wwPDB EM Validation Summary Report

Mar 19, 2024 – 04:04 PM JST

PDB ID	:	6A5P
EMDB ID	:	EMD-6982
Title	:	RNA polymerase II elongation complex stalled at SHL(-5) of the nucleosome
Authors	:	Kujirai, T.; Ehara, H.; Fujino, Y.; Shirouzu, M.; Sekine, S.; Kurumizaka, H.
Deposited on	:	2018-06-25
Resolution	:	7.00 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:

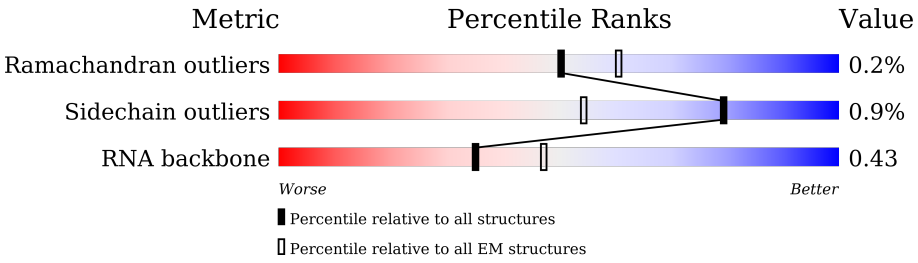
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 7.00 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)
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	1743	43% 80% • 19%
2	B	1227	60% 93% • 5%
3	C	304	46% 84% • 13%
4	D	186	84% 81% •• 16%
5	E	214	40% 97% •
6	F	155	30% 54% 46%
7	G	171	100% 98% •
8	H	145	54% 92% 8%

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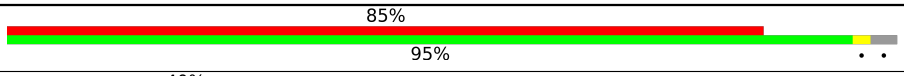
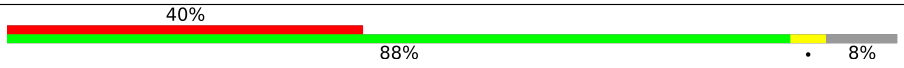
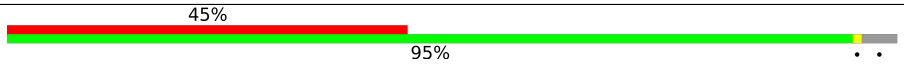
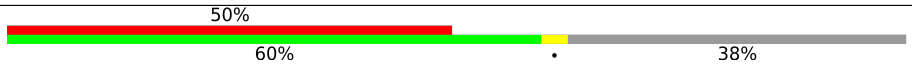
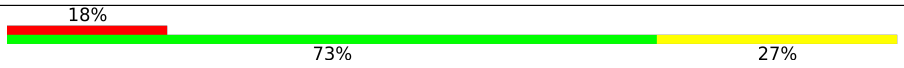
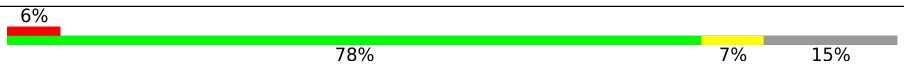
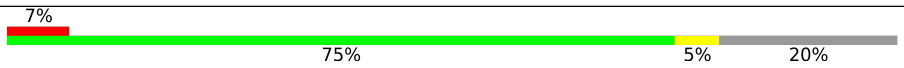
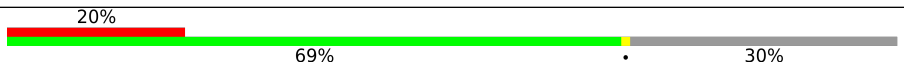
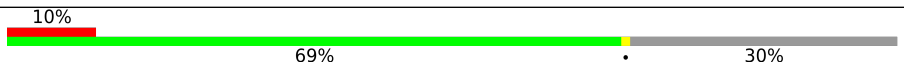
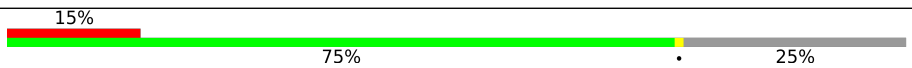
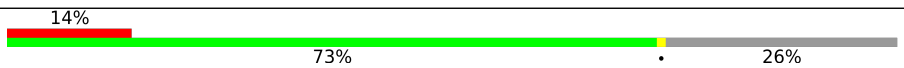
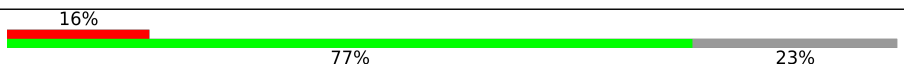
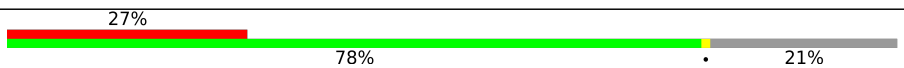
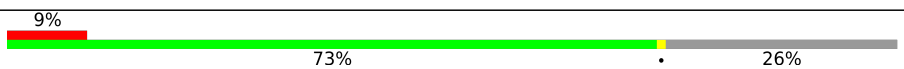
Mol	Chain	Length	Quality of chain
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	11	
14	T	198	
15	N	198	
16	a	139	
16	e	139	
17	b	106	
17	f	106	
18	c	133	
18	g	133	
19	d	129	
19	h	129	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 44084 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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1408	11095	6997	1935	2093	70	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1161	9261	5835	1636	1732	58	0	0

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	263	2098	1319	354	413	12	0	0

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	156	1210	753	210	245	2	0	0

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1740	1094	312	324	10	0	0

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a RNA chain called RNA (5'-R(P*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	11	Total	C	N	O	P	0	0
			241	106	44	80	11		

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	168	Total	C	N	O	P	0	0
			3424	1622	661	974	167		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	159	Total	C	N	O	P	0	0
			3273	1556	574	984	159		

- Molecule 16 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
16	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
17	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	103	Total	C	N	O	0	0
			796	502	155	139		
18	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
19	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

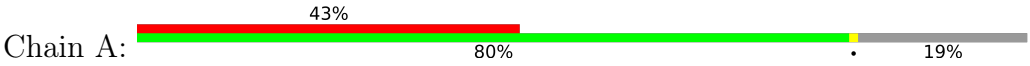
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total Mg 1 1	0

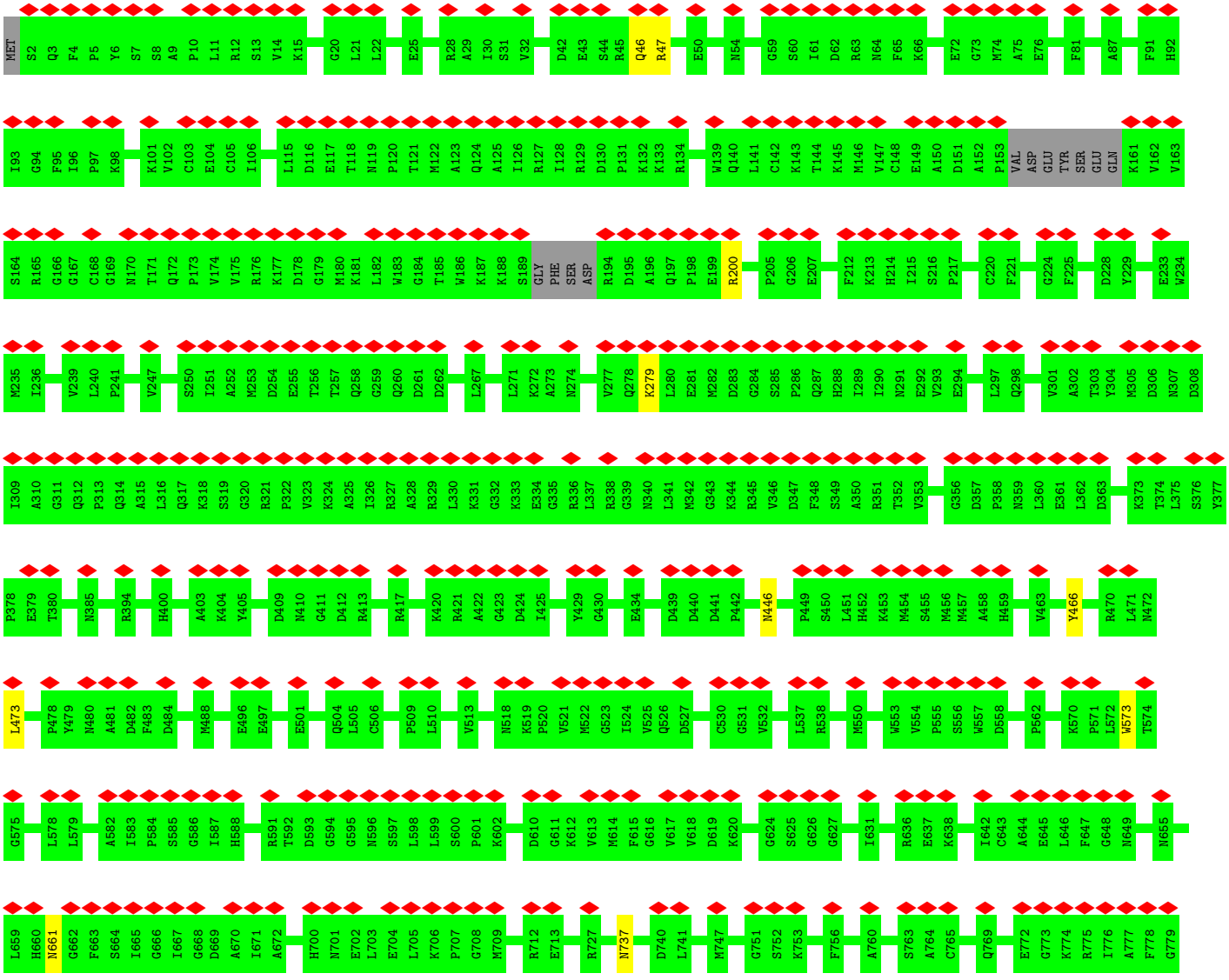
3 Residue-property plots (i)

