

Integrative Structure Validation Report ?

February 18, 2025 - 08:27 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

ATSAS Version 3.2.1 (r14885)

PDB ID	8ZZG
PDB-Dev ID	PDBDEV_00000016
Structure Title	Integrative structure-function mapping of the nucleoporin Nup133
Structure Authors	Kim SJ; Fernandez-Martinez J; Sampathkumar P; Martel A; Matsui T; Tsuruta H; Weiss TM; Shi Y; Markina-Inarrairaegui A; Bonanno JB; Sauder JM; Burley SK; Chait BT; Almo SC; Rout MP; Sali A
Deposited on	2018-03-23

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

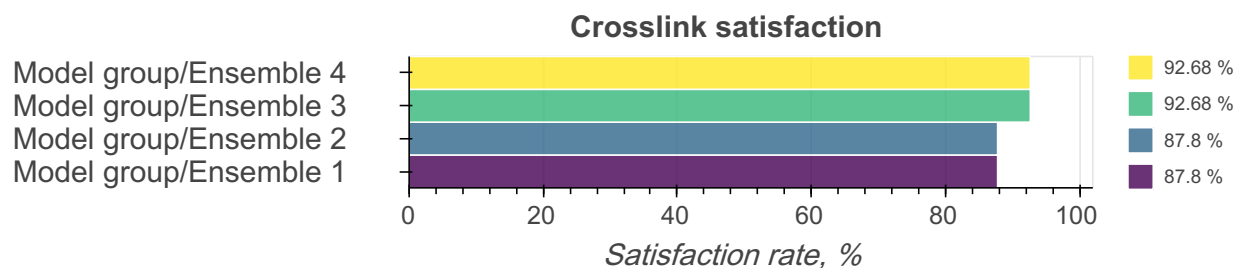
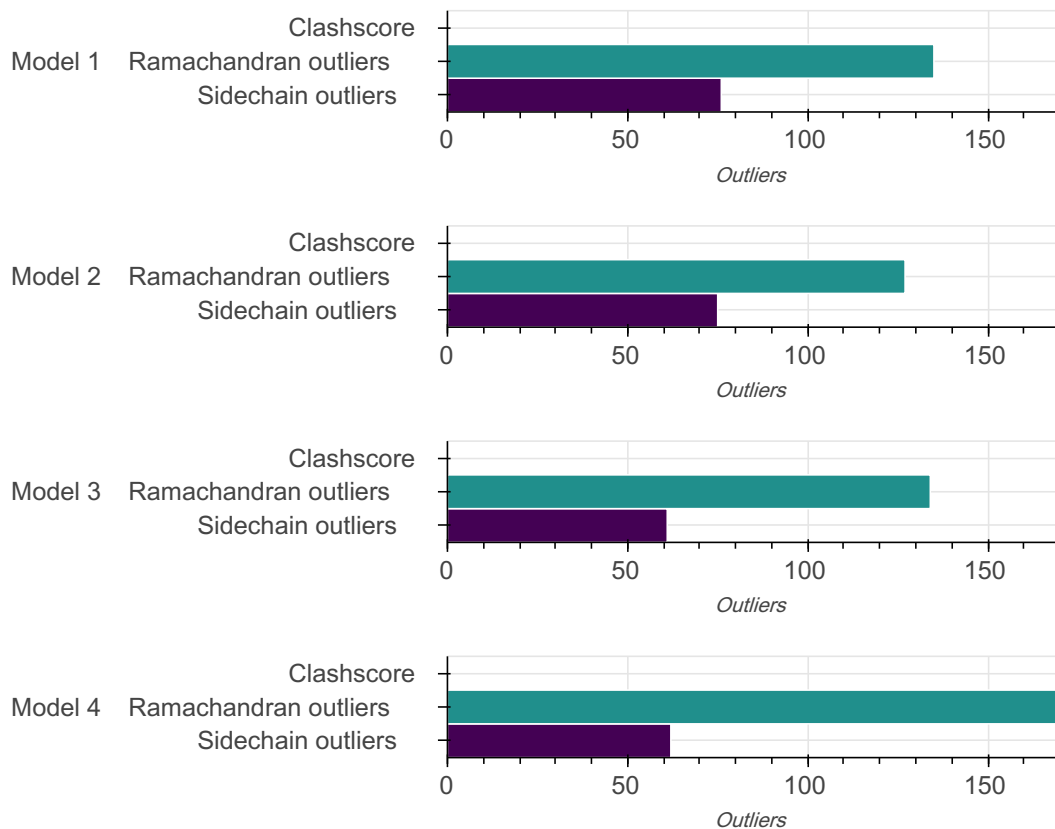
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 4 model(s). A total of 56 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	1-4	1	Nup133	A	1166	-	1-1166	100.00 / 100.00	Atomic

