

Integrative Structure Validation Report ?

February 18, 2025 - 08:32 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

PDB ID	9A1Q
PDB-Dev ID	PDBDEV_00000098
Structure Title	The structural models of alpha-synuclein dimer
Structure Authors	Zamel J; Chen J; Zaer S; Harris PD; Drori P; Lebendiker M; Kalisman N; Dokholyan NV; Lerner E
Deposited on	2021-12-15

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

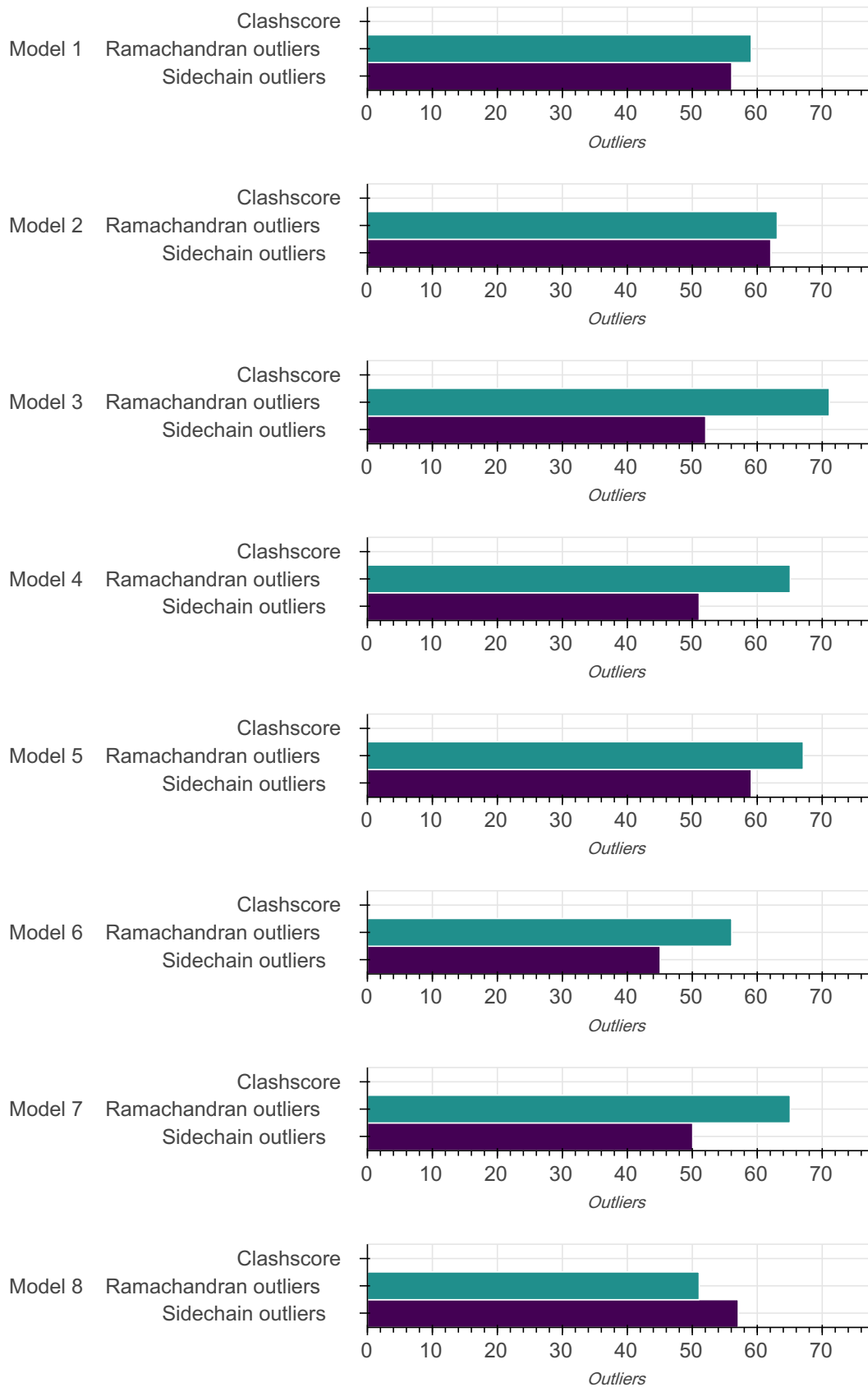
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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

Overall quality ?

