

Integrative Structure Validation Report ?

February 18, 2025 - 08:30 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	9A0N
PDB-Dev ID	PDBDEV_00000059
Structure Title	Integrative structure of Pg-cGMP-GAFab complex
Structure Authors	Gupta R; Liu Y; Wang H; Nordyke CT; Puterbaugh RZ; Cui W; Varga K; Chu F; Ke H; Vashisth H; Cote RH
Deposited on	2020-08-07

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

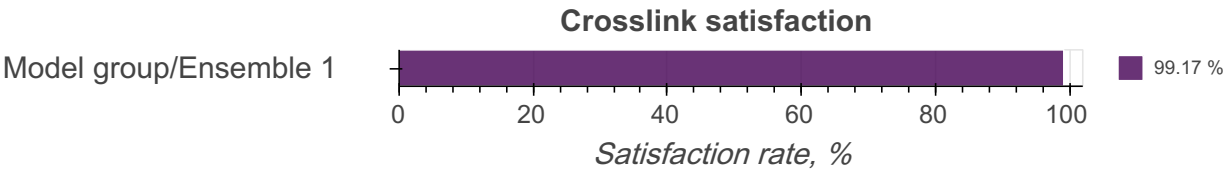
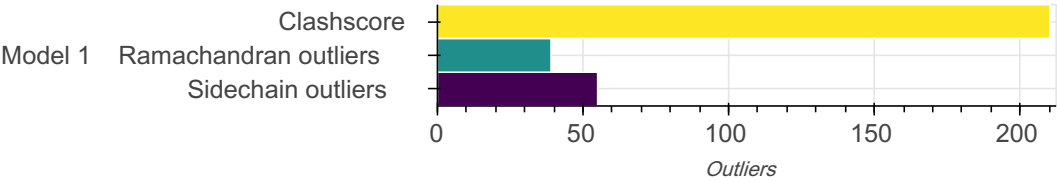
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	PDE GAFab	A	399	-	1-399	100.00 / 100.00	Atomic
				B					
		2	PDE gamma subunit	C	51	-	1-51	100.00 / 100.00	Atomic
				D					
		3	GUANOSINE-3',5'- MONOPHOSPHATE	E [A]	Non-polymeric	-	-	Not available / Not available	Atomic
				F [B]					

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	PXD020817
2	Experimental model	PDB	6X88
3	Experimental model	PDB	6MZB
4	Comparative model	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	None	None	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	Not available	integrative model building	https://integrativemodeling.org
2	Modeller	Not available	model building	https://salilab.org/modeller/