Datasets used for modeling

There are 56 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	SAS data	Zenodo	10.5281/zenodo.1209565
2	SAS data	Zenodo	10.5281/zenodo.1209565
3	SAS data	Zenodo	10.5281/zenodo.1209565
4	SAS data	Zenodo	10.5281/zenodo.1209565
5	SAS data	Zenodo	10.5281/zenodo.1209565
6	SAS data	Zenodo	10.5281/zenodo.1209565
7	SAS data	Zenodo	10.5281/zenodo.1209565
8	SAS data	Zenodo	10.5281/zenodo.1209565
9	SAS data	Zenodo	10.5281/zenodo.1209565
10	SAS data	Zenodo	10.5281/zenodo.1209565
11	SAS data	Zenodo	10.5281/zenodo.1209565
12	SAS data	Zenodo	10.5281/zenodo.1209565
13	SAS data	Zenodo	10.5281/zenodo.1209565
14	SAS data	Zenodo	10.5281/zenodo.1209565
15	SAS data	Zenodo	10.5281/zenodo.1209565
16	SAS data	Zenodo	10.5281/zenodo.1209565
17	SAS data	Zenodo	10.5281/zenodo.1209565
18	SAS data	Zenodo	10.5281/zenodo.1209565
19	SAS data	Zenodo	10.5281/zenodo.1209565
20	2DEM class average	Zenodo	10.5281/zenodo.1209565
21	2DEM class average	Zenodo	10.5281/zenodo.1209565
22	2DEM class average	Zenodo	10.5281/zenodo.1209565
23	2DEM class average	Zenodo	10.5281/zenodo.1209565
24	2DEM class average	Zenodo	10.5281/zenodo.1209565
25	2DEM class average	Zenodo	10.5281/zenodo.1209565
26	2DEM class average	Zenodo	10.5281/zenodo.1209565

ID	Dataset type	Database name	Data access code
27	2DEM class average	Zenodo	10.5281/zenodo.1209565
28	2DEM class average	Zenodo	10.5281/zenodo.1209565
29	2DEM class average	Zenodo	10.5281/zenodo.1209565
30	2DEM class average	Zenodo	10.5281/zenodo.1209565
31	2DEM class average	Zenodo	10.5281/zenodo.1209565
32	2DEM class average	Zenodo	10.5281/zenodo.1209565
33	2DEM class average	Zenodo	10.5281/zenodo.1209565
34	2DEM class average	Zenodo	10.5281/zenodo.1209565
35	2DEM class average	Zenodo	10.5281/zenodo.1209565
36	2DEM class average	Zenodo	10.5281/zenodo.1209565
37	2DEM class average	Zenodo	10.5281/zenodo.1209565
38	2DEM class average	Zenodo	10.5281/zenodo.1209565
39	2DEM class average	Zenodo	10.5281/zenodo.1209565
40	2DEM class average	Zenodo	10.5281/zenodo.1209565
41	2DEM class average	Zenodo	10.5281/zenodo.1209565
42	2DEM class average	Zenodo	10.5281/zenodo.1209565
43	Crosslinking-MS data	Zenodo	10.5281/zenodo.1209565
44	Experimental model	PDB	3I4R
45	Experimental model	PDB	3KFO
46	Experimental model	PDB	4Q9T
47	Experimental model	PDB	2JO8
48	Experimental model	PDB	2QIW
49	Experimental model	PDB	3CIG
50	Experimental model	PDB	2ELO
51	Experimental model	PDB	3GUZ
52	Experimental model	PDB	2CIW
53	Experimental model	PDB	1A92
54	Experimental model	PDB	1GDJ
55	Experimental model	PDB	1X4O
56	Comparative model	Zenodo	10.5281/zenodo.1209565

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	MD-based conformational sampling	AllosMod	None	7000	True	False
2	1	Minimal Ensemble Search	MES	None	4	True	False

There are 6 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HHpred	2.0.16	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred
2	PSIPRED	4.00	secondary structure prediction	http://bioinf.cs.ucl.ac.uk/psipred/
3	DISOPRED	3	disorder prediction	http://bioinf.cs.ucl.ac.uk/psipred/?disopred=1
4	Integrative Modeling Platform (IMP)	2.20	integrative model building	https://integrativemodeling.org
5	MODELLER	9.13	comparative modeling	https://salilab.org/modeller/
6	AllosMod	Not available	sampling	https://salilab.org/allosmod

Data quality ?

SAS:Scattering profile

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

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.

