wwPDB EM Validation Summary Report (i)

Mar 10, 2024 – 05:12 PM EDT

PDB ID	:	6OUL
EMDB ID	:	EMD-20203
Title	:	Cryo-EM structure of Escherichia coli RNAP polymerase bound to rpsTP2 promoter DNA
Authors	:	Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on	:	2019-05-04
Resolution	:	3.40 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 (i) 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 (1)) were used in the production of this report:

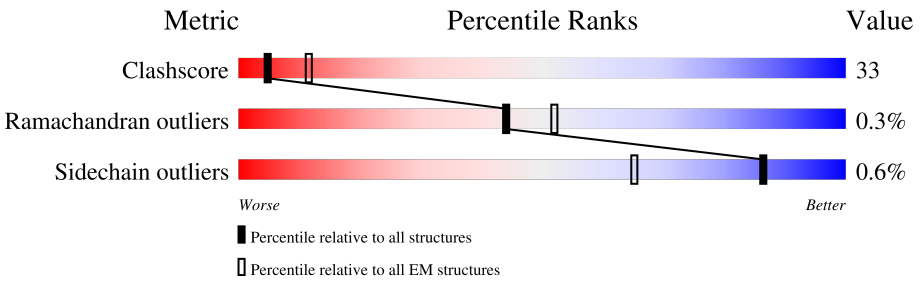
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.40 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	G	329	• 38% 32% • 30%
1	H	329	• 30% 36% 33%
1	R	329	21% 6% 16% 78%
2	I	1342	10% 50% 50%
3	J	1430	14% 42% 50% • 7%
4	K	91	11% 53% 34% 13%
5	L	616	30% 33% 43% 24%
6	P	85	20% 15% 56% 28%

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Mol	Chain	Length	Quality of chain
7	Q	85	24% 15% 51% 34%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 32044 atoms, of which 117 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	231	1785	1112	318	349	6	0	0
1	H	219	1681	1050	295	330	6	0	0
1	R	73	572	362	100	108	2	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	I	1341	10575	6634	1842	2056	43	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	J	1337	10386	6525	1851	1961	49	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP U9YPW3
J	1408	LEU	-	expression tag	UNP U9YPW3
J	1409	GLU	-	expression tag	UNP U9YPW3
J	1410	LEU	-	expression tag	UNP U9YPW3
J	1411	GLU	-	expression tag	UNP U9YPW3
J	1412	VAL	-	expression tag	UNP U9YPW3
J	1413	LEU	-	expression tag	UNP U9YPW3
J	1414	PHE	-	expression tag	UNP U9YPW3
J	1415	GLN	-	expression tag	UNP U9YPW3
J	1416	GLY	-	expression tag	UNP U9YPW3
J	1417	PRO	-	expression tag	UNP U9YPW3

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1418	SER	-	expression tag	UNP U9YPW3
J	1419	SER	-	expression tag	UNP U9YPW3
J	1420	GLY	-	expression tag	UNP U9YPW3
J	1421	HIS	-	expression tag	UNP U9YPW3
J	1422	HIS	-	expression tag	UNP U9YPW3
J	1423	HIS	-	expression tag	UNP U9YPW3
J	1424	HIS	-	expression tag	UNP U9YPW3
J	1425	HIS	-	expression tag	UNP U9YPW3
J	1426	HIS	-	expression tag	UNP U9YPW3
J	1427	HIS	-	expression tag	UNP U9YPW3
J	1428	HIS	-	expression tag	UNP U9YPW3
J	1429	HIS	-	expression tag	UNP U9YPW3
J	1430	HIS	-	expression tag	UNP U9YPW3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	79	627	382	118	126	1	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	471	3821	2397	681	720	23	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

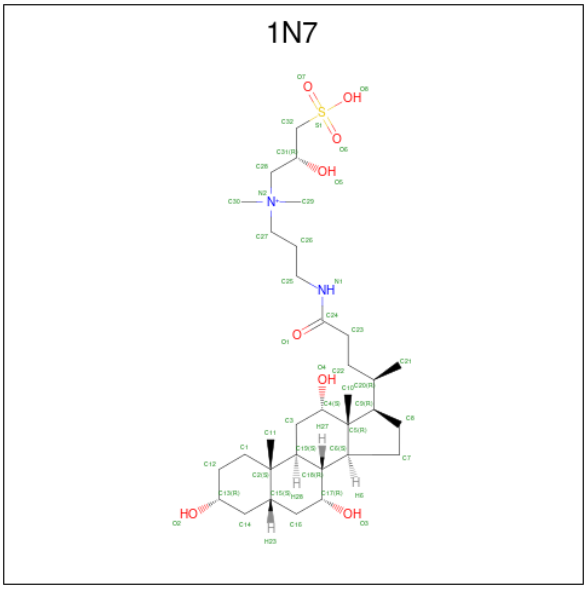
- Molecule 6 is a DNA chain called Non-template strand of rpsTP2 DNA promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	P	61	1253	599	235	358	61	0	0

- Molecule 7 is a DNA chain called Template strand of rpsTP2 DNA promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	Q	56	1143	549	192	346	56	0	0

- Molecule 8 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
8	I	1	66	24	39	3	0
8	J	1	66	24	39	3	0
8	L	1	66	24	39	3	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	J	1	1	1	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

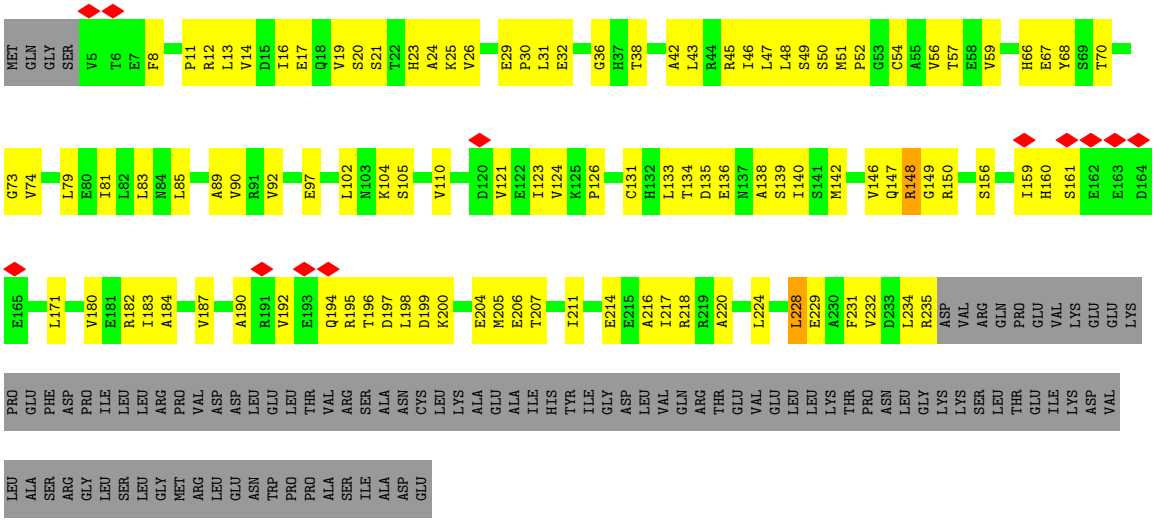
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	J	2	2	2	0

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.

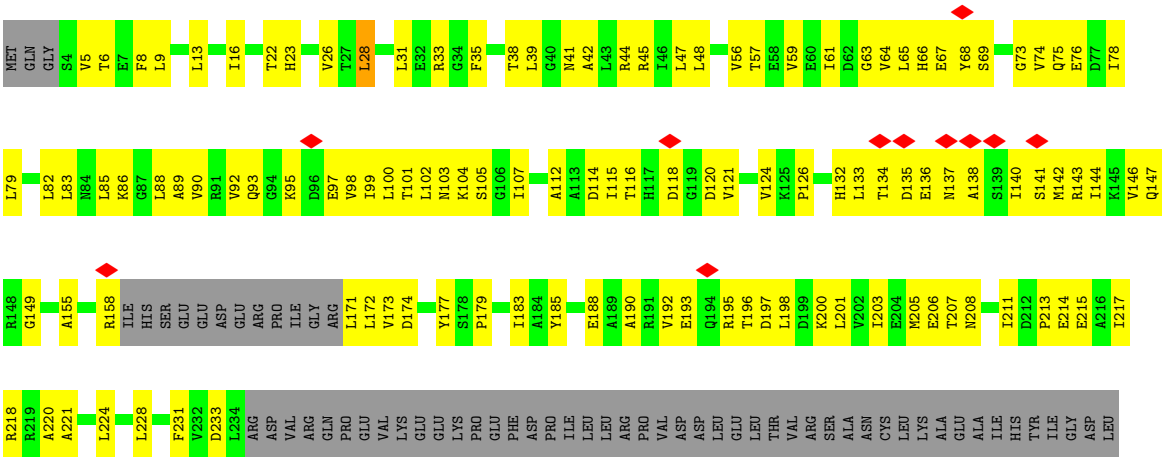
• Molecule 1: DNA-directed RNA polymerase subunit alpha

