

Summary of integrative structure determination of Invariant surface glycoprotein 65 of Trypanosoma brucei gambiense (PDB ID: 9A3G, PDB-Dev ID: PDBDEV_00000201)

1. Model Composition	
Entry composition	Invariant surface glycoprotein 65: Chain A (420 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - 3DEM volume, EMDB: EMD-14707 - Mass Spectrometry data, PRIDE: PXD033606 - Experimental model, PDB ID: 7ZGJ - De Novo model, Not available - De Novo model, Not available
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 7
Flexible units	A: 1-18, 19-129, 130-186, 187-210, 211-239, 240-296, 297-420
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique EM3DRestraint: SSM and convolution-based shape searches using Phenix Dock-in-map, Real-space refinement using Phenix, manual refinements using Coot (where applicable) - 1 unique CrossLinkRestraint: CYS, 3 cross-links
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 29.24, Number of Ramachandran outliers = 52, Number of sidechain outliers = 25
Model quality: assessment of excluded volume	Not applicable

<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Method</i>	AlphaFold model prediction
<i>Name</i>	None
2. <i>Method</i>	Modelling
<i>Name</i>	None
3. <i>Method</i>	Refinement
<i>Name</i>	None
<i>Software</i>	<ul style="list-style-type: none"> - AlphaFold2 (version Not available) - Coot (version Not available) - Phenix (version Not available)