2DEM class average

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 1671 bond length outliers in this entry (4.31% of 38736 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	138	ARG	NE-CZ	11.70	1.45	1.33	1	2
A	10	ARG	NE-CZ	10.90	1.45	1.33	1	2
A	1166	HIS	ND1-CE1	10.16	1.42	1.32	4	2
A	126	ARG	NE-CZ	10.03	1.44	1.33	3	2
A	541	HIS	C-N	9.26	1.46	1.33	2	1
A	855	HIS	ND1-CE1	9.07	1.41	1.32	1	3
A	629	HIS	ND1-CE1	9.02	1.41	1.32	4	3
A	1042	VAL	CA-C	8.93	1.34	1.52	2	1
A	541	HIS	ND1-CE1	8.62	1.41	1.32	2	1
A	119	PRO	C-N	8.61	1.45	1.33	2	1
A	850	GLU	C-N	8.59	1.45	1.33	3	1
A	310	ASP	CA-C	8.43	1.35	1.52	2	1
A	498	HIS	ND1-CE1	8.34	1.40	1.32	3	3
A	1163	HIS	ND1-CE1	8.28	1.40	1.32	3	2
A	195	HIS	ND1-CE1	8.23	1.40	1.32	3	4
A	982	ARG	NE-CZ	8.19	1.42	1.33	2	3
A	48	GLN	C-N	8.12	1.44	1.33	2	2
A	691	ARG	NE-CZ	8.09	1.42	1.33	2	2
A	51	ARG	NE-CZ	8.08	1.41	1.33	3	2
A	1161	HIS	CE1-NE2	7.97	1.40	1.32	3	1
A	249	LEU	C-N	7.93	1.44	1.33	2	1
A	557	HIS	ND1-CE1	7.91	1.40	1.32	2	1
A	557	HIS	CB-CG	7.87	1.61	1.50	3	2
A	165	LEU	C-N	7.75	1.44	1.33	4	1
A	864	ARG	CZ-NH2	7.71	1.43	1.33	1	3
A	8	HIS	ND1-CE1	7.64	1.40	1.32	2	2
A	5	LYS	C-N	7.60	1.44	1.33	1	1
A	32	TYR	C-N	7.33	1.43	1.33	2	1
A	1115	TYR	C-N	7.32	1.43	1.33	2	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	628	GLU	C-N	7.30	1.43	1.33	4	1
A	137	PRO	N-CD	7.27	1.37	1.47	2	2
A	1164	HIS	CE1-NE2	7.22	1.39	1.32	2	1
A	235	ARG	NE-CZ	7.22	1.41	1.33	4	1
A	45	MET	C-N	7.22	1.43	1.33	4	1
A	973	CYS	C-N	7.20	1.43	1.33	2	1
A	1162	HIS	ND1-CE1	7.19	1.39	1.32	4	3
A	795	LYS	C-N	7.18	1.43	1.33	1	1
A	329	HIS	ND1-CE1	7.16	1.39	1.32	2	4
A	263	ASN	CA-C	7.16	1.37	1.52	1	1
A	421	PHE	C-N	7.15	1.23	1.34	2	1
A	66	ASN	CA-CB	7.15	1.67	1.53	2	2
A	1161	HIS	ND1-CE1	7.14	1.39	1.32	4	2
A	1070	GLU	C-N	7.13	1.43	1.33	2	1
A	530	HIS	ND1-CE1	7.13	1.39	1.32	3	2
A	76	ASP	C-N	7.08	1.43	1.33	1	1
A	219	GLY	CA-C	7.08	1.39	1.52	1	1
A	736	LEU	CA-C	7.07	1.38	1.52	2	1
A	67	ARG	CD-NE	7.03	1.56	1.46	2	2
A	966	LYS	C-N	7.01	1.43	1.33	4	1
A	182	ILE	C-N	6.95	1.43	1.33	1	2
A	691	ARG	CZ-NH1	6.95	1.42	1.32	1	2
A	1018	ILE	C-N	6.95	1.23	1.34	4	1
A	1111	ARG	CZ-NH1	6.94	1.42	1.32	4	2
A	244	LYS	C-N	6.94	1.43	1.33	2	1
A	735	SER	C-N	6.93	1.43	1.33	4	1
A	1135	HIS	ND1-CE1	6.91	1.39	1.32	2	2
A	121	ILE	CA-C	6.89	1.38	1.52	1	1
A	577	ASN	C-N	6.88	1.43	1.33	1	1
A	195	HIS	C-N	6.88	1.43	1.33	2	1
A	1021	ARG	NE-CZ	6.88	1.40	1.33	4	3
A	707	LEU	CB-CG	6.87	1.67	1.53	2	1
A	324	LEU	C-N	6.86	1.43	1.33	1	2
A	67	ARG	NE-CZ	6.85	1.40	1.33	3	2
A	947	LYS	CA-CB	6.85	1.67	1.53	4	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	521	ILE	C-N	6.85	1.42	1.33	2	3
A	1102	ARG	CZ-NH1	6.82	1.42	1.32	3	2
A	584	LEU	C-N	6.82	1.42	1.33	1	1
A	51	ARG	CZ-NH2	6.79	1.42	1.33	2	3
A	502	ALA	C-N	6.78	1.42	1.33	4	3
A	275	PRO	N-CA	6.76	1.36	1.47	4	1
A	561	ARG	NE-CZ	6.75	1.40	1.33	1	1
A	337	SER	C-N	6.73	1.42	1.33	1	1
A	1033	GLU	N-CA	6.73	1.33	1.46	2	2
A	174	ILE	CA-C	6.72	1.38	1.52	3	1
A	272	ARG	CD-NE	6.71	1.55	1.46	1	2
A	317	ILE	C-N	6.71	1.42	1.33	3	2
A	701	GLU	C-N	6.70	1.42	1.33	2	1
A	696	GLU	CA-C	6.70	1.38	1.52	1	1
A	216	GLU	C-N	6.68	1.23	1.34	4	2
A	869	HIS	ND1-CE1	6.67	1.39	1.32	4	2
A	282	ARG	CD-NE	6.64	1.55	1.46	3	3
A	422	PRO	N-CA	6.62	1.37	1.47	4	1
A	960	ASN	C-N	6.62	1.42	1.33	2	1
A	812	LEU	C-N	6.59	1.42	1.33	3	1
A	874	GLN	C-N	6.59	1.42	1.33	3	2
A	784	ASP	C-N	6.59	1.42	1.33	4	2
A	546	TYR	C-N	6.59	1.42	1.33	2	1
A	119	PRO	CA-C	6.58	1.39	1.52	4	1
A	359	GLU	C-N	6.58	1.42	1.33	1	2
A	187	PHE	C-N	6.56	1.42	1.33	2	1
A	1043	TRP	NE1-CE2	6.56	1.44	1.37	2	3
A	383	ARG	CZ-NH1	6.56	1.41	1.32	4	1
A	403	PRO	N-CA	6.54	1.37	1.47	4	1
A	1113	GLU	C-N	6.54	1.42	1.33	3	1
A	549	PRO	CA-C	6.53	1.39	1.52	2	1
A	1	SER	CA-CB	6.53	1.66	1.53	2	1
A	304	HIS	ND1-CE1	6.53	1.39	1.32	1	1
A	877	GLN	C-N	6.53	1.42	1.33	2	1
A	195	HIS	CB-CG	6.51	1.59	1.50	2	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	170	GLY	N-CA	6.51	1.35	1.45	1	1

