

Integrative Structure Validation Report ?

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

IHMValidation Version 3.2

Python-IHM Version 2.9

MolProbity Version 4.5.2

PDB ID	9A8Z pdb_00009a8z
Structure Title	Integrative structure of Cyclin-dependent kinase 2-associated protein 1 inter-chain and intra-chain sulfur-pi states from NMR data
Structure Authors	Huang, Y.J.; Ramelot, T.A.; Spaman, L.E.; Montelione, G.T.
Deposited on	2025-01-24

This is a PDB-IHM Structure Validation Report.

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](#).

1. Overview ?

1.1. Summary ?

This entry consists of 10 model(s). A total of 1 dataset(s) were used to build this entry.

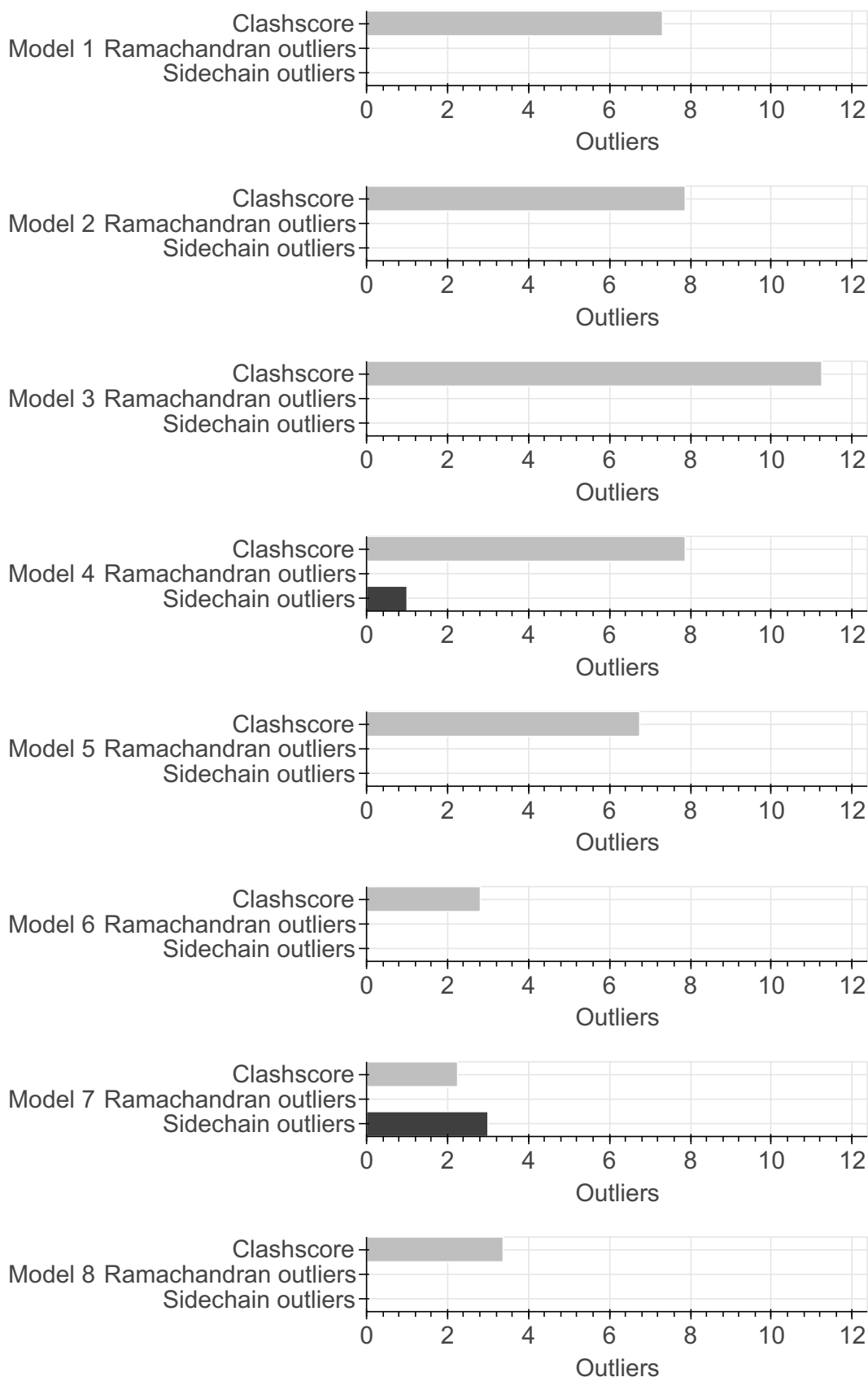
Name	Type	Count
NMR data	Experimental data	1

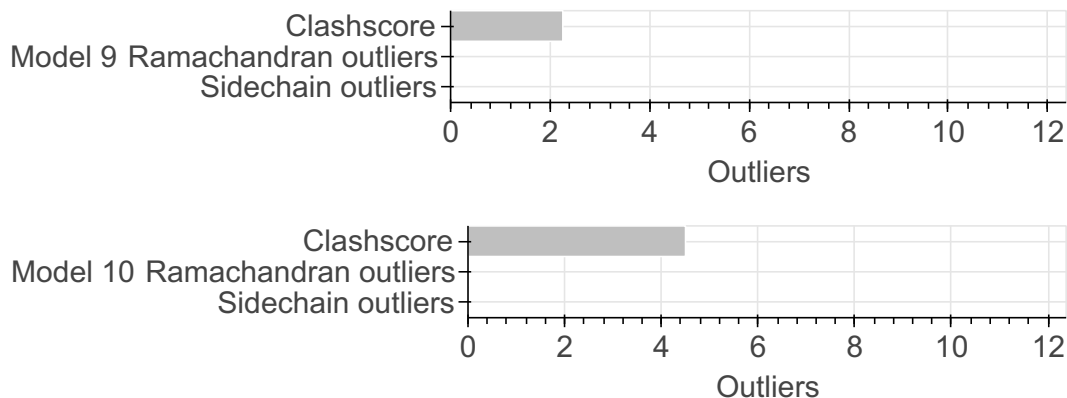
1.2. Overall quality ?