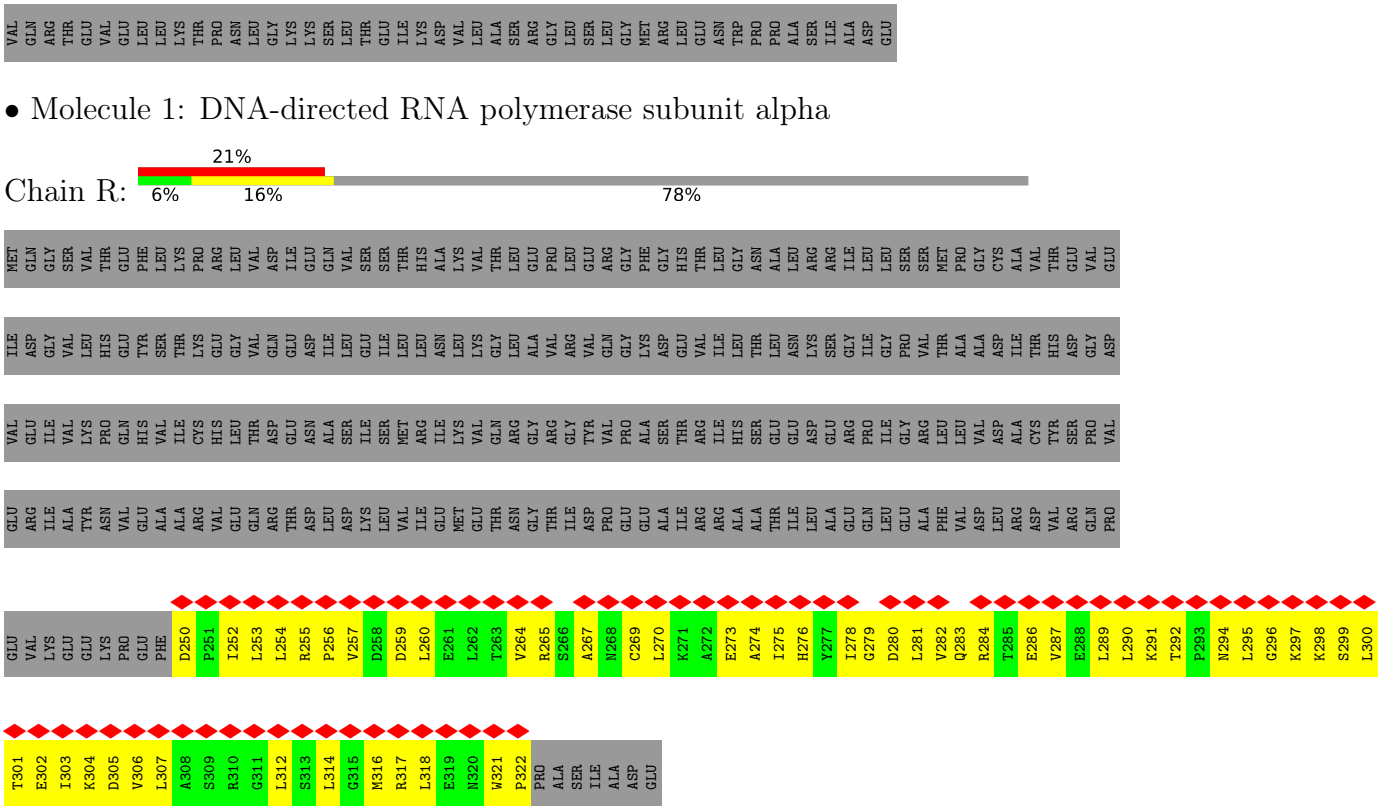
Chain G: 38% 32% 30%

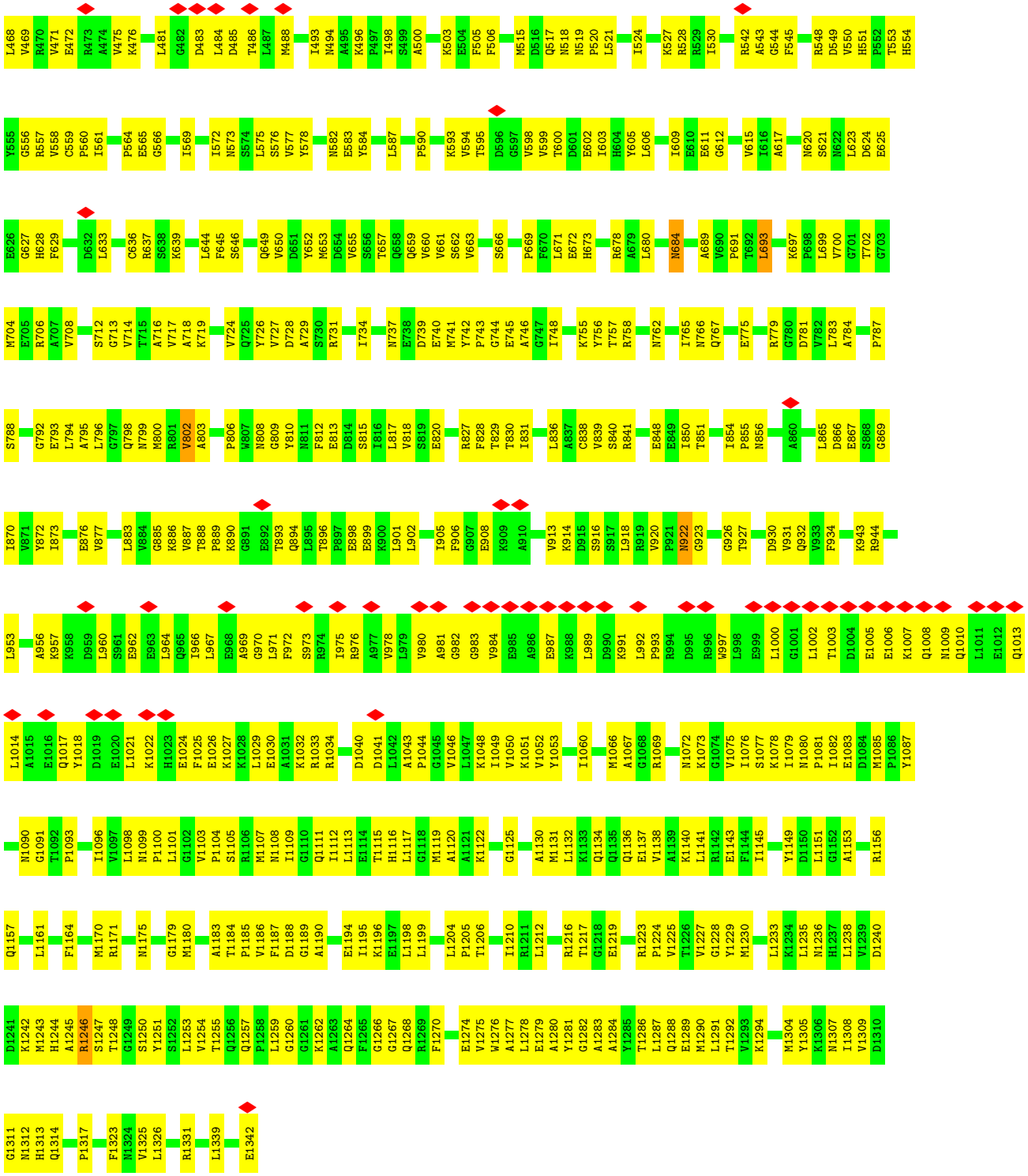


• Molecule 1: DNA-directed RNA polymerase subunit alpha

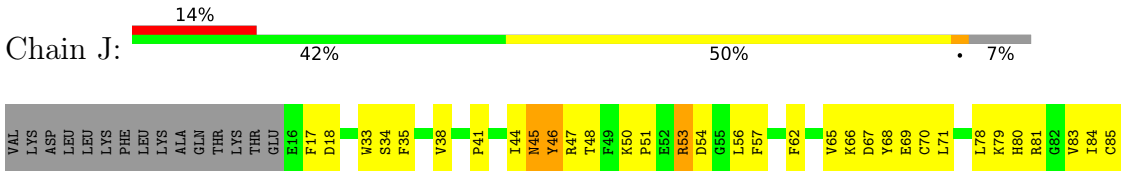
Chain H: 30% 36% 33%

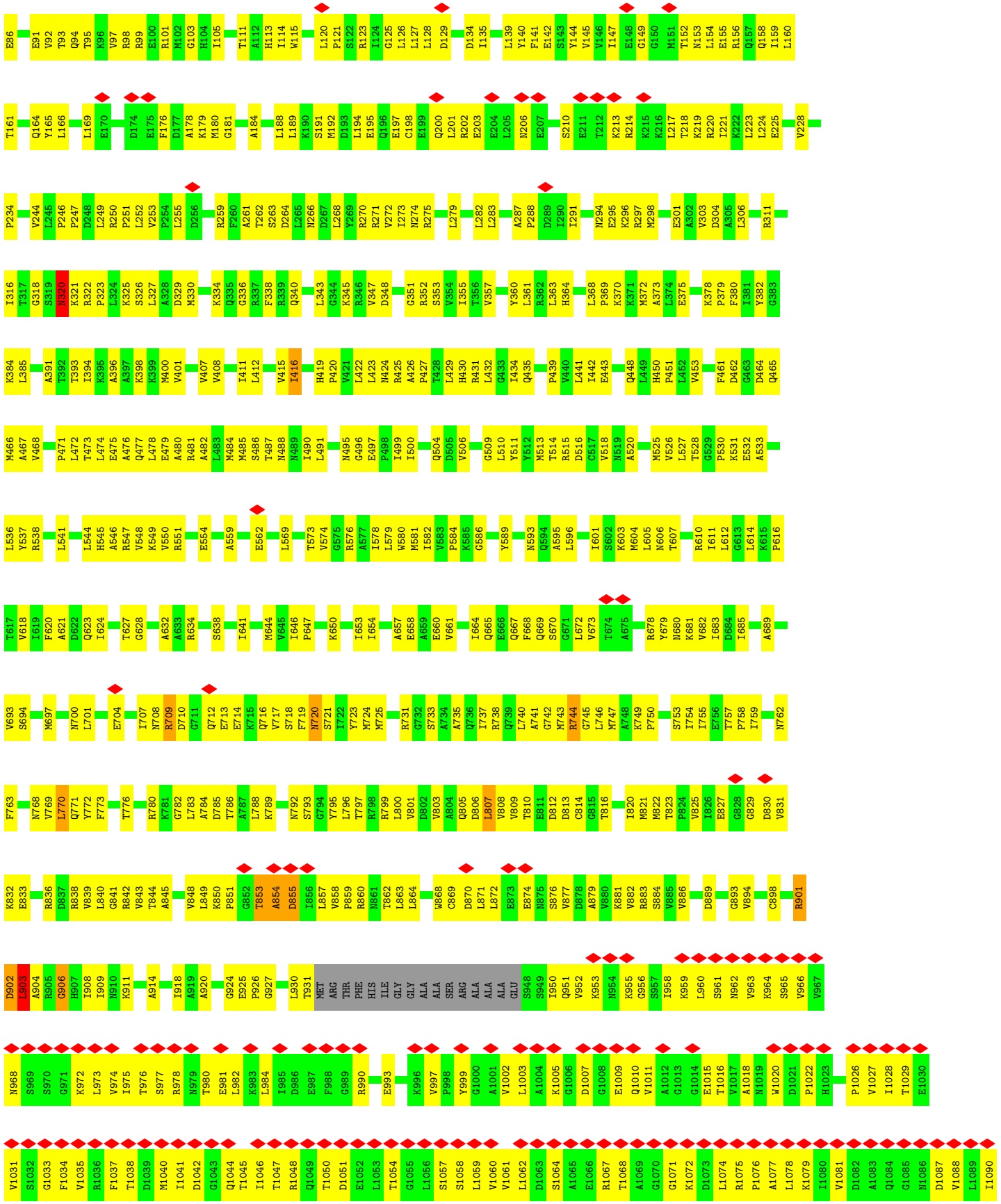


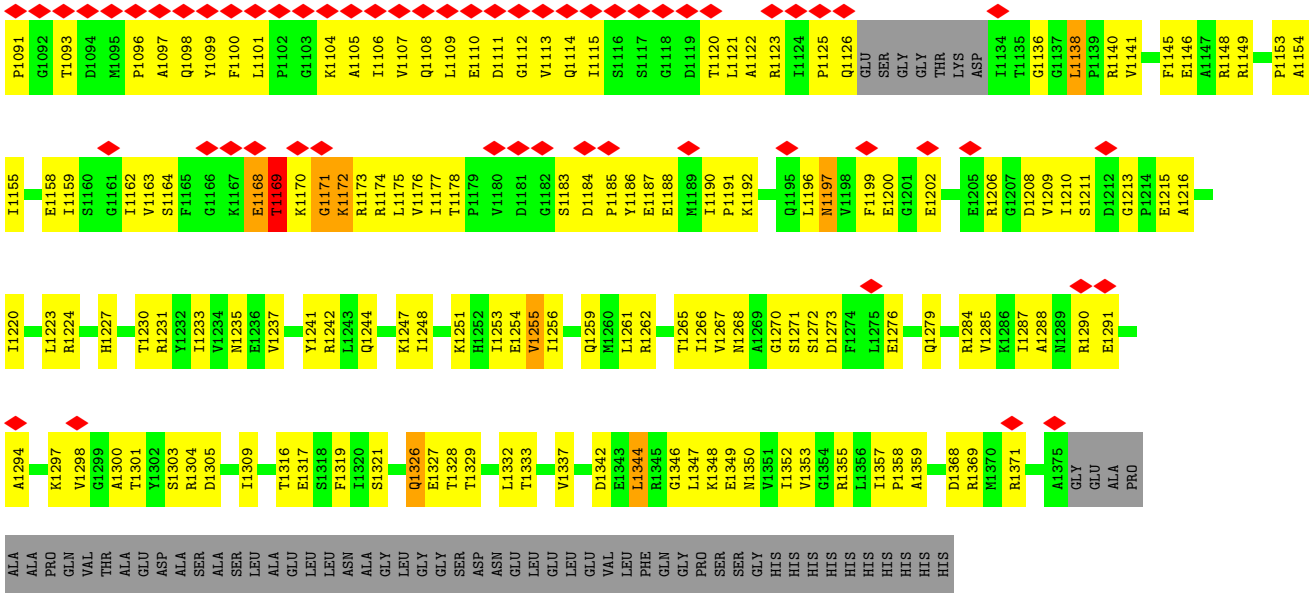

VAL GLN ARG THR GLU VAL GLU LEU LEU LYS LYS THR PRO ASN LEU GLY LYS LYS SER LEU THR GLU ILE LYS ASP VAL LEU ALA SER ARG GLY LEU SER LEU GLY MET ARG LEU GLU ASN TRP PRO PRO ALA SER ILE ALA ASP GLU
• Molecule 1: DNA-directed RNA polymerase subunit alpha
Chain R:
21%
6%
16%
78%
MET GLN GLY SER VAL THR GLU PHE LEU LYS PRO ARG LEU VAL ASP ILE GLU GLN VAL SER SER THR HIS ALA LYS VAL THR LEU GLU PRO LEU GLU ARG GLY PHE GLY HIS THR LEU GLY ASN ALA LEU ARG ARG ILE LEU LEU SER SER MET PRO GLY CYS ALA VAL THR GLU VAL GLU
ILE ASP GLY VAL LEU HIS GLU TYR SER THR LYS GLU GLY VAL GLN GLU ASP ILE LEU GLU ILE LEU LEU ASN LEU LYS GLY LEU ALA VAL ARG VAL GLN GLY LYS ASP GLU VAL ILE LEU THR LEU ASN LYS SER GLY ILE LEU GLY PRO VAL THR ALA ALA ASP ILE THR HIS ASP GLY ASP
VAL GLU ILE VAL LYS PRO GLN HIS VAL ILE CYS HIS LEU THR ASP GLU ASN ALA SER ILE SER MET ARG ILE LYS VAL GLN ARG GLY ARG GLY TYR VAL PRO ALA SER THR ARG ILE HIS SER GLU GLU ASP GLU ARG PRO ILE GLY ARG LEU LEU VAL ASP ALA CYS TYR SER PRO VAL
GLU ARG ILE ALA TYR ASN VAL GLU ALA ALA ARG VAL GLU GLN ARG THR ASP LEU ASP LYS LEU VAL ILE GLU MET GLU THR ASN GLY THR ILE ASP PRO GLU GLU ALA ILE ARG ARG ALA ALA THR ILE LEU ALA GLU GLN LEU GLU ALA PHE VAL ASP LEU ARG ASP VAL ARG GLN PRO
GLU VAL LYS GLU GLU LYS PRO GLU PHE D250 P251 I252 L253 L254 R255 P256 V257 D258 D259 L260 E261 L262 T263 V264 R265 S266 A267 N268 C269 L270 K271 A272 E273 A274 I275 H276 Y277 I278 G279 D280 L281 V282 Q283 R284 T285 E286 V287 E288 L289 L290 K291 T292 P293 N294 L295 G296 K297 K298 S299 L300
T301 E302 I303 K304 D305 V306 L307 A308 S309 R310 G311 L312 S313 L314 G315 M316 R317 L318 E319 N320 W321 P322 PRO ALA SER ILE ALA ASP GLU
• Molecule 2: DNA-directed RNA polymerase subunit beta
Chain I:
10%
50%
50%
MET V2 Y3 S4 Y5 T6 E7 K8 K9 R10 I11 R12 K13 D14 F15 G16 K17 R18 V21 L22 D23 V24 P25 Y26 L27 L28 S29 I30 Q31 L32 D33 K37 F38 I39 E44 G45 Q46 L49 E50 A51 A52 F53 V56 F57 Q60 S61 Y62 S63 E67 L68 Q69 Y70 V71
R74 L75 D81 E84 V90 T91 Y92 S93 A94 R97 V98 K99 L100 R101 L102 V103 E106 R107 E108 A109 P110 E111 G112 T113 V114 K115 D116 I117 K118 Y123 M124 G125 E126 I127 P128 L129 M130 T131 D132 N133 G134 T135 F136 V137 I138 T141 E142 R143 V144 I145 Q148
L149 H150 R151 V155 F156 F157 D158 S159 D160 K161 G162 K163 T164 H165 S166 S167 L171 R175 I176 L184 D185 F186 E187 F188 D189 D192 N193 L194 F195 L204 T207 I208 N214 Y215 T216 T217 E218 Q219 I220 L221 F224 I229 F230 E231 I232 R233 D234 N235 K236 L237
Q238 M239 E240 L241 V242 P243 E244 R245 L246 R247 G248 E249 T250 A251 S252 F253 D254 I255 E256 A257 N258 G259 K260 V261 Y262 V263 E264 K265 G266 R267 R268 I269 T270 A271 R272 H273 I274 R275 Q276 L277 E278 K279 D280 D281 V282 K283 L284 I285 E286 V287 P288 V289 I292 A293 V296 V297 A298 K299
D300 Y301 I302 D303 E304 S305 T306 G307 E308 L309 I310 C311 A312 A313 N314 M315 E316 L317 S318 L319 D320 L321 L322 A323 K324 L325 S326 Q327 S328 G329 H330 K331 R332 I333 E334 F337 T338 N339 D340 H343 G344 P345 Y346 I347 S348 E349 D354 R359 L360 L363 V364 E365 I366 Y367
R371 P372 G373 E374 P375 P376 T377 R378 E379 A380 L384 L388 F389 D396 L397 S398 A399 V400 G401 E412 E413 G418 K422 D423 D424 I425 V428 K431 L432 I435 V442 D443 D444 I445 D446 H447 N450 R451 R452 I453 R454 S455 V456 G457 E458 M459 Q463



- Molecule 3: DNA-directed RNA polymerase subunit beta'

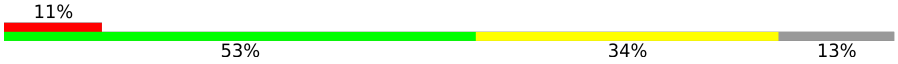


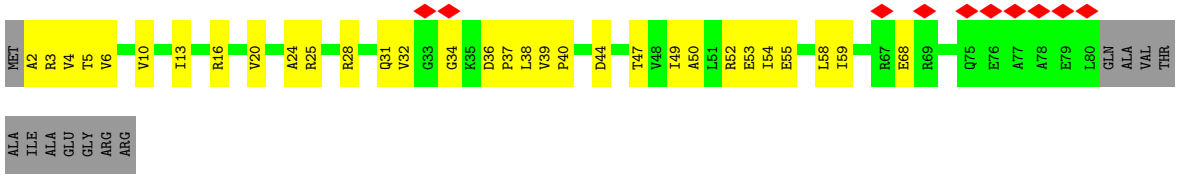

