

	<p>10.5281/zenodo.1209565</p> <ul style="list-style-type: none"> - 2DEM class average, File: 10.5281/zenodo.1209565 - 2DEM class average, File: 10.5281/zenodo.1209565 - 2DEM class average, File: 10.5281/zenodo.1209565 - 2DEM class average, File: 10.5281/zenodo.1209565 - 2DEM class average, File: 10.5281/zenodo.1209565 - 2DEM class average, File: 10.5281/zenodo.1209565 - 2DEM class average, File: 10.5281/zenodo.1209565 - 2DEM class average, File: 10.5281/zenodo.1209565 - Crosslinking-MS data, Linker name and number of cross-links: DSS, 18 cross-links - Experimental model, PDB ID: 3I4R - Experimental model, PDB ID: 3KFO - Experimental model, PDB ID: 4Q9T - Experimental model, PDB ID: 2JO8 - Experimental model, PDB ID: 2QIW - Experimental model, PDB ID: 3CIG - Experimental model, PDB ID: 2ELO - Experimental model, PDB ID: 3GUZ - Experimental model, PDB ID: 2CIW - Experimental model, PDB ID: 1A92 - Experimental model, PDB ID: 1GDJ - Experimental model, PDB ID: 1X4O - Comparative model, template PDB ID: Not available
2. Representation	
<i>Resolution</i>	Atomic
<i>Number of rigid bodies, flexible units</i>	0, 1
<i>Flexible units</i>	A: 1-1166
<i>Structural coverage (rigid bodies)</i>	100%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided

<p>Experimental data</p>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 18 cross-links - 1 unique CrossLinkRestraint: EDC, 23 cross-links - 1 unique EM2DRestraint: Number of micrographs: 103, Image resolution: 15.0 - 2 unique EM2DRestraint: Number of micrographs: 100, Image resolution: 15.0 - 3 unique EM2DRestraint: Number of micrographs: 88, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 64, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 60, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 111, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 51, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 70, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 49, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 32, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 76, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 77, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 44, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 56, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 86, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 120, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 16, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 34, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 6, Image resolution: 15.0 - 1 unique EM2DRestraint: Number of micrographs: 11, Image resolution: 15.0 - 19 unique SASRestraint: Assembly name: SAXS assembly Fitting method: FoXS Multi-state: True
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	4
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	<ul style="list-style-type: none"> - Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 135, Number of sidechain outliers = 76 - Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 127, Number of sidechain outliers = 75 - Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 134, Number of sidechain outliers = 61 - Model-4: Clashscore = 0.0, Number of Ramachandran outliers = 170, Number of sidechain outliers = 62
Model quality: assessment of excluded volume	Not applicable
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	MD-based conformational sampling
Name	AllosMod
Number of computed models	7000
2. Method	Minimal Ensemble Search
Name	MES
Number of computed models	4
Software	<ul style="list-style-type: none"> - HHpred (version 2.0.16) - PSIPRED (version 4.0) - DISOPRED (version 3) - Integrative Modeling Platform (IMP) (version 2.2) - MODELLER (version 9.13) - AllosMod (version Not available)