

Integrative Structure Validation Report ?

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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	9A1A
PDB-Dev ID	PDBDEV_00000082
Structure Title	The ensemble structure of alpha-synuclein monomer
Structure Authors	Chen J; Zaer S; Drori P; Zamel J; Joron K; Kalisman N; Lerner E; Dokholyan NV
Deposited on	2021-03-10

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

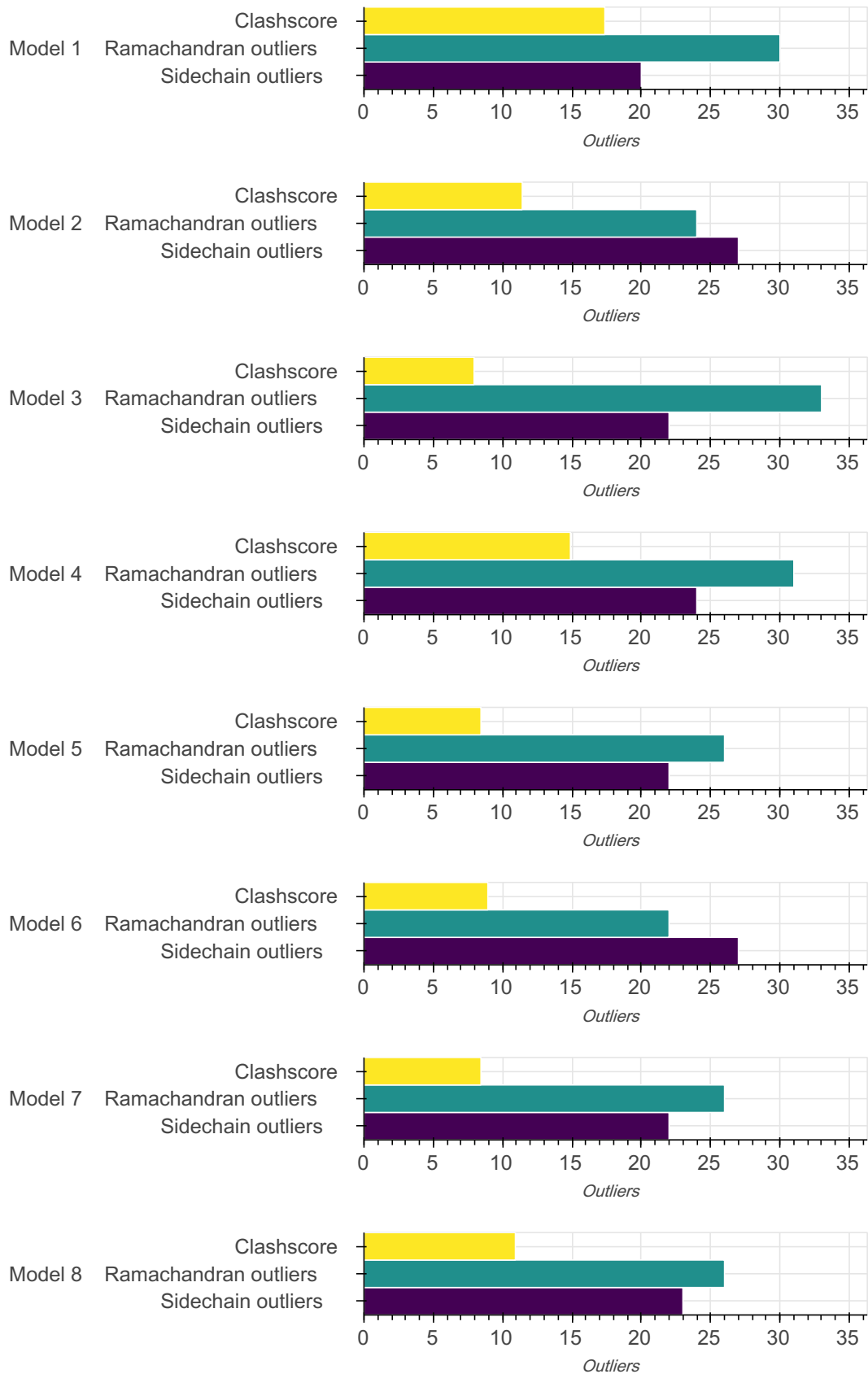
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 8 distinct ensemble(s).

Summary ?

This entry consists of 8 model(s). A total of 1 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 / 0.00	Atomic

Datasets used for modeling ?

There is 1 unique dataset used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Other	Not available	10.1016/j.jmb.2010.11.011

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	Discrete molecular dynamics simulations	None	None	30303	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	piDMD	Not available	model building	http://www.moleculesinaction.com/home.html
2	TTClust	Not available	structure clustering	https://github.com/tubiana/TTClust

Data quality ?

