

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	9A0R
PDB-Dev ID	PDBDEV_00000063
Structure Title	Integrative structure of transcriptional enhancer factor TEF-1 bound to C-MYC exon
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

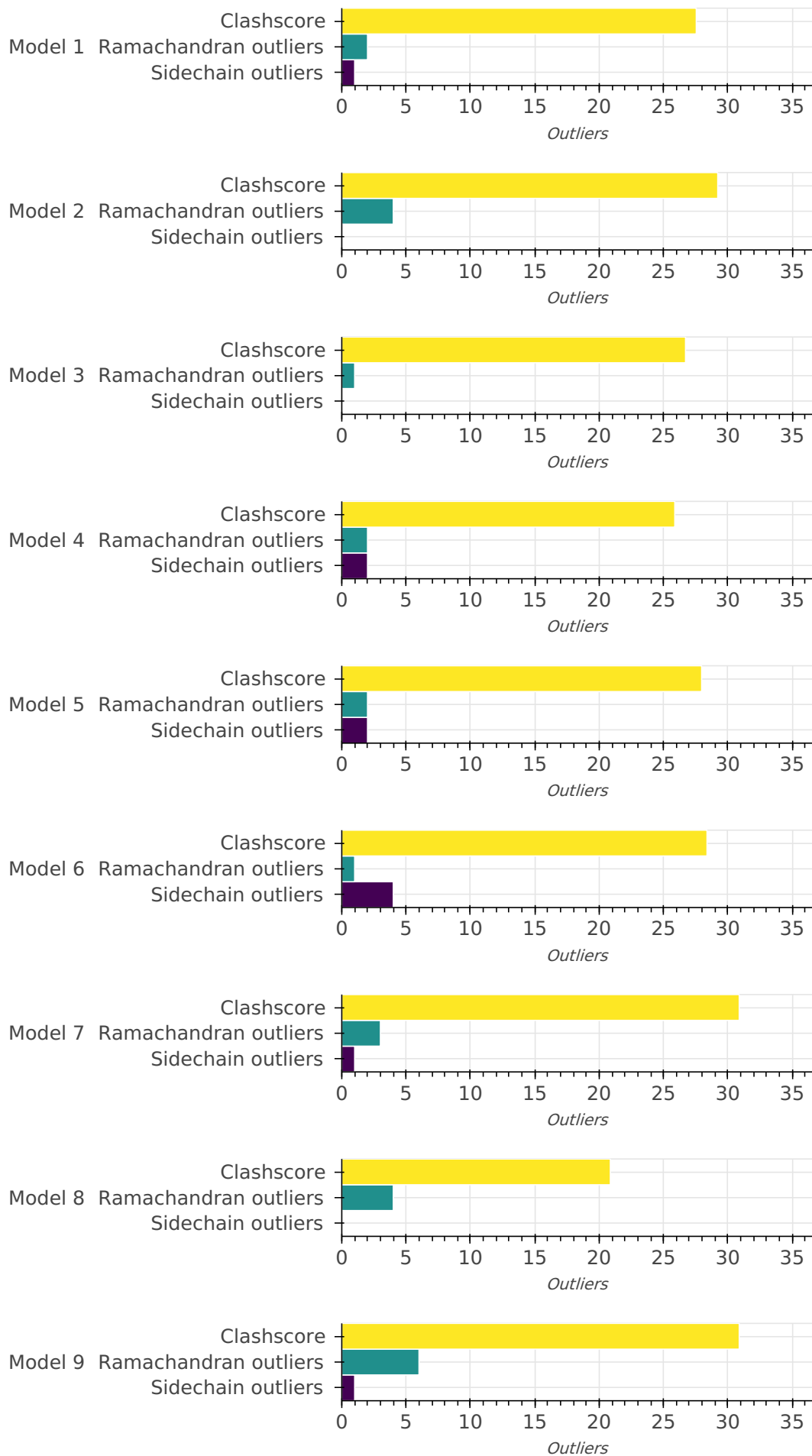
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

