



wwPDB EM Validation Summary Report ⓘ

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 ⓘ 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.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

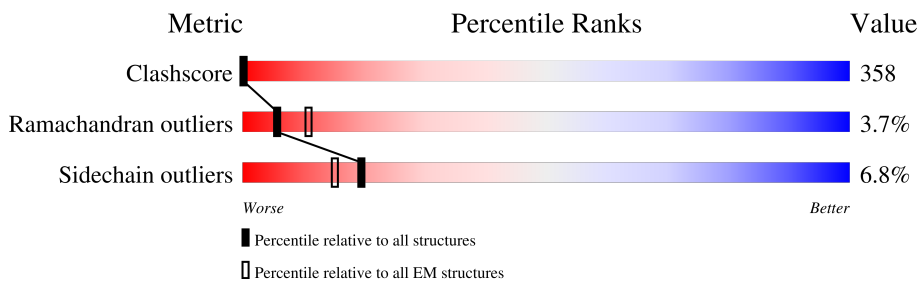
1 Overall quality at a glance i

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 $\leq 5\%$. 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	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>45%</p> </div> <div style="text-align: center;"> </div> </div>
1	B	1095	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>46%</p> </div> <div style="text-align: center;"> </div> </div>
1	C	1095	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>46%</p> </div> <div style="text-align: center;"> </div> </div>
1	D	1095	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>46%</p> </div> <div style="text-align: center;"> </div> </div>
1	E	1095	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>46%</p> </div> <div style="text-align: center;"> </div> </div>

2 Entry composition

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
			Total	C	N	O	S		
1	A	1071	8741	5604	1457	1642	38	10	0
1	B	1071	8741	5604	1457	1642	38	10	0
1	C	1071	8741	5604	1457	1642	38	10	0
1	D	1071	8741	5604	1457	1642	38	10	0
1	E	1071	8741	5604	1457	1642	38	10	0

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

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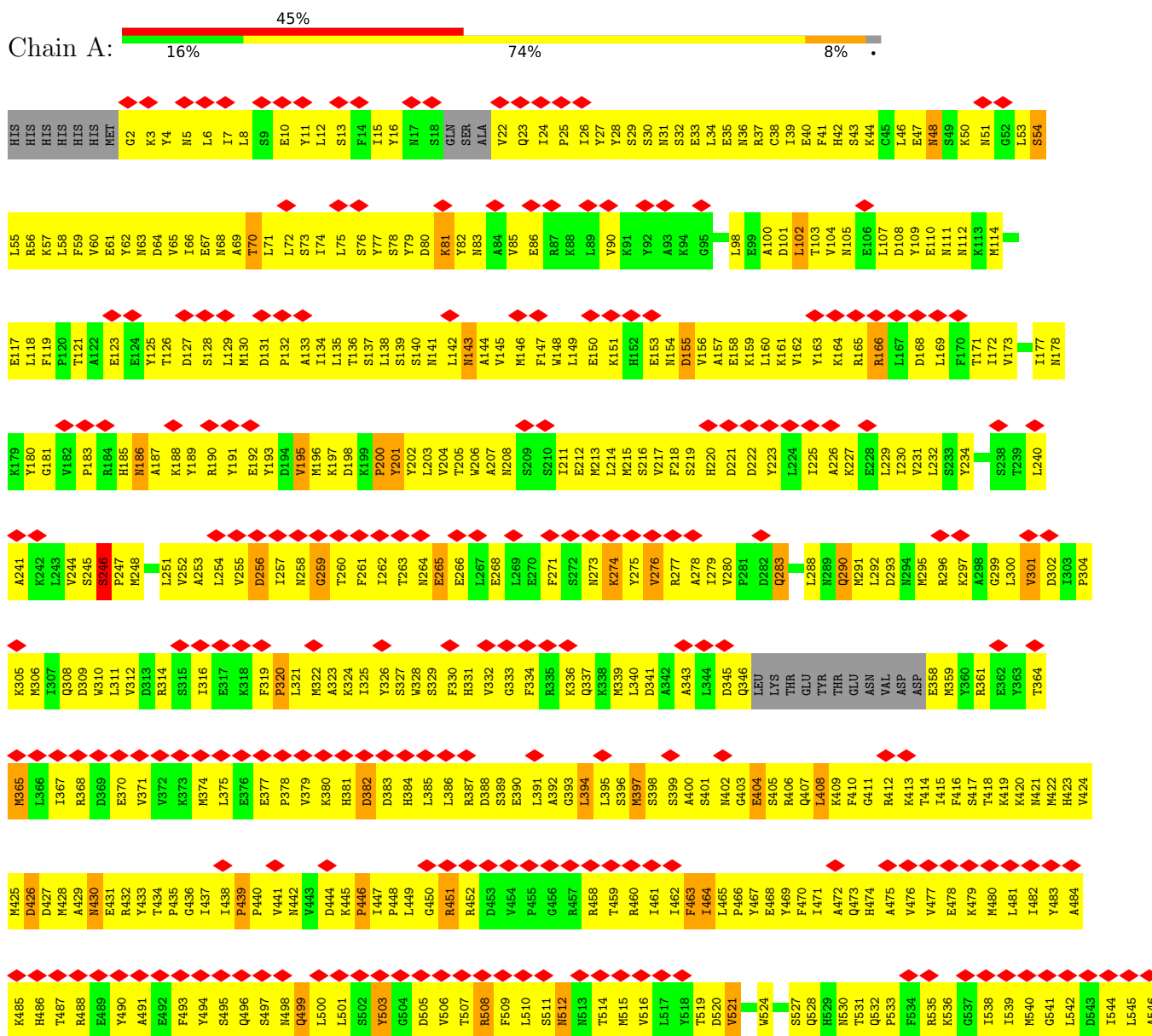
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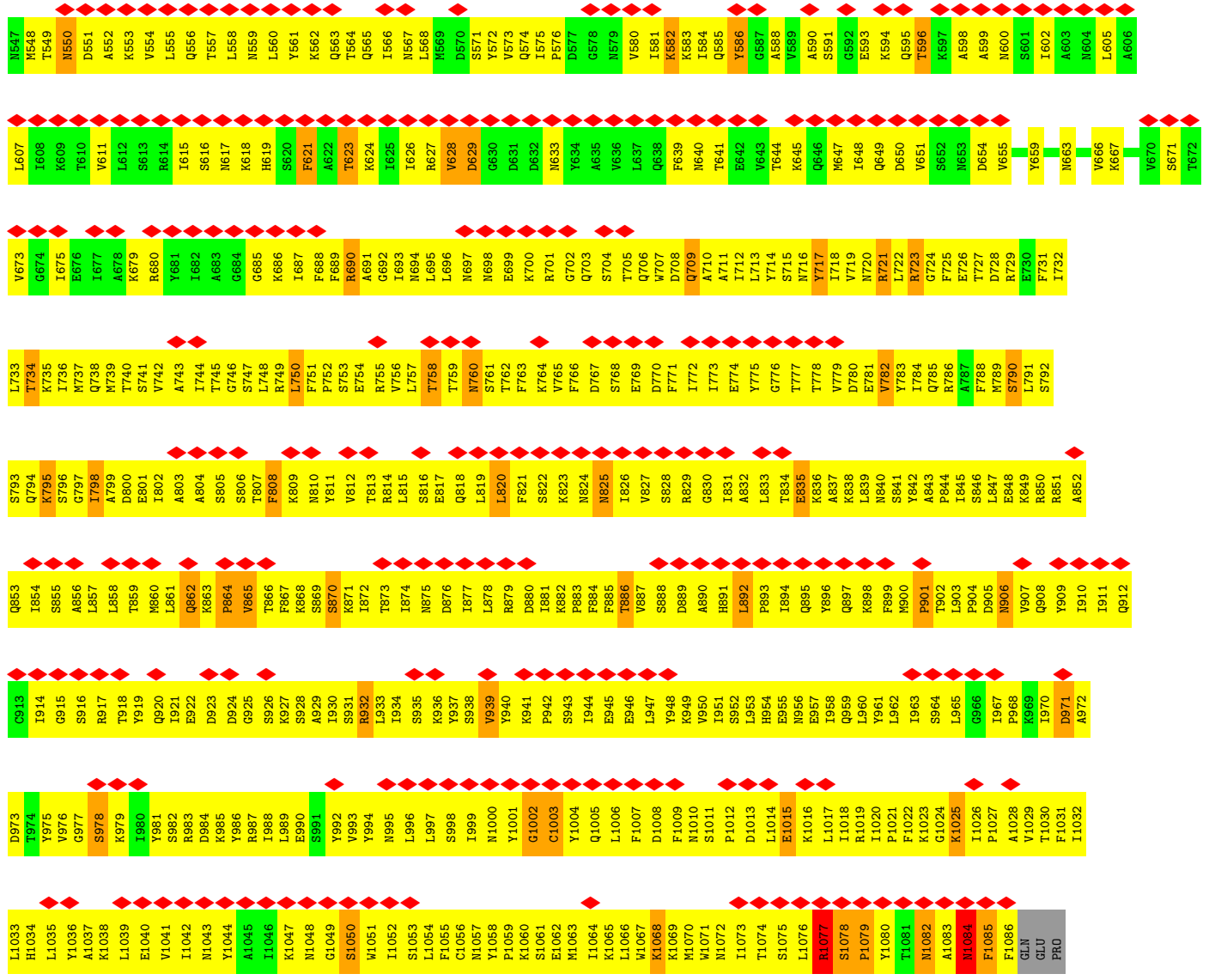
Chain	Residue	Modelled	Actual	Comment	Reference
C	1089	PRO	-	expression tag	UNP O37061
D	-5	HIS	-	expression tag	UNP O37061
D	-4	HIS	-	expression tag	UNP O37061
D	-3	HIS	-	expression tag	UNP O37061
D	-2	HIS	-	expression tag	UNP O37061
D	-1	HIS	-	expression tag	UNP O37061
D	0	HIS	-	expression tag	UNP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

