

Integrative Structure Validation Report ?

March 27, 2025 - 10:02 AM PDT

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	9A0P
PDB-Dev ID	PDBDEV_00000061
Structure Title	Driving Integrative Structural Modeling with Serial Capture Affinity Purification
Structure Authors	Liu X; Zhang Y; Wen Z; Hao Y; Banks CAS; Lange JJ; Slaughter BD; Unruh JR; Florens L; Abmayr SM; Workman JL; Washburn MP
Deposited on	2020-09-08

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

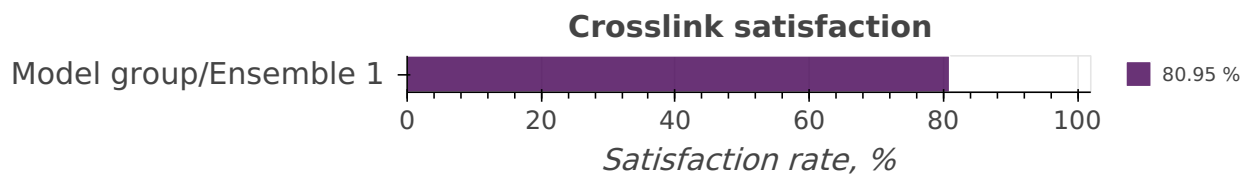
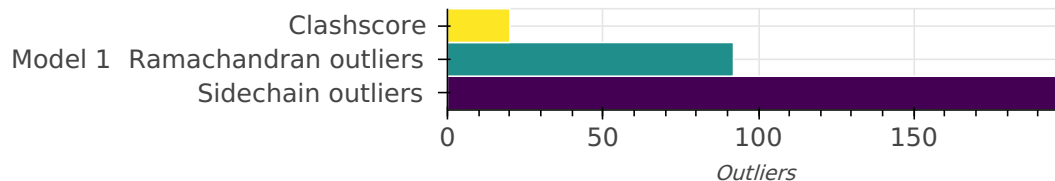
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 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	1	SPIN1	A	203	-	1-203	100.00 / 100.00	Atomic
		2	SPINDOC	B	381	-	1-381	100.00 / 100.00	Atomic
				C					

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	Crosslinking-MS data	MASSIVE	MSV000084719

ID	Dataset type	Database name	Data access code
2	Experimental model	PDB	4MZF
3	De Novo model	Not available	Not available

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	ab initio modeling of SPINDOC	None	None	None	False	False
2	1	integrative modeling of SPIN1-SPINDOC complex	None	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	Not available	model building	https://bianca.science.uu.nl/haddock2.4/
2	I-TASSER	Not available	model building	https://zhanglab.ccmb.med.umich.edu/I-TASSER/

Data quality ?

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

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 2 bond angle outliers in this entry (0.02% of 10351 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	312	ALA	C-CA-CB	4.77	117.65	110.50	1	1
B	312	ALA	C-CA-CB	4.62	117.43	110.50	1	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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	20.06	293