E86 E91 V92 T93 Q94 T95 K96 V97 R98 R99 E100 R101 M102 G103 H104 I105 T111 A112 H113 I114 W115 L120 P121 S122 R123 I124 G125 L126 L127 L128 D129 D134 I135 L139 Y140 F141 E142 S143 Y144 V145 V146 I147 E148 G149 G150 M151 T152 N153 L154 E155 R156 Q157 Q158 I159 L160
T161 Q164 Y165 L166 L169 E170 D174 E175 F176 D177 A178 K179 M180 G181 A184 L188 L189 K190 S191 M192 D193 L194 E195 Q196 E197 C198 E199 Q200 L201 R202 E203 E204 L205 N206 E207 S210 E211 T212 K213 R214 K215 K216 L217 T218 K219 R220 I221 K222 L223 L224 E225 V228
P234 V244 L245 P246 P247 D248 L249 R250 P251 L252 V253 P254 L255 D256 R259 F260 A261 T262 S263 D264 L265 N266 D267 L268 Y269 R270 R271 V272 I273 N274 R275 L279 L282 L283 A287 P288 D289 T290 I291 N294 E295 K296 R297 M298 E301 A302 V303 D304 A305 L306 R311
I316 T317 G318 S319 N320 K321 R322 P323 L324 K325 S326 L327 A328 D329 M330 K334 Q335 G336 R337 F338 R339 Q340 L343 G344 K345 R346 V347 D348 G351 R352 S353 V354 I355 T356 V357 Y360 L361 R362 L363 H364 L368 P369 K370 K371 M372 A373 L374 E375 K378 P379 F380 I381 Y382 G383
K384 L385 A391 T392 T393 I394 K395 A396 A397 K398 K399 M400 V401 V407 V408 I411 L412 V415 I416 H419 P420 V421 L422 L423 N424 R425 A426 P427 T428 L429 H430 R431 L432 G433 I434 Q435 P439 V440 L441 I442 E443 Q448 L449 H450 P451 L452 V453 F461 D462 G463 D464 Q465
M466 A467 V468 P471 L472 T473 L474 E475 A476 Q477 L478 E479 A480 R481 A482 L483 M484 M485 S486 T487 N488 N489 I490 L491 N495 G496 E497 P498 I499 I500 Q504 D505 V506 G509 L510 Y511 Y512 M513 T514 R515 D516 C517 V518 N519 A520 M525 V526 L527 T528 G529 P530 K531 E532 A533
L536 Y537 R538 L541 L544 H545 A546 R547 V548 K549 V550 R551 E554 A559 E562 L569 T573 V574 G575 R576 A577 I578 L579 W580 M581 I582 V583 P584 K585 G586 Y589 N593 Q594 A595 L596 I601 S602 K603 M604 L605 N606 T607 R610 I611 L612 G613 L614 K615 P616
T617 V618 I619 F620 A621 D622 Q623 I624 T627 G628 A632 A633 R634 S638 I641 M644 V645 I646 P647 K650 I653 I654 A657 E658 A659 E660 V661 I664 Q665 E666 Q667 F668 Q669 S670 G671 L672 V673 T674 A675 R678 Y679 N680 K681 V682 I683 D684 I685 A689
V693 S694 M697 N700 L701 E704 I707 N708 R709 D710 G711 Q712 E713 E714 K715 Q716 V717 S718 F719 N720 S721 I722 Y723 M724 M725 R731 G732 S733 A734 A735 Q736 I737 R738 Q739 L740 A741 G742 M743 R744 G745 L746 M747 A748 K749 P750 S753 I754 I755 E756 T757 P758 I759 N762
F763 N768 V769 L770 Q771 Y772 F773 T776 R780 K781 G782 L783 A784 D785 T786 A787 L788 K789 N792 S793 G794 Y795 L796 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 L807 V808 V809 T810 E811 D812 D813 C814 G815 T816 I820 M821 M822 T823 P824 V825 I826 E827 G828 G829 D830 V831
K832 E833 R836 D837 R838 V839 L840 G841 R842 V843 T844 A845 V848 L849 K850 P851 G852 T853 A854 D855 T856 L857 V858 P859 R860 N861 T862 L863 L864 W868 C869 D870 L871 L872 E873 E874 N875 S876 V877 D878 A879 V880 K881 V882 R883 S884 V885 V886 D889 G893 V894 C898 R901
D902 L903 A904 R905 G906 H907 I908 I909 N910 K911 A914 I918 A919 A920 G924 E925 P926 G927 L930 T931 MET ARG THR PHE HIS ILE GLY GLY ALA ALA SER ARG ALA ALA ALA GLU S948 S949 I950 Q951 V952 K953 N954 K955 G956 S957 I958 K959 L960 S961 N962 V963 K964 S965 V966 V967
N968 S969 S970 G971 K972 L973 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 F988 G989 R990 E993 K996 V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 Q1010 V1011 A1012 G1013 G1014 E1015 T1016 V1017 A1018 N1019 W1020 D1021 P1022 H1023 P1026 V1027 I1028 T1029 E1030
V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042 G1043 Q1044 T1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 G1055 L1056 S1057 S1058 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 T1068 A1069 G1070 G1071 K1072 D1073 L1074 R1075 P1076 A1077 L1078 K1079 I1080 V1081 D1082 A1083 Q1084 G1085 N1086 D1087 V1088 L1089 I1090