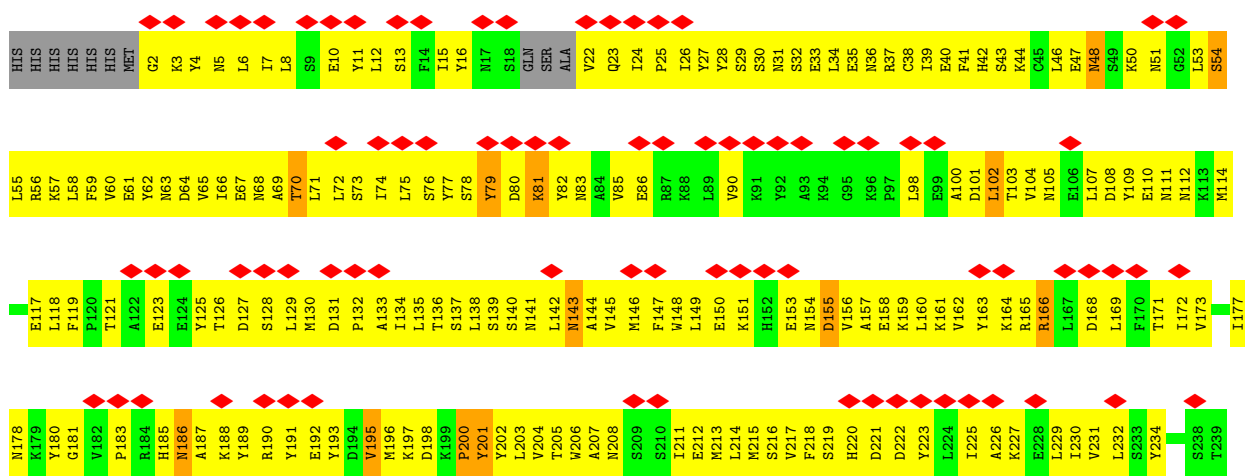
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

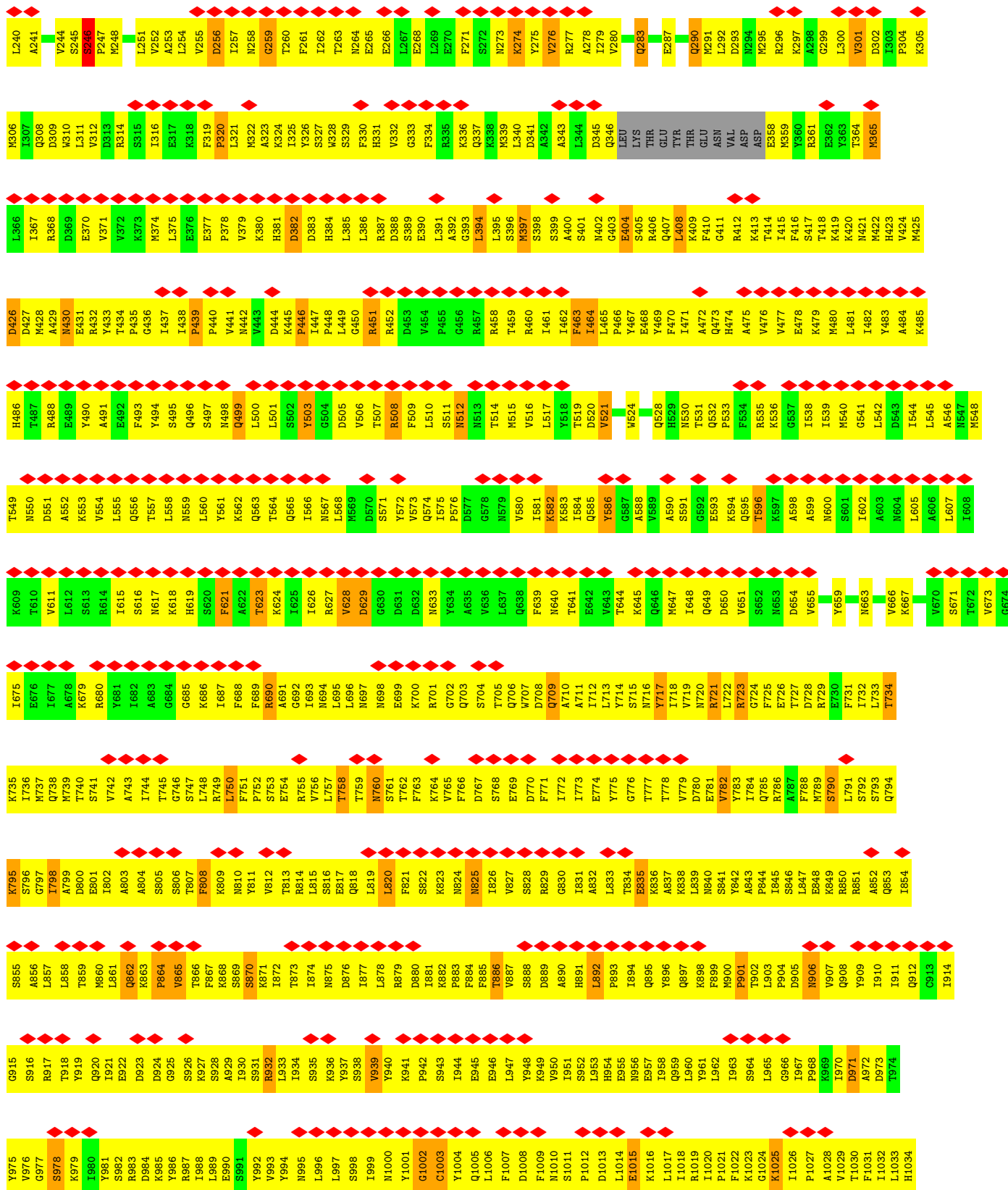
• Molecule 1: RNA-DEPENDENT RNA POLYMERASE





