

Integrative Structure Validation Report ?

February 18, 2025 - 08:32 AM PST

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	9A1R
PDB-Dev ID	PDBDEV_00000099
Structure Title	INTEGRATIVE STRUCTURE OF BTG2 IN COMPLEX WITH RRM1-2 OF PABPC1
Structure Authors	Ameerul, A.; Almasmoum, H.; Pavanello, L.; Dominguez, C.; Winkler, G.S.
Deposited on	2022-03-15

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

We welcome your comments at helpdesk@pdb-ihm.org

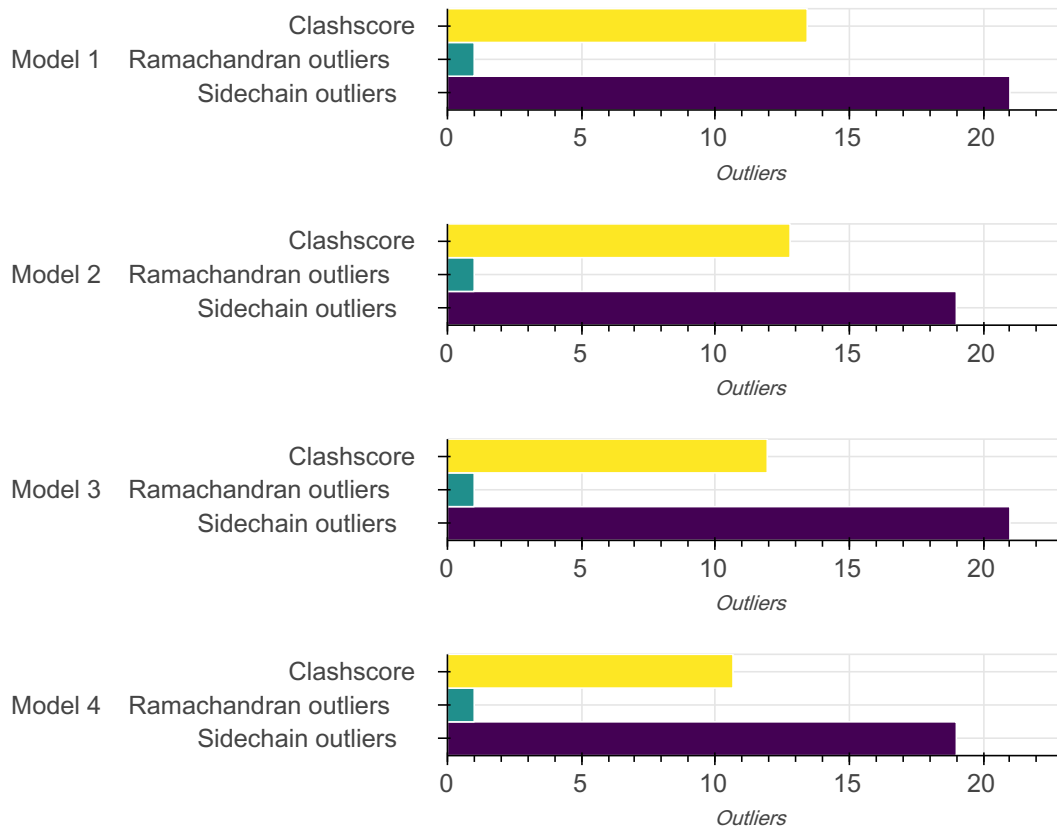
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 and fit to model assessments for SAS and crosslinking-MS 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 0 distinct ensemble(s).

Summary ?

This entry consists of 4 model(s). A total of 3 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1-4	1	POLY(A) BINDING PROTEIN CYTOPLASMIC 1	A	175	-	1-175	100.00 / 100.00	Atomic

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		2	PROTEIN BTG2	B	121	-	1-121	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	4F02
2	Experimental model	PDB	3DJU
3	NMR data	BMRB	50526

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	Rigid-body minimization	Rigid-body minimization in HADDOCK (it0)	None	1000	False	False
2	1	Simulated annealing	Semi-flexible SA in HADDOCK (it1)	None	200	False	False
3	1	Refinement	Water refinement in HADDOCK (itw)	None	200	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.40	Molecular docking	http://haddock.science.uu.nl/services/HADDOCK/

Data quality ?

NMR

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 no bond length outliers.

Standard geometry: angle outliers ?

There are no bond angle outliers.