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 63 bond length outliers in this entry (0.84% of 7472 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	392	GLU	CA-C	12.30	1.78	1.52	1	1
B	256	PRO	N-CA	11.61	1.29	1.47	1	1
A	392	GLU	CA-C	11.26	1.76	1.52	1	1
D	28	PHE	C-N	8.54	1.45	1.33	1	1
A	392	GLU	C-N	8.31	1.45	1.33	1	1
B	255	THR	C-N	8.10	1.47	1.34	1	1
B	392	GLU	C-N	7.96	1.44	1.33	1	1
C	28	PHE	CA-C	7.76	1.36	1.52	1	1
D	27	LYS	CA-C	7.22	1.68	1.52	1	1
A	313	ASP	C-N	6.98	1.43	1.33	1	1
C	24	GLY	C-N	6.83	1.23	1.34	1	1
D	26	PRO	C-N	6.28	1.42	1.33	1	1
B	313	ASP	C-N	6.21	1.42	1.33	1	1
A	300	GLU	CA-C	5.99	1.40	1.52	1	1
A	393	ASN	N-CA	5.98	1.57	1.46	1	1
C	26	PRO	CA-C	5.97	1.40	1.52	1	1
C	26	PRO	N-CD	5.88	1.39	1.47	1	1
D	28	PHE	CA-C	5.88	1.65	1.52	1	1
B	236	PHE	CB-CG	5.84	1.64	1.50	1	1
A	312	ALA	C-N	5.79	1.41	1.33	1	1
C	46	GLN	CA-C	5.72	1.40	1.52	1	1
B	393	ASN	N-CA	5.55	1.56	1.46	1	1
B	392	GLU	N-CA	5.22	1.36	1.46	1	1
D	27	LYS	N-CA	5.22	1.56	1.46	1	1
A	137	LEU	CA-C	5.22	1.42	1.52	1	1
B	137	LEU	CA-C	5.09	1.42	1.52	1	1
C	47	GLY	CA-C	5.08	1.42	1.52	1	1
A	257	ASP	C-N	5.06	1.40	1.33	1	1
B	312	ALA	C-N	5.05	1.40	1.33	1	1
B	257	ASP	C-N	5.03	1.40	1.33	1	1
B	256	PRO	C-N	5.02	1.26	1.33	1	1
A	209	LYS	CA-C	4.97	1.42	1.52	1	1
A	67	SER	C-N	4.96	1.40	1.33	1	1
B	256	PRO	N-CD	4.93	1.54	1.47	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	392	GLU	N-CA	4.90	1.36	1.46	1	1
C	48	PHE	C-N	4.80	1.40	1.33	1	1
B	258	GLY	N-CA	4.78	1.53	1.45	1	1
D	45	VAL	CA-C	4.78	1.42	1.52	1	1
A	341	LYS	C-N	4.76	1.40	1.33	1	1
B	67	SER	C-N	4.74	1.40	1.33	1	1
A	391	LEU	CA-C	4.69	1.43	1.52	1	1
D	29	LYS	N-CA	4.67	1.55	1.46	1	1
D	11	THR	N-CA	4.55	1.37	1.46	1	1
C	26	PRO	N-CA	4.55	1.40	1.47	1	1
B	341	LYS	C-N	4.54	1.39	1.33	1	1
C	23	LYS	CA-C	4.47	1.43	1.52	1	1
B	388	MET	CA-C	4.36	1.43	1.52	1	1
B	391	LEU	CA-C	4.32	1.43	1.52	1	1
D	24	GLY	C-N	4.30	1.27	1.34	1	1
B	75	ASN	C-N	4.25	1.27	1.34	1	1
B	73	LEU	CA-C	4.24	1.44	1.52	1	1
A	313	ASP	CA-C	4.23	1.61	1.52	1	1
D	23	LYS	CA-C	4.21	1.44	1.52	1	1
C	30	GLN	CA-C	4.21	1.44	1.52	1	1
B	135	GLU	C-N	4.17	1.39	1.33	1	1
D	29	LYS	C-N	4.14	1.39	1.33	1	1
B	257	ASP	N-CA	4.14	1.38	1.46	1	1
B	74	VAL	N-CA	4.13	1.38	1.46	1	1
B	209	LYS	CA-C	4.11	1.44	1.52	1	1
A	138	ALA	N-CA	4.09	1.38	1.46	1	1
A	388	MET	CA-C	4.07	1.44	1.52	1	1
B	138	ALA	N-CA	4.01	1.38	1.46	1	1
A	135	GLU	C-N	4.01	1.39	1.33	1	1

Standard geometry: angle outliers ?

