

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	9A0M
PDB-Dev ID	PDBDEV_00000058
Structure Title	Integrative structure of 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

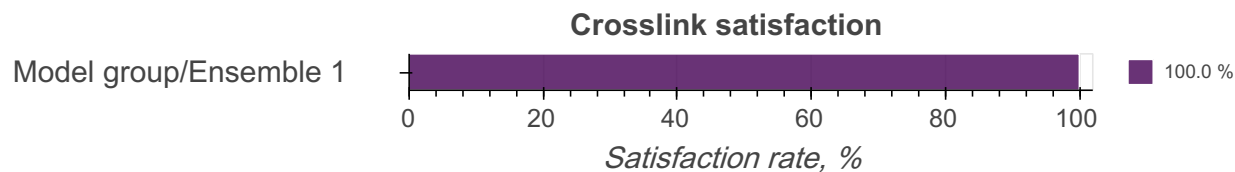
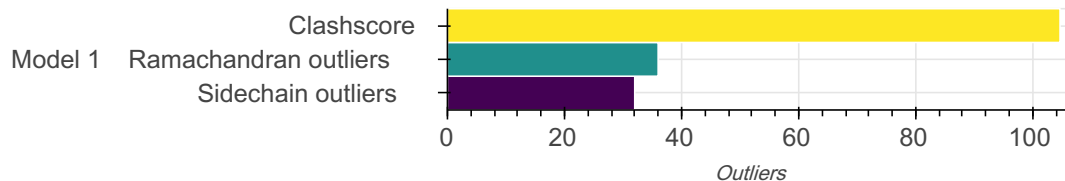
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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

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	PXD020817

ID	Dataset type	Database name	Data access code
2	Experimental model	PDB	6X88
3	Experimental model	PDB	6MZB

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 65 bond length outliers in this entry (0.97% of 6671 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	395	LYS	C-N	16.18	1.56	1.33	1	1
B	396	ASP	N-CA	12.38	1.69	1.46	1	1
A	254	LYS	C-N	12.37	1.50	1.33	1	1
B	254	LYS	C-N	12.34	1.50	1.33	1	1
A	256	PRO	C-N	11.68	1.49	1.33	1	1
B	256	PRO	C-N	11.38	1.49	1.33	1	1
A	256	PRO	N-CA	11.27	1.64	1.47	1	1
B	255	THR	C-N	11.27	1.52	1.34	1	1
B	256	PRO	N-CA	11.21	1.63	1.47	1	1
A	255	THR	C-N	11.09	1.52	1.34	1	1
B	396	ASP	CA-C	10.52	1.30	1.52	1	1
A	254	LYS	CA-C	10.43	1.74	1.52	1	1
B	254	LYS	CA-C	10.31	1.74	1.52	1	1
A	255	THR	CA-C	9.55	1.73	1.52	1	1
B	255	THR	CA-C	9.50	1.72	1.52	1	1
A	256	PRO	CA-C	8.80	1.71	1.52	1	1
A	114	LEU	CA-C	8.60	1.34	1.52	1	1
A	115	ASP	N-CA	8.59	1.29	1.46	1	1
A	255	THR	N-CA	8.58	1.62	1.46	1	1
B	256	PRO	CA-C	8.57	1.71	1.52	1	1
B	115	ASP	N-CA	8.56	1.30	1.46	1	1
B	255	THR	N-CA	8.52	1.62	1.46	1	1
B	396	ASP	C-N	8.50	1.21	1.33	1	1
B	341	LYS	C-N	8.36	1.45	1.33	1	1
B	388	MET	C-N	8.23	1.44	1.33	1	1
B	114	LEU	CA-C	8.11	1.35	1.52	1	1
A	341	LYS	C-N	7.72	1.44	1.33	1	1
A	257	ASP	CA-C	7.69	1.69	1.52	1	1
B	257	ASP	N-CA	7.60	1.60	1.46	1	1
A	257	ASP	N-CA	7.47	1.60	1.46	1	1
B	257	ASP	CA-C	7.22	1.68	1.52	1	1
A	395	LYS	C-N	7.05	1.43	1.33	1	1
B	342	LYS	N-CA	6.77	1.59	1.46	1	1
A	342	LYS	N-CA	5.83	1.57	1.46	1	1
A	396	ASP	CA-C	5.79	1.40	1.52	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	397	ILE	C-N	5.70	1.41	1.33	1	1
B	392	GLU	CA-C	5.65	1.41	1.52	1	1
A	387	LYS	N-CA	5.63	1.35	1.46	1	1
A	319	GLN	C-N	5.57	1.41	1.33	1	1
A	391	LEU	C-N	5.37	1.40	1.33	1	1
A	396	ASP	N-CA	5.35	1.56	1.46	1	1
A	257	ASP	C-N	5.17	1.40	1.33	1	1
A	388	MET	C-N	5.17	1.40	1.33	1	1
B	389	ASN	N-CA	4.94	1.55	1.46	1	1
B	257	ASP	C-N	4.90	1.40	1.33	1	1
B	395	LYS	N-CA	4.83	1.37	1.46	1	1
A	393	ASN	N-CA	4.79	1.37	1.46	1	1
B	387	LYS	N-CA	4.75	1.37	1.46	1	1
B	208	HIS	C-N	4.65	1.39	1.33	1	1
A	343	GLU	N-CA	4.57	1.37	1.46	1	1
A	397	ILE	N-CA	4.44	1.37	1.46	1	1
B	394	ARG	C-N	4.31	1.27	1.33	1	1
B	319	GLN	C-N	4.31	1.39	1.33	1	1
A	314	GLU	C-N	4.28	1.39	1.33	1	1
A	208	HIS	C-N	4.25	1.39	1.33	1	1
B	106	LYS	CA-C	4.22	1.44	1.52	1	1
B	384	THR	CA-C	4.20	1.44	1.52	1	1
B	320	LYS	N-CA	4.19	1.54	1.46	1	1
A	112	ASP	CA-C	4.16	1.44	1.52	1	1
B	388	MET	N-CA	4.14	1.38	1.46	1	1
A	320	LYS	N-CA	4.12	1.54	1.46	1	1
B	318	PHE	CA-C	4.08	1.44	1.52	1	1
B	105	LYS	CA-C	4.05	1.44	1.52	1	1
A	209	LYS	CA-C	4.04	1.61	1.52	1	1
B	112	ASP	CA-C	4.04	1.44	1.52	1	1

