

A Mutation identified in Neonatal Microcephaly Destabilizes Zika Virus NS1 Assembly *in vitro*

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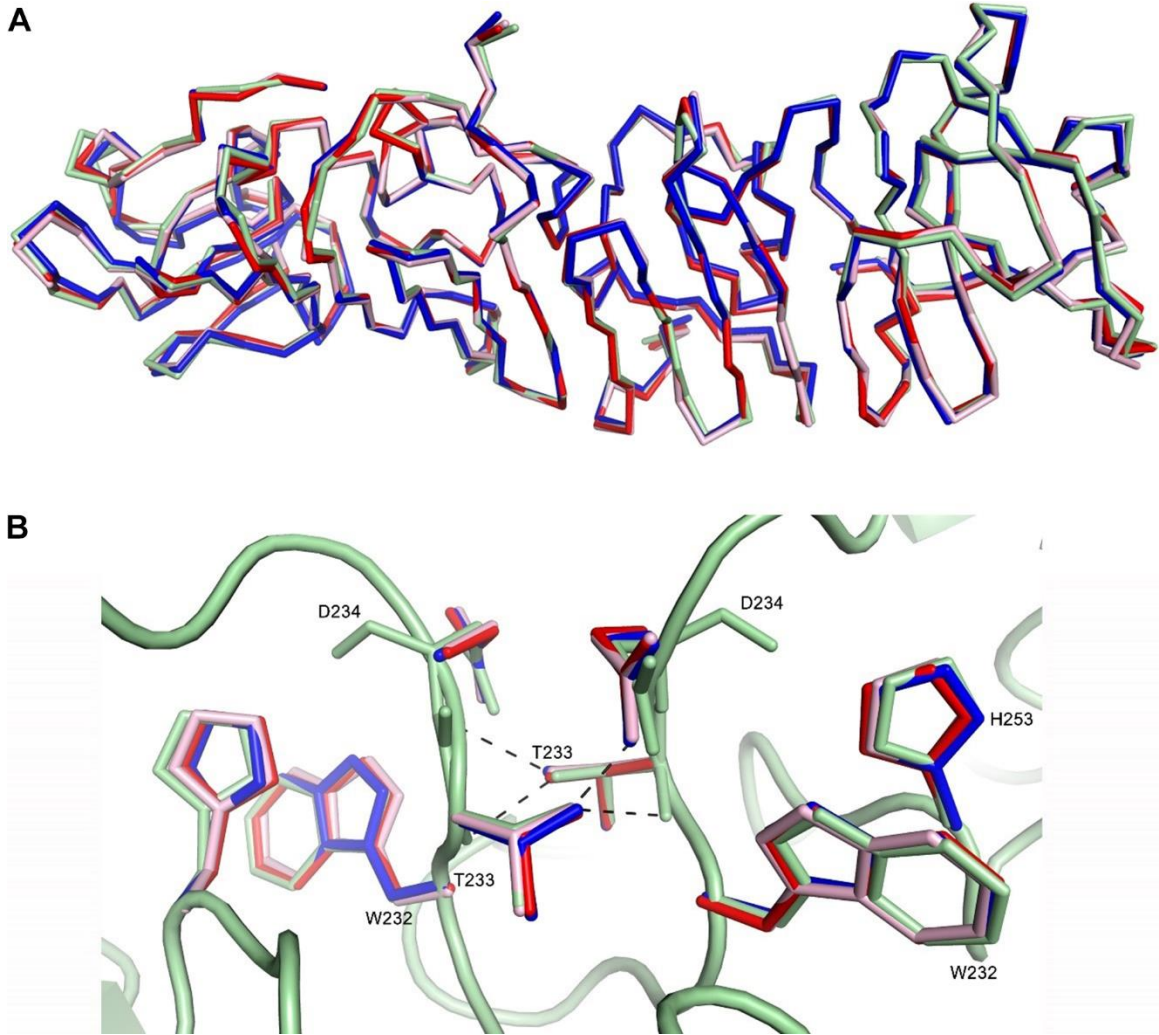
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Supplementary Figure 1. Comparison of the C-terminal structures from ZIKV NS1.

(A) The overlay of the main chain of four ZIKV NS1 C-terminal structures. The Suriname strain in green; PDB code: 5GS6 in red, PDB code: 5IY3 in blue, PDB code: 5K6K in pink^{1,2,3}.

(B) T233 plays a pivotal role in organizing a hydrogen-bonding network across the dimer interface among all ZIKV NS1 structures. The hydrogen bonds are shown in dash line.

Supplementary Table 1. Data collection and refinement statistics

NS1 ₁₇₂₋₃₅₂	
Data Collection	
X-ray Source	SSRF beamline BL19U1
Wavelength (Å)	0.97853 Å
Space group	C222 ₁
Unit cell a,b,c,α,β,γ (Å)	63.9, 100.8, 110.7, 90.0, 90.0, 90.0
Resolution range (Å)	50.0-2.80 (2.88-2.80) ^a
Unique reflections	8937 (705) ^a
Completeness (%)	99.4 (96.4) ^a
Redundancy	12.0 (9.6) ^a
<i>I</i> / σ <i>I</i>	15.9 (2.8) ^a
<i>R</i> _{merge} ^b	0.134 (0.653) ^a
Refinement	
Resolution range (Å)	37.27-2.82
No. of reflections (working/test)	7756/790
<i>R</i> _{work} / <i>R</i> _{free} ^c	0.210/0.259 (0.221/0.322)
Number of atoms	
Protein/water	2810/4
B-factors	
Protein	54.7
Water	20.3
r.m.s. deviations	
Bond lengths (Å)	0.004
Bond angles (°)	0.69
Ramachandran Plot ^d	
(% favored/allowed/outliers)	95/5/0
Rotamer Outliers (%) ^d	0.64
Clashscore ^d	6.88

^a Values in parentheses are the statistics for the highest resolution shell.

^b $R_{\text{merge}} = \frac{\sum_{\text{hkl}} \sum_j |\mathbf{I}_{\text{hkl}} - \mathbf{I}_{\text{hkl}}(j)|}{\sum_{\text{hkl}} \sum_j \mathbf{I}_{\text{hkl}}(j)}$. $\mathbf{I}_{\text{hkl}}(j)$ and \mathbf{I}_{hkl} represent the *j*th and mean intensity of reflection *hkl*.

^c $R_{\text{work}} = \frac{\sum_{\text{hkl}} (|\mathbf{F}_{\text{obs}}| - |\mathbf{F}_{\text{calc}}|)}{|\mathbf{F}_{\text{obs}}|}$. \mathbf{F}_{obs} and \mathbf{F}_{calc} represent the observed and calculated structure factors, respectively. *R*_{free} is the R factor calculated with 10 % of unique reflections as the test set.

^d The values are reported by PHENIX.

References

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- 3 Song, H., Qi, J., Haywood, J., Shi, Y. & Gao, G. F. Zika virus NS1 structure reveals diversity of electrostatic surfaces among flaviviruses. *Nat Struct Mol Biol* **23**, 456-458 (2016), doi: 10.1038/nsmb.3213.