wwPDB EM Validation Summary Report (i)

Apr 30, 2024 – 09:30 pm BST

PDB ID	:	4AU6
EMDB ID	:	EMD-2100
Title	:	Location of the dsRNA-dependent polymerase, VP1, in rotavirus particles
Authors	:	Estrozi, L.F.; Settembre, E.C.; Goret, G.; McClain, B.; Zhang, X.; Chen, J.Z.; Grigorieff, N.; Harrison, S.C.
Deposited on	:	2012-05-14
Resolution	:	6.00 Å(reported)
Based on initial model	:	2R7O

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 (i)) were used in the production of this report:

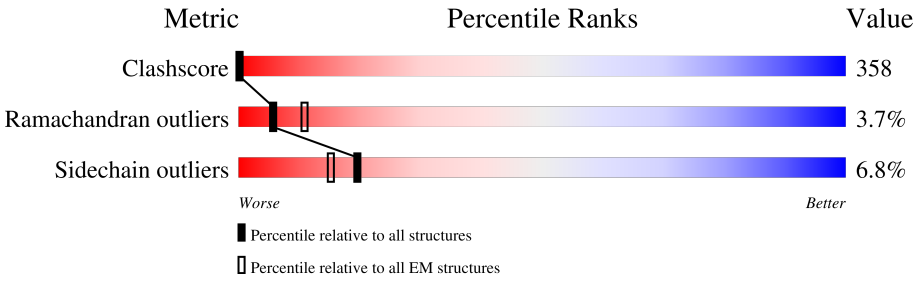
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 6.00 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)
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	A	1095	45% 16% 74% 8% .
1	B	1095	46% 15% 74% 8% .
1	C	1095	46% 15% 75% 8% .
1	D	1095	46% 15% 74% 8% .
1	E	1095	46% 15% 75% 8% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 43705 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 RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		
1	B	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		
1	C	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		
1	D	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		
1	E	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP O37061
A	-4	HIS	-	expression tag	UNP O37061
A	-3	HIS	-	expression tag	UNP O37061
A	-2	HIS	-	expression tag	UNP O37061
A	-1	HIS	-	expression tag	UNP O37061
A	0	HIS	-	expression tag	UNP O37061
A	1089	PRO	-	expression tag	UNP O37061
B	-5	HIS	-	expression tag	UNP O37061
B	-4	HIS	-	expression tag	UNP O37061
B	-3	HIS	-	expression tag	UNP O37061
B	-2	HIS	-	expression tag	UNP O37061
B	-1	HIS	-	expression tag	UNP O37061
B	0	HIS	-	expression tag	UNP O37061
B	1089	PRO	-	expression tag	UNP O37061
C	-5	HIS	-	expression tag	UNP O37061
C	-4	HIS	-	expression tag	UNP O37061
C	-3	HIS	-	expression tag	UNP O37061
C	-2	HIS	-	expression tag	UNP O37061
C	-1	HIS	-	expression tag	UNP O37061
C	0	HIS	-	expression tag	UNP O37061

Continued on next page...

Continued from previous page...

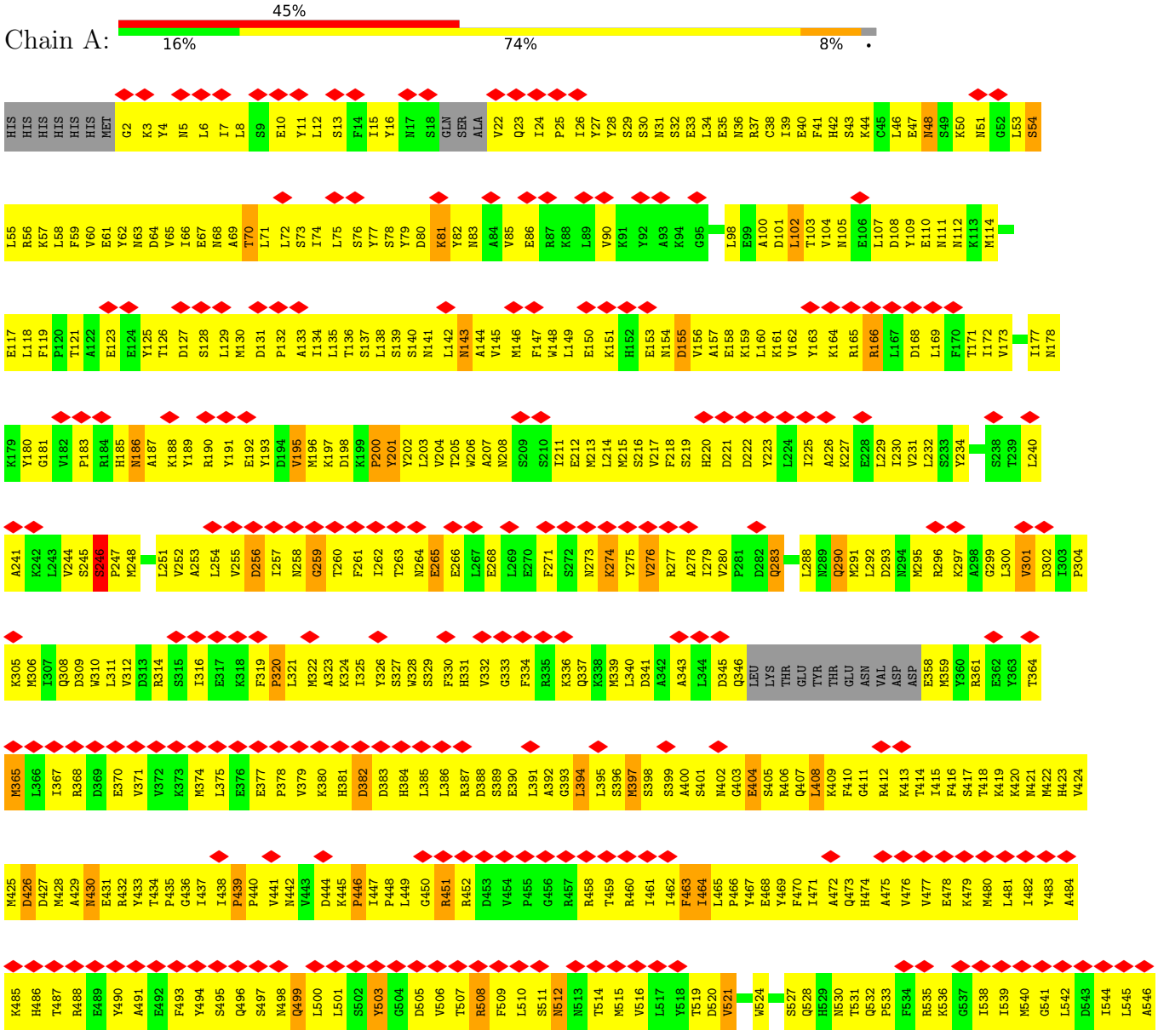
Chain	Residue	Modelled	Actual	Comment	Reference
C	1089	PRO	-	expression tag	UNP O37061
D	-5	HIS	-	expression tag	UNP O37061
D	-4	HIS	-	expression tag	UNP O37061
D	-3	HIS	-	expression tag	UNP O37061
D	-2	HIS	-	expression tag	UNP O37061
D	-1	HIS	-	expression tag	UNP O37061
D	0	HIS	-	expression tag	UNP O37061
D	1089	PRO	-	expression tag	UNP O37061
E	-5	HIS	-	expression tag	UNP O37061
E	-4	HIS	-	expression tag	UNP O37061
E	-3	HIS	-	expression tag	UNP O37061
E	-2	HIS	-	expression tag	UNP O37061
E	-1	HIS	-	expression tag	UNP O37061
E	0	HIS	-	expression tag	UNP O37061
E	1089	PRO	-	expression tag	UNP O37061

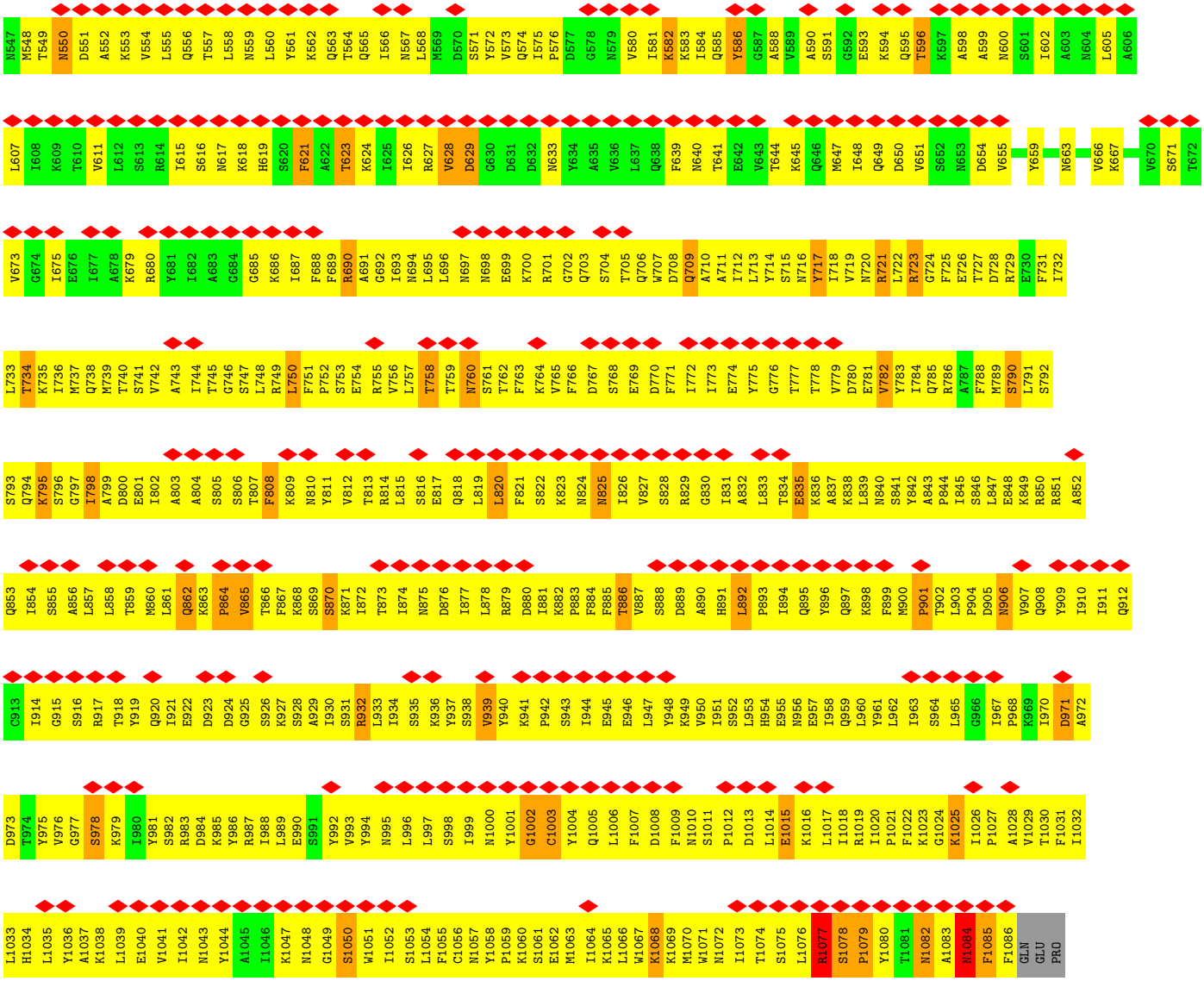
3 Residue-property plots (i)