Standard geometry: angle outliers ?

There are 304 bond angle outliers in this entry (3.37% of 9020 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	396	ASP	C-N-CA	20.24	85.27	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	395	LYS	C-N-CA	18.98	155.86	121.70	1	1
B	396	ASP	CA-C-N	17.77	80.66	116.20	1	1
B	341	LYS	C-N-CA	14.37	147.57	121.70	1	1
A	256	PRO	C-N-CA	13.75	146.44	121.70	1	1
B	256	PRO	C-N-CA	13.55	146.09	121.70	1	1
A	341	LYS	C-N-CA	12.98	145.07	121.70	1	1
B	392	GLU	C-N-CA	12.87	98.53	121.70	1	1
B	303	PHE	CA-CB-CG	12.39	101.41	113.80	1	1
A	396	ASP	C-N-CA	12.18	99.77	121.70	1	1
B	256	PRO	N-CA-C	12.15	142.48	112.10	1	1
A	256	PRO	N-CA-C	12.07	142.28	112.10	1	1
B	315	TYR	C-N-CA	12.03	143.35	121.70	1	1
A	105	LYS	C-N-CA	11.44	101.11	121.70	1	1
B	395	LYS	CA-C-O	11.34	101.53	120.80	1	1
A	395	LYS	C-N-CA	11.13	141.73	121.70	1	1
B	397	ILE	C-N-CA	10.76	141.06	121.70	1	1
A	392	GLU	C-N-CA	10.41	102.96	121.70	1	1
B	389	ASN	C-N-CA	10.33	103.11	121.70	1	1
B	388	MET	CA-C-O	10.30	103.29	120.80	1	1
B	148	ALA	C-N-CA	10.27	140.18	121.70	1	1
B	257	ASP	N-CA-C	10.26	139.73	111.00	1	1
B	396	ASP	CA-C-O	10.26	138.24	120.80	1	1
A	257	ASP	N-CA-C	10.25	139.71	111.00	1	1
B	197	PHE	CA-CB-CG	9.95	103.85	113.80	1	1
B	394	ARG	C-N-CA	9.93	103.83	121.70	1	1
B	318	PHE	C-CA-CB	9.92	91.25	110.10	1	1
B	388	MET	C-N-CA	9.91	139.54	121.70	1	1
B	316	PHE	CA-CB-CG	9.76	104.04	113.80	1	1
A	391	LEU	C-N-CA	9.62	139.02	121.70	1	1
A	254	LYS	CA-C-N	9.49	135.18	116.20	1	1
B	320	LYS	N-CA-C	9.37	84.75	111.00	1	1
B	257	ASP	CA-C-N	9.33	134.87	116.20	1	1
A	257	ASP	CA-C-N	9.29	134.79	116.20	1	1
B	254	LYS	CA-C-N	9.19	134.57	116.20	1	1
B	394	ARG	C-CA-CB	9.12	92.76	110.10	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	320	LYS	CA-CB-CG	8.99	96.11	114.10	1	1
A	320	LYS	N-CA-C	8.99	85.84	111.00	1	1
A	257	ASP	O-C-N	8.91	108.74	123.00	1	1
B	319	GLN	C-N-CA	8.83	137.59	121.70	1	1
A	315	TYR	C-CA-CB	8.74	93.49	110.10	1	1
A	82	PHE	CA-CB-CG	8.70	105.10	113.80	1	1
A	98	PHE	CA-CB-CG	8.70	105.10	113.80	1	1
B	315	TYR	C-CA-CB	8.66	93.65	110.10	1	1
B	318	PHE	N-CA-C	8.63	86.84	111.00	1	1
B	257	ASP	O-C-N	8.60	109.24	123.00	1	1
B	69	PHE	CA-CB-CG	8.26	105.54	113.80	1	1
B	397	ILE	CA-C-O	8.23	106.81	120.80	1	1