There are 293 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:329:ARG:HG3	B:332:GLU:HG3	0.92	1	1
C:329:ARG:HG3	C:332:GLU:HG3	0.92	1	1
A:148:LYS:HE2	C:208:GLU:HA	0.91	1	1
B:271:PRO:HB3	B:275:VAL:HB	0.90	1	1
C:271:PRO:HB3	C:275:VAL:HB	0.90	1	1
B:345:HIS:HB2	B:346:PRO:HA	0.88	1	1
B:126:SER:HA	B:129:LEU:HD23	0.88	1	1
C:345:HIS:HB2	C:346:PRO:HA	0.84	1	1
B:49:THR:HB	B:50:PRO:HD2	0.83	1	1
C:49:THR:HB	C:50:PRO:HD2	0.82	1	1
B:303:LEU:HB3	B:304:PRO:HD2	0.82	1	1
B:251:SER:HB2	B:252:PRO:HD3	0.79	1	1
B:167:ASP:HB3	B:171:MET:HB3	0.79	1	1
B:141:ASP:HA	B:175:ILE:HD11	0.78	1	1
C:251:SER:HB2	C:252:PRO:HD3	0.78	1	1
C:167:ASP:HB3	C:171:MET:HB3	0.78	1	1
C:141:ASP:HA	C:175:ILE:HD11	0.77	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
C:221:GLU:HB3	C:222:PRO:HD3	0.76	1	1
C:126:SER:HA	C:129:LEU:HD23	0.75	1	1
B:90:LEU:HG	B:97:GLU:HA	0.74	1	1
C:110:ILE:HG13	C:115:PRO:HD3	0.73	1	1
B:221:GLU:HB3	B:222:PRO:HD3	0.73	1	1
B:87:GLY:HA3	C:257:ALA:HA	0.71	1	1
C:312:ALA:HB3	C:313:PRO:HD3	0.71	1	1
B:312:ALA:HB3	B:313:PRO:HD3	0.68	1	1
C:155:GLY:HA2	C:159:HIS:HB2	0.68	1	1
B:155:GLY:HA2	B:159:HIS:HB2	0.68	1	1
C:312:ALA:CB	C:313:PRO:HD3	0.68	1	1
C:37:PRO:HB2	C:53:ARG:HA	0.67	1	1
B:77:PHE:HA	B:276:LEU:HD12	0.67	1	1
B:110:ILE:HG13	B:115:PRO:HD3	0.67	1	1
C:303:LEU:HB3	C:304:PRO:HD2	0.67	1	1
C:284:LEU:CB	C:323:LEU:HG	0.66	1	1
B:3:LEU:HG	B:4:LYS:HG2	0.66	1	1
C:90:LEU:HB2	C:276:LEU:HD13	0.66	1	1
B:37:PRO:HA	B:53:ARG:HG2	0.65	1	1
B:312:ALA:CB	B:313:PRO:HD3	0.65	1	1
C:90:LEU:HG	C:97:GLU:HG3	0.65	1	1
C:284:LEU:HB2	C:323:LEU:HG	0.65	1	1
B:222:PRO:N	B:223:PRO:HD2	0.64	1	1
C:184:ASN:N	C:185:PRO:HD3	0.64	1	1
C:37:PRO:HA	C:53:ARG:HG2	0.64	1	1
C:159:HIS:HB3	C:160:PRO:HA	0.64	1	1
B:37:PRO:HB2	B:53:ARG:HA	0.64	1	1
B:159:HIS:HB3	B:160:PRO:HA	0.64	1	1
A:53:TYR:HB2	A:56:PHE:HB2	0.64	1	1
B:184:ASN:N	B:185:PRO:HD3	0.64	1	1
C:197:ARG:NH1	C:228:VAL:HB	0.63	1	1
C:198:PRO:HB2	C:200:GLU:HG3	0.63	1	1
B:90:LEU:HB2	B:276:LEU:HD13	0.62	1	1
C:297:GLU:CD	C:297:GLU:H	0.62	1	1
C:288:ASP:OD1	C:290:LYS:HB3	0.62	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
C:18:LYS:HA	C:18:LYS:NZ	0.62	1	1
C:222:PRO:N	C:223:PRO:HD2	0.62	1	1
C:271:PRO:CB	C:275:VAL:HB	0.62	1	1
B:305:ARG:HD3	B:307:GLU:OE2	0.61	1	1
B:18:LYS:HA	B:18:LYS:NZ	0.61	1	1
B:336:VAL:O	B:355:GLY:HA3	0.61	1	1
B:49:THR:CB	B:50:PRO:HD2	0.60	1	1
C:313:PRO:HB2	C:314:PRO:HD2	0.60	1	1
C:344:ARG:HB2	C:356:ASP:OD2	0.60	1	1
A:63:GLU:OE1	A:66:LYS:HD2	0.59	1	1
C:275:VAL:HG11	C:284:LEU:HD21	0.59	1	1
C:143:ARG:HB3	C:143:ARG:NH1	0.58	1	1
C:132:TRP:CE3	C:132:TRP:HA	0.58	1	1
B:32:ALA:HB2	B:78:LEU:HD23	0.58	1	1
B:132:TRP:CE3	B:132:TRP:HA	0.57	1	1
C:3:LEU:HG	C:4:LYS:HG2	0.57	1	1
C:228:VAL:O	C:232:ARG:HB2	0.57	1	1
B:49:THR:HB	B:50:PRO:CD	0.57	1	1
B:296:ARG:HD2	B:300:GLU:OE2	0.57	1	1
A:95:ILE:HD12	A:119:ALA:HA	0.57	1	1
B:197:ARG:NH1	B:228:VAL:HB	0.57	1	1
B:37:PRO:HB2	B:54:PRO:HD2	0.57	1	1
B:228:VAL:O	B:232:ARG:HB2	0.57	1	1
B:262:VAL:HG23	B:335:ALA:HB2	0.57	1	1
C:374:LYS:N	C:375:PRO:HD2	0.57	1	1
A:1:GLY:HA2	A:65:ASN:OD1	0.57	1	1
C:37:PRO:HB2	C:54:PRO:HD2	0.56	1	1
A:39:LEU:HD11	A:52:LYS:HB2	0.56	1	1
C:31:VAL:HG12	C:115:PRO:HG3	0.56	1	1
B:374:LYS:N	B:375:PRO:HD2	0.56	1	1
C:279:PHE:O	C:280:SER:HB2	0.55	1	1
C:345:HIS:CB	C:346:PRO:HA	0.55	1	1
B:90:LEU:HD22	B:277:GLN:H	0.55	1	1
C:277:GLN:HG2	C:282:THR:OG1	0.55	1	1
C:336:VAL:O	C:355:GLY:HA3	0.55	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:288:ASP:OD1	B:290:LYS:HB3	0.55	1	1
A:52:LYS:NZ	A:57:ASP:HA	0.55	1	1
C:73:TRP:HB2	C:275:VAL:HG23	0.55	1	1
C:110:ILE:HA	C:114:HIS:HA	0.55	1	1
C:219:TRP:O	C:220:LYS:HD2	0.54	1	1
C:330:MET:HG2	C:331:GLU:H	0.54	1	1
B:192:ARG:O	B:194:ARG:HD3	0.54	1	1
C:174:GLU:HG3	C:176:VAL:H	0.54	1	1
C:349:THR:HB	C:351:ARG:HD3	0.54	1	1
C:49:THR:CB	C:50:PRO:HD2	0.54	1	1
A:21:GLN:NE2	A:76:LEU:HD11	0.53	1	1
A:148:LYS:HD3	C:207:THR:HB	0.53	1	1
A:167:GLU:CD	A:167:GLU:H	0.53	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	957	614	251	92