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: RNA-DEPENDENT RNA POLYMERASE

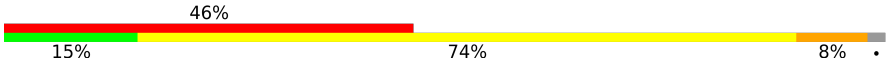
Chain A:

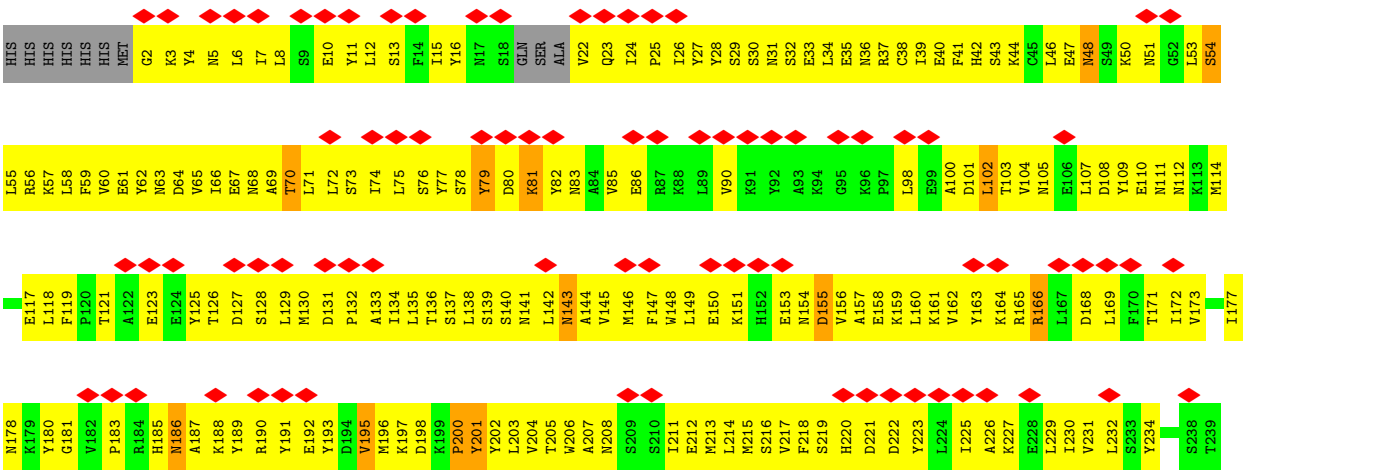


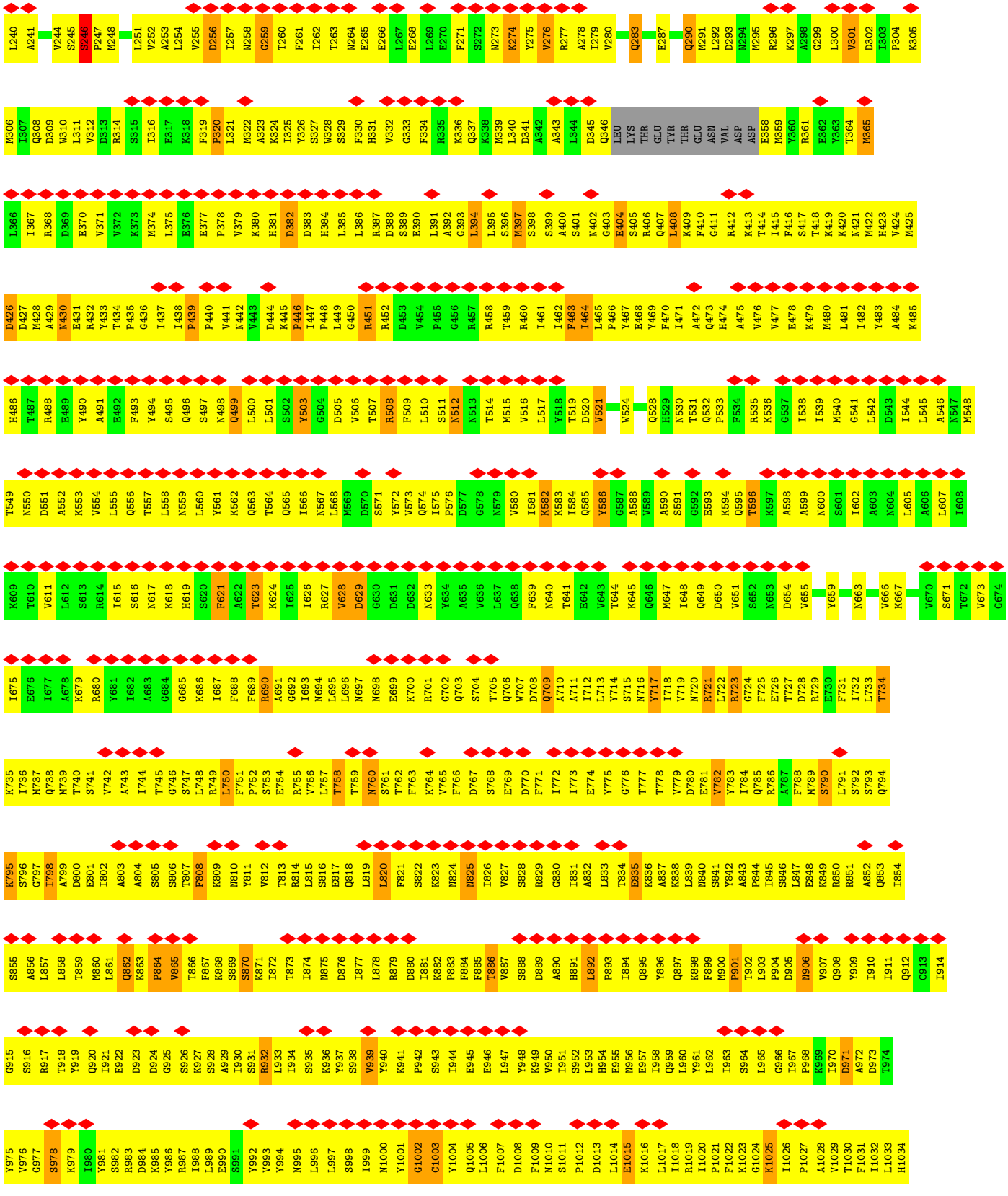


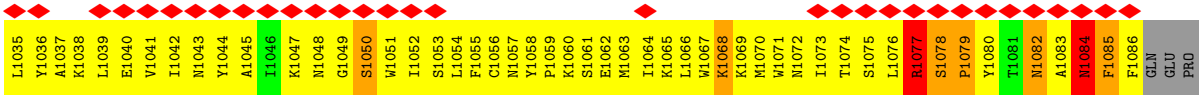
• Molecule 1: RNA-DEPENDENT RNA POLYMERASE

Chain B:



