

# Integrative Structure Validation Report ?

July 22, 2024 - 05:29 PM PDT

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

*Python-IHM* Version 1.3

*MolProbit* Version 4.5.2

*Integrative Modeling Validation* Version 1.2

PDB ID	9A3X
PDB-Dev ID	PDBDEV_00000218
Structure Title	Predicted model of tissue transglutaminase 2 (TG2) in complex with plasma fibronectin type I modules 2 and 3 (FNI2-3)
Structure Authors	Selcuk, K.; Leitner, A.; Le Blanc, F.

*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](mailto:pdb-dev@mail.wwpdb.org)

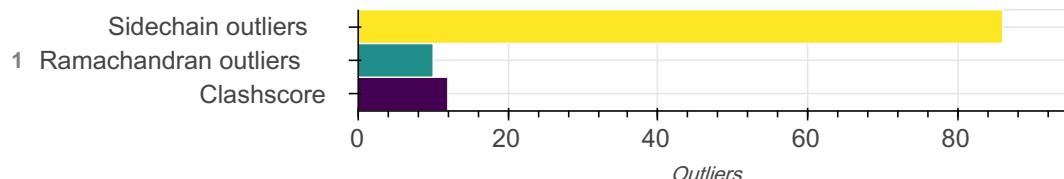
A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the ? symbol.

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: MolProbit Analysis



## Ensemble information ?

This entry consists of 0 distinct ensemble(s).

## Summary ?

This entry consists of 1 unique models, with 2 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 2 flexible or non-rigid units.

## Entry composition ?

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Protein-glutamine gamma-glutamyltransferase 2	A	A	687
1	2	2	Fibronectin	B	B	90

## 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	PRIDE	PXD043976
2	Experimental model	PDB	4PYG
3	Experimental model	PDB	2CG7

## Representation ?

This entry has only one representation and includes 0 rigid bodies and 2 flexible units

Chain ID	Rigid bodies	Non-rigid segments
B	-	1-90
A	-	1-687

## 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	Iterative Threading ASSEmble Refinement	Refinement	structural refinement of starting models guided by experimental crosslinks	None	False	False
2	1	Validate measured chemical cross-links on a protein 3D structure	satisfied/violated crosslinks identification	calculation of Euclidean distances between crosslinked residues	None	False	False
3	1	calculates the atomic accessible area when a probe is rolled around the Van der Waal's surface of a macromolecule	calculation of accessible area	calculation of accessible area	None	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
4	1	None	accessible interaction space	determine the number of complexes consistent with the restraints	None	False	False
5	1	data-driven biomolecular docking	docking	generates predicted model of a protein complex	None	False	False

There are 5 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	I-TASSER	Not available	structure refinement	<a href="https://zhanggroup.org/I-TASSER/">https://zhanggroup.org/I-TASSER/</a>
3	Xwalk	Not available	Euclidean distances calculation	<a href="https://www.xwalk.org/home.cgi">https://www.xwalk.org/home.cgi</a>
2	NACCESS	Not available	solvent accessibility	<a href="http://www.bioinf.manchester.ac.uk/naccess/">http://www.bioinf.manchester.ac.uk/naccess/</a>
4	DisVis	Not available	accessible interaction space	<a href="https://wenmr.science.uu.nl/disvis/">https://wenmr.science.uu.nl/disvis/</a>
5	HADDOCK	Not available	protein-protein docking	<a href="https://wenmr.science.uu.nl/haddock2.4/">https://wenmr.science.uu.nl/haddock2.4/</a>

## Data quality ?

### 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 1375 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
NE2--HE22	0.98	0.86	26
N--H	0.98	0.86	665
ND2--HD21	0.98	0.86	34
ND2--HD22	0.98	0.86	33
NE2--HE21	0.98	0.86	22
NE1--HE1	0.98	0.86	10
NE2--HE2	0.98	0.86	11
ND1--HD1	0.98	0.86	3
NE--HE	0.98	0.86	21
OG--HG	0.96	0.84	19
OH--HH	0.96	0.84	6
OG1--HG1	0.96	0.84	20
SG--HG	1.32	1.20	2
N--H	0.99	0.86	75
OG--HG	0.97	0.84	24
NE1--HE1	0.99	0.86	6
OH--HH	0.97	0.84	18
SG--HG	1.33	1.20	18
NE--HE	0.99	0.86	23
ND2--HD22	0.99	0.86	5
OG1--HG1	0.97	0.84	21
NE2--HE2	0.99	0.86	2

