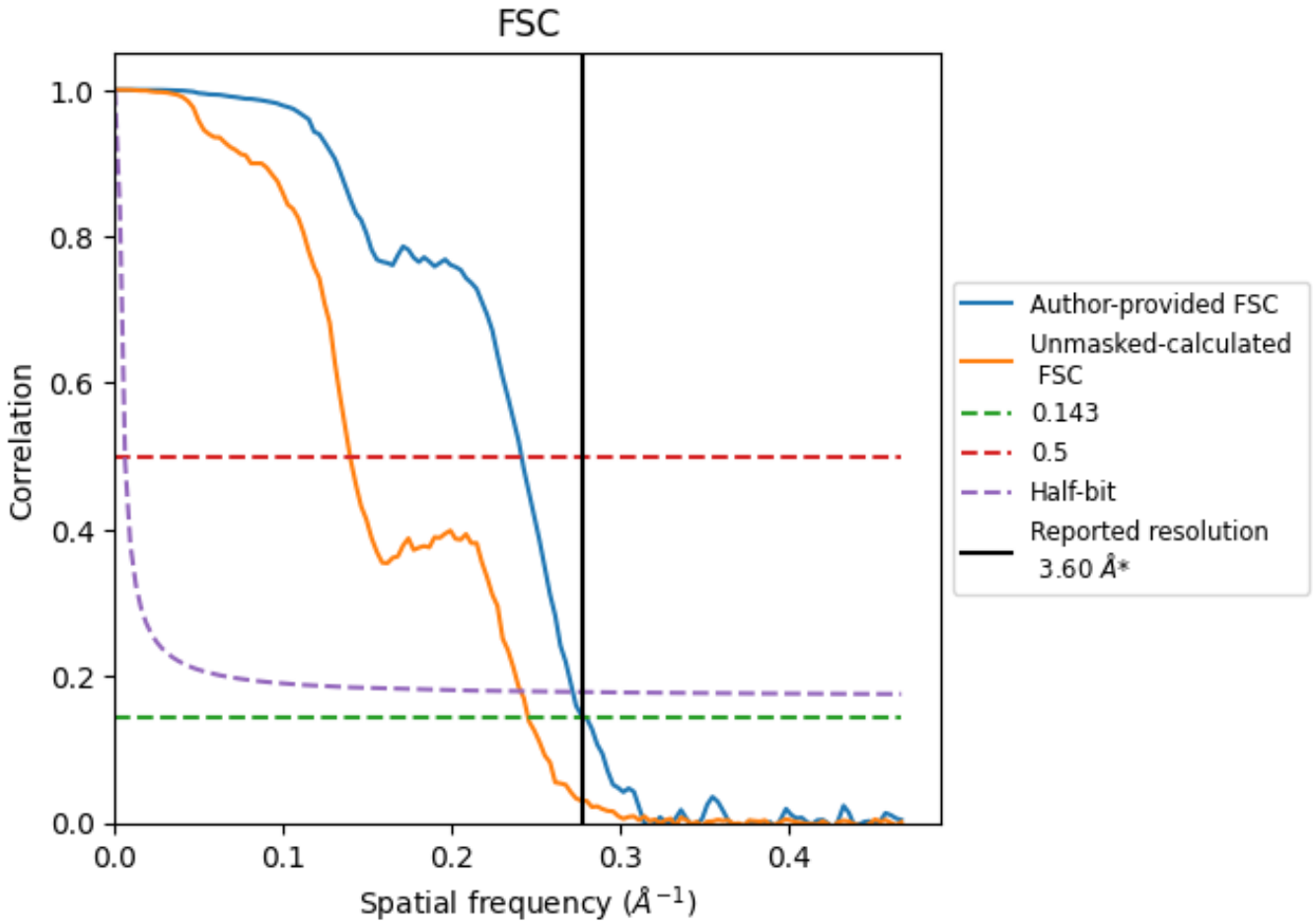


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 (i)

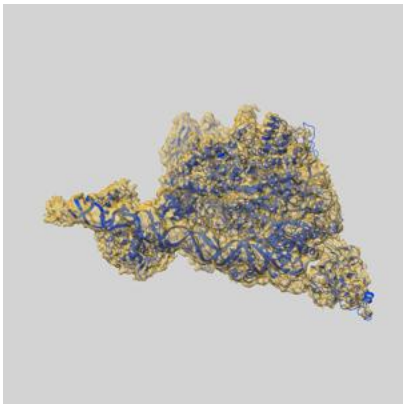
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.14	3.67
Unmasked-calculated*	4.07	7.15	4.15

