

Integrative Structure Validation Report ?

February 27, 2025 - 12:21 PM 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	9A8G
PDB-Dev ID	PDBDEV_00000380
Structure Title	Structural Basis for Mis18 Complex Assembly
Structure Authors	Thamkachy, R.; Medina-Pritchard, B.; Park, S.H.; Chiodi, C.G.; Zou, J.; de la Torre-Barranco, M.; Shimanaka, K.; Abad, M.A.; Paramo, C.G.; Feederle, R.; Ruksenaite, E.; Heun, P.; Davies, O.R.; Rappsilber, J.; Schneidman-Duhovny, D; Cho, U.; Jeyaprakash, A.A.
Deposited on	2024-04-26

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

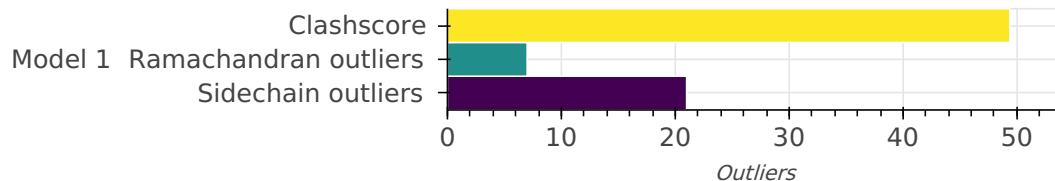
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 9 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	Protein Mis18-alpha	A	233	-	1-76, 77-190, 191-233	100.00 / 100.00	Atomic
				D					
				E					
				F					
		2	Protein Mis18-beta	B	229	-	1-187, 188-229	100.00 / 100.00	Atomic
				G					
		3	Mis18-binding protein 1	C	130	-	1-130	100.00 / 100.00	Atomic
				H					

Datasets used for modeling ?

There are 9 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	3DEM volume	EMDB	EMD-50218
6	3DEM volume	Not available	Not available
7	3DEM volume	Not available	Not available
1	Crosslinking-MS data	PRIDE	PXD047345
3	Experimental model	PDB	7sfz
4	Experimental model	PDB	7sfy
5	De Novo model	AlphaFoldDB	AF-Q9NYP9-F1
8	De Novo model	AlphaFoldDB	AF-O43482-F1
9	De Novo model	AlphaFoldDB	AF-Q6P0N0-F1

Methodology and software ?

This entry is a result of 2 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	docking	None	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaFold-Multimer	2.20	model building	https://github.com/google-deepmind/alphafold
2	CombDock	Not available	assembly	http://bioinfo3d.cs.tau.ac.il/CombDock/download/

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.