There are 451 bond angle outliers in this entry (4.47% of 10100 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)
B	236	PHE	CD1-CE1-CZ	58.06	15.48	120.00	1	1
B	236	PHE	CG-CD1-CE1	43.01	47.59	120.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	236	PHE	CE1-CZ-CE2	36.85	53.66	120.00	1	1
B	236	PHE	CD1-CG-CD2	29.92	73.72	118.60	1	1
B	236	PHE	CD2-CE2-CZ	22.73	79.09	120.00	1	1
B	236	PHE	CB-CG-CD1	18.80	152.66	120.70	1	1
C	22	ARG	C-N-CA	18.14	154.35	121.70	1	1
B	236	PHE	CG-CD2-CE2	17.78	90.47	120.70	1	1
D	22	ARG	C-N-CA	15.37	94.03	121.70	1	1
C	25	PRO	CA-C-N	15.00	139.40	116.90	1	1
C	47	GLY	C-N-CA	13.67	97.09	121.70	1	1
C	26	PRO	CA-N-CD	13.39	93.26	112.00	1	1
C	25	PRO	N-CA-CB	13.39	88.28	103.00	1	1
B	255	THR	CA-C-N	13.12	136.58	116.90	1	1
C	26	PRO	C-CA-CB	12.42	86.50	110.10	1	1
B	182	GLU	C-CA-CB	12.05	87.21	110.10	1	1
A	182	GLU	C-CA-CB	11.94	87.42	110.10	1	1
A	374	PHE	CA-CB-CG	11.91	101.89	113.80	1	1
B	313	ASP	C-N-CA	11.89	143.11	121.70	1	1
D	26	PRO	C-N-CA	11.85	143.03	121.70	1	1
B	256	PRO	CA-N-CD	11.39	96.06	112.00	1	1
A	82	PHE	CA-CB-CG	11.29	102.51	113.80	1	1
B	248	GLU	CA-C-N	11.22	133.73	116.90	1	1
D	12	GLY	N-CA-C	11.09	81.14	113.30	1	1
A	237	TYR	CA-CB-CG	11.06	93.99	113.90	1	1
C	24	GLY	CA-C-N	11.01	100.38	116.90	1	1
B	207	PHE	CA-CB-CG	10.84	102.96	113.80	1	1
B	317	THR	C-CA-CB	10.69	85.59	109.10	1	1
A	300	GLU	N-CA-CB	10.67	128.64	110.50	1	1
C	28	PHE	CA-C-O	10.24	103.39	120.80	1	1
B	67	SER	C-N-CA	10.17	140.00	121.70	1	1
A	261	VAL	C-CA-CB	10.13	92.15	111.40	1	1
D	27	LYS	O-C-N	10.03	106.96	123.00	1	1
A	256	PRO	C-CA-CB	9.98	129.07	110.10	1	1
C	46	GLN	N-CA-CB	9.96	127.44	110.50	1	1
B	360	PHE	CA-CB-CG	9.81	103.99	113.80	1	1
D	45	VAL	C-N-CA	9.81	104.04	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	101	ILE	CA-C-N	9.73	131.49	116.90	1	1
C	27	LYS	C-N-CA	9.52	104.56	121.70	1	1
D	23	LYS	N-CA-CB	9.46	126.57	110.50	1	1
C	21	PRO	C-N-CA	9.35	104.87	121.70	1	1
A	299	ALA	C-N-CA	9.32	104.93	121.70	1	1
A	313	ASP	C-N-CA	9.30	138.44	121.70	1	1
C	26	PRO	N-CA-CB	9.24	113.17	103.00	1	1
A	137	LEU	C-N-CA	9.24	105.07	121.70	1	1
C	25	PRO	O-C-N	9.17	108.32	123.00	1	1
D	46	GLN	C-CA-CB	9.14	127.47	110.10	1	1
A	191	TRP	N-CA-CB	9.10	95.04	110.50	1	1
