

Summary of integrative structure determination of Integrative model of full-length RAGE in complex with S100B (PDB ID: 9A18, PDB-Dev ID: PDBDEV_0000080)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - RAGE: Chain B (383 residues) - RAGE: Chain C (383 residues) - S100B: Chain G (91 residues) - RAGE: Chain A (383 residues) - S100B: Chain H (91 residues) - S100B: Chain E (91 residues) - RAGE: Chain D (383 residues) - S100B: Chain F (91 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB ID: 4ybh - Experimental model, PDB ID: 4xyn - Experimental model, PDB ID: 5d7f - Crosslinking-MS data, Linker name and number of cross-links: BS3, 27 cross-links - Crosslinking-MS data, Linker name and number of cross-links: BS3, 39 cross-links - H/D exchange data, MASSIVE: MSV000086718
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 12
Flexible units	<ul style="list-style-type: none"> - A: 1-301, 302-383 - B: 1-301, 302-383 - C: 1-301, 302-383 - D: 1-301, 302-383 - E: 1-91 - F: 1-91 - G: 1-91 - H: 1-91
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 CrossLinkRestraint: BS3, 27 cross-links - 1 unique CrossLinkRestraint: BS3, 39 cross-links
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1

<i>Model precision (uncertainty of models)</i>	Model precision can not be calculated with one structure
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	Model-1: Clashscore = 16.39, Number of Ramachandran outliers = 15, Number of sidechain outliers = 6
<i>Model quality: assessment of excluded volume</i>	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>	modeling
<i>Name</i>	?
<i>Description</i>	?
<i>Number of computed models</i>	?
<i>Software</i>	ROSETTA (version Not available)