Full wwPDB Integrative Structure Validation Report

November 05, 2019 -- 04:07 PM

PDB ID	*PDBDEV00000018*
Molecule Name	The molecular architecture of the BBSome and its implications for facilitated transition zone crossing
Title	The Molecular Architecture of Native BBSome Obtained by an Integrated Structural Approach
Authors	Chou H;Apelt L;Farrell DP;White SR;Woodsmith J;Svetlov V;Goldstein JS;Nager AR;Li Z;Muller J;Dollfus H;Nudler E;Stelzl U;DiMaio F;Nachury MV;Walz T

The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance

2. Ensemble information

This entry consists of 1 distinct ensemble.

Ensemble number	*Ensemble name*	*Model ID*	*Number of models*	*Clustering method*	*Clustering feature*	*Cluster precision*

1	None	None	1	None	None	None

3. Model composition

3.1 Summary

This entry consists of 1 unique models, with 8 subunits in each model. A total of 33 datasets or restraints was used to build this entry. Each model is represented by 8 rigid bodies and 0 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry.This model is titled Best scoring model respectively.

Model ID	*Subunit number*	*Subunit ID*	*Subunit name*	*Chain ID*	*Total residues*
1	1	1	BBS1	1	593
1	2	2	BBS2	2	721
1	3	3	BBS4	4	519
1	4	4	BBS5	5	341
1	5	5	BBS7	7	712
1	6	6	BBS8	8	506
1	7	7	BBS9	9	887
1	8	8	BBS18	IP	96

3.3 Datasets used for modeling

There are 33 unique datasets used to build the models in this entry.

ID	*Dataset type*	*Database name*	*Data access code*
1	Comparative model	Not listed	None
2	De Novo model	Not listed	None
3	De Novo model	Not listed	None
4	Comparative model	Not listed	None
5	De Novo model	Not listed	None
6	De Novo model	Not listed	None
7	De Novo model	Not listed	None

8	De Novo model	Not listed	None
9	Comparative model	Not listed	None
10	Comparative model	Not listed	None
11	Comparative model	Not listed	None
12	Comparative model	Not listed	None
13	De Novo model	Not listed	None
14	De Novo model	Not listed	None
15	De Novo model	Not listed	None
16	De Novo model	Not listed	None
17	Comparative model	Not listed	None
18	Comparative model	Not listed	None
19	Comparative model	Not listed	None
20	De Novo model	Not listed	None
21	De Novo model	Not listed	None
22	De Novo model	Not listed	None
23	De Novo model	Not listed	None
24	De Novo model	Not listed	None
25	3DEM volume	EMDB	7839
26	CX-MS data	Not listed	None
27	Experimental model	PDB	4V0N
28	Experimental model	PDB	1VYH
29	Experimental model	PDB	5G05
30	Experimental model	PDB	2CAY
31	Experimental model	PDB	3HSA
32	Experimental model	PDB	1W3B
33	Experimental model	PDB	4YHD

4. Representation

This entry has only one representation and includes 8 rigid bodies and 0 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
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.	-

5. Methodology and software

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification
1	Rosetta	Rosetta version unknown:839226a33c427862a8be7b4ca5554933f8c148 2017-09-18 10:39:53 -0700 from git@github.com:RosettaCommons/main.git	RosettaCM/hybridize, Rosetta Abinitio, and unpublished 'complex assembly'
2	HHpred	website	protein homology detection

6. Data quality

7. Model quality

7.1 Standard geometry

There are 13530 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--HD22	1.008	0.86	109

N--H	1.008	0.86	1609
NE2--HE2	1.008	0.86	39
NH1--HH12	1.008	0.86	89
CD2--HD2	1.078	0.93	199
CE1--HE1	1.078	0.93	199
CE2--HE2	1.078	0.93	159
NH1--HH11	1.009	0.86	89
ND2--HD21	1.009	0.86	109
NE2--HE22	1.009	0.86	99
CZ--HZ	1.079	0.93	49
NH2--HH22	1.009	0.86	89
NE2--HE21	1.008	0.86	99
NE--HE	1.009	0.86	89
CD1--HD1	1.078	0.93	159
NH2--HH21	1.009	0.86	89
CG--HG3	1.089	0.97	649
CA--HA	1.088	0.97	1659
CB--HB	1.088	0.97	149
CD--HD2	1.089	0.97	359
CB--HB2	1.088	0.97	1509
CD2--HD22	1.088	0.97	189
CE--HE1	1.088	0.97	59
CB--HB3	1.088	0.97	1509
CB--HB1	1.088	0.97	189
CG2--HG21	1.089	0.97	149
CA--HA2	1.089	0.97	179
CD2--HD21	1.088	0.97	189
CG--HG2	1.088	0.97	649