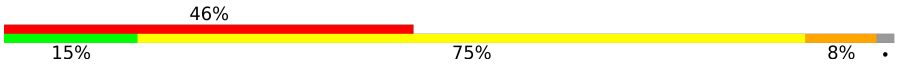


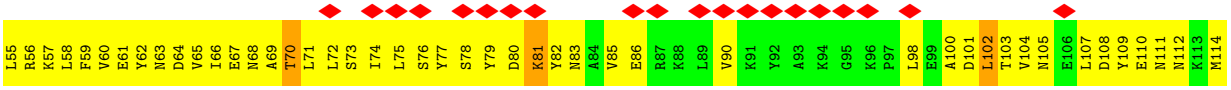

L240 A241 V244 S245 S246 P247 M248 L251 V252 A253 L254 V255 D256 I257 N258 G259 T260 F261 I262 T263 N264 E265 E266 L267 E268 L269 E270 F271 S272 N273 K274 Y275 V276 R277 A278 I279 V280 Q283 E287 Q290 M291 L292 D293 N294 M295 R296 K297 A298 G299 L300 V301 D302 I303 P304 K305
M306 I307 Q308 D309 W310 L311 V312 D313 R314 S315 I316 E317 K318 F319 P320 L321 M322 A323 K324 I325 Y326 S327 W328 S329 F330 H331 V332 G333 F334 R335 K336 Q337 K338 M339 L340 D341 A342 A343 L344 D345 Q346 LEU LYS THR GLU TYR THR GLU ASN VAL ASP ASP E358 M359 Y360 R361 E362 Y363 T364 M365
L366 I367 R368 D369 E370 V371 V372 K373 M374 L375 E376 E377 P378 V379 K380 H381 D382 D383 H384 L385 L386 R387 D388 S389 E390 L391 A392 G393 L394 L395 S396 M397 S398 S399 A400 S401 N402 G403 E404 S405 R406 Q407 L408 K409 F410 G411 R412 K413 T414 I415 F416 S417 T418 K419 K420 N421 M422 H423 V424 M425
D426 D427 M428 A429 N430 E431 R432 Y433 T434 P435 G436 I437 I438 P439 P440 V441 N442 V443 D444 K445 P446 I447 P448 L449 G450 R451 R452 D453 V454 P455 G456 R457 R458 T459 R460 I461 I462 F463 I464 L465 P466 Y467 E468 Y469 F470 I471 A472 Q473 H474 A475 V476 V477 E478 K479 M480 L481 I482 Y483 A484 K485
H486 T487 R488 E489 Y490 A491 E492 F493 Y494 S495 Q496 S497 N498 Q499 L500 L501 S502 Y503 G504 D505 V506 T507 R508 F509 L510 S511 N512 N513 T514 M515 V516 L517 Y518 T519 D520 V521 W524 Q528 H529 N530 T531 Q532 P533 F534 R535 K536 G537 I538 I539 M540 G541 L542 D543 I544 L545 A546 N547 M548
T549 N550 D551 A552 K553 V554 L555 Q556 T557 L558 N559 L560 Y561 K562 Q563 T564 Q565 I566 N567 L568 M569 D570 S571 Y572 V573 Q574 I575 P576 D577 G578 N579 V580 I581 K582 K583 I584 Q585 Y586 G587 A588 V589 A590 S591 G592 E593 K594 Q595 T596 K597 A598 A599 N600 S601 I602 A603 N604 L605 A606 L607 I608
K609 T610 V611 L612 S613 R614 I615 S616 N617 K618 H619 S620 F621 A622 T623 K624 I625 I626 R627 V628 D629 G630 D631 D632 N633 Y634 A635 V636 L637 Q638 F639 N640 T641 E642 V643 T644 K645 Q646 M647 I648 Q649 D650 V651 S652 N653 D654 V655 Y659 N663 V666 K667 V670 S671 T672 V673 G674
I675 E676 I677 A678 K679 R680 Y681 I682 A683 G684 G685 K686 I687 F688 F689 R690 A691 G692 I693 N694 L695 L696 N697 N698 E699 K700 R701 G702 Q703 S704 T705 Q706 W707 D708 Q709 A710 A711 I712 L713 Y714 S715 N716 Y717 I718 V719 N720 R721 L722 R723 G724 F725 E726 T727 D728 R729 E730 F731 I732 L733 T734
K735 I736 M737 Q738 M739 T740 S741 V742 A743 I744 T745 G746 S747 L748 R749 L750 F751 P752 S753 E754 R755 V756 L757 T758 T759 N760 S761 T762 F763 K764 V765 F766 D767 S768 E769 D770 F771 I772 I773 E774 Y775 G776 T777 T778 V779 D780 E781 V782 Y783 I784 Q785 R786 A787 F788 M789 S790 L791 S792 S793 Q794
K795 S796 G797 I798 A799 D800 E801 I802 A803 A804 S805 S806 T807 F808 K809 N810 Y811 V812 T813 R814 L815 S816 E817 Q818 L819 L820 F821 S822 K823 N824 N825 I826 V827 S828 R829 G830 I831 A832 L833 T834 E835 K836 A837 K838 L839 N840 S841 Y842 A843 P844 I845 S846 L847 E848 K849 R850 R851 A852 Q853 I854
S855 A856 L857 L858 T859 M860 L861 Q862 K863 P864 V865 T866 F867 K868 S869 S870 K871 I872 T873 I874 N875 D876 I877 L878 R879 D880 I881 K882 P883 F884 F885 T886 V887 S888 D889 A890 H891 L892 P893 I894 Q895 Y896 Q897 K898 F899 M900 P901 T902 L903 P904 D905 N906 Y907 Q908 Y909 I910 I911 Q912 C913 I914
G915 S916 R917 T918 Y919 Q920 I921 E922 D923 D924 G925 S926 K927 S928 A929 I930 S931 R932 L933 I934 S935 K936 Y937 S938 Y939 Y940 K941 P942 S943 I944 E945 E946 L947 Y948 K949 Y950 I951 S952 L953 H954 E955 N956 E957 I958 Q959 L960 Y961 L962 I963 S964 L965 G966 I967 P968 K969 I970 D971 A972 D973 I974
Y975 V976 G977 S978 K979 I980 Y981 S982 R983 D984 K985 Y986 R987 I988 L989 E990 S991 Y992 V993 Y994 N995 L996 L997 S998 I999 N1000 Y1001 G1002 C1003 Y1004 Q1005 L1006 F1007 D1008 F1009 N1010 S1011 P1012 D1013 L1014 E1015 K1016 L1017 I1018 R1019 I1020 P1021 F1022 K1023 G1024 K1025 I1026 P1027 A1028 V1029 T1030 F1031 I1032 L1033 H1034

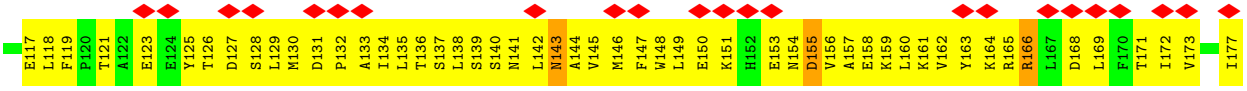


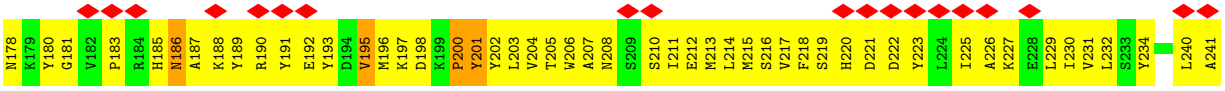
• Molecule 1: RNA-DEPENDENT RNA POLYMERASE

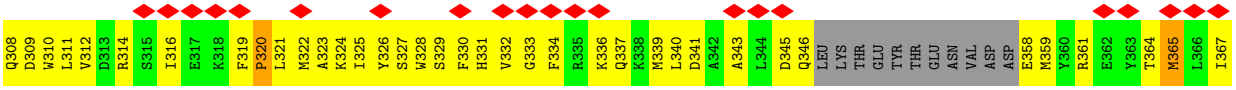
Chain C:

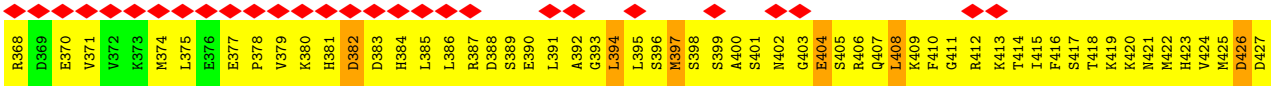


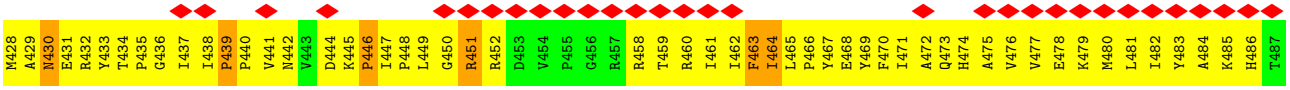


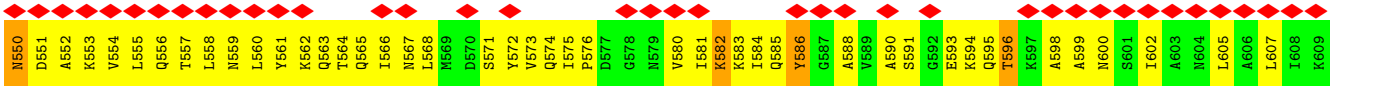


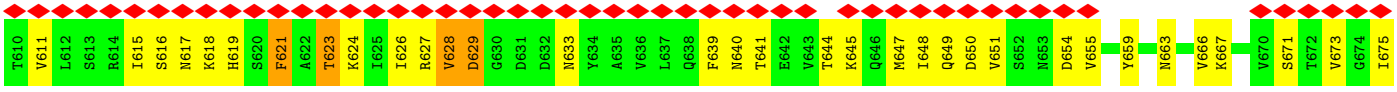


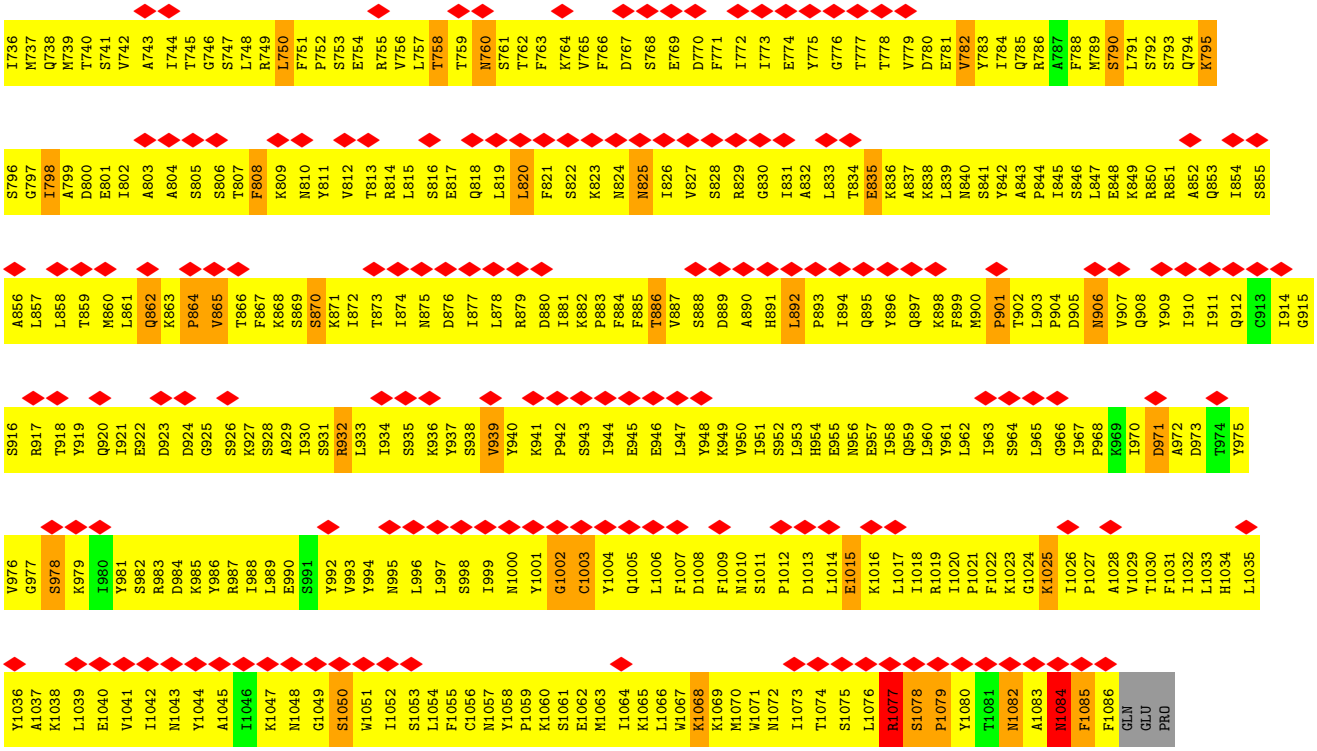






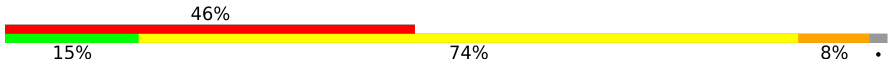


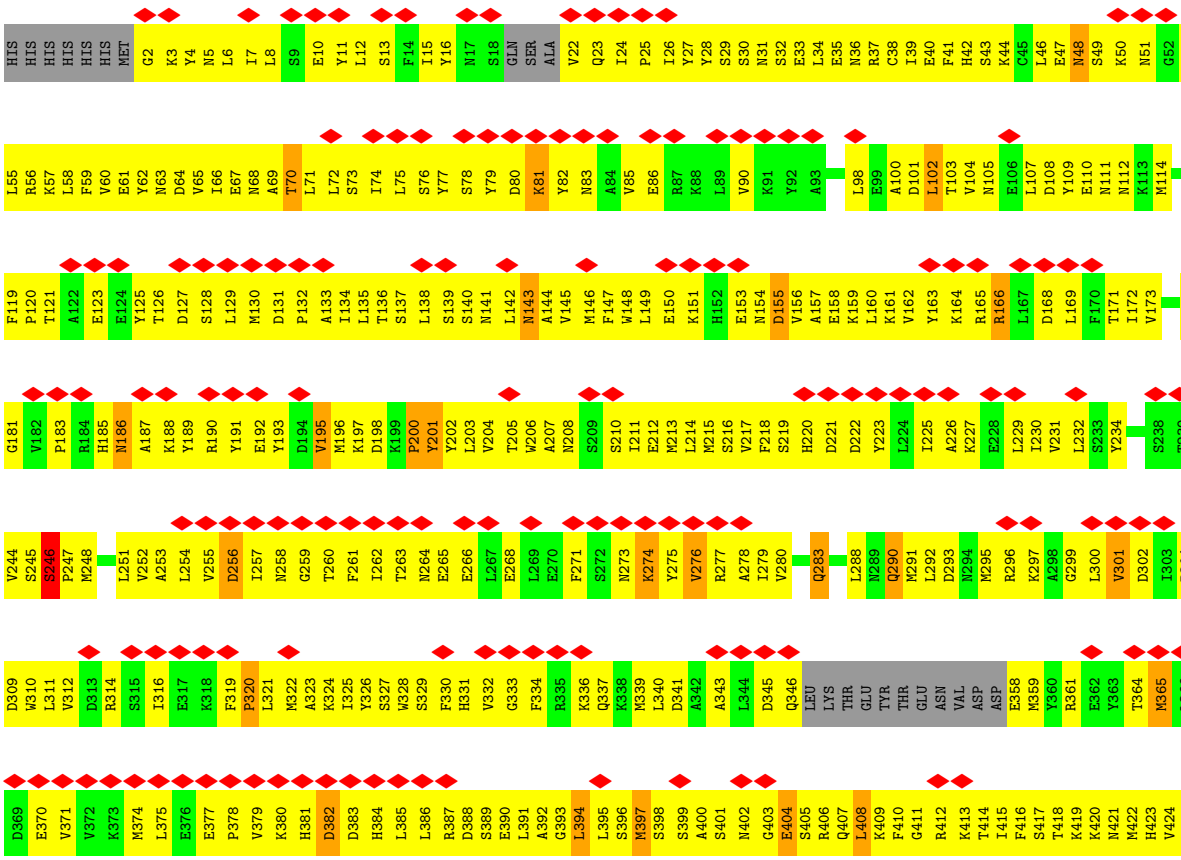


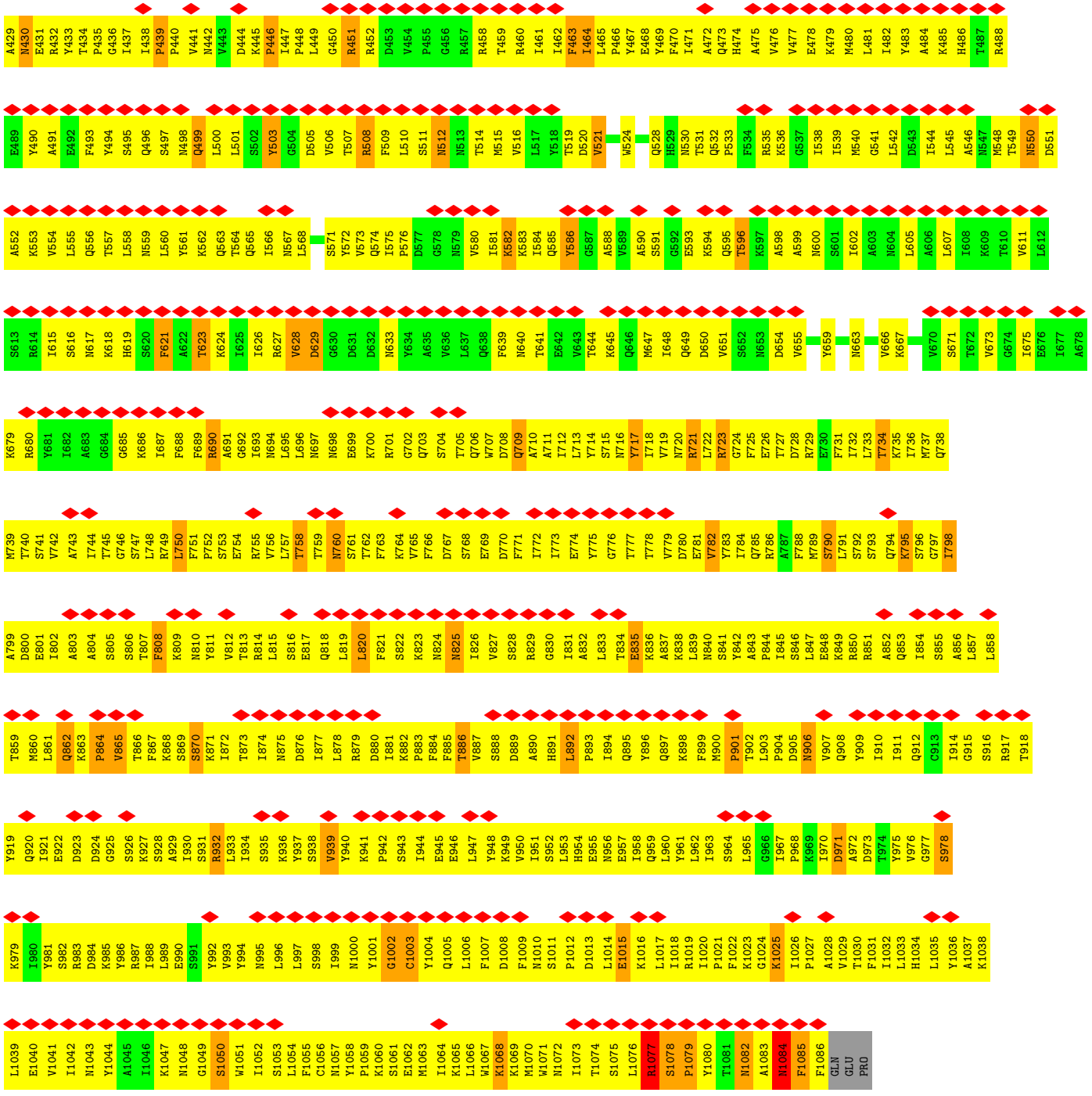


• Molecule 1: RNA-DEPENDENT RNA POLYMERASE

Chain D:

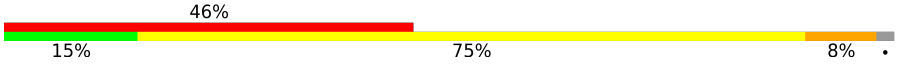


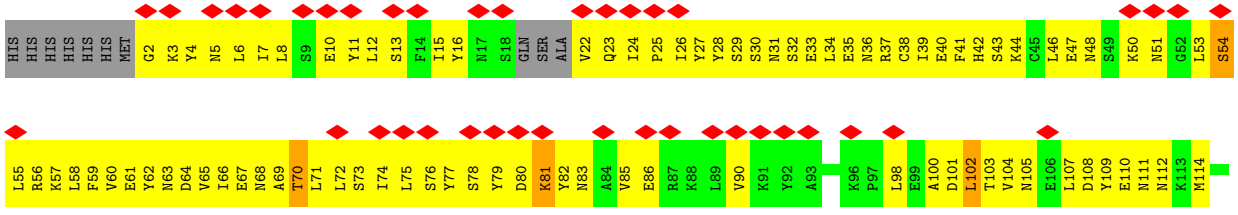


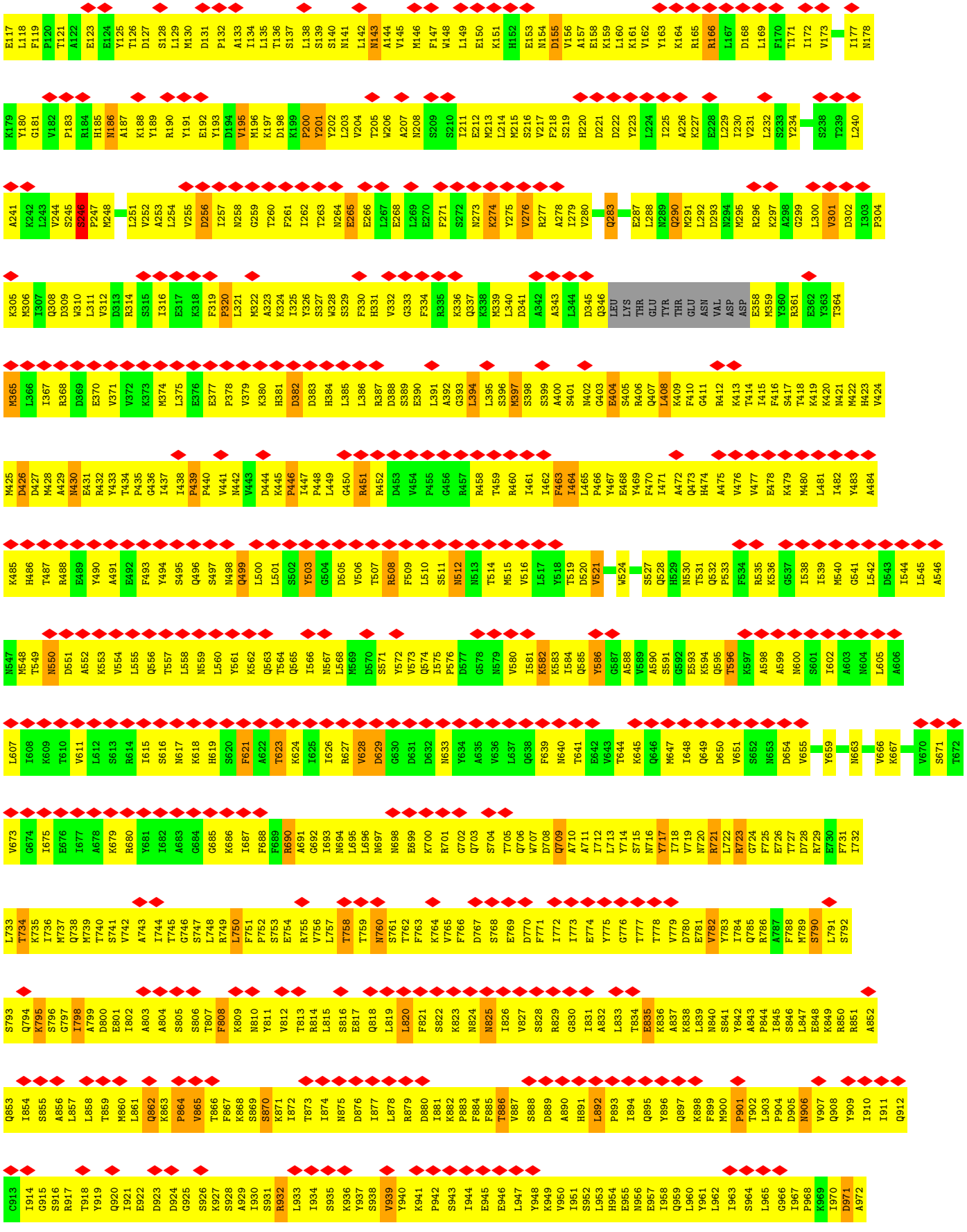


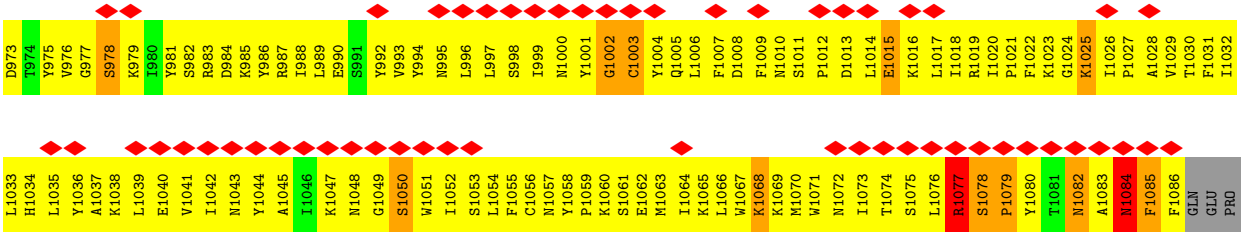
• Molecule 1: RNA-DEPENDENT RNA POLYMERASE

Chain E:






E117 L118 F119 P120 T121 A122 E123 E124 Y125 T126 D127 S128 L129 M130 D131 P132 A133 I134 L135 T136 S137 L138 S139 S140 N141 L142 N143 A144 V145 M146 F147 W148 L149 E150 K151 H152 E153 N154 D155 V156 A157 E158 K159 L160 K161 V162 Y163 K164 R165 R166 L167 D168 L169 F170 T171 I172 V173 I177 N178
K179 Y180 G181 V182 P183 R184 H185 N186 A187 K188 Y189 R190 Y191 E192 Y193 D194 V195 M196 K197 D198 K199 P200 Y201 Y202 L203 V204 T205 W206 A207 N208 S209 S210 I211 E212 M213 L214 M215 S216 V217 F218 S219 H220 D221 D222 Y223 L224 I225 A226 K227 E228 L229 I230 V231 L232 S233 Y234 S238 T239 L240
A241 K242 L243 V244 S245 S246 P247 M248 L251 V252 A253 L254 V255 D256 I257 N258 G259 T260 F261 I262 T263 N264 E265 E266 L267 E268 L269 E270 F271 S272 N273 K274 Y275 V276 R277 A278 I279 V280 Q283 E287 L288 N289 Q290 M291 L292 D293 N294 M295 R296 K297 A298 G299 L300 V301 D302 I303 P304
K305 M306 I307 Q308 D309 W310 L311 V312 D313 R314 S315 I316 E317 K318 F319 P320 L321 M322 A323 K324 I325 Y326 S327 W328 S329 F330 H331 V332 G333 F334 R335 K336 Q337 K338 M339 L340 D341 A342 A343 L344 D345 Q346 LEU LYS THR GLU TYR THR GLU ASN VAL ASP ASP E358 M359 Y360 R361 E362 Y363 T364
M365 L366 I367 R368 D369 E370 V371 V372 K373 M374 L375 E376 E377 P378 V379 K380 H381 D382 D383 H384 L385 L386 R387 D388 S389 E390 L391 A392 G393 L394 L395 S396 M397 S398 S399 A400 S401 N402 G403 E404 S405 R406 Q407 L408 K409 F410 G411 R412 K413 T414 I415 F416 S417 T418 K419 K420 N421 M422 H423 V424
M425 D426 D427 M428 A429 N430 E431 R432 Y433 T434 P435 G436 I437 I438 P439 P440 V441 N442 Y443 D444 K445 P446 I447 P448 L449 G450 R451 R452 D453 V454 P455 G456 R457 R458 T459 R460 I461 I462 F463 I464 L465 P466 Y467 E468 Y469 F470 I471 A472 Q473 H474 A475 V476 V477 E478 K479 M480 L481 I482 Y483 A484
K485 H486 T487 R488 E489 Y490 A491 E492 F493 Y494 S495 Q496 S497 N498 Q499 L500 L501 S502 Y503 G504 D505 V506 T507 R508 F509 L510 S511 N512 N513 T514 M515 V516 L517 Y518 T519 D520 V521 W524 S527 Q528 H529 N530 T531 Q532 P533 F534 R535 K536 G537 I538 I539 M540 G541 L542 D543 I544 L545 A546
N547 M548 T549 N550 D551 A552 K553 V554 L555 Q556 T557 L558 N559 L560 Y561 K562 Q563 T564 Q565 I566 N567 L568 N569 D570 S571 Y572 Y573 Q574 I575 P576 D577 G578 N579 V580 I581 K582 K583 I584 Q585 Y586 G587 A588 V589 A590 S591 G592 E593 K594 Q595 T596 K597 A598 A599 N600 S601 I602 A603 N604 L605 A606
L607 I608 K609 T610 V611 L612 S613 R614 I615 S616 N617 K618 H619 S620 F621 A622 T623 K624 I625 I626 R627 V628 D629 G630 D631 D632 N633 Y634 A635 V636 L637 Q638 F639 N640 T641 E642 V643 T644 K645 Q646 M647 I648 Q649 D650 V651 S652 N653 D654 V655 Y659 M663 V666 K667 V670 S671 T672
V673 G674 I675 E676 I677 A678 K679 R680 Y681 I682 A683 G684 G685 K686 I687 F688 F689 R690 A691 G692 I693 N694 L695 L696 N697 N698 E699 K700 R701 G702 Q703 S704 T705 Q706 W707 D708 Q709 A710 A711 I712 L713 Y714 S715 N716 Y717 I718 V719 N720 R721 L722 R723 G724 F725 E726 T727 D728 R729 E730 F731 I732
L733 T734 K735 I736 M737 Q738 M739 T740 S741 V742 A743 I744 T745 G746 S747 L748 R749 L750 F751 P752 S753 E754 R755 V756 L757 T758 T759 N760 S761 T762 F763 K764 V765 F766 D767 S768 E769 D770 F771 I772 I773 E774 Y775 G776 T777 T778 V779 D780 E781 V782 Y783 I784 Q785 R786 A787 F788 M789 S790 L791 S792
S793 Q794 K795 S796 G797 T798 A799 D800 E801 I802 A803 A804 S805 S806 T807 F808 K809 N810 Y811 V812 T813 R814 L815 S816 E817 Q818 L819 L820 F821 S822 K823 N824 N825 I826 V827 S828 R829 G830 I831 A832 L833 T834 E835 K836 A837 K838 L839 N840 S841 Y842 A843 P844 I845 S846 L847 E848 K849 R850 R851 A852
Q853 I854 S855 A856 L857 L858 T859 M860 L861 Q862 K863 P864 V865 T866 F867 K868 S869 S870 K871 I872 T873 I874 N875 D876 I877 L878 R879 D880 I881 K882 P883 F884 F885 T886 V887 S888 D889 A890 H891 L892 P893 I894 Q895 Y896 Q897 K898 F899 M900 P901 T902 L903 P904 D905 N906 V907 Q908 Y909 I910 I911 Q912
C913 I914 G915 S916 R917 T918 Y919 Q920 I921 E922 D923 D924 G925 S926 K927 S928 A929 I930 S931 R932 L933 I934 S935 K936 Y937 S938 V939 Y940 K941 P942 S943 I944 E945 E946 L947 Y948 K949 V950 I951 S952 L953 H954 E955 N956 E957 I958 Q959 L960 Y961 L962 I963 S964 L965 G966 I967 P968 K969 I970 D971 A972