Standard geometry: angle outliers ?

There are 3997 bond angle outliers in this entry (7.61% of 52504 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	157	ASN	CB-CG-OD1	42.48	35.84	120.80	4	1
A	552	ASN	CB-CG-OD1	39.49	41.81	120.80	3	1
A	951	ASN	CB-CG-OD1	38.89	43.01	120.80	3	1
A	971	GLN	CG-CD-OE1	38.82	43.17	120.80	1	1
A	322	GLN	CG-CD-OE1	35.93	48.94	120.80	4	1
A	643	PHE	CA-CB-CG	19.06	94.74	113.80	1	3
A	703	ASP	CA-CB-CG	18.57	94.03	112.60	2	3
A	875	PHE	CA-CB-CG	17.97	95.83	113.80	2	3
A	1067	PHE	CA-CB-CG	17.89	95.91	113.80	4	3
A	971	GLN	CG-CD-NE2	17.77	89.74	116.40	1	1
A	322	GLN	OE1-CD-NE2	17.46	140.06	122.60	4	2
A	396	PHE	CA-CB-CG	17.21	96.59	113.80	3	3
A	322	GLN	CG-CD-NE2	16.85	91.13	116.40	4	1
A	951	ASN	OD1-CG-ND2	16.76	139.36	122.60	3	1
A	576	PHE	CA-CB-CG	15.89	97.91	113.80	1	2
A	728	PHE	CA-CB-CG	15.30	98.50	113.80	2	3
A	647	PHE	CA-CB-CG	15.29	98.51	113.80	2	2
A	228	ARG	NE-CZ-NH2	15.27	105.46	119.20	2	2
A	665	ASN	CA-CB-CG	14.63	97.97	112.60	4	4
A	293	PHE	CA-CB-CG	14.43	99.37	113.80	1	3
A	552	ASN	OD1-CG-ND2	14.35	136.95	122.60	3	1
A	982	ARG	NE-CZ-NH2	14.25	106.38	119.20	1	2
A	552	ASN	CB-CG-ND2	13.91	95.54	116.40	3	2
A	401	PHE	CA-CB-CG	13.52	100.28	113.80	2	3
A	951	ASN	CB-CG-ND2	13.36	96.36	116.40	3	1
A	859	ASN	CA-CB-CG	13.19	99.41	112.60	4	2
A	193	PHE	CA-CB-CG	13.14	100.66	113.80	3	2
A	659	PHE	CA-CB-CG	13.08	100.72	113.80	3	2
A	774	ASN	CA-CB-CG	13.03	99.57	112.60	4	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	723	PHE	CA-CB-CG	13.01	100.79	113.80	3	3
A	777	ASN	CA-CB-CG	13.01	99.59	112.60	1	1
A	609	ASP	CA-CB-CG	12.89	99.71	112.60	1	2
A	10	ARG	NE-CZ-NH1	12.84	108.66	121.50	1	3
A	186	ASN	CA-CB-CG	12.71	99.89	112.60	2	2
A	138	ARG	NE-CZ-NH1	12.34	109.16	121.50	2	1
A	202	ASN	CA-CB-CG	12.32	100.28	112.60	4	4
A	567	ASN	CA-CB-CG	12.32	100.28	112.60	1	3
A	808	PHE	CA-CB-CG	12.28	101.52	113.80	2	4
A	596	ASN	CA-CB-CG	12.25	100.35	112.60	4	1
A	849	PHE	CA-CB-CG	12.24	101.56	113.80	2	3
A	864	ARG	CD-NE-CZ	12.09	107.47	124.40	3	3
A	926	ASN	CA-CB-CG	12.04	100.56	112.60	1	2
A	24	ASN	CA-CB-CG	11.96	100.64	112.60	1	1
A	157	ASN	OD1-CG-ND2	11.93	134.53	122.60	4	1
A	511	ASN	CA-CB-CG	11.89	124.49	112.60	2	3
A	1026	ASP	CA-CB-CG	11.88	100.72	112.60	3	3
A	12	ARG	NE-CZ-NH1	11.82	109.68	121.50	3	1
A	714	ASP	CA-CB-CG	11.79	100.81	112.60	3	1
A	976	PHE	CA-CB-CG	11.79	102.01	113.80	3	4
A	524	ASP	CA-CB-CG	11.73	100.87	112.60	3	3
A	575	ASN	CA-CB-CG	11.71	100.89	112.60	1	2
A	773	ASP	CA-CB-CG	11.69	100.91	112.60	2	2
A	157	ASN	CB-CG-ND2	11.67	98.90	116.40	4	1
A	1050	ASN	CA-CB-CG	11.65	100.95	112.60	3	3
A	911	ASP	CA-CB-CG	11.65	100.95	112.60	4	2
A	110	ASN	CA-CB-CG	11.53	101.07	112.60	1	3
A	160	ASP	CA-CB-CG	11.50	101.10	112.60	1	3
A	1075	ASN	CA-CB-CG	11.47	101.13	112.60	3	3
A	455	ASP	CA-CB-CG	11.41	101.19	112.60	2	2
A	724	PHE	CA-CB-CG	11.41	102.39	113.80	3	3
A	423	ASN	CA-CB-CG	11.35	101.25	112.60	2	2
A	825	ASN	CA-CB-CG	11.32	101.28	112.60	1	2
A	1127	ASP	CA-CB-CG	11.24	101.36	112.60	1	4
A	1044	ARG	NE-CZ-NH2	11.22	109.10	119.20	3	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	369	PHE	CA-CB-CG	11.22	102.58	113.80	4	4
A	565	PHE	CA-CB-CG	11.07	102.73	113.80	2	4
A	379	PHE	CA-CB-CG	10.86	102.94	113.80	2	3
A	148	ASP	CA-CB-CG	10.86	101.74	112.60	2	3
A	1108	ASN	CA-CB-CG	10.85	101.75	112.60	3	3
A	641	ASP	CA-CB-CG	10.80	101.80	112.60	1	1
A	157	ASN	CA-CB-CG	10.73	101.87	112.60	4	4
A	1128	ASN	CA-CB-CG	10.72	101.88	112.60	3	1
A	178	ASP	CA-CB-CG	10.72	101.88	112.60	1	1
A	66	ASN	CA-CB-CG	10.69	101.91	112.60	2	3
A	130	ASN	CA-CB-CG	10.69	101.91	112.60	3	3
A	552	ASN	CA-CB-CG	10.64	101.96	112.60	2	4
A	695	LEU	C-N-CA	10.60	102.63	121.70	3	2
A	56	PHE	CA-CB-CG	10.52	103.28	113.80	3	2
A	253	PHE	CA-CB-CG	10.50	103.30	113.80	4	4
A	57	ASP	CA-CB-CG	10.49	102.11	112.60	1	2
A	1037	PHE	CA-CB-CG	10.45	103.35	113.80	4	1
A	864	ARG	NE-CZ-NH1	10.44	111.06	121.50	4	1
A	762	ASN	CA-CB-CG	10.38	102.22	112.60	4	4
A	338	HIS	CD2-NE2-CE1	10.37	98.63	109.00	2	4
A	370	ASP	CA-CB-CG	10.32	102.28	112.60	2	3
A	184	ASN	CA-CB-CG	10.31	102.29	112.60	2	2
A	960	ASN	CA-CB-CG	10.30	102.30	112.60	3	3
A	302	ASN	CA-CB-CG	10.30	102.30	112.60	2	4
A	158	ASP	CA-CB-CG	10.23	102.37	112.60	3	1
A	1083	ASP	CA-CB-CG	10.19	102.41	112.60	3	3
A	1162	HIS	CD2-NE2-CE1	10.17	98.83	109.00	2	2
A	1146	ASN	CA-CB-CG	10.15	102.45	112.60	3	4
A	410	ASP	CA-CB-CG	10.15	102.45	112.60	2	3
A	184	ASN	C-CA-CB	10.11	90.89	110.10	1	1
A	865	PHE	CA-CB-CG	10.07	103.73	113.80	4	3
A	216	GLU	CB-CG-CD	9.94	95.70	112.60	2	1
A	712	ASN	CA-CB-CG	9.94	102.66	112.60	2	3
A	864	ARG	NE-CZ-NH2	9.93	128.14	119.20	4	2
A	273	ASN	CA-CB-CG	9.88	102.72	112.60	4	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	876	PHE	CA-CB-CG	9.88	103.92	113.80	2	3

