

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	9A3Z
PDB-Dev ID	PDBDEV_00000220
Structure Title	A predicted model of tissue transglutaminase 2 (TG2) in complex with plasma fibronectin's gelatin binding domain (FNI6FNII1-2FNI7-9).
Structure Authors	Selcuk, K.; Leitner, A.; Le Blanc, F.
Deposited on	2023-10-04

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

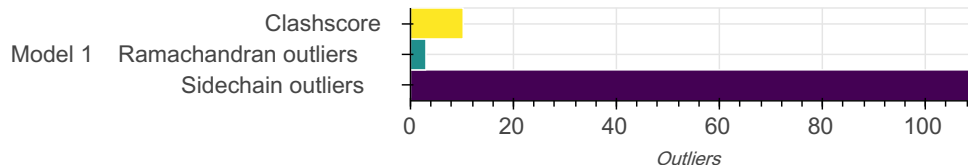
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

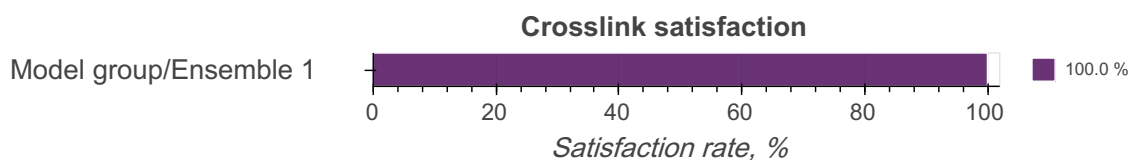
List of references used to build this report is available [here](#).

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 4 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	Protein-glutamine gamma-glutamyltransferase 2	A	687	-	1-687	100.00 / 100.00	Atomic
		2	Fibronectin	B	297	-	1-297	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD043976
2	Experimental model	PDB	4PYG
3	De Novo model	Not available	Not available
4	Experimental model	PDB	3EJH

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	Refinement	Iterative Threading ASSEmbly Refinement	structural refinement of starting models guided by experimental crosslinks	None	False	False
2	1	structure prediction	AI prediction of protein 3D structure from its amino acid sequence	structure prediction of fibronectin's gelatin binding domain	None	False	False
3	1	satisfied/violated crosslinks identification	Validate measured chemical crosslinks on a protein 3D structure	calculation of Euclidean distances between crosslinked residues	None	False	False
4	1	calculation of accessible area	calculates the atomic accessible area when a probe is rolled around the Van der Waal's surface of a macromolecule	calculation of accessible area	None	False	False
5	1	quality assessment	composite scoring function which is able to derive both global (i.e. for the entire structure) and local (i.e. per residue) absolute quality estimates on the basis of one single model	None	None	False	False
6	1	accessible interaction space	None	determine the number of complexes consistent with the restraints	None	False	False
7	1	docking	data-driven biomolecular docking	generates predicted model of a protein complex	None	False	False

There are 7 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	I-TASSER	Not available	structure refinement	https://zhanggroup.org/I-TASSER/
2	AlphaFold2	Not available	structure prediction	https://colab.research.google.com/github/sokrypton/ColabFold/blob/main/AlphaFold2.ipynb

ID	Software name	Software version	Software classification	Software location
3	Xwalk	Not available	calculation of Euclidean distances	https://www.xwalk.org/home.cgi
4	NACCESS	Not available	solvent accessibility	http://www.bioinf.manchester.ac.uk/naccess/
5	QMEAN	Not available	Estimation of the quality of protein structure models	https://swissmodel.expasy.org/qmean/
6	DisVis	Not available	accessible interaction space	https://wenmr.science.uu.nl/disvis/
7	HADDOCK	Not available	protein-protein docking	https://wenmr.science.uu.nl/haddock2.4/