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE21	0.99	0.86	4
ND2--HD21	0.99	0.86	4
NE--HE	1.00	0.86	2
OG1--HG1	0.98	0.84	2
OH--HH	0.98	0.84	4
NH2--HH21	1.00	0.86	22
NH2--HH22	1.00	0.86	28
NH1--HH12	1.00	0.86	32
NH1--HH11	1.00	0.86	30
NH1--HH11	1.01	0.86	16
NH2--HH22	1.01	0.86	15
NZ--HZ3	1.04	0.89	28
NH1--HH12	1.01	0.86	14
NH2--HH21	1.01	0.86	21
NZ--HZ2	1.04	0.89	32
NZ--HZ1	1.04	0.89	30
NH2--HH22	1.02	0.86	3
NZ--HZ1	1.05	0.89	7
NH2--HH21	1.02	0.86	3
NZ--HZ3	1.05	0.89	9
NZ--HZ2	1.05	0.89	5

### Standard geometry: angle outliers

*Bond angle outliers do not exist or can not be evaluated for this model*

### 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	11.96	145

All 145 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:249:VAL:HG22	B:24:ASP:HA	0.955
1	A:11:ASP:HB3	A:42:THR:HB	0.888
1	A:361:PRO:HA	A:369:TYR:HB3	0.881
1	A:514:VAL:HG21	A:562:LYS:HB2	0.828
1	A:641:PRO:HG3	B:39:ARG:HG3	0.815
1	A:62:VAL:HG13	A:67:PRO:HB3	0.738
1	A:483:MET:HB2	A:584:LEU:HD23	0.729
1	A:12:LEU:HB3	A:31:LEU:HD22	0.728
1	A:499:THR:HG23	A:501:GLU:H	0.717
1	B:27:ILE:HG12	B:54:SER:HB3	0.685
1	A:379:ILE:HD13	A:393:VAL:HG12	0.683
1	A:514:VAL:HG13	A:518:GLY:HA2	0.662
1	A:606:GLU:HB3	A:651:ARG:HG3	0.652
1	A:81:ASP:HA	A:92:VAL:HG22	0.648
1	A:617:LEU:HD11	A:668:PHE:HZ	0.645
1	A:200:ASN:HA	A:227:MET:SD	0.643
1	A:460:ASN:HB3	A:464:LYS:HB2	0.633
1	A:158:GLU:HA	A:162:THR:OG1	0.622
1	A:599:GLN:HG3	A:600:LYS:HG2	0.621

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:262:ARG:HD2	A:632:GLU:HG2	0.620
1	A:504:VAL:HA	A:533:ASN:HA	0.612
1	A:374:VAL:HG21	A:390:ALA:HA	0.611
1	A:259:ASP:O	A:263:ARG:HG2	0.596
1	A:668:PHE:HB3	A:676:VAL:HB	0.585
1	A:495:ILE:HD11	A:507:LEU:HD22	0.584
1	A:276:GLN:HG2	A:278:TRP:CZ3	0.583
1	A:196:LEU:HD12	A:227:MET:HB3	0.581
1	A:167:ILE:HB	A:178:ILE:HG23	0.576
1	A:559:ASN:HB3	A:584:LEU:HB2	0.571
1	A:355:GLN:HB3	A:373:PRO:HB2	0.568
1	A:236:VAL:HG23	A:237:LEU:HD12	0.565
1	A:260:ILE:HG23	A:272:VAL:HG21	0.562
1	A:567:LEU:HB3	A:576:LEU:HB2	0.560
1	A:343:THR:HG22	A:352:GLU:HG3	0.559
1	A:565:ALA:HB3	A:578:ALA:HB3	0.555
1	B:72:LEU:HB3	B:86:CYS:SG	0.547
1	A:186:GLU:HB3	A:189:ILE:HG12	0.546
1	A:26:LEU:HD22	A:185:PHE:HA	0.543
1	A:59:PHE:HB2	A:77:PHE:CE1	0.538
1	A:179:PRO:HG3	A:679:PHE:HB3	0.538
1	A:416:ILE:HD12	A:469:GLU:HG2	0.534
1	A:9:ARG:HB2	A:44:HIS:HB3	0.529

