Integrative Structure Validation Report

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	8ZZI
PDB-Dev ID	PDBDEV_00000018
Structure Title	The molecular architecture of the BBSome and its implications for facilitated transition zone crossing
Structure 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

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

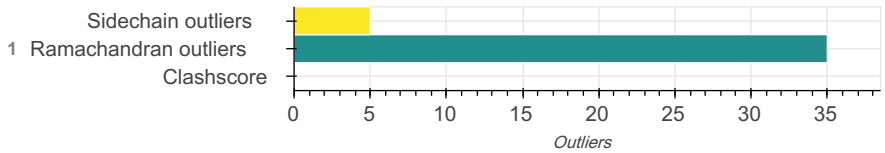
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information

This entry consists of 1 distinct ensemble(s).

Summary

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

Entry composition

There is 1 unique type of models in this entry. This model is titled None/Best scoring model.

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

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	File	10.5281/zenodo.1255360
2	De Novo model	File	10.5281/zenodo.1255360
3	De Novo model	File	10.5281/zenodo.1255360
4	Comparative model	File	10.5281/zenodo.1255360
5	De Novo model	File	10.5281/zenodo.1255360
6	De Novo model	File	10.5281/zenodo.1255360
7	De Novo model	File	10.5281/zenodo.1255360
8	De Novo model	File	10.5281/zenodo.1255360
9	Comparative model	File	10.5281/zenodo.1255360
10	Comparative model	File	10.5281/zenodo.1255360
11	Comparative model	File	10.5281/zenodo.1255360
12	Comparative model	File	10.5281/zenodo.1255360

ID	Dataset type	Database name	Data access code
13	De Novo model	File	10.5281/zenodo.1255360
14	De Novo model	File	10.5281/zenodo.1255360
15	De Novo model	File	10.5281/zenodo.1255360
16	De Novo model	File	10.5281/zenodo.1255360
17	Comparative model	File	10.5281/zenodo.1255360
18	Comparative model	File	10.5281/zenodo.1255360
19	Comparative model	File	10.5281/zenodo.1255360
20	De Novo model	File	10.5281/zenodo.1255360
21	De Novo model	File	10.5281/zenodo.1255360
22	De Novo model	File	10.5281/zenodo.1255360
23	De Novo model	File	10.5281/zenodo.1255360
24	De Novo model	File	10.5281/zenodo.1255360
25	3DEM volume	EMDB	EMD-7839
26	Crosslinking-MS data	File	10.5281/zenodo.1255360
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

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	-

Chain ID	Rigid bodies	Non-rigid segments
5	1-341:None	-
7	1-712:None	-
8	1-506:None	-
9	1-887:None	-
IP	1-96:None	-

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Monte Carlo	Production sampling	None	None	False	False
2	1	Rosetta Hybridize	Rosetta Hybridize	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Rosetta	Rosetta version unknown:839226a33c427862a8be7b4ca555493368c1485c 2017-09-18 10:39:53 -0700 from git@github.com:RosettaCommons/main.git	RosettaCM/hybridize, Rosetta Abinitio, and unpublished 'complex assembly'	https://www.rosettacommons.org/
2	HHpred	website	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred

Data quality

3DEM volume

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 27890 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--2HB	1.05	0.97	17
CD1--2HD1	1.05	0.97	3
CG--1HG	1.05	0.97	2
CG1--3HG1	1.05	0.97	1
CD2--2HD2	1.05	0.97	2
CB--1HB	1.05	0.97	19
CG2--3HG2	1.05	0.97	4
CG1--1HG1	1.05	0.97	6
CG2--1HG2	1.05	0.97	4
CG--HG	1.05	0.97	3
CB--HB	1.05	0.97	8
CD2--3HD2	1.05	0.97	5
CD1--3HD1	1.05	0.97	4
CG2--2HG2	1.05	0.97	2
N--1H	1.04	0.96	1
CB--3HB	1.05	0.97	1
CE--2HE	1.05	0.97	1
CG--2HG	1.05	0.97	1
CD--2HD	1.05	0.97	2
CD--1HD	1.05	0.97	1
CB--3HB	1.06	0.97	9
CB--1HB	1.06	0.97	53
CG1--2HG1	1.06	0.97	11
CA--HA	1.06	0.97	6
CD1--1HD1	1.06	0.97	8
CD1--2HD1	1.06	0.97	16
CD--2HD	1.06	0.97	7
CB--2HB	1.06	0.97	61

