

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	9A0Q
PDB-Dev ID	PDBDEV_00000062
Structure Title	Integrative structure of transcriptional enhancer factor TEF-1
Structure Authors	Filandrova R; Valis K; Cerny J; Chmelik J; Slavata L; Fiala J; Rosulek M; Kavan D; Man P; Chum T; Cebecauer M; Fabris D; Novak P
Deposited on	2020-10-08

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

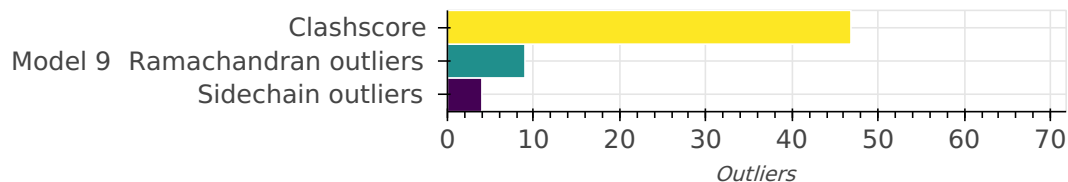
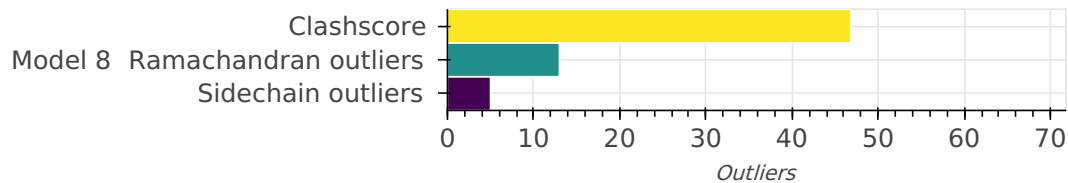
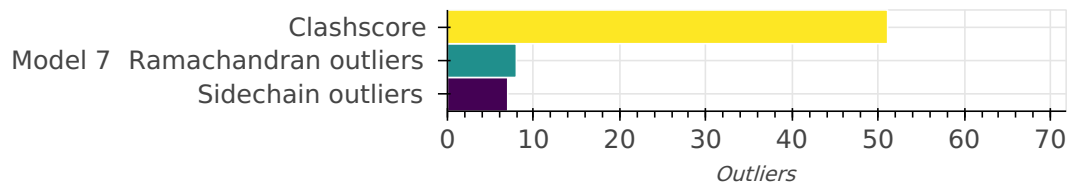
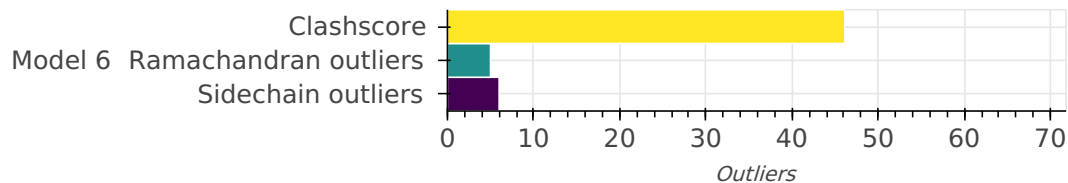
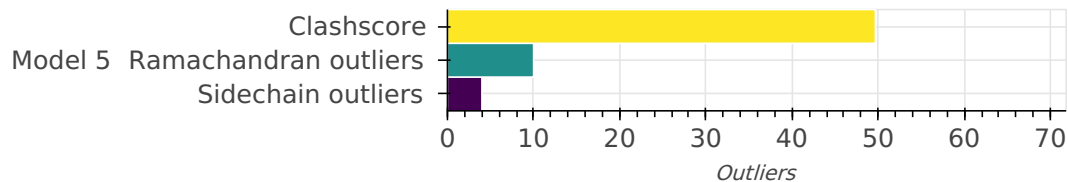
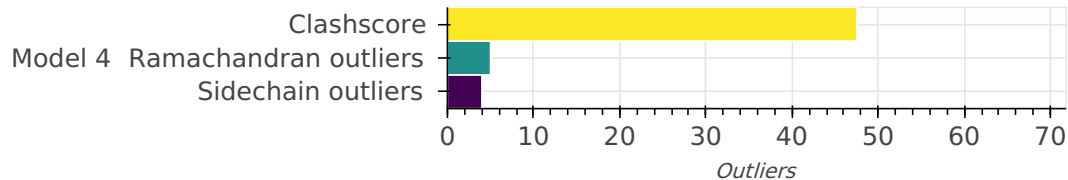
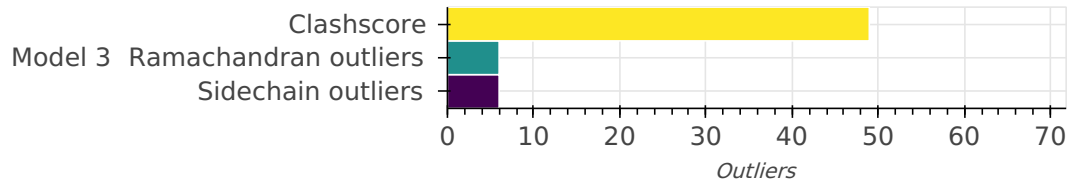
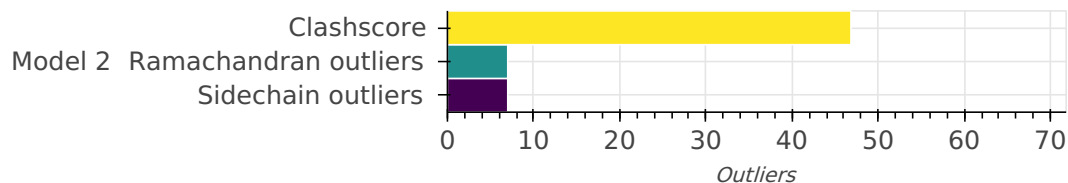
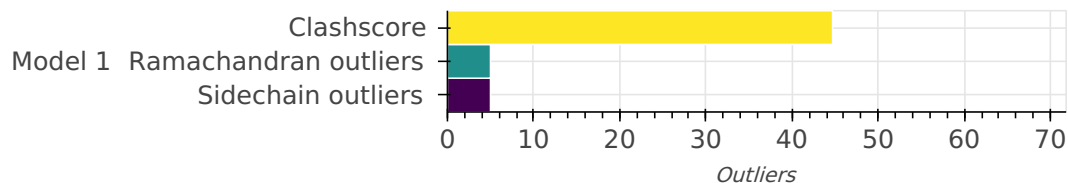
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