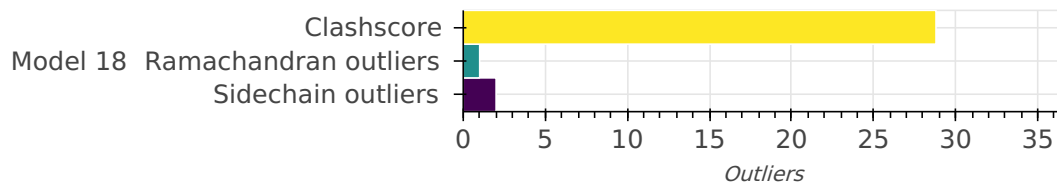
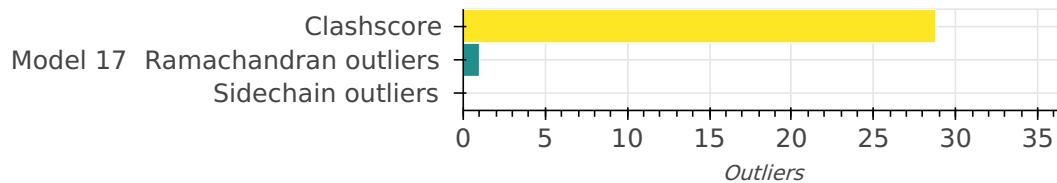
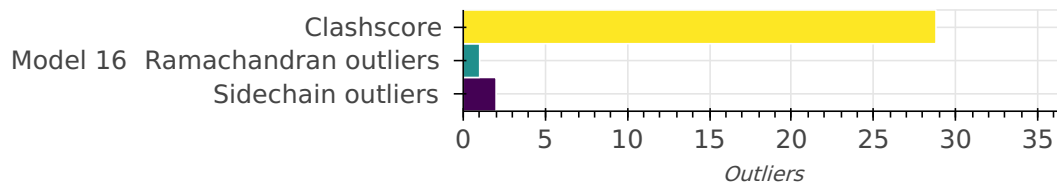
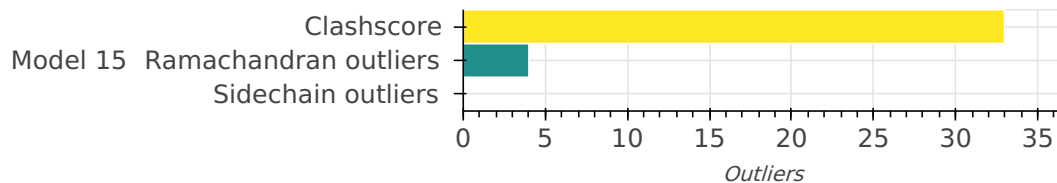
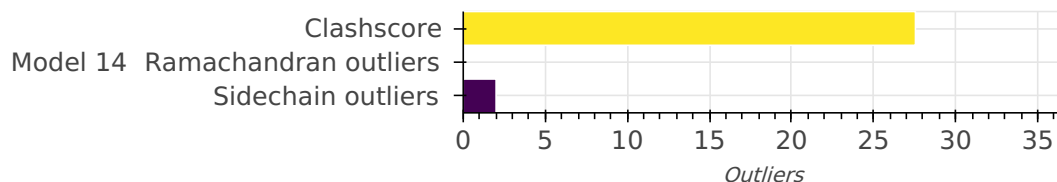
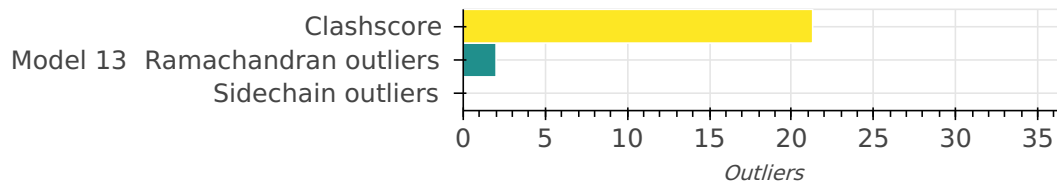
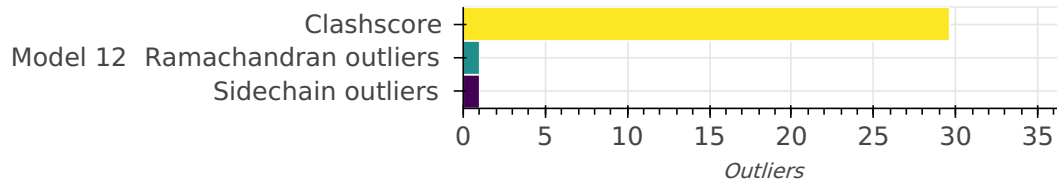
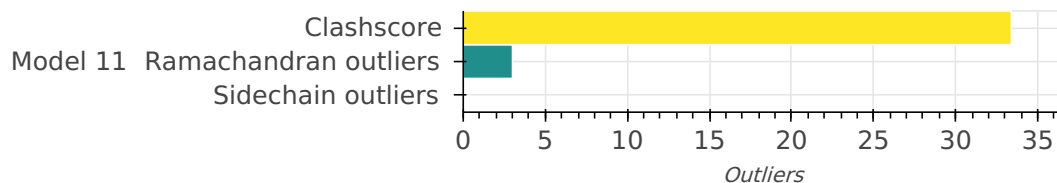
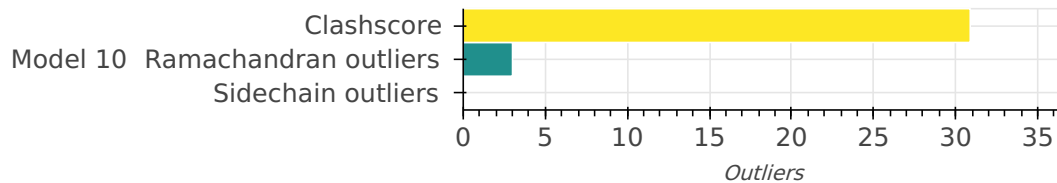
List of references used to build this report is available [here](#).