There are 92 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	6	HIS	1
A	27	GLY	1
A	30	PRO	1
A	86	SER	1
B	5	ALA	1
B	20	GLU	1
B	26	GLU	1
B	31	VAL	1
B	37	PRO	1
B	43	VAL	1
B	51	PRO	1
B	54	PRO	1
B	77	PHE	1
B	79	VAL	1

Chain	Res	Type	Models (Total)
B	92	MET	1
B	93	VAL	1
B	114	HIS	1
B	126	SER	1
B	141	ASP	1
B	144	ALA	1
B	161	ASP	1
B	162	PRO	1
B	166	PRO	1
B	172	PRO	1
B	179	LEU	1
B	202	PRO	1
B	217	GLN	1
B	218	ARG	1
B	221	GLU	1
B	247	PRO	1
B	251	SER	1
B	259	PRO	1
B	262	VAL	1
B	266	THR	1
B	268	GLY	1
B	270	PHE	1
B	275	VAL	1
B	280	SER	1
B	286	GLY	1
B	288	ASP	1
B	304	PRO	1
B	310	SER	1
B	312	ALA	1
B	328	VAL	1
B	336	VAL	1
B	346	PRO	1
B	354	ALA	1
B	358	SER	1
C	5	ALA	1

Chain	Res	Type	Models (Total)
C	20	GLU	1
C	26	GLU	1
C	31	VAL	1
C	37	PRO	1
C	43	VAL	1
C	51	PRO	1
C	54	PRO	1
C	77	PHE	1
C	79	VAL	1
C	92	MET	1
C	93	VAL	1
C	114	HIS	1
C	126	SER	1
C	141	ASP	1
C	144	ALA	1
C	161	ASP	1
C	162	PRO	1
C	166	PRO	1
C	172	PRO	1
C	179	LEU	1
C	201	LEU	1
C	202	PRO	1
C	206	ALA	1
C	207	THR	1
C	221	GLU	1
C	247	PRO	1
C	251	SER	1
C	259	PRO	1
C	262	VAL	1
C	268	GLY	1
C	270	PHE	1
C	275	VAL	1
C	280	SER	1
C	286	GLY	1
C	288	ASP	1

Chain	Res	Type	Models (Total)
C	294	LYS	1
C	304	PRO	1
C	312	ALA	1
C	313	PRO	1
C	328	VAL	1
C	346	PRO	1
C	354	ALA	1
C	358	SER	1

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	818	507	114	197

There are 197 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	5	HIS	1
A	6	HIS	1
A	9	HIS	1
A	11	SER	1
A	32	THR	1
A	37	THR	1
A	47	SER	1
A	58	CYS	1
A	71	SER	1
A	82	THR	1
A	83	SER	1
A	100	GLU	1
A	105	THR	1
A	110	LYS	1
A	120	ARG	1
A	126	THR	1
A	162	VAL	1
A	163	GLU	1