D973 T974 Y975 V976 G977 S978 K979 I980 Y981 S982 R983 D984 K985 Y986 R987 I988 L989 E990 S991 Y992 V993 Y994 N995 L996 L997 S998 I999 N1000 Y1001 G1002 C1003 Y1004 Q1005 L1006 F1007 D1008 F1009 M1010 S1011 P1012 D1013 L1014 E1015 K1016 L1017 I1018 R1019 I1020 P1021 F1022 K1023 G1024 K1025 I1026 P1027 A1028 V1029 T1030 F1031 I1032

L1033 H1034 L1035 Y1036 A1037 K1038 L1039 E1040 V1041 I1042 N1043 Y1044 A1045 I1046 K1047 N1048 G1049 S1050 W1051 I1052 S1053 L1054 F1055 C1056 N1057 Y1058 P1059 K1060 S1061 E1062 M1063 I1064 K1065 L1066 W1067 K1068 K1069 M1070 W1071 N1072 I1073 T1074 S1075 L1076 R1077 S1078 P1079 Y1080 T1081 N1082 A1083 N1084 F1085 F1086 GLN GLU PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	7000	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL PARTICLE PHASE FLIPPING	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	56540	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.008	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0004844	Depositor
Map size (Å)	237.5, 473.30356, 237.5	wwPDB
Map dimensions	140, 279, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.696428571, 1.696428571, 1.696428571	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	A	0.41	0/8914	0.62	5/12052 (0.0%)
1	B	0.41	0/8914	0.62	5/12052 (0.0%)
1	C	0.40	0/8914	0.62	5/12052 (0.0%)
1	D	0.41	0/8914	0.62	5/12052 (0.0%)
1	E	0.40	0/8914	0.62	5/12052 (0.0%)
All	All	0.40	0/44570	0.62	25/60260 (0.0%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1082[A]	ASN	N-CA-C	6.33	128.08	111.00
1	E	1082[B]	ASN	N-CA-C	6.33	128.08	111.00
1	C	1082[A]	ASN	N-CA-C	6.31	128.04	111.00
1	C	1082[B]	ASN	N-CA-C	6.31	128.04	111.00
1	A	1082[A]	ASN	N-CA-C	6.30	128.01	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8741	0	8343	11726	0
1	B	8741	0	8344	11702	0
1	C	8741	0	8343	11680	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	8741	0	8341	11771	0
1	E	8741	0	8341	11762	0
All	All	43705	0	41712	30580	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 358.

The worst 5 of 30580 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:MET:SD	1:C:786:ARG:HD3	1.25	1.77
1:A:786:ARG:HD3	1:D:789:MET:SD	1.25	1.77
1:B:786:ARG:HD3	1:E:789:MET:SD	1.25	1.75
1:C:789:MET:SD	1:E:786:ARG:HD3	1.25	1.75
1:B:789:MET:SD	1:D:786:ARG:HD3	1.25	1.73

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	A	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	3	23
1	B	1073/1095 (98%)	927 (86%)	104 (10%)	42 (4%)	3	23
1	C	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	3	23
1	D	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	3	23
1	E	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	3	23
All	All	5365/5475 (98%)	4631 (86%)	524 (10%)	210 (4%)	6	23

5 of 210 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	397	MET
1	A	401	SER
1	A	864	PRO
1	A	978	SER

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	979/996 (98%)	911 (93%)	68 (7%)	15	40
1	B	979/996 (98%)	912 (93%)	67 (7%)	16	41
1	C	979/996 (98%)	911 (93%)	68 (7%)	15	40
1	D	979/996 (98%)	911 (93%)	68 (7%)	15	40
1	E	979/996 (98%)	911 (93%)	68 (7%)	15	40
All	All	4895/4980 (98%)	4556 (93%)	339 (7%)	19	40

5 of 339 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	426	ASP
1	E	274	LYS
1	D	550	ASN
1	D	932	ARG
1	E	430	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	308	GLN
1	E	498	ASN
1	C	853	GLN
1	E	473	GLN
1	E	709	GLN

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)

There are no chain breaks in this entry.

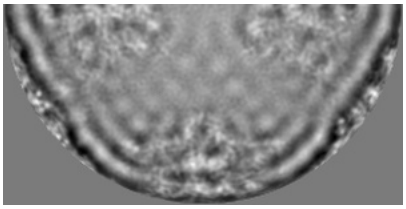
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2100. These allow visual inspection of the internal detail of the map and identification of artifacts.

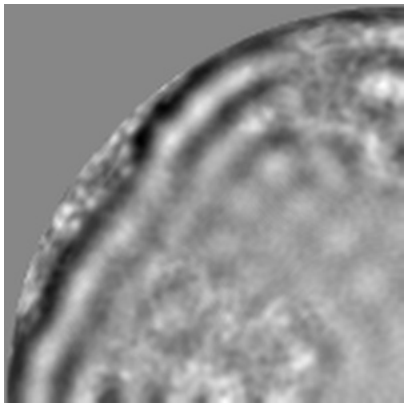
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

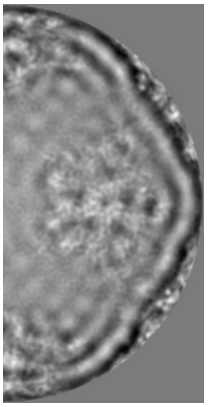
6.1.1 Primary map



X



Y

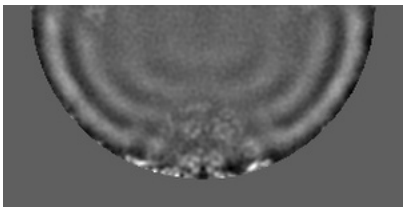


Z

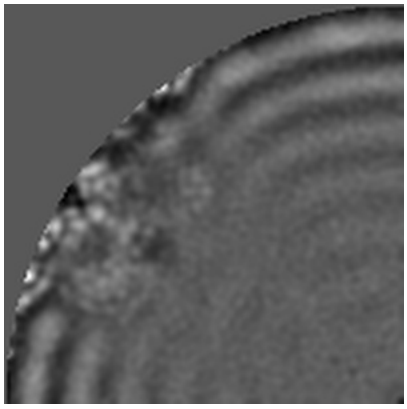
The images above show the map projected in three orthogonal directions.

6.2 Central slices

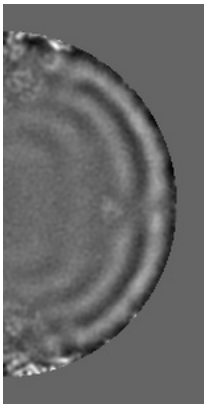
6.2.1 Primary map



X Index: 70



Y Index: 139

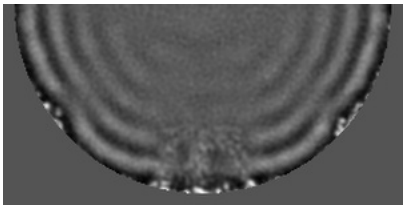


Z Index: 70

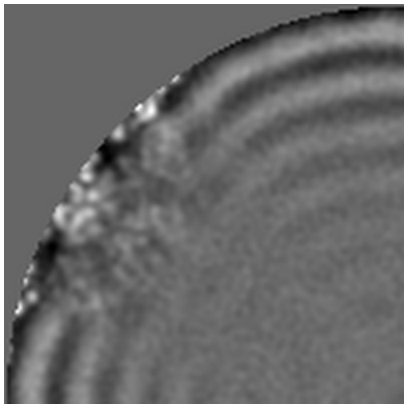
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

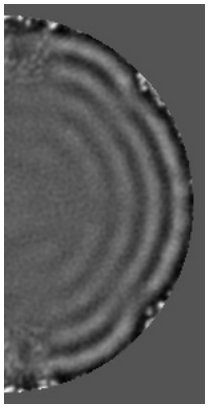
6.3.1 Primary map



X Index: 45



Y Index: 145

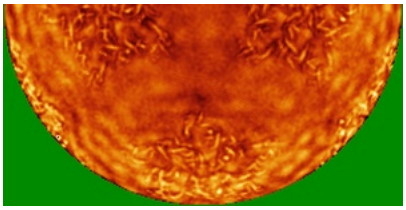


Z Index: 94

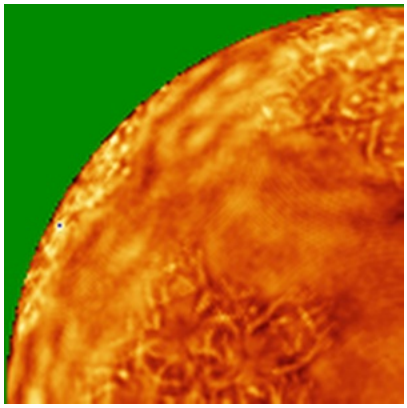
The images above show the largest variance slices of the map in three orthogonal directions.