CA--HA3	1.089	0.97	179
CD--HD3	1.089	0.97	359
CD1--HD11	1.089	0.97	209
CD1--HD13	1.088	0.97	209
NZ--HZ3	1.009	0.89	49
CG1--HG12	1.089	0.97	79
CG2--HG22	1.088	0.97	149
N--H3	1.009	0.89	9
CG2--HG23	1.089	0.97	149
OG--HG	0.959	0.84	139
CE--HE2	1.089	0.97	109
CD1--HD12	1.089	0.97	209
CG1--HG11	1.089	0.97	59
NZ--HZ2	1.009	0.89	49
CG1--HG13	1.088	0.97	79
CD2--HD23	1.089	0.97	189
OG1--HG1	0.959	0.84	69
CE--HE3	1.089	0.97	109
NZ--HZ1	1.009	0.89	49
OH--HH	0.959	0.84	109
CG--HG	1.089	0.97	189
N--H2	1.009	0.89	9
N--H1	1.009	0.89	9

There are 316 angle outliers in this entry.

Angle type	*Observed angle (°)*	*Ideal angle (°)*	*Number of outliers*
C-N-H	112.269	124.3	122
HG2-CG-HG3	97.708	110	8

CG-CB-HB2	120.202	108	7
HD22-CD2-HD23	97.918	110	2
HG12-CG1-HG13	92.282	110	0
HB2-CB-HB3	97.993	110	31
HZ1-NZ-HZ3	122.371	109	2
CA-N-H	126.273	114	7
CB-OG1-HG1	93.037	110	0
CB-CA-HA	96.938	109	3
N-CA-HA	97.858	110	6
HD21-CD2-HD22	97.003	110	1
HB1-CB-HB2	96.99	110	5
CG-CB-HB3	95.827	108	7
HD2-CD-HD3	122.233	110	7
C-CA-HA	96.951	109	10
CE-NZ-HZ2	94.864	110	0
CA-CB-HB3	96.927	109	9
CA-CB-HB2	121.002	109	4
HD12-CD1-HD13	97.874	110	1
HD11-CD1-HD12	95.703	110	0
HG22-CG2-HG23	96.722	109	3
SD-CE-HE1	95.744	109	1
HG21-CG2-HG23	95.829	110	0
CB-CG-HG3	121.179	109	2
CB-CG1-HG11	122.984	109	0
CG-CD2-HD23	121.251	109	1
NZ-CE-HE2	121.714	108	0
HD21-CD2-HD23	96.708	110	1
N-CA-HA2	96.384	110	0

HE2-CE-HE3	96.468	110	0
CB-CG-HG2	121.139	109	2
CD-CG-HG2	121.262	108	0
CB-CG2-HG22	97.308	110	1
HG11-CG1-HG13	97.438	110	3
SD-CE-HE2	121.941	109	0
HE1-CE-HE3	97.073	110	0
CZ-CE2-HE2	107.364	120.2	0
HG11-CG1-HG12	97.195	110	0
CZ-OH-HH	122.334	110	1
HH21-NH2-HH22	107.333	120	0
HB1-CB-HB3	97.473	110	1
OG-CB-HB2	121.604	109	0
CD-CG-HG3	97.925	110	2
N-CD-HD3	121.548	109	0
CG-CD1-HD12	121.475	109	0
N-CD-HD2	121.456	109	0
CG-CD2-HD22	121.003	109	1
CD2-CG-HG	95.7	108	0
CZ-NH2-HH22	107.711	120	0
CG2-CB-HB	95.715	108	0
HZ2-NZ-HZ3	121.179	109	1
OG-CB-HB3	96.789	109	0
CB-CG2-HG23	121.082	109	1
CG-CD-HD3	121.18	109	0
HD11-CD1-HD13	97.867	110	0
C-CA-HA3	96.869	109	0
HA2-CA-HA3	96.936	109	1

CZ-NH1-HH11	107.88	120	0
CG-ND2-HD21	107.932	120	0
CA-CB-HB1	121.049	109	0
NZ-CE-HE3	120.023	108	0

7.2 Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	*Clash score*	*Number of clashes*
Model 1	0.00	0
Model 10	0.00	0
Model 2	0.00	0
Model 3	0.00	0
Model 4	0.00	0
Model 5	0.00	0
Model 6	0.00	0
Model 7	0.00	0
Model 8	0.00	0
Model 9	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

7.3 Torsion angles

7.3.1 Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation wasanalysed.