B	74	VAL	C-N-CA	9.09	105.33	121.70	1	1
B	73	LEU	N-CA-CB	8.95	125.72	110.50	1	1
A	256	PRO	C-N-CA	8.94	137.80	121.70	1	1
A	195	LYS	N-CA-CB	8.88	125.60	110.50	1	1
A	360	PHE	CA-CB-CG	8.84	104.96	113.80	1	1
B	256	PRO	N-CA-CB	8.78	112.66	103.00	1	1
A	313	ASP	N-CA-C	8.78	86.42	111.00	1	1
B	217	TYR	CA-CB-CG	8.72	98.20	113.90	1	1
B	300	GLU	C-CA-CB	8.67	93.63	110.10	1	1
A	212	TYR	C-N-CA	8.57	106.28	121.70	1	1
A	75	ASN	CA-C-N	8.51	129.66	116.90	1	1
A	257	ASP	CA-CB-CG	8.33	104.27	112.60	1	1
B	238	ASP	CA-CB-CG	8.32	104.28	112.60	1	1
B	137	LEU	C-N-CA	8.27	106.81	121.70	1	1
B	318	PHE	CA-CB-CG	8.26	105.54	113.80	1	1
B	74	VAL	C-CA-CB	8.24	95.75	111.40	1	1
C	46	GLN	C-CA-CB	8.20	94.53	110.10	1	1
D	27	LYS	CA-C-N	8.16	132.51	116.20	1	1
B	313	ASP	N-CA-C	8.08	88.36	111.00	1	1
B	217	TYR	N-CA-CB	8.07	124.22	110.50	1	1
A	351	PHE	CA-CB-CG	8.04	105.76	113.80	1	1
D	28	PHE	C-N-CA	8.00	136.10	121.70	1	1
A	67	SER	C-N-CA	8.00	136.10	121.70	1	1
A	235	GLU	C-N-CA	7.98	107.34	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	237	TYR	CA-CB-CG	7.94	99.61	113.90	1	1
A	191	TRP	C-CA-CB	7.93	125.16	110.10	1	1
C	23	LYS	N-CA-CB	7.89	123.91	110.50	1	1
A	69	PHE	CA-CB-CG	7.75	106.05	113.80	1	1
A	392	GLU	C-N-CA	7.74	135.64	121.70	1	1
B	313	ASP	CA-CB-CG	7.69	104.91	112.60	1	1
B	229	ASP	CA-CB-CG	7.63	104.97	112.60	1	1
C	49	GLY	N-CA-C	7.63	91.18	113.30	1	1
B	236	PHE	CB-CG-CD2	7.59	133.61	120.70	1	1
A	318	PHE	CA-CB-CG	7.47	106.33	113.80	1	1
D	14	ALA	C-CA-CB	7.40	99.40	110.50	1	1
B	236	PHE	CA-CB-CG	7.37	106.43	113.80	1	1
C	23	LYS	N-CA-C	7.34	90.44	111.00	1	1
A	313	ASP	CA-CB-CG	7.29	105.31	112.60	1	1
A	78	LYS	C-CA-CB	7.26	96.31	110.10	1	1
D	47	GLY	C-N-CA	7.25	134.75	121.70	1	1
A	74	VAL	N-CA-CB	7.25	99.17	111.50	1	1
A	303	PHE	N-CA-CB	7.23	122.79	110.50	1	1
B	136	VAL	N-CA-C	7.20	90.83	111.00	1	1
A	136	VAL	N-CA-C	7.20	90.84	111.00	1	1
B	256	PRO	N-CD-CG	7.19	113.99	103.20	1	1
B	110	PHE	CA-CB-CG	7.18	106.62	113.80	1	1
D	27	LYS	N-CA-C	7.15	131.02	111.00	1	1
C	30	GLN	CB-CG-CD	7.15	100.45	112.60	1	1
B	255	THR	CA-C-O	7.10	108.72	120.80	1	1
B	256	PRO	C-N-CA	7.09	134.47	121.70	1	1
B	392	GLU	O-C-N	7.09	111.65	123.00	1	1
B	374	PHE	CA-CB-CG	7.06	106.74	113.80	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	210.32	3074