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

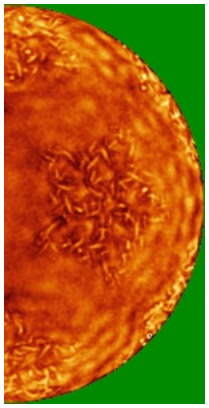
6.4.1 Primary map



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 0.0004844. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

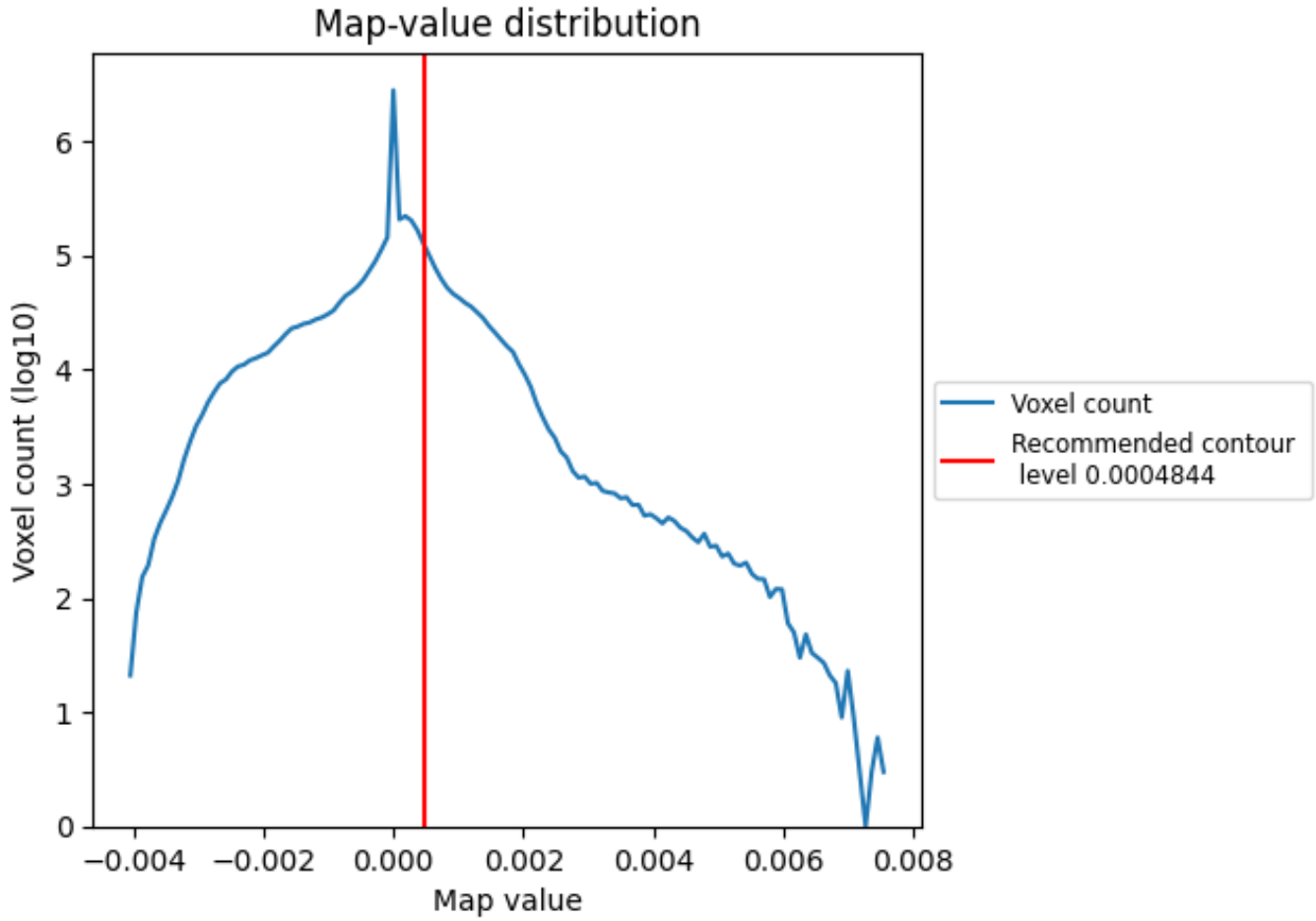
6.6 Mask visualisation (i)

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

7 Map analysis

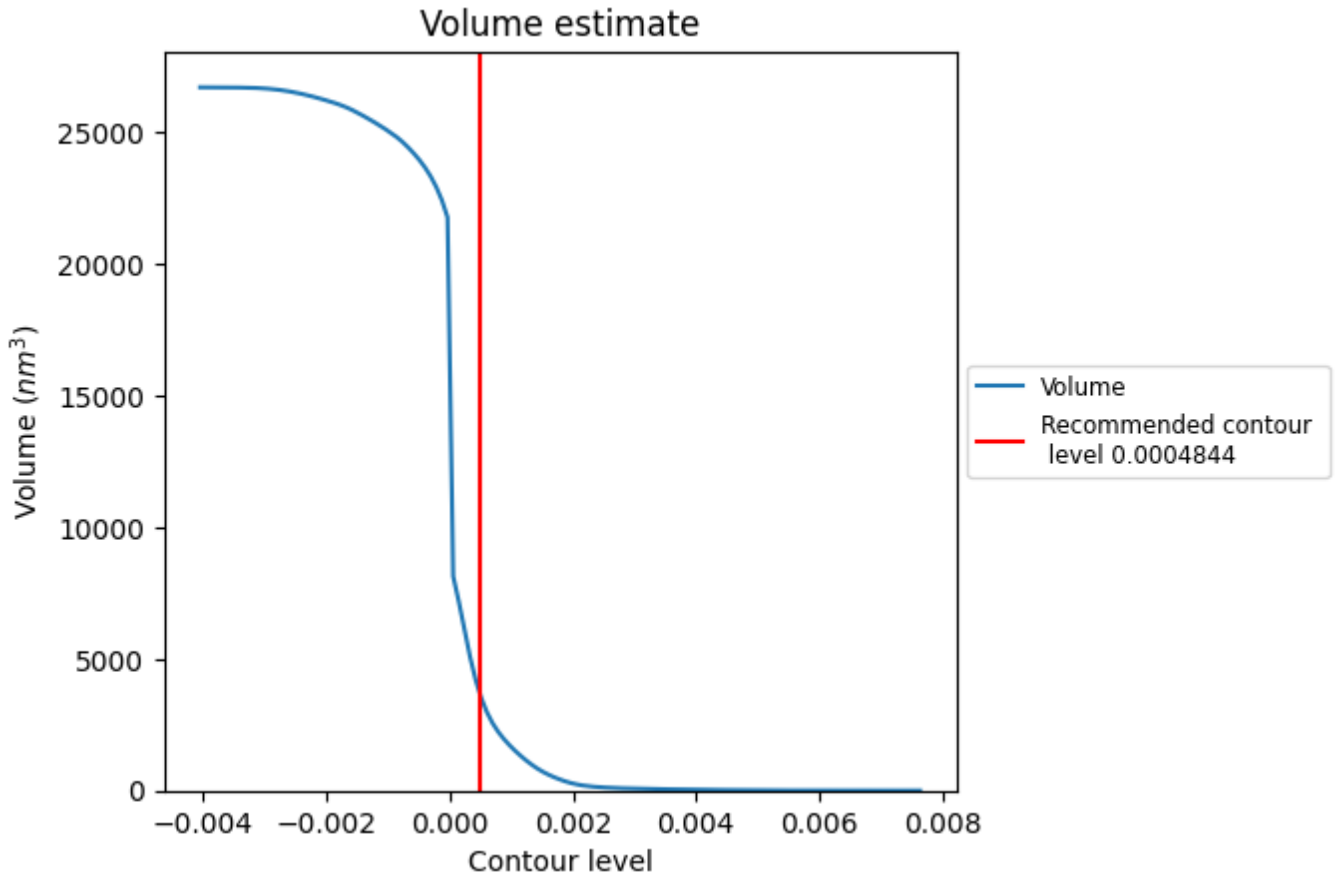
This section contains the results of statistical analysis of the map.

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



The volume at the recommended contour level is 3732 nm^3; this corresponds to an approximate mass of 3371 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.

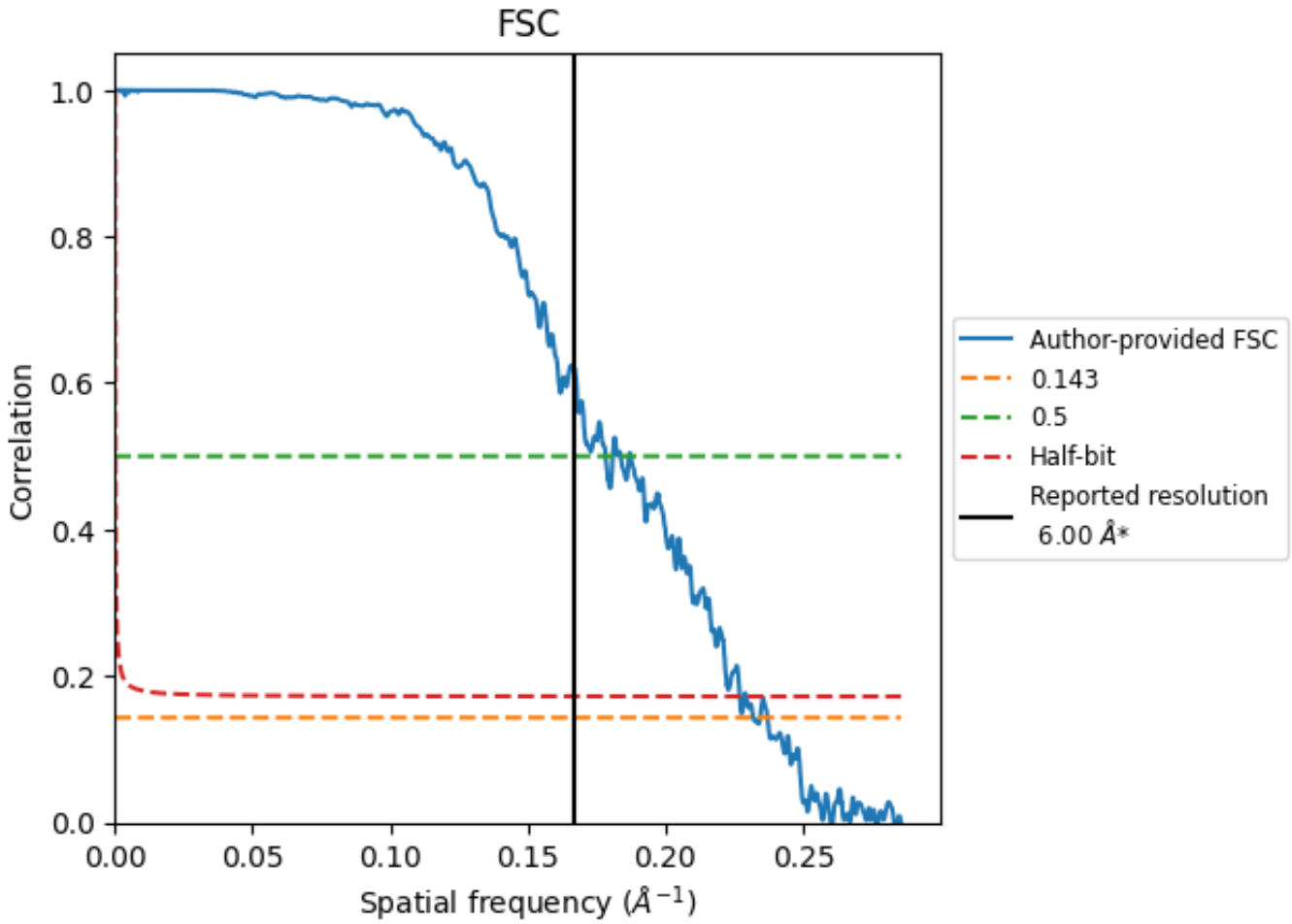
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.167 Å^{-1}