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 1 bond length outliers in this entry (0.01% of 8184 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	21	LYS	CE-NZ	19.75	2.08	1.49	1	1

Standard geometry: angle outliers ?

There are 6 bond angle outliers in this entry (0.05% of 11032 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	21	LYS	CD-CE-NZ	7.95	86.45	111.90	1	1
A	49	VAL	CA-CB-CG1	4.30	117.71	110.40	1	1
A	122	ASN	CA-CB-CG	4.21	116.81	112.60	3	1
A	103	ASN	CA-CB-CG	4.16	116.76	112.60	4	1
A	77	VAL	CA-CB-CG2	4.11	117.38	110.40	3	1
A	119	ASP	CA-CB-CG	4.10	116.70	112.60	5	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	17.37	35
2	11.41	23
3	7.94	16
4	14.89	30
5	8.44	17
6	8.93	18
7	8.44	17
8	10.92	22

There are 178 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:21:LYS:CE	A:21:LYS:NZ	1.16	1	1
A:36:GLY:HA3	A:76:ALA:HB3	1.04	7	1
A:40:VAL:HG12	A:47:GLY:HA2	0.95	4	1
A:18:ALA:HB2	A:49:VAL:HG13	0.95	1	1
A:119:ASP:HB2	A:125:TYR:HD2	0.89	2	1
A:1:MET:HE3	A:6:LYS:HB3	0.85	2	2
A:30:ALA:HB1	A:99:GLN:HB2	0.81	1	1
A:19:ALA:HB1	A:34:LYS:HE3	0.79	1	1
A:4:PHE:HB2	A:70:VAL:HG13	0.77	1	1
A:10:LYS:HG3	A:18:ALA:HB3	0.76	8	1
A:77:VAL:HG11	A:121:ASP:HB2	0.76	7	1
A:21:LYS:CD	A:21:LYS:NZ	0.74	1	1
A:117:PRO:HG2	A:128:PRO:HA	0.73	4	1
A:49:VAL:HG23	A:87:SER:HB2	0.72	1	1
A:4:PHE:HB3	A:7:GLY:HA2	0.72	5	1
A:49:VAL:HG12	A:66:VAL:HA	0.72	7	1
A:99:GLN:HA	A:110:GLU:HB2	0.72	8	1
A:18:ALA:HB1	A:22:THR:HG22	0.70	3	1
A:4:PHE:HD2	A:71:VAL:HA	0.70	1	1
A:70:VAL:HG22	A:94:PHE:HE1	0.69	6	1
A:30:ALA:HB3	A:95:VAL:HG22	0.69	1	1
A:120:PRO:HA	A:124:ALA:HB3	0.69	3	1
A:94:PHE:HE2	A:100:LEU:HD12	0.68	6	1
A:26:VAL:HB	A:113:LEU:HD13	0.68	8	1
A:99:GLN:HG3	A:112:ILE:HD11	0.67	2	1
A:11:ALA:HA	A:56:ALA:HA	0.66	1	1
A:56:ALA:HA	A:95:VAL:HG11	0.66	8	1
A:71:VAL:HG22	A:88:ILE:HD12	0.66	8	1
A:130:GLU:HA	A:134:GLN:HB2	0.65	1	1
A:9:SER:HB3	A:76:ALA:HB1	0.65	1	1
A:130:GLU:HB2	A:134:GLN:HE22	0.65	8	1
A:15:VAL:HG22	A:134:GLN:HG2	0.65	3	1
A:4:PHE:HE2	A:72:THR:HG22	0.65	1	1
A:15:VAL:HG21	A:82:VAL:HG22	0.64	4	1
A:15:VAL:HG22	A:138:PRO:HG2	0.64	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:95:VAL:HA	A:98:ASP:HB2	0.64	1	1
A:108:PRO:HA	A:112:ILE:HB	0.63	4	1
A:74:VAL:HG12	A:75:THR:HG23	0.62	6	1
A:95:VAL:HG12	A:97:LYS:HG3	0.62	3	1
A:26:VAL:HA	A:30:ALA:HB3	0.62	6	1
A:16:VAL:HA	A:22:THR:HG22	0.62	2	1
A:131:GLU:HG2	A:135:ASP:HB2	0.62	4	1
