Integrative Structure Validation Report

March 27, 2025 - 09:59 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	8ZZX
PDB-Dev ID	PDBDEV_00000033
Structure Title	Insight into the structure of the unstructured tau protein
Structure Authors	Popov KI; Makepeace KA; Petrotchenko EV; Dokholyan NV; Borchers CH
Deposited on	2019-08-12

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

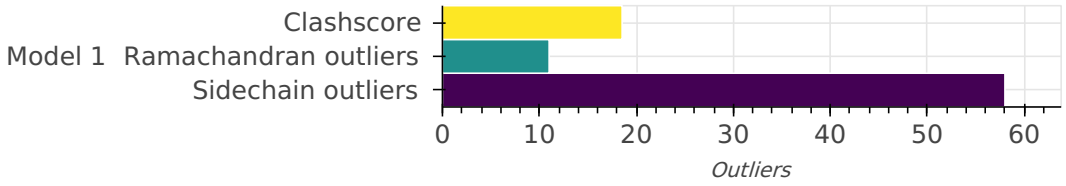
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

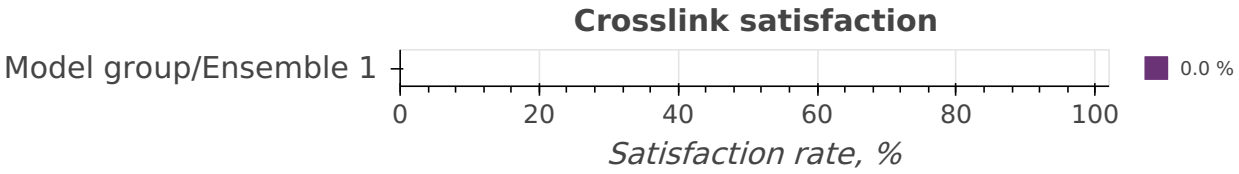
List of references used to build this report is available here.

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	tau protein	A	441	-	1-441	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
1	Crosslinking-MS data	PRIDE	PXD015044
2	Other	PRIDE	PXD015044
3	Other	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	Discrete Molecular Dynamics	Protein folding	None	–	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	piDMD	Not available	model building	http://www.moleculesinaction.com/pdmd.html
2	GROMACS	2018	model building	http://www.gromacs.org