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--1HG1	1.06	0.97	11
CB--HB	1.06	0.97	26
CG2--3HG2	1.06	0.97	13
CG2--2HG2	1.06	0.97	19
CD1--3HD1	1.06	0.97	18
CD2--1HD2	1.06	0.97	7
CD2--2HD2	1.06	0.97	9
CD2--3HD2	1.06	0.97	6
CG--1HG	1.06	0.97	10
CG1--3HG1	1.06	0.97	6
CG--2HG	1.06	0.97	14
CG2--1HG2	1.06	0.97	7
CG--HG	1.06	0.97	12
CD--1HD	1.06	0.97	8
CE--2HE	1.06	0.97	1
CE--3HE	1.06	0.97	1
CD1--3HD1	1.07	0.97	44
CD1--2HD1	1.07	0.97	55
CB--1HB	1.07	0.97	184
CB--2HB	1.07	0.97	208
CB--3HB	1.07	0.97	28
CG1--2HG1	1.07	0.97	38
CG2--3HG2	1.07	0.97	43
CG2--2HG2	1.07	0.97	58
CD2--1HD2	1.07	0.97	23
CG--1HG	1.07	0.97	38
CA--HA	1.07	0.97	53
CD--2HD	1.07	0.97	17

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--2HD2	1.07	0.97	21
CB--HB	1.07	0.97	54
CG--HG	1.07	0.97	33
CG--2HG	1.07	0.97	24
CG2--1HG2	1.07	0.97	36
CG1--1HG1	1.07	0.97	39
CD2--3HD2	1.07	0.97	33
CA--1HA	1.07	0.97	7
CD1--1HD1	1.07	0.97	40
CG1--3HG1	1.07	0.97	20
CE--2HE	1.07	0.97	6
CE--3HE	1.07	0.97	4
CD--1HD	1.07	0.97	16
CE--1HE	1.07	0.97	7
CB--HB	1.08	0.97	184
CD1--2HD1	1.08	0.97	221
CB--2HB	1.08	0.97	600
CA--2HA	1.08	0.97	39
CD1--1HD1	1.08	0.97	162
CB--1HB	1.08	0.97	559
CG2--1HG2	1.08	0.97	197
CG--HG	1.08	0.97	132
CG--1HG	1.08	0.97	174
CG1--2HG1	1.08	0.97	113
CA--HA	1.08	0.97	618
CG2--2HG2	1.08	0.97	170
CD2--3HD2	1.08	0.97	190
CB--3HB	1.08	0.97	95

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--1HG1	1.08	0.97	110
CG2--3HG2	1.08	0.97	186
CD2--1HD2	1.08	0.97	102
CD2--2HD2	1.08	0.97	117
CG--2HG	1.08	0.97	177
CD--2HD	1.08	0.97	68
CG1--3HG1	1.08	0.97	68
CD1--3HD1	1.08	0.97	248
CD--1HD	1.08	0.97	67
CA--1HA	1.08	0.97	38
CE--1HE	1.08	0.97	39
CE--2HE	1.08	0.97	46
CE--3HE	1.08	0.97	18
NZ--3HZ	1.00	0.89	9
NZ--1HZ	1.00	0.89	7
OG--HG	0.95	0.84	2
OH--HH	0.95	0.84	2
NZ--2HZ	1.00	0.89	2
OG1--HG1	0.95	0.84	2
CD--2HD	1.09	0.97	332
CD--1HD	1.09	0.97	348
CD2--1HD2	1.09	0.97	309
CA--HA	1.09	0.97	2537
CB--1HB	1.09	0.97	1768
CG--1HG	1.09	0.97	635
CB--2HB	1.09	0.97	1699
CG2--1HG2	1.09	0.97	360
CD1--2HD1	1.09	0.97	330