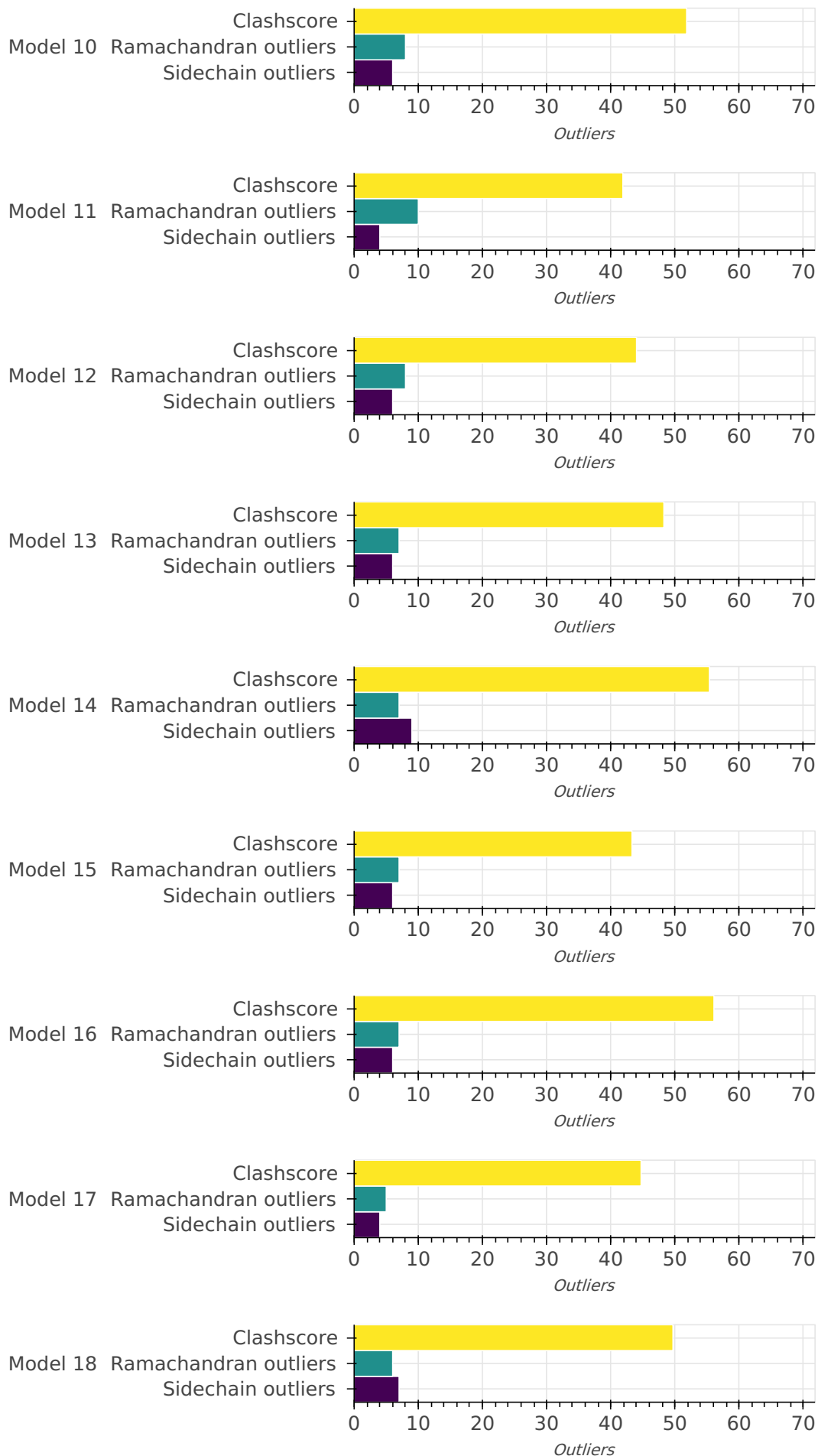
List of references used to build this report is available [here](#).