3DEM volume

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 98 bond length outliers in this entry (1.05% of 9302 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D	58	ASP	C-N	27.77	0.94	1.33	1	1
A	58	ASP	C-N	27.75	0.94	1.33	1	1
E	76	ALA	C-N	17.05	1.09	1.33	1	1
F	76	ALA	C-N	17.02	1.09	1.33	1	1
D	63	ASP	C-N	15.47	1.11	1.33	1	1
A	63	ASP	C-N	15.45	1.11	1.33	1	1
A	54	SER	C-N	15.04	1.12	1.33	1	1
D	54	SER	C-N	14.98	1.12	1.33	1	1
A	67	ALA	C-N	14.61	1.12	1.33	1	1
D	67	ALA	C-N	14.57	1.13	1.33	1	1
A	62	ALA	C-N	14.10	1.13	1.33	1	1
D	62	ALA	C-N	14.03	1.13	1.33	1	1
D	71	GLU	C-N	12.59	1.15	1.33	1	1
A	71	GLU	C-N	12.54	1.15	1.33	1	1
A	70	GLU	C-N	12.32	1.16	1.33	1	1
D	70	GLU	C-N	12.29	1.16	1.33	1	1
F	55	MET	C-N	12.26	1.50	1.33	1	1
A	34	ARG	C-N	11.71	1.17	1.33	1	1
D	34	ARG	C-N	11.64	1.17	1.33	1	1
A	66	ARG	C-N	10.73	1.18	1.33	1	1
D	66	ARG	C-N	10.66	1.18	1.33	1	1
D	44	LEU	C-N	10.53	1.48	1.33	1	1
A	44	LEU	C-N	10.52	1.48	1.33	1	1
E	61	VAL	C-N	10.38	1.18	1.33	1	1
F	61	VAL	C-N	10.36	1.18	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	39	SER	C-N	10.28	1.19	1.33	1	1
D	65	GLU	C-N	10.24	1.19	1.33	1	1
A	65	GLU	C-N	10.19	1.19	1.33	1	1
D	52	TRP	C-N	10.18	1.19	1.33	1	1
D	39	SER	C-N	10.14	1.19	1.33	1	1
A	52	TRP	C-N	10.14	1.19	1.33	1	1
A	57	GLU	C-N	9.65	1.46	1.33	1	1
D	57	GLU	C-N	9.63	1.46	1.33	1	1
A	74	ALA	C-N	8.99	1.20	1.33	1	1
D	74	ALA	C-N	8.98	1.20	1.33	1	1
D	53	SER	C-N	8.84	1.21	1.33	1	1
A	53	SER	C-N	8.84	1.21	1.33	1	1
F	37	GLU	C-N	8.74	1.45	1.33	1	1
E	37	GLU	C-N	8.70	1.45	1.33	1	1
F	67	ALA	C-N	8.29	1.21	1.33	1	1
E	67	ALA	C-N	8.29	1.21	1.33	1	1
F	65	GLU	C-N	7.97	1.22	1.33	1	1
E	65	GLU	C-N	7.96	1.22	1.33	1	1
D	37	GLU	C-N	7.78	1.22	1.33	1	1
A	37	GLU	C-N	7.77	1.22	1.33	1	1
E	64	MET	C-N	7.65	1.22	1.33	1	1
F	64	MET	C-N	7.63	1.22	1.33	1	1
E	47	LYS	C-N	7.62	1.22	1.33	1	1
F	47	LYS	C-N	7.61	1.22	1.33	1	1
E	58	ASP	C-N	7.40	1.23	1.33	1	1
F	58	ASP	C-N	7.38	1.23	1.33	1	1
F	44	LEU	C-N	6.86	1.42	1.33	1	1
E	44	LEU	C-N	6.81	1.42	1.33	1	1
F	33	LYS	C-N	6.69	1.42	1.33	1	1
E	33	LYS	C-N	6.63	1.42	1.33	1	1
E	73	ALA	C-N	6.61	1.42	1.33	1	1
F	73	ALA	C-N	6.53	1.42	1.33	1	1
E	75	ALA	C-N	6.49	1.42	1.33	1	1
F	75	ALA	C-N	6.45	1.42	1.33	1	1
A	33	LYS	C-N	6.45	1.24	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D	46	GLN	C-N	6.37	1.42	1.33	1	1
D	33	LYS	C-N	6.36	1.24	1.33	1	1
E	68	GLN	C-N	6.29	1.24	1.33	1	1
F	68	GLN	C-N	6.29	1.24	1.33	1	1
F	48	TRP	C-N	6.27	1.42	1.33	1	1
A	46	GLN	C-N	6.26	1.42	1.33	1	1
E	48	TRP	C-N	6.20	1.42	1.33	1	1
D	69	LEU	C-N	6.20	1.24	1.33	1	1
A	69	LEU	C-N	6.15	1.24	1.33	1	1
D	68	GLN	C-N	5.93	1.25	1.33	1	1
A	68	GLN	C-N	5.90	1.25	1.33	1	1
D	47	LYS	C-N	5.90	1.25	1.33	1	1
A	47	LYS	C-N	5.88	1.25	1.33	1	1
F	30	LEU	C-N	5.86	1.41	1.33	1	1
A	59	ALA	C-N	5.81	1.25	1.33	1	1
E	63	ASP	C-N	5.78	1.25	1.33	1	1
F	63	ASP	C-N	5.76	1.25	1.33	1	1
D	59	ALA	C-N	5.74	1.25	1.33	1	1
E	30	LEU	C-N	5.71	1.41	1.33	1	1
A	64	MET	C-N	5.63	1.25	1.33	1	1
D	64	MET	C-N	5.53	1.25	1.33	1	1
D	56	SER	C-N	5.44	1.41	1.33	1	1
A	56	SER	C-N	5.39	1.40	1.33	1	1
D	76	ALA	C-N	5.27	1.26	1.33	1	1
A	76	ALA	C-N	5.25	1.26	1.33	1	1
E	74	ALA	C-N	5.22	1.40	1.33	1	1
F	74	ALA	C-N	5.20	1.40	1.33	1	1
A	35	LEU	C-N	5.08	1.40	1.33	1	1
D	35	LEU	C-N	5.07	1.40	1.33	1	1
E	57	GLU	C-N	4.72	1.26	1.33	1	1
F	57	GLU	C-N	4.66	1.26	1.33	1	1
E	34	ARG	C-N	4.61	1.39	1.33	1	1
F	34	ARG	C-N	4.59	1.39	1.33	1	1
E	60	SER	C-N	4.52	1.27	1.33	1	1
F	60	SER	C-N	4.48	1.27	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D	51	MET	C-N	4.23	1.27	1.33	1	1
A	51	MET	C-N	4.19	1.27	1.33	1	1
D	31	LEU	C-N	4.03	1.27	1.33	1	1