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	10.24	156

There are 156 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:87:ASP:HA	A:107:PRO:HB3	0.90	1	1
A:155:GLU:HG2	A:431:VAL:HG21	0.82	1	1
A:328:SER:HB3	A:519:ILE:HA	0.79	1	1
A:298:VAL:HG21	A:439:ILE:HD11	0.77	1	1
A:298:VAL:HG23	A:428:THR:HB	0.75	1	1
A:343:THR:HA	A:352:GLU:HG3	0.73	1	1
A:509:LEU:HB2	A:527:LYS:HB2	0.71	1	1
A:624:VAL:HG12	A:666:VAL:HG12	0.70	1	1
A:57:LEU:HD11	A:119:LEU:HD12	0.68	1	1
B:223:THR:HG23	B:237:THR:HG23	0.66	1	1
A:668:PHE:HB3	A:676:VAL:HB	0.66	1	1
A:11:ASP:HB3	A:42:THR:HB	0.64	1	1
A:311:LEU:HD13	A:395:ALA:HA	0.64	1	1
A:344:ARG:HB3	A:347:LEU:HB2	0.64	1	1
A:460:ASN:HA	A:463:ASN:HB2	0.64	1	1
B:69:THR:HG23	B:77:LEU:HD23	0.64	1	1
A:298:VAL:HG22	A:426:ILE:HG22	0.63	1	1
B:157:ALA:HB3	B:160:GLU:HG3	0.62	1	1
A:426:ILE:HG13	A:440:THR:HG23	0.62	1	1
A:567:LEU:HB3	A:576:LEU:HB2	0.62	1	1
A:512:ARG:HB3	A:523:GLU:HA	0.61	1	1
A:500:ALA:HA	A:536:PRO:HB3	0.61	1	1
A:589:ILE:HA	A:609:LEU:HD13	0.60	1	1
A:491:VAL:HB	A:544:LEU:HB2	0.59	1	1
A:213:ARG:HA	A:213:ARG:NE	0.58	1	1
A:179:PRO:HG3	A:679:PHE:HB3	0.58	1	1
A:277:CYS:HA	A:280:PHE:CD2	0.57	1	1
A:599:GLN:HG3	A:600:LYS:HG2	0.57	1	1
A:63:THR:HG23	A:73:THR:HG22	0.57	1	1
A:229:ASN:HD21	A:361:PRO:HG3	0.57	1	1
B:127:CYS:HB3	B:137:LYS:HB3	0.57	1	1
A:587:PRO:HD2	A:673:LEU:HD21	0.56	1	1
B:240:GLY:HA2	B:244:GLY:HA2	0.56	1	1
A:240:ARG:HD3	A:274:TYR:CE1	0.56	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:294:PRO:HB2	A:341:TRP:HB3	0.56	1	1
A:196:LEU:HD12	A:227:MET:HB3	0.56	1	1
A:598:LYS:HB3	A:601:ARG:HD2	0.56	1	1
A:26:LEU:HD22	A:185:PHE:HA	0.56	1	1
B:187:MET:HG2	B:203:ALA:HA	0.56	1	1
A:8:GLU:HG3	A:46:GLU:HA	0.55	1	1
B:278:TYR:HB3	B:292:CYS:HB3	0.55	1	1
A:623:THR:HB	A:635:THR:HG23	0.55	1	1
B:2:VAL:HG22	B:8:VAL:HG22	0.55	1	1
B:205:SER:HA	B:210:GLN:HB2	0.55	1	1
A:559:ASN:CB	A:584:LEU:HB2	0.54	1	1
A:445:TYR:HB2	A:452:GLU:HB3	0.54	1	1
B:99:VAL:HB	B:115:PHE:HD2	0.53	1	1
A:497:ASN:O	A:537:PHE:HA	0.53	1	1
B:254:CYS:HB3	B:290:TRP:CD1	0.53	1	1
A:116:ARG:HD2	A:134:HIS:HB3	0.52	1	1
A:548:TYR:HA	A:551:TYR:CE2	0.52	1	1
A:61:VAL:O	A:74:LYS:HA	0.51	1	1
A:201:PRO:HA	B:176:GLN:NE2	0.51	1	1
A:213:ARG:HA	A:213:ARG:HE	0.51	1	1
A:203:PHE:HD1	A:210:ASP:HB3	0.51	1	1
B:280:CYS:HA	B:292:CYS:HA	0.51	1	1
B:176:GLN:HG2	B:190:THR:HG23	0.51	1	1
A:4:GLU:HB3	A:123:THR:HG21	0.51	1	1
B:172:ARG:O	B:175:ASP:HB2	0.51	1	1
A:240:ARG:HD3	A:274:TYR:HE1	0.51	1	1
A:374:VAL:HG21	A:393:VAL:HG21	0.51	1	1
B:25:LEU:HD23	B:36:GLN:HE21	0.50	1	1
A:69:GLN:H	A:69:GLN:NE2	0.50	1	1
B:236:CYS:HA	B:248:CYS:HA	0.50	1	1
B:53:CYS:HA	B:81:THR:HA	0.49	1	1
A:243:ASN:HB2	A:556:THR:HG23	0.49	1	1
A:315:TYR:HE1	A:323:ILE:HG13	0.49	1	1
B:189:CYS:HA	B:201:CYS:HA	0.49	1	1
A:559:ASN:HB3	A:584:LEU:HB2	0.49	1	1
A:280:PHE:HB3	A:359:PRO:HG2	0.49	1	1
A:612:PRO:HD2	A:613:LEU:HD12	0.49	1	1
A:611:ASN:OD1	A:644:ALA:HA	0.49	1	1
A:298:VAL:CG2	A:426:ILE:HG22	0.49	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:183:MET:HE3	B:185:HIS:HE1	0.49	1	1
A:305:HIS:HB3	A:329:GLU:HB3	0.48	1	1
B:163:CYS:O	B:170:MET:HA	0.48	1	1
A:618:GLU:HG2	A:641:PRO:HB3	0.48	1	1
A:68:SER:HB2	A:71:ALA:HB3	0.47	1	1
A:606:GLU:HB3	A:651:ARG:HG3	0.47	1	1
A:84:GLU:CD	A:84:GLU:H	0.47	1	1
A:251:PRO:HB3	A:275:GLY:HA2	0.47	1	1
A:12:LEU:HB3	A:31:LEU:HD22	0.47	1	1
B:72:ARG:HG3	B:78:TRP:CD1	0.47	1	1
A:447:GLU:CD	A:447:GLU:H	0.47	1	1
A:313:ILE:HD12	A:330:MET:HG2	0.46	1	1
A:384:LEU:HG	A:391:PRO:HG3	0.46	1	1
A:384:LEU:HD13	A:459:ALA:HB1	0.46	1	1
A:499:THR:HG21	A:503:TYR:CE1	0.46	1	1
A:61:VAL:HB	A:115:TYR:HD2	0.46	1	1
B:148:ASP:HB3	B:150:LYS:HG2	0.46	1	1
A:608:SER:HA	A:648:VAL:O	0.46	1	1
A:251:PRO:HD3	A:274:TYR:HB3	0.46	1	1
A:276:GLN:O	A:279:VAL:HG22	0.46	1	1
A:569:GLU:OE1	A:571:VAL:HG13	0.45	1	1
A:344:ARG:CB	A:347:LEU:HB2	0.45	1	1
A:447:GLU:HA	A:452:GLU:CD	0.45	1	1
B:43:THR:HA	B:93:PHE:O	0.45	1	1
A:158:GLU:HA	A:162:THR:OG1	0.45	1	1
A:512:ARG:CB	A:523:GLU:HA	0.45	1	1
A:224:VAL:O	A:228:VAL:HG23	0.45	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	980	897	80	3