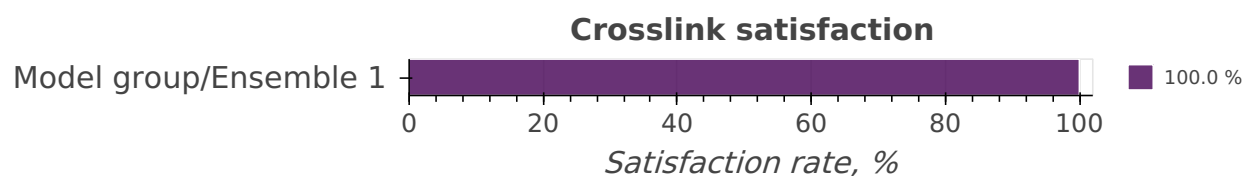
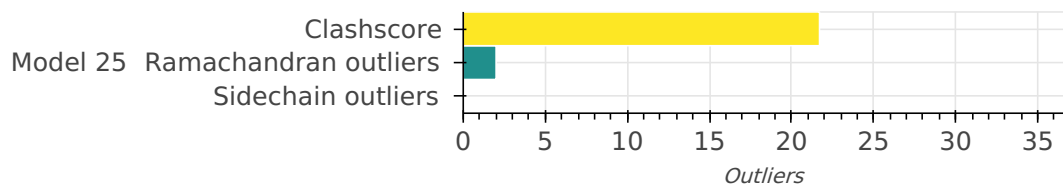
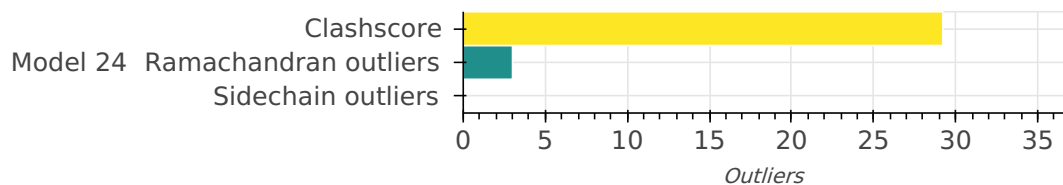
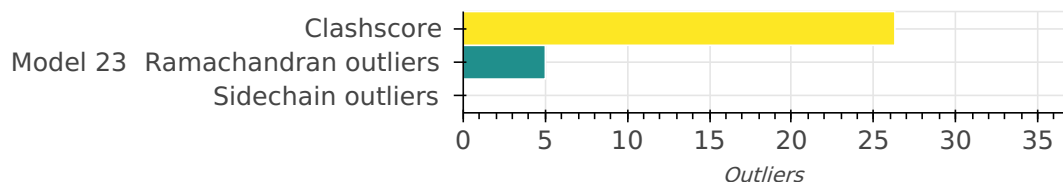
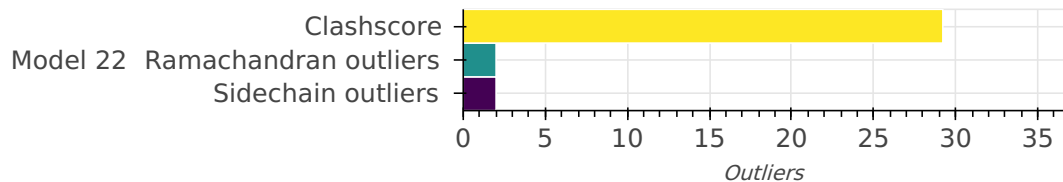
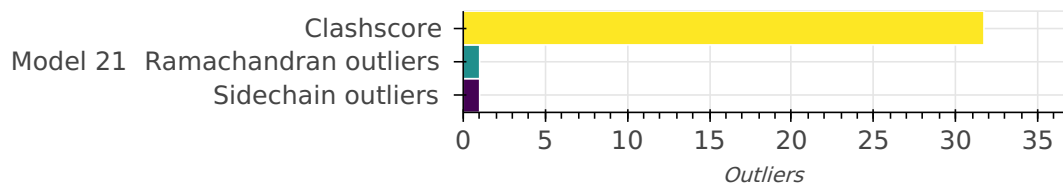
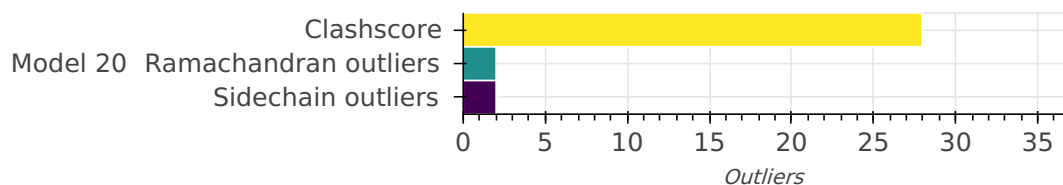
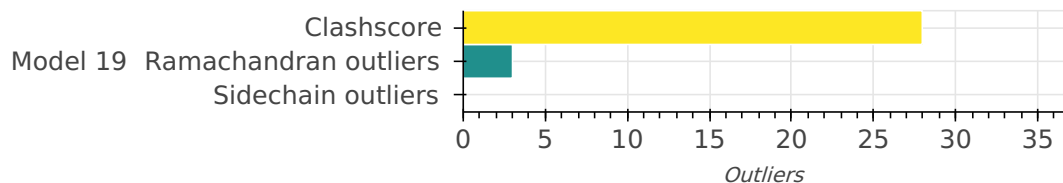
Overall quality ?