Standard geometry: angle outliers ?

There are 136 bond angle outliers in this entry (1.09% of 12494 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)
F	55	MET	O-C-N	48.86	44.82	123.00	1	1
F	55	MET	CA-C-N	23.48	163.17	116.20	1	1
C	51	SER	CA-C-O	14.25	163.74	121.00	1	1
C	51	SER	CA-C-OXT	12.83	82.52	121.00	1	1
C	51	SER	O-C-OXT	12.25	81.24	118.00	1	1
D	56	SER	O-C-N	11.85	104.04	123.00	1	1
A	56	SER	O-C-N	11.83	104.06	123.00	1	1
A	54	SER	O-C-N	11.10	105.25	123.00	1	1
D	54	SER	O-C-N	11.07	105.28	123.00	1	1
D	59	ALA	O-C-N	10.56	106.10	123.00	1	1
A	59	ALA	O-C-N	10.55	106.12	123.00	1	1
A	30	LEU	C-N-CA	9.91	139.54	121.70	1	1
D	30	LEU	C-N-CA	9.90	139.51	121.70	1	1
D	55	MET	O-C-N	9.41	107.95	123.00	1	1
A	55	MET	O-C-N	9.38	107.99	123.00	1	1
A	57	GLU	C-N-CA	9.04	137.97	121.70	1	1
D	57	GLU	C-N-CA	9.00	137.89	121.70	1	1
A	56	SER	CA-C-N	8.89	133.98	116.20	1	1
D	56	SER	CA-C-N	8.88	133.96	116.20	1	1
E	73	ALA	O-C-N	8.82	137.11	123.00	1	1
F	73	ALA	O-C-N	8.79	137.06	123.00	1	1
A	58	ASP	O-C-N	8.27	109.78	123.00	1	1
D	58	ASP	O-C-N	8.26	109.78	123.00	1	1
A	43	GLN	C-N-CA	8.00	107.30	121.70	1	1
D	43	GLN	C-N-CA	7.96	107.37	121.70	1	1
E	73	ALA	C-N-CA	7.79	107.68	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
F	73	ALA	C-N-CA	7.76	107.73	121.70	1	1
D	53	SER	O-C-N	7.59	110.86	123.00	1	1
A	53	SER	O-C-N	7.58	110.87	123.00	1	1
D	52	TRP	O-C-N	7.45	111.07	123.00	1	1
A	52	TRP	O-C-N	7.45	111.08	123.00	1	1
D	55	MET	CA-C-N	7.27	130.74	116.20	1	1
A	55	MET	CA-C-N	7.26	130.72	116.20	1	1
E	73	ALA	CA-C-N	7.10	101.99	116.20	1	1
F	73	ALA	CA-C-N	7.10	102.00	116.20	1	1
A	57	GLU	O-C-N	6.97	111.85	123.00	1	1
D	57	GLU	O-C-N	6.92	111.93	123.00	1	1
A	54	SER	CA-C-N	6.78	129.75	116.20	1	1
D	54	SER	CA-C-N	6.75	129.71	116.20	1	1
A	76	ALA	C-N-CA	6.25	110.46	121.70	1	1
A	37	GLU	CA-C-N	6.24	103.72	116.20	1	1
D	37	GLU	CA-C-N	6.24	103.72	116.20	1	1
D	76	ALA	C-N-CA	6.24	110.47	121.70	1	1
F	55	MET	C-N-CA	6.23	132.91	121.70	1	1
E	63	ASP	C-N-CA	6.11	110.69	121.70	1	1
F	63	ASP	C-N-CA	6.09	110.74	121.70	1	1
A	33	LYS	C-N-CA	6.08	132.65	121.70	1	1
D	33	LYS	C-N-CA	6.08	132.64	121.70	1	1
D	58	ASP	CA-C-N	6.02	128.25	116.20	1	1
A	58	ASP	CA-C-N	6.00	128.20	116.20	1	1