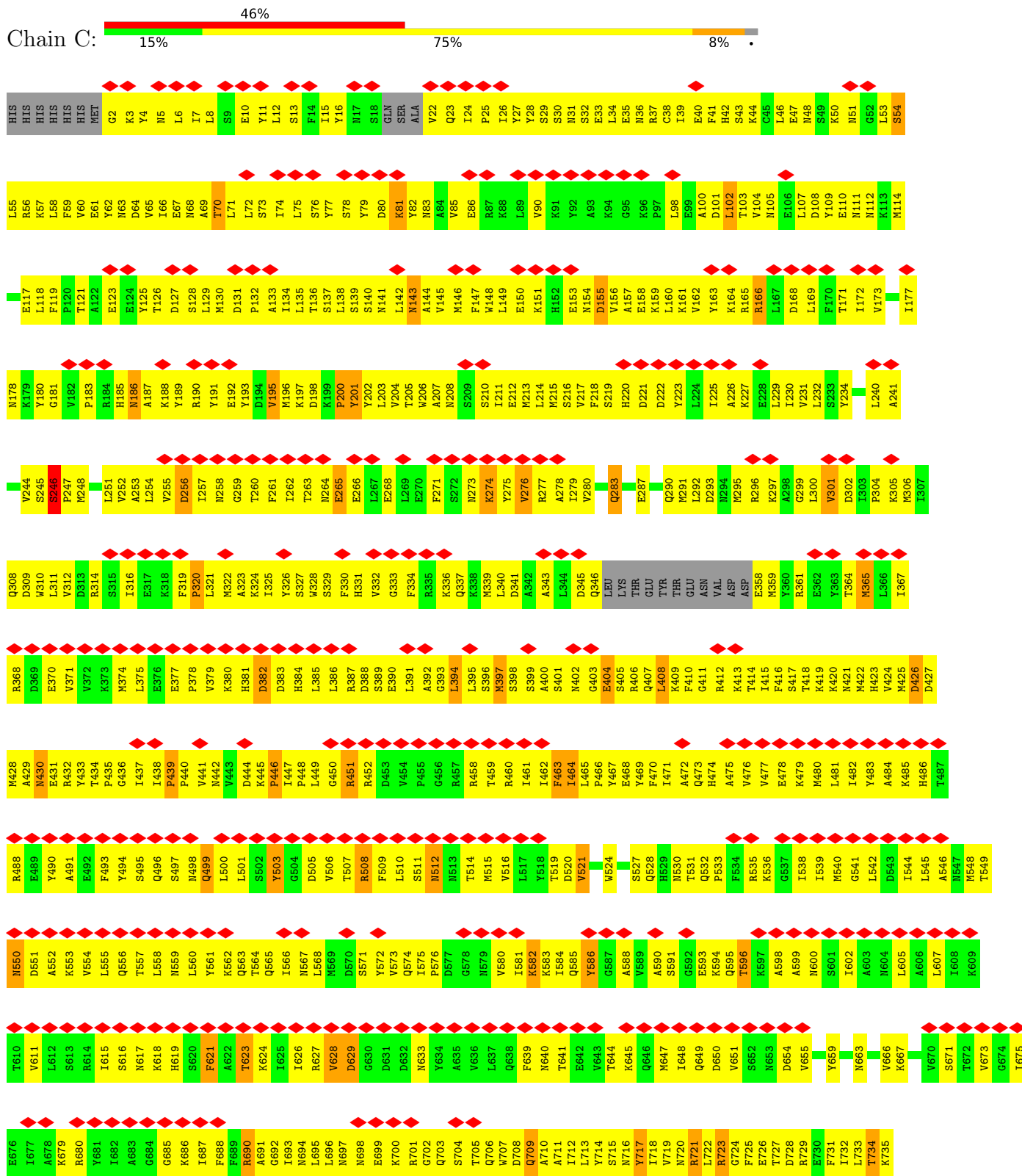
● Molecule 1: RNA-DEPENDENT RNA POLYMERASE

