

Integrative Structure Validation Report ?

July 10, 2025 - 01:38 PM PDT

The following software was used in the production of this report:

Integrative Modeling Validation Version 2.1

Python-IHM Version 2.5

MolProbity Version 4.5.2

PyMOL Version 2.5.0

PDB ID	9A96
Structure Title	PTEN model. Model restrained with crosslinking-MS data from "eased" conformation and CTT. RoseTTAFold-generated initial structure
Structure Authors	Dawson, J.E.; Eng, C.
Deposited on	2025-01-02

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

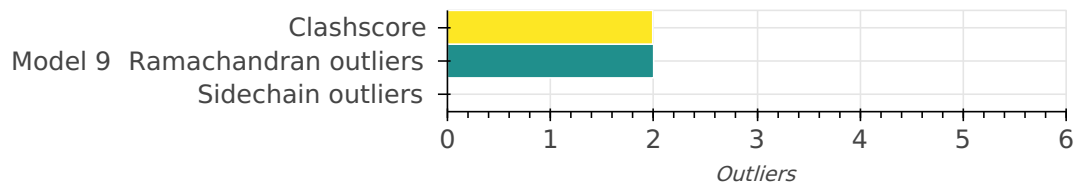
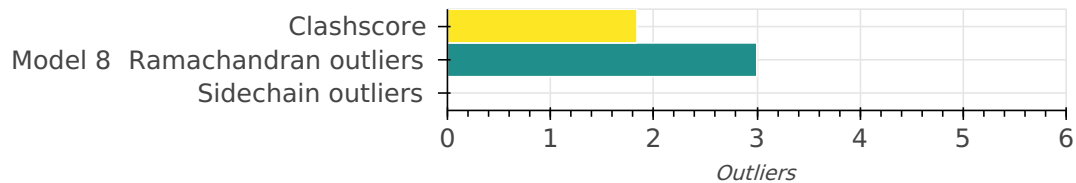
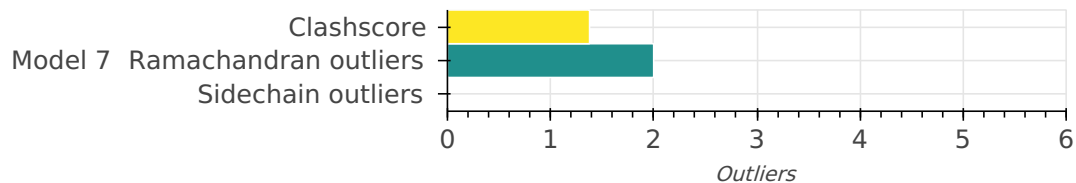
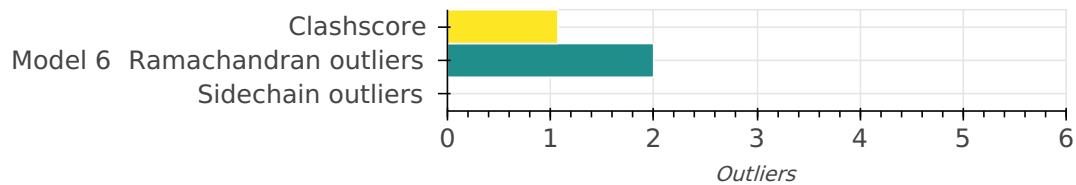
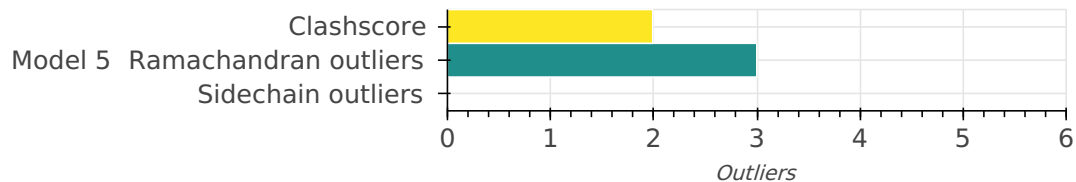
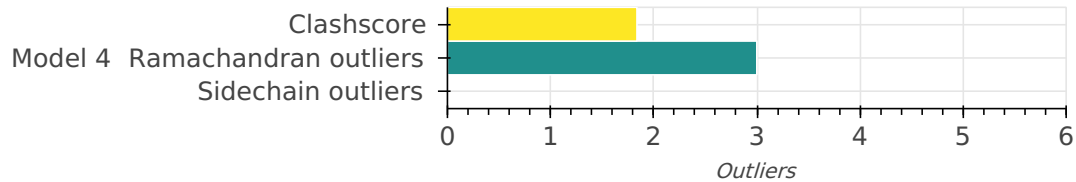
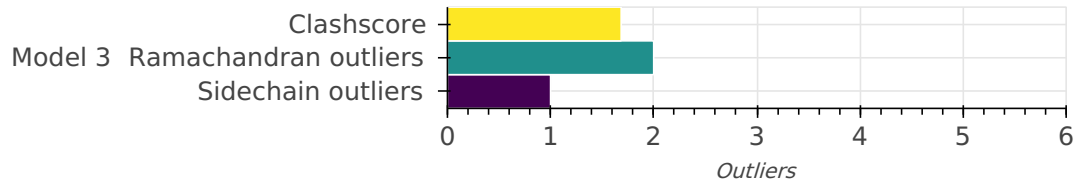
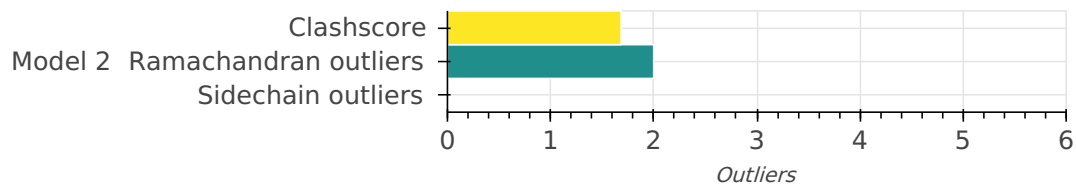
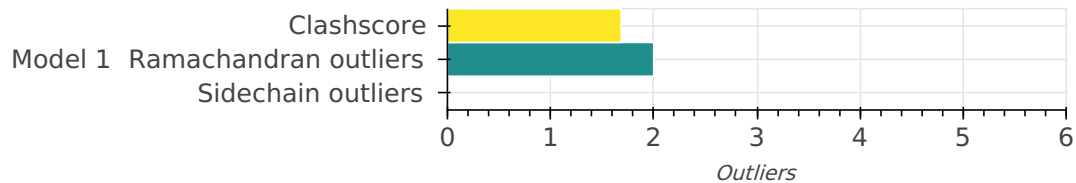
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

