

3D MODELS OF PROTEINS AND PUTATIVE G-QUADRUPLLEXES IN PORCINE CIRCOVIRUS TYPE 3 SINGLE-STRANDED CIRCULAR DNA

The problem

Until now, there is no information about 3D structure of proteins and putative G-quadruplexes (G4s) in porcine circovirus 3 (PCV-3) genome.

Methods

QGRS Mapper software was used for searching motifs of G4s. 3D models of G4s and proteins were built by the AlphaFold 3 (J. Abramson et al, 2024). For a reliability of the 3D model prediction in AlphaFold 3 the pLDDT parameter was used. A pLDDT value for a high level of model confidence should be over 90 on a scale from 0 to 100.

Fig. 4. Intramolecular anti-parallel G-quadruplex structure formed by stacking of three G-quartets with length of 15 nt in 1164-1178 position of PP067099 PCV-3 isolate.

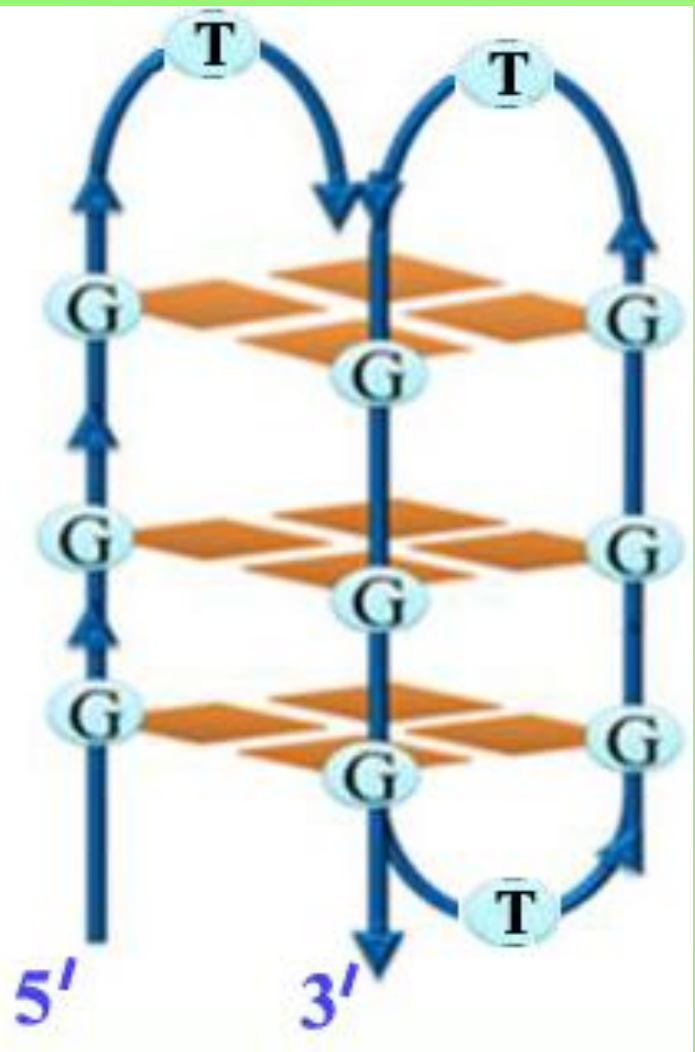


Table 1. Conservative sequences of putative G-quadruplexes in DNA of the *Porcine circovirus 3* PP067099 isolate. G-rich fragments of sequences for G4s are underlined.

Position	Gene/Product	G-quadruplex motif	G-score	pLDDT	Number of PCV-3 isolates with 100% identity by BLAST
645	Replicase	<u>GGG</u> TTTGC GTGATTTTTCG <u>GGG</u> TGAT <u>GGG</u> GTT <u>GGG</u>	59	90 > pLDDT > 70	1172
802	Replicase	<u>GGG</u> CCTTG GT <u>GGG</u> ATG GTTATAAT <u>GGG</u> GAG <u>GGG</u>	63	70 > pLDDT > 50	1117
893	Replicase	<u>GGG</u> ACAGGTACCCTCTGAG <u>GGG</u> TTCCTGTTAAG <u>GGG</u> T <u>GGG</u>	58	70 > pLDDT > 50	1011
1164	Intergenic region	<u>GGG</u> T <u>GGG</u> T <u>GGG</u> T <u>GGG</u> (Fig. 4)	72	pLDDT > 90	1998

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Results

4 conserved putative G-quadruplexes formed by three G-tetrads were found in the DNA of PCV-3 PP067099 isolate with complete genome (Table 1).