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 107 bond length outliers in this entry (3.26% of 3280 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	407	HIS	ND1-CE1	88.24	2.20	1.32	1	1
A	329	HIS	ND1-CE1	88.06	2.20	1.32	1	1
A	268	HIS	ND1-CE1	88.05	2.20	1.32	1	1
A	32	HIS	ND1-CE1	87.36	2.19	1.32	1	1
A	374	HIS	ND1-CE1	87.12	2.19	1.32	1	1
A	14	HIS	ND1-CE1	87.03	2.19	1.32	1	1
A	121	HIS	ND1-CE1	86.91	2.19	1.32	1	1
A	94	HIS	ND1-CE1	86.86	2.19	1.32	1	1
A	299	HIS	ND1-CE1	86.78	2.19	1.32	1	1
A	388	HIS	ND1-CE1	86.47	2.19	1.32	1	1
A	362	HIS	ND1-CE1	86.43	2.19	1.32	1	1
A	330	HIS	ND1-CE1	85.98	2.18	1.32	1	1
A	121	HIS	CD2-NE2	71.87	2.16	1.37	1	1
A	362	HIS	CD2-NE2	71.45	2.16	1.37	1	1
A	94	HIS	CD2-NE2	71.11	2.16	1.37	1	1
A	329	HIS	CD2-NE2	70.69	2.15	1.37	1	1
A	407	HIS	CD2-NE2	70.47	2.15	1.37	1	1
A	14	HIS	CD2-NE2	70.31	2.15	1.37	1	1
A	32	HIS	CD2-NE2	70.17	2.15	1.37	1	1
A	268	HIS	CD2-NE2	70.13	2.15	1.37	1	1
A	299	HIS	CD2-NE2	70.01	2.14	1.37	1	1
A	388	HIS	CD2-NE2	69.91	2.14	1.37	1	1
A	330	HIS	CD2-NE2	69.81	2.14	1.37	1	1
A	374	HIS	CD2-NE2	69.30	2.14	1.37	1	1
A	52	THR	CB-OG1	6.79	1.54	1.43	1	1
A	76	THR	CB-OG1	6.24	1.53	1.43	1	1
A	17	THR	CB-OG1	6.22	1.53	1.43	1	1
A	231	THR	CB-OG1	6.20	1.53	1.43	1	1
A	111	THR	CB-OG1	6.18	1.53	1.43	1	1
A	50	THR	CB-OG1	6.00	1.53	1.43	1	1
A	149	THR	CB-OG1	5.99	1.53	1.43	1	1
A	35	GLN	CD-OE1	5.81	1.34	1.23	1	1
A	319	THR	CB-OG1	5.80	1.53	1.43	1	1
A	220	THR	CB-OG1	5.78	1.53	1.43	1	1
A	153	THR	CB-OG1	5.71	1.52	1.43	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	205	THR	CB-OG1	5.65	1.52	1.43	1	1
A	123	THR	CB-OG1	5.64	1.52	1.43	1	1
A	212	THR	CB-OG1	5.63	1.52	1.43	1	1
A	26	GLN	CD-OE1	5.59	1.34	1.23	1	1
A	427	THR	CB-OG1	5.58	1.52	1.43	1	1
A	102	THR	CB-OG1	5.58	1.52	1.43	1	1
A	71	THR	CB-OG1	5.57	1.52	1.43	1	1
A	217	THR	CB-OG1	5.56	1.52	1.43	1	1
A	6	GLN	CD-OE1	5.55	1.34	1.23	1	1
A	296	ASN	CG-OD1	5.55	1.34	1.23	1	1
A	439	GLN	CD-OE1	5.52	1.34	1.23	1	1
A	30	THR	CB-OG1	5.49	1.52	1.43	1	1
