

Integrative Structure Validation Report ?

February 18, 2025 - 08:38 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	9A3T
PDB-Dev ID	PDBDEV_00000214
Structure Title	Bovine adenylyl cyclase 8 in complex with the G protein heterodimer G beta gamma
Structure Authors	Schuster, D.; Khanppnavar, B.; Korkhov, V.M.
Deposited on	2023-06-06

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

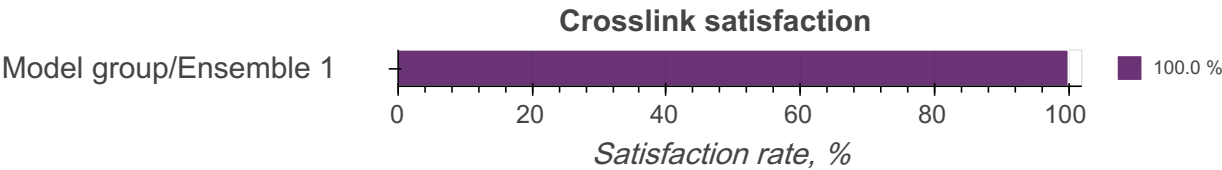
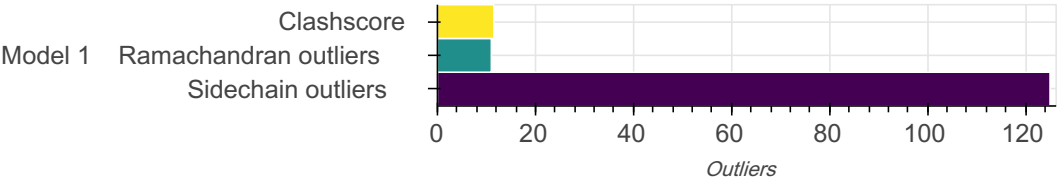
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	Adenylate cyclase type 8	A	890	-	1-890	100.00 / 100.00	Atomic
		2	Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1	B	339	-	1-339	100.00 / 100.00	Atomic
		3	Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2	C	46	-	1-46	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
3	Crosslinking-MS data	PRIDE	PXD040374
1	Experimental model	PDB	1XHM
2	Experimental model	PDB	8BUZ

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	Identification of crosslinked residues	Crosslinked residues were identified from the acquired mass spectrometry data based on the presence of heavy/light pairs of linked peptides.	None	None	False	False
2	1	Docking	Accessible interaction space was assessed with DisVis, solvent accessible residues were determined with GetArea. The information from these steps was used for docking with HADDOCK.	None	1	False	False

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	xQuest	2.1.5	crosslink identification	https://gitlab.ethz.ch/leitner_lab/xquest_xprophet
4	HADDOCK	2.40	docking	https://wenmr.science.uu.nl/haddock2.4/
2	DisVis	Not available	assessing of accessible interaction space	https://wenmr.science.uu.nl/disvis/
3	GetArea	Not available	calculation of solvent accessible surface area and residues	https://curie.utmb.edu/getarea.html

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 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	11.50	232