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
2	0.00	0
3	0.00	0
4	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	1164	703	326	135
2	1164	702	335	127
3	1164	714	316	134
4	1164	648	346	170

There are 439 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	145	ALA	4
A	766	VAL	4
A	882	LYS	4
A	24	ASN	3
A	31	SER	3
A	39	SER	3
A	47	GLN	3
A	300	ALA	3
A	324	LEU	3
A	403	PRO	3
A	436	SER	3
A	437	SER	3

Chain	Res	Type	Models (Total)
A	473	MET	3
A	512	PRO	3
A	714	ASP	3
A	776	ILE	3
A	797	ASN	3
A	894	ASP	3
A	967	LYS	3
A	994	SER	3
A	998	VAL	3
A	1071	LEU	3
A	1127	ASP	3
A	1161	HIS	3
A	7	VAL	2
A	19	ILE	2
A	22	VAL	2
A	29	GLN	2
A	48	GLN	2
A	50	LEU	2
A	65	ASN	2
A	67	ARG	2
A	69	ILE	2
A	80	GLY	2
A	81	PHE	2
A	97	TYR	2
A	111	ILE	2
A	112	HIS	2
A	114	THR	2
A	119	PRO	2
A	122	THR	2
A	125	PHE	2
A	160	ASP	2
A	169	LYS	2
A	184	ASN	2
A	201	ILE	2
A	216	GLU	2

