

Summary of integrative structure determination of The molecular architecture of the BBSome and its implications for facilitated transition zone crossing (PDB ID: 8ZZI, PDB-Dev ID: PDBDEV_00000018)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - BBS9: Chain 9 (887 residues) - BBS2: Chain 2 (721 residues) - BBS18: Chain 1P (96 residues) - BBS5: Chain 5 (341 residues) - BBS4: Chain 4 (519 residues) - BBS7: Chain 7 (712 residues) - BBS8: Chain 8 (506 residues) - BBS1: Chain 1 (593 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Comparative model, template PDB ID: Not available - De Novo model, File: 10.5281/zenodo.1255360 - De Novo model, File: 10.5281/zenodo.1255360 - Comparative model, template PDB ID: Not available - De Novo model, File: 10.5281/zenodo.1255360 - Comparative model, template PDB ID: Not available - 3DEM volume, EMDB: EMD-7839 - Crosslinking-MS data, Linker name and number of cross-links: DSS, 103 cross-links - Experimental model, PDB ID: 4V0N - Experimental model, PDB ID: 1VYH - Experimental model, PDB ID: 5G05 - Experimental model, PDB ID: 2CAY - Experimental model, PDB ID: 3HSA - Experimental model, PDB ID: 1W3B - Experimental model, PDB ID: 4YHD
2. Representation	
<u>Resolution</u>	Atomic

<u>Number of rigid bodies, flexible units</u>	8, 0
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - 1: 1-593:None - 2: 1-721:None - 4: 1-519:None - 5: 1-341:None - 7: 1-712:None - 8: 1-506:None - 9: 1-887:None - IP: 1-96:None
<u>Structural coverage (rigid bodies)</u>	100%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 103 cross-links - 1 unique CrossLinkRestraint: BS3, 19 cross-links - 1 unique EM3DRestraint: None
4. Validation	
<u>Number of ensembles</u>	1
<u>Number of models in ensembles</u>	1
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	None, Å
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 35, Number of sidechain outliers = 5
<u>Model quality: assessment of excluded volume</u>	Not applicable
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	Production sampling
<u>Name</u>	Monte Carlo
2. Method	Rosetta Hybridize
<u>Name</u>	Rosetta Hybridize

Software

- [Rosetta](#) (version Rosetta version
unknown:839226a33c427862a8be7b4ca555493368c148f
2017-09-18 10:39:53 -0700 from
git@github.com:RosettaCommons/main.git)
- [HHpred](#) (version website)