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:307:GLN:HE22	A:311:LEU:HA	0.526
1	A:85:GLU:H	A:89:THR:HG21	0.519
1	A:153:GLU:O	A:156:ARG:HG2	0.516
1	A:513:THR:HG23	A:555:LEU:HD23	0.515
1	A:249:VAL:HG13	B:24:ASP:HB3	0.511
1	A:311:LEU:HD22	A:395:ALA:HB2	0.510
1	A:624:VAL:HG12	A:666:VAL:HG12	0.508
1	B:5:PHE:HD2	B:7:LYS:HE2	0.506
1	A:445:TYR:HB2	A:452:GLU:HB3	0.505
1	A:4:GLU:HG2	A:123:THR:HB	0.502
1	A:50:TYR:HE2	A:57:LEU:HB2	0.502
1	A:323:ILE:HG12	A:325:GLY:H	0.500
1	A:342:MET:HG2	A:355:GLN:HG3	0.498
1	A:343:THR:HA	A:352:GLU:HG3	0.496
1	A:14:LEU:H	A:14:LEU:HD12	0.495
1	A:112:ILE:H	A:112:ILE:HD13	0.494
1	B:60:THR:HG23	B:75:VAL:HB	0.493
1	A:433:ARG:HB2	A:435:GLU:OE1	0.492
1	A:56:SER:HB3	A:122:SER:HB2	0.490
1	A:548:TYR:HA	A:551:TYR:CE2	0.490
1	A:67:PRO:HB2	A:74:LYS:HB2	0.489
1	A:36:GLY:H	A:106:THR:HB	0.486
1	A:491:VAL:HB	A:544:LEU:HB2	0.482

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:587:PRO:HG2	A:673:LEU:HD21	0.480
1	A:509:LEU:HB2	A:527:LYS:HB2	0.479
1	A:154:GLU:HB2	A:431:VAL:HG11	0.475
1	A:445:TYR:HB3	A:446:PRO:HD2	0.474
1	A:61:VAL:O	A:74:LYS:HA	0.473
1	A:532:LEU:H	A:532:LEU:HD22	0.472
1	A:639:PRO:HA	B:43:THR:OG1	0.472
1	A:623:THR:HB	A:635:THR:HG23	0.471
1	A:21:HIS:CE1	A:37:GLN:HB3	0.469
1	A:618:GLU:CB	B:40:ILE:HG13	0.467
1	A:425:LYS:HA	A:425:LYS:HD3	0.466
1	A:430:SER:HB2	A:433:ARG:HG3	0.465
1	A:255:ILE:HD12	A:625:GLU:HG2	0.464
1	A:623:THR:HA	A:635:THR:HA	0.463
1	A:244:ASN:HD21	B:10:GLY:HA3	0.460
1	A:13:GLU:HG3	A:16:THR:HB	0.458
1	A:294:PRO:HB2	A:341:TRP:HB3	0.458
1	A:201:PRO:O	A:205:LYS:HG2	0.457
1	A:195:ILE:O	A:199:VAL:HG23	0.454
1	A:193:CYS:HB3	A:287:VAL:HG13	0.453
1	A:328:SER:HB3	A:519:ILE:HA	0.449
1	A:593:ILE:HD13	A:680:ARG:HD2	0.449
1	A:387:LYS:O	A:388:TYR:HB2	0.446

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:497:ASN:OD1	A:499:THR:HG22	0.446
1	A:471:THR:HG22	A:574:SER:HB3	0.445
1	A:61:VAL:HB	A:115:TYR:HD2	0.444
1	A:447:GLU:HA	A:452:GLU:OE1	0.440
1	A:343:THR:HG22	A:352:GLU:CG	0.439
1	A:362:GLN:HG3	A:392:PHE:CZ	0.439
1	A:456:PHE:O	A:460:ASN:HB2	0.439
1	A:492:PHE:CZ	A:543:PRO:HB3	0.439
1	A:299:THR:HG23	A:336:CYS:SG	0.437
1	A:505:CYS:HB2	A:567:LEU:HD11	0.437
1	A:569:GLU:OE1	A:571:VAL:HG13	0.436
1	A:81:ASP:CG	A:82:ALA:H	0.435
1	A:347:LEU:HB3	A:348:GLN:H	0.434
1	B:28:TRP:CD1	B:44:ILE:HG13	0.432
1	A:569:GLU:HG3	A:572:ILE:O	0.431
1	A:461:HIS:HB3	A:462:LEU:HD22	0.430
1	A:291:LEU:HA	A:291:LEU:HD23	0.429
1	A:500:ALA:HA	A:536:PRO:HB3	0.429
1	A:307:GLN:NE2	A:395:ALA:HB1	0.428
1	A:497:ASN:O	A:537:PHE:HA	0.427
1	A:276:GLN:O	A:279:VAL:HG22	0.426
1	A:88:TRP:HA	A:105:THR:O	0.425
1	A:320:PHE:HA	A:508:LEU:HD22	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:15:GLU:O	A:19:ARG:HD3	0.423
1	A:166:PHE:HE1	A:177:ASN:HB2	0.423
1	A:315:TYR:HB2	A:330:MET:SD	0.422
1	A:475:MET:HA	A:494:HIS:O	0.422
1	A:51:GLU:HB2	A:55:ASP:HB2	0.419
1	A:246:GLY:HA2	B:9:THR:HA	0.419
1	A:615:VAL:HG22	A:616:ALA:H	0.419
1	A:167:ILE:HD13	A:278:TRP:HB2	0.417
1	A:401:VAL:HB	A:418:ARG:O	0.415
1	A:522:PRO:HB2	A:554:CYS:SG	0.415
1	A:303:SER:HB3	A:396:GLU:HG2	0.414
1	A:315:TYR:HB2	A:330:MET:CE	0.414
1	A:407:GLN:HB2	A:409:ASP:OD2	0.413
1	A:508:LEU:HG	A:529:LEU:HB3	0.413
1	A:390:ALA:N	A:391:PRO:HD2	0.412
1	A:590:LYS:HD2	A:610:GLN:HE22	0.412
1	A:357:LEU:HB2	A:373:PRO:HB3	0.411
1	A:374:VAL:HA	A:375:PRO:HD3	0.410
1	A:497:ASN:HB2	A:534:LEU:HD13	0.410
1	A:228:VAL:HA	A:236:VAL:HG22	0.409
1	A:298:VAL:HG11	A:339:GLU:HG3	0.409
1	A:608:SER:HA	A:648:VAL:O	0.408
1	A:68:SER:HB2	A:71:ALA:HB3	0.406