There are 3 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	108	ALA	1
A	525	GLY	1
A	632	GLU	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	855	623	123	109

There are 109 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	7	LEU	1
A	13	GLU	1
A	26	LEU	1
A	29	GLU	1
A	42	THR	1
A	58	THR	1
A	68	SER	1
A	73	THR	1
A	84	GLU	1
A	89	THR	1
A	96	GLN	1
A	98	CYS	1
A	99	THR	1
A	100	LEU	1
A	106	THR	1
A	112	ILE	1
A	114	LEU	1
A	123	THR	1
A	129	SER	1
A	150	LEU	1
A	166	PHE	1
A	184	GLN	1
A	186	GLU	1
A	204	LEU	1
A	205	LYS	1
A	211	CYS	1
A	215	SER	1
A	223	VAL	1
A	225	SER	1
A	232	ASP	1
A	234	GLN	1
A	238	LEU	1

Chain	Res	Type	Models (Total)
A	255	ILE	1
A	257	SER	1
A	271	ARG	1
A	278	TRP	1
A	307	GLN	1
A	312	LEU	1
A	313	ILE	1
A	314	GLU	1
A	324	GLN	1
A	326	ASP	1
A	344	ARG	1
A	347	LEU	1
A	362	GLN	1
A	364	LYS	1
A	384	LEU	1
A	398	ASN	1
A	400	ASP	1
A	403	ASP	1
A	414	LYS	1
A	440	THR	1
A	441	HIS	1
A	442	THR	1
A	447	GLU	1
A	468	LYS	1
A	478	ARG	1
A	483	MET	1
A	485	MET	1
A	490	ASP	1
A	491	VAL	1
A	496	THR	1
A	507	LEU	1
A	526	THR	1
A	529	LEU	1
A	532	LEU	1
A	533	ASN	1
A	534	LEU	1
A	552	ARG	1
A	556	THR	1
A	557	GLU	1