There are 232 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)
A:461:ASP:HB3	A:464:PHE:HB2	0.92	1	1
A:873:ASP:HA	A:882:GLY:HA2	0.85	1	1
B:293:CYS:HB2	B:307:LEU:HB2	0.82	1	1
A:875:ARG:HA	A:880:VAL:HA	0.78	1	1
B:50:LEU:HB2	B:335:LEU:HB2	0.78	1	1
A:814:ILE:HB	A:855:ILE:HG23	0.76	1	1
B:46:THR:HG21	B:336:LYS:HE2	0.74	1	1
A:424:GLU:HA	A:427:ILE:HG12	0.74	1	1
A:857:VAL:HG22	A:858:PRO:HD2	0.73	1	1
A:251:VAL:HG21	A:353:VAL:HG22	0.71	1	1
B:309:GLY:HA3	B:338:TRP:HH2	0.70	1	1
B:319:VAL:HG13	B:326:VAL:HG22	0.70	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:120:CYS:HB3	B:138:LEU:HB2	0.69	1	1
A:147:VAL:HG13	A:148:ILE:HG13	0.69	1	1
A:460:ARG:HD2	A:532:GLU:OE2	0.69	1	1
B:94:LEU:HD13	B:99:VAL:HG21	0.69	1	1
B:24:CYS:HA	C:23:LYS:HE3	0.67	1	1
A:792:SER:HB3	A:814:ILE:HG21	0.66	1	1
A:514:GLU:HA	A:524:ARG:HG2	0.64	1	1
A:50:LYS:HG2	A:102:TYR:HB3	0.64	1	1
B:50:LEU:HD23	B:86:THR:HG23	0.64	1	1
A:358:LEU:HD22	A:743:ASN:HB2	0.63	1	1
C:29:ALA:HA	C:32:MET:HE2	0.63	1	1
C:8:LYS:HD3	C:11:GLU:OE1	0.63	1	1
A:206:GLN:HG3	A:210:ARG:HH21	0.62	1	1
A:424:GLU:HA	A:427:ILE:CG1	0.62	1	1
B:24:CYS:HA	C:23:LYS:CE	0.62	1	1
A:279:GLU:OE2	A:283:ARG:HD2	0.61	1	1
A:34:LEU:HD23	A:104:LEU:HD22	0.61	1	1
A:516:TYR:HB3	A:519:LEU:HD23	0.60	1	1
B:191:LEU:HD23	B:198:PHE:HB3	0.60	1	1
A:582:LEU:HD22	A:650:LEU:HD13	0.60	1	1
B:70:VAL:HG12	B:80:ILE:HG12	0.60	1	1
A:309:LEU:HB3	A:310:PRO:HD3	0.59	1	1
A:409:LYS:HA	A:409:LYS:HE2	0.59	1	1
A:846:MET:HE1	A:858:PRO:HB3	0.59	1	1
A:530:ILE:HG21	A:540:ILE:HD12	0.59	1	1
A:112:VAL:HG21	A:141:GLN:HE21	0.58	1	1
A:339:LYS:HG3	A:340:HIS:H	0.58	1	1
A:694:PHE:HA	A:699:ARG:HG3	0.57	1	1
A:717:ALA:HA	A:813:ARG:O	0.57	1	1
B:165:CYS:HB2	B:179:PHE:HB2	0.57	1	1
A:405:GLU:O	A:420:ILE:HA	0.57	1	1
A:161:ALA:HB2	A:484:LEU:HD11	0.56	1	1
A:122:MET:HE1	A:645:TYR:HB3	0.56	1	1
B:250:ARG:HD3	B:259:GLU:OE1	0.56	1	1
A:435:LEU:HA	A:438:GLU:HB2	0.55	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:99:GLY:HA2	A:148:ILE:HD11	0.55	1	1
A:25:VAL:O	A:28:VAL:HG12	0.55	1	1
A:491:MET:HB2	A:492:PRO:HD3	0.55	1	1
A:71:ARG:HG2	A:79:TYR:HB2	0.55	1	1
A:53:LEU:HD13	A:97:ALA:HB1	0.55	1	1
A:346:ILE:HB	A:387:ILE:HG22	0.55	1	1
A:593:LEU:HB3	A:640:LEU:HD11	0.55	1	1
B:319:VAL:HG12	B:323:GLY:HA2	0.55	1	1
A:376:ASN:OD1	A:377:LYS:HE3	0.54	1	1
C:28:ALA:O	C:32:MET:HG3	0.54	1	1
A:19:SER:HB2	A:122:MET:HG2	0.54	1	1
A:817:SER:HB2	A:843:ALA:HB2	0.54	1	1
A:98:ALA:HA	A:102:TYR:O	0.54	1	1
B:293:CYS:SG	B:314:VAL:HG21	0.54	1	1
A:816:ILE:O	A:858:PRO:HD3	0.53	1	1
A:883:ILE:HG22	A:884:SER:H	0.53	1	1
B:230:ALA:HB2	B:274:SER:HA	0.53	1	1
B:232:CYS:SG	B:276:SER:HA	0.53	1	1
A:435:LEU:HD12	A:440:ILE:HG12	0.53	1	1
B:48:ARG:HD2	B:86:THR:OG1	0.53	1	1
A:537:ARG:O	A:541:ILE:HG12	0.52	1	1
A:331:ILE:O	A:335:ARG:HG2	0.52	1	1
A:11:TYR:O	A:15:GLN:HG2	0.52	1	1
A:635:LEU:HA	A:638:MET:HE2	0.52	1	1
B:288:TYR:HE1	B:294:ASN:HB2	0.52	1	1
A:109:ILE:HB	A:569:PHE:CZ	0.52	1	1
A:88:TRP:HA	A:91:MET:HE2	0.51	1	1
A:272:GLU:HG3	A:275:ARG:HH21	0.51	1	1
A:479:THR:HA	A:497:PHE:HE2	0.51	1	1
A:697:LYS:HG2	A:698:ASP:OD1	0.51	1	1
A:335:ARG:HH22	A:342:VAL:HG23	0.51	1	1
A:474:VAL:HG21	A:577:THR:HG22	0.51	1	1
A:3:ASP:HA	A:6:ARG:HH21	0.51	1	1
B:52:GLY:HA3	B:81:TRP:HH2	0.51	1	1
A:592:VAL:HG22	A:596:MET:HE2	0.51	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:209:LEU:HD22	B:254:LEU:HD22	0.51	1	1
B:73:SER:HB3	B:75:ASP:OD1	0.51	1	1
A:13:LEU:O	A:17:ARG:HB2	0.50	1	1
A:369:SER:O	A:372:VAL:HG22	0.50	1	1
B:47:ARG:HG3	B:339:ASN:OD1	0.50	1	1
B:24:CYS:SG	C:21:ARG:HB3	0.50	1	1
A:264:LEU:HA	A:267:THR:OG1	0.50	1	1
A:514:GLU:HB3	A:527:CYS:SG	0.50	1	1
A:378:LEU:HA	A:417:LYS:NZ	0.50	1	1
A:105:LEU:H	A:105:LEU:HD23	0.50	1	1
A:269:SER:HB3	A:272:GLU:OE1	0.50	1	1
A:275:ARG:HA	A:704:LEU:HD22	0.50	1	1
B:232:CYS:HB2	B:275:VAL:HG23	0.50	1	1
A:422:ARG:O	A:425:HIS:HB2	0.50	1	1
A:355:CYS:HB2	A:365:PHE:CZ	0.49	1	1
A:506:ALA:O	A:509:LEU:HG	0.49	1	1
A:467:ASN:HD21	A:581:PHE:HA	0.49	1	1
B:101:THR:HB	B:146:SER:O	0.49	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	1263	1161	91	11