A:17:ALA:HA	A:21:LYS:HD3	0.61	5	1
A:8:LEU:HD22	A:128:PRO:HB3	0.61	4	1
A:60:LYS:HB3	A:95:VAL:HG11	0.61	2	1
A:35:GLU:HG2	A:48:VAL:HG21	0.60	7	1
A:52:VAL:HG21	A:136:TYR:HE1	0.60	1	1
A:55:VAL:HG21	A:102:LYS:HG2	0.60	7	1
A:55:VAL:HG21	A:88:ILE:HG22	0.60	3	1
A:19:ALA:HB3	A:24:GLN:HB2	0.60	1	2
A:55:VAL:HG13	A:60:LYS:HB2	0.60	6	1
A:107:ALA:HB3	A:116:MET:HB3	0.60	7	1
A:19:ALA:HB3	A:22:THR:HB	0.59	2	1
A:45:LYS:HA	A:48:VAL:HB	0.59	8	1
A:21:LYS:HB2	A:90:ALA:HB3	0.59	2	1
A:80:LYS:HB3	A:82:VAL:CG1	0.59	8	1
A:94:PHE:CZ	A:96:LYS:HB3	0.59	8	1
A:8:LEU:HD21	A:74:VAL:HG11	0.58	5	1
A:87:SER:HB3	A:95:VAL:HG12	0.58	1	1
A:91:ALA:HB3	A:118:VAL:HB	0.58	4	1
A:50:HIS:HB2	A:106:GLY:HA3	0.57	8	1
A:64:THR:HG23	A:112:ILE:HG23	0.57	3	1
A:15:VAL:HG21	A:59:THR:HG21	0.57	5	1
A:116:MET:SD	A:128:PRO:HG3	0.56	7	1
A:52:VAL:HG11	A:88:ILE:HD11	0.55	1	1
A:88:ILE:HA	A:93:GLY:HA2	0.55	2	1
A:94:PHE:CE2	A:100:LEU:HD12	0.55	6	1
A:66:VAL:HG13	A:70:VAL:HB	0.55	5	1
A:58:LYS:HD2	A:67:GLY:HA2	0.55	1	1
A:55:VAL:HG13	A:95:VAL:HG13	0.55	2	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:62:GLN:HG3	A:63:VAL:HG12	0.54	1	1
A:8:LEU:HD23	A:16:VAL:HB	0.54	4	1
A:95:VAL:HG13	A:99:GLN:HB2	0.54	6	1
A:74:VAL:HG12	A:138:PRO:HG3	0.54	4	1
A:26:VAL:HG11	A:37:VAL:HG21	0.54	5	1
A:91:ALA:HB2	A:114:GLU:HB2	0.54	5	1
A:70:VAL:HG22	A:94:PHE:CE1	0.54	6	1
A:133:TYR:HB2	A:136:TYR:HB2	0.54	8	1
A:23:LYS:HE3	A:64:THR:HG22	0.54	4	1
A:89:ALA:HB2	A:96:LYS:HB2	0.54	7	1
A:72:THR:HG22	A:94:PHE:HE2	0.54	2	1
A:108:PRO:HG2	A:120:PRO:HB3	0.54	3	1
A:103:ASN:HB2	A:110:GLU:HG3	0.53	4	1
A:44:THR:HG23	A:87:SER:HB2	0.53	3	1
A:80:LYS:HB3	A:82:VAL:HG12	0.52	8	1
A:130:GLU:HA	A:134:GLN:CB	0.52	1	1
A:26:VAL:HG21	A:37:VAL:HG11	0.52	5	1
A:119:ASP:HB2	A:125:TYR:CD2	0.52	2	1
A:102:LYS:HB2	A:110:GLU:HB2	0.52	4	1
A:1:MET:HE1	A:8:LEU:HD23	0.52	5	1
A:30:ALA:CB	A:95:VAL:HG22	0.51	1	1
A:56:ALA:HB3	A:79:GLN:H	0.51	1	1
A:83:GLU:HB3	A:89:ALA:HB3	0.51	5	1
A:77:VAL:CG1	A:121:ASP:HB2	0.51	7	1
A:116:MET:HE1	A:133:TYR:CE2	0.51	6	1
A:130:GLU:HB2	A:134:GLN:NE2	0.51	8	1
A:12:LYS:HA	A:37:VAL:HG11	0.50	3	1
A:49:VAL:HG21	A:113:LEU:HD21	0.50	1	1
A:39:TYR:HD2	A:46:GLU:HB3	0.50	7	1
A:30:ALA:HB3	A:48:VAL:HG21	0.50	4	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	138	81	27	30

Model ID	Analysed	Favored	Allowed	Outliers
2	138	90	24	24
3	138	83	22	33
4	138	76	31	31
5	138	89	23	26
6	138	84	32	22
7	138	88	24	26
8	138	82	30	26