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--3HD2	1.09	0.97	207
CE--1HE	1.09	0.97	250
CD1--1HD1	1.09	0.97	417
CG1--1HG1	1.09	0.97	256
CE--2HE	1.09	0.97	243
CG--2HG	1.09	0.97	643
CB--3HB	1.09	0.97	105
CB--HB	1.09	0.97	327
CG2--2HG2	1.09	0.97	352
CG--HG	1.09	0.97	259
CG1--2HG1	1.09	0.97	261
CA--2HA	1.09	0.97	173
CG2--3HG2	1.09	0.97	358
CD2--2HD2	1.09	0.97	292
CD1--3HD1	1.09	0.97	310
CG1--3HG1	1.09	0.97	143
NZ--1HZ	1.01	0.89	191
OH--HH	0.96	0.84	85
CE--3HE	1.09	0.97	53
NZ--3HZ	1.01	0.89	177
NZ--2HZ	1.01	0.89	172
CA--1HA	1.09	0.97	167
OG--HG	0.96	0.84	163
OG1--HG1	0.96	0.84	90
N--3H	1.01	0.89	16
N--1H	1.01	0.89	16
N--2H	1.01	0.89	16
CE2--HE2	1.05	0.93	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE1--HE1	1.05	0.93	1
CD2--HD2	1.05	0.93	1
CE3--HE3	1.05	0.93	1
OG1--HG1	0.97	0.84	71
OG--HG	0.97	0.84	45
NZ--3HZ	1.02	0.89	27
CA--HA	1.10	0.97	96
NZ--2HZ	1.02	0.89	33
CG--2HG	1.10	0.97	110
CB--1HB	1.10	0.97	105
CB--2HB	1.10	0.97	105
CD--2HD	1.10	0.97	65
CD1--1HD1	1.10	0.97	1
OH--HH	0.97	0.84	29
CG--1HG	1.10	0.97	111
CD2--HD2	1.06	0.93	8
SG--HG	1.33	1.20	34
CD--1HD	1.10	0.97	56
CD1--HD1	1.06	0.93	9
NZ--1HZ	1.02	0.89	16
CG--HG	1.10	0.97	1
CE1--HE1	1.06	0.93	2
ND2--1HD2	0.99	0.86	1
CE2--HE2	1.06	0.93	3
CZ--HZ	1.06	0.93	3
NE2--1HE2	0.99	0.86	1
CH2--HH2	1.06	0.93	1
ND2--2HD2	0.99	0.86	2

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--2HE2	0.99	0.86	3
OG--HG	0.98	0.84	18
NZ--2HZ	1.03	0.89	14
CE2--HE2	1.07	0.93	14
CD--2HD	1.11	0.97	5
NE2--1HE2	1.00	0.86	144
CG--1HG	1.11	0.97	1
NZ--1HZ	1.03	0.89	6
NZ--3HZ	1.03	0.89	8
CE1--HE1	1.07	0.93	13
OG1--HG1	0.98	0.84	15
CE3--HE3	1.07	0.93	4
CD1--HD1	1.07	0.93	21
ND2--2HD2	1.00	0.86	137
NE2--2HE2	1.00	0.86	115
OH--HH	0.98	0.84	10
CD2--HD2	1.07	0.93	19
CZ--HZ	1.07	0.93	10
ND2--1HD2	1.00	0.86	144
SG--HG	1.34	1.20	28
CB--1HB	1.11	0.97	1
ND1--HD1	1.00	0.86	36
CG--2HG	1.11	0.97	1
CZ3--HZ3	1.07	0.93	3
N--H	1.00	0.86	19
NH2--1HH2	1.00	0.86	2
NE1--HE1	1.00	0.86	4
NH2--2HH2	1.00	0.86	2