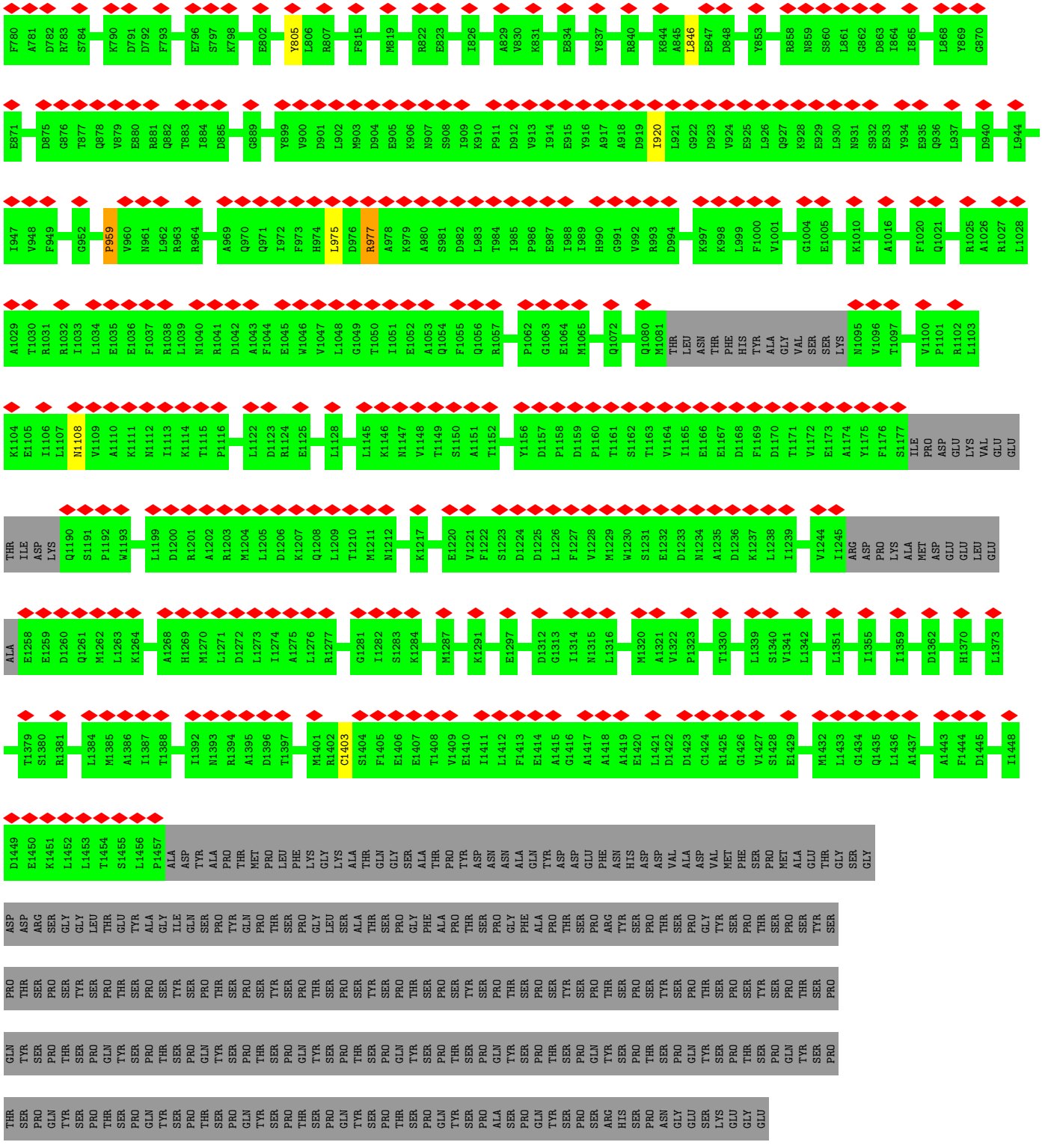
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-directed RNA polymerase subunit

Chain A:

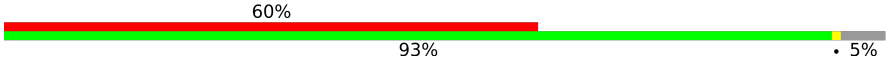


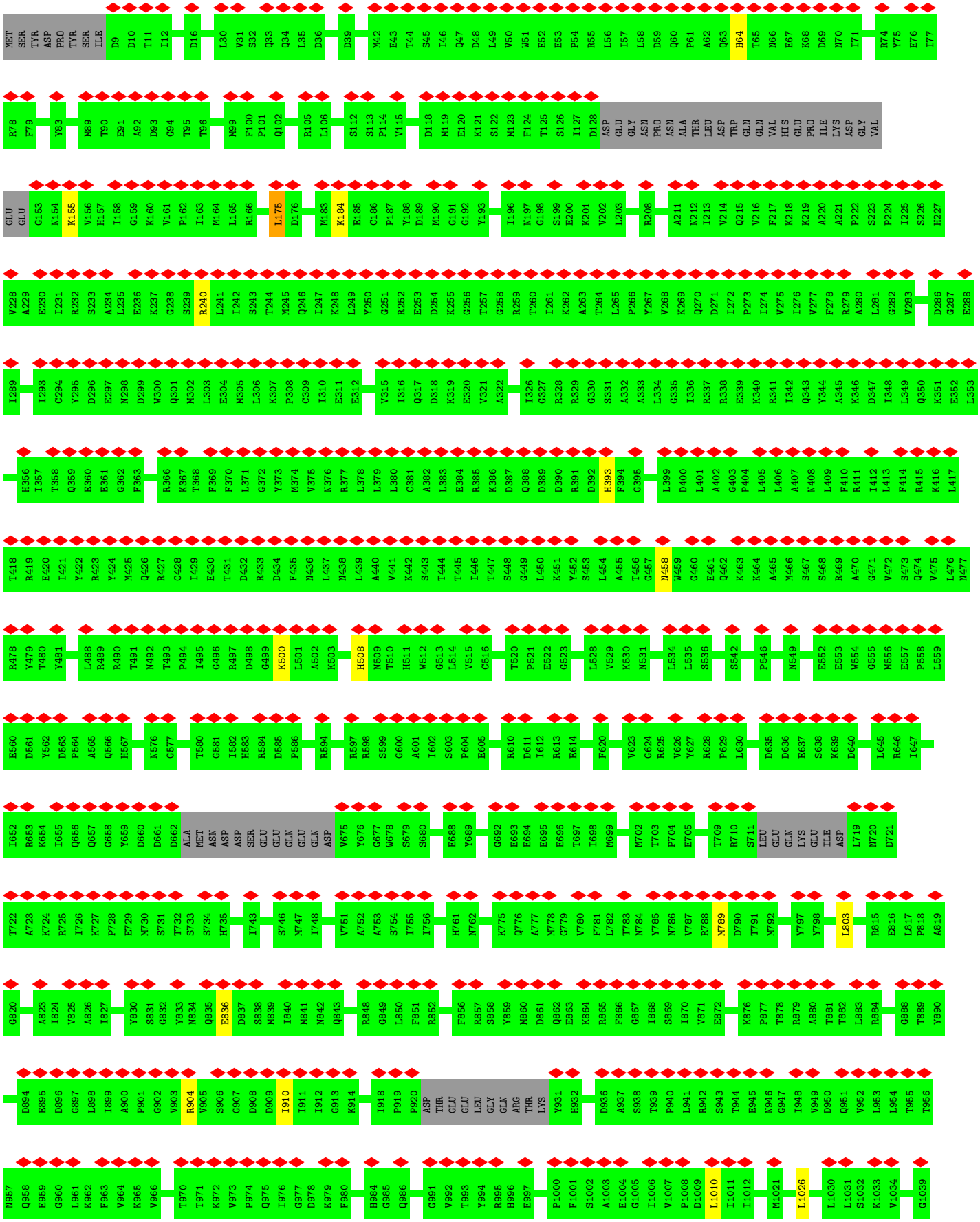


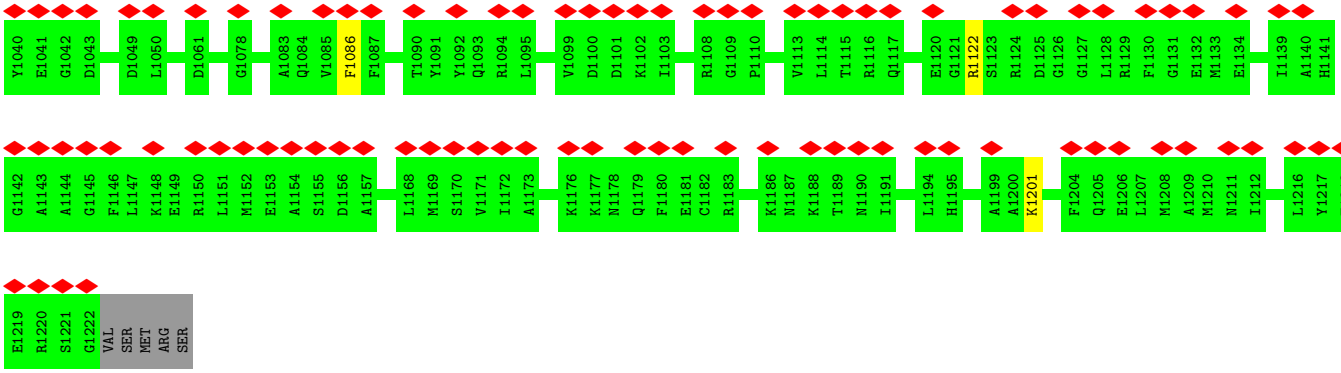


• Molecule 2: DNA-directed RNA polymerase subunit beta

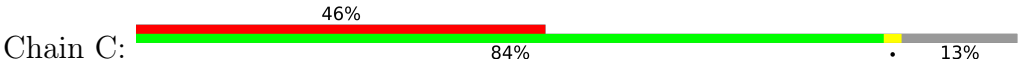
Chain B:

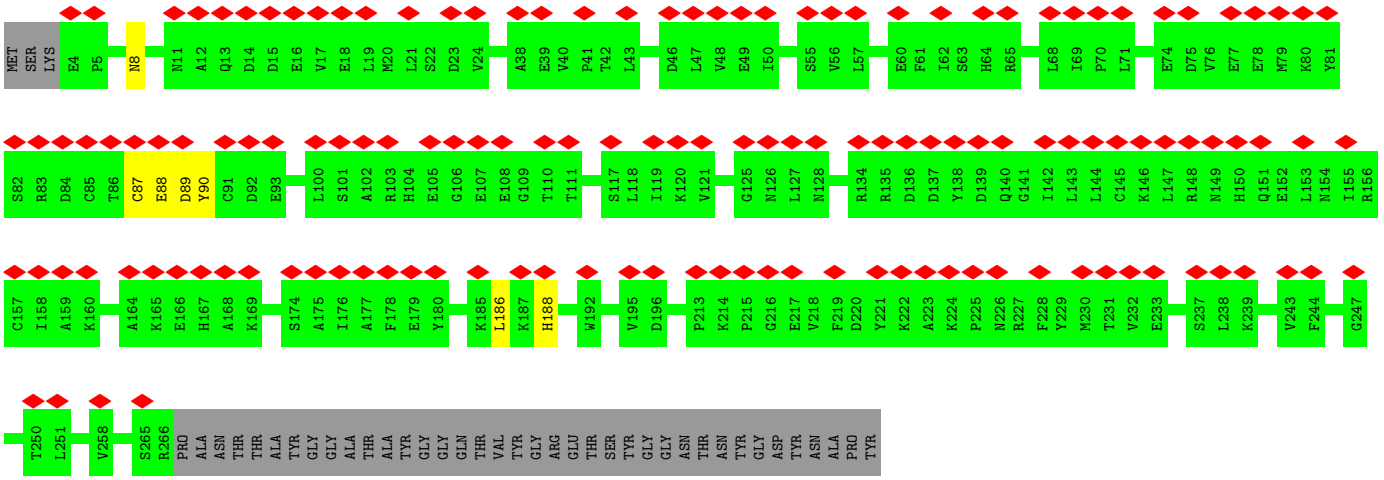



MET SER TYR ASP PRO TYR SER ILE D9 D10 T11 I12 D16 L30 V31 S32 Q33 Q34 L35 D36 D39 M42 E43 T44 S45 I46 Q47 D48 L49 V50 W51 E52 E53 P54 R55 L56 I57 L58 D59 Q60 P61 A62 Q63 H64 T65 N66 E67 K68 D69 N70 I71 R74 Y75 E76 I77
R78 F79 Y83 M89 T90 E91 A92 D93 G94 T95 T96 M99 F100 P101 Q102 R105 L106 S112 S113 P114 V115 D118 M119 E120 K121 S122 M123 F124 T125 S126 I127 D128 ASP GLU GLY ASN PRO ASN ALA THR LEU ASP TRP GLN GLN VAL HIS GLU PRO ILE LYS ASP GLY VAL
GLU GLU G153 N154 K155 V156 H157 I158 G159 K160 V161 P162 I163 M164 L165 R166 L175 D176 M183 K184 E185 C186 P187 Y188 D189 M190 G191 G192 Y193 I196 N197 G198 S199 E200 K201 V202 L203 R208 A211 N212 I213 V214 Q215 V216 F217 K218 K219 A220 A221 P222 S223 P224 I225 S226 H227
V228 A229 E230 I231 R232 S233 A234 L235 E236 K237 G238 S239 R240 L241 I242 S243 T244 M245 Q246 I247 K248 L249 Y250 G251 R252 E253 D254 K255 G256 T257 G258 R259 T260 I261 K262 A263 T264 L265 P266 Y267 V268 K269 Q270 D271 I272 P273 I274 V275 I276 V277 F278 R279 A280 L281 G282 V283 D286 G287 E288
I289 I293 C294 Y295 D296 E297 N298 D299 W300 Q301 M302 L303 E304 M305 L306 K307 P308 C309 I310 E311 E312 V315 I316 Q317 D318 K319 E320 V321 A322 I326 G327 R328 R329 G330 S331 A332 A333 L334 G335 I336 R337 R338 E339 K340 R341 I342 Q343 Y344 A345 K346 D347 I348 L349 Q350 K351 E352 L353
H356 I357 T358 Q359 E360 E361 G362 F363 R366 K367 T368 F369 F370 L371 G372 Y373 N374 V375 N376 R377 L378 L379 L380 C381 A382 L383 E384 R385 K386 D387 Q388 D389 D390 R391 D392 H393 F394 G395 L399 D400 L401 A402 G403 P404 L405 L406 A407 N408 L409 F410 R411 I412 L413 F414 R415 K416 L417
T418 R419 E420 I421 Y422 R423 Y424 M425 Q426 R427 C428 I429 E430 T431 D432 R433 D434 F435 N436 L437 N438 L439 A440 V441 K442 S443 T444 T445 I446 T447 S448 G449 L450 K451 Y452 S453 L454 A455 T456 G457 N458 W459 G460 E461 Q462 K463 K464 A465 M466 S467 S468 R469 A470 G471 V472 S473 Q474 V475 L476 N477
R478 Y479 T480 Y481 L488 R489 R490 T491 N492 T493 P494 I495 G496 R497 D498 G499 K500 L501 A502 K503 H508 N509 T510 H511 W512 G513 L514 V515 C516 T520 P521 E522 G523 L528 V529 K530 M531 L534 L535 S536 S542 P546 N549 E552 E553 W554 G555 M556 E557 P558 L559
E560 D561 Y562 D563 P564 A565 Q566 H567 N576 G577 T580 G581 I582 H583 R584 D585 P586 R594 R597 R598 S599 G600 A601 I602 S603 P604 E605 R610 D611 I612 R613 E614 F620 V623 G624 R625 V626 Y627 R628 P629 L630 D635 D636 E637 S638 K639 D640 L645 R646 I647
I652 R653 K654 I655 Q656 Q657 G658 Y659 D660 D661 D662 ALA MET ASN ASP ASP SER GLU GLU GLN GLN ASP V675 Y676 G677 W678 S679 S680 E688 Y689 G692 E693 E694 E695 E696 T697 I698 M699 M702 T703 P704 E705 T709 R710 S711 LEU GLU GLN LYS GLU ILE ASP L719 N720 D721
T722 A723 K724 R725 I726 K727 P728 E729 M730 S731 T732 S733 S734 H735 I743 S746 M747 I748 V751 A752 A753 S754 I755 I756 H761 N762 K775 Q776 A777 M778 G779 V780 F781 L782 T783 N784 Y785 N786 V787 R788 M789 D790 T791 M792 Y797 Y798 L803 R815 E816 L817 P818 A819
G820 A823 I824 V825 A826 I827 Y830 S831 G832 Y833 N834 Q835 E836 D837 S838 M839 I840 M841 N842 Q843 R848 G849 L850 F851 R852 P856 R857 S858 Y859 M860 D861 Q862 E863 K864 R865 F866 G867 I868 S869 I870 V871 E872 K876 P877 T878 R879 A880 T881 T882 L883 R884 G888 T889 Y890
D894 E895 D896 G897 L898 I899 A900 P901 G902 V903 R904 V905 S906 G907 D908 D909 I910 I911 I912 G913 K914 I918 P919 P920 ASP THR GLU GLU LEU GLY GLN ARG THR LYS Y931 H932 D936 A937 S938 T939 P940 L941 R942 S943 T944 E945 N946 G947 I948 V949 D950 Q951 V952 L953 L954 T955 T956
N957 Q958 E959 G960 L961 K962 F963 V964 K965 V966 T970 T971 K972 V973 P974 Q975 I976 G977 D978 K979 F980 H984 G985 Q986 G991 V992 T993 Y994 R995 H996 E997 P1000 F1001 S1002 A1003 E1004 G1005 I1006 V1007 P1008 D1009 L1010 I1011 I1012 M1021 L1026 L1030 L1031 S1032 K1033 V1034 G1039

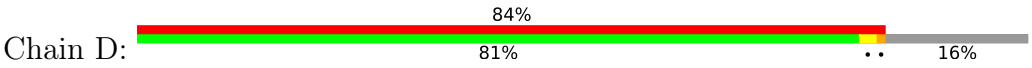


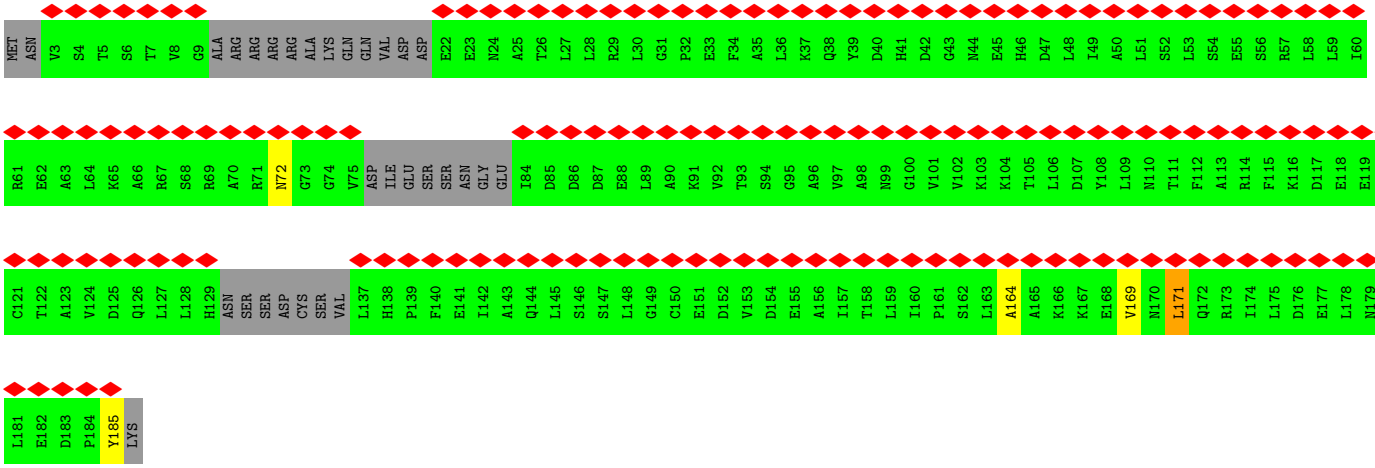
• Molecule 3: RNA polymerase II third largest subunit B44, part of central core





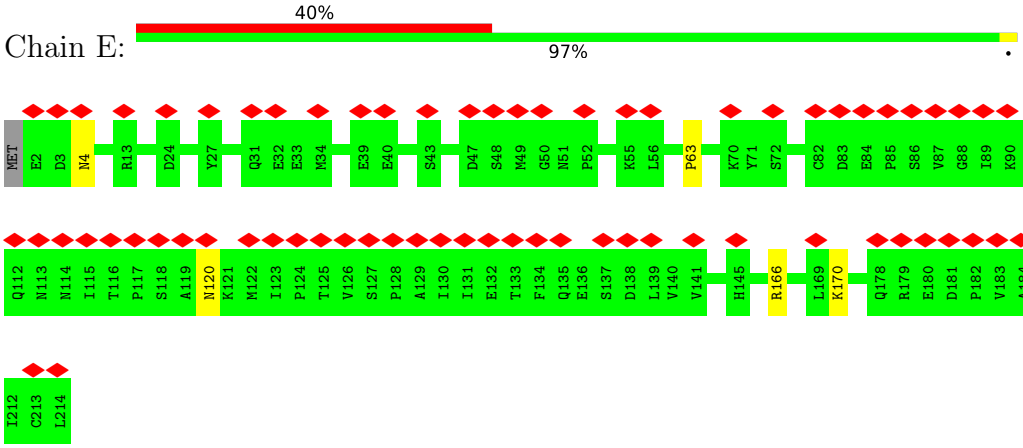
• Molecule 4: RNA polymerase II subunit B32





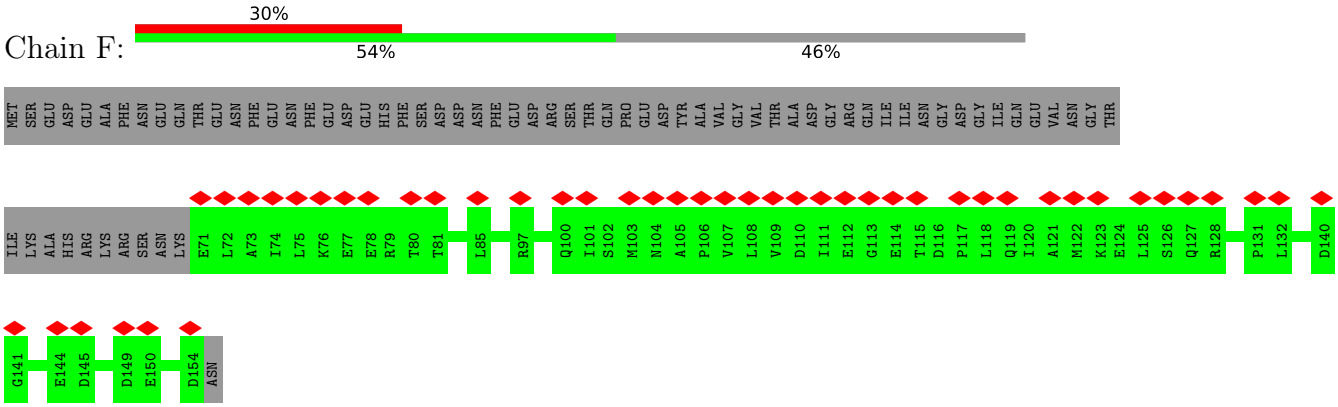
• Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