*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 4.07 differs from the reported value 3.6 by more than 10 %

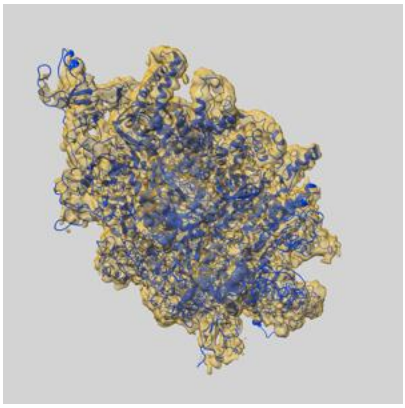
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34476 and PDB model 8H40. Per-residue inclusion information can be found in section 3 on page 6.

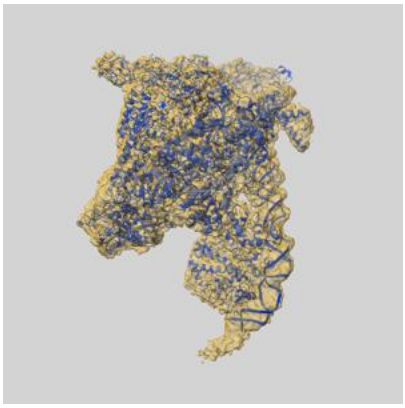
9.1 Map-model overlay



X



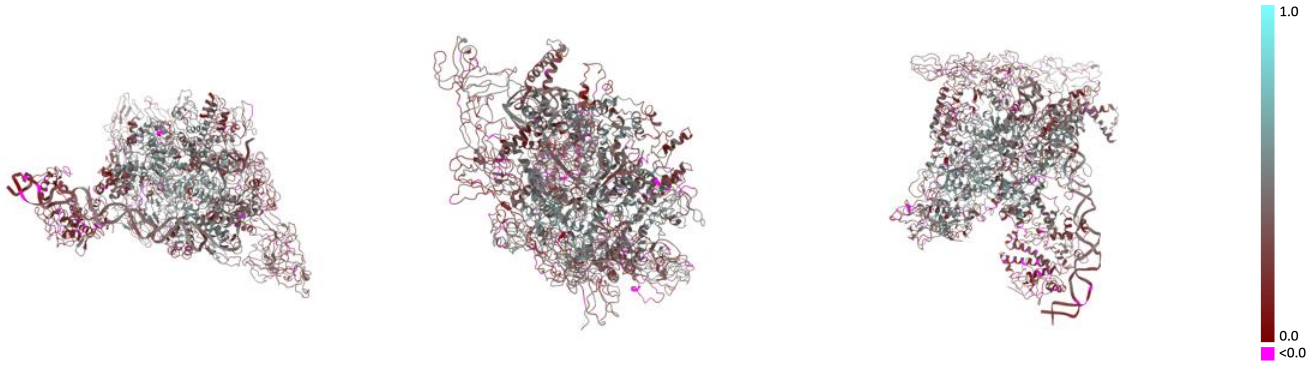
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

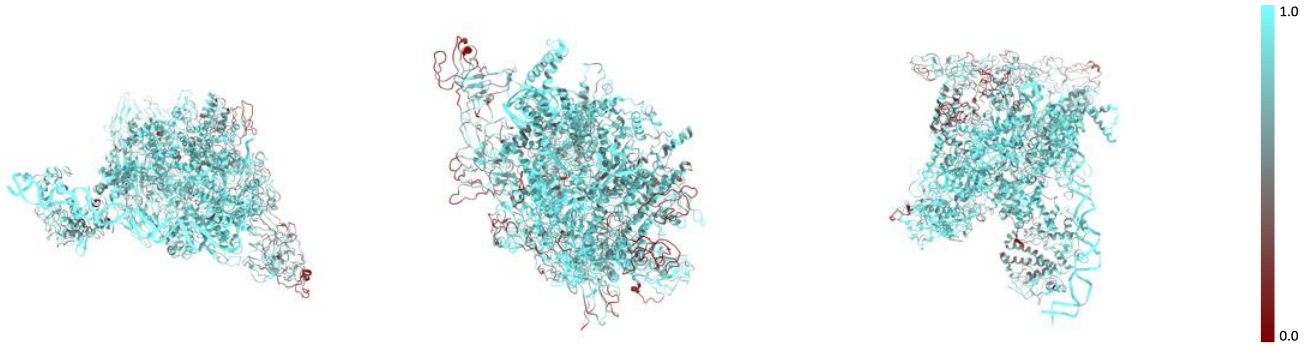
9.2 Q-score mapped to coordinate model



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.

