

Integrative Structure Validation Report ?

March 27, 2025 - 10:02 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	9A00
PDB-Dev ID	PDBDEV_00000060
Structure Title	Integrative structure of Pg-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

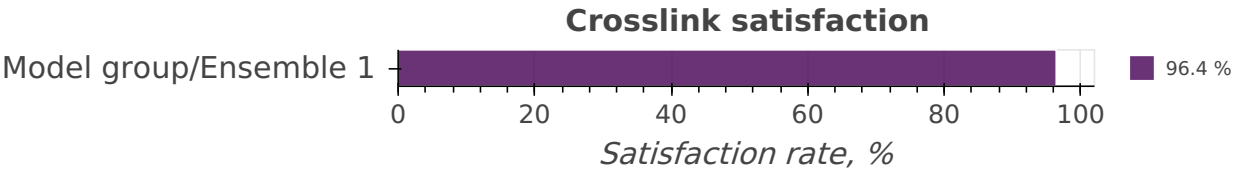
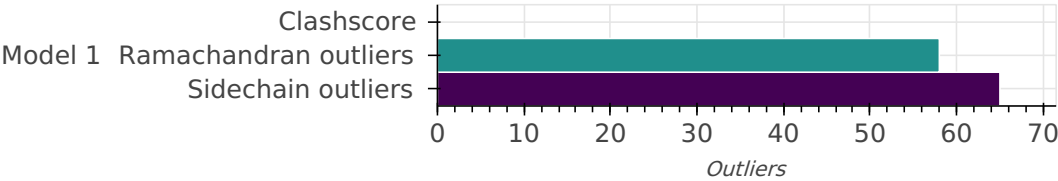
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	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					

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
2	Experimental model	PDB	6X88
3	Integrative model	PDB	9A0N