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 6 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-3	A	87	-	1-87	100.00 / 100.00	Atomic
		2	DNA (30-MER)	B	30	-	1-30	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 6 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	5GZB
4	Comparative model	Not available	Not available
5	Comparative model	Not available	Not available
6	H/D exchange data	Not available	10.17632/27zkz3v729.1

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
2	1	None	molecular docking	None	200	False	False
3	1	None	molecular dynamics	None	300	False	False

There are 5 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	Make-na	Not available	nucleic acid builder	http://structure.usc.edu/make-na/
3	Modeller	9.24	homology modeling	https://salilab.org/modeller/
4	Haddock	2.20	docking	https://alcazar.science.uu.nl/services/HADDOCK2.2/
5	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.

H/D exchange

Validation for this section is under development.

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 no bond angle outliers.

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	27.55	66
2	29.22	70
3	26.71	64
4	25.88	62
5	27.96	67
6	28.38	68
7	30.88	74
8	20.87	50
9	30.88	74
10	30.88	74
11	33.39	80
12	29.63	71
13	21.29	51
14	27.55	66
15	32.97	79
16	28.80	69
17	28.80	69
18	28.80	69
19	27.96	67
20	27.96	67
21	31.72	76
22	29.22	70
23	26.29	63
24	29.22	70

Model ID	Clash score	Number of clashes
25	21.70	52

There are 1688 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:8:DT:H3'	B:9:DT:H71	0.95	17	6
B:19:DT:H2'	B:20:DG:C8	0.94	15	19
B:9:DT:H2'	B:10:DC:O4'	0.93	3	21
B:26:DA:H2'	B:27:DC:C6	0.91	22	24
B:18:DC:H2'	B:19:DT:C6	0.90	17	17
B:19:DT:H2'	B:20:DG:H8	0.90	10	12
B:10:DC:H2'	B:11:DC:C6	0.89	10	21
A:35:PRO:HA	A:52:ARG:HE	0.89	10	10
A:72:GLN:HB3	B:8:DT:H73	0.89	19	9
B:4:DG:H2'	B:5:DT:O4'	0.88	4	11
B:21:DG:H2'	B:22:DA:O4'	0.87	6	6