D	37	GLU	O-C-N	6.00	132.60	123.00	1	1
A	37	GLU	O-C-N	6.00	132.59	123.00	1	1
D	59	ALA	CA-C-N	5.92	128.04	116.20	1	1
A	59	ALA	CA-C-N	5.92	128.04	116.20	1	1
D	38	ASP	C-N-CA	5.88	111.11	121.70	1	1
A	38	ASP	C-N-CA	5.85	111.17	121.70	1	1
A	52	TRP	CA-C-N	5.70	127.60	116.20	1	1
D	52	TRP	CA-C-N	5.69	127.57	116.20	1	1
A	62	ALA	O-C-N	5.48	114.23	123.00	1	1
D	62	ALA	O-C-N	5.48	114.23	123.00	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
H	49	GLN	OE1-CD-NE2	5.47	117.13	122.60	1	1
E	55	MET	C-N-CA	5.44	111.91	121.70	1	1
D	76	ALA	O-C-N	5.43	114.31	123.00	1	1
A	76	ALA	O-C-N	5.40	114.37	123.00	1	1
E	70	GLU	O-C-N	5.34	131.54	123.00	1	1
F	70	GLU	O-C-N	5.33	131.53	123.00	1	1
D	60	SER	O-C-N	5.21	114.66	123.00	1	1
F	63	ASP	O-C-N	5.20	131.32	123.00	1	1
A	60	SER	O-C-N	5.20	114.68	123.00	1	1
E	63	ASP	O-C-N	5.19	131.31	123.00	1	1
D	40	SER	O-C-N	5.15	131.24	123.00	1	1
A	53	SER	CA-C-N	5.15	126.49	116.20	1	1
D	53	SER	CA-C-N	5.14	126.47	116.20	1	1
E	66	ARG	C-N-CA	5.12	112.48	121.70	1	1
F	66	ARG	C-N-CA	5.09	112.55	121.70	1	1
F	70	GLU	C-N-CA	5.08	112.56	121.70	1	1
A	40	SER	O-C-N	5.07	131.11	123.00	1	1
E	70	GLU	C-N-CA	5.07	112.58	121.70	1	1
A	68	GLN	C-N-CA	5.04	112.63	121.70	1	1
D	68	GLN	C-N-CA	5.03	112.65	121.70	1	1
G	188	GLN	OE1-CD-NE2	4.98	117.62	122.60	1	1
D	52	TRP	C-N-CA	4.97	130.65	121.70	1	1
A	52	TRP	C-N-CA	4.96	130.64	121.70	1	1
C	49	GLN	OE1-CD-NE2	4.90	117.70	122.60	1	1
C	129	GLN	OE1-CD-NE2	4.86	117.74	122.60	1	1
C	127	GLN	OE1-CD-NE2	4.78	117.82	122.60	1	1
D	56	SER	C-N-CA	4.76	130.28	121.70	1	1
F	30	LEU	C-N-CA	4.75	130.25	121.70	1	1
E	30	LEU	C-N-CA	4.75	130.25	121.70	1	1
A	56	SER	C-N-CA	4.74	130.23	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
H	129	GLN	OE1-CD-NE2	4.73	117.87	122.60	1	1
A	35	LEU	C-N-CA	4.70	113.23	121.70	1	1
E	66	ARG	O-C-N	4.69	130.51	123.00	1	1
H	127	GLN	OE1-CD-NE2	4.69	117.91	122.60	1	1
D	35	LEU	C-N-CA	4.67	113.29	121.70	1	1
F	66	ARG	O-C-N	4.65	130.44	123.00	1	1
D	40	SER	CA-C-N	4.61	106.97	116.20	1	1
G	71	GLN	OE1-CD-NE2	4.58	118.02	122.60	1	1
A	40	SER	CA-C-N	4.57	107.05	116.20	1	1
A	38	ASP	CA-C-N	4.52	107.17	116.20	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	49.39	905