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 113 bond length outliers in this entry (1.51% of 7465 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)
C	37	LYS	CA-C	14.93	1.84	1.52	1	1
C	37	LYS	C-N	14.47	1.53	1.33	1	1
B	397	ILE	C-N	13.63	1.52	1.33	1	1
B	341	LYS	C-N	13.27	1.51	1.33	1	1
A	67	SER	C-N	13.08	1.51	1.33	1	1
A	341	LYS	C-N	12.98	1.51	1.33	1	1
D	37	LYS	C-N	12.53	1.50	1.33	1	1
D	37	LYS	CA-C	12.43	1.79	1.52	1	1
B	67	SER	C-N	12.32	1.50	1.33	1	1
C	21	PRO	C-N	10.83	1.48	1.33	1	1
B	324	ASP	C-N	10.19	1.47	1.33	1	1
D	38	SER	C-N	10.09	1.47	1.33	1	1
A	68	LYS	N-CA	9.99	1.65	1.46	1	1
B	342	LYS	N-CA	9.84	1.64	1.46	1	1
B	68	LYS	N-CA	9.66	1.64	1.46	1	1
B	341	LYS	CA-C	9.61	1.73	1.52	1	1
A	341	LYS	CA-C	9.53	1.73	1.52	1	1
A	342	LYS	N-CA	9.37	1.64	1.46	1	1
D	38	SER	N-CA	9.33	1.64	1.46	1	1
B	324	ASP	CA-C	9.19	1.72	1.52	1	1
A	324	ASP	C-N	8.73	1.45	1.33	1	1
C	15	PRO	CA-C	8.63	1.34	1.52	1	1
C	38	SER	N-CA	8.44	1.62	1.46	1	1
B	66	THR	C-N	8.44	1.45	1.33	1	1
A	324	ASP	CA-C	8.37	1.70	1.52	1	1
C	22	ARG	C-N	8.31	1.45	1.33	1	1
A	66	THR	C-N	8.28	1.44	1.33	1	1
B	393	ASN	CA-C	8.21	1.35	1.52	1	1
B	398	ALA	N-CA	8.17	1.61	1.46	1	1
C	38	SER	C-N	7.72	1.44	1.33	1	1
B	325	GLU	N-CA	7.49	1.60	1.46	1	1
D	38	SER	CA-C	7.27	1.68	1.52	1	1
A	75	ASN	C-N	7.25	1.22	1.34	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	67	SER	CA-C	7.23	1.68	1.52	1	1
A	264	TYR	C-N	7.06	1.43	1.33	1	1
C	16	THR	CA-C	7.00	1.38	1.52	1	1
D	36	PHE	C-N	6.98	1.43	1.33	1	1
C	21	PRO	CA-C	6.88	1.67	1.52	1	1
A	312	ALA	C-N	6.70	1.42	1.33	1	1
A	67	SER	CA-C	6.57	1.66	1.52	1	1
B	388	MET	C-N	6.53	1.42	1.33	1	1
B	319	GLN	C-N	6.41	1.42	1.33	1	1
D	39	LYS	N-CA	6.39	1.58	1.46	1	1
A	340	ASN	C-N	6.36	1.42	1.33	1	1
C	15	PRO	C-N	6.34	1.42	1.33	1	1
C	38	SER	CA-C	6.30	1.66	1.52	1	1
A	325	GLU	N-CA	6.29	1.58	1.46	1	1
B	340	ASN	C-N	6.17	1.42	1.33	1	1
D	50	ASP	C-N	6.09	1.41	1.33	1	1
C	22	ARG	N-CA	5.96	1.57	1.46	1	1
C	23	LYS	N-CA	5.95	1.57	1.46	1	1
C	10	THR	C-N	5.87	1.41	1.33	1	1
A	319	GLN	C-N	5.82	1.41	1.33	1	1
B	75	ASN	CA-C	5.72	1.40	1.52	1	1
B	397	ILE	N-CA	5.65	1.35	1.46	1	1
B	72	ASN	CA-C	5.62	1.41	1.52	1	1
A	117	LYS	C-N	5.57	1.41	1.33	1	1
C	36	PHE	C-N	5.56	1.41	1.33	1	1
B	76	PRO	N-CA	5.52	1.38	1.47	1	1
B	320	LYS	C-N	5.50	1.41	1.33	1	1
C	50	ASP	C-N	5.34	1.40	1.33	1	1
B	117	LYS	C-N	5.24	1.40	1.33	1	1
C	22	ARG	CA-C	5.22	1.63	1.52	1	1
A	52	GLY	CA-C	5.07	1.42	1.52	1	1
A	397	ILE	C-N	5.05	1.40	1.33	1	1
A	317	THR	N-CA	5.05	1.36	1.46	1	1
D	39	LYS	CA-C	5.04	1.42	1.52	1	1
A	317	THR	CA-CB	4.95	1.41	1.54	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	379	VAL	CA-CB	4.90	1.41	1.54	1	1
B	379	VAL	CA-CB	4.88	1.41	1.54	1	1
B	392	GLU	CA-C	4.88	1.42	1.52	1	1
B	396	ASP	CA-C	4.87	1.42	1.52	1	1
A	248	GLU	C-N	4.86	1.26	1.34	1	1
A	315	TYR	C-N	4.83	1.40	1.33	1	1
B	67	SER	N-CA	4.81	1.55	1.46	1	1
C	25	PRO	C-N	4.78	1.26	1.34	1	1
A	251	LYS	C-N	4.72	1.40	1.33	1	1
A	342	LYS	C-N	4.71	1.39	1.33	1	1
B	67	SER	CA-CB	4.68	1.44	1.53	1	1
A	323	VAL	C-N	4.68	1.39	1.33	1	1
B	68	LYS	C-N	4.65	1.39	1.33	1	1
A	388	MET	C-N	4.65	1.39	1.33	1	1
B	264	TYR	C-N	4.63	1.39	1.33	1	1
B	313	ASP	C-N	4.60	1.39	1.33	1	1
A	320	LYS	CA-C	4.55	1.62	1.52	1	1
A	307	MET	CA-C	4.54	1.43	1.52	1	1
C	39	LYS	N-CA	4.51	1.54	1.46	1	1
A	312	ALA	CA-C	4.51	1.43	1.52	1	1
B	323	VAL	C-N	4.45	1.39	1.33	1	1
B	66	THR	CA-C	4.39	1.62	1.52	1	1
B	394	ARG	N-CA	4.39	1.37	1.46	1	1
B	321	GLY	C-N	4.36	1.27	1.34	1	1
D	40	PRO	N-CA	4.36	1.40	1.47	1	1
A	308	MET	N-CA	4.36	1.38	1.46	1	1
A	117	LYS	CA-C	4.33	1.62	1.52	1	1
B	117	LYS	CA-C	4.30	1.62	1.52	1	1
A	391	LEU	C-N	4.30	1.39	1.33	1	1
B	396	ASP	N-CA	4.28	1.38	1.46	1	1
A	73	LEU	CA-C	4.26	1.44	1.52	1	1
A	116	LYS	C-N	4.24	1.39	1.33	1	1

