Integrative Structure Validation Report

July 22, 2024 - 05:28 PM PDT

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	9A3V
PDB-Dev ID	PDBDEV_00000216
Structure Title	Predicted model of tissue transglutaminase 2 (TG2) in complex with plasma fibronectin type III modules 14 and 15 (FNIII14-15)
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

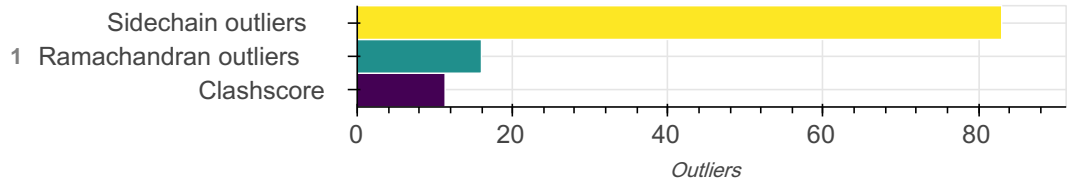
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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: MolProbity 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	180

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	1FNH

Representation

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

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-687
B	-	1-180

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 ASSEmbly 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	https://zhanggroup.org/I-TASSER/
2	Xwalk	Not available	calculation of Euclidean distances	https://www.xwalk.org/home.cgi
3	NACCESS	Not available	solvent accessibility	http://www.bioinf.manchester.ac.uk/naccess/
4	DisVis	Not available	accessible interaction space	https://wenmr.science.uu.nl/disvis/
5	HADDOCK	Not available	protein-protein docking	https://wenmr.science.uu.nl/haddock2.4/

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 1537 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
N--H	0.97	0.86	1
N--H	0.98	0.86	751
ND2--HD21	0.98	0.86	34
NE2--HE22	0.98	0.86	30
ND2--HD22	0.98	0.86	37
NE2--HE21	0.98	0.86	27
NE--HE	0.98	0.86	23
NE1--HE1	0.98	0.86	10
ND1--HD1	0.98	0.86	1
NE2--HE2	0.98	0.86	10
OG1--HG1	0.96	0.84	21
OG--HG	0.96	0.84	17
OH--HH	0.96	0.84	9
SG--HG	1.32	1.20	1
OH--HH	0.97	0.84	19
OG1--HG1	0.97	0.84	34
N--H	0.99	0.86	62
OG--HG	0.97	0.84	30
NE--HE	0.99	0.86	29
NE1--HE1	0.99	0.86	5
NE2--HE2	0.99	0.86	2
ND2--HD22	0.99	0.86	5

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
SG--HG	1.33	1.20	19
ND2--HD21	0.99	0.86	8
NE2--HE21	0.99	0.86	4
ND1--HD1	0.99	0.86	1
NE2--HE22	0.99	0.86	1
OH--HH	0.98	0.84	3
OG1--HG1	0.98	0.84	4
OG--HG	0.98	0.84	3
NE--HE	1.00	0.86	1
NH2--HH22	1.00	0.86	29
NH2--HH21	1.00	0.86	21
NH1--HH11	1.00	0.86	40
NH1--HH12	1.00	0.86	34
NH1--HH12	1.01	0.86	19
NH2--HH22	1.01	0.86	22
NH2--HH21	1.01	0.86	31
NZ--HZ1	1.04	0.89	36
NH1--HH11	1.01	0.86	13
NZ--HZ3	1.04	0.89	32
NZ--HZ2	1.04	0.89	33
NZ--HZ2	1.05	0.89	8
NH2--HH22	1.02	0.86	2
NZ--HZ3	1.05	0.89	9

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH21	1.02	0.86	1
NZ--HZ1	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	11.32	154

All 154 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:87:ASP:HA	A:107:PRO:HB3	0.859
1	A:514:VAL:HG21	A:562:LYS:HB2	0.837
1	A:179:PRO:HG3	A:679:PHE:HB3	0.830
1	A:620:CYS:HB2	A:638:ILE:HG12	0.816
1	A:116:ARG:HD2	A:134:HIS:HB3	0.788
1	A:11:ASP:HB3	A:42:THR:HB	0.782
1	A:646:GLU:HA	A:544:LEU:HD22	0.729
1	A:509:LEU:HD22	A:428:THR:HB	0.717
1	A:298:VAL:HG12	A:676:VAL:HB	0.704
1	A:643:GLU:OE1	A:373:PRO:HB2	0.695
1	A:668:PHE:HB3	A:604:VAL:HB	0.685
1	A:639:PRO:HB3	A:413:HIS:HB2	0.679
1	A:355:GLN:HB3	A:422:VAL:HG21	0.670