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH1--1HH1	1.00	0.86	4
NH1--2HH1	1.00	0.86	1
NE--HE	1.00	0.86	1
N--H	1.01	0.86	1769
ND1--HD1	1.01	0.86	17
CE1--HE1	1.08	0.93	65
CD2--HD2	1.08	0.93	79
ND2--1HD2	1.01	0.86	13
NH1--1HH1	1.01	0.86	105
NE2--2HE2	1.01	0.86	39
CE2--HE2	1.08	0.93	58
CD1--HD1	1.08	0.93	104
NE2--HE2	1.01	0.86	27
NH2--2HH2	1.01	0.86	111
OG1--HG1	0.99	0.84	4
NE2--1HE2	1.01	0.86	24
ND2--2HD2	1.01	0.86	21
NH1--2HH1	1.01	0.86	124
CZ--HZ	1.08	0.93	38
NE--HE	1.01	0.86	93
NH2--1HH2	1.01	0.86	98
CZ2--HZ2	1.08	0.93	6
SG--HG	1.35	1.20	8
CE3--HE3	1.08	0.93	8
NE1--HE1	1.01	0.86	19
CH2--HH2	1.08	0.93	5
CZ3--HZ3	1.08	0.93	5
OG--HG	0.99	0.84	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--1HZ	1.04	0.89	1
N--H	1.02	0.86	1583
CD1--HD1	1.09	0.93	174
CZ3--HZ3	1.09	0.93	22
NH1--1HH1	1.02	0.86	31
CE1--HE1	1.09	0.93	289
CE2--HE2	1.09	0.93	203
CZ--HZ	1.09	0.93	102
NE--HE	1.02	0.86	39
CD2--HD2	1.09	0.93	263
NH2--1HH2	1.02	0.86	36
ND2--1HD2	1.02	0.86	7
CE3--HE3	1.09	0.93	17
NH1--2HH1	1.02	0.86	13
NH2--2HH2	1.02	0.86	27
ND1--HD1	1.02	0.86	6
NE2--2HE2	1.02	0.86	22
CH2--HH2	1.09	0.93	24
NE2--1HE2	1.02	0.86	10
ND2--2HD2	1.02	0.86	5
CZ2--HZ2	1.09	0.93	24
NE1--HE1	1.02	0.86	5
NE2--HE2	1.02	0.86	4
NH2--1HH2	1.03	0.86	5
NH1--2HH1	1.03	0.86	3
CD1--HD1	1.10	0.93	1
N--H	1.03	0.86	1
NE--HE	1.03	0.86	8

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--2HH2	1.03	0.86	1
NE2--HE2	1.03	0.86	1
NE1--HE1	1.03	0.86	2
NH1--1HH1	1.03	0.86	1

Standard geometry: angle outliers

There are 14 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	156.46	1
C-N-CA	121.70	134.19	1
C-N-CA	121.70	134.06	1
C-N-CA	121.70	133.16	1
C-N-CA	121.70	131.64	1
C-N-CA	121.70	130.67	1
C-N-CA	121.70	130.59	1
CA-CB-CG	112.60	107.84	1
CA-CB-CG	113.80	118.56	1
CA-CB-CG	113.80	118.06	1
CA-CB-CG	113.80	117.88	1
C-N-CA	121.70	129.04	1
CA-N-H	78.89	114.00	1
C-N-H	77.58	124.30	1

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
1	0.00	0

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

Torsion angles: Protein backbone

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

Model ID	Analyzed	Favored	Allowed	Outliers

Model ID	Analyzed	Favored	Allowed	Outliers
1	3488	3257	196	35

Detailed list of outliers are tabulated below.

Torsion angles: 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	3068	3007	56	5

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	1	47	HIS
1	1	72	LYS
1	1	251	LEU
1	4	229	LEU
1	4	306	ILE

Fit of model to data used for modeling

3DEM volume

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

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