A	269	GLN	CD-OE1	5.47	1.33	1.23	1	1
A	288	GLN	CD-OE1	5.46	1.33	1.23	1	1
A	403	THR	CB-OG1	5.43	1.52	1.43	1	1
A	327	ASN	CG-OD1	5.41	1.33	1.23	1	1
A	381	ASN	CG-OD1	5.38	1.33	1.23	1	1
A	101	THR	CB-OG1	5.36	1.52	1.43	1	1
A	351	GLN	CD-OE1	5.32	1.33	1.23	1	1
A	124	GLN	CD-OE1	5.29	1.33	1.23	1	1
A	175	THR	CB-OG1	5.28	1.52	1.43	1	1
A	39	THR	CB-OG1	5.28	1.52	1.43	1	1
A	424	GLN	CD-OE1	5.27	1.33	1.23	1	1
A	165	GLN	CD-OE1	5.21	1.33	1.23	1	1
A	167	ASN	CG-OD1	5.21	1.33	1.23	1	1
A	410	ASN	CG-OD1	5.20	1.33	1.23	1	1
A	181	THR	CB-OG1	5.17	1.52	1.43	1	1
A	286	ASN	CG-OD1	5.16	1.33	1.23	1	1
A	359	ASN	CG-OD1	5.16	1.33	1.23	1	1
A	63	THR	CB-OG1	5.15	1.52	1.43	1	1
A	386	THR	CB-OG1	5.15	1.52	1.43	1	1
A	92	GLN	CD-OE1	5.14	1.33	1.23	1	1
A	265	ASN	CG-OD1	5.13	1.33	1.23	1	1
A	69	THR	CB-OG1	5.11	1.51	1.43	1	1
A	95	THR	CB-OG1	5.09	1.51	1.43	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	361	THR	CB-OG1	5.08	1.51	1.43	1	1
A	336	GLN	CD-OE1	5.06	1.33	1.23	1	1
A	244	GLN	CD-OE1	5.04	1.33	1.23	1	1
A	276	GLN	CD-OE1	5.04	1.33	1.23	1	1
A	162	GLN	CD-OE1	5.00	1.33	1.23	1	1
A	88	GLN	CD-OE1	4.99	1.33	1.23	1	1
A	169	THR	CB-OG1	4.99	1.51	1.43	1	1
A	49	GLN	CD-OE1	4.94	1.32	1.23	1	1
A	368	ASN	CG-OD1	4.90	1.32	1.23	1	1
A	33	GLN	CD-OE1	4.89	1.32	1.23	1	1
A	307	GLN	CD-OE1	4.88	1.32	1.23	1	1
A	414	THR	CB-OG1	4.87	1.51	1.43	1	1
A	373	THR	CB-OG1	4.85	1.51	1.43	1	1
A	255	ASN	CG-OD1	4.84	1.32	1.23	1	1
A	167	ASN	CG-ND2	4.83	1.23	1.33	1	1
A	377	THR	CB-OG1	4.82	1.51	1.43	1	1
A	263	THR	CB-OG1	4.82	1.51	1.43	1	1
A	245	THR	CB-OG1	4.79	1.51	1.43	1	1
A	276	GLN	CD-NE2	4.78	1.23	1.33	1	1
A	135	THR	CB-OG1	4.75	1.51	1.43	1	1
A	26	GLN	CD-NE2	4.72	1.23	1.33	1	1
A	265	ASN	CG-ND2	4.66	1.23	1.33	1	1
A	244	GLN	CD-NE2	4.63	1.23	1.33	1	1
A	269	GLN	CD-NE2	4.60	1.23	1.33	1	1
A	424	GLN	CD-NE2	4.59	1.23	1.33	1	1
A	124	GLN	CD-NE2	4.56	1.23	1.33	1	1
A	288	GLN	CD-NE2	4.46	1.23	1.33	1	1
A	410	ASN	CG-ND2	4.37	1.24	1.33	1	1
A	49	GLN	CD-NE2	4.36	1.24	1.33	1	1
A	279	ASN	CG-OD1	4.35	1.31	1.23	1	1