B	312	ALA	N-CA-C	7.97	133.33	111.00	1	1
A	386	ASP	C-N-CA	7.63	107.96	121.70	1	1
B	96	LYS	C-N-CA	7.63	135.43	121.70	1	1
A	338	ILE	C-N-CA	7.55	108.11	121.70	1	1
B	393	ASN	CA-C-N	7.52	101.16	116.20	1	1
B	392	GLU	CB-CG-CD	7.51	99.83	112.60	1	1
A	388	MET	CG-SD-CE	7.50	84.41	100.90	1	1
B	234	LYS	C-N-CA	7.49	135.18	121.70	1	1
A	197	PHE	CA-CB-CG	7.45	106.35	113.80	1	1
B	313	ASP	CA-CB-CG	7.43	105.17	112.60	1	1
B	320	LYS	C-CA-CB	7.42	124.20	110.10	1	1
B	255	THR	N-CA-C	7.32	131.51	111.00	1	1
A	255	THR	N-CA-C	7.29	131.42	111.00	1	1
A	96	LYS	C-N-CA	7.17	134.61	121.70	1	1
B	394	ARG	CA-C-O	7.17	132.99	120.80	1	1
B	114	LEU	CA-C-N	7.13	101.93	116.20	1	1
A	114	LEU	CA-C-N	7.10	102.00	116.20	1	1
B	98	PHE	CA-CB-CG	7.08	106.72	113.80	1	1
B	311	PRO	N-CA-C	7.01	129.64	112.10	1	1
A	363	TYR	CA-CB-CG	6.96	101.37	113.90	1	1
B	9	PHE	CA-CB-CG	6.86	106.94	113.80	1	1
B	391	LEU	C-N-CA	6.82	133.98	121.70	1	1
B	397	ILE	N-CA-C	6.70	129.77	111.00	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	395	LYS	CA-C-N	6.70	129.59	116.20	1	1
A	318	PHE	N-CA-C	6.69	92.26	111.00	1	1
A	72	ASN	CA-CB-CG	6.68	105.92	112.60	1	1
B	321	GLY	CA-C-N	6.63	126.84	116.90	1	1
A	311	PRO	N-CA-C	6.61	128.62	112.10	1	1
A	374	PHE	CA-CB-CG	6.58	107.22	113.80	1	1
B	393	ASN	C-N-CA	6.57	109.88	121.70	1	1
A	207	PHE	CA-CB-CG	6.53	107.27	113.80	1	1
A	391	LEU	C-CA-CB	6.51	97.74	110.10	1	1
B	352	TYR	CA-CB-CG	6.45	102.28	113.90	1	1
B	360	PHE	CA-CB-CG	6.43	107.37	113.80	1	1
B	162	TYR	CA-CB-CG	6.42	102.35	113.90	1	1
A	389	ASN	C-N-CA	6.40	110.18	121.70	1	1
A	9	PHE	CA-CB-CG	6.38	107.42	113.80	1	1
B	363	TYR	CA-CB-CG	6.34	102.49	113.90	1	1
A	380	LEU	C-CA-CB	6.31	98.11	110.10	1	1
A	351	PHE	CA-CB-CG	6.29	107.51	113.80	1	1
B	380	LEU	C-CA-CB	6.25	98.22	110.10	1	1
B	147	ASN	CA-CB-CG	6.16	106.44	112.60	1	1
B	338	ILE	C-N-CA	6.13	110.67	121.70	1	1
A	236	PHE	C-CA-CB	6.12	98.47	110.10	1	1
B	48	ARG	C-CA-CB	6.11	98.49	110.10	1	1
B	312	ALA	C-CA-CB	6.11	101.34	110.50	1	1
B	255	THR	CA-C-N	6.07	126.01	116.90	1	1
B	386	ASP	C-N-CA	6.05	110.81	121.70	1	1
A	391	LEU	CA-C-O	6.01	110.58	120.80	1	1
A	254	LYS	O-C-N	6.00	113.39	123.00	1	1
A	255	THR	CA-C-N	5.91	125.77	116.90	1	1
A	235	GLU	C-N-CA	5.90	132.32	121.70	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	104.67	1365