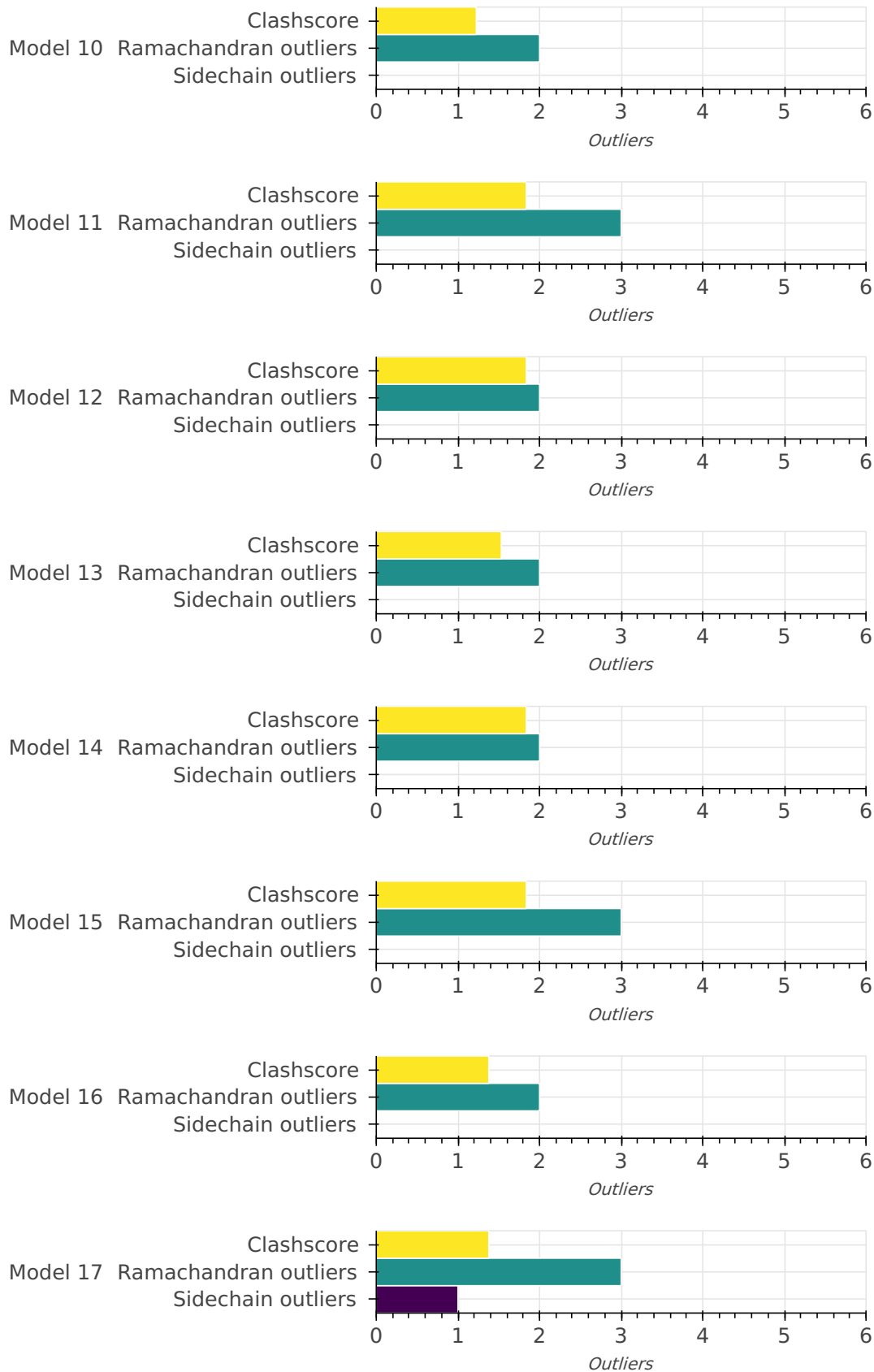
List of references used to build this report is available [here](#).