Standard geometry: angle outliers ?

There are 614 bond angle outliers in this entry (6.08% of 10102 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)
C	13	ASP	CA-CB-CG	23.72	136.32	112.60	1	1
A	309	ASN	CA-CB-CG	19.45	93.15	112.60	1	1
B	397	ILE	C-N-CA	18.49	154.98	121.70	1	1
B	67	SER	C-N-CA	17.97	154.05	121.70	1	1
C	22	ARG	C-N-CA	17.78	153.70	121.70	1	1
A	197	PHE	CA-CB-CG	17.71	96.09	113.80	1	1
D	37	LYS	C-N-CA	17.56	153.31	121.70	1	1
C	37	LYS	N-CA-C	16.45	64.94	111.00	1	1
A	76	PRO	C-CA-CB	14.59	137.83	110.10	1	1
B	197	PHE	CA-CB-CG	14.57	99.23	113.80	1	1
B	397	ILE	CA-C-O	14.15	96.75	120.80	1	1
A	320	LYS	C-N-CA	14.07	147.02	121.70	1	1
A	67	SER	C-N-CA	13.83	146.60	121.70	1	1
D	8	ASN	C-N-CA	13.36	145.74	121.70	1	1
B	320	LYS	N-CA-C	13.00	74.59	111.00	1	1
C	46	GLN	C-CA-CB	12.66	86.04	110.10	1	1
C	13	ASP	C-CA-CB	12.53	133.91	110.10	1	1
C	37	LYS	C-CA-CB	12.40	86.54	110.10	1	1
B	395	LYS	C-N-CA	12.27	99.61	121.70	1	1
B	207	PHE	CA-CB-CG	11.93	101.87	113.80	1	1
C	21	PRO	N-CA-C	11.79	141.57	112.10	1	1
A	324	ASP	N-CA-C	11.74	78.13	111.00	1	1
C	37	LYS	CA-C-N	11.65	139.50	116.20	1	1
A	340	ASN	CA-CB-CG	10.87	123.47	112.60	1	1
B	342	LYS	C-N-CA	10.72	141.00	121.70	1	1
D	9	LEU	C-N-CA	10.68	102.48	121.70	1	1
A	313	ASP	CA-CB-CG	10.61	101.99	112.60	1	1
A	52	GLY	C-N-CA	10.59	102.64	121.70	1	1
D	11	THR	N-CA-CB	10.58	93.52	111.50	1	1
B	340	ASN	C-N-CA	10.50	140.61	121.70	1	1
A	317	THR	CA-CB-CG2	10.43	92.77	110.50	1	1
C	46	GLN	N-CA-CB	10.41	128.20	110.50	1	1
B	66	THR	N-CA-C	10.39	140.08	111.00	1	1
A	82	PHE	C-CA-CB	10.39	90.37	110.10	1	1
B	338	ILE	C-CA-CB	10.38	132.36	111.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	68	LYS	N-CA-C	10.34	82.06	111.00	1	1
C	14	ALA	CA-C-N	10.23	132.24	116.90	1	1
A	68	LYS	C-N-CA	10.22	140.10	121.70	1	1
C	15	PRO	O-C-N	10.13	139.21	123.00	1	1
C	38	SER	C-N-CA	10.12	139.92	121.70	1	1
A	309	ASN	C-N-CA	10.11	139.90	121.70	1	1
A	249	PRO	C-CA-CB	10.11	90.89	110.10	1	1
B	340	ASN	CA-CB-CG	10.07	122.67	112.60	1	1
A	319	GLN	C-N-CA	10.01	139.71	121.70	1	1
B	374	PHE	CA-CB-CG	10.00	103.80	113.80	1	1
A	207	PHE	CA-CB-CG	9.90	103.90	113.80	1	1
A	318	PHE	CA-CB-CG	9.86	103.94	113.80	1	1
A	324	ASP	CA-C-N	9.85	135.90	116.20	1	1
C	39	LYS	N-CA-C	9.73	138.24	111.00	1	1