There are 1365 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:254:LYS:C	B:254:LYS:CA	1.59	1	1
A:254:LYS:C	A:254:LYS:CA	1.57	1	1
B:396:ASP:CA	B:396:ASP:N	1.54	1	1
A:122:THR:HG23	C:1:35G:C2	1.51	1	1
B:110:PHE:CZ	D:1:35G:O2'	1.36	1	1
B:111:SER:O	D:1:35G:H4'	1.33	1	1
B:143:LEU:CD2	D:1:35G:O6	1.33	1	1
B:396:ASP:N	B:397:ILE:N	1.29	1	1
B:143:LEU:HD21	D:1:35G:O6	1.27	1	1
A:122:THR:HG21	C:1:35G:C6	1.26	1	1
A:115:ASP:OD2	C:1:35G:C1'	1.26	1	1
A:115:ASP:OD2	C:1:35G:H1'	1.19	1	1
A:122:THR:CG2	C:1:35G:N1	1.18	1	1
A:115:ASP:CG	C:1:35G:N3	1.17	1	1
A:115:ASP:OD2	C:1:35G:N3	1.17	1	1
A:122:THR:CG2	C:1:35G:C2	1.14	1	1
B:188:MET:HG2	B:214:ILE:HD11	1.13	1	1
B:396:ASP:N	B:397:ILE:H	1.13	1	1
B:128:ILE:HG21	B:163:LEU:HD13	1.13	1	1
A:342:LYS:H	A:342:LYS:HD2	1.13	1	1
B:88:ILE:N	D:1:35G:O2P	1.12	1	1
A:232:LYS:HB2	A:260:GLU:HG2	1.12	1	1
A:181:ILE:HG23	A:367:ILE:HD11	1.11	1	1
A:340:ASN:HD21	A:343:GLU:HB2	1.10	1	1
B:289:CYS:HA	B:320:LYS:HE2	1.10	1	1
A:338:ILE:HG22	A:372:THR:HG23	1.09	1	1
A:126:MET:HE1	A:156:GLU:HA	1.08	1	1
B:230:MET:HA	B:230:MET:HE2	1.08	1	1
A:395:LYS:HB2	B:391:LEU:HD23	1.07	1	1
B:240:TRP:HB2	B:243:ARG:HD2	1.07	1	1
B:257:ASP:HB2	B:301:ASN:HA	1.07	1	1
A:64:THR:HG23	A:67:SER:H	1.06	1	1
B:286:ASP:HA	B:291:ILE:HD11	1.06	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:181:ILE:HD13	B:363:TYR:HB3	1.05	1	1
A:115:ASP:HB2	C:1:35G:O4'	1.03	1	1
A:115:ASP:OD1	C:1:35G:N3	1.03	1	1
A:339:VAL:HG11	A:342:LYS:HA	1.02	1	1
B:340:ASN:HD21	B:343:GLU:HB2	1.02	1	1
A:122:THR:HG21	A:143:LEU:HD23	1.02	1	1
B:392:GLU:HG3	B:398:ALA:HB3	1.02	1	1
A:195:LYS:HD2	A:209:LYS:HG2	1.01	1	1
A:294:LEU:HD11	A:307:MET:HE1	1.01	1	1
A:395:LYS:HG2	A:398:ALA:HB2	1.00	1	1
A:257:ASP:HB2	A:301:ASN:HA	1.00	1	1
A:288:TRP:HE3	A:320:LYS:HA	0.99	1	1
A:289:CYS:HA	A:320:LYS:HE2	0.99	1	1
B:87:GLY:HA2	B:111:SER:HB3	0.99	1	1
B:319:GLN:HG2	B:330:ILE:H	0.98	1	1
B:110:PHE:CE1	D:1:35G:O2'	0.97	1	1
A:288:TRP:CE3	A:320:LYS:HA	0.97	1	1