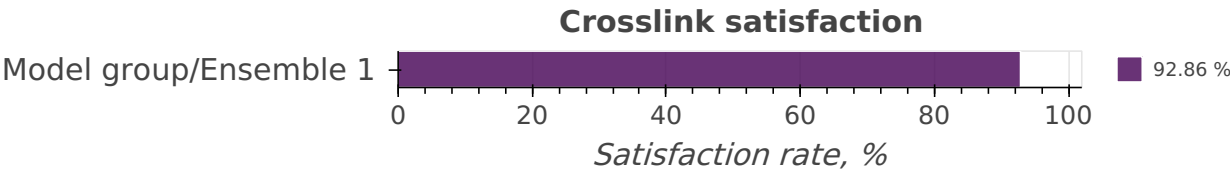
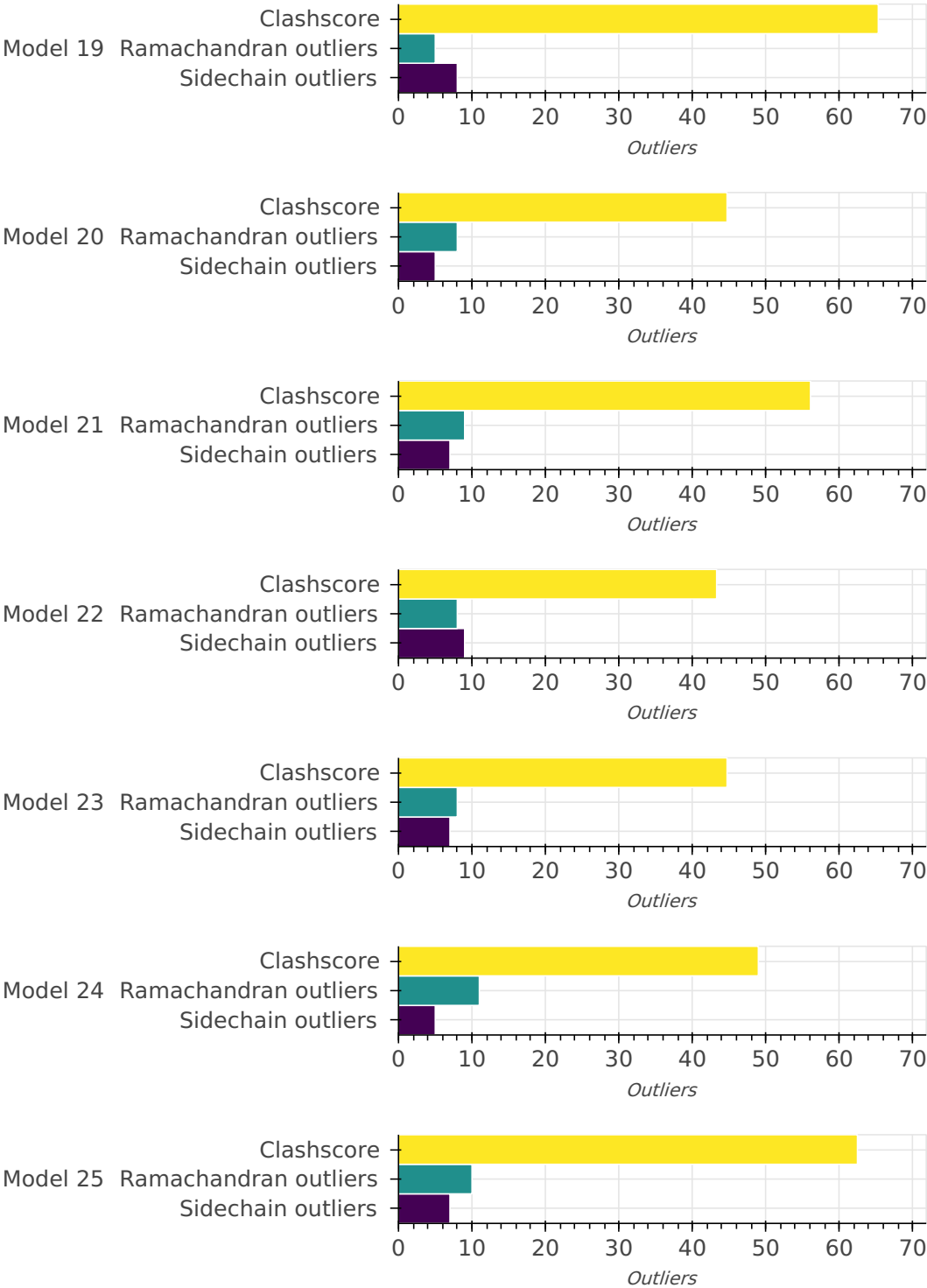
Overall quality ?