Chain	Res	Type	Models (Total)
A	167	GLU	1
A	168	ASP	1
A	173	THR	1
A	183	LYS	1
A	192	ASP	1
B	16	THR	1
B	18	LYS	1
B	25	GLU	1
B	27	GLU	1
B	30	VAL	1
B	33	VAL	1
B	36	ARG	1
B	42	ARG	1
B	43	VAL	1
B	44	THR	1
B	48	LYS	1
B	49	THR	1
B	66	GLU	1
B	68	LYS	1
B	69	GLN	1
B	70	GLN	1
B	71	VAL	1
B	74	GLU	1
B	76	GLU	1
B	77	PHE	1
B	79	VAL	1
B	81	SER	1
B	93	VAL	1
B	94	CYS	1
B	97	GLU	1
B	99	ARG	1
B	104	ASP	1
B	105	THR	1
B	109	HIS	1
B	110	ILE	1

Chain	Res	Type	Models (Total)
B	116	HIS	1
B	121	SER	1
B	126	SER	1
B	129	LEU	1
B	132	TRP	1
B	142	VAL	1
B	145	GLU	1
B	146	GLN	1
B	152	SER	1
B	170	ARG	1
B	171	MET	1
B	178	LEU	1
B	186	SER	1
B	187	LEU	1
B	190	ARG	1
B	191	SER	1
B	194	ARG	1
B	197	ARG	1
B	200	GLU	1
B	215	ARG	1
B	219	TRP	1
B	225	GLU	1
B	226	GLU	1
B	232	ARG	1
B	239	ASN	1
B	243	ASP	1
B	245	GLU	1
B	248	SER	1
B	250	ASP	1
B	253	THR	1
B	254	GLU	1
B	255	THR	1
B	262	VAL	1
B	265	PHE	1
B	266	THR	1

Chain	Res	Type	Models (Total)
B	269	SER	1
B	270	PHE	1
B	275	VAL	1
B	282	THR	1
B	289	SER	1
B	290	LYS	1
B	295	ASP	1
B	296	ARG	1
B	298	VAL	1
B	300	GLU	1
B	305	ARG	1
B	307	GLU	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*".

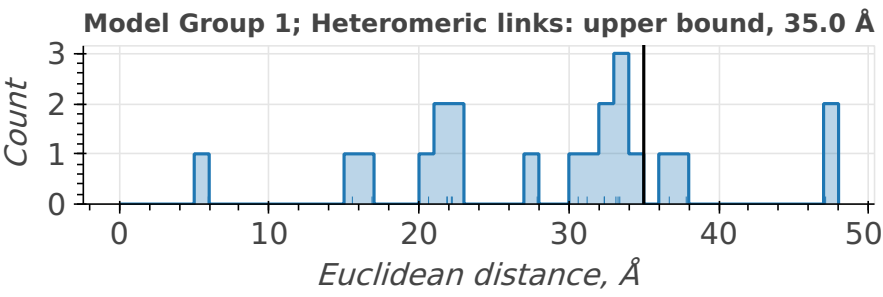
Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 21 crosslinking restraints combined in 21 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	CA	LYS	CA	upper bound	35.0	21

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



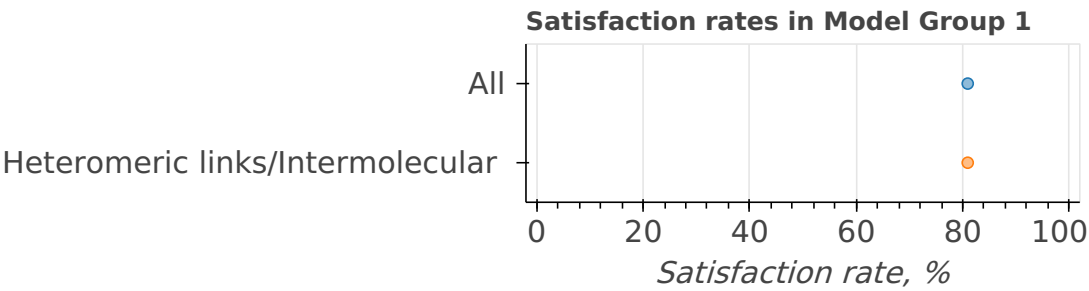
Satisfaction of restraints

Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=21)
1	1	1	1/1	All	80.95	19.05	21
				Heteromeric links/ Intermolecular	80.95	19.05	21

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



Fit of model to data used for validation ?

Validation for this section is under development.

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

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