B:321:GLY:HA3	B:328:TRP:CE3	0.96	1	1
A:294:LEU:HA	A:315:TYR:CE1	0.96	1	1
A:395:LYS:HG2	B:391:LEU:HB2	0.96	1	1
B:200:LEU:HD12	B:385:TYR:HD1	0.95	1	1
B:58:THR:HG21	B:61:LEU:HD11	0.95	1	1
A:82:PHE:HZ	A:114:LEU:HB2	0.95	1	1
A:388:MET:HA	A:391:LEU:CD1	0.95	1	1
A:118:THR:HG23	A:120:TYR:H	0.95	1	1
A:87:GLY:HA2	A:111:SER:HB3	0.94	1	1
B:225:VAL:HG12	B:267:ILE:HG12	0.94	1	1
A:297:TYR:CD1	A:314:GLU:HB2	0.94	1	1
B:291:ILE:HB	B:318:PHE:CE1	0.94	1	1
A:175:THR:HG23	B:175:THR:HG21	0.94	1	1
B:392:GLU:HG3	B:398:ALA:CB	0.94	1	1
A:339:VAL:CG1	A:342:LYS:HA	0.93	1	1
A:187:GLN:HA	A:187:GLN:HE21	0.93	1	1
A:267:ILE:CD1	A:279:VAL:HG22	0.92	1	1
A:319:GLN:HB3	A:330:ILE:HB	0.92	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:388:MET:HA	A:391:LEU:HD12	0.92	1	1
B:313:ASP:HB2	B:315:TYR:CE2	0.92	1	1
A:181:ILE:HG23	A:367:ILE:CD1	0.92	1	1
B:95:THR:CB	B:97:LYS:HG2	0.92	1	1
A:111:SER:O	C:1:35G:H4'	0.92	1	1
A:122:THR:HG21	C:1:35G:N1	0.91	1	1
B:294:LEU:HB3	B:295:PRO:HD3	0.91	1	1
A:122:THR:CG2	C:1:35G:C6	0.91	1	1
A:319:GLN:HG2	A:330:ILE:H	0.91	1	1
B:297:TYR:CD2	B:314:GLU:HB2	0.91	1	1
B:235:GLU:HB2	B:257:ASP:CA	0.90	1	1
B:319:GLN:HB2	B:322:PRO:HG3	0.90	1	1
A:95:THR:HB	A:97:LYS:HG2	0.90	1	1
A:95:THR:CB	A:97:LYS:HG2	0.89	1	1
B:339:VAL:HG11	B:342:LYS:HA	0.89	1	1
A:371:LEU:HD13	A:375:LEU:HD23	0.89	1	1
A:294:LEU:HB3	A:295:PRO:HD3	0.89	1	1
A:128:ILE:CD1	A:163:LEU:HD13	0.89	1	1
B:111:SER:O	D:1:35G:C4'	0.89	1	1
A:321:GLY:HA3	A:328:TRP:CE3	0.88	1	1
B:319:GLN:HG2	B:330:ILE:N	0.88	1	1
A:291:ILE:HD13	A:318:PHE:CE1	0.88	1	1
B:159:PHE:CE2	B:163:LEU:HD11	0.88	1	1
A:9:PHE:CG	B:161:LYS:HD2	0.88	1	1
B:339:VAL:CG1	B:342:LYS:HA	0.88	1	1
A:340:ASN:ND2	A:343:GLU:HB2	0.88	1	1
A:98:PHE:CD1	A:128:ILE:HG22	0.87	1	1
A:228:LEU:HD22	A:261:VAL:HG13	0.87	1	1
A:82:PHE:CZ	A:114:LEU:HB2	0.87	1	1
B:87:GLY:CA	B:111:SER:HB3	0.87	1	1
A:395:LYS:CG	B:391:LEU:HB2	0.87	1	1
B:304:ILE:HG12	B:336:LEU:HD12	0.87	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	794	716	42	36