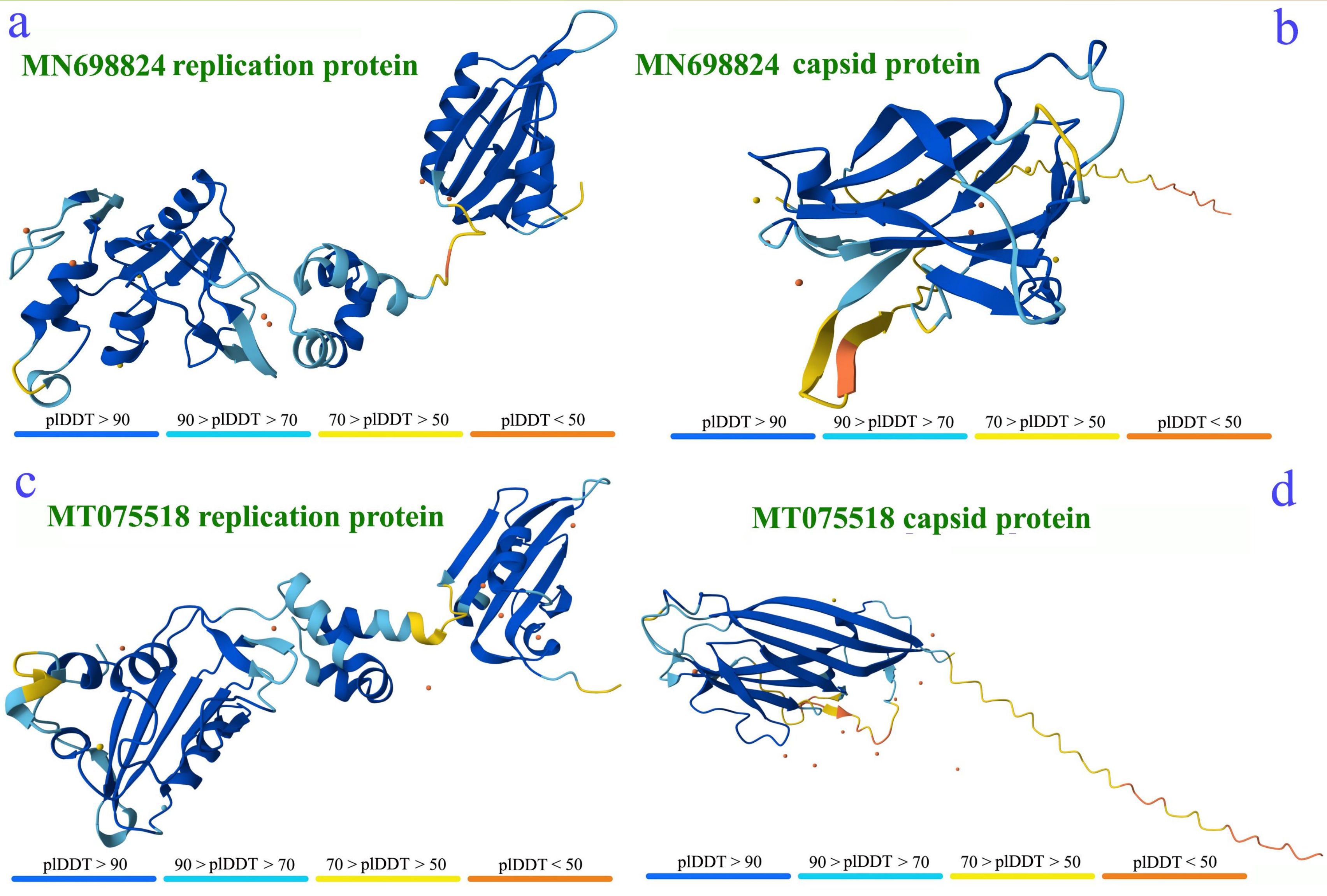


Fig. 3. 3D models of replication and capsid proteins for two phylogenetically most distant PCV-3 isolates. Number of β -sheets is 17 for MT075518 PCV-3 isolate comparing with 10 ones for MN698824 isolate.

