

Summary of integrative structure determination of USP7 TRAF domain in complex with DNA polymerase iota peptide 573-584 (PDB ID: 9A0Y, PDB-Dev ID: PDBDEV_0000070)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - DNA polymerase iota peptide 573-584: Chain A (12 residues) - USP7 TRAF domain: Chain B (145 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 2fop - NMR data, BMRB: 50080 - Mutagenesis data, File: 10.1016/j.jmb.2020.166733
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	2, 0
Rigid bodies	<ul style="list-style-type: none"> - A: 1-12 - B: 1-145
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 96 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	20
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 7.28, Number of Ramachandran outliers = 1, Number of sidechain outliers = 19 - Model-2: Clashscore = 12.14, Number of Ramachandran outliers = 2, Number of sidechain outliers = 15 - Model-3: Clashscore = 12.94, Number of Ramachandran outliers = 0, Number of sidechain outliers = 5 - Model-4: Clashscore = 13.75, Number of Ramachandran outliers = 2, Number of sidechain outliers = 16 - Model-5: Clashscore = 8.5, Number of Ramachandran outliers = 2, Number of sidechain outliers = 11 - Model-6: Clashscore = 9.3, Number of Ramachandran outliers = 2, Number of sidechain outliers = 15 - Model-7: Clashscore = 8.5, Number of Ramachandran outliers = 1, Number of sidechain outliers = 16 - Model-8: Clashscore = 9.3, Number of Ramachandran outliers = 3, Number of sidechain outliers = 12 - Model-9: Clashscore = 11.73, Number of Ramachandran outliers = 2, Number of sidechain outliers = 12 - Model-10: Clashscore = 5.66, Number of Ramachandran outliers = 1, Number of sidechain outliers = 10 - Model-11: Clashscore = 7.28, Number of Ramachandran outliers = 1, Number of sidechain outliers = 16 - Model-12: Clashscore = 8.09, Number of Ramachandran outliers = 2, Number of sidechain outliers = 12 - Model-13: Clashscore = 11.33, Number of Ramachandran outliers = 2, Number of sidechain outliers = 10 - Model-14: Clashscore = 7.28, Number of Ramachandran outliers = 2, Number of sidechain outliers = 10 - Model-15: Clashscore = 7.69, Number of Ramachandran outliers = 2, Number of sidechain outliers = 15 - Model-16: Clashscore = 10.92, Number of Ramachandran outliers = 2, Number of sidechain outliers = 12 - Model-17: Clashscore = 12.94, Number of Ramachandran outliers = 2, Number of sidechain outliers = 13 - Model-18: Clashscore = 10.52, Number of Ramachandran outliers = 2, Number of sidechain outliers = 13 - Model-19: Clashscore = 11.33, Number of Ramachandran outliers = 1, Number of sidechain outliers = 7 - Model-20: Clashscore = 10.11, Number of Ramachandran outliers = 1, Number of sidechain outliers = 12
<p><i>Model quality: assessment of excluded volume</i></p>	<p>Not applicable</p>

<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>	None
<i>Name</i>	docking
<i>Number of computed models</i>	?
<i>Software</i>	<ul style="list-style-type: none">- MODELLER (version Not available)- HADDOCK (version Not available)- PYMOL (version Not available)