B:4:DG:N2	B:28:DT:H1'	0.86	8	18
B:5:DT:H2'	B:6:DA:C8	0.86	12	13
B:8:DT:H2'	B:9:DT:H6	0.86	11	15
B:8:DT:H2'	B:9:DT:C6	0.86	11	20
B:17:DG:H2'	B:18:DC:O4'	0.85	17	15
B:24:DT:H2'	B:25:DT:C6	0.85	10	20
A:40:LYS:HE3	B:20:DG:H5''	0.83	24	2
B:5:DT:H2'	B:6:DA:O4'	0.82	24	9
B:6:DA:H2'	B:7:DA:C8	0.82	5	23
B:12:DA:H2'	B:13:DG:H8	0.81	16	4
B:2:DT:H2'	B:3:DA:C8	0.81	6	6
B:12:DA:H1'	B:20:DG:N2	0.80	1	18
A:10:ILE:H	A:10:ILE:HD13	0.80	4	3
B:24:DT:H3'	B:25:DT:H71	0.79	9	7
B:4:DG:H3'	B:5:DT:H71	0.79	17	3
B:5:DT:H71	B:5:DT:OP1	0.79	5	5
B:12:DA:H2'	B:13:DG:C8	0.79	22	4
B:27:DC:H2'	B:28:DT:H6	0.79	1	23
B:23:DA:H3'	B:24:DT:H71	0.77	21	12
B:24:DT:H2'	B:25:DT:O4'	0.77	25	5

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:58:ARG:HA	A:61:LYS:HE2	0.76	22	2
A:40:LYS:HZ3	A:52:ARG:HB3	0.76	16	3
B:10:DC:H2'	B:11:DC:H6	0.76	23	18
B:2:DT:H2'	B:3:DA:H8	0.76	6	2
B:7:DA:H2'	B:8:DT:C6	0.76	2	16
B:20:DG:H2'	B:21:DG:O4'	0.76	6	9
A:49:MET:HE1	B:19:DT:H5''	0.76	22	1
A:40:LYS:HZ2	A:52:ARG:HB3	0.75	4	8
B:13:DG:O2'	B:14:DC:H5'	0.74	24	21
B:9:DT:H2'	B:10:DC:C6	0.74	20	10
B:23:DA:H2'	B:24:DT:O4'	0.74	15	19
B:23:DA:H2'	B:24:DT:C6	0.74	6	15
B:17:DG:H2'	B:18:DC:C6	0.74	22	7
B:24:DT:H2'	B:25:DT:H6	0.72	22	20
B:25:DT:H2'	B:26:DA:O4'	0.72	17	16
A:4:MET:HG3	A:5:SER:H	0.72	10	2
A:40:LYS:CE	B:20:DG:H5''	0.72	24	2
B:28:DT:H2'	B:29:DA:C8	0.72	22	17
B:27:DC:H3'	B:28:DT:H71	0.72	22	5
B:23:DA:H2'	B:24:DT:H6	0.72	6	15
A:19:SER:H	A:20:PRO:HD2	0.72	9	2
B:22:DA:H2'	B:23:DA:O4'	0.71	23	11
B:22:DA:H2'	B:23:DA:H8	0.71	22	4
B:20:DG:H2'	B:21:DG:C8	0.71	24	4
B:4:DG:H2'	B:5:DT:H5'	0.71	16	4
A:51:GLY:H	A:54:GLU:HG3	0.70	6	1
B:6:DA:H2'	B:7:DA:H8	0.70	6	11
B:18:DC:H3'	B:19:DT:H71	0.70	1	6
A:70:ARG:H	A:70:ARG:HD2	0.70	6	1
B:21:DG:H2'	B:22:DA:H8	0.70	12	8
A:48:LYS:HB3	A:48:LYS:HZ2	0.70	5	2
A:40:LYS:HZ1	A:53:ASN:H	0.70	24	2
B:27:DC:H2'	B:28:DT:C6	0.70	16	21
A:70:ARG:HH22	B:19:DT:H5''	0.70	24	1
B:12:DA:H1'	B:20:DG:H22	0.69	24	10