There are 36 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	21	SER	1
A	102	PRO	1
A	144	ASN	1
A	234	LYS	1
A	241	PRO	1
A	258	GLY	1
A	261	VAL	1
A	262	ASN	1
A	301	ASN	1
A	302	GLY	1
A	309	ASN	1
A	312	ALA	1
A	313	ASP	1
A	318	PHE	1
A	320	LYS	1
A	324	ASP	1
A	340	ASN	1
A	342	LYS	1
A	353	ASN	1
A	396	ASP	1
B	144	ASN	1
B	148	ALA	1
B	234	LYS	1
B	235	GLU	1
B	238	ASP	1
B	242	ILE	1
B	258	GLY	1
B	261	VAL	1
B	262	ASN	1
B	313	ASP	1
B	320	LYS	1

Chain	Res	Type	Models (Total)
B	340	ASN	1
B	341	LYS	1
B	342	LYS	1
B	353	ASN	1
B	396	ASP	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	724	620	72	32

There are 32 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	22	MET	1
A	28	LYS	1
A	50	ARG	1
A	56	VAL	1
A	187	GLN	1
A	209	LYS	1
A	222	ARG	1
A	235	GLU	1
A	251	LYS	1
A	254	LYS	1
A	260	GLU	1
A	315	TYR	1
A	320	LYS	1
A	342	LYS	1
A	388	MET	1
A	399	GLN	1
B	107	ASN	1
B	200	LEU	1
B	233	GLU	1
B	242	ILE	1
B	251	LYS	1
B	254	LYS	1

Chain	Res	Type	Models (Total)
B	267	ILE	1
B	274	LYS	1
B	315	TYR	1
B	320	LYS	1
B	336	LEU	1
B	390	LYS	1
B	391	LEU	1
B	395	LYS	1
B	397	ILE	1
B	399	GLN	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.