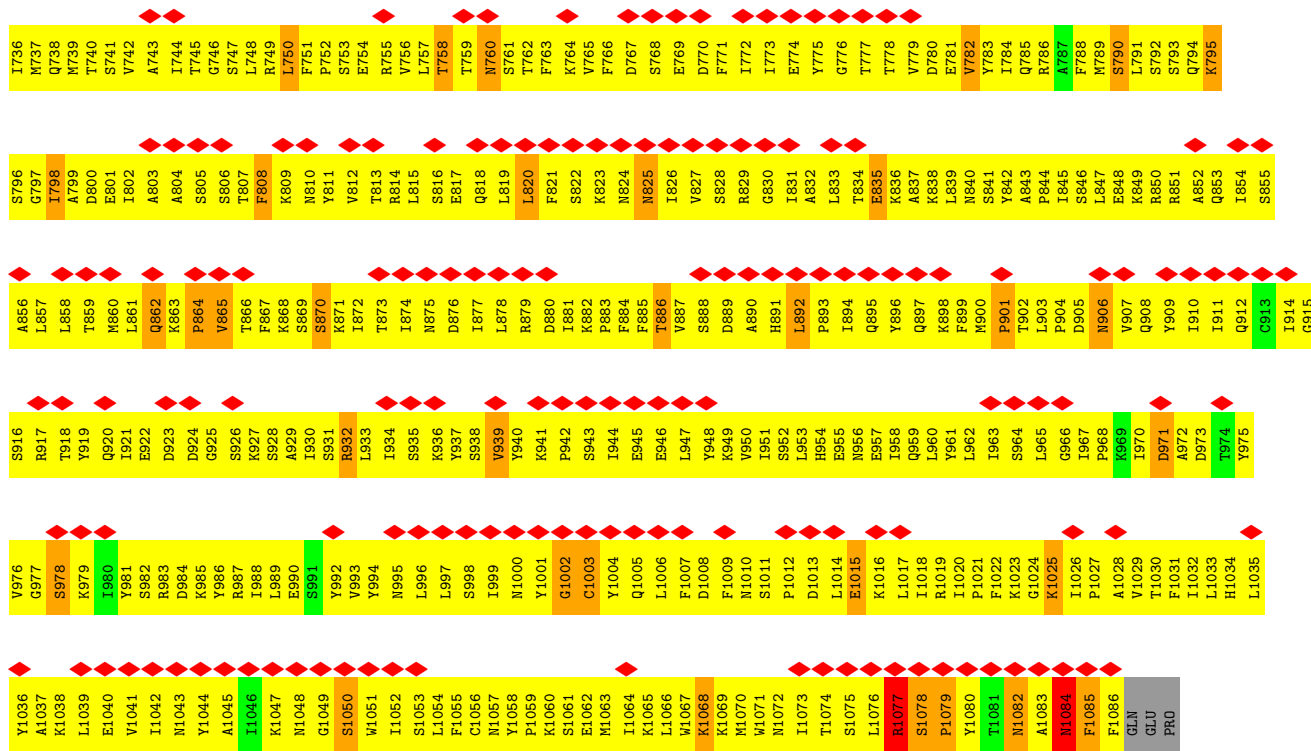




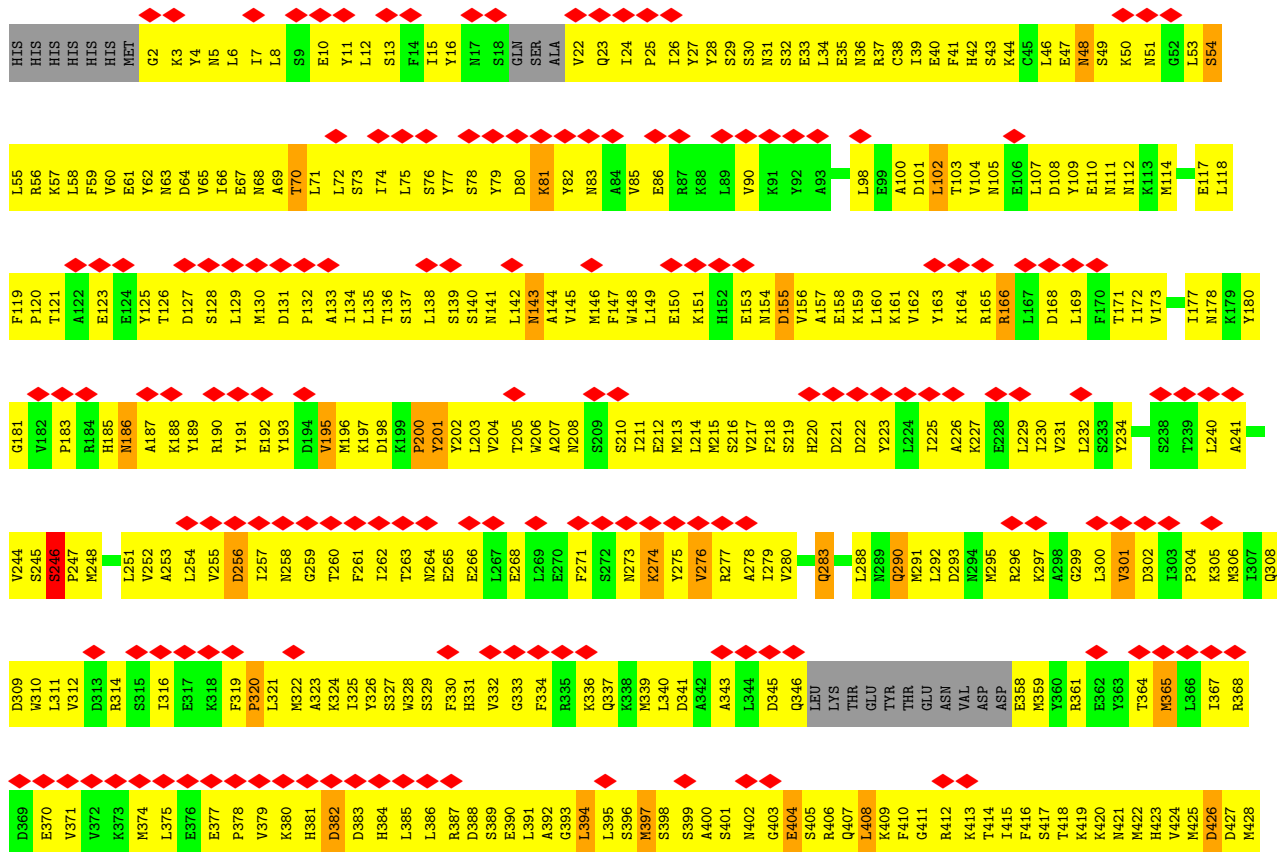


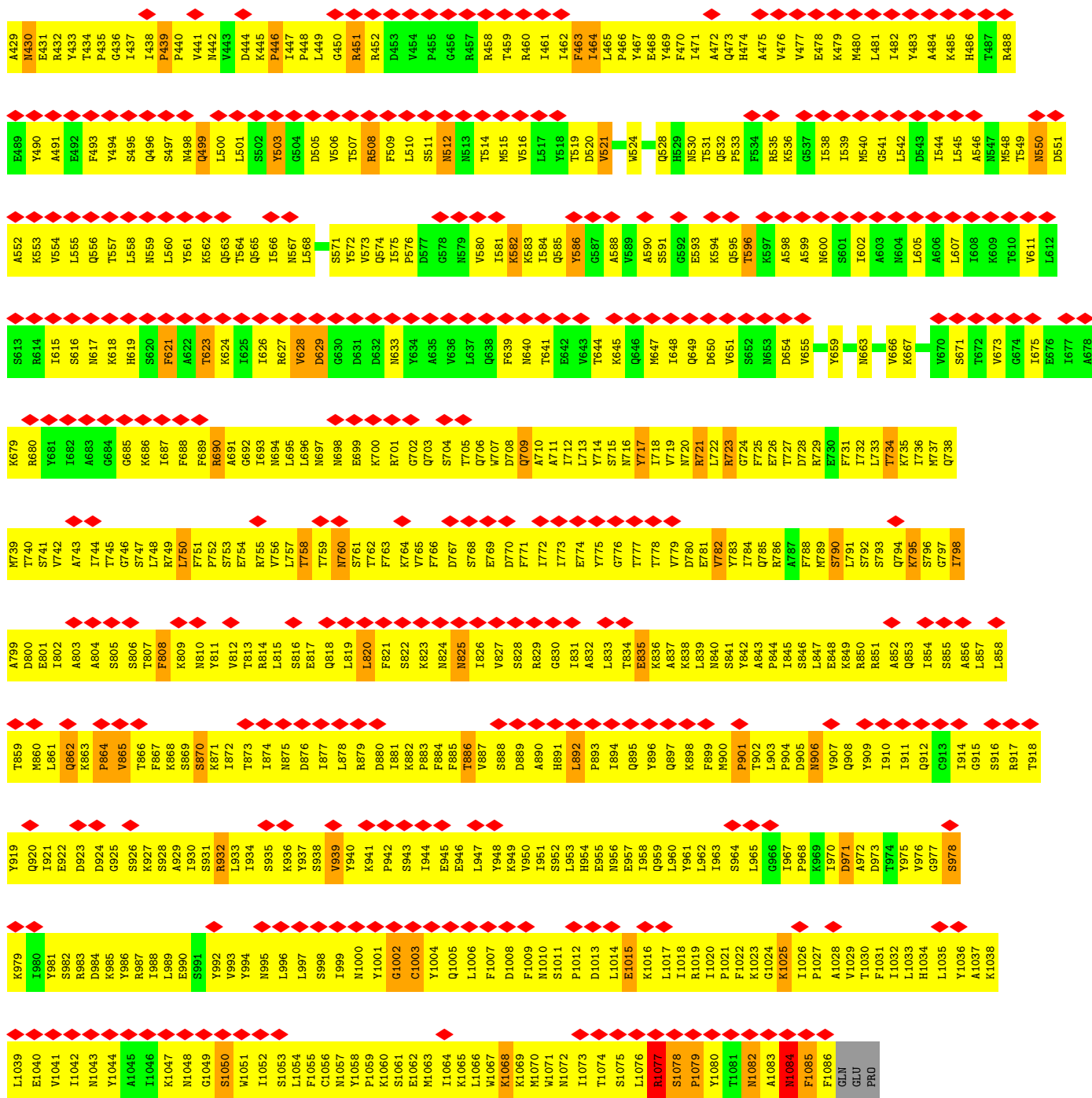
● Molecule 1: RNA-DEPENDENT RNA POLYMERASE