Chain E:



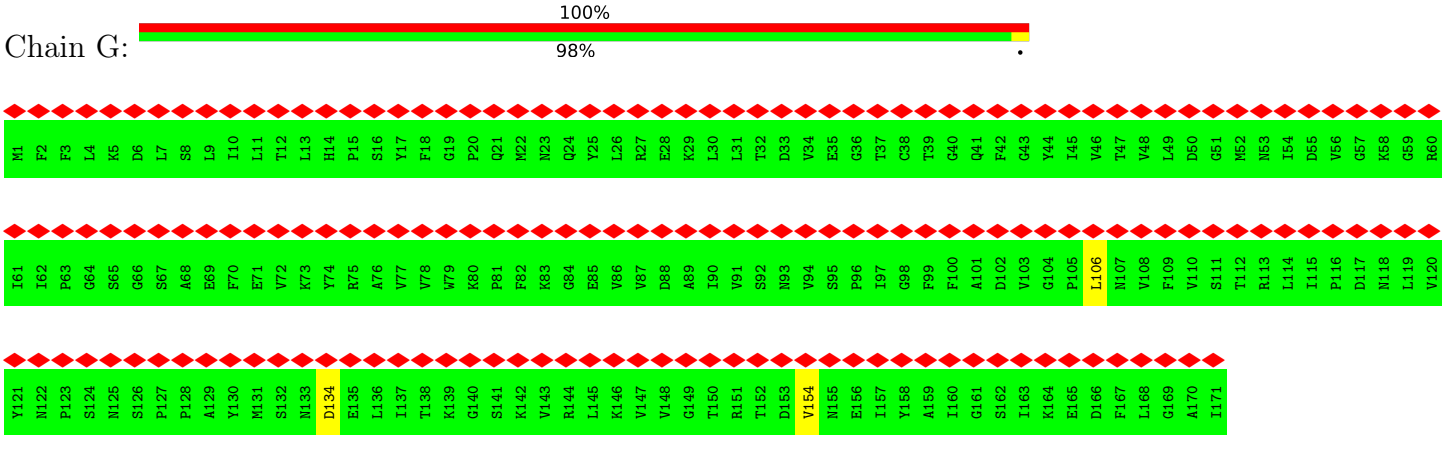
• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F:



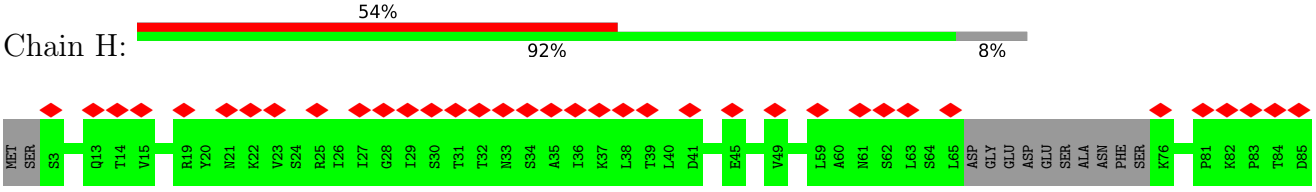
• Molecule 7: RNA polymerase II subunit

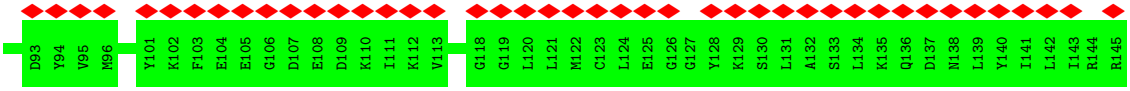
Chain G:



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

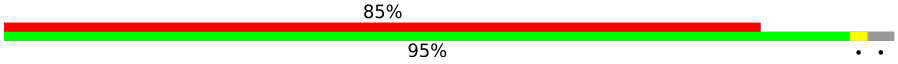
Chain H:

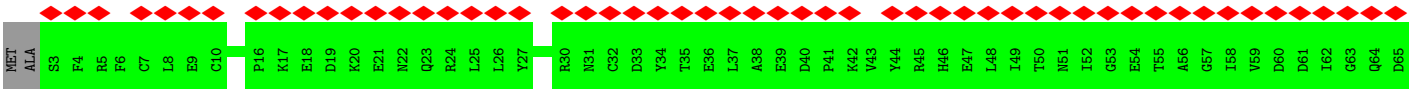


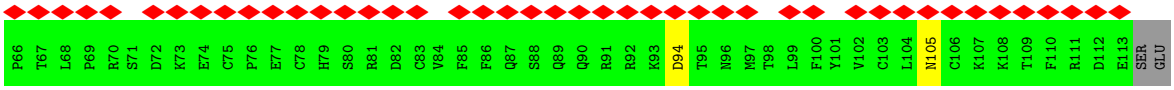


• Molecule 9: DNA-directed RNA polymerase subunit

Chain I:

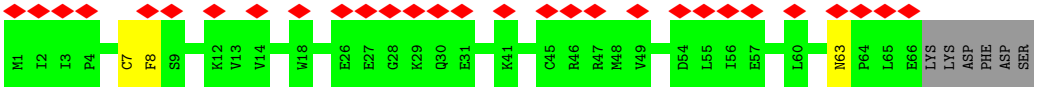






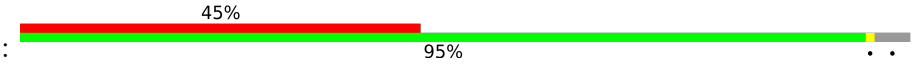
• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

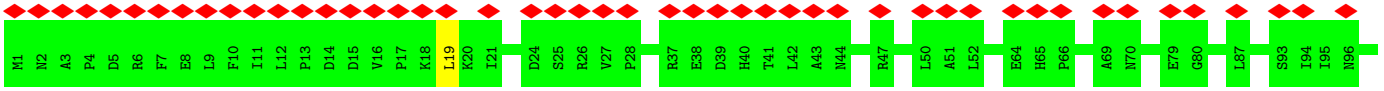
Chain J:

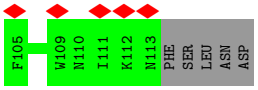


• Molecule 11: RNA polymerase II subunit B12.5

Chain K:

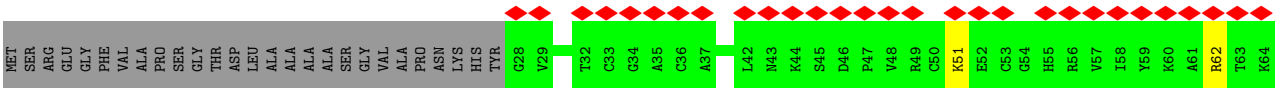


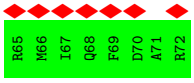




• Molecule 12: RNA polymerase subunit ABC10-alpha

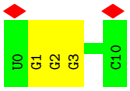
Chain L:





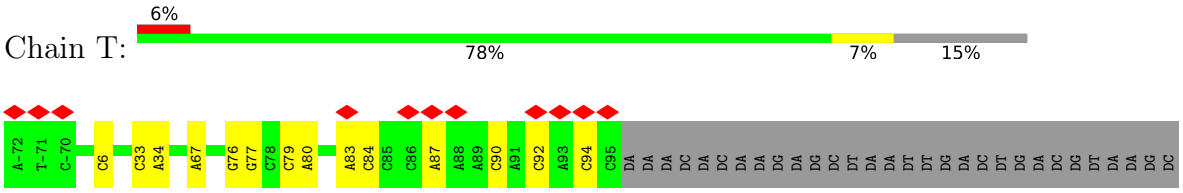
• Molecule 13: RNA (5'-R(P*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*C)-3')

Chain P:



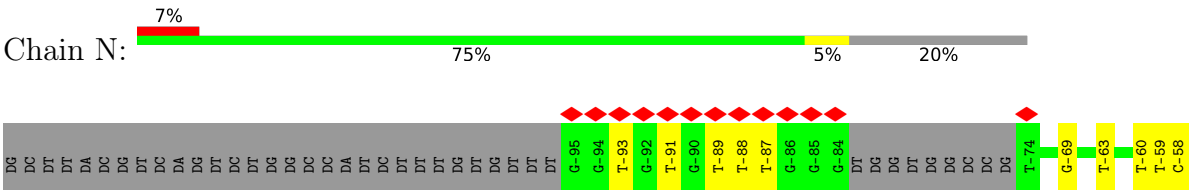
• Molecule 14: DNA (198-MER)

Chain T:



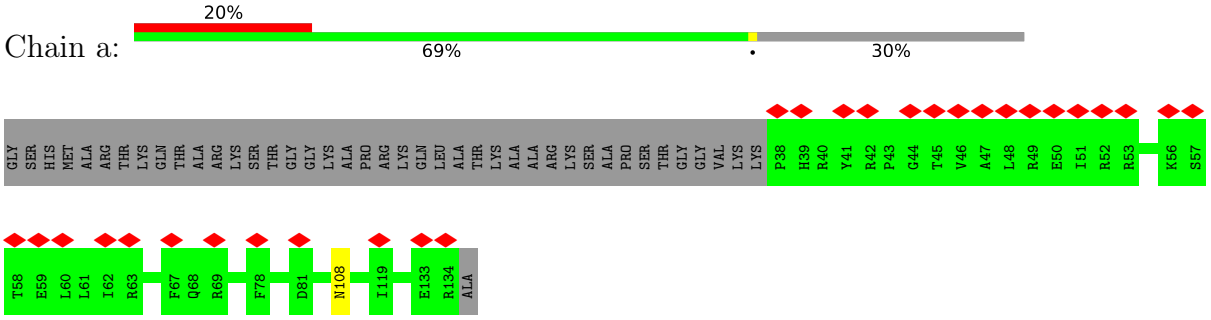
• Molecule 15: DNA (198-MER)

Chain N:



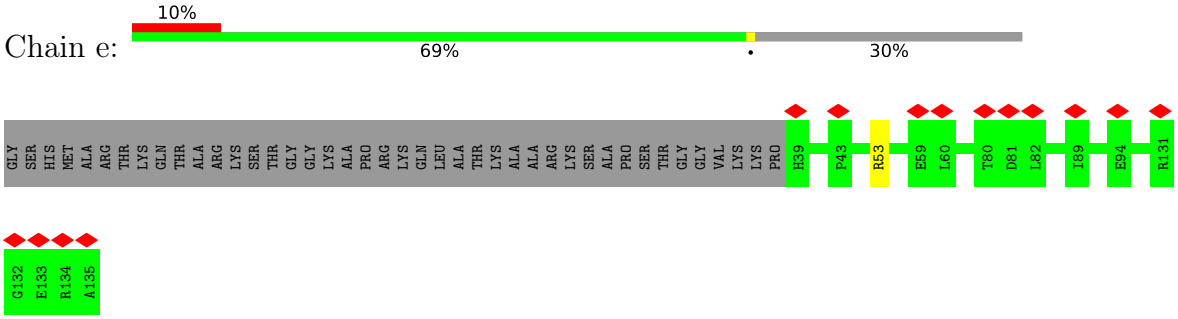
• Molecule 16: Histone H3.3

Chain a:



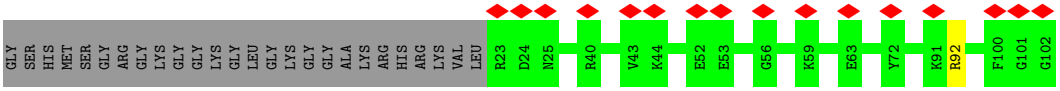
• Molecule 16: Histone H3.3

Chain e:



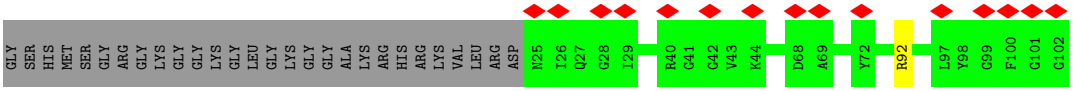
• Molecule 17: Histone H4

Chain b:



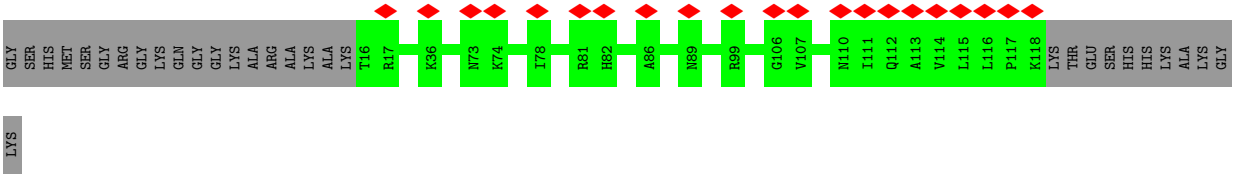
• Molecule 17: Histone H4

Chain f:



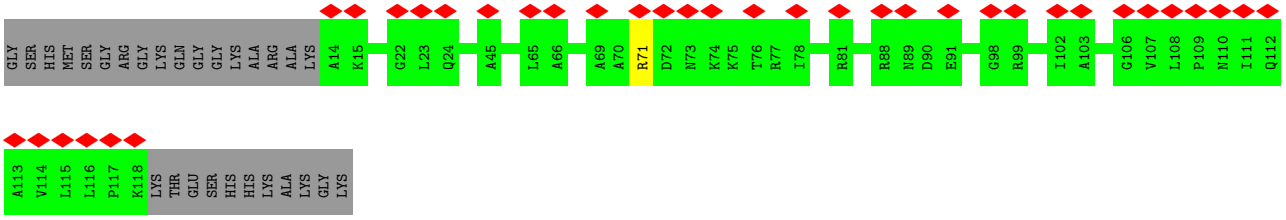
• Molecule 18: Histone H2A type 1-B/E

Chain c:



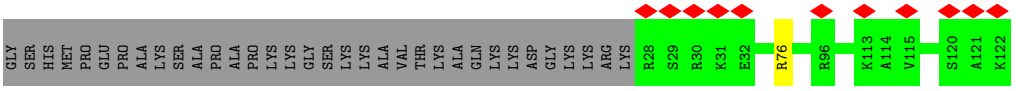
• Molecule 18: Histone H2A type 1-B/E

Chain g:



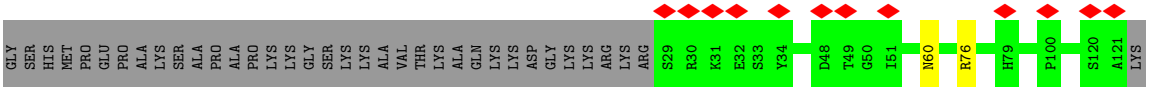
• Molecule 19: Histone H2B type 1-J

Chain d:



• Molecule 19: Histone H2B type 1-J

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	91888	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49, 1.49, 1.49	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: MG, ZN

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	0.62	1/11299 (0.0%)	0.73	3/15266 (0.0%)
2	B	0.65	1/9441 (0.0%)	0.76	2/12732 (0.0%)
3	C	0.66	0/2139	0.76	1/2895 (0.0%)
4	D	0.28	0/1221	0.52	0/1648
5	E	0.59	0/1772	0.66	0/2385
6	F	0.58	0/687	0.64	0/931
7	G	0.33	0/1353	0.61	0/1837
8	H	0.61	0/1069	0.67	0/1444
9	I	0.42	0/934	0.70	0/1257
10	J	0.89	1/554 (0.2%)	0.82	0/742
11	K	0.56	0/953	0.66	0/1291
12	L	0.60	0/365	0.71	0/484
13	P	1.15	2/269 (0.7%)	1.37	2/419 (0.5%)
14	T	1.00	9/3848 (0.2%)	1.06	7/5927 (0.1%)
15	N	0.94	10/3663 (0.3%)	1.06	0/5658
16	a	0.34	0/809	0.54	0/1085
16	e	0.38	0/807	0.52	0/1081
17	b	0.38	0/645	0.57	0/862
17	f	0.40	0/626	0.56	0/837
18	c	0.35	0/806	0.52	0/1089
18	g	0.35	0/820	0.52	0/1107
19	d	0.38	0/757	0.54	0/1015
19	h	0.37	0/736	0.55	0/990
All	All	0.66	24/45573 (0.1%)	0.78	15/62982 (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	8
2	B	0	8
3	C	0	3
5	E	0	2
9	I	0	1
10	J	0	1
All	All	0	23

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	-69	DG	C1'-N9	-9.49	1.33	1.47
14	T	76	DG	C1'-N9	-8.05	1.35	1.47
14	T	80	DA	C1'-N9	-7.29	1.37	1.47
14	T	83	DA	C1'-N9	-6.75	1.37	1.47
14	T	87	DA	C1'-N9	-6.32	1.38	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	2	G	C4-N9-C1'	6.66	135.16	126.50
2	B	1026	LEU	CA-CB-CG	-6.66	99.98	115.30
14	T	84	DC	O4'-C1'-N1	5.81	112.06	108.00
14	T	80	DA	O4'-C4'-C3'	-5.79	102.18	104.50
1	A	279	LYS	CB-CA-C	5.78	121.95	110.40

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	GLN	Peptide
1	A	466	TYR	Peptide
1	A	846	LEU	Peptide
1	A	920	ILE	Peptide
1	A	959	PRO	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1396/1743 (80%)	1252 (90%)	142 (10%)	2 (0%)	51 86
2	B	1151/1227 (94%)	1020 (89%)	129 (11%)	2 (0%)	47 81
3	C	261/304 (86%)	231 (88%)	29 (11%)	1 (0%)	34 72
4	D	148/186 (80%)	136 (92%)	9 (6%)	3 (2%)	7 38
5	E	211/214 (99%)	195 (92%)	16 (8%)	0	100 100
6	F	82/155 (53%)	73 (89%)	9 (11%)	0	100 100
7	G	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	13 50
8	H	129/145 (89%)	113 (88%)	16 (12%)	0	100 100
9	I	109/115 (95%)	94 (86%)	15 (14%)	0	100 100
10	J	64/72 (89%)	57 (89%)	7 (11%)	0	100 100
11	K	111/118 (94%)	100 (90%)	11 (10%)	0	100 100
12	L	43/72 (60%)	40 (93%)	3 (7%)	0	100 100
16	a	95/139 (68%)	92 (97%)	3 (3%)	0	100 100
16	e	95/139 (68%)	90 (95%)	5 (5%)	0	100 100
17	b	78/106 (74%)	75 (96%)	3 (4%)	0	100 100
17	f	76/106 (72%)	72 (95%)	4 (5%)	0	100 100
18	c	101/133 (76%)	95 (94%)	6 (6%)	0	100 100
18	g	103/133 (77%)	97 (94%)	6 (6%)	0	100 100
19	d	93/129 (72%)	90 (97%)	3 (3%)	0	100 100
19	h	91/129 (70%)	88 (97%)	3 (3%)	0	100 100
All	All	4606/5536 (83%)	4169 (90%)	427 (9%)	10 (0%)	50 81

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	171	LEU

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Mol	Chain	Res	Type
7	G	134	ASP
4	D	169	VAL
7	G	154	VAL
4	D	164	ALA

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
1	A	1223/1528 (80%)	1217 (100%)	6 (0%)	88 93
2	B	1016/1077 (94%)	1009 (99%)	7 (1%)	84 90
3	C	236/264 (89%)	234 (99%)	2 (1%)	81 89
4	D	133/160 (83%)	130 (98%)	3 (2%)	50 70
5	E	196/197 (100%)	193 (98%)	3 (2%)	65 80
6	F	75/137 (55%)	75 (100%)	0	100 100
7	G	148/148 (100%)	147 (99%)	1 (1%)	84 90
8	H	120/130 (92%)	120 (100%)	0	100 100
9	I	106/109 (97%)	105 (99%)	1 (1%)	78 87
10	J	60/66 (91%)	59 (98%)	1 (2%)	60 78
11	K	104/109 (95%)	103 (99%)	1 (1%)	76 86
12	L	38/56 (68%)	36 (95%)	2 (5%)	22 47
16	a	83/112 (74%)	82 (99%)	1 (1%)	71 83
16	e	82/112 (73%)	81 (99%)	1 (1%)	71 83
17	b	65/81 (80%)	64 (98%)	1 (2%)	65 80
17	f	63/81 (78%)	62 (98%)	1 (2%)	62 79
18	c	82/102 (80%)	82 (100%)	0	100 100
18	g	83/102 (81%)	82 (99%)	1 (1%)	71 83
19	d	81/107 (76%)	80 (99%)	1 (1%)	71 83
19	h	79/107 (74%)	77 (98%)	2 (2%)	47 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4073/4785 (85%)	4038 (99%)	35 (1%)	79 87

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	b	92	ARG
19	d	76	ARG
18	g	71	ARG
2	B	1201	LYS
2	B	1122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	112	GLN
16	a	68	GLN
5	E	120	ASN
11	K	2	ASN
1	A	927	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	10/11 (90%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	1	G

There are no RNA pucker outliers to report.

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)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

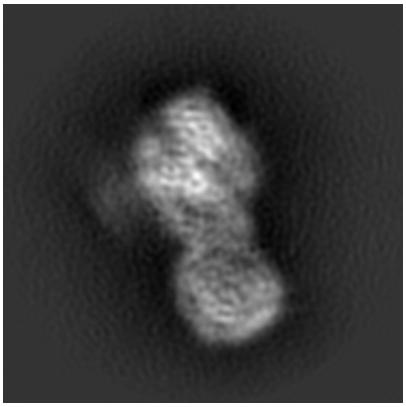
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6982. These allow visual inspection of the internal detail of the map and identification of artifacts.