There are 905 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)
D:215:LEU:HD21	F:52:TRP:CZ3	1.69	1	1
E:48:TRP:CE2	E:211:VAL:HG13	1.65	1	1
D:193:PHE:CD2	F:44:LEU:HB2	1.64	1	1
E:191:GLU:HB3	G:105:VAL:CG1	1.63	1	1
F:51:MET:HE3	F:211:VAL:CA	1.62	1	1
B:95:TRP:CE3	F:198:ARG:CD	1.61	1	1
A:211:VAL:HG13	E:48:TRP:CH2	1.60	1	1
B:95:TRP:CZ3	F:198:ARG:CD	1.59	1	1
F:59:ALA:HB1	F:203:LYS:CG	1.58	1	1
D:215:LEU:CD2	F:52:TRP:CH2	1.58	1	1
D:215:LEU:CD2	F:52:TRP:CZ3	1.57	1	1
B:105:VAL:CG1	F:191:GLU:HB3	1.56	1	1
E:77:GLU:HG3	G:162:PHE:CZ	1.56	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
D:211:VAL:CG2	F:48:TRP:CZ3	1.55	1	1
E:191:GLU:CD	G:105:VAL:HG21	1.55	1	1
E:77:GLU:CG	G:162:PHE:CZ	1.55	1	1
B:105:VAL:HG21	F:191:GLU:CD	1.53	1	1
F:59:ALA:CB	F:203:LYS:HG3	1.52	1	1
E:62:ALA:CB	E:203:LYS:HD2	1.51	1	1
A:48:TRP:HH2	G:214:MET:SD	1.51	1	1
F:51:MET:CE	F:211:VAL:HA	1.51	1	1
E:62:ALA:HB3	E:203:LYS:CD	1.49	1	1
E:191:GLU:CG	G:163:CYS:SG	1.47	1	1
D:215:LEU:HD23	F:52:TRP:CH2	1.47	1	1
A:211:VAL:CG1	E:48:TRP:CH2	1.46	1	1
E:191:GLU:HG3	G:163:CYS:SG	1.45	1	1
E:48:TRP:NE1	E:211:VAL:HG13	1.45	1	1
A:48:TRP:CH2	G:214:MET:SD	1.43	1	1
B:105:VAL:CG2	F:191:GLU:CD	1.43	1	1
B:95:TRP:CD2	F:198:ARG:HD3	1.42	1	1
D:211:VAL:HG22	F:48:TRP:CZ3	1.42	1	1
B:163:CYS:SG	F:191:GLU:CG	1.41	1	1
F:48:TRP:CE2	F:211:VAL:CG1	1.41	1	1
B:163:CYS:SG	F:191:GLU:HG3	1.41	1	1
F:48:TRP:NE1	F:211:VAL:HG13	1.40	1	1
E:191:GLU:CD	G:105:VAL:CG2	1.40	1	1
D:77:GLU:OE2	D:79:ARG:CD	1.40	1	1
B:95:TRP:CE3	F:198:ARG:HD3	1.40	1	1
B:95:TRP:CZ3	F:198:ARG:HD3	1.39	1	1
E:48:TRP:CZ2	E:211:VAL:CG1	1.39	1	1
F:54:SER:CA	F:57:GLU:HB3	1.39	1	1
D:193:PHE:CD2	F:44:LEU:CB	1.39	1	1
F:59:ALA:CB	F:203:LYS:CG	1.37	1	1
F:59:ALA:O	F:63:ASP:HB2	1.36	1	1
D:194:ASN:CB	F:37:GLU:HB3	1.34	1	1
F:48:TRP:CE2	F:211:VAL:HG13	1.34	1	1
D:207:GLN:OE1	F:41:ARG:NH1	1.33	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
E:54:SER:O	E:58:ASP:N	1.33	1	1
E:77:GLU:HG3	G:162:PHE:CE1	1.32	1	1