• Molecule 4: DNA-directed RNA polymerase subunit omega

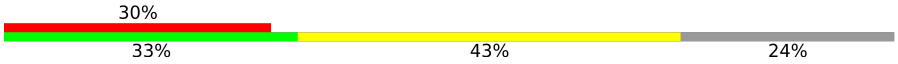
Chain K:

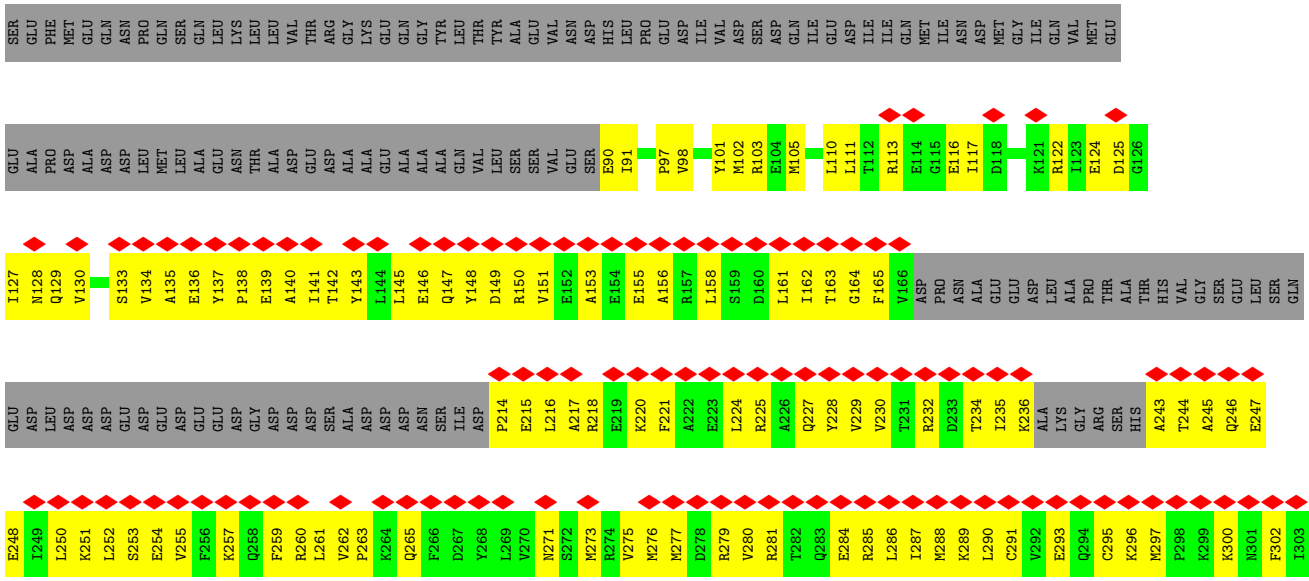


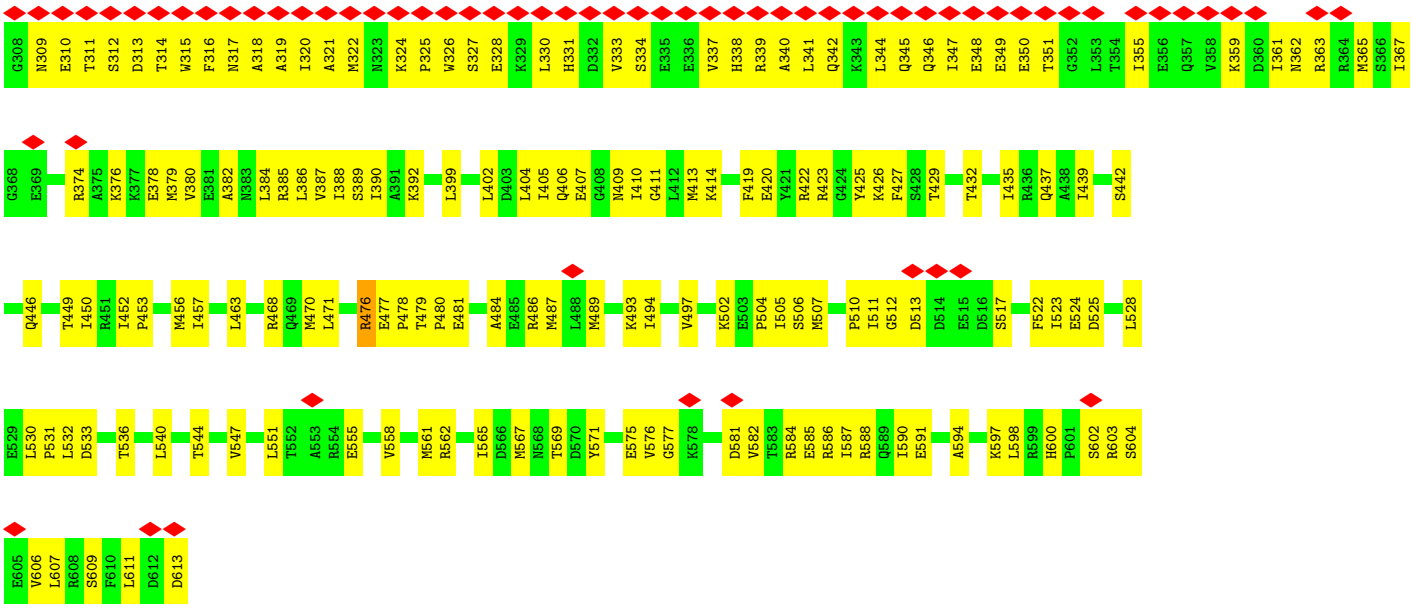


• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:

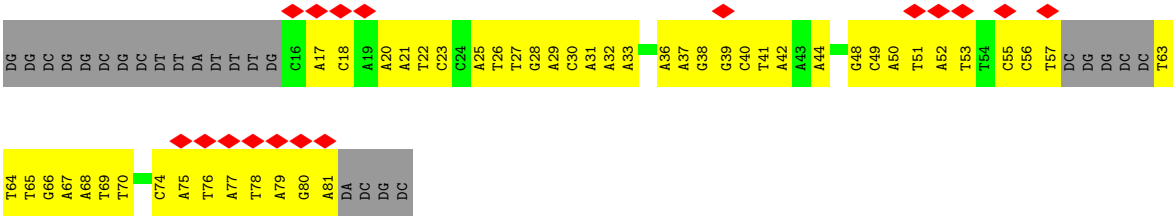






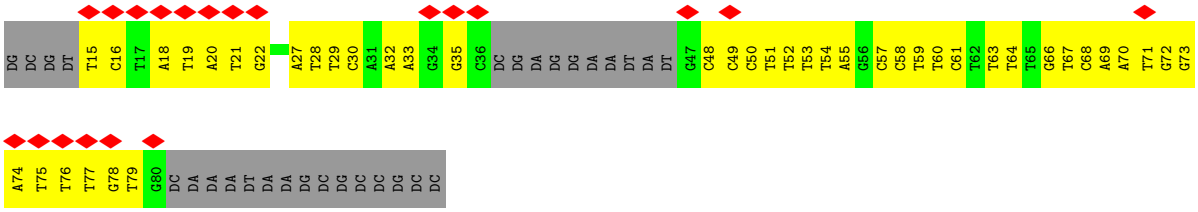
• Molecule 6: Non-template strand of rpsTP2 DNA promoter

Chain P:



• Molecule 7: Template strand of rpsTP2 DNA promoter

Chain Q:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	289670	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 ($e^-/Å^2$)	1.0	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	0.251	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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: 1N7, ZN, MG

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	G	0.71	0/1807	0.69	1/2449 (0.0%)
1	H	0.55	0/1700	0.65	1/2305 (0.0%)
1	R	0.26	0/579	0.51	0/784
2	I	0.75	0/10744	0.68	3/14496 (0.0%)
3	J	0.70	2/10543 (0.0%)	0.69	3/14239 (0.0%)
4	K	0.50	0/629	0.59	0/847
5	L	0.42	0/3872	0.55	0/5204
6	P	0.75	0/1407	0.97	0/2166
7	Q	0.73	0/1276	0.99	0/1965
All	All	0.68	2/32557 (0.0%)	0.70	8/44455 (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
2	I	0	1
3	J	0	10
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1255	VAL	CB-CG1	-5.31	1.41	1.52
3	J	453	VAL	CB-CG1	-5.03	1.42	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1344	LEU	CA-CB-CG	-6.66	99.97	115.30
3	J	903	LEU	CA-CB-CG	6.38	129.96	115.30
2	I	693	LEU	CA-CB-CG	5.57	128.10	115.30
3	J	807	LEU	CA-CB-CG	-5.45	102.77	115.30
2	I	28	LEU	CA-CB-CG	-5.36	102.98	115.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	1185	PRO	Peptide
3	J	320	ASN	Peptide
3	J	416	ILE	Peptide
3	J	853	THR	Peptide
3	J	855	ASP	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	G	1785	0	1806	120	0
1	H	1681	0	1708	148	0
1	R	572	0	602	84	0
2	I	10575	0	10584	682	0
3	J	10386	0	10594	791	0
4	K	627	0	634	39	0
5	L	3821	0	3891	312	0
6	P	1253	0	689	72	0
7	Q	1143	0	640	50	0
8	I	27	39	37	6	0
8	J	27	39	37	4	0
8	L	27	39	38	4	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	31927	117	31260	2115	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 33.

