Integrative Structure Validation Report

February 18, 2025 - 08:37 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	9A3R
PDB-Dev ID	PDBDEV_00000212
Structure Title	Vimentin intermediate filament tetramer
Structure Authors	Eibauer, M.; Medalia, O.
Deposited on	2023-06-05

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

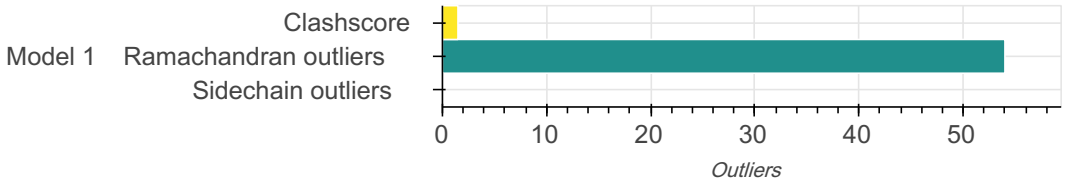
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 model(s). A total of 5 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	1	Vimentin	A	466	-	1-466	100.00 / 100.00	Atomic
				B					
				C					
				D					

Datasets used for modeling

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
3	Mass Spectrometry data	Not available	Not available
1	3DEM volume	EMDB	EMD-16844
2	3DEM volume	Not available	Not available
4	De Novo model	Not available	Not available
5	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	Molecular dynamics flexible fitting	Molecular dynamics flexible fitting	The vimentin dimer starting model was fitted by molecular dynamics flexible fitting to an elongated version of the electron density map EMD-16844. Spatial restraints derived from chemical crosslinking and from an electron density map indicating the position of the vimentin tail domains were applied in the modelling procedure.	1	False	False

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaFold	2.1.2	model building	https://alphafold.ebi.ac.uk/
2	ClusPro	2.00	model docking	https://cluspro.org/
3	Namdinator	Not available	molecular dynamics flexible fitting	https://namdinator.au.dk/
4	UCSF Chimera	1.15	model visualization	https://www.cgl.ucsf.edu/chimerax/

Data quality

3DEM volume

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 7 bond length outliers in this entry (0.09% of 7452 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	263	PRO	C-N	64.93	2.24	1.33	1	1
C	261	SER	C-N	35.78	0.83	1.33	1	1
D	413	LEU	CA-C	5.45	1.64	1.52	1	1
D	413	LEU	N-CA	5.29	1.56	1.46	1	1
D	412	SER	C-N	5.17	1.40	1.33	1	1
A	252	GLN	CA-C	4.06	1.61	1.52	1	1
D	413	LEU	C-N	4.02	1.41	1.34	1	1