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 25 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	1-25	1	Transcriptional enhancer factor TEF-1	A	87	-	1-87	100.00 / 100.00	Atomic

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	Mass Spectrometry data	PRIDE	PXD012127
2	Crosslinking-MS data	Not available	10.17632/27zkz3v729.1
3	Experimental model	PDB	2HZD
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	homology modeling	None	25	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
2	1	None	molecular dynamics	None	100	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	MODELLER	9.20	comparative modeling	https://salilab.org/modeller/
2	Modeller	9.24	homology modeling	https://salilab.org/modeller/
3	CNS	1.30	simulated annealing	http://cns-online.org

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.

Mass Spectrometry

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 no bond length outliers.

Standard geometry: angle outliers ?

There are 77 bond angle outliers in this entry (0.32% of 23750 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	47	GLY	N-CA-C	7.15	92.58	113.30	20	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	38	ARG	C-N-CA	6.71	133.77	121.70	24	1
A	51	GLY	N-CA-C	6.03	130.78	113.30	14	1
A	42	ILE	N-CA-C	5.86	94.60	111.00	24	1
A	71	LYS	C-CA-CB	5.78	121.07	110.10	16	25
A	68	ARG	C-CA-CB	5.50	120.54	110.10	24	5
A	66	LYS	C-CA-CB	5.46	99.73	110.10	9	18
A	69	THR	N-CA-CB	4.93	119.88	111.50	17	5
A	38	ARG	CA-C-N	4.86	106.48	116.20	24	1
A	51	GLY	CA-C-N	4.82	125.84	116.20	14	1
A	39	ARG	C-N-CA	4.79	130.33	121.70	25	3
A	45	ASP	N-CA-C	4.77	97.64	111.00	20	2
A	45	ASP	C-N-CA	4.68	130.12	121.70	18	1
A	39	ARG	N-CA-C	4.59	123.86	111.00	24	1
A	68	ARG	C-N-CA	4.57	129.92	121.70	14	5
A	66	LYS	N-CA-C	4.50	123.59	111.00	17	1
A	51	GLY	CA-C-O	4.49	111.37	120.80	14	1
A	37	GLY	N-CA-C	4.45	100.39	113.30	24	1
A	39	ARG	CA-C-N	4.26	107.67	116.20	24	1
A	37	GLY	C-N-CA	4.21	129.28	121.70	24	1
A	47	GLY	C-N-CA	4.17	129.20	121.70	18	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	44.71	63
2	46.84	66
3	48.97	69
4	47.55	67
5	49.68	70
6	46.13	65
7	51.10	72
8	46.84	66
9	46.84	66
10	51.81	73

Model ID	Clash score	Number of clashes
11	41.87	59
12	44.00	62
13	48.26	68
14	55.36	78
15	43.29	61
16	56.07	79
17	44.71	63
18	49.68	70
19	65.29	92
20	44.71	63
21	56.07	79
22	43.29	61
23	44.71	63
24	48.97	69
25	62.46	88