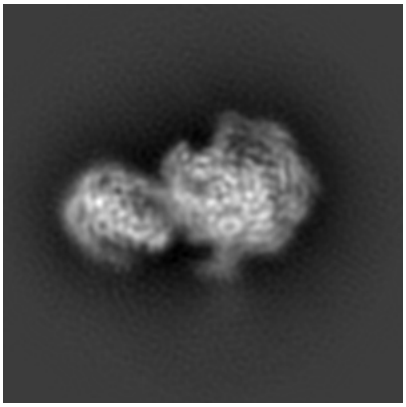
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

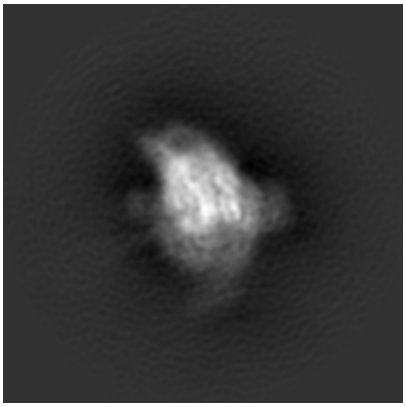
6.1.1 Primary map



X



Y

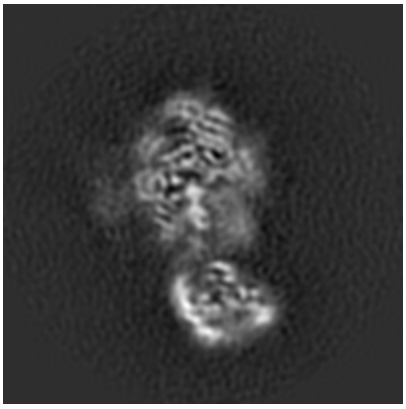


Z

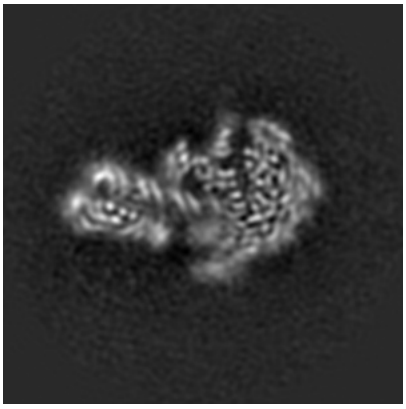
The images above show the map projected in three orthogonal directions.

6.2 Central slices

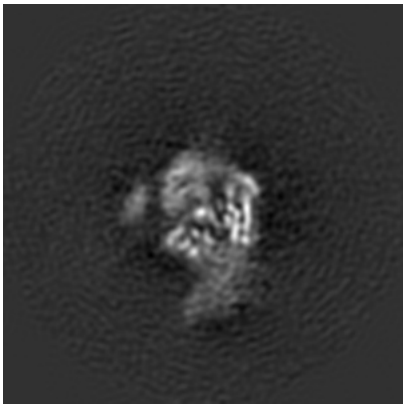
6.2.1 Primary map



X Index: 120



Y Index: 120

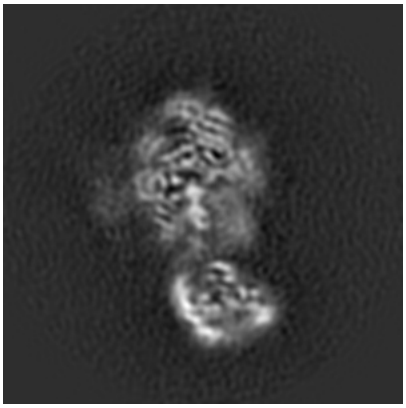


Z Index: 120

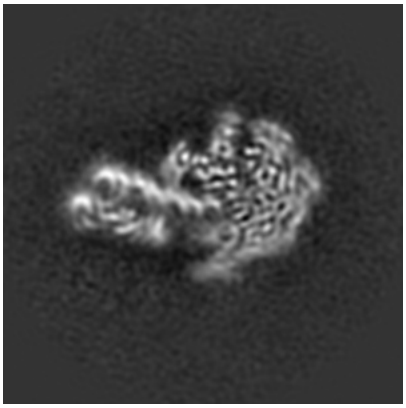
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

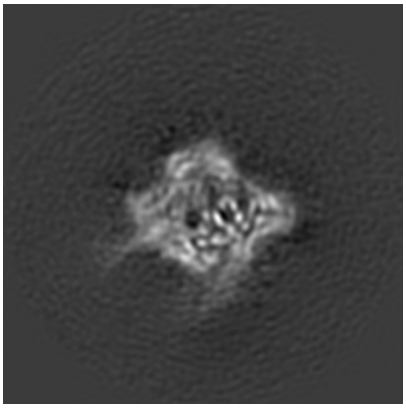
6.3.1 Primary map



X Index: 120



Y Index: 117

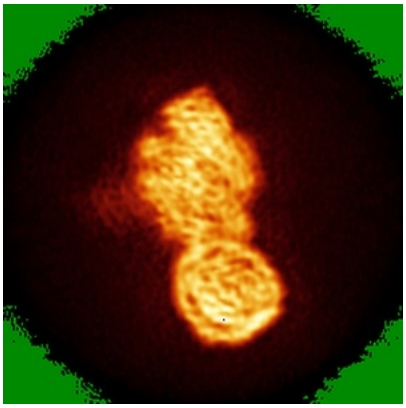


Z Index: 132

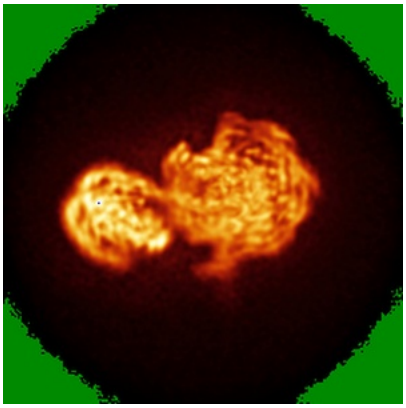
The images above show the largest variance slices of the map in three orthogonal directions.

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

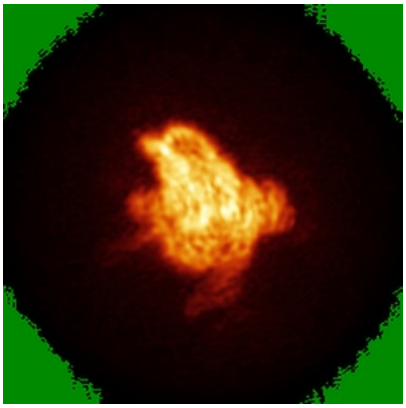
6.4.1 Primary map



X



Y

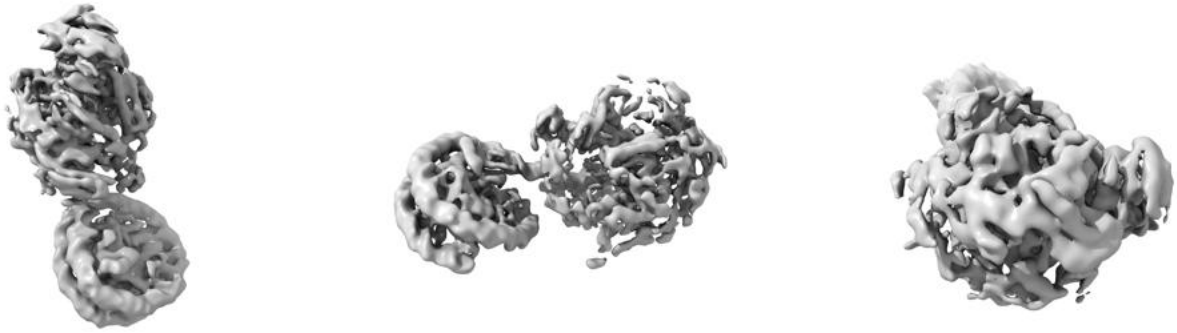


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

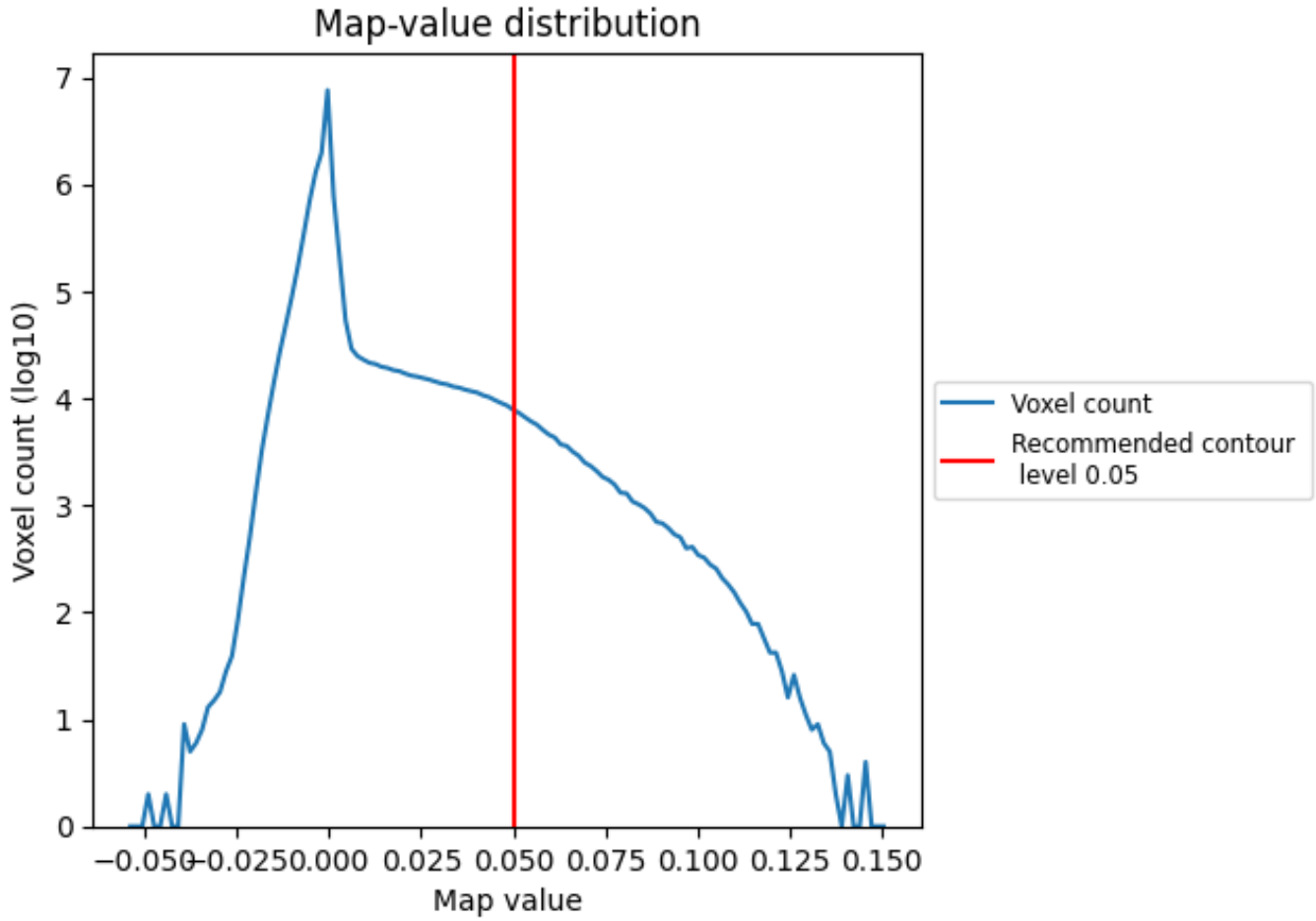
6.6 Mask visualisation (i)