Standard geometry: angle outliers

There are 77 bond angle outliers in this entry (1.73% of 4442 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	362	HIS	CD2-NE2-CE1	73.82	35.18	109.00	1	1
A	121	HIS	CD2-NE2-CE1	73.55	35.45	109.00	1	1
A	388	HIS	CD2-NE2-CE1	73.31	35.69	109.00	1	1
A	329	HIS	CD2-NE2-CE1	73.28	35.72	109.00	1	1
A	14	HIS	CD2-NE2-CE1	73.26	35.74	109.00	1	1
A	330	HIS	CD2-NE2-CE1	73.25	35.75	109.00	1	1
A	407	HIS	CD2-NE2-CE1	73.20	35.80	109.00	1	1
A	268	HIS	CD2-NE2-CE1	73.16	35.84	109.00	1	1
A	299	HIS	CD2-NE2-CE1	73.05	35.95	109.00	1	1
A	32	HIS	CD2-NE2-CE1	72.97	36.03	109.00	1	1
A	94	HIS	CD2-NE2-CE1	72.95	36.05	109.00	1	1
A	374	HIS	CD2-NE2-CE1	72.63	36.37	109.00	1	1
A	299	HIS	ND1-CE1-NE2	72.55	35.85	108.40	1	1
A	329	HIS	ND1-CE1-NE2	72.24	36.16	108.40	1	1
A	374	HIS	ND1-CE1-NE2	72.17	36.23	108.40	1	1
A	14	HIS	ND1-CE1-NE2	71.98	36.42	108.40	1	1
A	32	HIS	ND1-CE1-NE2	71.88	36.52	108.40	1	1
A	362	HIS	ND1-CE1-NE2	71.87	36.53	108.40	1	1
A	268	HIS	ND1-CE1-NE2	71.82	36.58	108.40	1	1
A	407	HIS	ND1-CE1-NE2	71.76	36.64	108.40	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	94	HIS	ND1-CE1-NE2	71.60	36.80	108.40	1	1
A	121	HIS	ND1-CE1-NE2	71.46	36.94	108.40	1	1
A	388	HIS	ND1-CE1-NE2	71.27	37.13	108.40	1	1
A	330	HIS	ND1-CE1-NE2	71.12	37.28	108.40	1	1
A	268	HIS	CG-CD2-NE2	34.54	72.66	107.20	1	1
A	14	HIS	CG-CD2-NE2	34.44	72.76	107.20	1	1
A	121	HIS	CG-CD2-NE2	34.44	72.76	107.20	1	1
A	362	HIS	CG-CD2-NE2	34.30	72.90	107.20	1	1
A	299	HIS	CG-CD2-NE2	34.12	73.08	107.20	1	1
A	329	HIS	CG-CD2-NE2	33.85	73.35	107.20	1	1
A	32	HIS	CG-CD2-NE2	33.82	73.38	107.20	1	1
A	94	HIS	CG-CD2-NE2	33.79	73.41	107.20	1	1
A	407	HIS	CG-CD2-NE2	33.62	73.58	107.20	1	1
A	330	HIS	CG-CD2-NE2	33.62	73.58	107.20	1	1
A	374	HIS	CG-CD2-NE2	33.28	73.92	107.20	1	1
A	388	HIS	CG-CD2-NE2	32.87	74.33	107.20	1	1
A	268	HIS	CG-ND1-CE1	22.37	71.27	109.30	1	1
A	407	HIS	CG-ND1-CE1	22.16	71.63	109.30	1	1
A	121	HIS	CG-ND1-CE1	22.15	71.65	109.30	1	1
A	362	HIS	CG-ND1-CE1	22.11	71.70	109.30	1	1
A	32	HIS	CG-ND1-CE1	22.03	71.85	109.30	1	1
A	14	HIS	CG-ND1-CE1	21.93	72.02	109.30	1	1
A	330	HIS	CG-ND1-CE1	21.85	72.16	109.30	1	1
A	329	HIS	CG-ND1-CE1	21.79	72.27	109.30	1	1
A	94	HIS	CG-ND1-CE1	21.76	72.32	109.30	1	1
A	299	HIS	CG-ND1-CE1	21.62	72.54	109.30	1	1
A	388	HIS	CG-ND1-CE1	21.56	72.65	109.30	1	1
A	374	HIS	CG-ND1-CE1	21.28	73.13	109.30	1	1
A	362	HIS	CB-CG-CD2	8.78	119.78	131.20	1	1
A	121	HIS	CB-CG-CD2	8.44	120.22	131.20	1	1
A	299	HIS	CB-CG-CD2	8.38	120.31	131.20	1	1
A	268	HIS	CB-CG-CD2	8.20	120.54	131.20	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	374	HIS	CB-CG-CD2	7.46	121.50	131.20	1	1
A	407	HIS	CB-CG-CD2	6.90	122.23	131.20	1	1
A	14	HIS	CB-CG-CD2	6.86	122.29	131.20	1	1
A	330	HIS	CB-CG-CD2	6.59	122.64	131.20	1	1
A	329	HIS	CB-CG-CD2	6.36	122.94	131.20	1	1
A	94	HIS	CB-CG-CD2	6.27	123.05	131.20	1	1
A	388	HIS	CB-CG-CD2	5.75	123.72	131.20	1	1
A	32	HIS	CB-CG-CD2	5.28	124.33	131.20	1	1
A	374	HIS	CB-CG-ND1	5.24	130.56	122.70	1	1
A	299	HIS	CB-CG-ND1	4.60	129.59	122.70	1	1
A	94	HIS	CB-CG-ND1	4.48	129.43	122.70	1	1
A	14	HIS	CB-CG-ND1	4.38	129.27	122.70	1	1
A	329	HIS	CB-CG-ND1	4.34	129.21	122.70	1	1
A	359	ASN	CB-CG-ND2	4.30	122.85	116.40	1	1
A	296	ASN	CB-CG-ND2	4.25	122.77	116.40	1	1
A	330	HIS	CB-CG-ND1	4.21	129.01	122.70	1	1
A	327	ASN	OD1-CG-ND2	4.19	118.41	122.60	1	1
A	388	HIS	CB-CG-ND1	4.19	128.98	122.70	1	1
A	215	LEU	CD1-CG-CD2	4.15	101.67	110.80	1	1
A	32	HIS	CB-CG-ND1	4.11	128.87	122.70	1	1
A	124	GLN	CG-CD-NE2	4.09	122.54	116.40	1	1
A	325	LEU	CD1-CG-CD2	4.07	101.84	110.80	1	1
A	424	GLN	CG-CD-NE2	4.07	122.50	116.40	1	1
A	35	GLN	CG-CD-NE2	4.02	122.43	116.40	1	1
A	81	ASP	CA-CB-CG	4.00	116.60	112.60	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	18.53	119