There are 1732 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)
A:48:LYS:NZ	A:50:TYR:HA	1.13	20	21
A:29:ALA:CB	A:56:ILE:HG23	1.12	1	2
A:29:ALA:HB1	A:56:ILE:CG2	1.12	1	25
A:58:ARG:HG2	A:61:LYS:HZ1	1.12	23	1
A:68:ARG:O	A:69:THR:O	1.06	25	1
A:35:PRO:HD3	A:84:LYS:HD2	1.00	5	1
A:76:HIS:O	A:79:VAL:HG22	0.99	18	1
A:79:VAL:HG13	A:82:ARG:HH21	0.99	12	3
A:58:ARG:HG2	A:61:LYS:NZ	0.97	23	1
A:70:ARG:HB2	A:71:LYS:HZ2	0.96	17	4
A:80:LEU:O	A:84:LYS:N	0.95	25	25
A:48:LYS:HZ3	A:49:MET:HA	0.95	14	2
A:58:ARG:HB3	A:61:LYS:HZ3	0.93	18	5
A:70:ARG:HH11	A:73:VAL:HB	0.92	16	1
A:29:ALA:HB1	A:56:ILE:HG23	0.92	1	2
A:66:LYS:HZ1	A:68:ARG:NH1	0.91	8	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:57:ALA:HB2	A:70:ARG:HG2	0.91	16	20
A:70:ARG:HB2	A:71:LYS:NZ	0.91	5	4
A:81:ALA:HB1	A:86:ARG:HE	0.90	19	1
A:69:THR:HG21	A:72:GLN:HE21	0.90	20	1
A:68:ARG:H	A:68:ARG:HE	0.90	21	4
A:48:LYS:HZ2	A:50:TYR:HA	0.90	20	10
A:56:ILE:HG21	A:73:VAL:HG21	0.89	1	1
A:57:ALA:O	A:61:LYS:HG3	0.88	17	6
A:60:ILE:HD12	A:66:LYS:HZ1	0.88	24	3
A:48:LYS:NZ	A:50:TYR:H	0.87	14	2
A:77:ILE:HG22	A:84:LYS:NZ	0.87	25	5
A:58:ARG:HB3	A:61:LYS:HZ1	0.87	16	11
A:81:ALA:HA	A:84:LYS:HG2	0.87	25	6
A:22:ILE:HG23	A:23:GLU:H	0.86	11	3
A:40:LYS:HZ3	A:55:LEU:HD11	0.85	2	9
A:48:LYS:HZ1	A:50:TYR:HA	0.85	20	8
A:56:ILE:CG2	A:73:VAL:HG21	0.84	1	1
A:40:LYS:HZ2	A:55:LEU:HD13	0.84	24	1
A:58:ARG:HB3	A:61:LYS:NZ	0.82	9	15
A:66:LYS:NZ	A:67:THR:O	0.82	20	6
A:70:ARG:HB3	A:71:LYS:NZ	0.82	25	10
A:53:ASN:HB2	A:70:ARG:HE	0.81	16	1
A:58:ARG:N	A:61:LYS:HZ2	0.81	12	5
A:53:ASN:HB3	A:71:LYS:HZ1	0.81	14	12
A:48:LYS:HZ2	A:50:TYR:CA	0.80	20	14
A:58:ARG:HB3	A:61:LYS:HZ2	0.80	9	1
A:22:ILE:HD11	A:65:GLY:HA3	0.80	19	1
A:58:ARG:HB2	A:61:LYS:HZ3	0.80	14	3
A:66:LYS:HZ3	A:68:ARG:HD3	0.80	8	5
A:75:SER:HA	A:78:GLN:HE21	0.80	4	2
A:8:LYS:H	A:9:PRO:HD2	0.80	21	2
A:70:ARG:NH2	A:74:SER:HB2	0.79	16	1
A:22:ILE:O	A:24:GLN:N	0.79	11	2
A:48:LYS:HZ2	A:50:TYR:N	0.79	16	9