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:594:LEU:HB3	A:415:SER:HB2	0.654
1	A:405:ILE:HG23	A:293:ILE:HD12	0.652
1	A:399:ALA:H	A:529:LEU:HB3	0.617
1	A:262:ARG:HB3	A:272:VAL:HG21	0.616
1	A:403:ASP:HB3	A:55:ASP:HB3	0.602
1	A:288:LEU:HD22	A:412:VAL:HG22	0.602
1	A:508:LEU:HG	A:617:LEU:HD21	0.600
1	A:260:ILE:HG23	A:637:GLU:HB2	0.600
1	A:51:GLU:HB2	A:636:VAL:HG23	0.599
1	A:406:GLN:HG3	A:162:THR:OG1	0.590
1	A:613:LEU:HD12	A:31:LEU:HD13	0.585
1	A:621:THR:HG23	A:533:ASN:HA	0.581
1	A:622:PHE:HB2	A:641:PRO:HG3	0.565
1	A:158:GLU:HA	A:459:ALA:HB1	0.563
1	A:14:LEU:HA	A:79:LEU:HD22	0.561
1	A:504:VAL:HA	A:460:ASN:CG	0.559
1	A:618:GLU:HG3	A:391:PRO:HG3	0.555
1	A:384:LEU:HD13	A:254:TRP:CD1	0.553
1	A:57:LEU:HD23	A:74:LYS:HB2	0.551
1	A:311:LEU:HG	A:557:GLU:HB2	0.544
1	A:262:ARG:HD3	A:496:THR:HB	0.538
1	A:384:LEU:HG	A:347:LEU:HB2	0.529
1	A:251:PRO:HA	A:497:ASN:HA	0.528

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:67:PRO:HB2	A:272:VAL:HB	0.522
1	A:252:MET:HG3	A:44:HIS:HB3	0.517
1	A:474:ALA:HB3	A:665:VAL:HG13	0.513
1	A:344:ARG:HB3	A:606:GLU:HB2	0.513
1	A:473:MET:SD	A:55:ASP:CB	0.511
1	A:639:PRO:HA	A:673:LEU:HD21	0.509
1	A:237:LEU:HD23	A:93:VAL:HG11	0.505
1	A:9:ARG:HB2	A:34:ARG:HG2	0.504
1	A:179:PRO:HG2	A:557:GLU:H	0.504
1	A:592:ARG:HB2	A:103:GLN:O	0.503
1	A:51:GLU:HB2	A:452:GLU:CD	0.503
1	A:587:PRO:HG2	A:178:ILE:HG23	0.502
1	A:40:TRP:HZ3	A:544:LEU:HB2	0.501
1	A:21:HIS:HB3	A:199:VAL:HG23	0.498
1	A:557:GLU:CD	A:684:ILE:HB	0.498
1	A:90:ALA:HA	A:156:ARG:HG2	0.492
1	A:447:GLU:HA	A:433:ARG:HG3	0.490
1	A:167:ILE:HB	A:184:GLN:OE1	0.485
1	A:491:VAL:HB	A:564:ARG:HG2	0.485
1	A:195:ILE:O	A:258:VAL:HG11	0.484
1	A:659:MET:HA	A:571:VAL:HG13	0.484
1	A:153:GLU:O	A:369:TYR:HB3	0.482
1	A:430:SER:HB2	A:393:VAL:HG21	0.482

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:163:GLN:HA	A:580:ARG:HD2	0.481
1	A:510:CYS:HB3	A:601:ARG:HD2	0.476
1	A:186:GLU:HG3	A:675:ALA:HB2	0.475
1	A:569:GLU:OE1	A:230:CYS:HB2	0.474
1	A:361:PRO:HA	A:396:GLU:OE2	0.469
1	A:374:VAL:HG21	A:187:ASP:HA	0.468
1	A:477:ILE:O	A:325:GLY:H	0.463
1	A:639:PRO:HB2	A:446:PRO:HD2	0.463
1	A:598:LYS:HB3	A:74:LYS:HA	0.461
1	A:252:MET:HB3	A:494:HIS:O	0.460
1	A:226:GLY:O	A:263:ARG:HG2	0.459
1	A:303:SER:HB3	A:93:VAL:HG11	0.458
1	A:27:CYS:HB2	A:404:TRP:CD1	0.457
1	A:323:ILE:HG12	A:460:ASN:HD21	0.457
1	A:445:TYR:HB3	A:44:HIS:ND1	0.456
1	A:61:VAL:O	A:262:ARG:HG3	0.454
1	A:475:MET:HA	A:155:GLU:HB2	0.451
1	A:259:ASP:O	A:123:THR:HG21	0.450
1	A:40:TRP:CZ3	A:420:LEU:HB2	0.449
1	A:314:GLU:HB3	A:391:PRO:HA	0.447
1	A:394:PHE:HE2	A:536:PRO:HB3	0.445
1	A:9:ARG:HD2	A:641:PRO:HA	0.444
1	A:258:VAL:O	A:75:ALA:O	0.441