There are 119 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:229:VAL:HG12	A:399:VAL:HB	1.08	1	1
A:35:GLN:H	A:39:THR:HG22	0.92	1	1
A:234:LYS:HG2	A:405:PRO:HB3	0.91	1	1
A:346:PHE:HB3	A:352:SER:HB2	0.90	1	1
A:169:THR:HG22	A:173:ALA:HA	0.89	1	1
A:373:THR:HG22	A:384:ALA:H	0.88	1	1
A:169:THR:HG21	A:174:LYS:H	0.87	1	1
A:23:ARG:HD2	A:93:PRO:HB3	0.84	1	1
A:92:GLN:H	A:95:THR:HG22	0.81	1	1
A:169:THR:CG2	A:173:ALA:HA	0.80	1	1
A:280:LYS:HE3	A:283:ASP:HB3	0.76	1	1
A:233:PRO:HA	A:403:THR:HG21	0.75	1	1
A:19:GLY:HA2	A:24:LYS:HB2	0.75	1	1
A:212:THR:HG23	A:213:PRO:N	0.74	1	1
A:131:SER:H	A:135:THR:CG2	0.74	1	1
A:284:LEU:HB3	A:423:PRO:HB3	0.73	1	1
A:71:THR:HA	A:265:ASN:HB3	0.72	1	1
A:373:THR:CG2	A:384:ALA:H	0.71	1	1
A:231:THR:HG22	A:401:GLY:H	0.70	1	1
A:57:GLU:HG3	A:426:ALA:HB2	0.69	1	1
A:419:MET:HE3	A:420:VAL:HG23	0.67	1	1
A:245:THR:O	A:245:THR:HG23	0.66	1	1
A:361:THR:HG22	A:366:GLY:HA3	0.66	1	1
A:111:THR:HG22	A:226:VAL:HG22	0.66	1	1
A:361:THR:HG23	A:363:VAL:H	0.62	1	1
A:35:GLN:N	A:39:THR:HG22	0.62	1	1
A:79:LEU:HB2	A:315:LEU:HD11	0.61	1	1
A:427:THR:HG23	A:429:ALA:H	0.61	1	1
A:34:ASP:HB3	A:437:ALA:HB3	0.60	1	1
A:357:LEU:HB2	A:370:LYS:HG3	0.60	1	1
A:363:VAL:HG21	A:408:LEU:HG	0.59	1	1
A:352:SER:HA	A:376:LEU:HD23	0.58	1	1
A:123:THR:HB	A:214:SER:HB2	0.57	1	1
A:169:THR:O	A:169:THR:HG22	0.57	1	1
A:275:VAL:HG13	A:344:LEU:HG	0.56	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:351:GLN:H	A:377:THR:CG2	0.56	1	1
A:386:THR:HB	A:388:HIS:CE1	0.56	1	1
A:200:PRO:HB3	A:215:LEU:HD12	0.55	1	1
A:386:THR:HB	A:388:HIS:HE1	0.55	1	1
A:110:ASP:HB3	A:224:LYS:HD2	0.55	1	1
A:166:ALA:HB3	A:183:PRO:HD3	0.54	1	1
A:10:VAL:HG23	A:157:ALA:HB1	0.54	1	1
A:182:PRO:HG3	A:188:PRO:HG3	0.54	1	1
A:351:GLN:H	A:377:THR:HG23	0.54	1	1
A:427:THR:HG23	A:429:ALA:N	0.54	1	1
A:131:SER:H	A:135:THR:HG22	0.53	1	1
A:420:VAL:HG13	A:434:ALA:HB1	0.53	1	1
A:69:THR:HG22	A:71:THR:O	0.53	1	1
A:234:LYS:H	A:403:THR:HG21	0.53	1	1
A:29:TYR:HB2	A:46:SER:HB3	0.53	1	1
A:9:GLU:HB3	A:157:ALA:HB3	0.51	1	1
A:101:THR:HG22	A:394:TYR:O	0.51	1	1
A:14:HIS:HD2	A:91:ALA:O	0.51	1	1
A:436:LEU:HB3	A:438:LYS:HG3	0.51	1	1
A:212:THR:HG23	A:214:SER:H	0.51	1	1
A:63:THR:HG22	A:65:ASP:O	0.51	1	1
A:197:TYR:CE1	A:203:PRO:HG3	0.50	1	1
A:211:ARG:HG3	A:215:LEU:HD11	0.50	1	1
A:378:PHE:CD2	A:379:ARG:HB2	0.50	1	1
A:424:GLN:NE2	A:428:LEU:HD21	0.50	1	1
A:160:PRO:HB2	A:394:TYR:HB2	0.49	1	1
A:79:LEU:HD22	A:315:LEU:HD11	0.49	1	1
A:111:THR:HG21	A:150:LYS:NZ	0.48	1	1
A:344:LEU:O	A:353:LYS:HA	0.48	1	1
A:35:GLN:H	A:39:THR:CG2	0.48	1	1
A:277:ILE:HG21	A:280:LYS:HD2	0.48	1	1
A:288:GLN:HA	A:424:GLN:CB	0.48	1	1
A:288:GLN:HA	A:424:GLN:HB2	0.48	1	1
A:244:GLN:O	A:249:PRO:HA	0.48	1	1
A:310:TYR:CG	A:315:LEU:HD13	0.48	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:94:HIS:HD2	A:259:LYS:O	0.48	1	1
A:361:THR:CG2	A:366:GLY:HA3	0.47	1	1
A:6:GLN:HB2	A:390:ALA:O	0.47	1	1
A:75:VAL:HG13	A:309:VAL:HG22	0.47	1	1
A:386:THR:O	A:386:THR:HG23	0.47	1	1
A:95:THR:CG2	A:95:THR:O	0.47	1	1
A:52:THR:O	A:52:THR:HG23	0.47	1	1
A:340:LYS:HD2	A:358:ASP:HB3	0.47	1	1
A:34:ASP:HA	A:39:THR:HG22	0.46	1	1
A:102:THR:HG23	A:104:GLU:H	0.46	1	1
A:420:VAL:CG1	A:434:ALA:HB1	0.46	1	1
A:424:GLN:HE21	A:428:LEU:HD21	0.46	1	1
A:147:GLY:HA2	A:151:ILE:HA	0.46	1	1
A:231:THR:HA	A:232:PRO:HD3	0.45	1	1
A:95:THR:O	A:95:THR:HG23	0.45	1	1
A:267:LYS:HD3	A:305:SER:OG	0.45	1	1
A:234:LYS:N	A:403:THR:HG21	0.45	1	1
A:102:THR:HG21	A:105:GLU:HA	0.45	1	1
A:219:PRO:HB3	A:243:LEU:HD21	0.45	1	1
A:282:LEU:HD21	A:337:VAL:CG1	0.45	1	1
A:235:SER:OG	A:245:THR:HG22	0.45	1	1
A:94:HIS:CD2	A:259:LYS:O	0.45	1	1
A:353:LYS:HB3	A:375:LYS:HB2	0.45	1	1
A:341:SER:HB3	A:360:ILE:HA	0.44	1	1
A:420:VAL:HG21	A:428:LEU:HD22	0.44	1	1
A:422:SER:HB2	A:434:ALA:O	0.44	1	1
A:212:THR:CG2	A:214:SER:H	0.44	1	1
A:215:LEU:HA	A:216:PRO:HA	0.44	1	1
A:273:GLY:HA2	A:346:PHE:HA	0.44	1	1
A:275:VAL:HG22	A:344:LEU:HD23	0.44	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	439	358	70	11