A:35:PRO:HB3	A:84:LYS:HD2	0.79	25	14

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:70:ARG:HB2	A:71:LYS:HZ3	0.79	5	1
A:40:LYS:NZ	A:55:LEU:HD11	0.79	2	9
A:21:ASP:HB2	A:24:GLN:HE21	0.78	18	1
A:22:ILE:HD11	A:24:GLN:HE21	0.78	3	1
A:53:ASN:HB3	A:71:LYS:NZ	0.78	14	17
A:35:PRO:HB3	A:84:LYS:HE2	0.78	24	9
A:68:ARG:O	A:69:THR:HG22	0.77	17	2
A:58:ARG:HA	A:61:LYS:HB2	0.77	7	24
A:48:LYS:NZ	A:50:TYR:CA	0.77	24	23
A:19:SER:H	A:20:PRO:HD2	0.77	7	1
A:66:LYS:HZ3	A:67:THR:HA	0.77	6	3
A:68:ARG:HE	A:68:ARG:N	0.77	19	4
A:52:ARG:HA	A:55:LEU:HD23	0.77	25	7
A:42:ILE:O	A:43:LEU:HB2	0.76	24	1
A:44:SER:C	A:46:GLU:H	0.76	20	2
A:70:ARG:NH1	A:73:VAL:HB	0.76	16	1
A:53:ASN:O	A:70:ARG:CD	0.75	16	1
A:55:LEU:HD23	A:58:ARG:HH21	0.75	11	3
A:60:ILE:HD12	A:66:LYS:NZ	0.75	24	5
A:66:LYS:NZ	A:67:THR:HA	0.75	19	17
A:53:ASN:O	A:70:ARG:HD3	0.75	16	1
A:84:LYS:HE3	A:86:ARG:HG3	0.75	25	1
A:20:PRO:HB2	A:67:THR:HG21	0.74	22	2
A:48:LYS:HZ3	A:49:MET:CA	0.74	14	2
A:66:LYS:HD2	A:67:THR:N	0.74	1	3
A:66:LYS:HZ1	A:68:ARG:HH11	0.74	8	1
A:8:LYS:HE2	A:75:SER:HB2	0.74	18	1
A:52:ARG:HA	A:55:LEU:HD13	0.74	1	6
A:24:GLN:HA	A:27:GLN:HE21	0.73	24	17
A:66:LYS:HZ1	A:67:THR:HA	0.73	15	4
A:61:LYS:HD3	A:68:ARG:HD3	0.73	17	1
A:48:LYS:HZ3	A:50:TYR:HA	0.73	24	6
A:68:ARG:H	A:68:ARG:NE	0.73	19	4
A:61:LYS:HG3	A:68:ARG:HE	0.73	6	1
A:44:SER:C	A:46:GLU:N	0.72	18	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:70:ARG:HB2	A:71:LYS:HZ1	0.72	18	3
A:69:THR:HG21	A:72:GLN:NE2	0.72	20	2
A:28:GLU:O	A:32:ILE:HG22	0.72	22	3
A:22:ILE:HD11	A:24:GLN:NE2	0.71	3	1
A:76:HIS:O	A:79:VAL:HG12	0.71	14	1
A:35:PRO:HG2	A:80:LEU:HD22	0.71	21	1
A:81:ALA:C	A:83:ARG:H	0.71	14	23
A:43:LEU:C	A:46:GLU:HB3	0.71	18	2
A:66:LYS:CG	A:67:THR:N	0.70	19	2
A:54:GLU:O	A:58:ARG:HG3	0.70	23	1
A:40:LYS:O	A:41:ILE:HG23	0.70	4	6
A:30:LEU:HD13	A:76:HIS:NE2	0.70	1	2
A:10:ILE:HG22	A:12:ASN:HD22	0.70	19	1
A:57:ALA:O	A:61:LYS:HD3	0.70	14	17