8.2 Resolution estimates (i)

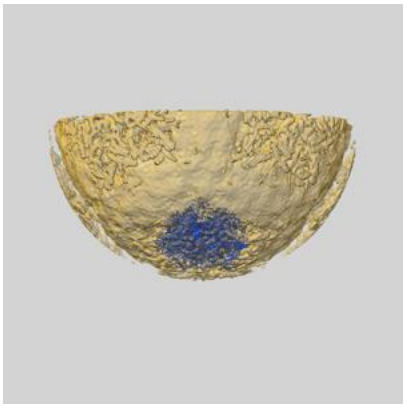
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.31	5.61	4.40
Unmasked-calculated*	-	-	-

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

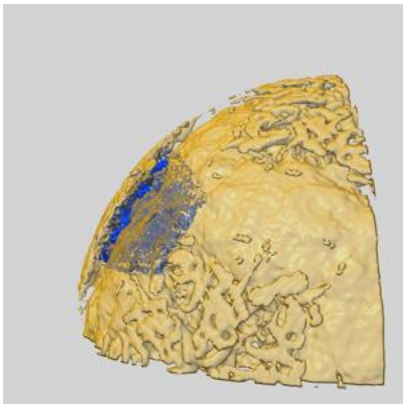
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2100 and PDB model 4AU6. Per-residue inclusion information can be found in section 3 on page 5.

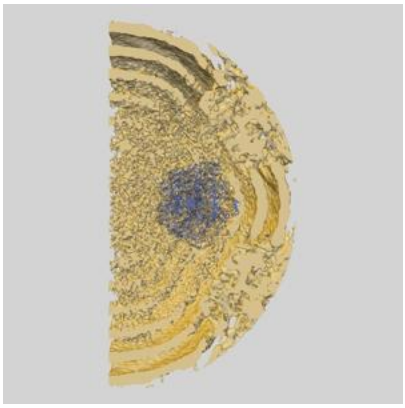
9.1 Map-model overlay



X



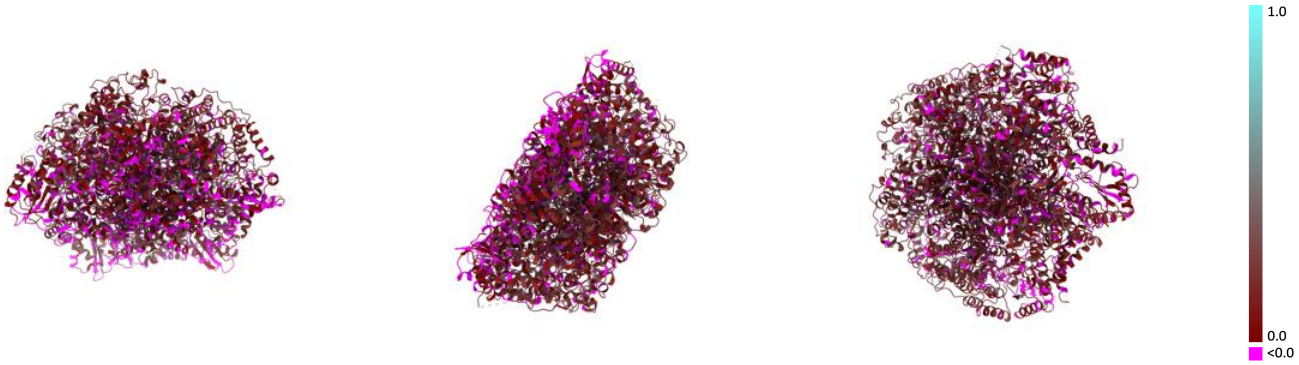
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0004844 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.

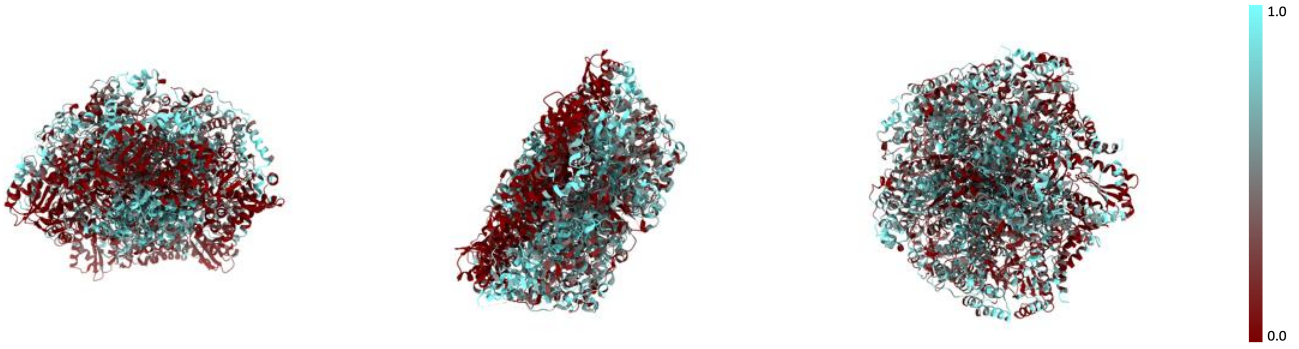
9.2 Q-score mapped to coordinate model (i)



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.

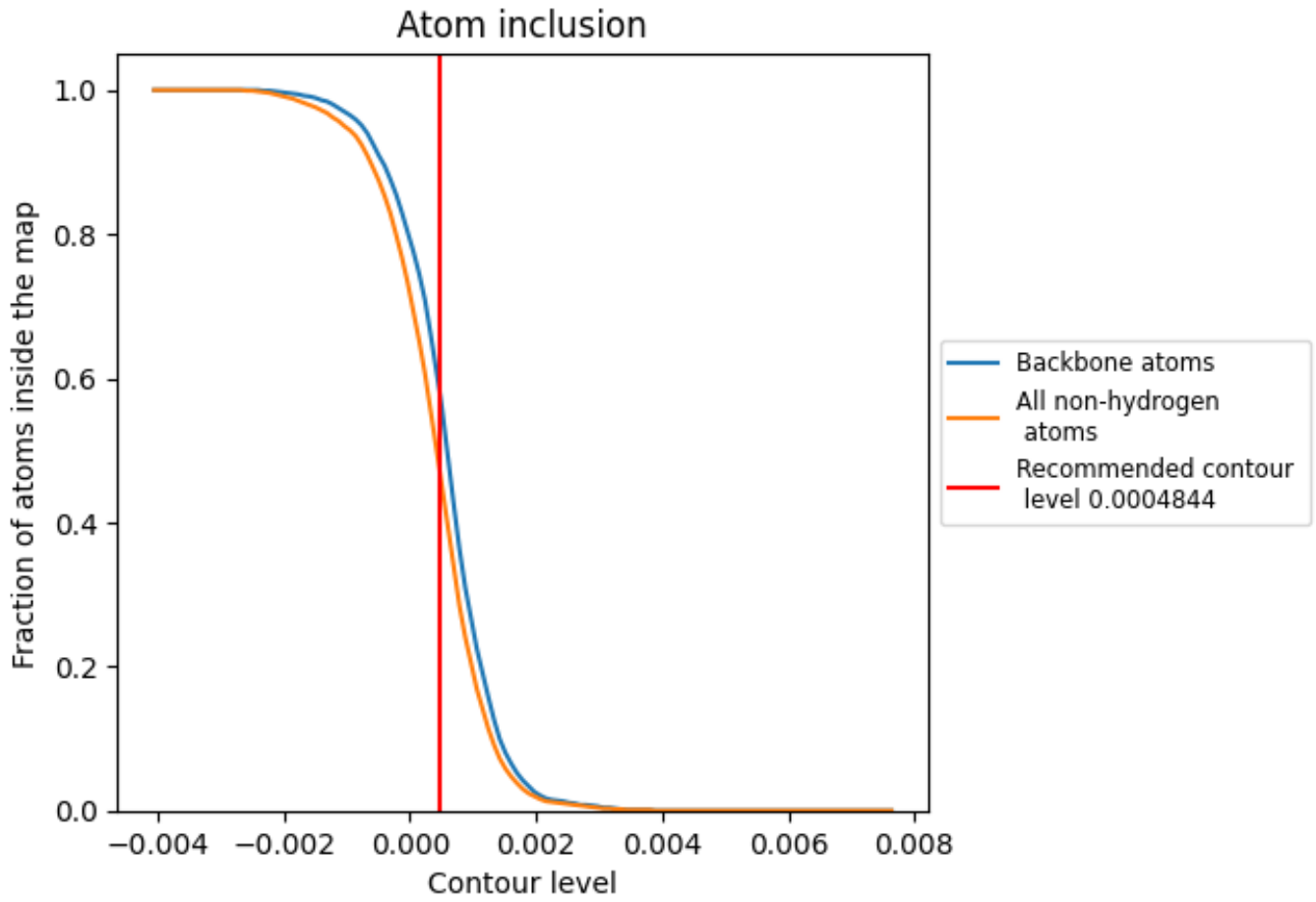
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0004844).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 47% 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 (0.0004844) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4660	0.1190
A	0.4680	0.1180
B	0.4670	0.1190
C	0.4700	0.1180
D	0.4640	0.1190
E	0.4640	0.1200