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

7 Map analysis

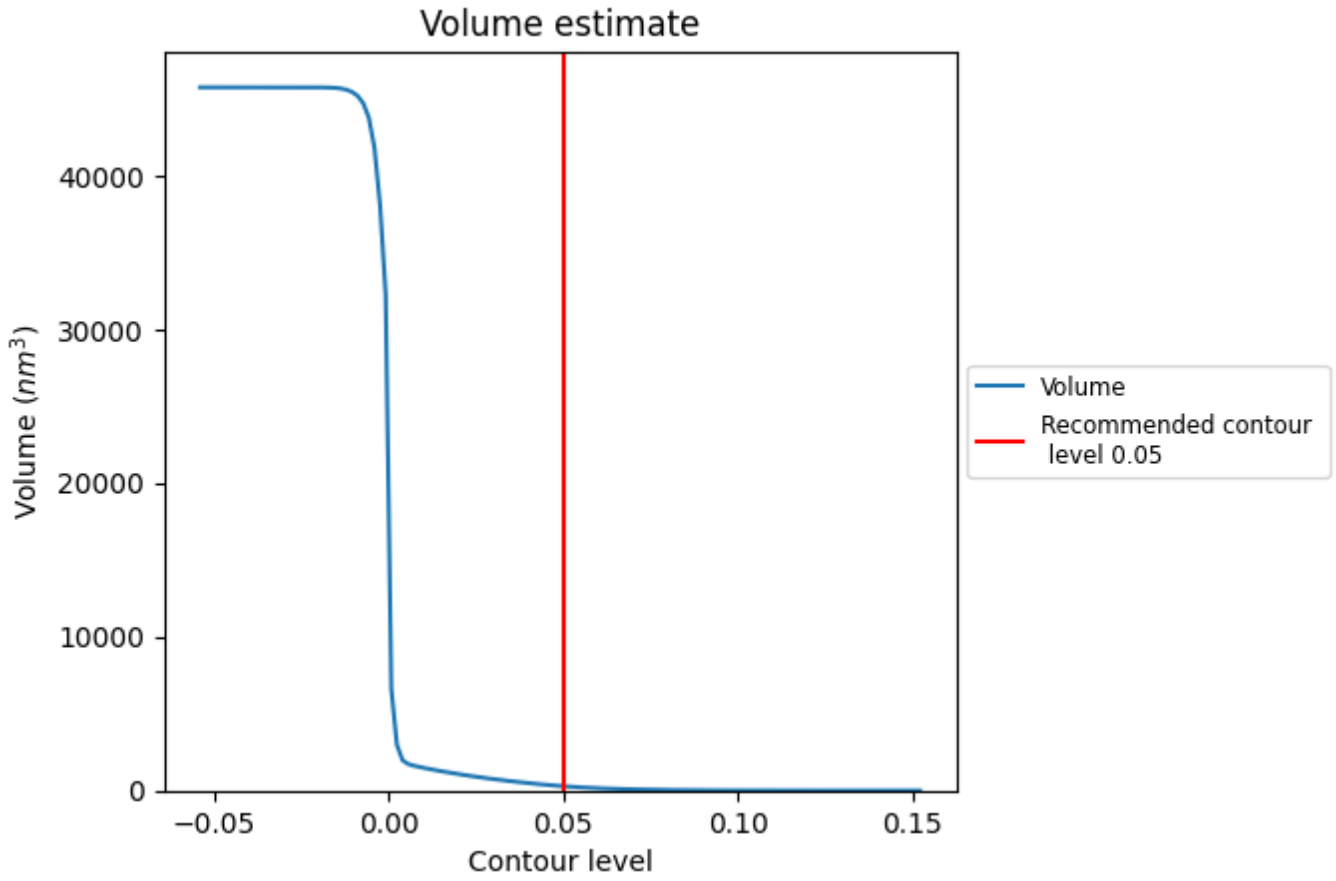
This section contains the results of statistical analysis of the map.

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.

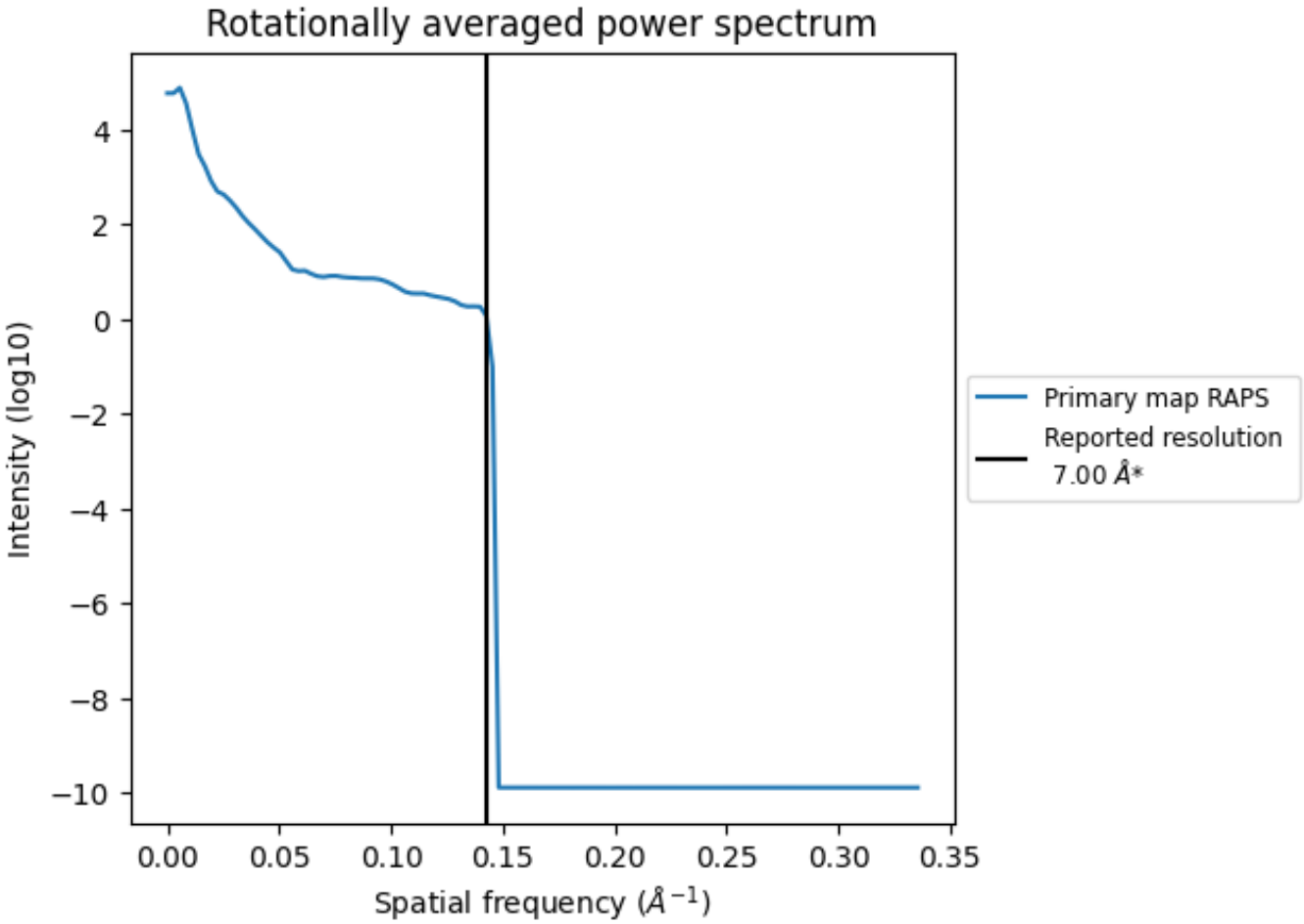
7.2 Volume estimate (i)



The volume at the recommended contour level is 283 nm^3; this corresponds to an approximate mass of 256 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)