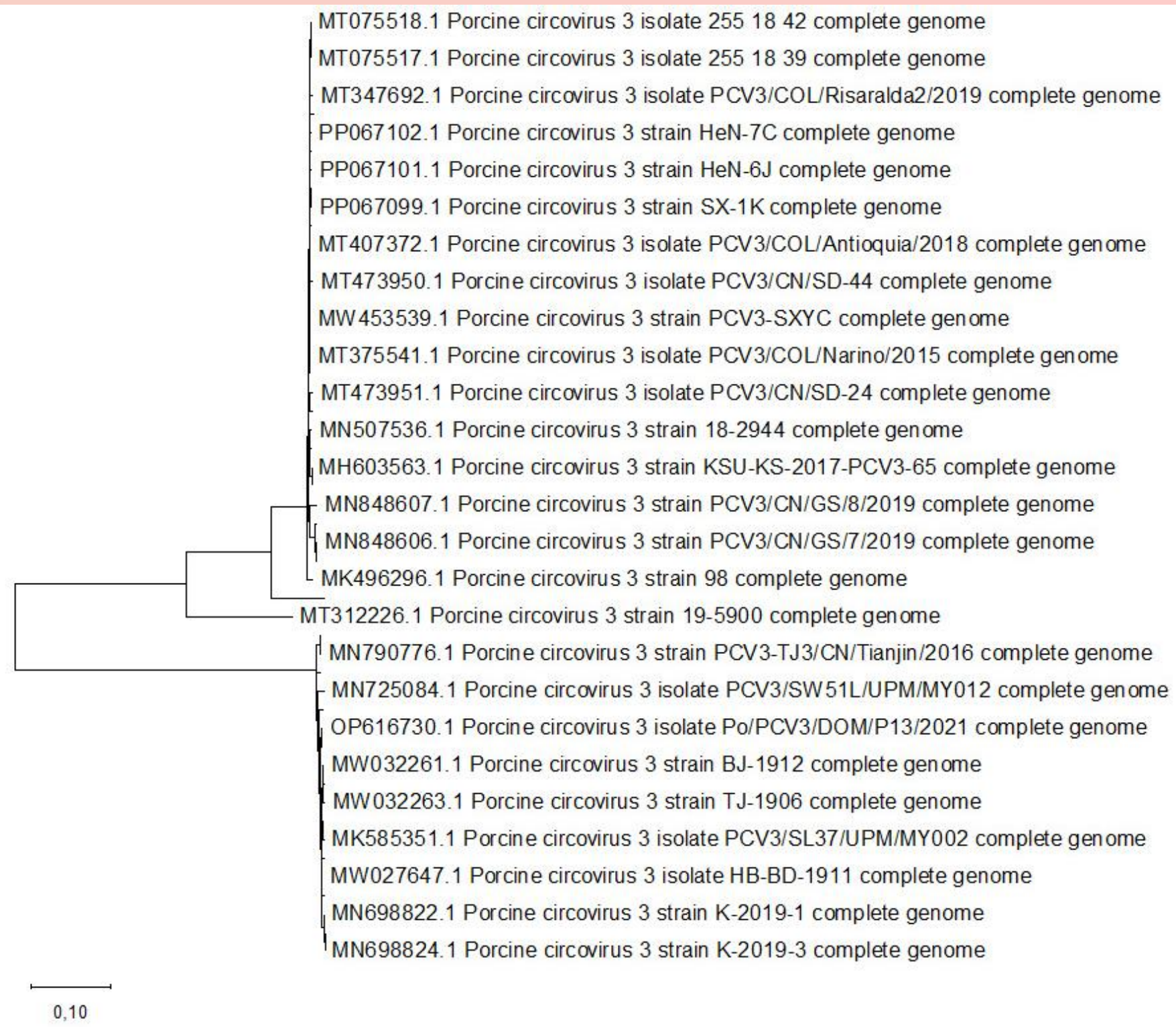


Fig. 1. Phylogenetic tree of 51 PCV-3 isolates with complete genome for determination of the most distant isolates.