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	85	64	16	5
2	85	64	14	7
3	85	67	12	6
4	85	63	17	5
5	85	63	12	10
6	85	66	14	5
7	85	68	9	8
8	85	63	9	13
9	85	61	15	9
10	85	67	10	8
11	85	62	13	10
12	85	66	11	8
13	85	59	19	7
14	85	65	13	7
15	85	66	12	7
16	85	67	11	7
17	85	66	14	5

Model ID	Analysed	Favored	Allowed	Outliers
18	85	64	15	6
19	85	67	13	5
20	85	64	13	8
21	85	62	14	9
22	85	63	14	8
23	85	64	13	8
24	85	64	10	11
25	85	64	11	10

There are 38 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	41	ILE	25
A	64	THR	19
A	66	LYS	16
A	67	THR	16
A	16	GLY	9
A	8	LYS	8
A	22	ILE	8
A	3	HIS	7
A	6	ALA	6
A	10	ILE	6
A	7	ASP	5
A	13	ASP	5
A	17	VAL	5
A	19	SER	5
A	21	ASP	5
A	20	PRO	4
A	49	MET	4
A	84	LYS	4
A	4	MET	3
A	11	ASP	3
A	15	GLU	3
A	23	GLU	3
A	86	ARG	3
A	2	SER	2

Chain	Res	Type	Models (Total)
A	14	ALA	2
A	48	LYS	2
A	69	THR	2
A	85	SER	2
A	5	SER	1
A	12	ASN	1
A	38	ARG	1
A	40	LYS	1
A	42	ILE	1
A	43	LEU	1
A	46	GLU	1
A	51	GLY	1
A	52	ARG	1
A	70	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	75	64	6	5
2	75	60	8	7
3	75	57	12	6
4	75	64	7	4
5	75	61	10	4
6	75	61	8	6
7	75	61	7	7
8	75	58	12	5
9	75	61	10	4
10	75	58	11	6
11	75	63	8	4
12	75	60	9	6
13	75	63	6	6
14	75	61	5	9
15	75	61	8	6
16	75	59	10	6
17	75	63	8	4

Model ID	Analysed	Favored	Allowed	Outliers
18	75	62	6	7
19	75	55	12	8
20	75	63	7	5
21	75	61	7	7
22	75	61	5	9
23	75	59	9	7
24	75	63	7	5
25	75	61	7	7