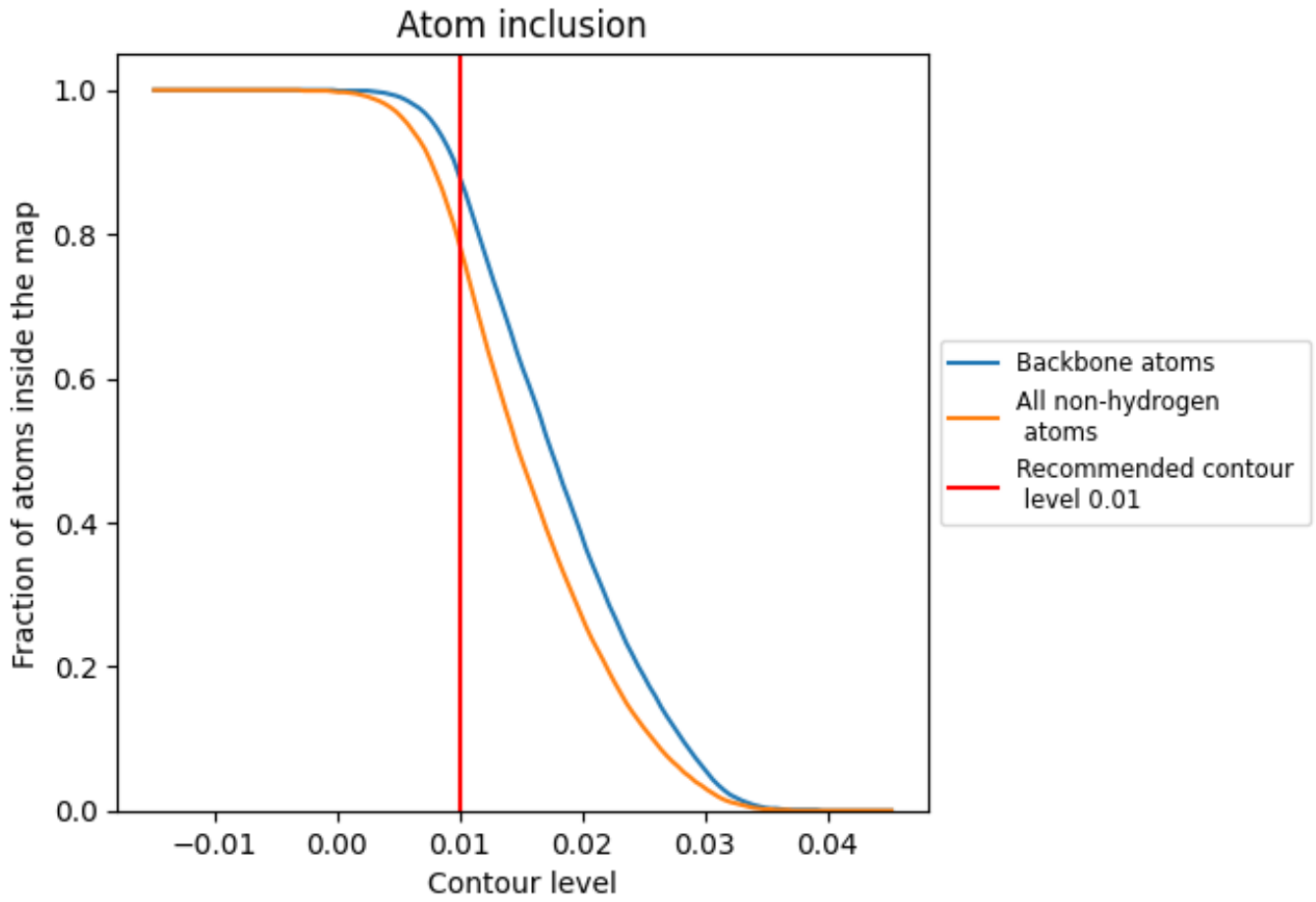
9.3 Atom inclusion mapped to coordinate model



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.3530
1	0.9600	0.3610
2	0.9420	0.3390
A	0.8800	0.4270
B	0.6250	0.3320
C	0.8400	0.3720
D	0.8060	0.3160
E	0.8600	0.4120
F	0.7460	0.3130
G	0.8080	0.3080
X	0.7120	0.2080
Y	0.6830	0.1450