Chain	Res	Type	Models (Total)
A	564	ARG	1
A	569	GLU	1
A	571	VAL	1
A	577	LEU	1
A	580	ARG	1
A	588	GLU	1
A	592	ARG	1
A	632	GLU	1
A	637	GLU	1
A	640	ASP	1
A	646	GLU	1
A	658	HIS	1
A	659	MET	1
B	5	SER	1
B	36	GLN	1
B	41	THR	1
B	53	CYS	1
B	63	THR	1
B	69	THR	1
B	82	THR	1
B	83	SER	1
B	95	THR	1
B	98	THR	1
B	122	HIS	1
B	125	THR	1
B	141	THR	1
B	142	THR	1
B	146	ASP	1
B	164	THR	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

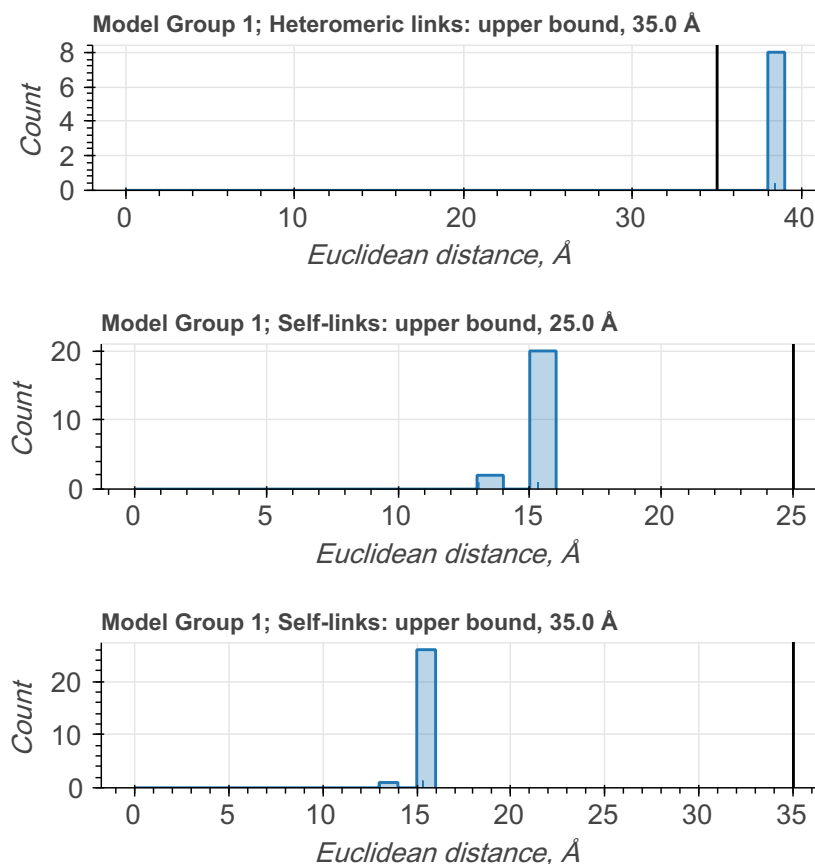
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". **Restraint group** represents a set of crosslinking restraints applied collectively in the modeling.

There are 57 crosslinking restraints combined in 1 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DMTMM	GLU	CA	LYS	CA	upper bound	25.0	22
DMTMM	GLU	CA	LYS	CA	upper bound	35.0	35

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.



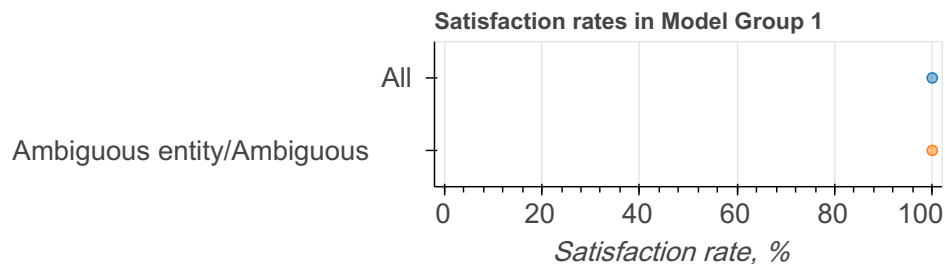
Satisfaction of restraints

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=1)
1	1	1	1/1	All	100.00	0.00	1
				Ambiguous entity/ Ambiguous	100.00	0.00	1

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.