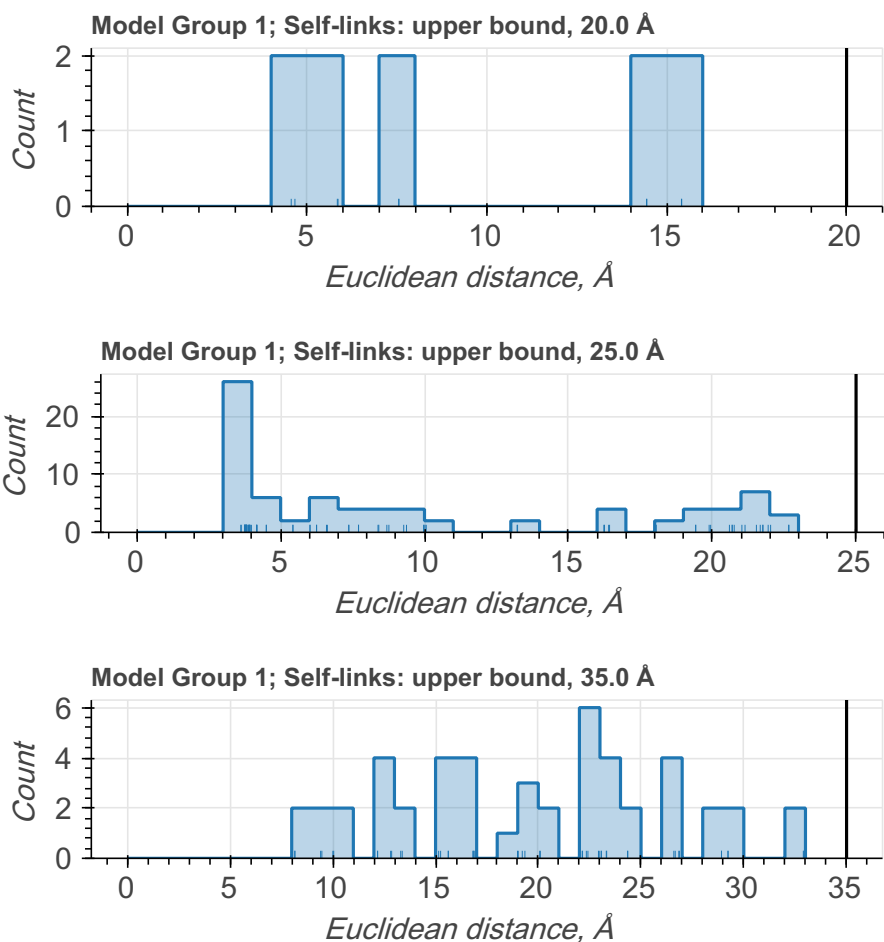
There are 138 crosslinking restraints combined in 69 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
sulfo-SDA	LYS	CA	VAL	CA	upper bound	25.0	10
sulfo-SDA	ILE	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	ARG	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	LYS	CA	PHE	CA	upper bound	25.0	2
sulfo-SDA	GLU	CA	LYS	CA	upper bound	25.0	16
sulfo-SDA	LEU	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	LYS	CA	THR	CA	upper bound	25.0	6
sulfo-SDA	LYS	CA	LYS	CA	upper bound	25.0	10
sulfo-SDA	ASP	CA	LYS	CA	upper bound	25.0	12
sulfo-SDA	ALA	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	LYS	CA	TYR	CA	upper bound	25.0	2
sulfo-SDA	GLY	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	ASN	CA	LYS	CA	upper bound	25.0	2
BS3	LYS	CA	LYS	CA	upper bound	35.0	46

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	MET	CA	upper bound	35.0	2
EDC	ASP	CA	LYS	CA	upper bound	20.0	4
EDC	GLU	CA	LYS	CA	upper bound	20.0	6

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.



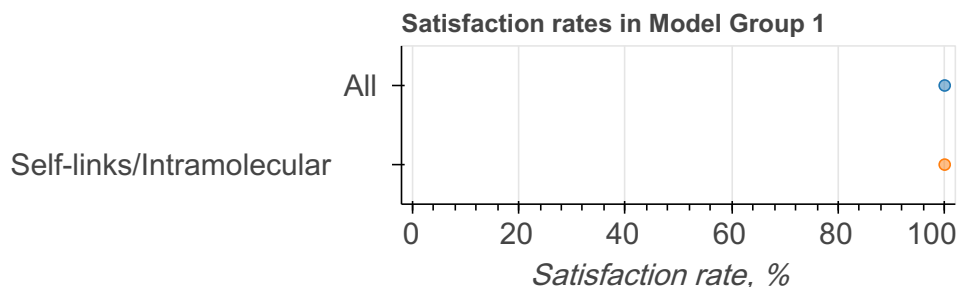
Satisfaction of restraints

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=69)
1	1	1	1/1	All	100.00	0.00	69
				Self-links/ Intramolecular	100.00	0.00	69

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.

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