E:52:TRP:CE3	E:211:VAL:HG21	1.31	1	1
D:193:PHE:HE2	F:44:LEU:C	1.31	1	1
D:193:PHE:CE2	F:45:LEU:N	1.31	1	1
E:48:TRP:CE2	E:211:VAL:CG1	1.31	1	1
F:51:MET:CE	F:211:VAL:CA	1.30	1	1
F:55:MET:CA	F:58:ASP:HB2	1.30	1	1
E:62:ALA:N	E:203:LYS:HZ2	1.30	1	1
A:38:ASP:O	A:42:HIS:ND1	1.30	1	1
E:63:ASP:H	E:203:LYS:NZ	1.29	1	1
E:191:GLU:HA	G:158:LEU:CD2	1.29	1	1
E:53:SER:O	E:57:GLU:N	1.29	1	1
F:48:TRP:NE1	F:211:VAL:CG1	1.29	1	1
F:51:MET:HE3	F:211:VAL:N	1.29	1	1
E:59:ALA:O	E:63:ASP:HB2	1.28	1	1
B:95:TRP:CE3	F:198:ARG:HD2	1.28	1	1
B:158:LEU:CD2	F:191:GLU:HA	1.28	1	1
D:193:PHE:HE2	F:45:LEU:N	1.27	1	1
F:56:SER:O	F:203:LYS:HE3	1.26	1	1
B:105:VAL:CG1	F:191:GLU:CB	1.26	1	1
A:52:TRP:CH2	G:218:SER:OG	1.26	1	1
D:194:ASN:ND2	F:38:ASP:N	1.25	1	1
E:191:GLU:OE1	G:105:VAL:CG2	1.25	1	1
B:95:TRP:CH2	F:198:ARG:HD3	1.25	1	1
D:38:ASP:O	D:42:HIS:ND1	1.24	1	1
A:211:VAL:CG1	E:48:TRP:CZ2	1.24	1	1
B:95:TRP:CE2	F:198:ARG:HD3	1.24	1	1
F:54:SER:HA	F:57:GLU:CB	1.22	1	1
A:36:SER:O	A:39:SER:OG	1.21	1	1
D:36:SER:O	D:39:SER:OG	1.21	1	1
D:194:ASN:HD21	F:38:ASP:CA	1.20	1	1
D:38:ASP:HB3	D:42:HIS:CE1	1.20	1	1
A:38:ASP:HB3	A:42:HIS:CE1	1.20	1	1
B:105:VAL:CG2	F:191:GLU:OE1	1.20	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
E:191:GLU:CG	G:158:LEU:HD13	1.19	1	1
A:38:ASP:O	A:70:GLU:OE2	1.19	1	1
A:211:VAL:HG13	E:48:TRP:CZ2	1.18	1	1
D:38:ASP:O	D:70:GLU:OE2	1.18	1	1
E:191:GLU:CB	G:105:VAL:CG1	1.18	1	1
B:158:LEU:HD13	F:191:GLU:CG	1.17	1	1
D:53:SER:CB	D:59:ALA:O	1.17	1	1
D:194:ASN:HD21	F:38:ASP:N	1.17	1	1
E:57:GLU:HA	E:60:SER:HB3	1.17	1	1
B:95:TRP:CZ2	F:198:ARG:HD3	1.17	1	1
A:53:SER:CB	A:59:ALA:O	1.16	1	1
E:59:ALA:CB	E:207:GLN:NE2	1.16	1	1
A:215:LEU:HD23	E:52:TRP:HH2	1.16	1	1
E:191:GLU:CA	G:158:LEU:HD22	1.16	1	1
E:59:ALA:HB3	E:207:GLN:HE22	1.14	1	1
B:95:TRP:CH2	F:198:ARG:CD	1.14	1	1
F:57:GLU:HA	F:60:SER:HB3	1.14	1	1
B:97:LEU:HD12	F:191:GLU:OE2	1.14	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	1132	1094	31	7