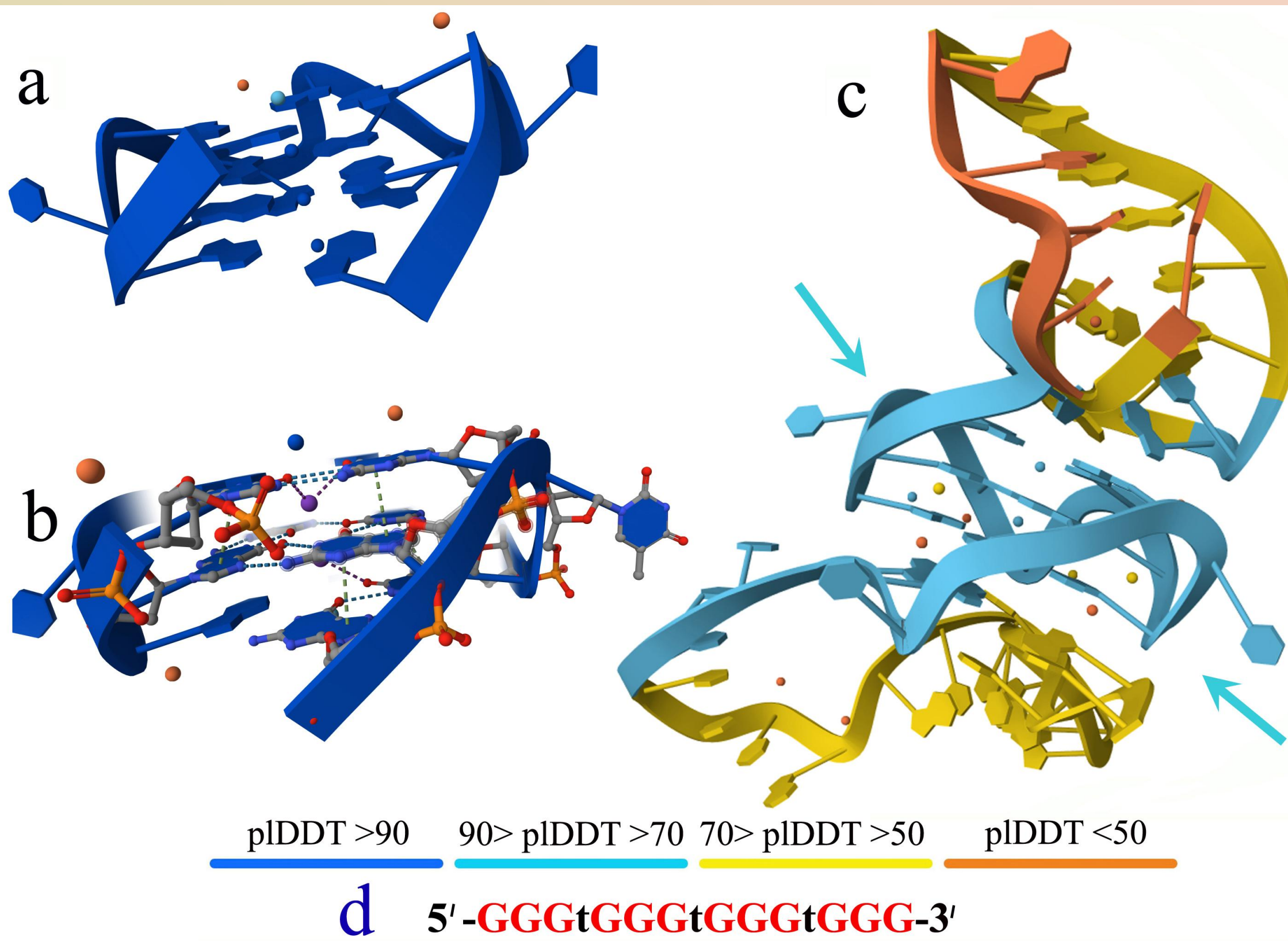


Fig. 2. 3D models of G-quadruplexes formed by three G-tetrads in single-stranded DNA of PP067099 isolate of the PCV-3 for a fragment of 15 nucleotides (nt) at positions 1164-1178 for 8 Na⁺ (a, b) and 57 nt at positions 1144-1200 for 20 Na⁺ (c; arrows indicate G4) in the intergenic region. (a, b) – pLDDT > 90, (c) – 90 > pLDDT > 70. (d) – G4 motif.

Conclusion

Main difference between two phylogenetically distant PCV-3 isolates is the number of β -sheets of capsid proteins.