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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	13.43	63
2	12.79	60
3	11.94	56
4	10.66	50

There are 229 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:104:SER:HB3	B:115:VAL:HG22	0.79	2	1
A:10:HIS:HB3	A:13:VAL:HG23	0.74	1	4
B:3:MET:HE1	B:45:LYS:HA	0.74	4	4
A:5:TYR:HD2	A:76:MET:HB2	0.74	4	4
A:15:GLU:HG2	A:33:VAL:HG23	0.71	2	2
B:39:ALA:HA	B:42:GLU:OE1	0.69	2	4
A:21:LYS:HG2	A:68:ILE:HD11	0.69	2	4
B:103:VAL:HB	B:117:TYR:HB3	0.67	3	2
A:91:ASN:HA	A:135:HIS:HA	0.66	1	4
A:60:LEU:O	A:64:ASN:HB2	0.66	2	4
B:106:ARG:HG3	B:113:ILE:HD13	0.64	3	1
B:106:ARG:NH2	B:109:GLU:HA	0.63	3	2
A:31:ILE:O	B:114:CYS:HA	0.62	2	3
A:40:ARG:HH22	B:118:GLU:HG2	0.62	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:106:ARG:NH1	B:109:GLU:HA	0.62	1	2
A:15:GLU:HG3	A:33:VAL:HG23	0.61	3	2
B:107:ILE:O	B:111:GLY:HA3	0.60	4	4
A:68:ILE:HD12	A:73:VAL:HG11	0.59	2	4
A:35:ARG:HG2	A:42:SER:HA	0.59	2	3
A:11:PRO:HA	A:42:SER:HB3	0.59	3	2
A:33:VAL:HG22	A:46:ALA:HB2	0.59	4	3
B:93:GLU:HB2	B:108:GLY:HA2	0.58	3	2
A:9:LEU:HD22	A:13:VAL:HG11	0.57	4	1
A:17:MET:SD	A:69:LYS:HD2	0.57	3	1
B:7:ILE:HG22	B:37:GLN:HG2	0.57	2	4
A:122:VAL:HG21	A:131:TYR:CE1	0.56	4	1
A:74:ARG:HD2	A:120:LYS:HB2	0.56	3	4
B:64:ILE:HD12	B:94:LEU:HD23	0.55	4	3
B:32:PHE:HB2	B:79:ILE:HD13	0.55	2	4
A:94:ILE:HG23	A:161:VAL:HG22	0.55	1	4
A:76:MET:SD	A:118:SER:HB2	0.55	4	4
A:140:GLU:CD	A:140:GLU:H	0.55	1	4
A:9:LEU:HD23	A:73:VAL:HG12	0.53	1	4
A:15:GLU:HG2	A:33:VAL:CG2	0.53	1	1
A:87:SER:HB2	A:89:VAL:HG23	0.52	2	4
B:68:MET:HE3	B:86:LEU:HB3	0.52	3	4
A:52:GLN:HB2	A:55:ASP:OD2	0.52	3	2
A:12:ASP:CB	A:69:LYS:HE2	0.52	2	1
A:3:SER:HB2	A:78:SER:HB2	0.52	3	3
A:144:ARG:HA	A:147:GLU:OE1	0.52	2	3
B:11:VAL:HG21	B:37:GLN:HG3	0.51	1	4
A:122:VAL:HG21	A:131:TYR:CE2	0.51	3	3
B:101:TYR:CZ	B:121:PRO:HA	0.51	4	2
B:93:GLU:HB3	B:108:GLY:HA2	0.50	2	1
B:94:LEU:HD13	B:107:ILE:HG12	0.50	4	2
A:122:VAL:HG21	A:131:TYR:CZ	0.50	4	4
B:75:VAL:HA	B:78:GLN:OE1	0.50	2	4
B:101:TYR:O	B:118:GLU:HA	0.49	1	3
B:28:ARG:HD2	B:79:ILE:O	0.49	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:140:GLU:HA	A:143:GLU:OE1	0.48	1	3
A:74:ARG:HD2	A:120:LYS:HD2	0.48	2	1
A:3:SER:HB2	A:78:SER:CB	0.48	3	3
A:12:ASP:HB3	A:69:LYS:HE2	0.48	2	1
A:36:ASP:O	A:40:ARG:HA	0.47	2	4
B:106:ARG:HH12	B:109:GLU:HA	0.47	1	1
A:22:PHE:HB3	A:50:PHE:CZ	0.47	1	1
B:36:LEU:O	B:40:LEU:HG	0.47	2	3
A:32:ARG:NH2	B:118:GLU:HG2	0.47	2	1
A:10:HIS:O	A:13:VAL:HB	0.47	3	1
B:76:ALA:HB1	B:81:LEU:HB2	0.47	3	4
A:97:LEU:HD23	A:159:VAL:HG11	0.46	2	3
A:140:GLU:O	A:144:ARG:HG3	0.46	4	4
B:93:GLU:CB	B:108:GLY:HA2	0.46	2	1
A:97:LEU:O	A:130:GLY:HA2	0.46	2	4
A:15:GLU:OE1	A:32:ARG:HA	0.46	1	1
A:19:TYR:HE1	B:111:GLY:HA2	0.46	1	1
A:27:PRO:HD2	A:55:ASP:OD2	0.46	3	3
B:49:PHE:O	B:100:PRO:HG2	0.46	1	3
A:92:ILE:HG23	A:142:ALA:HB1	0.45	2	3
A:23:SER:HB3	A:24:PRO:HD3	0.45	4	4
A:22:PHE:HB3	A:50:PHE:HZ	0.45	1	1
A:122:VAL:HG22	A:131:TYR:O	0.45	4	1
B:41:THR:O	B:45:LYS:HB2	0.45	2	3
A:15:GLU:CD	B:114:CYS:HB3	0.45	2	2
B:60:ARG:HH21	B:99:ASP:CG	0.45	3	3
B:106:ARG:HH21	B:109:GLU:HA	0.44	3	1
A:8:ASP:OD2	A:74:ARG:HD3	0.44	1	1
A:71:LYS:HB3	A:71:LYS:HE2	0.44	1	3
B:3:MET:HB3	B:48:TRP:CE2	0.44	4	2
A:37:MET:HB3	B:119:GLU:OE1	0.43	2	1
A:20:GLU:H	A:20:GLU:HG2	0.43	1	1
A:15:GLU:HG2	A:32:ARG:HA	0.43	4	1
B:38:GLU:O	B:42:GLU:HG3	0.43	4	1
B:11:VAL:HG13	B:36:LEU:HD23	0.43	1	3