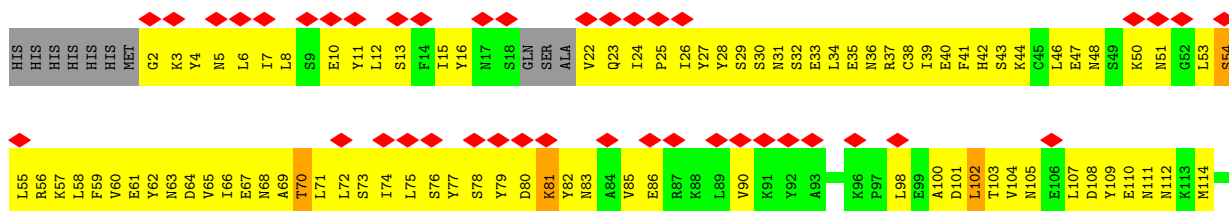


● Molecule 1: RNA-DEPENDENT RNA POLYMERASE





• Molecule 1: RNA-DEPENDENT RNA POLYMERASE



D973	Y974	Y975	Y976	G977	S978	K979	Y980	Y981	S982	R983	D984	K985	Y986	R987	I988	L989	E990	S991	Y992	Y993	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	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	M1069	M1070	W1071	N1072	I1073	T1074	S1075	L1076	R1077	S1078	P1079	Y1080	T1081	N1082	A1083	N1084	F1085	F1086	GLN	GLU	PRO			

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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($^{\circ}$)	Ideal($^{\circ}$)
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 [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	A	8741	0	8343	11726	0
1	B	8741	0	8344	11702	0
1	C	8741	0	8343	11680	0

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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.

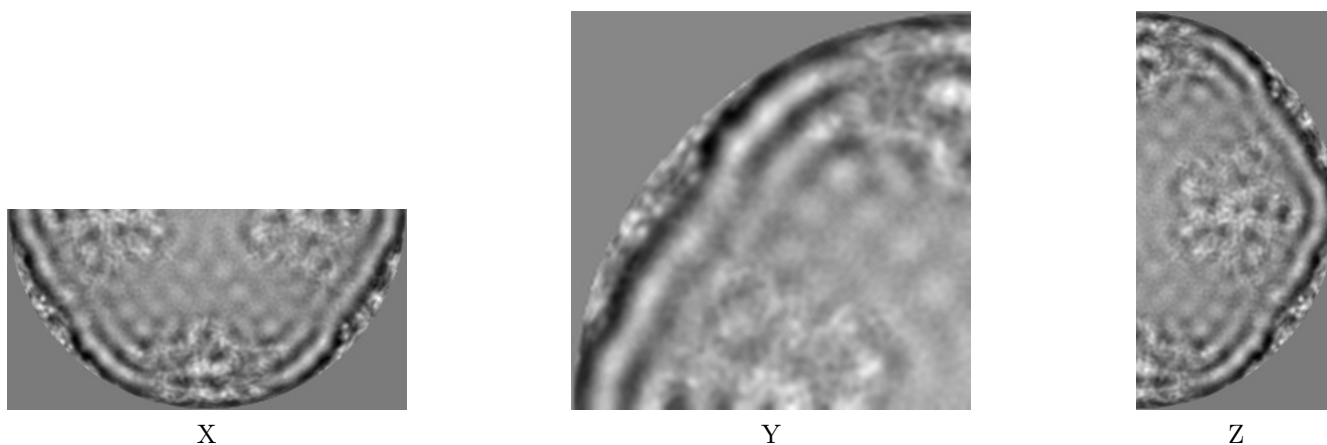
6 Map visualisation [i](#)

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 [i](#)

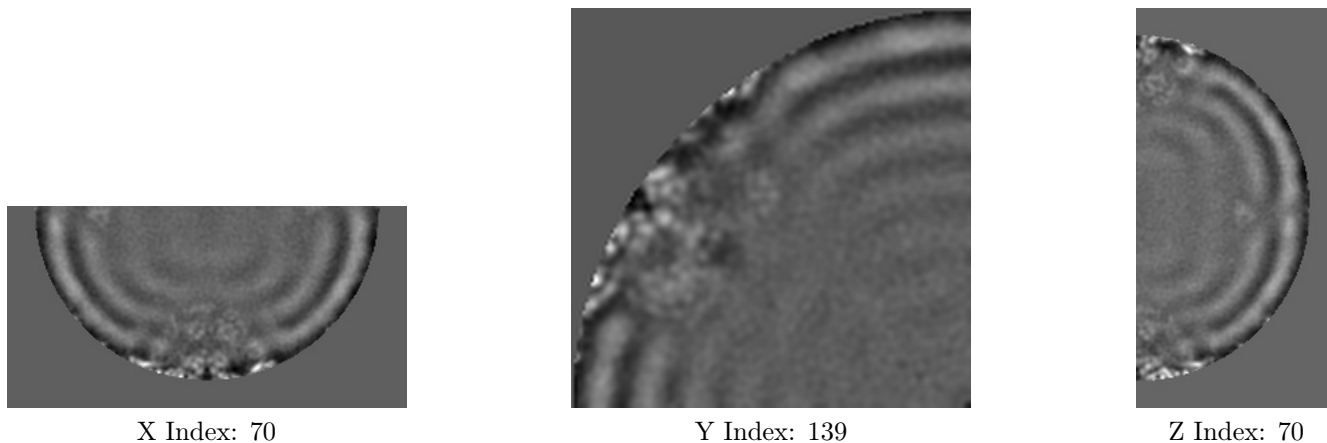
6.1.1 Primary map



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

6.2 Central slices [i](#)

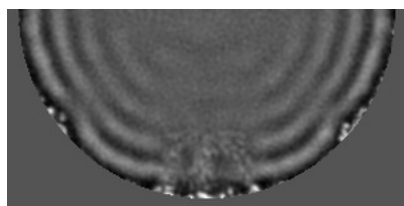
6.2.1 Primary map



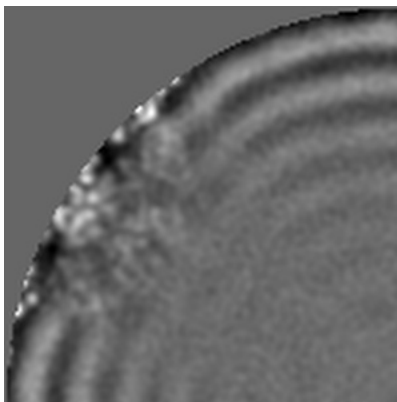
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

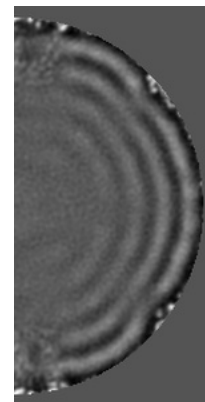
6.3.1 Primary map



X Index: 45



Y Index: 145

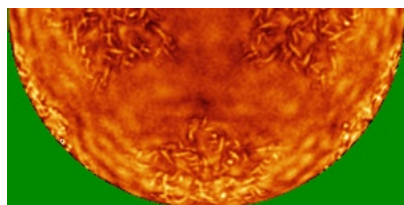


Z Index: 94

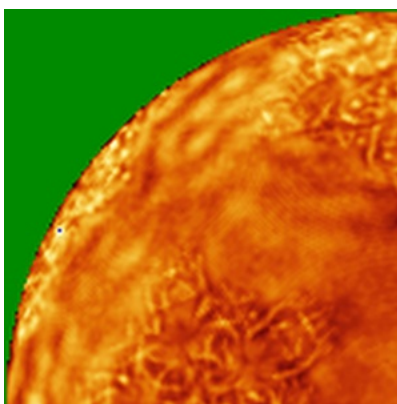
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