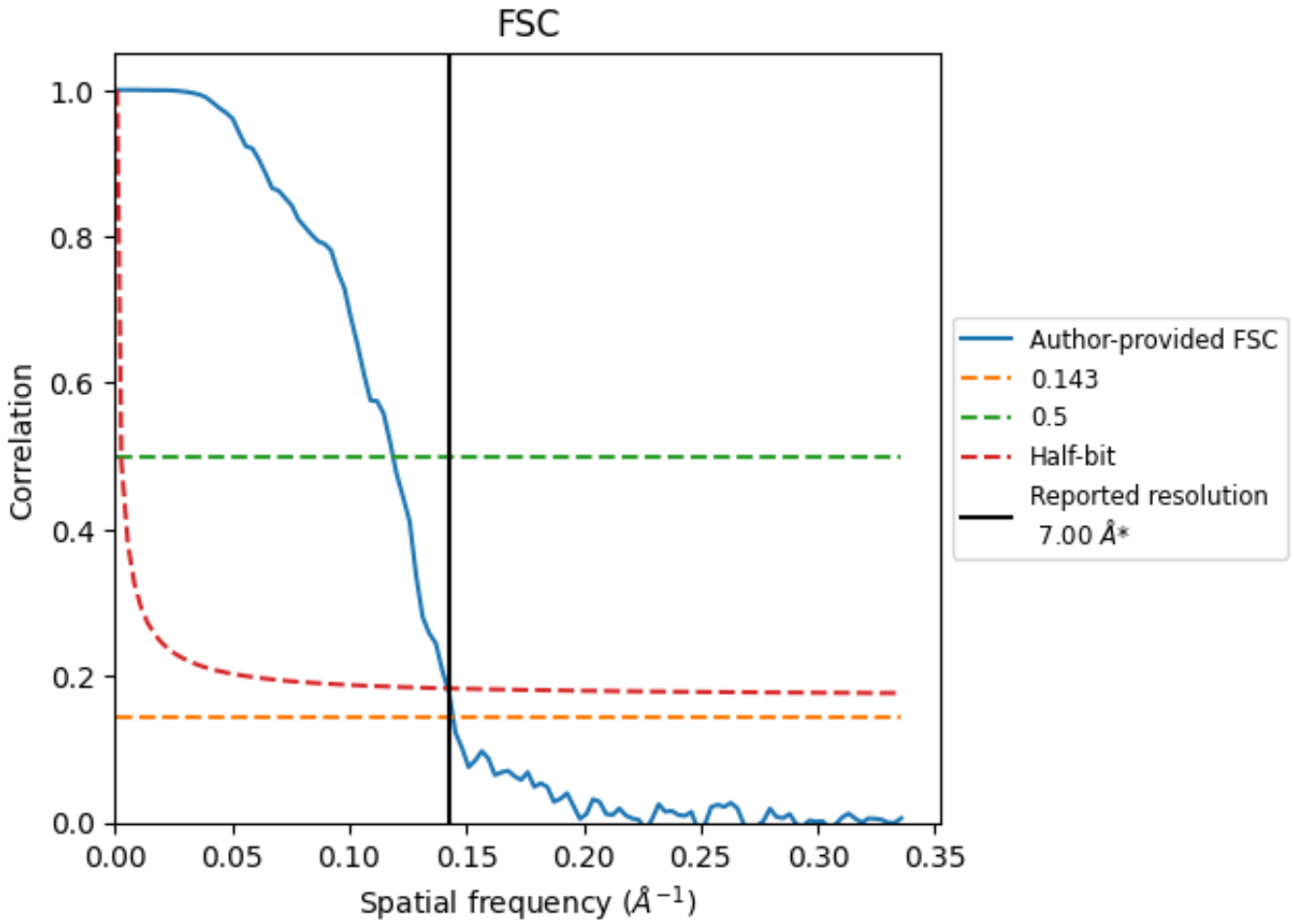


*Reported resolution corresponds to spatial frequency of 0.143 Å^{-1}

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 0.143 Å^{-1}

8.2 Resolution estimates (i)

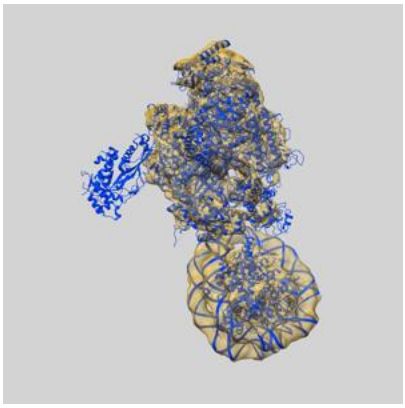
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.00	-	-
Author-provided FSC curve	6.93	8.42	7.04
Unmasked-calculated*	-	-	-

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

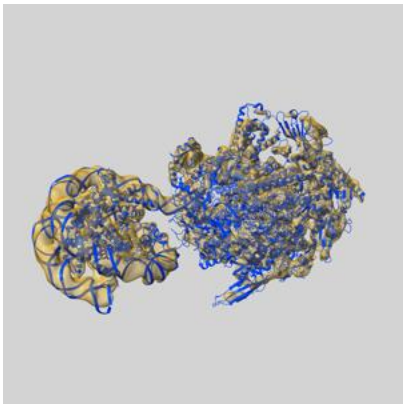
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6982 and PDB model 6A5P. Per-residue inclusion information can be found in section 3 on page 9.

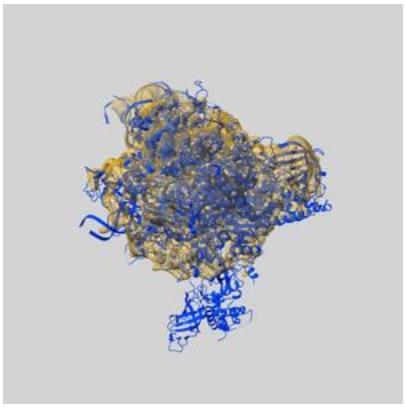
9.1 Map-model overlay



X



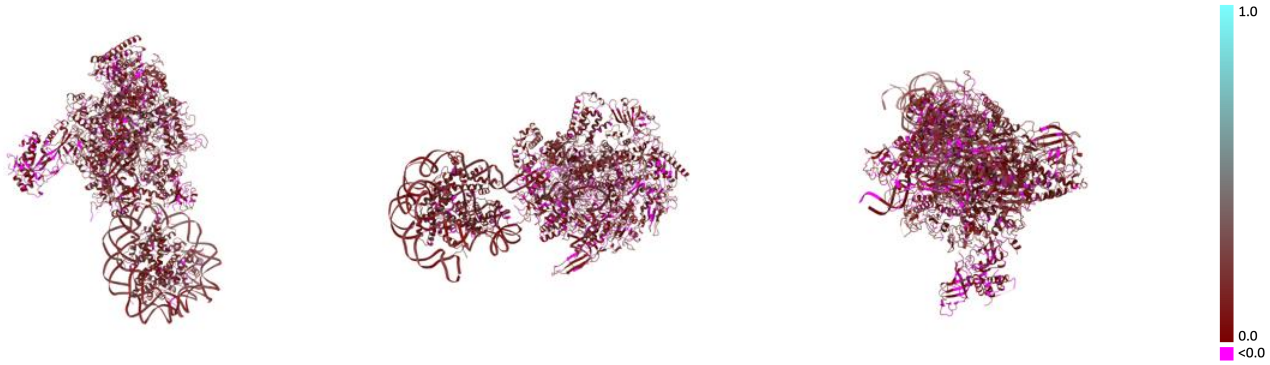
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

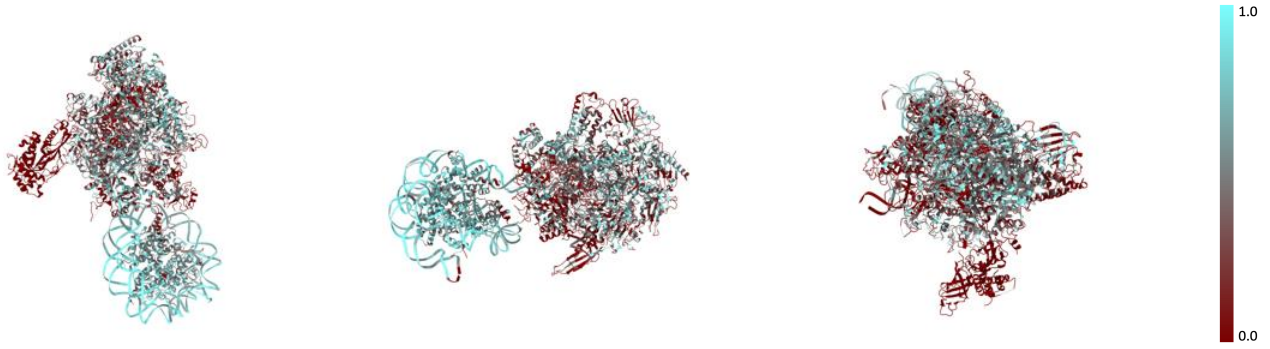
9.2 Q-score mapped to coordinate model



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.

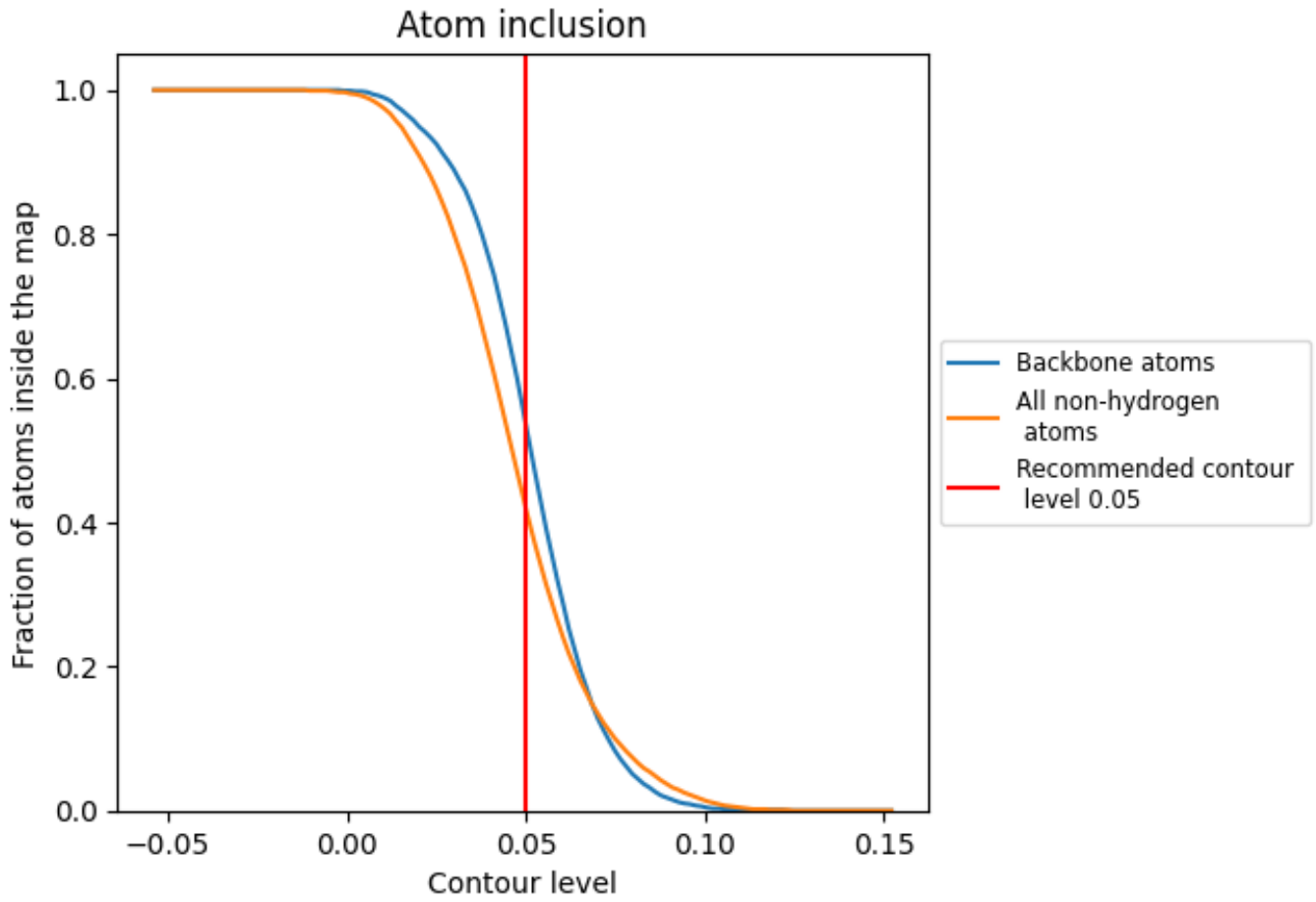
9.3 Atom inclusion mapped to coordinate model



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 42% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4190	0.1380
A	0.3670	0.1470
B	0.3080	0.1180
C	0.3780	0.1300
D	0.0000	0.0500
E	0.4720	0.1570
F	0.3530	0.1540
G	0.0000	0.0740
H	0.3150	0.1460
I	0.1120	0.0800
J	0.5020	0.1280
K	0.4070	0.1220
L	0.2040	0.1300
N	0.7280	0.1730
P	0.6800	0.2310
T	0.7370	0.1800
a	0.4870	0.1360
b	0.6030	0.1360
c	0.6260	0.1600
d	0.6160	0.1370
e	0.6340	0.1590
f	0.6190	0.1300
g	0.4900	0.1520
h	0.5950	0.1510