Chain	Res	Type	Models (Total)
A	227	GLY	2
A	231	PHE	2
A	238	MET	2
A	239	GLY	2
A	243	LEU	2
A	246	GLY	2
A	247	LYS	2
A	251	LYS	2
A	255	LEU	2
A	269	VAL	2
A	279	LYS	2
A	302	ASN	2
A	313	ILE	2
A	358	ASN	2
A	371	SER	2
A	405	MET	2
A	421	PHE	2
A	423	ASN	2
A	427	ILE	2
A	433	LYS	2
A	463	SER	2
A	470	THR	2
A	507	LYS	2
A	546	TYR	2
A	548	PRO	2
A	554	LEU	2
A	577	ASN	2
A	582	PRO	2
A	604	ILE	2
A	620	SER	2
A	640	PRO	2
A	655	VAL	2
A	693	GLU	2
A	698	ASP	2
A	718	CYS	2

Chain	Res	Type	Models (Total)
A	732	GLU	2
A	763	THR	2
A	778	ILE	2
A	809	TYR	2
A	857	LYS	2
A	883	TYR	2
A	913	LYS	2
A	916	GLU	2
A	949	GLN	2
A	995	THR	2
A	1011	ASP	2
A	1024	SER	2
A	1042	VAL	2
A	1077	PHE	2
A	1102	ARG	2
A	1125	ASN	2
A	1126	SER	2
A	1150	ASN	2

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	1096	895	125	76
2	1096	907	114	75
3	1096	910	125	61
4	1096	909	125	62

There are 223 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	489	LYS	4
A	174	ILE	3
A	588	LEU	3
A	630	LEU	3
A	948	ILE	3

Chain	Res	Type	Models (Total)
A	952	LEU	3
A	972	ILE	3
A	1028	ASN	3
A	1046	ILE	3
A	41	MET	2
A	52	LEU	2
A	88	ASN	2
A	104	LYS	2
A	141	LEU	2
A	189	LEU	2
A	211	LEU	2
A	222	LEU	2
A	298	LEU	2
A	391	ILE	2
A	397	LYS	2
A	431	ASN	2
A	473	MET	2
A	517	LEU	2
A	579	LYS	2
A	648	LYS	2
A	691	ARG	2
A	719	ILE	2
A	746	ILE	2
A	759	ILE	2
A	805	ILE	2
A	832	LEU	2
A	842	LYS	2
A	857	LYS	2
A	861	LEU	2
A	872	LEU	2
A	907	ILE	2
A	940	LEU	2
A	955	ILE	2
A	988	LEU	2
A	993	LYS	2

Chain	Res	Type	Models (Total)
A	1085	LEU	2
A	6	LYS	1
A	9	LEU	1
A	10	ARG	1
A	11	LEU	1
A	13	LYS	1
A	15	LEU	1
A	25	GLU	1
A	50	LEU	1
A	51	ARG	1
A	60	LYS	1
A	65	ASN	1
A	69	ILE	1
A	70	VAL	1
A	73	LEU	1
A	75	THR	1
A	79	SER	1
A	95	ILE	1
A	99	LEU	1
A	105	LYS	1
A	108	ILE	1
A	111	ILE	1
A	121	ILE	1
A	140	ILE	1
A	149	GLU	1
A	160	ASP	1
A	167	ILE	1
A	168	ILE	1
A	169	LYS	1
A	179	ILE	1
A	188	LYS	1
A	199	LEU	1
A	201	ILE	1
A	208	LYS	1
A	234	ILE	1

Chain	Res	Type	Models (Total)
A	240	LYS	1
A	243	LEU	1
A	244	LYS	1
A	247	LYS	1
A	249	LEU	1
A	250	ASN	1
A	251	LYS	1
A	260	LYS	1
A	261	ILE	1
A	263	ASN	1
A	268	VAL	1
A	269	VAL	1
A	271	LEU	1
A	272	ARG	1
A	276	ILE	1
A	290	LYS	1
A	292	ILE	1
A	307	LYS	1
A	309	ILE	1
A	317	ILE	1
A	321	LEU	1
A	324	LEU	1
A	333	LYS	1
A	334	ILE	1
A	349	LEU	1

Fit of model to data used for modeling ?