There are 3074 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)
B:392:GLU:C	B:392:GLU:CA	1.54	1	1
A:392:GLU:C	A:392:GLU:CA	1.53	1	1
A:41:ARG:HD3	E:1:35G:N1	1.40	1	1
A:41:ARG:CD	E:1:35G:HN1	1.36	1	1
A:197:PHE:HB2	B:380:LEU:HD13	1.19	1	1
B:255:THR:CA	D:27:LYS:HA	1.19	1	1
A:110:PHE:CE1	E:1:35G:O1P	1.17	1	1
A:257:ASP:N	C:26:PRO:HD3	1.17	1	1
A:11:LEU:HD21	A:28:LYS:HE2	1.16	1	1
A:101:ILE:HG23	A:102:PRO:HA	1.15	1	1
B:29:THR:HG21	B:166:ILE:HG12	1.14	1	1
B:255:THR:HA	D:27:LYS:HA	1.13	1	1
B:210:ALA:HA	C:46:GLN:HG2	1.13	1	1
B:225:VAL:HG12	B:267:ILE:HG22	1.13	1	1
A:130:ILE:HG12	A:163:LEU:HD11	1.13	1	1
C:45:VAL:HG21	C:50:ASP:H	1.13	1	1
B:255:THR:HG23	D:26:PRO:HB2	1.12	1	1
A:120:TYR:HB2	C:3:GLU:HG3	1.12	1	1
A:22:MET:HG3	A:173:HIS:HB2	1.12	1	1
D:3:GLU:HG2	D:5:PRO:HD2	1.12	1	1
B:74:VAL:HA	B:78:LYS:HB2	1.12	1	1
B:361:ASP:H	B:364:ASP:HB2	1.12	1	1
A:126:MET:HE1	A:156:GLU:HG3	1.11	1	1
B:227:LEU:HB3	B:265:LYS:HB3	1.11	1	1
B:82:PHE:HZ	B:89:ALA:HB3	1.11	1	1
A:59:ARG:HA	A:78:LYS:HG3	1.11	1	1
B:228:LEU:HD21	B:261:VAL:HB	1.10	1	1
B:30:LEU:HD21	B:44:MET:HE3	1.10	1	1
A:361:ASP:H	A:364:ASP:HB3	1.10	1	1
A:43:SER:HA	A:60:LEU:HD12	1.09	1	1
B:188:MET:HE2	B:214:ILE:HA	1.09	1	1
B:63:VAL:HG13	B:67:SER:HB2	1.09	1	1
A:130:ILE:HG21	A:170:LEU:HD11	1.09	1	1
B:307:MET:HG2	B:312:ALA:HB3	1.09	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:64:THR:HG23	A:66:THR:H	1.09	1	1
B:295:PRO:HB3	B:348:VAL:HG11	1.09	1	1
A:258:GLY:HA2	A:297:TYR:HB2	1.09	1	1
A:307:MET:HB3	A:312:ALA:HB3	1.09	1	1
B:57:ALA:HB1	B:79:GLU:HB3	1.09	1	1
A:213:THR:HB	D:45:VAL:HA	1.08	1	1
A:61:LEU:HB2	A:72:ASN:HD22	1.08	1	1
B:258:GLY:HA2	B:297:TYR:HB2	1.07	1	1
A:230:MET:HE3	A:342:LYS:HE2	1.07	1	1
B:44:MET:H	B:60:LEU:HB3	1.07	1	1
B:122:THR:HA	F:1:35G:N3	1.07	1	1
A:26:VAL:HG13	A:166:ILE:HD11	1.07	1	1
A:385:TYR:HA	A:388:MET:HE2	1.07	1	1
A:79:GLU:HG3	C:11:THR:HG23	1.07	1	1
B:96:LYS:HE3	B:136:VAL:HG13	1.07	1	1
A:41:ARG:HD3	E:1:35G:C6	1.06	1	1
B:46:ILE:HG23	B:59:ARG:HB3	1.06	1	1
B:25:ILE:HG21	B:169:VAL:HG11	1.06	1	1
A:319:GLN:HB2	A:330:ILE:HB	1.06	1	1
B:213:THR:HB	C:46:GLN:HG3	1.06	1	1
A:63:VAL:HG13	A:67:SER:HB2	1.05	1	1
A:331:LYS:HG2	C:9:LEU:HB2	1.05	1	1
A:60:LEU:HD23	A:68:LYS:HG2	1.05	1	1
A:221:GLU:HG3	A:272:HIS:HB2	1.05	1	1
A:214:ILE:HG23	A:217:TYR:HD2	1.04	1	1
B:41:ARG:HD3	B:62:ASN:HB3	1.04	1	1
B:88:ILE:HD11	B:104:VAL:HG13	1.04	1	1
A:195:LYS:HB3	D:46:GLN:HB3	1.04	1	1
B:259:ARG:HB2	D:22:ARG:HB2	1.04	1	1
B:257:ASP:H	B:300:GLU:HB3	1.04	1	1
B:257:ASP:N	B:300:GLU:HB3	1.03	1	1
B:336:LEU:HB2	B:372:THR:HG21	1.03	1	1
A:295:PRO:HA	A:348:VAL:HG11	1.03	1	1
A:181:ILE:HD11	A:367:ILE:HG21	1.02	1	1
A:307:MET:HE2	A:333:VAL:HG22	1.02	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:92:VAL:HG11	A:139:VAL:HG21	1.02	1	1
A:286:ASP:HA	A:291:ILE:HD11	1.02	1	1
C:23:LYS:HG2	C:27:LYS:HE3	1.01	1	1
A:342:LYS:HB3	A:346:VAL:HG11	1.01	1	1
B:215:ARG:HG2	B:271:LEU:HD11	1.00	1	1
B:310:ALA:HB2	D:9:LEU:HD22	1.00	1	1
B:266:ILE:HD13	B:283:PRO:HG3	1.00	1	1
A:122:THR:HA	E:1:35G:N3	1.00	1	1
C:23:LYS:HD3	C:27:LYS:HG2	1.00	1	1
A:164:ASN:HB3	B:12:LEU:HD22	1.00	1	1
A:188:MET:HE2	A:371:LEU:HB2	1.00	1	1
B:191:TRP:CZ3	C:43:LYS:HA	0.99	1	1
A:37:LEU:HD11	A:151:PHE:CE1	0.99	1	1
A:213:THR:CB	D:45:VAL:HA	0.99	1	1
B:78:LYS:HA	B:78:LYS:HE3	0.99	1	1
B:299:ALA:HB1	B:345:ILE:HG21	0.99	1	1
B:221:GLU:HB2	B:352:TYR:CD2	0.99	1	1
B:295:PRO:HA	B:348:VAL:HG21	0.98	1	1
B:76:PRO:HD2	B:358:LYS:HG2	0.98	1	1
A:165:PHE:HA	B:12:LEU:HD11	0.98	1	1
A:322:PRO:HG3	A:329:VAL:HA	0.98	1	1
A:214:ILE:HG23	A:217:TYR:CD2	0.98	1	1
B:98:PHE:HD1	B:128:ILE:HG13	0.98	1	1
B:49:SER:HB2	B:362:GLU:HB3	0.98	1	1
A:299:ALA:HA	A:345:ILE:HD13	0.98	1	1
A:82:PHE:CE1	A:114:LEU:HA	0.97	1	1
B:82:PHE:CZ	B:89:ALA:HB3	0.97	1	1
A:59:ARG:HA	A:78:LYS:CG	0.97	1	1
A:59:ARG:CA	A:78:LYS:HG3	0.97	1	1
B:341:LYS:HD2	B:380:LEU:HD12	0.97	1	1
A:59:ARG:HB2	A:78:LYS:HE2	0.97	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	892	766	87	39

