
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	
Entry composition	<ul style="list-style-type: none">- BBS1: chain(s) 1 (593 residues)- BBS2: chain(s) 2 (721 residues)- BBS4: chain(s) 4 (519 residues)- BBS5: chain(s) 5 (341 residues)- BBS7: chain(s) 7 (712 residues)- BBS8: chain(s) 8 (506 residues)- BBS9: chain(s) 9 (887 residues)- BBS18: chain(s) IP (96 residues)

[Datasets used for modeling](#)

- Comparative model, Zenodo: [10.5281/zenodo.1255360](https://zenodo.org/record/1255360/files/10.5281/zenodo.1255360)
- De Novo model, Zenodo: [10.5281/zenodo.1255360](https://zenodo.org/record/1255360/files/10.5281/zenodo.1255360)
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- De Novo model, Zenodo: [10.5281/zenodo.1255360](https://zenodo.org/record/1255360/files/10.5281/zenodo.1255360)
- 3DEM volume, EMDB: [EMD-7839](https://www.ebi.ac.uk/EMDB/entry/EMD-7839)
- Crosslinking-MS data, Zenodo: [10.5281/zenodo.1255360](https://zenodo.org/record/1255360/files/10.5281/zenodo.1255360)
- Experimental model, PDB: [4V0N](https://www.rcsb.org/structure/4V0N)
- Experimental model, PDB: [1VYH](https://www.rcsb.org/structure/1VYH)
- Experimental model, PDB: [5G05](https://www.rcsb.org/structure/5G05)
- Experimental model, PDB: [2CAY](https://www.rcsb.org/structure/2CAY)
- Experimental model, PDB: [3HSA](https://www.rcsb.org/structure/3HSA)
- Experimental model, PDB: [1W3B](https://www.rcsb.org/structure/1W3B)
- Experimental model, PDB: [4YHD](https://www.rcsb.org/structure/4YHD)

2. Representation

[Number of representations](#)

1

[Scale](#)

Atomic

Number of [rigid](#) and [flexible](#) segments

42, 0

3. Restraints

<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 103 crosslinks - 1 unique CrossLinkRestraint: BS3, 19 crosslinks - 1 unique EM3DRestraint: None
4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	1
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	Not available
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 0.00 - Ramachandran outliers: 35 - Sidechain outliers: 5
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 55.79%
<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>Name</i>	Production sampling
2. <i>Name</i>	Rosetta Hybridize
<i>Software</i>	<ul style="list-style-type: none"> - Rosetta (version Rosetta version unknown:839226a33c427862a8be7b4ca555493368c1 2017-09-18 10:39:53 -0700 from git@github.com:RosettaCommons/main.git) - HHpred (version website)