B	364	ASP	CA-CB-CG	9.73	102.87	112.60	1	1
D	38	SER	C-N-CA	9.65	139.07	121.70	1	1
A	74	VAL	N-CA-C	9.59	84.14	111.00	1	1
C	35	GLN	C-N-CA	9.53	138.85	121.70	1	1
C	9	LEU	C-N-CA	9.52	138.83	121.70	1	1
C	21	PRO	CA-C-N	9.47	135.14	116.20	1	1
A	174	HIS	CA-CB-CG	9.41	104.39	113.80	1	1
B	67	SER	N-CA-C	9.39	137.28	111.00	1	1
A	374	PHE	CA-CB-CG	9.33	104.47	113.80	1	1
B	311	PRO	CA-N-CD	9.23	99.08	112.00	1	1
A	341	LYS	C-N-CA	9.22	138.29	121.70	1	1
A	79	GLU	N-CA-CB	9.18	126.10	110.50	1	1
D	39	LYS	CA-C-N	9.14	103.19	116.90	1	1
A	195	LYS	N-CA-CB	9.13	126.01	110.50	1	1
C	37	LYS	O-C-N	9.02	108.57	123.00	1	1
B	396	ASP	C-N-CA	8.98	105.54	121.70	1	1
A	320	LYS	N-CA-C	8.97	85.89	111.00	1	1
A	76	PRO	C-N-CA	8.93	137.78	121.70	1	1
A	78	LYS	C-N-CA	8.82	137.57	121.70	1	1
B	341	LYS	C-N-CA	8.77	137.48	121.70	1	1
A	346	VAL	CA-CB-CG2	8.75	95.52	110.40	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	388	MET	CA-C-O	8.74	105.94	120.80	1	1
A	74	VAL	C-N-CA	8.64	137.26	121.70	1	1
A	340	ASN	C-CA-CB	8.63	93.71	110.10	1	1
A	69	PHE	C-N-CA	8.59	106.24	121.70	1	1
B	342	LYS	N-CA-C	8.56	87.03	111.00	1	1
A	342	LYS	N-CA-C	8.50	87.21	111.00	1	1
A	379	VAL	CA-CB-CG2	8.48	124.82	110.40	1	1
C	23	LYS	N-CA-C	8.44	87.36	111.00	1	1
A	310	ALA	N-CA-CB	8.44	97.75	110.40	1	1
A	136	VAL	N-CA-C	8.38	87.54	111.00	1	1
B	82	PHE	CA-CB-CG	8.37	105.43	113.80	1	1
A	396	ASP	C-N-CA	8.28	106.79	121.70	1	1
C	10	THR	C-N-CA	8.25	136.55	121.70	1	1
A	346	VAL	N-CA-CB	8.16	97.63	111.50	1	1
B	136	VAL	N-CA-C	8.16	88.16	111.00	1	1
B	66	THR	CA-C-N	8.12	132.43	116.20	1	1
B	379	VAL	CA-CB-CG2	8.06	124.11	110.40	1	1
B	346	VAL	CA-CB-CG1	8.03	96.75	110.40	1	1
D	38	SER	N-CA-C	8.01	133.44	111.00	1	1
D	37	LYS	CA-C-N	8.00	132.19	116.20	1	1
A	379	VAL	CA-CB-CG1	7.98	96.83	110.40	1	1
B	73	LEU	C-CA-CB	7.97	94.95	110.10	1	1
B	341	LYS	CA-C-N	7.94	132.07	116.20	1	1
A	340	ASN	C-N-CA	7.91	135.95	121.70	1	1
C	38	SER	C-CA-CB	7.85	95.18	110.10	1	1
B	379	VAL	C-CA-CB	7.83	96.52	111.40	1	1
C	48	PHE	C-N-CA	7.82	107.63	121.70	1	1
A	304	ILE	C-N-CA	7.81	107.64	121.70	1	1
A	212	TYR	C-N-CA	7.76	107.73	121.70	1	1
A	249	PRO	C-N-CA	7.75	135.66	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	0.00	0

There are no too-close contacts.