Overall quality ?

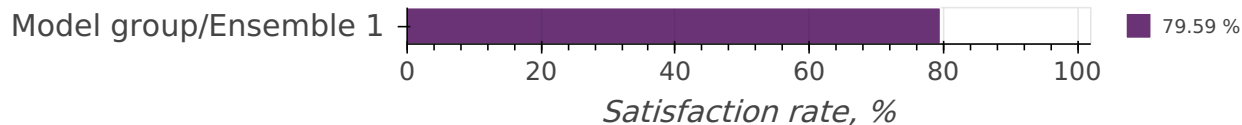
This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis





Crosslink satisfaction



Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 17 model(s). A total of 2 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	1-17	1	Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN	A	403	-	1-403	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	Crosslinking-MS data	PRIDE	PXD059974
1	De Novo 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	Protein structure prediction	RoseTTAFold	Not available	1	False	False
2	1	Rosetta pre-relaxation	Rosetta relax protocol. Unrestrained. Lowest energy model of 200 used in next step	Not available	200	False	False
3	1	Restrained modeling	Rosetta, crosslinking-MS distance restraints	The individual models were restrained with subsets of experimental crosslink data in order to parse out specific restraints that correspond to a particular model. The crosslink list table provides the full set of experimental data obtained and the crosslink restraint table identifies the subset of crosslink restraints used in the modeling.	2000	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
2	RoseTTAFold	Not available	Protein Structure Prediction	https://github.com/RosettaCommons/RoseTTAFold
1	Rosetta	2020.08	Model building and refinement	https://rosettacommons.org/software/
3	Rosetta	3.12	Model building and refinement	https://rosettacommons.org/software/

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 16 bond length outliers in this entry (0.03% of 57970 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	134	MET	SD-CE	4.58	1.68	1.79	15	11
A	200	PHE	CB-CG	4.47	1.40	1.50	16	5

Standard geometry: angle outliers ?