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 ?





2. Model Details ?

2.1. Ensemble information ?

This entry consists of 0 distinct ensemble(s).

2.2. 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	1-10	1	Cyclin-dependent kinase 2-associated protein 1	A	55	-	1-55	100.00 / 0.00	Atomic
				B					

2.3. 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	NMR data	BMRB	16808

2.4. Methodology and software ?

This entry is a result of 2 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
2	1	modeling	Not available	AFsample modeling calculations were carried out using modified version of AlphaFold v2.2.0. AFsample calculations, which use six different settings with network dropouts to create conformational heterogeneity, were carried out to generate ~6000 models	6000	True	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	modeling	Not available	A modified version of AlphaFold v2.2.0 used by AFsample. AF2 was trained using the PDB database of 2018-04-30 and did not include any NMR structures in the training data.	Not available	True	False

There are 7 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Protein Structure Validation Software	2.00	Validation	https://montelionelab.chem.rpi.edu/PSVS/PSVS2/
3	RPF	ASDP ver 1.0	Validation	https://montelionelab.chem.rpi.edu/rpf/
6	DoubleRecall	1.00	Validation	https://github.rpi.edu/RPIBioinformatics/AlphaFold-NMR
7	AISAR	1.00	Model Selection	https://github.com/MontelioneLab/AISAR
5	AFsample	Not available	Enhanced Sampling	https://github.com/bjornwallner/alphafoldv2.2.0
4	AlphaFold2	2.2.0	Model Building	https://github.com/google-deepmind/alphafold
2	RCI	Not available	Other	https://www.randomcoilindex.ca/cgi-bin/rci CGI_current.py

3. Data quality ?

3.4. NMR ?

Validation for this section is under development.

4. 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.

4.1b. MolProbity Analysis ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

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	7.31	13
2	7.87	14
3	11.25	20
4	7.87	14
5	6.75	12
6	2.81	5
7	2.25	4
8	3.37	6
9	2.26	4
10	4.50	8

There are 100 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:35:ILE:HD12	B:17:ILE:HD11	0.85	3	10
A:21:TYR:CG	B:28:MET:HE2	0.79	5	4
A:6:LEU:HD21	B:6:LEU:HD21	0.74	1	5
A:28:MET:HE2	B:21:TYR:CG	0.71	5	4
A:17:ILE:HD11	B:35:ILE:HD12	0.71	5	10
A:45:CYS:HB3	B:3:TYR:CE1	0.64	5	4
A:31:LEU:HD21	B:31:LEU:HD21	0.64	9	7
A:3:TYR:CE1	B:45:CYS:HB3	0.61	3	5
A:3:TYR:CZ	B:3:TYR:CZ	0.60	5	5
A:13:LEU:HD22	A:31:LEU:HD12	0.57	3	1
A:45:CYS:HB3	B:3:TYR:CZ	0.55	2	5
A:21:TYR:CD1	B:28:MET:HE2	0.55	3	2
A:3:TYR:CZ	B:45:CYS:HB3	0.55	2	3
A:28:MET:HE3	B:21:TYR:CG	0.52	10	1
A:21:TYR:CG	B:28:MET:HE3	0.52	8	3
B:13:LEU:HD22	B:31:LEU:HD12	0.51	3	3
A:28:MET:CE	B:21:TYR:CG	0.49	4	5
A:21:TYR:CG	B:28:MET:CE	0.48	2	5
B:38:ALA:O	B:42:VAL:HG23	0.48	3	1
A:28:MET:HE2	B:21:TYR:CE1	0.48	7	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:13:LEU:HD21	A:34:GLY:HA3	0.47	3	1
A:28:MET:HE2	B:21:TYR:CD1	0.46	7	1
B:13:LEU:HD21	B:34:GLY:HA3	0.46	3	3
A:46:LEU:HD21	B:3:TYR:CB	0.46	10	2
A:3:TYR:CE1	B:45:CYS:CB	0.46	3	1
A:46:LEU:HD21	B:3:TYR:HB2	0.45	10	2
A:3:TYR:CE1	B:3:TYR:CE1	0.43	5	1
A:3:TYR:HB2	B:46:LEU:HD21	0.42	9	1
A:3:TYR:CE1	B:3:TYR:CZ	0.42	3	1
A:3:TYR:CB	B:46:LEU:HD21	0.41	10	1
A:38:ALA:O	A:42:VAL:HG23	0.40	2	1
A:3:TYR:CZ	B:3:TYR:OH	0.40	3	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	106	106	0	0
2	106	106	0	0
3	106	105	1	0
4	106	106	0	0
5	106	104	2	0
6	106	105	1	0
7	106	106	0	0
8	106	106	0	0
9	106	106	0	0
10	106	106	0	0

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	88	86	2	0
2	88	86	2	0
3	88	87	1	0
4	88	83	4	1

Model ID	Analysed	Favored	Allowed	Outliers
5	88	87	1	0
6	88	88	0	0
7	88	82	3	3
8	88	88	0	0
9	87	87	0	0
10	88	87	1	0

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

Chain	Res	Type	Models (Total)
A	26	SER	1
A	46	LEU	1
B	28	MET	1
B	31	LEU	1

5. Fit to Data Used for Modeling Assessment ?

5.4. NMR ?

Validation for this section is under development.

6. Fit to Data Used for Validation Assessment ?

Validation for this section is under development.

Acknowledgments

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