There are 39 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	51	ASN	1
A	60	LEU	1
A	69	PHE	1
A	123	VAL	1
A	238	ASP	1
A	286	ASP	1
A	301	ASN	1
A	302	GLY	1
A	312	ALA	1
A	314	GLU	1
A	315	TYR	1
A	322	PRO	1
A	342	LYS	1
B	60	LEU	1
B	69	PHE	1
B	75	ASN	1
B	79	GLU	1
B	103	ASP	1
B	123	VAL	1
B	218	LEU	1
B	256	PRO	1
B	312	ALA	1
B	314	GLU	1
B	315	TYR	1
B	342	LYS	1
C	6	THR	1
C	10	THR	1
C	11	THR	1
C	23	LYS	1
C	25	PRO	1
C	26	PRO	1

Chain	Res	Type	Models (Total)
C	27	LYS	1
C	30	GLN	1
C	44	GLY	1
D	11	THR	1
D	15	PRO	1
D	26	PRO	1
D	39	LYS	1
D	48	PHE	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	812	683	74	55

There are 55 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	27	HIS	1
A	37	LEU	1
A	41	ARG	1
A	70	GLU	1
A	78	LYS	1
A	84	LEU	1
A	134	LYS	1
A	162	TYR	1
A	170	LEU	1
A	174	HIS	1
A	181	ILE	1
A	184	ARG	1
A	185	ARG	1
A	217	TYR	1
A	218	LEU	1
A	240	TRP	1
A	254	LYS	1
A	280	ILE	1
A	294	LEU	1

Chain	Res	Type	Models (Total)
A	304	ILE	1
A	319	GLN	1
A	320	LYS	1
A	336	LEU	1
A	340	ASN	1
A	341	LYS	1
A	342	LYS	1
A	368	ILE	1
A	380	LEU	1
A	393	ASN	1
B	22	MET	1
B	25	ILE	1
B	27	HIS	1
B	78	LYS	1
B	86	ILE	1
B	105	LYS	1
B	182	GLU	1
B	206	GLN	1
B	294	LEU	1
B	301	ASN	1
B	304	ILE	1
B	308	MET	1
B	331	LYS	1
B	332	ASN	1
B	336	LEU	1
B	341	LYS	1
B	342	LYS	1
B	345	ILE	1
B	367	ILE	1
B	393	ASN	1
B	394	ARG	1
C	23	LYS	1
C	25	PRO	1
C	28	PHE	1
C	34	ARG	1

Chain	Res	Type	Models (Total)
C	37	LYS	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.