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:147:ALA:HB3	A:217:PRO:HG3	0.406
1	A:431:VAL:HB	A:432:GLY:H	0.406
1	A:467:GLU:H	A:467:GLU:HG2	0.406
1	A:566:LEU:HD11	A:575:TYR:HD2	0.405
1	A:69:GLN:H	A:69:GLN:NE2	0.405
1	A:618:GLU:HB2	B:40:ILE:HG13	0.404
1	B:9:THR:OG1	B:21:ARG:HG3	0.403
1	A:529:LEU:H	A:529:LEU:HD23	0.403
1	A:337:TRP:HB2	A:357:LEU:O	0.403
1	A:664:LEU:HA	A:664:LEU:HD22	0.401
1	B:21:ARG:HA	B:22:PRO:HD3	0.400

#### 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
1	773	682	81	10

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	671	460	125	86

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	26	LEU
1	A	29	GLU

Model ID	Chain	Residue ID	Residue type
1	A	46	GLU
1	A	56	SER
1	A	58	THR
1	A	73	THR
1	A	84	GLU
1	A	94	ASP
1	A	100	LEU
1	A	103	GLN
1	A	112	ILE
1	A	118	SER
1	A	129	SER
1	A	151	ASP
1	A	157	GLN
1	A	163	GLN
1	A	164	GLN
1	A	166	PHE
1	A	184	GLN
1	A	186	GLU
1	A	209	ARG
1	A	211	CYS
1	A	215	SER
1	A	216	SER
1	A	225	SER

Model ID	Chain	Residue ID	Residue type
1	A	238	LEU
1	A	250	SER
1	A	255	ILE
1	A	257	SER
1	A	271	ARG
1	A	279	VAL
1	A	298	VAL
1	A	305	HIS
1	A	307	GLN
1	A	312	LEU
1	A	313	ILE
1	A	314	GLU
1	A	347	LEU
1	A	362	GLN
1	A	364	LYS
1	A	365	SER
1	A	381	GLU
1	A	419	SER
1	A	422	VAL
1	A	431	VAL
1	A	442	THR
1	A	447	GLU
1	A	478	ARG

Model ID	Chain	Residue ID	Residue type
1	A	483	MET
1	A	491	VAL
1	A	496	THR
1	A	503	TYR
1	A	524	CYS
1	A	526	THR
1	A	531	ASN
1	A	532	LEU
1	A	533	ASN
1	A	549	GLU
1	A	556	THR
1	A	560	LEU
1	A	571	VAL
1	A	577	LEU
1	A	608	SER
1	A	617	LEU
1	A	618	GLU
1	A	621	THR
1	A	631	GLU
1	A	632	GLU
1	A	653	ASP
1	A	657	LEU
1	A	659	MET

Model ID	Chain	Residue ID	Residue type
1	A	664	LEU
1	B	3	THR
1	B	7	LYS
1	B	9	THR
1	B	12	THR
1	B	13	TYR
1	B	24	ASP
1	B	29	ASP
1	B	40	ILE
1	B	56	LYS
1	B	60	THR
1	B	63	ARG
1	B	67	THR
1	B	74	CYS
1	B	85	THR

### Fit of model to data used for modeling ?

#### 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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