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

Chain	Res	Type	Models (Total)
A	16	GLY	1
A	17	THR	1
A	28	GLY	1
A	73	GLU	1
A	100	GLY	1
A	154	PRO	1
A	176	PRO	1
A	177	PRO	1
A	183	PRO	1
A	206	PRO	1
A	301	PRO	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	358	249	51	58

There are 58 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	3	GLU	1
A	20	LEU	1
A	22	ASP	1
A	25	ASP	1
A	32	HIS	1
A	39	THR	1
A	49	GLN	1
A	50	THR	1
A	51	PRO	1
A	62	GLU	1
A	64	SER	1
A	75	VAL	1
A	93	PRO	1
A	97	ILE	1
A	102	THR	1

Chain	Res	Type	Models (Total)
A	109	VAL	1
A	111	THR	1
A	122	VAL	1
A	138	ASP	1
A	141	LYS	1
A	146	ASP	1
A	162	GLN	1
A	163	LYS	1
A	169	THR	1
A	211	ARG	1
A	212	THR	1
A	213	PRO	1
A	217	THR	1
A	221	ARG	1
A	228	VAL	1
A	231	THR	1
A	237	SER	1
A	250	MET	1
A	252	ASP	1
A	255	ASN	1
A	258	SER	1
A	264	GLU	1
A	269	GLN	1
A	275	VAL	1
A	277	ILE	1
A	278	ILE	1
A	279	ASN	1
A	280	LYS	1
A	288	GLN	1
A	291	CYS	1
A	308	ILE	1
A	327	ASN	1
A	328	ILE	1
A	339	VAL	1
A	356	SER	1

Chain	Res	Type	Models (Total)
A	361	THR	1
A	370	LYS	1
A	393	VAL	1
A	394	TYR	1
A	396	SER	1
A	412	SER	1
A	422	SER	1
A	427	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.

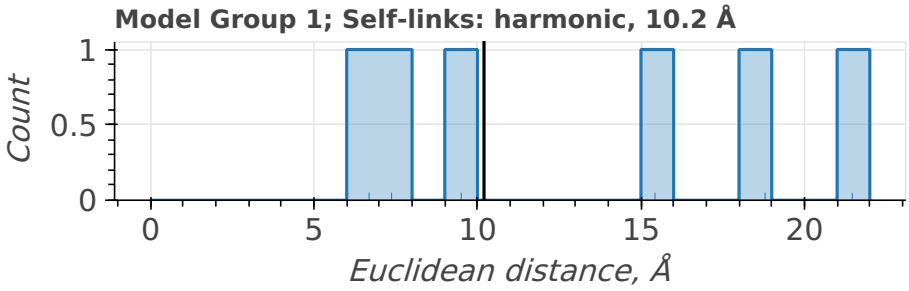
There are 105 crosslinking restraints combined in 103 restraint groups.