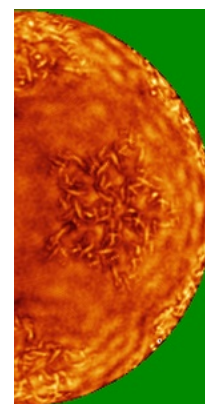
6.4.1 Primary map



X



Y

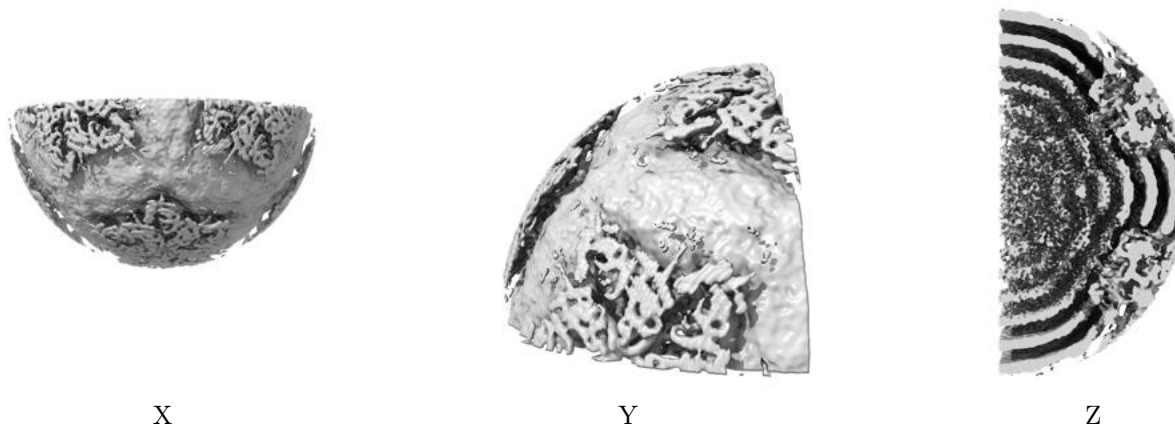


Z

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



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.

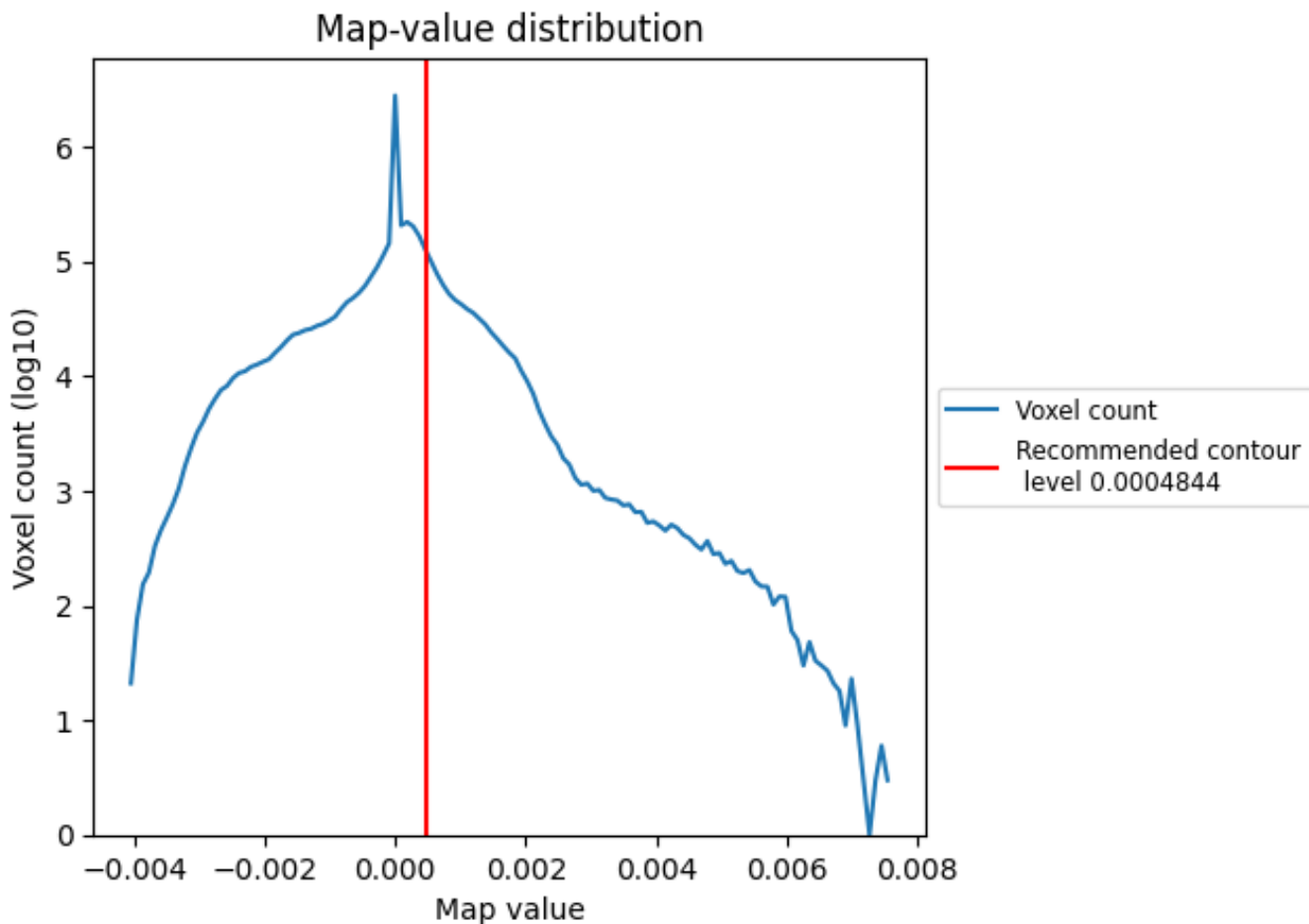
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

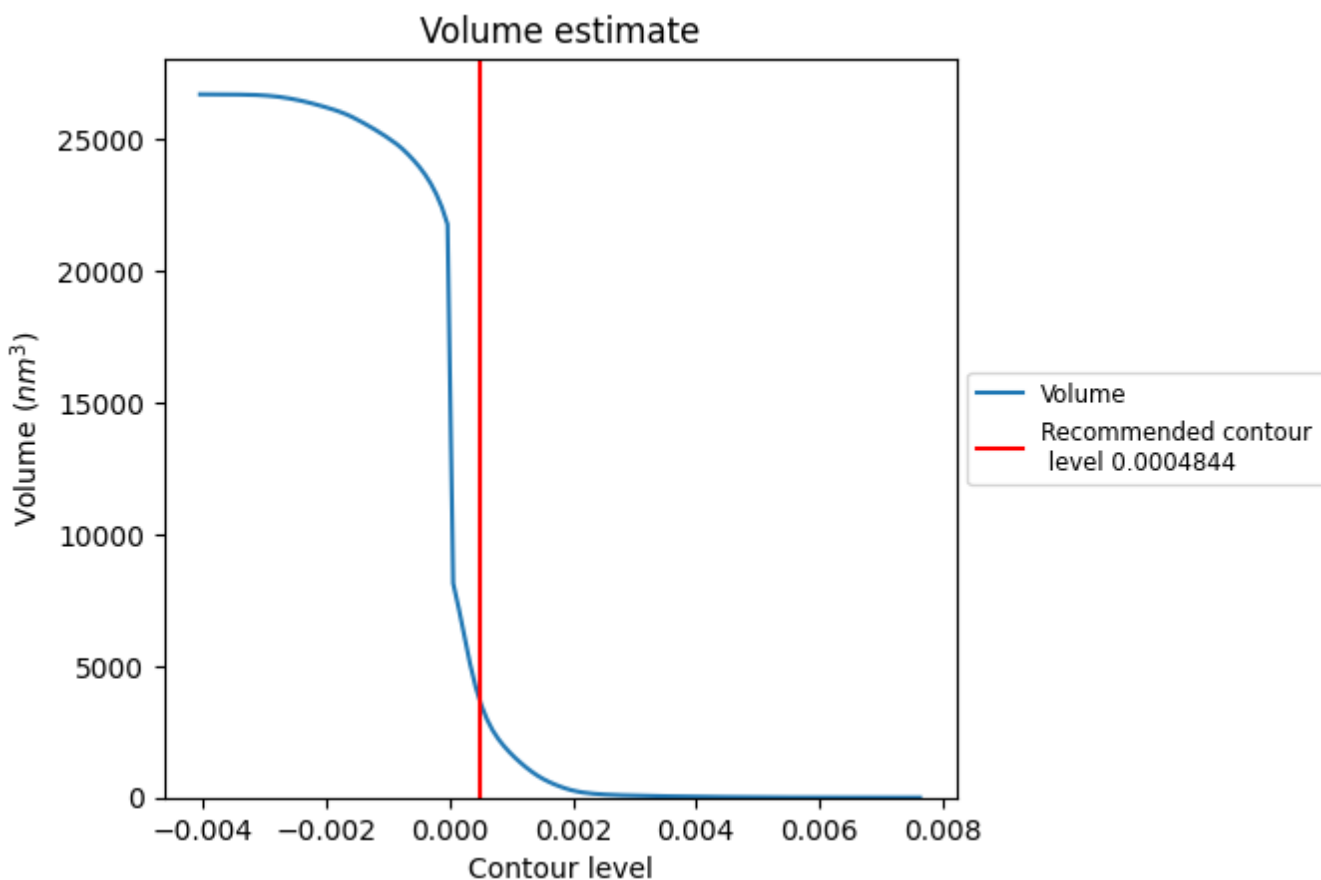
This section contains the results of statistical analysis of the map.