There are 7 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	57	GLU	1
B	191	PRO	1
C	21	ARG	1
D	57	GLU	1
F	56	SER	1
G	191	PRO	1
H	21	ARG	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	1038	956	61	21

There are 21 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	30	LEU	1
A	38	ASP	1
B	101	LEU	1
B	201	GLU	1
B	214	MET	1
B	218	SER	1
C	24	LEU	1
D	30	LEU	1
D	38	ASP	1
E	30	LEU	1
E	56	SER	1
E	64	MET	1
F	30	LEU	1
F	56	SER	1
F	64	MET	1
G	101	LEU	1
G	187	ILE	1
G	201	GLU	1
G	214	MET	1
G	218	SER	1
H	24	LEU	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 2336 crosslinking restraints combined in 231 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
sulfo-SDA	GLU	None	LYS	None	upper bound	22.0	80
sulfo-SDA	LYS	None	SER	None	upper bound	22.0	16
sulfo-SDA	GLU	None	SER	None	upper bound	22.0	40
sulfo-SDA	HIS	None	LYS	None	upper bound	22.0	12
sulfo-SDA	LYS	None	THR	None	upper bound	22.0	16
sulfo-SDA	HIS	None	SER	None	upper bound	22.0	16
sulfo-SDA	LEU	None	LYS	None	upper bound	22.0	60
sulfo-SDA	LYS	None	MET	None	upper bound	22.0	8
sulfo-SDA	MET	None	SER	None	upper bound	22.0	4
sulfo-SDA	LYS	None	VAL	None	upper bound	22.0	48
sulfo-SDA	GLN	None	SER	None	upper bound	22.0	16
sulfo-SDA	ILE	None	LYS	None	upper bound	22.0	20
sulfo-SDA	LYS	None	PHE	None	upper bound	22.0	8
sulfo-SDA	LYS	None	LYS	None	upper bound	22.0	8
sulfo-SDA	GLN	None	LYS	None	upper bound	22.0	8
sulfo-SDA	SER	None	SER	None	upper bound	22.0	16
sulfo-SDA	SER	None	VAL	None	upper bound	22.0	16
sulfo-SDA	ASP	None	SER	None	upper bound	22.0	16
sulfo-SDA	ASP	None	LYS	None	upper bound	22.0	8
sulfo-SDA	ARG	None	SER	None	upper bound	22.0	32
sulfo-SDA	CYS	None	LYS	None	upper bound	22.0	8
EDC	GLU	None	LYS	None	upper bound	22.0	1264
EDC	ASP	None	LYS	None	upper bound	22.0	208
EDC	ASP	None	SER	None	upper bound	22.0	56
EDC	ASP	None	TYR	None	upper bound	22.0	16
EDC	GLU	None	SER	None	upper bound	22.0	216
EDC	GLU	None	THR	None	upper bound	22.0	32
EDC	ASN	None	LYS	None	upper bound	22.0	36
EDC	LYS	None	PRO	None	upper bound	22.0	12
EDC	ARG	None	SER	None	upper bound	22.0	16
EDC	ASP	None	THR	None	upper bound	22.0	8
EDC	SER	None	SER	None	upper bound	22.0	16

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=231)
1	1	1	1/1	All	Not available	Not available	0

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.

3DEM volume

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

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