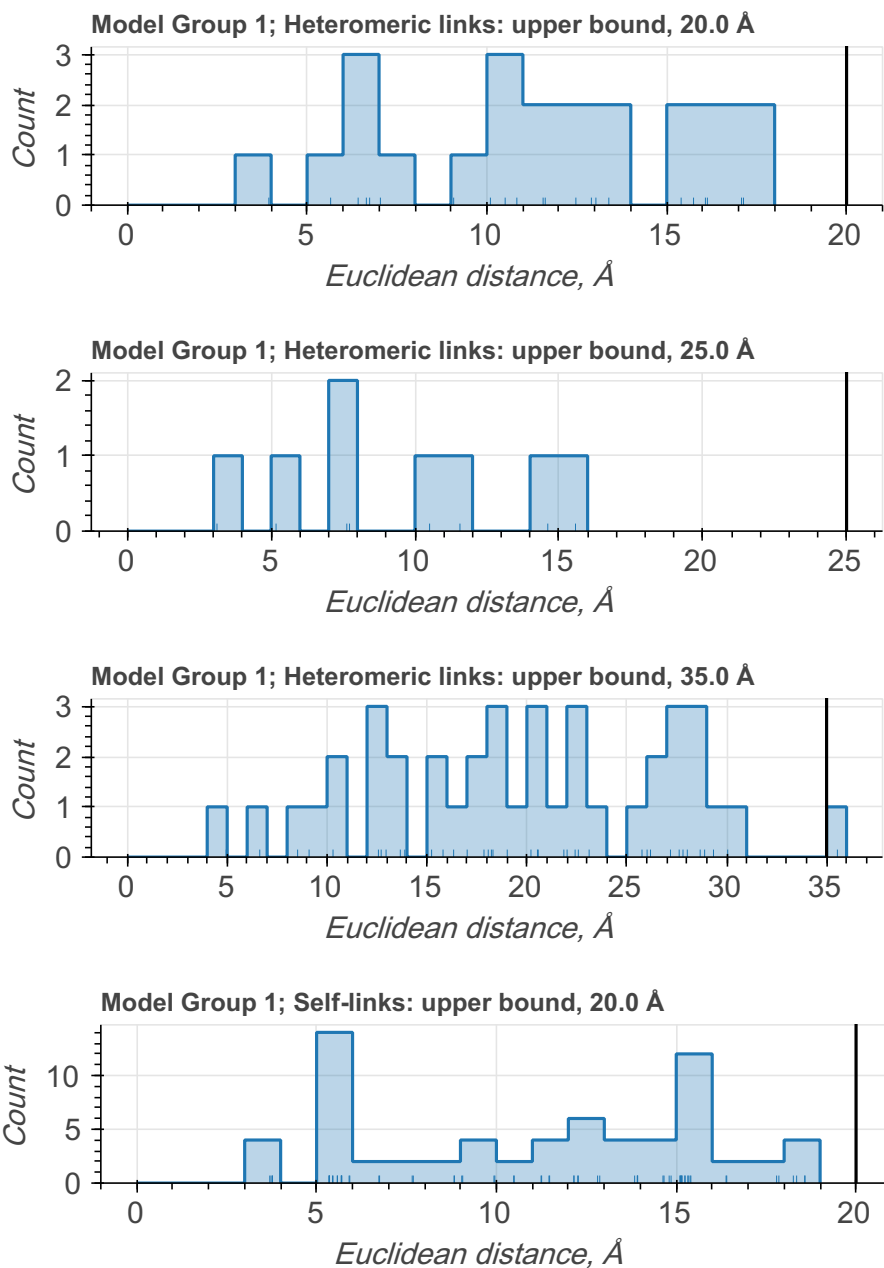
There are 242 crosslinking restraints combined in 121 restraint groups.