The worst 5 of 2115 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)
8:I:1401:1N7:C3	8:I:1401:1N7:C19	1.83	1.55
8:J:1504:1N7:C19	8:J:1504:1N7:C3	1.84	1.54
8:L:701:1N7:C19	8:L:701:1N7:C3	1.84	1.52
1:H:105:SER:HA	1:H:138:ALA:HB2	1.42	1.01
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.43	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	229/329 (70%)	194 (85%)	35 (15%)	0	100	100
1	H	215/329 (65%)	185 (86%)	30 (14%)	0	100	100
1	R	71/329 (22%)	62 (87%)	9 (13%)	0	100	100
2	I	1339/1342 (100%)	1161 (87%)	175 (13%)	3 (0%)	47	78
3	J	1331/1430 (93%)	1167 (88%)	157 (12%)	7 (0%)	29	61
4	K	77/91 (85%)	67 (87%)	10 (13%)	0	100	100
5	L	465/616 (76%)	428 (92%)	37 (8%)	0	100	100
All	All	3727/4466 (84%)	3264 (88%)	453 (12%)	10 (0%)	44	72

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	854	ALA
3	J	1169	THR
2	I	399	ALA
3	J	320	ASN
3	J	1172	LYS

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	G	196/286 (68%)	195 (100%)	1 (0%)	88	94
1	H	186/286 (65%)	186 (100%)	0	100	100
1	R	65/286 (23%)	65 (100%)	0	100	100
2	I	1155/1157 (100%)	1149 (100%)	6 (0%)	88	94
3	J	1118/1189 (94%)	1108 (99%)	10 (1%)	78	90
4	K	67/75 (89%)	67 (100%)	0	100	100
5	L	415/543 (76%)	414 (100%)	1 (0%)	93	98
All	All	3202/3822 (84%)	3184 (99%)	18 (1%)	86	94

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	901	ARG
5	L	476	ARG
3	J	1197	ASN
3	J	53	ARG
3	J	770	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	817	HIS
5	L	265	GLN
3	J	1010	GLN
3	J	1326	GLN
5	L	331	HIS

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)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
8	1N7	I	1401	-	30,30,46	5.03	16 (53%)	47,48,72	2.59	17 (36%)
8	1N7	J	1504	-	30,30,46	5.12	15 (50%)	47,48,72	2.84	25 (53%)
8	1N7	L	701	-	30,30,46	5.03	14 (46%)	47,48,72	2.67	16 (34%)

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
8	1N7	I	1401	-	-	1/7/72/92	0/4/4/4
8	1N7	J	1504	-	-	7/7/72/92	0/4/4/4
8	1N7	L	701	-	-	0/7/72/92	0/4/4/4

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	1N7	C3-C19	18.52	1.84	1.53
8	L	701	1N7	C3-C19	18.49	1.84	1.53
8	I	1401	1N7	C3-C19	17.99	1.83	1.53
8	I	1401	1N7	C3-C4	12.22	1.73	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	701	1N7	C3-C4	11.66	1.73	1.53

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	1504	1N7	C9-C5-C4	-8.57	109.84	117.67
8	L	701	1N7	C7-C6-C18	-7.10	108.40	118.33
8	L	701	1N7	C9-C5-C6	6.82	106.97	100.09
8	I	1401	1N7	C9-C5-C6	6.44	106.59	100.09
8	L	701	1N7	C9-C5-C4	-6.15	112.05	117.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

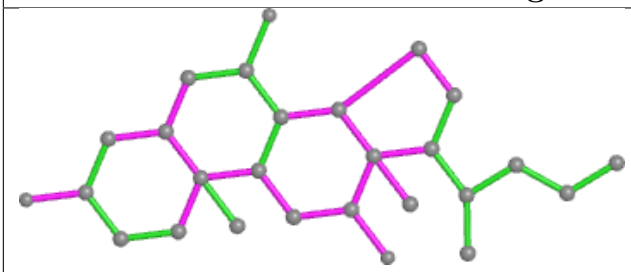
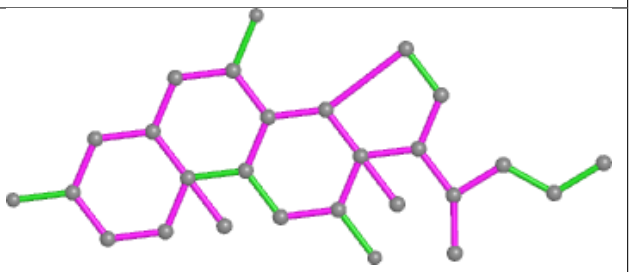
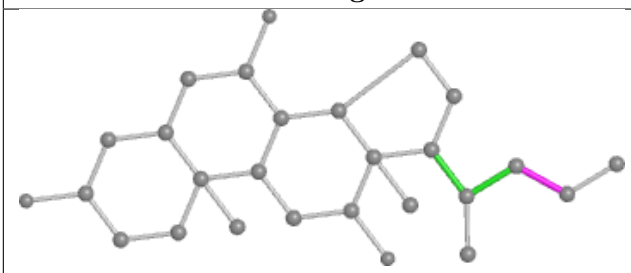
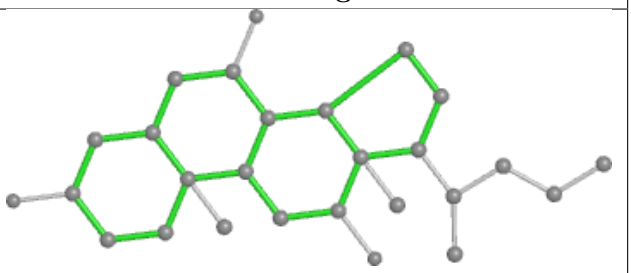
Mol	Chain	Res	Type	Atoms
8	J	1504	1N7	C21-C20-C9-C5
8	J	1504	1N7	C21-C20-C9-C8
8	J	1504	1N7	C22-C20-C9-C5
8	J	1504	1N7	C22-C20-C9-C8
8	J	1504	1N7	C9-C20-C22-C23

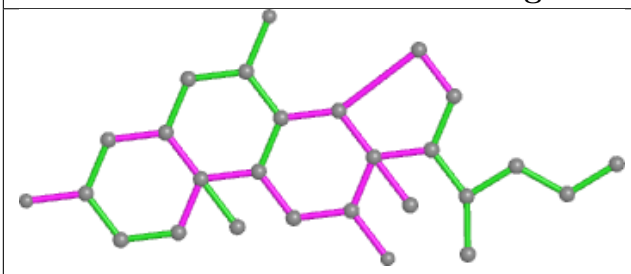
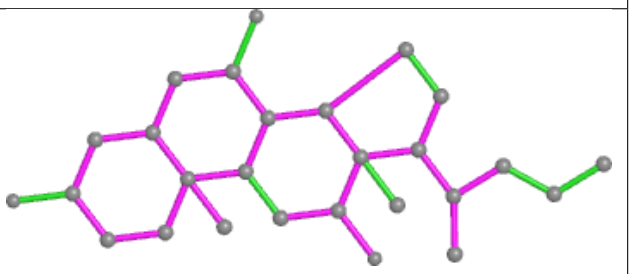
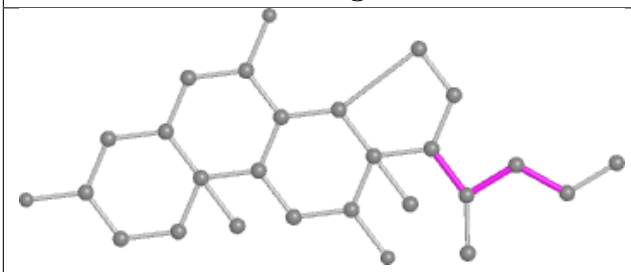
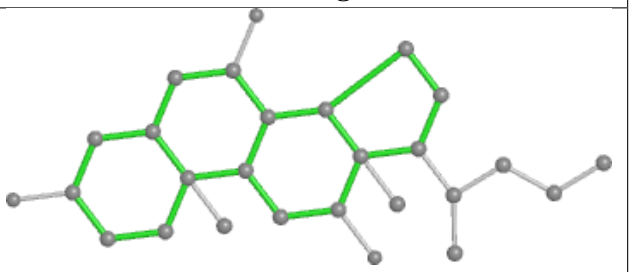
There are no ring outliers.

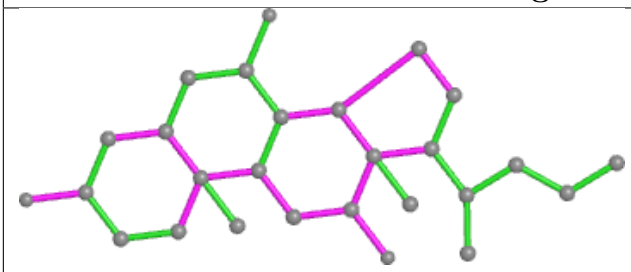
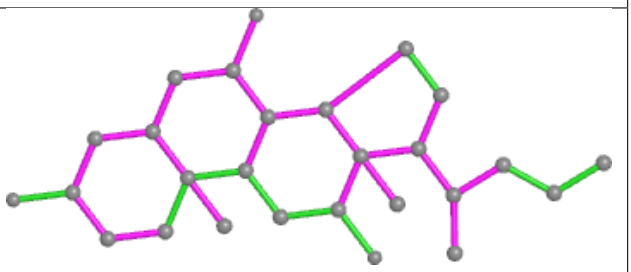
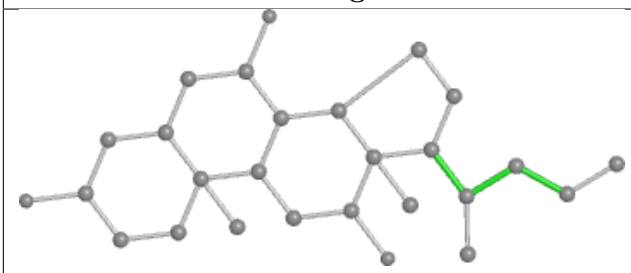
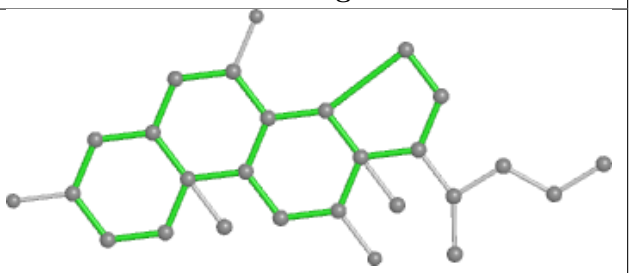
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1401	1N7	6	0
8	J	1504	1N7	4	0
8	L	701	1N7	4	0

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 1N7 I 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 1N7 J 1504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 1N7 L 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

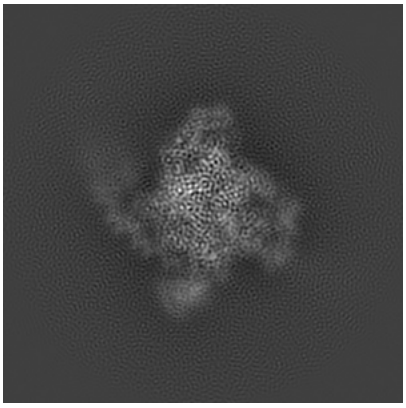
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20203. These allow visual inspection of the internal detail of the map and identification of artifacts.