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 3732 nm³; 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.

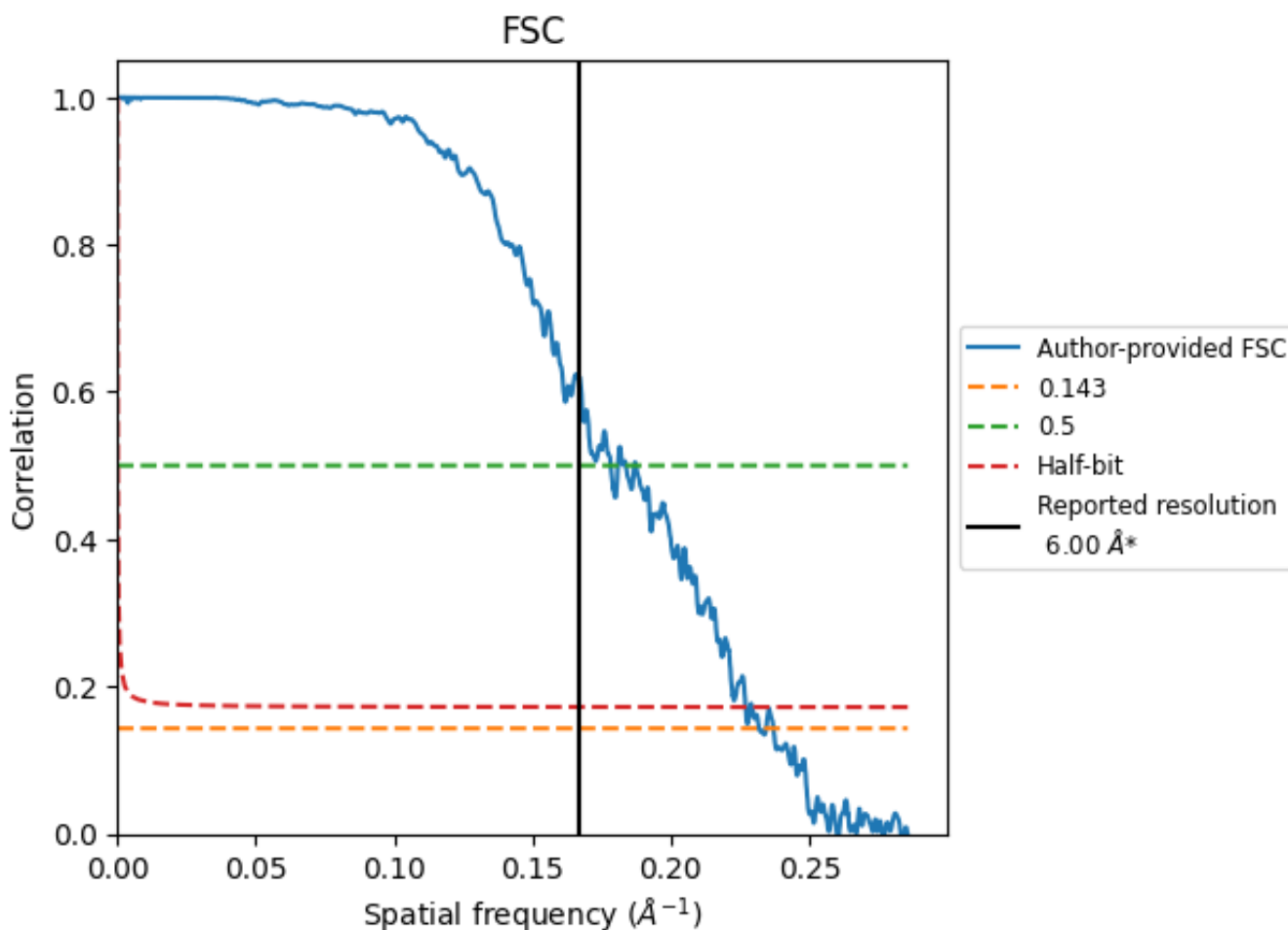
7.3 Rotationally averaged power spectrum [i](#)

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

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 0.167 Å⁻¹

8.2 Resolution estimates [i](#)

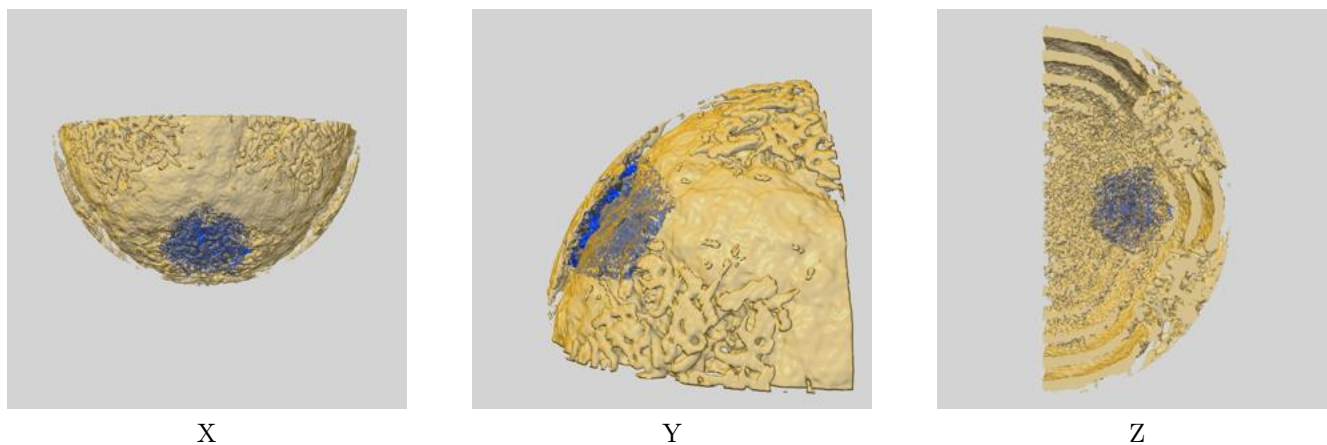
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.31	5.61	4.40
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