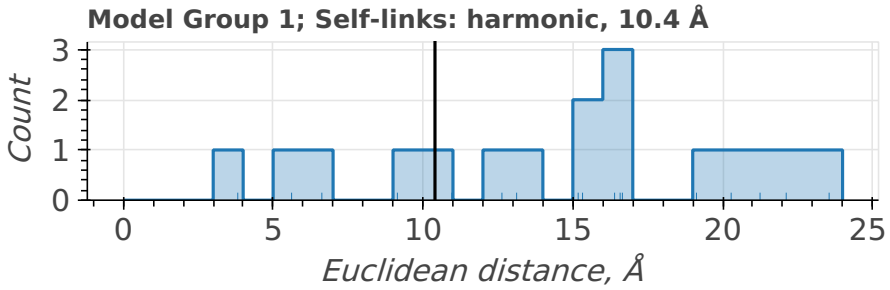
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
SDA	GLN	CA	LYS	CA	harmonic	10.2	2
SDA	GLU	CA	LYS	CA	harmonic	10.2	2
SDA	ASP	CA	LYS	CA	harmonic	9.5	2
SDA	GLY	CA	LYS	CA	harmonic	8.2	3
SDA	LYS	CA	THR	CA	harmonic	9.5	3
SDA	ASP	CA	LYS	CA	harmonic	9.4	1
SDA	LYS	CA	PRO	CA	harmonic	8.95	1
SDA	LYS	CA	SER	CA	harmonic	10.4	1
SDA	LYS	CA	PRO	CA	harmonic	10.2	1
SDA	GLY	CA	LYS	CA	harmonic	9.4	1
SDA	LYS	CA	LYS	CA	harmonic	8.2	1
SDA	LYS	CA	LYS	CA	harmonic	12.4	4
SDA	LYS	CA	LYS	CA	harmonic	10.4	3
SDA	ASN	CA	LYS	CA	harmonic	12.4	1
SDA	ALA	CA	LYS	CA	harmonic	12.4	1
DSA	LYS	CA	LYS	CA	harmonic	12.4	42

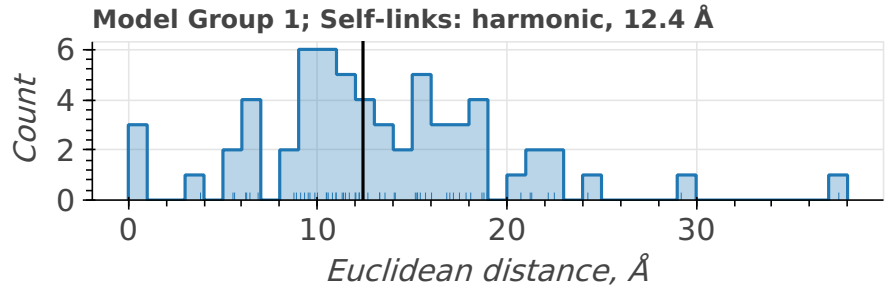
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSA	LYS	CA	LYS	CA	harmonic	10.4	9
DSA	ALA	CA	LYS	CA	harmonic	10.4	1
DSA	ALA	CA	LYS	CA	harmonic	8.95	1
DSA	LYS	CA	LYS	CA	harmonic	8.95	2
DSA	LYS	CA	PRO	CA	harmonic	12.4	1
DSA	LYS	CA	LYS	CA	harmonic	9.5	3
DSA	LYS	CA	SER	CA	harmonic	12.4	1
DSA	ASN	CA	LYS	CA	harmonic	10.2	1
DSG	LYS	CA	LYS	CA	harmonic	10.4	2
DSG	LYS	CA	LYS	CA	harmonic	12.4	9
DSG	GLN	CA	LYS	CA	harmonic	8.95	1
DSG	LYS	CA	SER	CA	harmonic	10.4	1
DSG	LYS	CA	THR	CA	harmonic	9.4	1
DSG	LYS	CA	THR	CA	harmonic	12.4	1
DSG	LYS	CA	LYS	CA	harmonic	8.95	1
DSG	GLU	CA	LYS	CA	harmonic	12.4	1