Standard geometry: angle outliers

There are 68 bond angle outliers in this entry (0.73% of 9308 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	261	SER	O-C-N	53.53	37.35	123.00	1	1
C	263	PRO	O-C-N	20.46	155.74	123.00	1	1
C	263	PRO	CA-C-N	18.39	79.43	116.20	1	1
C	261	SER	CA-C-N	16.49	149.18	116.20	1	1
C	261	SER	C-N-CA	13.30	97.77	121.70	1	1
C	263	PRO	C-N-CA	10.68	102.48	121.70	1	1
D	253	HIS	C-N-CA	9.73	139.22	121.70	1	1
D	413	LEU	CA-C-N	9.66	131.39	116.90	1	1
D	410	ARG	C-N-CA	8.92	137.76	121.70	1	1
A	253	HIS	O-C-N	7.80	110.53	123.00	1	1
C	424	ARG	C-N-CA	7.77	135.68	121.70	1	1
D	86	PHE	C-N-CA	7.51	135.21	121.70	1	1
D	412	SER	C-N-CA	7.36	134.95	121.70	1	1
A	256	ILE	C-N-CA	7.19	134.64	121.70	1	1
C	454	VAL	C-N-CA	6.78	133.91	121.70	1	1
A	436	THR	C-N-CA	6.72	133.79	121.70	1	1
D	253	HIS	CA-C-N	6.65	129.51	116.20	1	1
B	435	ASP	C-N-CA	6.50	133.40	121.70	1	1
B	85	ASP	C-N-CA	6.50	133.40	121.70	1	1
C	435	ASP	C-N-CA	6.50	133.40	121.70	1	1
C	413	LEU	CA-C-N	6.37	126.46	116.90	1	1
D	447	VAL	C-N-CA	6.34	133.10	121.70	1	1
D	253	HIS	O-C-N	6.29	112.93	123.00	1	1
C	85	ASP	C-N-CA	6.02	132.54	121.70	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	436	THR	O-C-N	5.94	113.50	123.00	1	1
C	264	ASP	C-N-CA	5.79	132.13	121.70	1	1
D	412	SER	CA-C-O	5.66	111.17	120.80	1	1
D	254	VAL	C-N-CA	5.53	131.66	121.70	1	1
A	252	GLN	C-N-CA	5.49	131.58	121.70	1	1
D	412	SER	CA-C-N	5.48	127.15	116.20	1	1
C	417	ASN	C-N-CA	5.45	131.50	121.70	1	1
B	263	PRO	C-N-CA	5.42	131.46	121.70	1	1
D	414	PRO	N-CA-C	5.38	125.56	112.10	1	1
D	465	LEU	C-N-CA	5.35	131.34	121.70	1	1
A	250	GLN	C-N-CA	5.31	131.26	121.70	1	1
D	413	LEU	O-C-N	5.24	114.61	123.00	1	1
A	253	HIS	C-N-CA	5.07	130.83	121.70	1	1
D	447	VAL	CA-C-N	5.06	126.32	116.20	1	1
A	254	VAL	C-N-CA	4.94	130.58	121.70	1	1
C	454	VAL	O-C-N	4.88	115.20	123.00	1	1
C	436	THR	C-N-CA	4.77	130.29	121.70	1	1
A	257	ASP	N-CA-C	4.70	124.17	111.00	1	1
A	255	GLN	CA-C-N	4.65	106.89	116.20	1	1
A	426	THR	CA-C-O	4.64	112.91	120.80	1	1
D	414	PRO	C-N-CA	4.63	130.04	121.70	1	1
D	418	PHE	C-N-CA	4.54	129.86	121.70	1	1
A	436	THR	CA-C-N	4.51	125.23	116.20	1	1
C	423	LEU	C-N-CA	4.49	129.79	121.70	1	1
D	413	LEU	CA-C-O	4.47	113.20	120.80	1	1
C	415	LEU	CA-C-N	4.45	123.57	116.90	1	1
A	421	LEU	C-N-CA	4.40	129.62	121.70	1	1
B	264	ASP	C-N-CA	4.38	129.59	121.70	1	1
D	447	VAL	O-C-N	4.37	116.01	123.00	1	1
C	68	VAL	C-N-CA	4.34	129.52	121.70	1	1
A	264	ASP	C-N-CA	4.32	129.48	121.70	1	1
C	436	THR	O-C-N	4.26	116.18	123.00	1	1
C	435	ASP	O-C-N	4.25	116.20	123.00	1	1
A	260	VAL	C-N-CA	4.23	129.31	121.70	1	1
B	253	HIS	CA-C-N	4.20	124.59	116.20	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	435	ASP	CA-C-N	4.19	124.59	116.20	1	1
A	239	GLU	C-N-CA	4.18	129.22	121.70	1	1
C	24	PRO	C-N-CA	4.16	129.19	121.70	1	1
B	466	GLU	CA-C-O	4.09	113.85	120.80	1	1
D	96	PHE	C-N-CA	4.08	129.05	121.70	1	1
B	412	SER	O-C-N	4.07	116.48	123.00	1	1
A	2	SER	C-N-CA	4.07	129.02	121.70	1	1
A	10	SER	C-N-CA	4.04	128.97	121.70	1	1
A	18	PRO	C-N-CA	4.01	128.92	121.70	1	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	1.49	14

There are 14 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)
C:261:SER:C	C:262:LYS:CA	1.52	1	1
C:263:PRO:C	C:264:ASP:N	0.96	1	1
C:261:SER:CA	C:262:LYS:N	0.95	1	1
C:261:SER:C	C:262:LYS:N	0.93	1	1
C:261:SER:O	C:262:LYS:CA	0.80	1	1
C:263:PRO:CA	C:264:ASP:N	0.77	1	1
C:261:SER:O	C:262:LYS:N	0.64	1	1
C:261:SER:CA	C:262:LYS:CA	0.53	1	1
D:409:SER:C	D:411:ILE:H	0.47	1	1
B:431:LEU:C	B:433:LEU:H	0.46	1	1
C:261:SER:C	C:262:LYS:C	0.46	1	1
D:95:GLU:C	D:97:LYS:H	0.43	1	1
C:17:GLY:C	C:19:GLY:HA3	0.41	1	1
C:263:PRO:C	C:264:ASP:CA	0.40	1	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	1854	1607	193	54

There are 54 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	9	SER	1
A	19	GLY	1
A	85	ASP	1
A	144	SER	1
A	257	ASP	1
A	258	VAL	1
A	263	PRO	1
A	265	LEU	1
A	413	LEU	1
A	414	PRO	1
A	437	HIS	1
B	4	ARG	1
B	21	ALA	1
B	34	SER	1
B	76	GLY	1
B	79	LEU	1
B	264	ASP	1
B	420	SER	1
B	431	LEU	1
B	435	ASP	1
B	437	HIS	1
B	438	SER	1
C	6	VAL	1
C	18	PRO	1
C	25	SER	1
C	62	ALA	1
C	69	ARG	1
C	71	ARG	1
C	85	ASP	1
C	200	GLU	1
C	265	LEU	1

Chain	Res	Type	Models (Total)
C	413	LEU	1
C	414	PRO	1
C	418	PHE	1
C	420	SER	1
C	455	ILE	1
C	463	ASP	1
D	31	VAL	1
D	77	VAL	1
D	84	VAL	1
D	87	SER	1
D	142	GLY	1
D	252	GLN	1
D	254	VAL	1
D	255	GLN	1
D	259	ASP	1
D	411	ILE	1
D	412	SER	1
D	413	LEU	1
D	414	PRO	1
D	439	LYS	1
D	441	THR	1
D	446	THR	1
D	447	VAL	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	0	0	0	0

Fit of model to data used for modeling

3DEM volume

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

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