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

Fit of model(s) to crosslinking-MS data

Restraint types

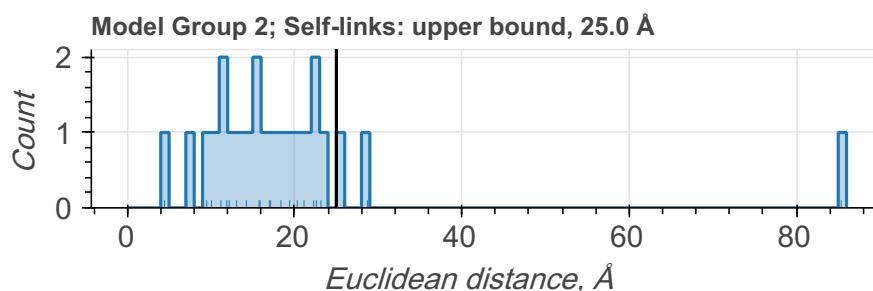
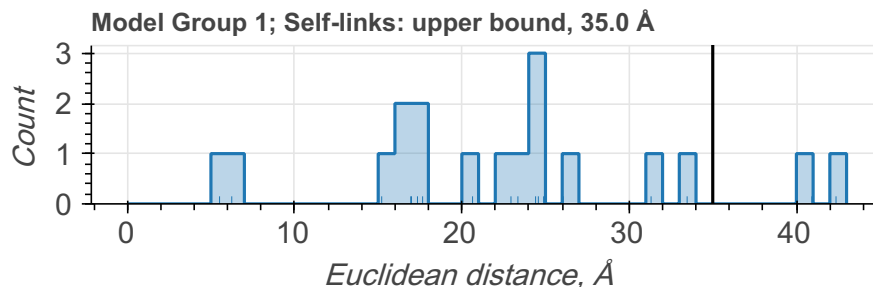
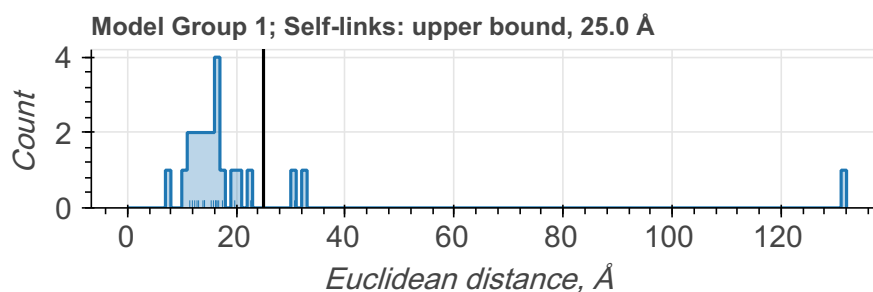
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

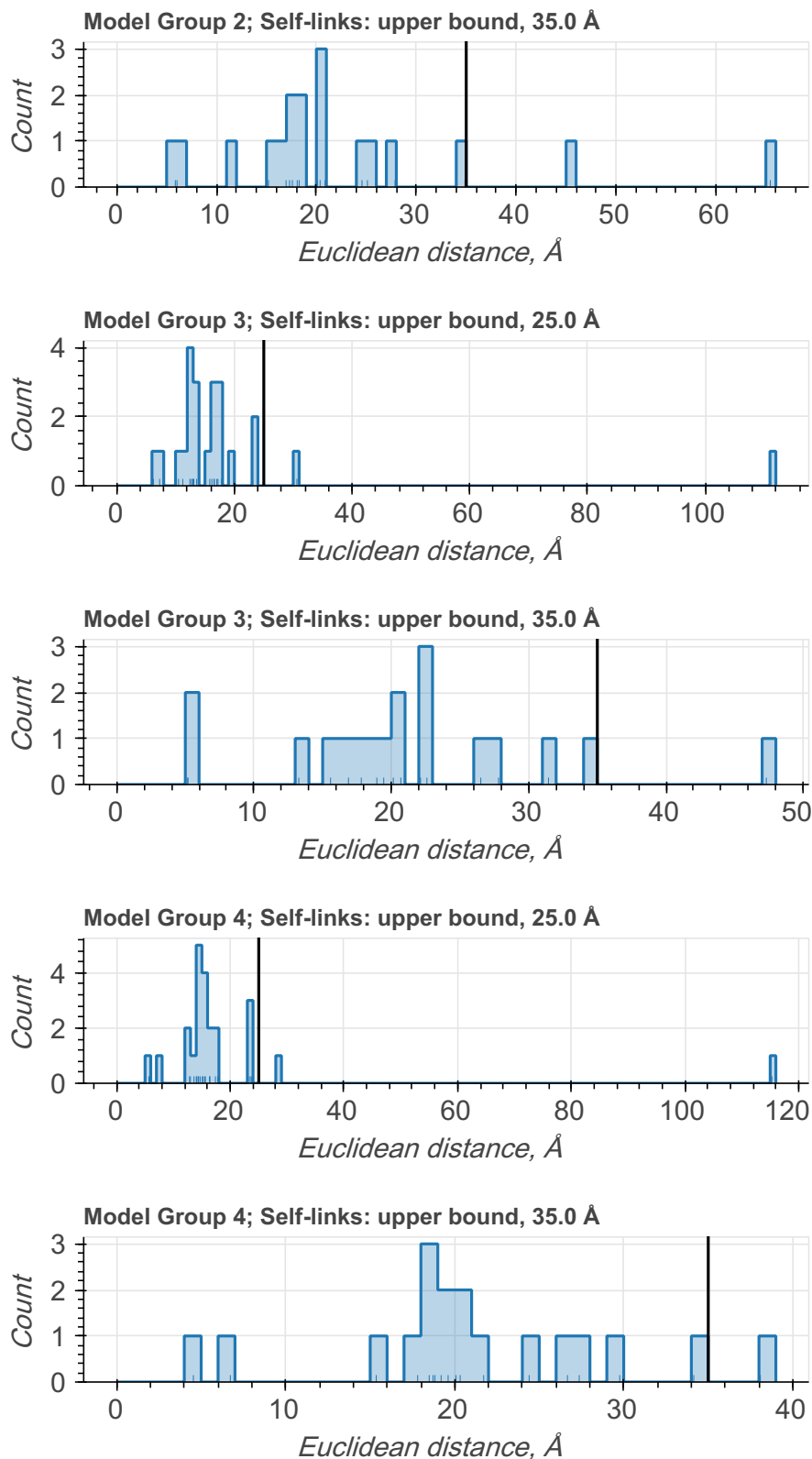
There are 41 crosslinking restraints combined in 41 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	LYS	CA	LYS	CA	upper bound	35.0	18
EDC	ASP	CA	LYS	CA	upper bound	25.0	6
EDC	GLU	CA	LYS	CA	upper bound	25.0	16
EDC	ASN	CA	LYS	CA	upper bound	25.0	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.