There are 93 bond angle outliers in this entry (0.12% of 78387 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	292	ASN	CA-CB-CG	6.51	119.11	112.60	10	17
A	347	PHE	CA-CB-CG	5.56	119.36	113.80	1	15
A	200	PHE	CA-CB-CG	4.75	109.05	113.80	15	5
A	341	PHE	CA-CB-CG	4.46	118.26	113.80	16	13
A	312	ASP	CA-CB-CG	4.37	116.97	112.60	12	10
A	241	PHE	CA-CB-CG	4.30	118.10	113.80	8	16
A	148	ALA	C-CA-CB	4.15	104.27	110.50	7	17

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	1.68	11
2	1.68	11
3	1.68	11
4	1.84	12
5	1.99	13
6	1.07	7
7	1.38	9
8	1.84	12
9	1.99	13
10	1.23	8
11	1.84	12
12	1.84	12
13	1.53	10
14	1.84	12
15	1.84	12
16	1.38	9
17	1.38	9

There are 183 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:188:TYR:CD2	A:188:TYR:O	0.73	4	16
A:60:LYS:HA	A:60:LYS:HE2	0.70	1	14
A:403:VAL:OXT	A:403:VAL:HG12	0.61	3	17
A:188:TYR:CG	A:188:TYR:O	0.57	14	9
A:19:ASP:OD2	A:60:LYS:NZ	0.56	8	14
A:10:SER:OG	A:15:ARG:NE	0.52	13	5
A:295:LEU:C	A:295:LEU:HD12	0.51	1	17
A:354:PRO:O	A:355:SER:C	0.50	8	17
A:124:CYS:O	A:125:LYS:C	0.49	4	8
A:66:LYS:NZ	A:107:ASP:OD2	0.49	8	7
A:92:ASP:OD1	A:130:ARG:NH2	0.49	5	6
A:318:LEU:C	A:318:LEU:HD13	0.48	2	1
A:60:LYS:CE	A:60:LYS:HA	0.48	8	5
A:32:ILE:O	A:32:ILE:HG23	0.48	15	1
A:48:ASN:C	A:48:ASN:HD22	0.47	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:316:LEU:N	A:316:LEU:HD22	0.47	5	1
A:125:LYS:NZ	A:382:THR:O	0.45	15	2
A:292:ASN:OD1	A:293:GLY:N	0.44	9	4
A:43:GLU:O	A:47:ARG:NH1	0.43	15	1
A:48:ASN:O	A:49:ASN:C	0.43	3	5
A:199:MET:C	A:199:MET:SD	0.43	1	8
A:260:LYS:O	A:261:GLN:C	0.43	11	1
A:292:ASN:CG	A:293:GLY:H	0.43	17	10
A:14:ARG:O	A:15:ARG:C	0.42	1	4
A:345:LEU:N	A:345:LEU:HD12	0.42	15	1
A:173:ARG:NH1	A:274:TRP:O	0.41	8	2
A:332:LYS:NZ	A:392:PHE:O	0.41	11	1
A:122:ILE:N	A:122:ILE:HD12	0.41	15	1
A:317:VAL:HG22	A:346:TYR:CD2	0.41	7	1
A:5:ILE:CG2	A:46:TYR:H	0.41	10	1
A:45:VAL:O	A:46:TYR:C	0.41	5	1
A:257:PHE:CD1	A:271:PHE:CE1	0.40	5	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	401	371	28	2
2	401	374	25	2
3	401	377	22	2
4	401	372	26	3
5	401	373	25	3
6	401	375	24	2
7	401	372	27	2
8	401	375	23	3
9	401	376	23	2
10	401	375	24	2
11	401	372	26	3
12	401	377	22	2
13	401	377	22	2
14	401	373	26	2