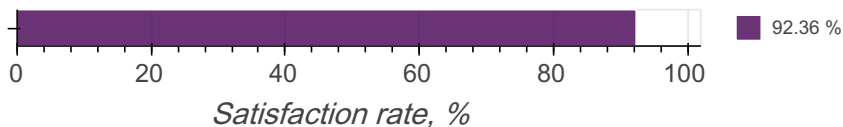
This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Crosslink satisfaction

Model group/Ensemble 1



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 8 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	1-8	1	alpha-synuclein	A	140	-	1-140	100.00 / 100.00	Atomic
				B					

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
1	Crosslinking-MS data	PRIDE	PXD030299
2	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	Design square-well functions based on cross-linking constraints	None	At this step, cross-linking constraints are collected from experiments and used to design square-well functions for DMD simulations.	None	False	False
2	1	Perform DMD simulations	None	At this step, the designed square-well functions are incorporated into the force field. Start DMD simulations.	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	DMD software	Not available	model building	http://www.moleculesinaction.com/pdmd.html

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 no bond length outliers.

Standard geometry: angle outliers ?

There are 22 bond angle outliers in this entry (0.10% of 22064 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	122	ASN	CA-CB-CG	4.94	117.54	112.60	4	1
B	65	ASN	CA-CB-CG	4.39	116.99	112.60	4	1
A	113	LEU	CD1-CG-CD2	4.37	101.18	110.80	7	2
A	38	LEU	CD1-CG-CD2	4.32	101.31	110.80	7	2
A	126	GLU	CA-C-O	4.23	113.62	120.80	3	1
B	103	ASN	OD1-CG-ND2	4.21	118.39	122.60	6	1
A	55	VAL	CA-CB-CG2	4.21	117.56	110.40	5	2
B	8	LEU	CD1-CG-CD2	4.21	101.54	110.80	8	1
A	46	GLU	CA-C-O	4.15	113.74	120.80	5	1
B	100	LEU	CD1-CG-CD2	4.14	101.70	110.80	4	1
B	26	VAL	CA-CB-CG2	4.12	117.41	110.40	7	1
A	8	LEU	CD1-CG-CD2	4.12	101.74	110.80	3	1
A	135	ASP	CA-CB-CG	4.12	116.72	112.60	6	1
A	100	LEU	CD1-CG-CD2	4.11	101.76	110.80	5	2
B	38	LEU	CD1-CG-CD2	4.10	101.78	110.80	7	1
A	103	ASN	CA-CB-CG	4.09	116.69	112.60	1	1
B	71	VAL	CA-CB-CG1	4.09	117.35	110.40	7	1
A	15	VAL	CA-CB-CG2	4.03	117.26	110.40	8	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	0.00	0
2	0.00	0
3	0.00	0
4	0.00	0
5	0.00	0
6	0.00	0
7	0.00	0
8	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	276	162	55	59
2	276	159	54	63
3	276	157	48	71
4	276	167	44	65
5	276	160	49	67
6	276	161	59	56
7	276	152	59	65
8	276	168	57	51

There are 188 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	2	ASP	8
A	13	GLU	7
A	43	LYS	7
B	42	SER	7
B	74	VAL	7
A	33	THR	6
A	42	SER	6
A	88	ILE	6
A	94	PHE	6
A	95	VAL	6
B	5	MET	6
B	35	GLU	6
B	71	VAL	6
B	82	VAL	6
B	102	LYS	6
B	123	GLU	6
B	133	TYR	6
A	21	LYS	5
A	34	LYS	5
A	35	GLU	5
A	37	VAL	5
A	82	VAL	5
A	115	ASP	5
A	121	ASP	5

Chain	Res	Type	Models (Total)
A	127	MET	5
A	137	GLU	5
B	87	SER	5
B	92	THR	5
B	105	GLU	5
B	115	ASP	5
B	130	GLU	5
B	138	PRO	5
A	8	LEU	4
A	9	SER	4
A	15	VAL	4
A	17	ALA	4
A	26	VAL	4
A	29	ALA	4
A	39	TYR	4
A	64	THR	4
A	66	VAL	4
A	90	ALA	4
A	123	GLU	4
B	2	ASP	4
B	4	PHE	4
B	17	ALA	4
B	24	GLN	4
B	28	GLU	4
B	29	ALA	4
B	30	ALA	4
B	39	TYR	4
B	57	GLU	4
B	70	VAL	4
B	94	PHE	4
A	18	ALA	3
A	27	ALA	3
A	28	GLU	3
A	30	ALA	3
A	58	LYS	3