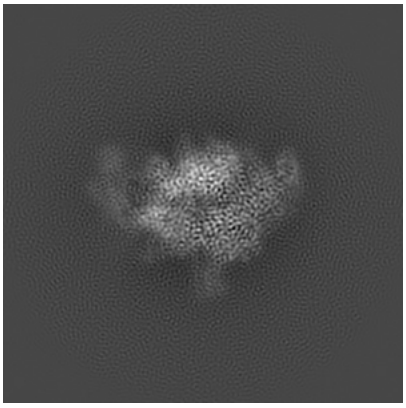
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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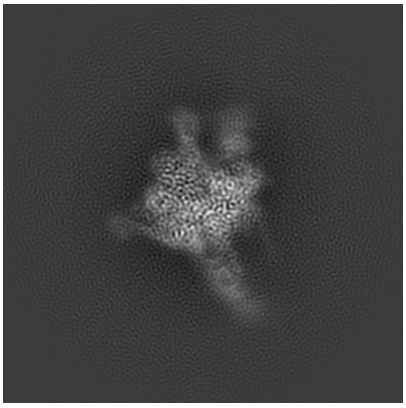
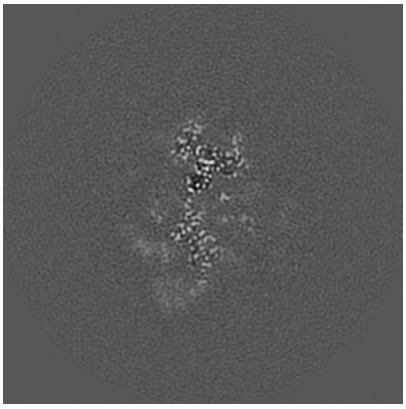


Z

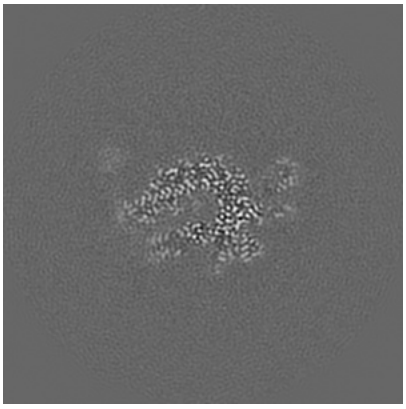
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

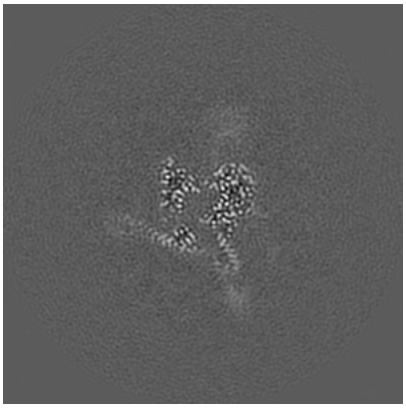
6.2.1 Primary map



X Index: 128



Y Index: 128

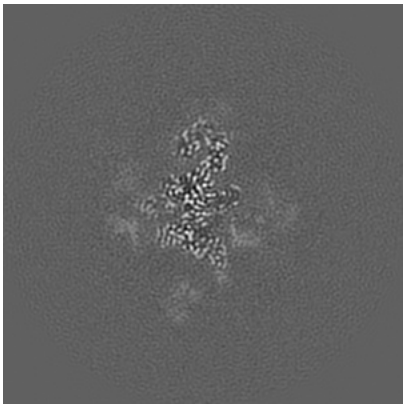


Z Index: 128

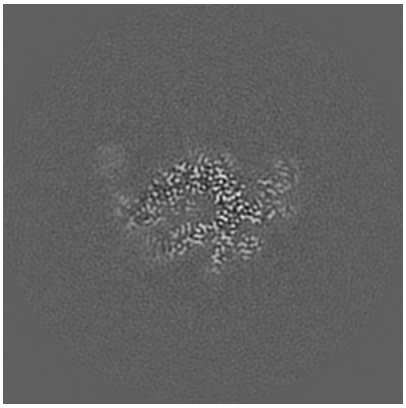
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

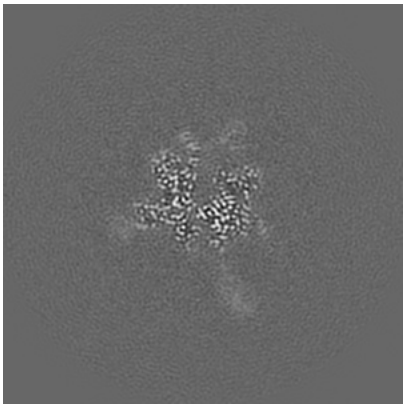
6.3.1 Primary map



X Index: 138



Y Index: 126

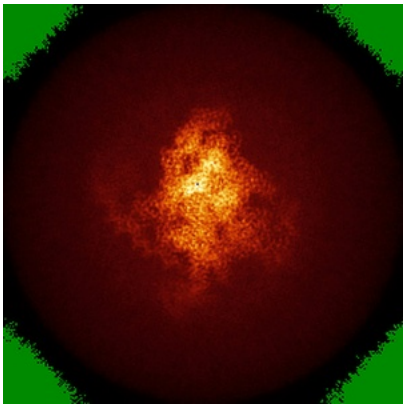


Z Index: 136

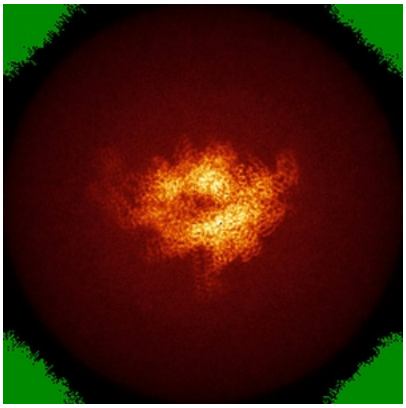
The images above show the largest variance slices of the map in three orthogonal directions.

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

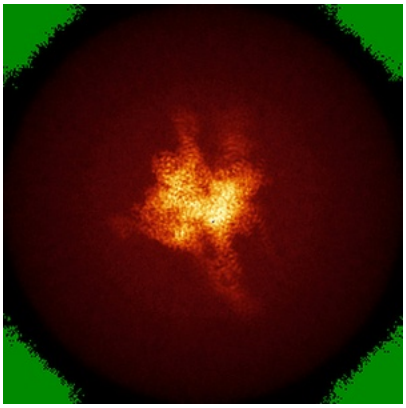
6.4.1 Primary map



X



Y

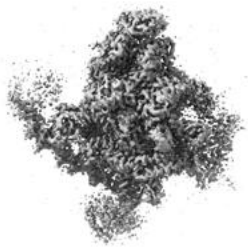


Z

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

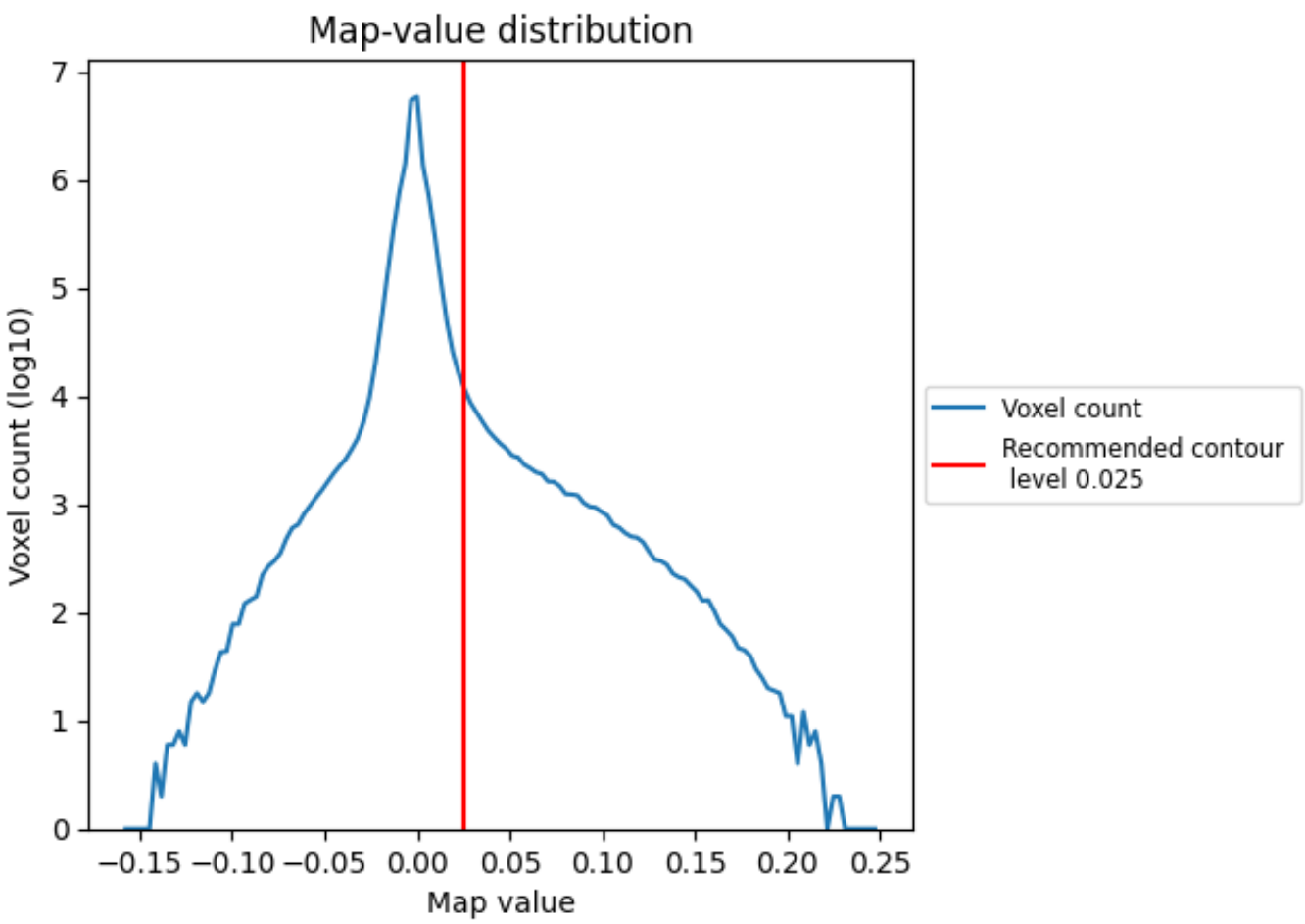
6.6 Mask visualisation (i)