There are 95 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	133	TYR	8
A	115	ASP	6
A	30	ALA	5
A	82	VAL	5
A	137	GLU	5
A	8	LEU	4
A	21	LYS	4
A	24	GLN	4
A	34	LYS	4
A	42	SER	4
A	49	VAL	4
A	91	ALA	4
A	92	THR	4
A	94	PHE	4
A	102	LYS	4
A	123	GLU	4
A	128	PRO	4
A	5	MET	3
A	16	VAL	3
A	22	THR	3
A	27	ALA	3
A	32	LYS	3
A	53	ALA	3
A	62	GLN	3
A	71	VAL	3

Chain	Res	Type	Models (Total)
A	74	VAL	3
A	75	THR	3
A	77	VAL	3
A	83	GLU	3
A	85	ALA	3
A	88	ILE	3
A	89	ALA	3
A	95	VAL	3
A	127	MET	3
A	130	GLU	3
A	138	PRO	3
A	3	VAL	2
A	4	PHE	2
A	15	VAL	2
A	18	ALA	2
A	20	GLU	2
A	26	VAL	2
A	28	GLU	2
A	29	ALA	2
A	37	VAL	2
A	39	TYR	2
A	40	VAL	2
A	43	LYS	2
A	48	VAL	2
A	54	THR	2
A	56	ALA	2
A	58	LYS	2
A	72	THR	2
A	76	ALA	2
A	79	GLN	2
A	87	SER	2
A	97	LYS	2
A	98	ASP	2
A	103	ASN	2
A	108	PRO	2

Chain	Res	Type	Models (Total)
A	120	PRO	2
A	2	ASP	1
A	7	GLY	1
A	9	SER	1
A	10	LYS	1
A	11	ALA	1
A	12	LYS	1
A	13	GLU	1
A	19	ALA	1
A	31	GLY	1
A	33	THR	1
A	35	GLU	1
A	46	GLU	1
A	52	VAL	1
A	55	VAL	1
A	57	GLU	1
A	60	LYS	1
A	61	GLU	1
A	63	VAL	1
A	65	ASN	1
A	69	ALA	1
A	70	VAL	1
A	80	LYS	1
A	81	THR	1
A	84	GLY	1
A	86	GLY	1
A	90	ALA	1
A	99	GLN	1
A	100	LEU	1
A	105	GLU	1
A	107	ALA	1
A	109	GLN	1
A	113	LEU	1
A	117	PRO	1
A	122	ASN	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	103	66	17	20
2	103	59	17	27
3	103	59	22	22
4	103	57	22	24
5	103	59	22	22
6	103	64	12	27
7	103	63	18	22
8	103	62	18	23

There are 78 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	16	VAL	6
A	71	VAL	6
A	88	ILE	6
A	3	VAL	5
A	48	VAL	5
A	59	THR	5
A	64	THR	5
A	66	VAL	5
A	115	ASP	5
A	8	LEU	4
A	15	VAL	4
A	55	VAL	4
A	77	VAL	4
A	82	VAL	4
A	95	VAL	4
A	112	ILE	4
A	4	PHE	3
A	26	VAL	3
A	32	LYS	3
A	40	VAL	3
A	49	VAL	3

Chain	Res	Type	Models (Total)
A	52	VAL	3
A	54	THR	3
A	62	GLN	3
A	72	THR	3
A	74	VAL	3
A	81	THR	3
A	92	THR	3
A	118	VAL	3
A	1	MET	2
A	2	ASP	2
A	12	LYS	2
A	13	GLU	2
A	21	LYS	2
A	22	THR	2
A	33	THR	2
A	37	VAL	2
A	38	LEU	2
A	44	THR	2
A	70	VAL	2
A	79	GLN	2
A	98	ASP	2
A	100	LEU	2
A	109	GLN	2
A	116	MET	2
A	121	ASP	2
A	122	ASN	2
A	126	GLU	2
A	131	GLU	2
A	133	TYR	2
A	134	GLN	2
A	136	TYR	2
A	9	SER	1
A	20	GLU	1
A	34	LYS	1
A	43	LYS	1

Chain	Res	Type	Models (Total)
A	57	GLU	1
A	60	LYS	1
A	63	VAL	1
A	65	ASN	1
A	80	LYS	1
A	83	GLU	1
A	94	PHE	1
A	99	GLN	1
A	102	LYS	1
A	103	ASN	1
A	104	GLU	1
A	105	GLU	1
A	110	GLU	1
A	113	LEU	1
A	114	GLU	1
A	123	GLU	1
A	125	TYR	1
A	128	PRO	1
A	130	GLU	1
A	135	ASP	1
A	137	GLU	1
A	139	GLU	1

Fit of model to data used for modeling ?

Fit of model to data used for validation ?

Validation for this section is under development.

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