Model ID	Analysed	Favored	Allowed	Outliers
15	401	376	22	3
16	401	375	24	2
17	401	375	23	3

There are 4 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	46	TYR	17
A	210	THR	17
A	392	PHE	5
A	38	PRO	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	371	366	5	0
2	371	365	6	0
3	371	364	6	1
4	371	368	3	0
5	371	364	7	0
6	371	362	9	0
7	371	366	5	0
8	371	367	4	0
9	371	365	6	0
10	371	367	4	0
11	371	367	4	0
12	371	364	7	0
13	371	368	3	0
14	371	364	7	0
15	371	367	4	0
16	371	365	6	0
17	371	365	5	1

There are 2 unique sidechain outliers. Detailed list of outliers are tabulated below.

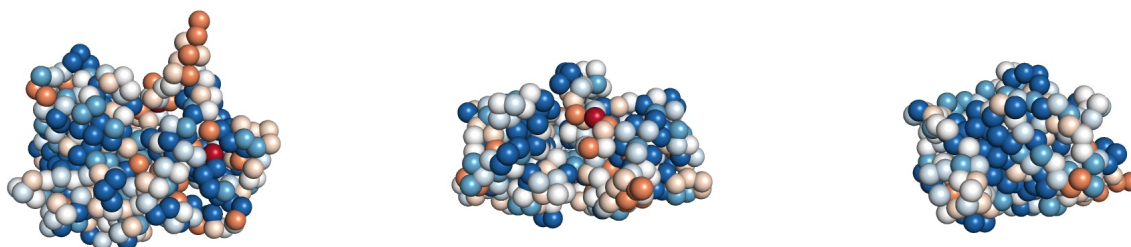
Chain	Res	Type	Models (Total)
A	48	ASN	1

Chain	Res	Type	Models (Total)
A	325	LEU	1

PrISM precision analysis ?

Regions of **low**  **high** precision, defined as the variability among the models that satisfy the input data and calculated as the density-weighted root mean-square fluctuation (RMSF) from the bead/atom center of density, annotated and visualized using PrISM. The per-bead precision is computed from the deposited ensemble of superposed integrative models. High- and low-precision regions are then determined by clustering beads of similar precision based on their proximity in the structure. Only coarse-grained beads (or CA atoms for atomic models) of deposited models are used for assessment and visualization, and three projections for each representative model are generated.

PrISM analysis for Ensemble 1 (models deposited/total: 17/17).



Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

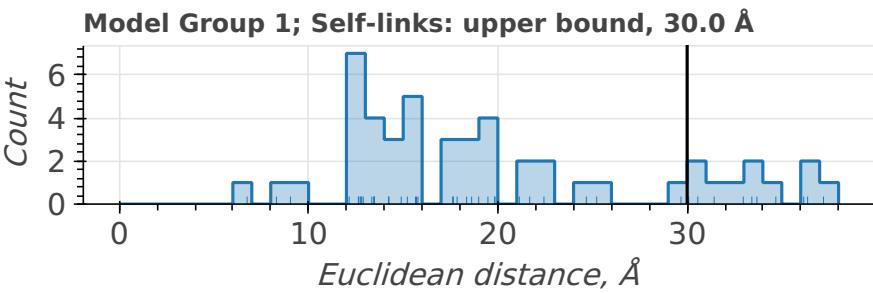
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 49 crosslinking restraints combined in 49 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	CA	LYS	CA	upper bound	30.0	39
DHSO	GLU	CA	GLU	CA	upper bound	30.0	6
DHSO	ASP	CA	GLU	CA	upper bound	30.0	3
DHSO	ASP	CA	ASP	CA	upper bound	30.0	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=49)
1	1	1	17/17	All	79.59	20.41	49
				Self-links/Intramolecular	79.59	20.41	49

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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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.

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