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

7 Map analysis (i)

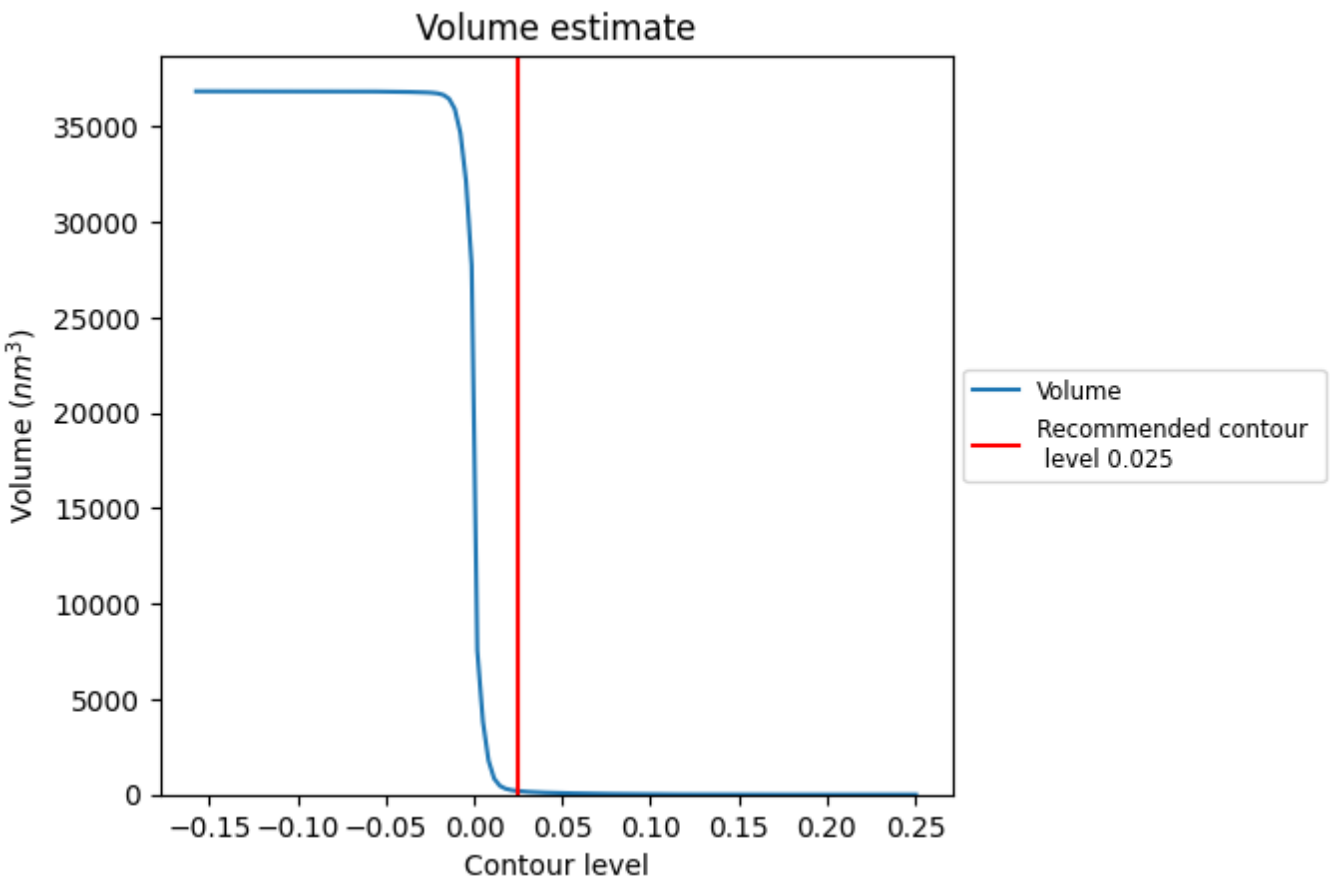
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

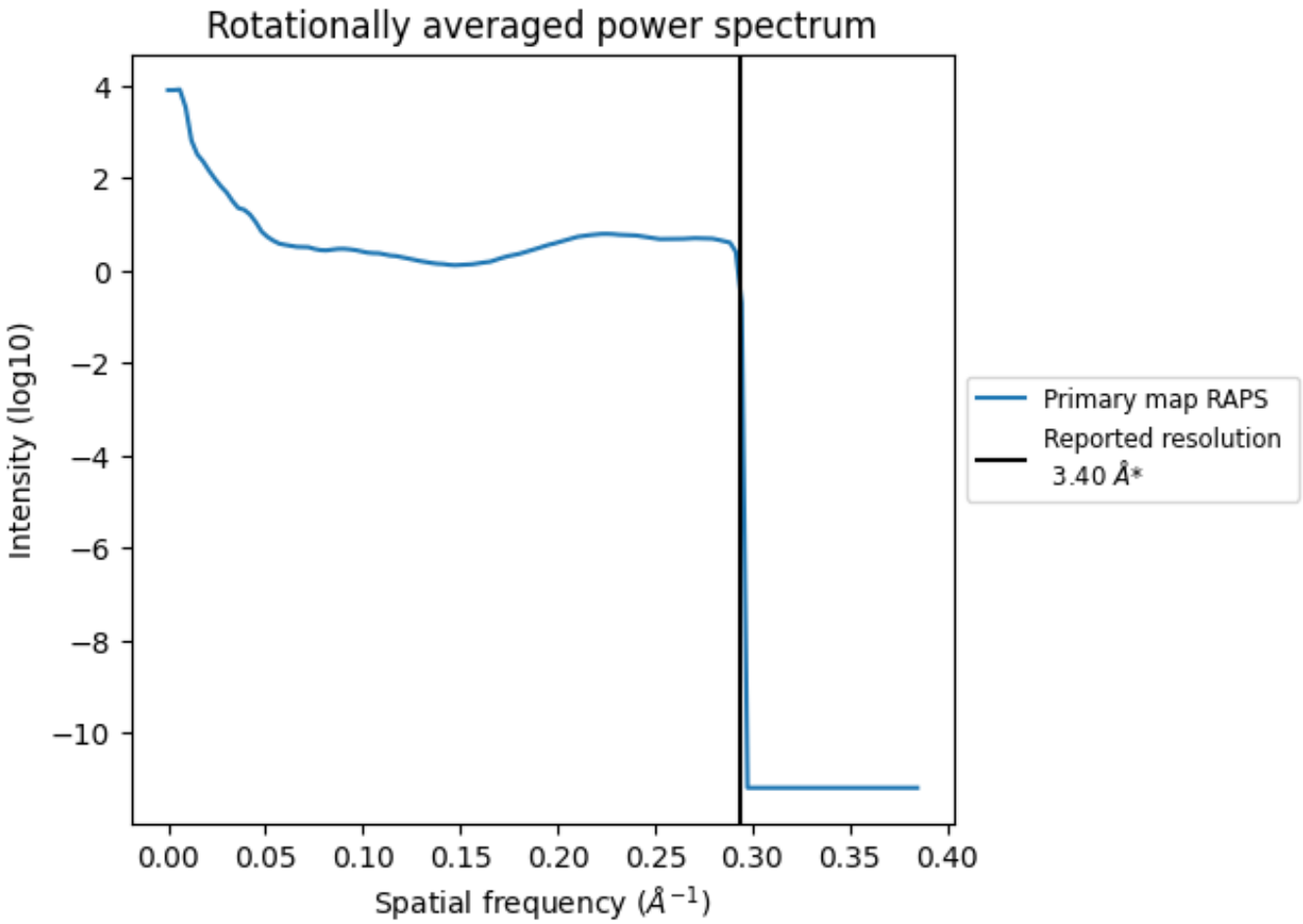
7.2 Volume estimate (i)



The volume at the recommended contour level is 187 nm^3; this corresponds to an approximate mass of 169 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)