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	755	79	58

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

Chain	Res	Type	Models (Total)
A	21	SER	1
A	64	THR	1
A	67	SER	1
A	69	PHE	1
A	75	ASN	1
A	144	ASN	1
A	148	ALA	1
A	237	TYR	1
A	249	PRO	1
A	261	VAL	1
A	262	ASN	1
A	301	ASN	1
A	309	ASN	1
A	311	PRO	1
A	313	ASP	1
A	316	PHE	1
A	318	PHE	1
A	331	LYS	1
A	343	GLU	1
A	397	ILE	1
B	64	THR	1
B	67	SER	1
B	73	LEU	1
B	79	GLU	1
B	144	ASN	1

Chain	Res	Type	Models (Total)
B	148	ALA	1
B	236	PHE	1
B	261	VAL	1
B	262	ASN	1
B	309	ASN	1
B	311	PRO	1
B	312	ALA	1
B	318	PHE	1
B	322	PRO	1
B	325	GLU	1
B	327	GLY	1
B	343	GLU	1
B	397	ILE	1
C	4	ASN	1
C	6	THR	1
C	10	THR	1
C	11	THR	1
C	12	GLY	1
C	13	ASP	1
C	14	ALA	1
C	16	THR	1
C	25	PRO	1
C	30	GLN	1
C	32	GLN	1
C	34	ARG	1
C	35	GLN	1
C	38	SER	1
C	42	LYS	1
D	11	THR	1
D	12	GLY	1
D	18	PRO	1
D	37	LYS	1
D	38	SER	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	676	71	65

There are 65 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	22	MET	1
A	24	LYS	1
A	27	HIS	1
A	41	ARG	1
A	60	LEU	1
A	79	GLU	1
A	96	LYS	1
A	117	LYS	1
A	132	GLN	1
A	134	LYS	1
A	143	LEU	1
A	191	TRP	1
A	194	ASN	1
A	203	ILE	1
A	251	LYS	1
A	260	GLU	1
A	294	LEU	1
A	300	GLU	1
A	316	PHE	1
A	320	LYS	1
A	328	TRP	1
A	330	ILE	1
A	332	ASN	1
A	333	VAL	1
A	334	LEU	1
A	338	ILE	1
A	352	TYR	1
A	354	ARG	1
A	358	LYS	1
A	379	VAL	1

Chain	Res	Type	Models (Total)
B	27	HIS	1
B	48	ARG	1
B	50	ARG	1
B	60	LEU	1
B	72	ASN	1
B	96	LYS	1
B	117	LYS	1
B	125	MET	1
B	179	TYR	1
B	185	ARG	1
B	195	LYS	1
B	255	THR	1
B	309	ASN	1
B	320	LYS	1
B	325	GLU	1
B	328	TRP	1
B	334	LEU	1
B	341	LYS	1
B	342	LYS	1
B	352	TYR	1
B	379	VAL	1
B	395	LYS	1
C	3	GLU	1
C	16	THR	1
C	23	LYS	1
C	32	GLN	1
C	35	GLN	1
C	37	LYS	1
C	39	LYS	1
C	42	LYS	1
D	4	ASN	1
D	22	ARG	1
D	23	LYS	1
D	37	LYS	1
D	45	VAL	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.