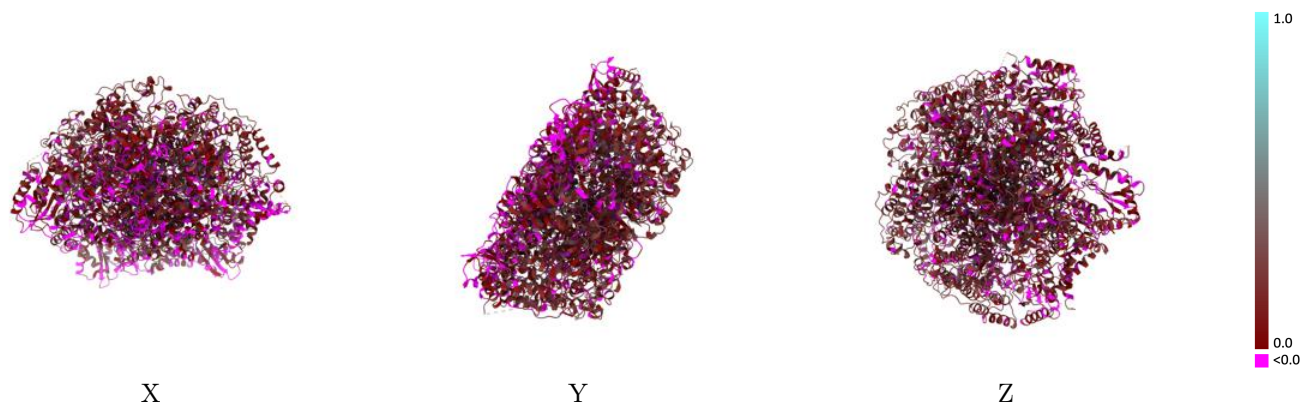
This section contains information regarding the fit between EMDB map EMD-2100 and PDB model 4AU6. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



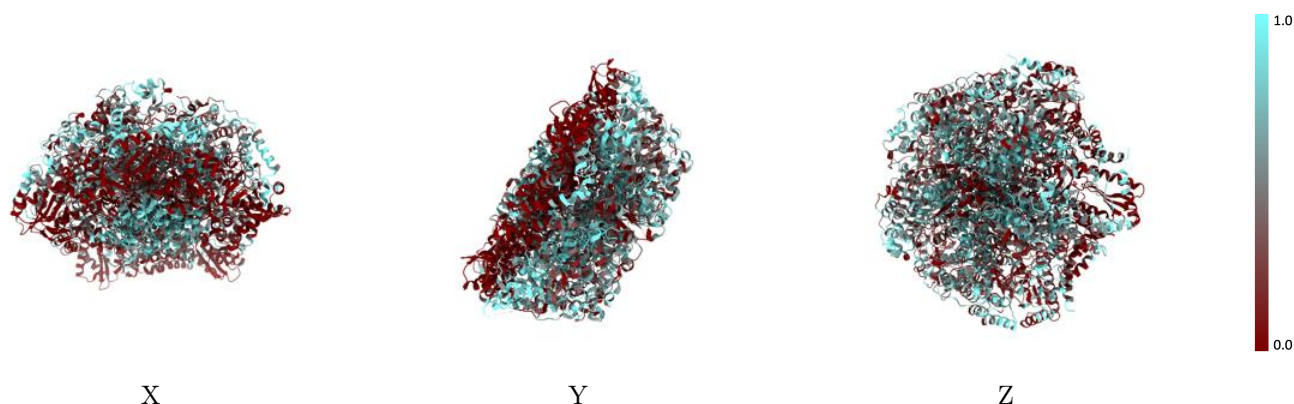
The images above show the 3D surface view of the map at the recommended contour level 0.0004844 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



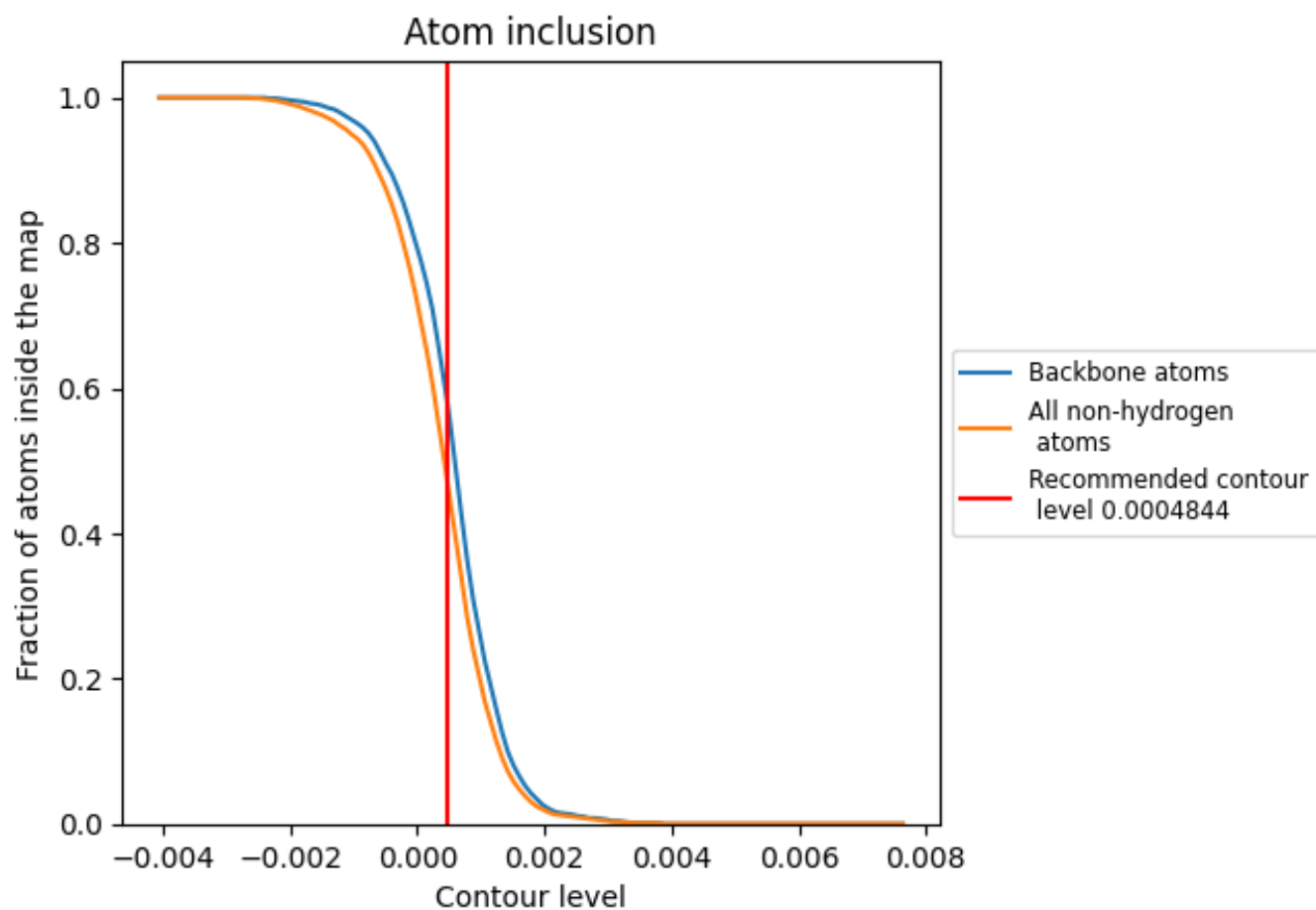
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0004844).

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 [i](#)

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