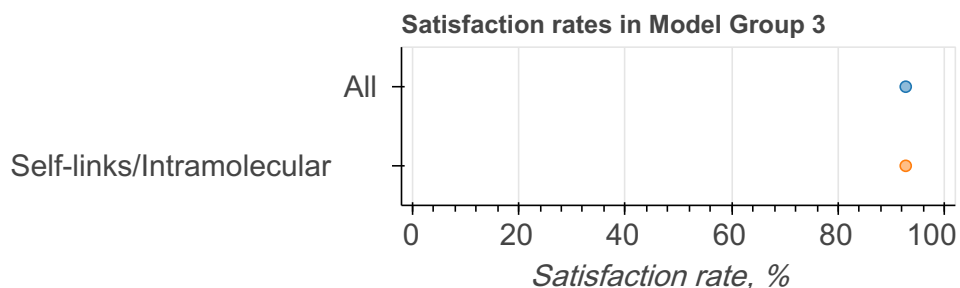
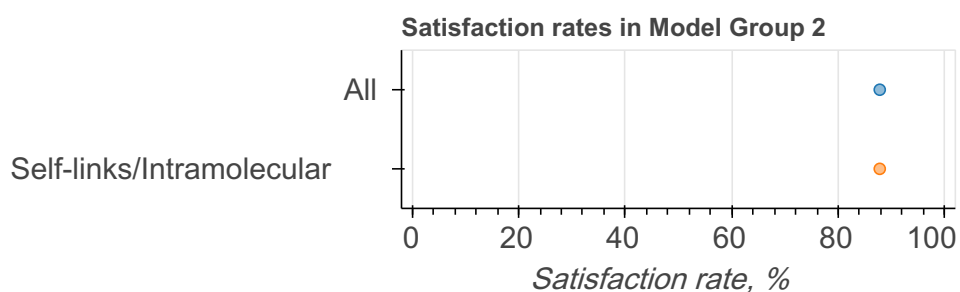
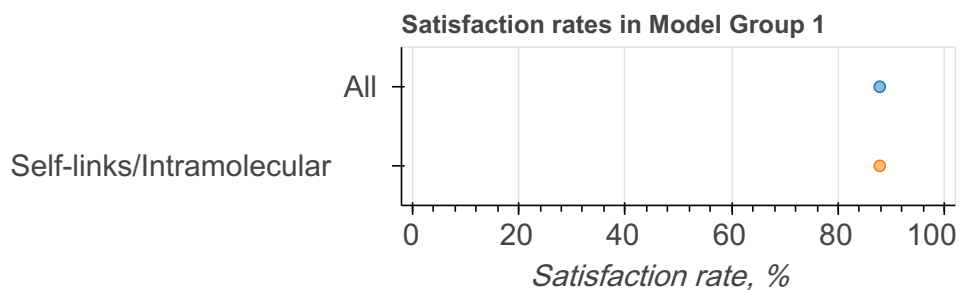
Satisfaction of restraints

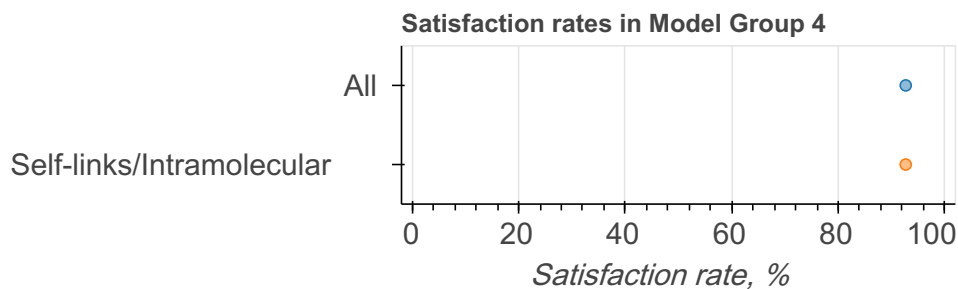
Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=41)
1	1	1	1/1	All	87.80	12.20	41
				Self-links/Intramolecular	87.80	12.20	41
1	2	2	1/1	All	87.80	12.20	41
				Self-links/Intramolecular	87.80	12.20	41
1	3	3	1/1	All	92.68	7.32	41
				Self-links/Intramolecular	92.68	7.32	41
1	4	4	1/1	All	92.68	7.32	41
				Self-links/Intramolecular	92.68	7.32	41

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.





2DEM class average

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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