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:49:MET:HE1	B:18:DC:H4'	0.69	17	1
B:27:DC:O2'	B:28:DT:H5'	0.69	20	24
A:81:ALA:HA	A:84:LYS:HE2	0.69	15	6
A:40:LYS:HE3	A:52:ARG:HB3	0.69	2	3
B:13:DG:H1	B:17:DG:H1	0.69	10	3
B:28:DT:H2'	B:29:DA:H8	0.68	22	10
A:83:ARG:HH22	B:5:DT:H3'	0.68	16	2
B:7:DA:H3'	B:8:DT:H71	0.68	6	2
B:22:DA:H2'	B:23:DA:C8	0.68	25	9
B:26:DA:H2'	B:27:DC:H6	0.67	16	16
B:21:DG:C2	B:22:DA:H1'	0.67	1	11
B:21:DG:H2'	B:22:DA:C8	0.67	12	10
B:3:DA:H2'	B:4:DG:O4'	0.67	15	18
B:13:DG:H2'	B:14:DC:H6	0.67	10	11
A:72:GLN:HB3	B:8:DT:C7	0.67	3	10
B:9:DT:H3	B:22:DA:H61	0.67	23	1
A:8:LYS:H	A:9:PRO:HD2	0.67	11	1
B:17:DG:O2'	B:18:DC:H5'	0.66	6	3
A:72:GLN:HE22	B:7:DA:H3'	0.66	15	1
B:14:DC:H2'	B:15:DG:H8	0.66	1	8
B:18:DC:H2'	B:19:DT:H6	0.66	11	13
B:4:DG:H22	B:28:DT:H1'	0.66	8	16
B:7:DA:H2	B:25:DT:H3	0.66	24	1
B:4:DG:C2'	B:5:DT:H5'	0.65	16	4
B:11:DC:H2'	B:12:DA:O4'	0.65	24	22
A:10:ILE:HG13	A:11:ASP:H	0.65	20	1
A:36:CYS:H	A:52:ARG:HD2	0.65	25	11
B:26:DA:H2'	B:27:DC:O4'	0.65	20	9
A:10:ILE:HG22	A:12:ASN:H	0.65	14	1
A:58:ARG:HA	A:61:LYS:HD2	0.65	18	7
B:28:DT:O2'	B:29:DA:H5'	0.64	25	21
B:8:DT:O2'	B:9:DT:H5'	0.64	22	8
B:18:DC:H2'	B:19:DT:O4'	0.64	6	2
B:8:DT:H73	B:8:DT:OP1	0.64	22	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	85	71	12	2
2	85	74	7	4
3	85	74	10	1
4	85	70	13	2
5	85	72	11	2
6	85	75	9	1
7	85	71	11	3
8	85	65	16	4
9	85	66	13	6
10	85	70	12	3
11	85	70	12	3
12	85	72	12	1
13	85	71	12	2
14	85	72	13	0
15	85	67	14	4
16	85	76	8	1
17	85	73	11	1
18	85	75	9	1
19	85	67	15	3
20	85	75	8	2
21	85	72	12	1
22	85	71	12	2
23	85	71	9	5
24	85	72	10	3
25	85	68	15	2

There are 22 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	47	GLY	13
A	16	GLY	6
A	14	ALA	5
A	22	ILE	5
A	2	SER	3
A	9	PRO	3