There are 25 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	71	LYS	24
A	66	LYS	23
A	48	LYS	20
A	61	LYS	19
A	84	LYS	11
A	64	THR	9
A	63	ARG	6
A	68	ARG	5
A	73	VAL	5
A	26	PHE	4
A	49	MET	3
A	56	ILE	3
A	22	ILE	2
A	43	LEU	2
A	44	SER	2
A	52	ARG	2
A	80	LEU	2
A	4	MET	1
A	25	SER	1
A	28	GLU	1
A	42	ILE	1
A	70	ARG	1
A	72	GLN	1
A	76	HIS	1

Chain	Res	Type	Models (Total)
A	79	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*".

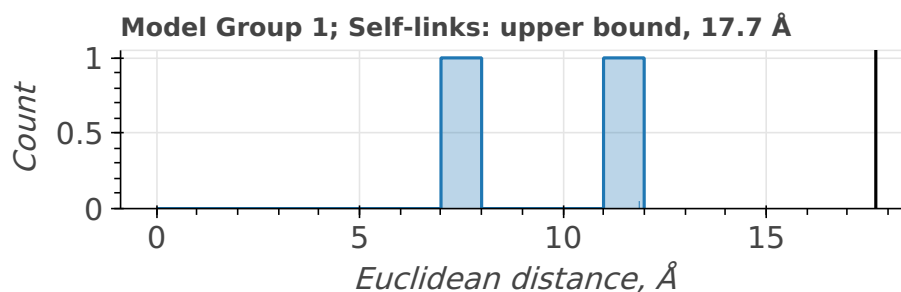
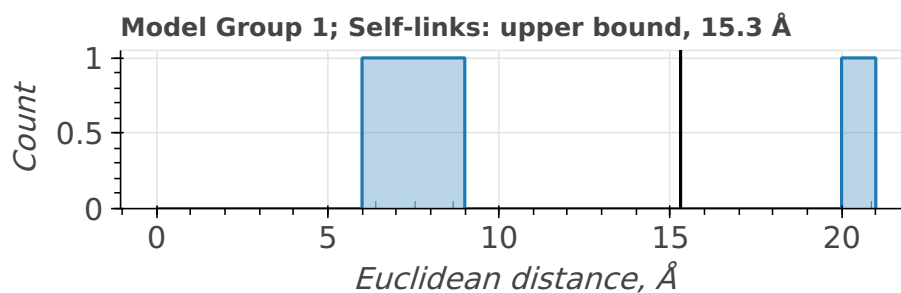
Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

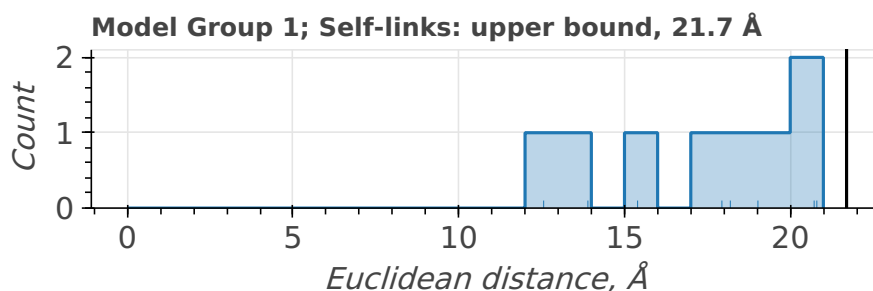
There are 14 crosslinking restraints combined in 14 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSA	GLY	CA	LYS	CA	upper bound	15.3	3
DSA	LYS	CA	LYS	CA	upper bound	21.7	8
DSA	LYS	CA	SER	CA	upper bound	17.7	1
DSA	LYS	CA	LYS	CA	upper bound	15.3	1
DSA	LYS	CA	THR	CA	upper bound	17.7	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=14)
1	1	1	25/25	All	92.86	7.14	14
				Self-links/Intramolecular	92.86	7.14	14

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.



Mass Spectrometry

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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