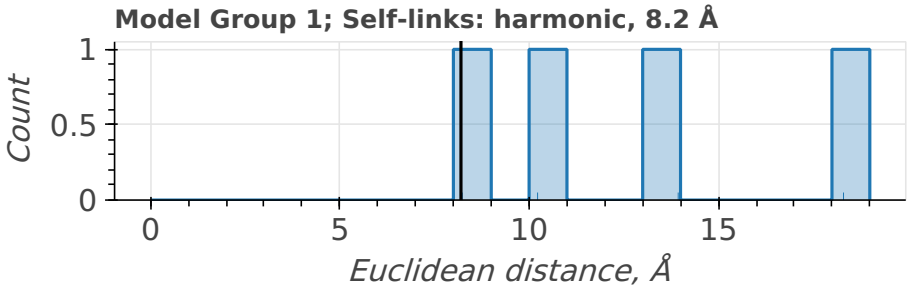
Distograms of individual restraints

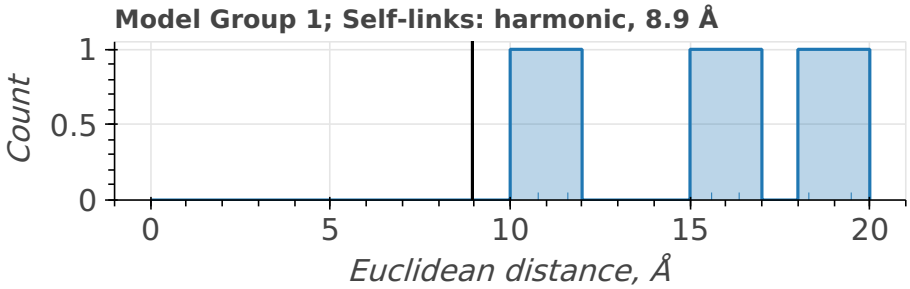
Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as 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.

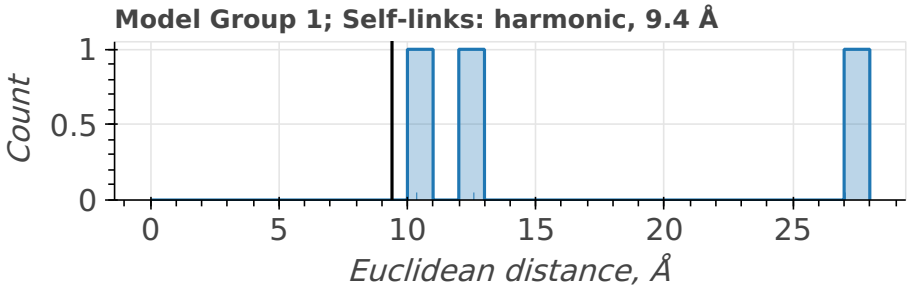


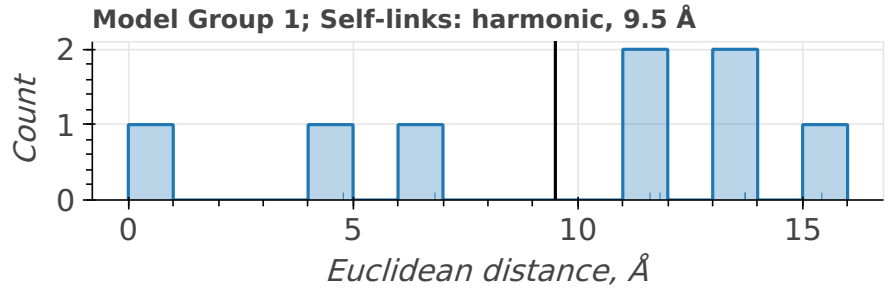












Satisfaction of restraints

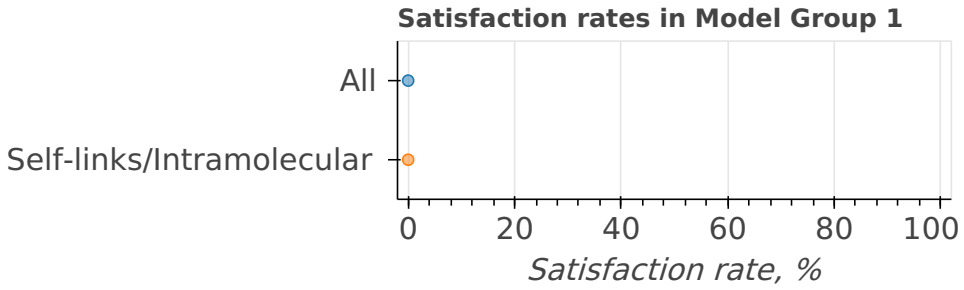
Satisfaction of restraints is calculated on a restraint group (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=103)
1	1	1	1/1	All	0.00	100.00	103
				Self-links/ Intramolecular	0.00	100.00	103

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 Trewhella, 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.