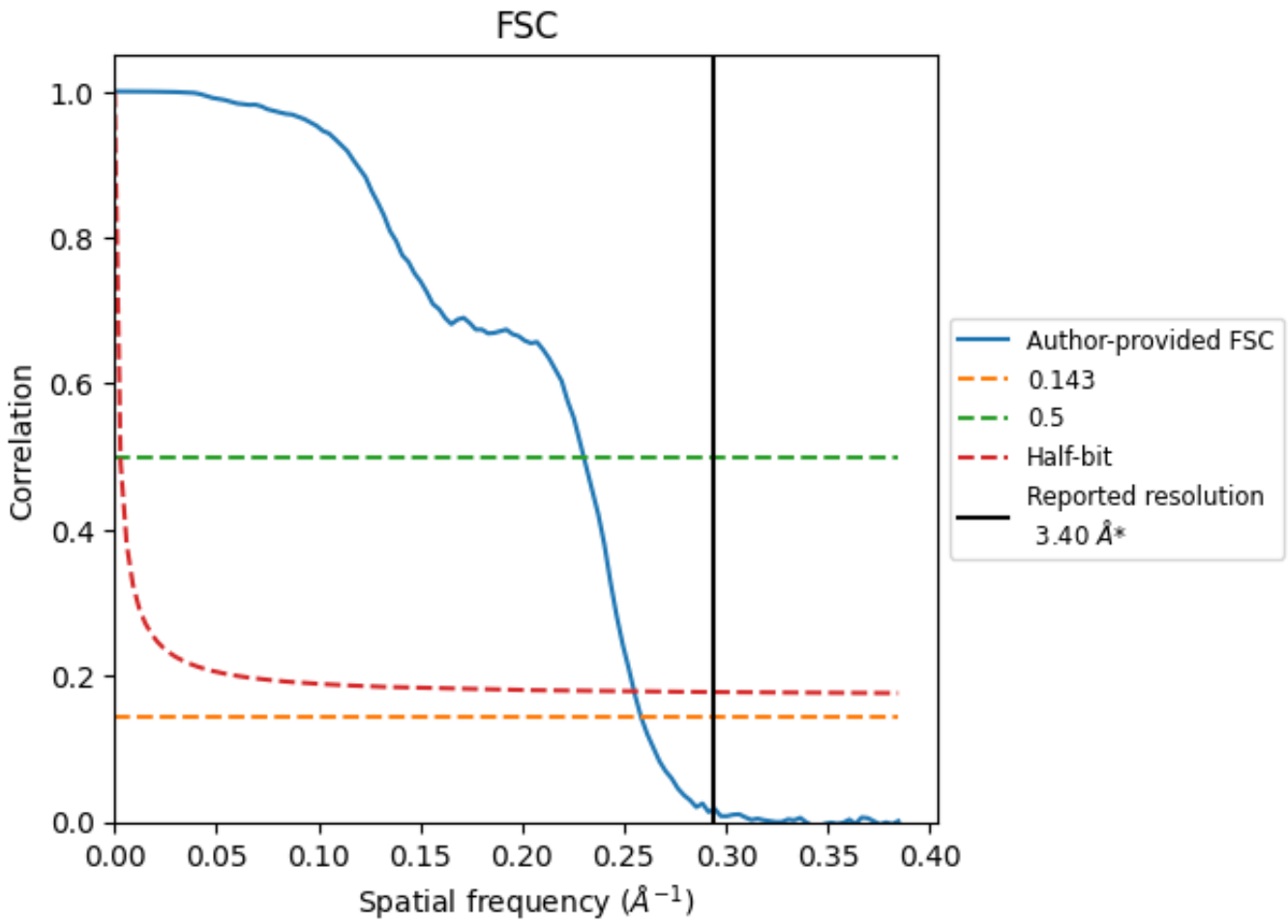


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

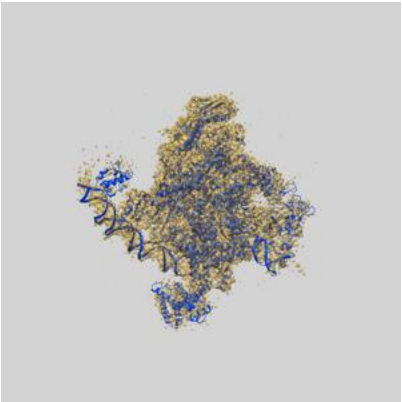
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.87	4.34	3.92
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.4 by more than 10 %

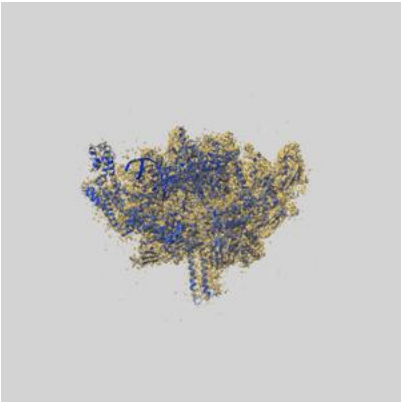
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20203 and PDB model 6OUL. Per-residue inclusion information can be found in section 3 on page 7.

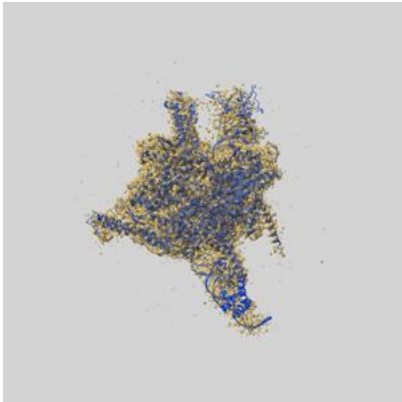
9.1 Map-model overlay (i)



X



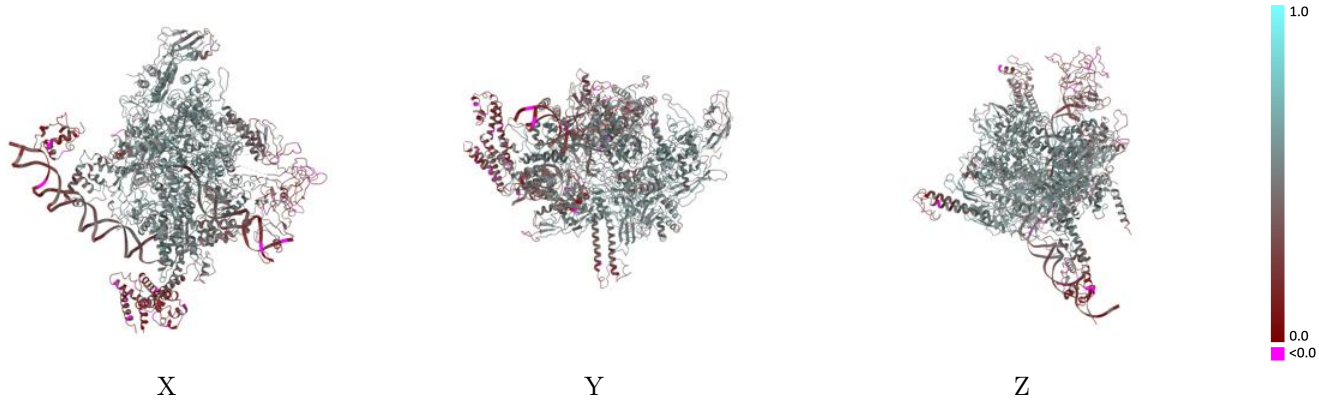
Y



Z

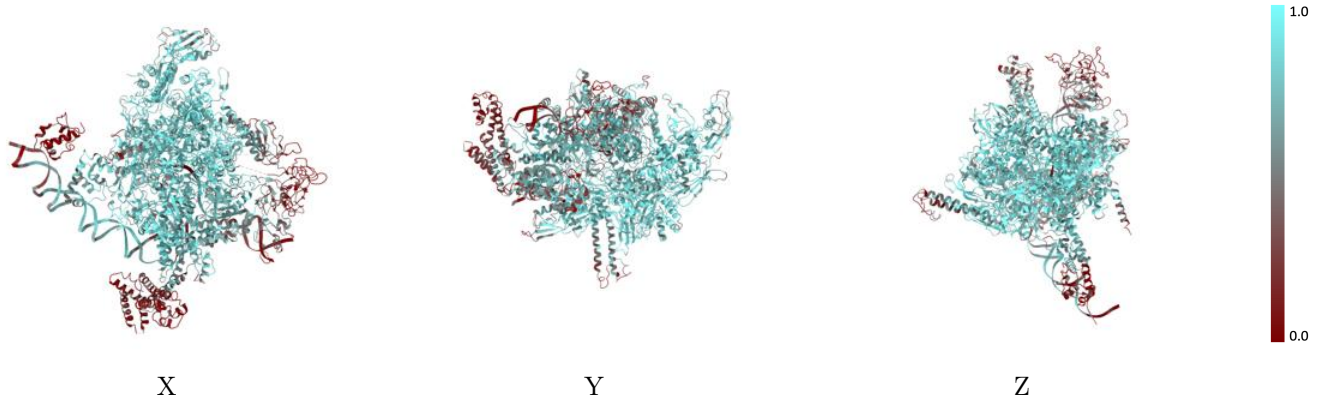
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



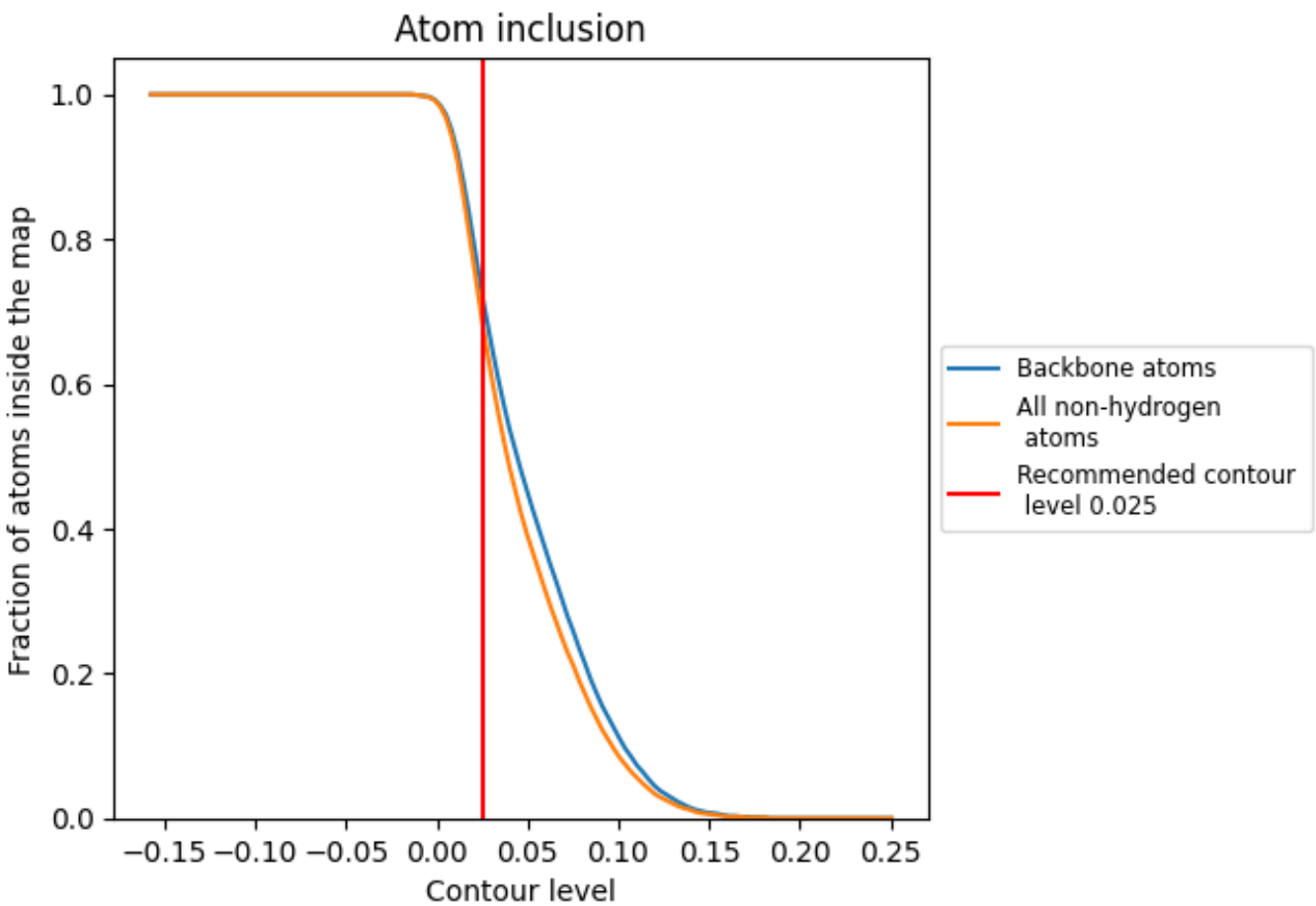
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.4600
G	0.7840	0.5150
H	0.7480	0.4900
I	0.7640	0.4990
J	0.7240	0.4850
K	0.6790	0.4830
L	0.5050	0.3730
P	0.5540	0.3180
Q	0.5380	0.2950
R	0.0770	0.2020