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:152:SER:HB3	A:529:LEU:HA	0.437
1	A:5:LEU:H	A:519:ILE:HB	0.436
1	A:419:SER:O	A:520:LEU:HD23	0.435
1	A:646:GLU:HG3	A:572:ILE:HG12	0.435
1	A:384:LEU:HD11	A:523:GLU:HA	0.434
1	A:500:ALA:HA	A:452:GLU:HB3	0.433
1	A:617:LEU:O	A:271:ARG:HD3	0.432
1	A:60:SER:HA	A:330:MET:SD	0.432
1	A:507:LEU:O	A:236:VAL:HG22	0.424
1	A:517:ASN:HD21	A:551:TYR:CE2	0.424
1	A:520:LEU:H	A:334:PHE:HA	0.423
1	A:571:VAL:HG22	A:291:LEU:HA	0.422
1	A:512:ARG:HB3	A:469:GLU:CD	0.421
1	A:445:TYR:HB2	A:59:PHE:HZ	0.419
1	A:235:GLY:O	A:214:ARG:HG3	0.419
1	A:315:TYR:HB2	A:400:ASP:HB2	0.419
1	A:228:VAL:HA	A:289:ARG:HB3	0.416
1	A:548:TYR:HA	A:463:ASN:HB2	0.416
1	A:300:ASN:O	A:634:LYS:HB2	0.416
1	A:138:LEU:HD22	A:510:CYS:N	0.415
1	A:414:LYS:HZ1	A:352:GLU:OE1	0.412
1	A:43:LEU:HD11	A:520:LEU:HD23	0.412
1	A:210:ASP:O	A:584:LEU:HD23	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:312:LEU:HB3	A:620:CYS:SG	0.407
1	A:184:GLN:HG2	A:213:ARG:NE	0.406
1	A:460:ASN:HB3	A:17:ASN:HB2	0.405
1	A:624:VAL:HG22	A:423:GLY:HA2	0.405
1	A:509:LEU:HG	A:529:LEU:CB	0.405
1	A:349:PRO:HA	A:541:SER:HA	0.402
1	A:519:ILE:HG12	A:215:SER:H	0.402
1	A:485:MET:HA	A:329:GLU:O	0.402
1	A:617:LEU:HB3	A:259:ASP:H	0.401

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	863	780	67	16

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	755	520	152	83

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	4	GLU
1	A	26	LEU
1	A	29	GLU

Model ID	Chain	Residue ID	Residue type
1	A	42	THR
1	A	56	SER
1	A	58	THR
1	A	73	THR
1	A	81	ASP
1	A	84	GLU
1	A	97	ASP
1	A	98	CYS
1	A	112	ILE
1	A	129	SER
1	A	164	GLN
1	A	184	GLN
1	A	196	LEU
1	A	215	SER
1	A	223	VAL
1	A	225	SER
1	A	238	LEU
1	A	264	TRP
1	A	271	ARG
1	A	279	VAL
1	A	303	SER
1	A	311	LEU
1	A	312	LEU

Model ID	Chain	Residue ID	Residue type
1	A	343	THR
1	A	346	ASP
1	A	347	LEU
1	A	362	GLN
1	A	363	GLU
1	A	365	SER
1	A	383	ASP
1	A	384	LEU
1	A	385	SER
1	A	403	ASP
1	A	442	THR
1	A	462	LEU
1	A	470	GLU
1	A	471	THR
1	A	478	ARG
1	A	483	MET
1	A	485	MET
1	A	526	THR
1	A	533	ASN
1	A	537	PHE
1	A	553	ASP
1	A	557	GLU
1	A	564	ARG

Model ID	Chain	Residue ID	Residue type
1	A	567	LEU
1	A	571	VAL
1	A	574	SER
1	A	577	LEU
1	A	588	GLU
1	A	618	GLU
1	A	621	THR
1	A	635	THR
1	A	636	VAL
1	A	640	ASP
1	A	649	LYS
1	A	664	LEU
1	A	666	VAL
1	A	671	ASP
1	B	4	ARG
1	B	9	ASP
1	B	11	THR
1	B	12	GLU
1	B	14	THR
1	B	16	THR
1	B	32	ASP
1	B	46	ILE
1	B	56	THR

Model ID	Chain	Residue ID	Residue type
1	B	59	GLN
1	B	70	THR
1	B	73	ASP
1	B	85	SER
1	B	99	THR
1	B	100	THR
1	B	104	LEU
1	B	114	ARG
1	B	146	THR
1	B	161	LEU
1	B	174	LYS

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

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 ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The PDB-Dev team and members of Sali labcontributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded byRCSB PDB (grant number

DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from RCSB PDB, Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the SASBDB repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the wwPDB Integrative/Hybrid Methods Task Force provided recommendations and community support for the project.