There are 11 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	107	ASP	1
A	310	PRO	1
A	383	ILE	1
A	442	PRO	1
A	621	SER	1
A	733	ASN	1
A	858	PRO	1
A	873	ASP	1
A	878	ILE	1

Chain	Res	Type	Models (Total)
B	181	GLY	1
B	309	GLY	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	1099	820	154	125

There are 125 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	17	ARG	1
A	41	LEU	1
A	49	LEU	1
A	58	THR	1
A	72	LYS	1
A	128	THR	1
A	155	SER	1
A	168	CYS	1
A	171	THR	1
A	190	GLU	1
A	194	CYS	1
A	196	GLU	1
A	209	GLU	1
A	222	LEU	1
A	224	MET	1
A	229	THR	1
A	234	GLU	1
A	262	THR	1
A	265	SER	1
A	267	THR	1
A	268	LEU	1
A	278	ASN	1
A	299	LEU	1
A	343	ASP	1

Chain	Res	Type	Models (Total)
A	350	SER	1
A	352	SER	1
A	369	SER	1
A	390	SER	1
A	393	THR	1
A	397	LEU	1
A	407	HIS	1
A	413	GLU	1
A	422	ARG	1
A	431	SER	1
A	433	ASP	1
A	434	LYS	1
A	437	ARG	1
A	446	MET	1
A	450	SER	1
A	451	SER	1
A	453	GLU	1
A	468	LEU	1
A	484	LEU	1
A	485	LEU	1
A	498	SER	1
A	500	LEU	1
A	515	ASP	1
A	526	THR	1
A	532	GLU	1
A	544	SER	1
A	550	LEU	1
A	562	SER	1
A	565	GLU	1
A	576	VAL	1
A	586	SER	1
A	605	GLU	1
A	616	ASP	1
A	618	LEU	1
A	620	HIS	1

Chain	Res	Type	Models (Total)
A	656	LEU	1
A	657	ASP	1
A	678	ASN	1
A	688	SER	1
A	700	ASP	1
A	724	ASP	1
A	727	SER	1
A	733	ASN	1
A	755	GLU	1
A	756	ASP	1
A	760	ASP	1
A	762	GLU	1
A	765	LYS	1
A	769	SER	1
A	775	SER	1
A	792	SER	1
A	797	GLU	1
A	803	ASN	1
A	806	SER	1
A	820	SER	1
A	852	SER	1
A	856	GLN	1
A	857	VAL	1
A	861	THR	1
A	865	LEU	1
A	883	ILE	1
B	8	GLN	1
B	30	SER	1
B	37	ASP	1
B	51	ARG	1
B	64	THR	1
B	69	LEU	1
B	97	SER	1
B	125	LEU	1
B	126	LYS	1

Chain	Res	Type	Models (Total)
B	127	THR	1
B	128	ARG	1
B	135	SER	1
B	142	THR	1
B	145	LEU	1
B	146	SER	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

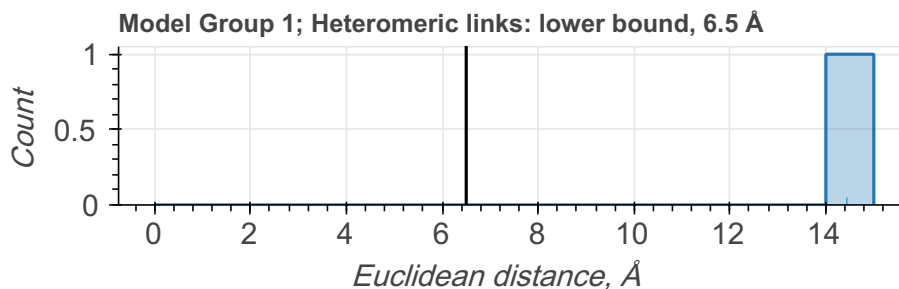
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