Chain	Res	Type	Models (Total)
A	60	LYS	3
A	71	VAL	3
A	86	GLY	3
A	89	ALA	3
A	91	ALA	3
A	92	THR	3
A	120	PRO	3
A	133	TYR	3
A	138	PRO	3
B	21	LYS	3
B	27	ALA	3
B	40	VAL	3
B	43	LYS	3
B	48	VAL	3
B	55	VAL	3
B	64	THR	3
B	76	ALA	3
B	88	ILE	3
B	89	ALA	3
B	90	ALA	3
B	95	VAL	3
B	121	ASP	3
B	129	SER	3
B	137	GLU	3
A	4	PHE	2
A	12	LYS	2
A	16	VAL	2
A	24	GLN	2
A	32	LYS	2
A	50	HIS	2
A	52	VAL	2
A	74	VAL	2
A	85	ALA	2
A	96	LYS	2
A	98	ASP	2

Chain	Res	Type	Models (Total)
A	102	LYS	2
A	107	ALA	2
A	128	PRO	2
A	129	SER	2
A	130	GLU	2
A	132	GLY	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	206	116	34	56
2	206	110	34	62
3	206	123	31	52
4	206	114	41	51
5	206	117	30	59
6	206	125	36	45
7	206	104	52	50
8	206	118	31	57

There are 157 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
B	26	VAL	8
B	16	VAL	7
B	71	VAL	7
A	34	LYS	6
A	55	VAL	6
A	59	THR	6
B	79	GLN	6
A	3	VAL	5
A	33	THR	5
A	38	LEU	5
A	43	LYS	5
A	49	VAL	5
A	71	VAL	5

Chain	Res	Type	Models (Total)
A	72	THR	5
A	75	THR	5
A	88	ILE	5
A	112	ILE	5
A	121	ASP	5
B	3	VAL	5
B	40	VAL	5
B	88	ILE	5
B	92	THR	5
A	15	VAL	4
A	16	VAL	4
A	26	VAL	4
A	40	VAL	4
A	46	GLU	4
A	64	THR	4
A	66	VAL	4
A	70	VAL	4
A	77	VAL	4
A	81	THR	4
A	95	VAL	4
A	115	ASP	4
A	118	VAL	4
B	2	ASP	4
B	8	LEU	4
B	21	LYS	4
B	48	VAL	4
B	49	VAL	4
B	55	VAL	4
B	63	VAL	4
B	74	VAL	4
B	82	VAL	4
B	95	VAL	4
B	100	LEU	4
A	2	ASP	3
A	12	LYS	3

Chain	Res	Type	Models (Total)
A	13	GLU	3
A	24	GLN	3
A	39	TYR	3
A	52	VAL	3
A	58	LYS	3
A	63	VAL	3
A	94	PHE	3
A	99	GLN	3
A	127	MET	3
A	133	TYR	3
B	15	VAL	3
B	22	THR	3
B	24	GLN	3
B	35	GLU	3
B	37	VAL	3
B	44	THR	3
B	59	THR	3
B	62	GLN	3
B	64	THR	3
B	70	VAL	3
B	72	THR	3
B	77	VAL	3
B	98	ASP	3
B	112	ILE	3
B	115	ASP	3
B	135	ASP	3
A	4	PHE	2
A	8	LEU	2
A	9	SER	2
A	32	LYS	2
A	37	VAL	2
A	42	SER	2
A	44	THR	2
A	45	LYS	2
A	48	VAL	2

Chain	Res	Type	Models (Total)
A	50	HIS	2
A	65	ASN	2
A	74	VAL	2
A	83	GLU	2
A	87	SER	2
A	92	THR	2
A	100	LEU	2
A	103	ASN	2
A	105	GLU	2
A	116	MET	2
A	119	ASP	2
A	122	ASN	2
A	123	GLU	2
A	130	GLU	2
A	135	ASP	2
B	1	MET	2
B	4	PHE	2

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.