Model ID	*Analyzed*	*Favored*	*Allowed*	*Outliers*
1	182	147	32	3
2	182	150	28	4
3	182	169	10	3

4	182	154	26	2
5	182	161	14	7
6	182	153	23	6
7	182	159	19	4
8	182	153	23	6
9	182	156	19	7
10	182	155	23	4

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*
1	A:55	PRO
1	A:74	GLY
1	A:136	PRO
2	A:21	1ASN
2	A:35	1LEU
2	A:55	1PRO
2	A:129	1PRO
3	A:55	PRO
3	A:72	VAL
3	A:124	HIS
4	A:55	PRO
4	A:99	PRO
5	A:10	SER
5	A:11	GLY
5	A:14	LEU
5	A:55	PRO
5	A:76	THR
5	A:117	LEU

5	A:144	ALA
6	A:55	PRO
6	A:70	ALA
6	A:103	VAL
6	A:126	GLN
6	A:146	PRO
6	A:163	GLU
7	A:44	LEU
7	A:47	SER
7	A:55	PRO
7	A:110	LEU
8	A:32	LYS
8	A:55	PRO
8	A:79	PRO
8	A:86	ALA
8	A:90	GLY
8	A:144	ALA
9	A:55	PRO
9	A:57	GLY
9	A:69	ASN
9	A:70	ALA
9	A:88	ALA
9	A:96	GLY
9	A:126	GLN
10	A:42	VAL
10	A:55	PRO
10	A:57	GLY
10	A:141	VAL

7.3.2 Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	147	123	14	10
2	147	133	12	2
3	147	132	9	6
4	147	125	16	6
5	147	108	24	15
6	147	126	13	8
7	147	116	19	12
8	147	119	21	7
9	147	124	15	8
10	147	119	21	7

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:2	THR
1	A:18	ILE
1	A:26	LEU
1	A:72	VAL
1	A:109	MET
1	A:116	GLN
1	A:151	ARG
1	A:165	LEU
1	A:168	THR
1	A:184	TYR
2	A:106	SER
2	A:177	GLU

3	A:17	GLN
3	A:26	LEU
3	A:33	ILE
3	A:99	PRO
3	A:102	SER
3	A:140	THR
4	A:12	MET
4	A:51	VAL
4	A:91	SER
4	A:97	PHE
4	A:112	HIS
4	A:140	THR
5	A:14	LEU
5	A:39	LEU
5	A:42	VAL
5	A:43	TYR
5	A:60	TYR
5	A:97	PHE
5	A:103	VAL
5	A:117	LEU
5	A:120	PHE
5	A:135	GLU
5	A:154	SER
5	A:164	ARG
5	A:168	THR
5	A:169	ASN
5	A:181	GLU
6	A:4	THR

6	A:52	TYR
6	A:85	GLU
6	A:110	LEU
6	A:134	ASN
6	A:140	THR
6	A:165	LEU
6	A:177	GLU
7	A:1	MET
7	A:4	THR
7	A:31	LEU
7	A:35	LEU
7	A:45	ASP
7	A:91	SER
7	A:126	GLN
7	A:128	VAL
7	A:132	LEU
7	A:165	LEU
7	A:180	LYS
7	A:183	ARG
8	A:44	LEU
8	A:72	VAL
8	A:108	LEU
8	A:140	THR
8	A:143	GLU
8	A:159	GLN
8	A:168	THR
9	A:6	HIS
9	A:15	LEU

9	A:19	GLN
9	A:104	SER
9	A:126	GLN
9	A:127	GLN
9	A:174	MET
9	A:178	SER
10	A:35	LEU
10	A:39	LEU
10	A:42	VAL
10	A:78	LEU
10	A:100	LEU
10	A:129	PRO
10	A:176	MET

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model