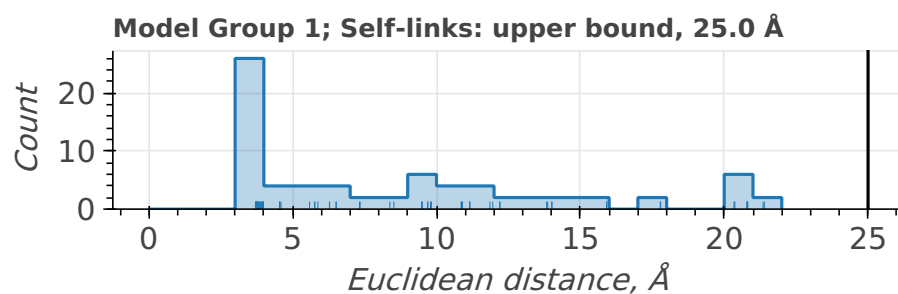
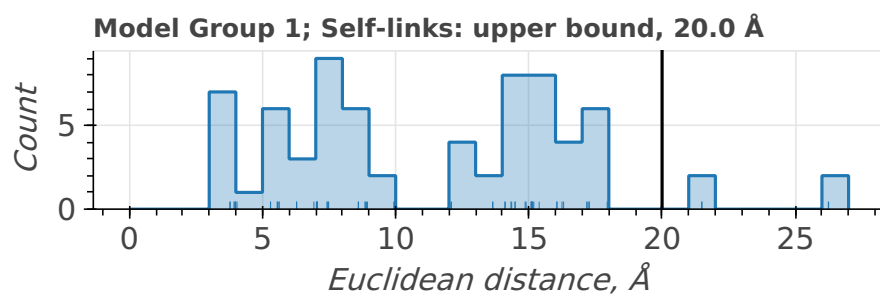
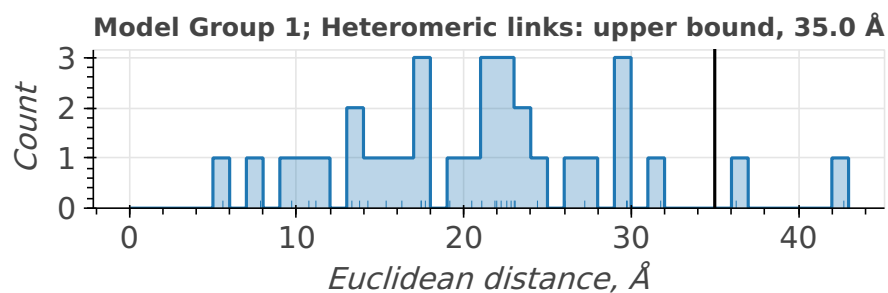
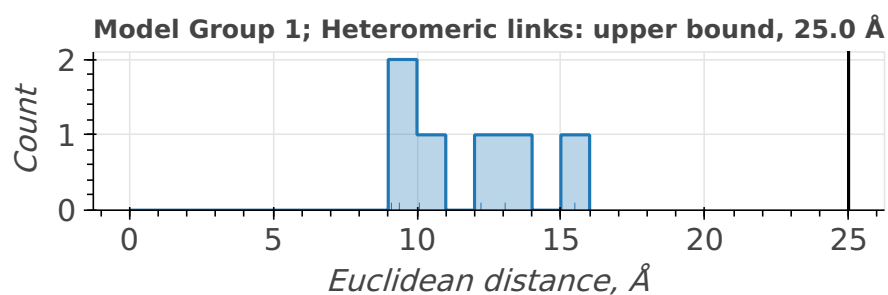
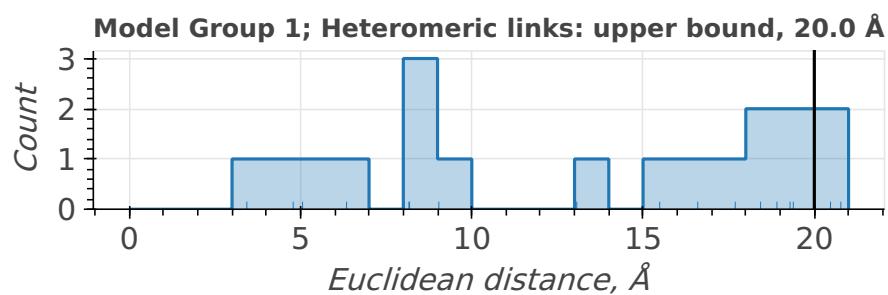
There are 222 crosslinking restraints combined in 111 restraint groups.