Chain	Res	Type	Models (Total)
A	20	PRO	3
A	3	HIS	2
A	5	SER	2
A	10	ILE	2
A	17	VAL	2
A	19	SER	2
A	38	ARG	2
A	6	ALA	1
A	13	ASP	1
A	15	GLU	1
A	18	TRP	1
A	21	ASP	1
A	37	GLY	1
A	61	LYS	1
A	85	SER	1
A	86	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	68	6	1
2	75	69	6	0
3	75	66	9	0
4	75	71	2	2
5	75	72	1	2
6	75	67	4	4
7	75	68	6	1
8	75	69	6	0
9	75	69	5	1
10	75	71	4	0
11	75	68	7	0
12	75	70	4	1
13	75	69	6	0
14	75	71	2	2
15	75	67	8	0

Model ID	Analysed	Favored	Allowed	Outliers
16	75	66	7	2
17	75	72	3	0
18	75	70	3	2
19	75	69	6	0
20	75	72	1	2
21	75	68	6	1
22	75	69	4	2
23	75	68	7	0
24	75	70	5	0
25	75	70	5	0

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

Chain	Res	Type	Models (Total)
A	48	LYS	11
A	10	ILE	3
A	55	LEU	3
A	70	ARG	2
A	77	ILE	2
A	3	HIS	1
A	66	LYS	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*".

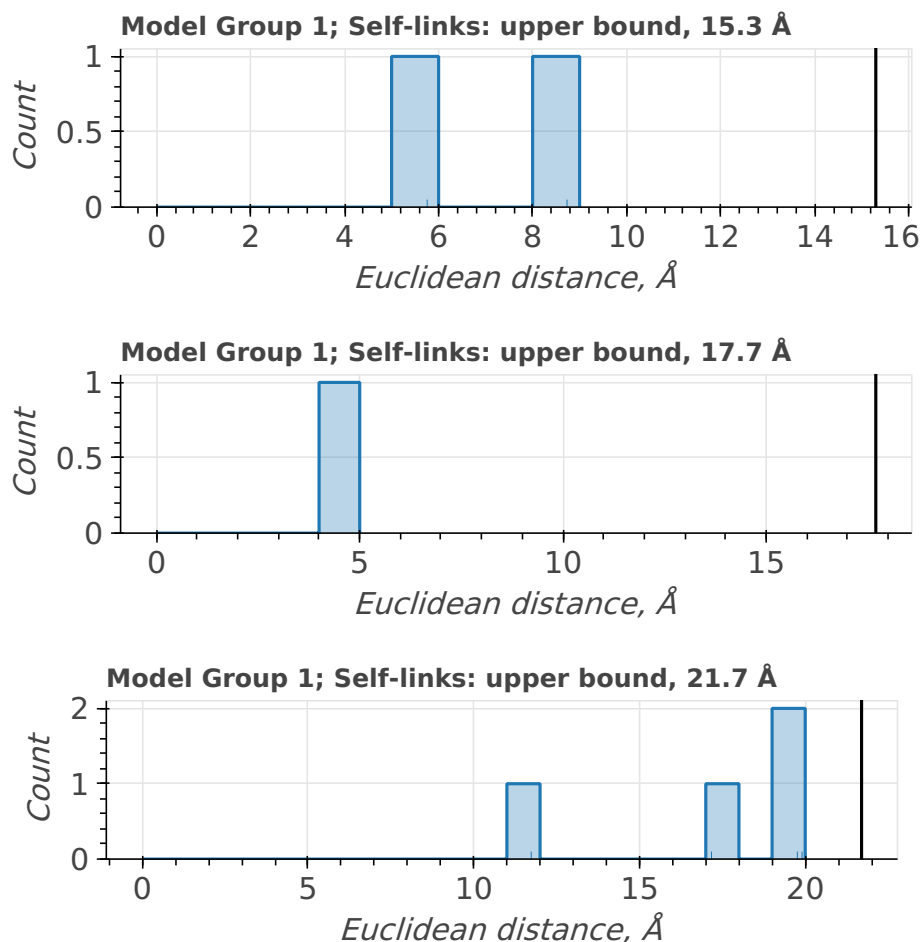
Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 7 crosslinking restraints combined in 7 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	2
DSA	LYS	CA	LYS	CA	upper bound	21.7	4
DSA	LYS	CA	SER	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=7)
1	1	1	25/25	All	100.00	0.00	7
				Self-links/ Intramolecular	100.00	0.00	7

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.



H/D exchange

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.