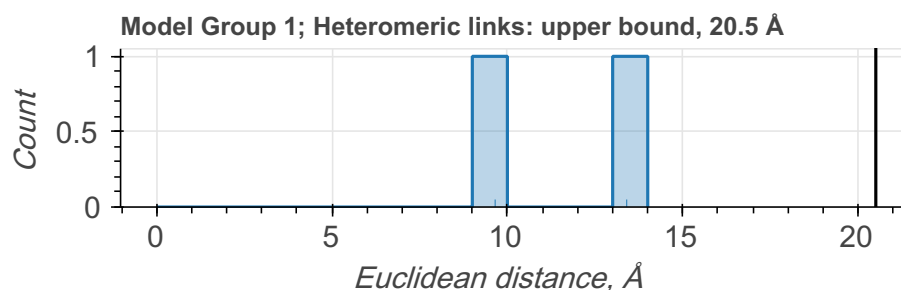
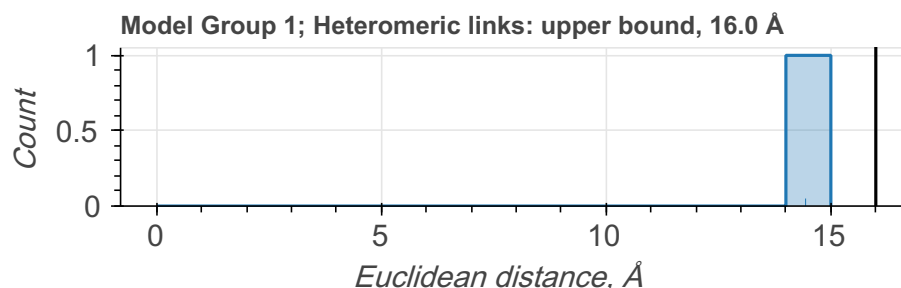
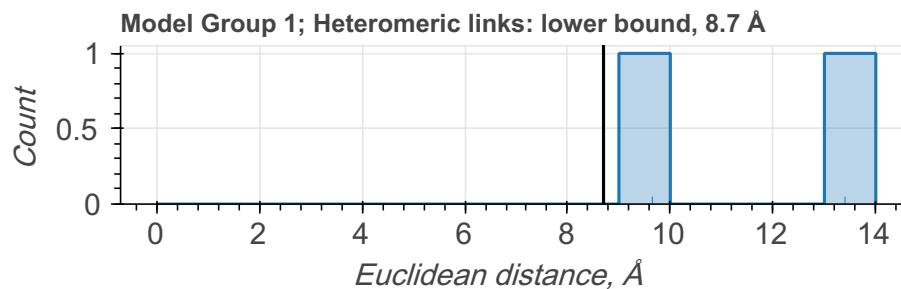
There are 6 crosslinking restraints combined in 3 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
PDH	ASP	CA	ASP	CA	upper bound	20.5	1
PDH	ASP	CA	GLU	CA	upper bound	20.5	1
PDH	ASP	CA	ASP	CA	lower bound	8.7	1
PDH	ASP	CA	GLU	CA	lower bound	8.7	1
DMTMM	ASP	CA	LYS	CA	upper bound	16.0	1
DMTMM	ASP	CA	LYS	CA	lower bound	6.5	1

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.





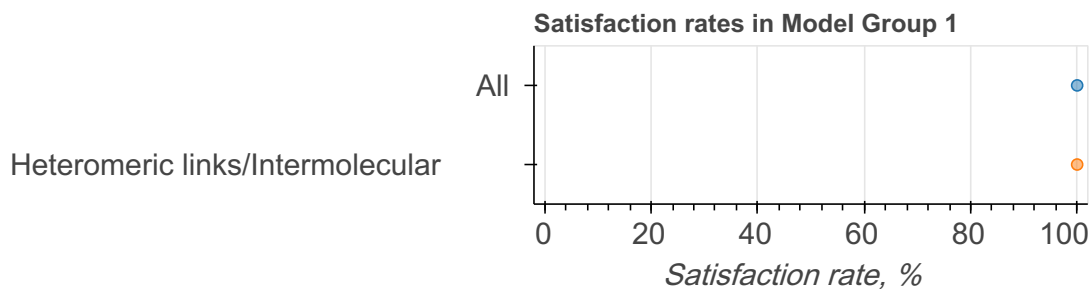
Satisfaction of restraints

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=3)
1	1	1	1/1	All	100.00	0.00	3
				Heteromeric links/ Intermolecular	100.00	0.00	3

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.

Acknowledgments

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.

Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.