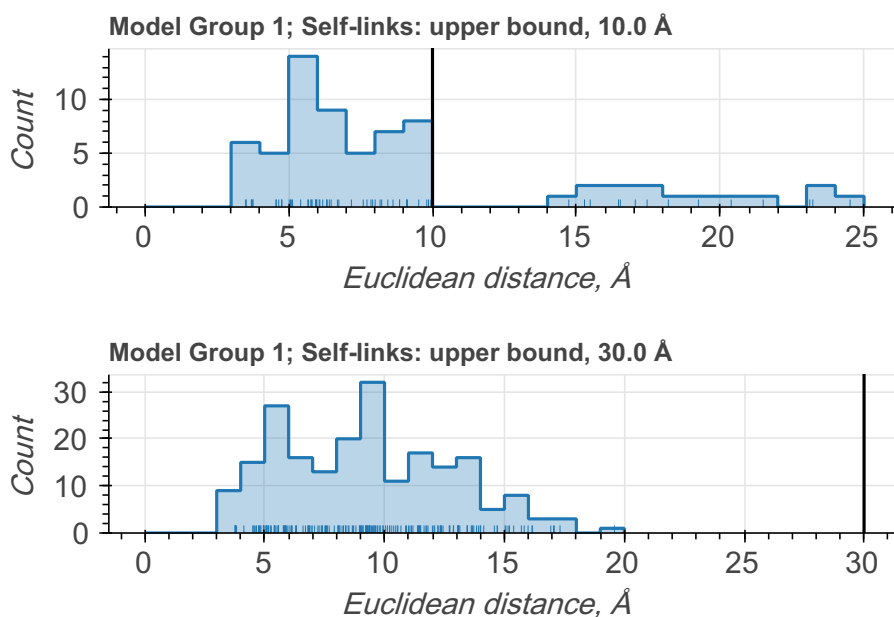
There are 278 crosslinking restraints combined in 157 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	MET	CA	upper bound	30.0	23
BS3	MET	CA	THR	CA	upper bound	30.0	2
BS3	LYS	CA	LYS	CA	upper bound	30.0	123
BS3	LYS	CA	SER	CA	upper bound	30.0	16
BS3	LYS	CA	THR	CA	upper bound	30.0	32
BS3	LYS	CA	TYR	CA	upper bound	30.0	14
BS3	GLU	CA	MET	CA	upper bound	10.0	10

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	ASP	CA	MET	CA	upper bound	10.0	2
BS3	ASP	CA	LYS	CA	upper bound	10.0	4
BS3	GLU	CA	LYS	CA	upper bound	10.0	44
BS3	GLU	CA	THR	CA	upper bound	10.0	4
BS3	GLU	CA	TYR	CA	upper bound	10.0	2
BS3	GLU	CA	SER	CA	upper bound	10.0	2

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.



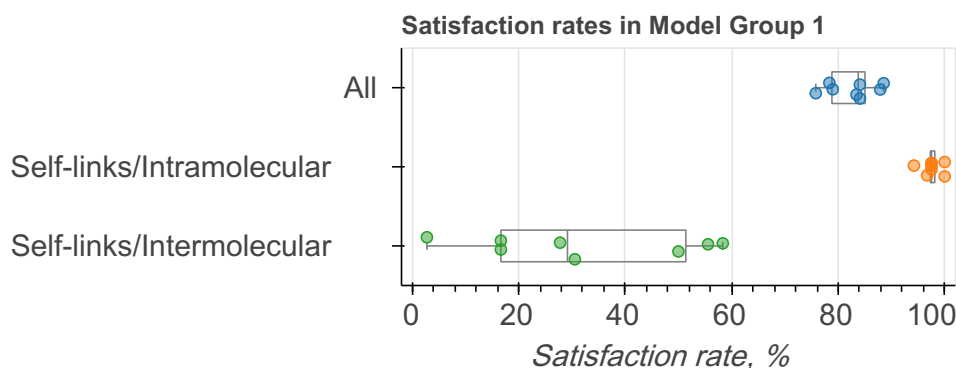
Satisfaction of restraints

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=157)
1	1	1	8/8	All	92.36	7.64	157
				Self-links/ Intramolecular	100.00	0.00	121
				Self-links/ Intermolecular	66.67	33.33	36

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

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.