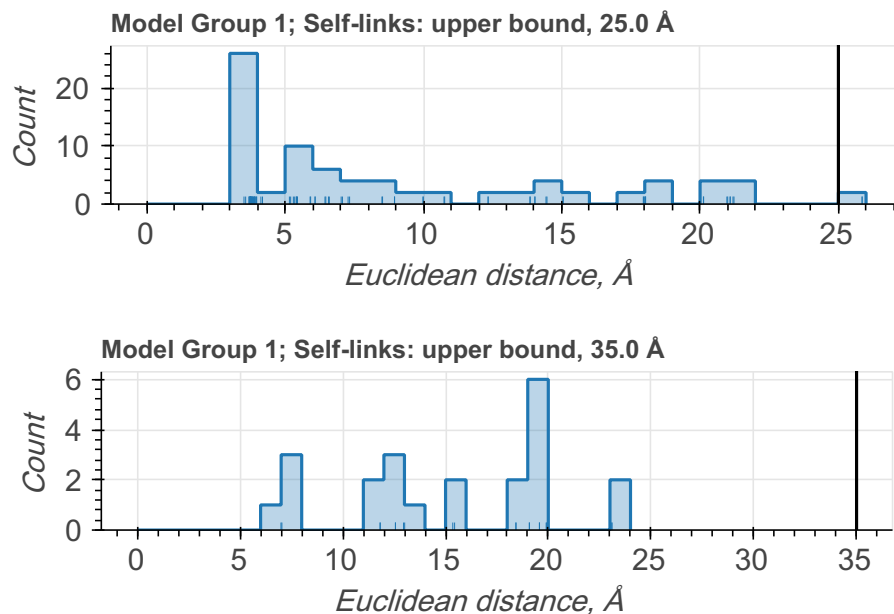
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
EDC	GLU	CA	LYS	CA	upper bound	20.0	58
EDC	LYS	CA	MET	CA	upper bound	20.0	2
EDC	ASP	CA	LYS	CA	upper bound	20.0	26
EDC	ASP	CA	THR	CA	upper bound	20.0	4
BS3	LYS	CA	LYS	CA	upper bound	35.0	56
BS3	LYS	CA	THR	CA	upper bound	35.0	4
BS3	GLN	CA	LYS	CA	upper bound	35.0	2
sulfo-SDA	ILE	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	LYS	CA	THR	CA	upper bound	25.0	6
sulfo-SDA	ARG	CA	LYS	CA	upper bound	25.0	2
sulfo-SDA	LYS	CA	SER	CA	upper bound	25.0	2
sulfo-SDA	LYS	CA	PHE	CA	upper bound	25.0	4
sulfo-SDA	ASN	CA	LYS	CA	upper bound	25.0	6
sulfo-SDA	LYS	CA	PRO	CA	upper bound	25.0	2
sulfo-SDA	LYS	CA	TYR	CA	upper bound	25.0	4
sulfo-SDA	GLU	CA	LYS	CA	upper bound	25.0	16
sulfo-SDA	LYS	CA	VAL	CA	upper bound	25.0	10
sulfo-SDA	HIS	CA	LYS	CA	upper bound	25.0	2
sulfo-SDA	LEU	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	GLY	CA	LYS	CA	upper bound	25.0	10
sulfo-SDA	ALA	CA	LYS	CA	upper bound	25.0	2
sulfo-SDA	LYS	CA	LYS	CA	upper bound	25.0	6
sulfo-SDA	ASP	CA	LYS	CA	upper bound	25.0	6

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
sulfo-SDA	THR	CA	TYR	CA	upper bound	25.0	2
sulfo-SDA	ALA	CA	GLN	CA	upper bound	25.0	2

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.





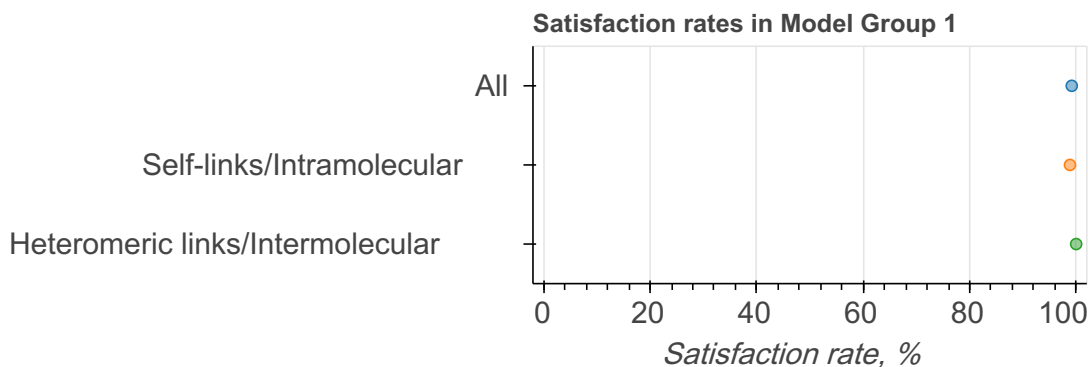
Satisfaction of restraints

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=121)
1	1	1	1/1	All	99.17	0.83	121
				Self-links/ Intramolecular	98.84	1.16	86
				Heteromeric links/ Intermolecular	100.00	0.00	35

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.