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:120:ALA:HA	B:121:PRO:HD3	0.42	4	2
B:39:ALA:HB1	B:74:ARG:NH2	0.42	2	1
A:32:ARG:HG3	B:115:VAL:HB	0.42	3	1
A:10:HIS:ND1	A:12:ASP:HB2	0.42	4	1
A:123:CYS:HA	A:127:GLY:O	0.41	3	4
A:27:PRO:HB2	A:51:GLN:CD	0.41	4	1
A:52:GLN:HA	A:53:PRO:HD3	0.41	4	2
A:95:LYS:HB3	A:95:LYS:HE2	0.41	3	1
A:147:GLU:HG2	A:148:LYS:HG3	0.40	2	1
A:170:ARG:HH21	A:174:LEU:HD21	0.40	1	2
B:63:ARG:HD3	B:95:THR:HG23	0.40	1	1

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	Analysed	Favored	Allowed	Outliers
1	292	277	14	1
2	292	276	15	1
3	292	279	12	1
4	292	277	14	1

There are 1 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	78	SER	4

Torsion angles : Protein sidechains ?

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

Model ID	Analysed	Favored	Allowed	Outliers
1	255	205	29	21
2	255	204	32	19
3	255	204	30	21
4	255	203	33	19

There are 32 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	102	ASP	4

Chain	Res	Type	Models (Total)
A	138	THR	4
A	140	GLU	4
A	147	GLU	4
B	25	SER	4
B	30	LYS	4
B	41	THR	4
B	54	SER	4
B	92	SER	4
B	96	LEU	4
B	104	SER	4
A	62	THR	3
A	87	SER	3
A	171	GLU	3
B	102	GLU	3
B	116	LEU	3
A	32	ARG	2
B	18	LEU	2
B	19	ARG	2
B	95	THR	2
B	112	SER	2
A	8	ASP	1
A	12	ASP	1
A	14	THR	1
A	20	GLU	1
A	28	ILE	1
A	30	SER	1
A	94	ILE	1
B	20	THR	1
B	110	ASP	1
B	118	GLU	1
B	119	GLU	1

Fit of model to data used for modeling ?

NMR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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