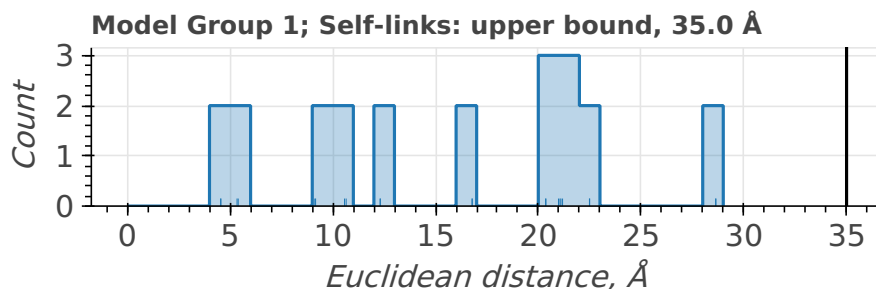
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
EDC	GLU	CA	LYS	CA	upper bound	20.0	56
EDC	ASP	CA	LYS	CA	upper bound	20.0	30
EDC	ASP	CA	THR	CA	upper bound	20.0	2
BS3	LYS	CA	LYS	CA	upper bound	35.0	46
BS3	ASP	CA	LYS	CA	upper bound	35.0	2
BS3	LYS	CA	THR	CA	upper bound	35.0	4
BS3	GLN	CA	LYS	CA	upper bound	35.0	2
sulfo-SDA	ILE	CA	LYS	CA	upper bound	25.0	2
sulfo-SDA	LYS	CA	THR	CA	upper bound	25.0	6
sulfo-SDA	LYS	CA	PHE	CA	upper bound	25.0	2
sulfo-SDA	LYS	CA	VAL	CA	upper bound	25.0	12
sulfo-SDA	LYS	CA	PRO	CA	upper bound	25.0	4
sulfo-SDA	ASN	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	LYS	CA	LYS	CA	upper bound	25.0	6
sulfo-SDA	ASP	CA	LYS	CA	upper bound	25.0	6
sulfo-SDA	GLU	CA	LYS	CA	upper bound	25.0	14
sulfo-SDA	LEU	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	ALA	CA	LYS	CA	upper bound	25.0	4
sulfo-SDA	LYS	CA	TYR	CA	upper bound	25.0	6
sulfo-SDA	GLY	CA	LYS	CA	upper bound	25.0	8
sulfo-SDA	ARG	CA	LYS	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.





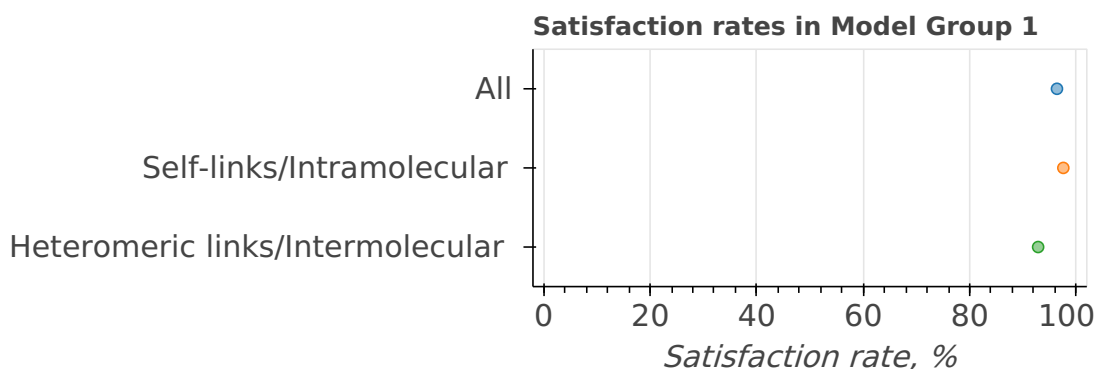
Satisfaction of restraints

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=111)
1	1	1	1/1	All	96.40	3.60	111
				Self-links/ Intramolecular	97.59	2.41	83
				Heteromeric links/ Intermolecular	92.86	7.14	28

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

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