

# 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	9A2D
PDB-Dev ID	PDBDEV_00000156
Structure Title	Modeling of the ciliary Intraflagellar transport-A complex
Structure Authors	McCafferty, C.L.; Papoulas, O.; Jordan, M.A.; Hoogerbrugge, G.; Nichols, C.; Pigino, G.; Taylor, D.W.; Wallingford, J.B.; Marcotte, E.M.
Deposited on	2022-08-03

*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](mailto:helpdesk@pdb-ihm.org)*

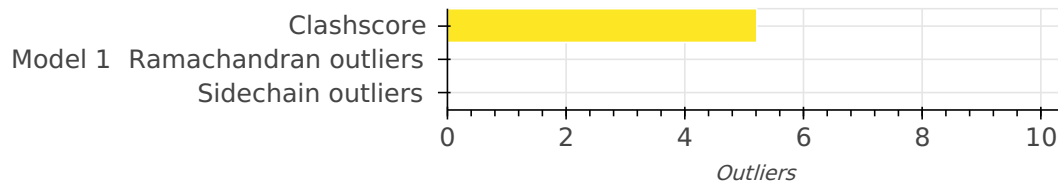
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 3 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	Intraflagellar transport protein 43	A	146	70-80, 90-130	1-69, 81-89, 131-146	100.00 / 35.62	Coarse-grained: 1 residue(s) per bead
		2	Intraflagellar transport protein 121	B	1195	1-341, 342-655, 656-799, 800-895, 896-978, 979-1004, 1005-1195	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
		3	Intraflagellar transport protein 122	C	1251	1-319, 320-581, 582-811, 812-1251	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		4	Intraflagellar transport protein 139	D	1334	1-1334	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
		5	Intraflagellar transport protein 140	E	1407	1-376, 377-713, 714-979, 980-1080, 1081-1407	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
		6	Intraflagellar transport protein 144	F	1387	1-655, 656-985, 986-1114, 1115-1387	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead

### Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	Crosslinking-MS data	Zenodo	<a href="https://zenodo.org/record/7222413">10.5281/zenodo.7222413</a>
1	De Novo model	Zenodo	<a href="https://zenodo.org/record/7222413">10.5281/zenodo.7222413</a>
3	3DEM volume	EMDB	<a href="https://www.ebi.ac.uk/emdb/EMD-26791">EMD-26791</a>

### 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	Sampling	Replica exchange monte carlo	None	200000	False	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
3	<a href="#">AlphaFold2</a>	Not available	structure prediction	<a href="https://alphafold.ebi.ac.uk/">https://alphafold.ebi.ac.uk/</a>
1	<a href="#">IMP PMI module</a>	2.11.1	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
2	<a href="#">Integrative Modeling Platform (IMP)</a>	2.11.1	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>

## 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.

### 3DEM volume

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 ?

*Bond length outliers can not be evaluated for this model*

### Standard geometry: angle outliers ?

*Bond angle outliers can not be evaluated for this model*

### 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	5.21	35

There are 35 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:102:PRO:CA	D:1048:ASN:CA	1.47	1	1
E:51:TYR:CA	F:1067:ALA:CA	1.43	1	1
A:48:GLN:CA	A:49:GLU:CA	1.34	1	1
F:290:ILE:CA	F:630:ARG:CA	1.22	1	1
C:905:LEU:CA	E:1081:LYS:CA	1.13	1	1
C:710:PRO:CA	E:1369:LEU:CA	1.11	1	1
C:899:MET:CA	E:1078:GLN:CA	1.11	1	1
C:682:ASN:CA	E:1376:GLU:CA	1.09	1	1
D:862:GLY:CA	D:954:GLU:CA	1.05	1	1
C:706:THR:CA	E:1393:ASN:CA	1.03	1	1
C:901:ALA:CA	E:1079:ARG:CA	0.92	1	1
F:764:GLU:CA	F:791:LEU:CA	0.83	1	1
A:132:GLY:CA	A:133:ASN:CA	0.82	1	1
C:1240:GLU:CA	E:1045:LYS:CA	0.76	1	1
C:1190:CYS:CA	E:1083:ARG:CA	0.74	1	1
C:702:ARG:CA	E:1394:LYS:CA	0.72	1	1
C:902:THR:CA	E:1079:ARG:CA	0.69	1	1
F:786:LEU:CA	F:808:ALA:CA	0.68	1	1
C:712:ASN:CA	E:1372:TYR:CA	0.66	1	1
F:785:TYR:CA	F:806:ARG:CA	0.63	1	1
F:787:THR:CA	F:806:ARG:CA	0.59	1	1
C:901:ALA:CA	E:1080:ASN:CA	0.58	1	1
F:290:ILE:CA	F:631:GLY:CA	0.51	1	1
C:902:THR:CA	E:1076:GLU:CA	0.49	1	1
A:5:GLY:CA	A:9:TRP:CA	0.49	1	1
F:786:LEU:CA	F:805:ARG:CA	0.49	1	1
C:902:THR:CA	E:1078:GLN:CA	0.48	1	1
F:600:ILE:CA	F:716:ASP:CA	0.48	1	1
F:618:LYS:CA	F:703:LEU:CA	0.48	1	1
C:910:ASN:CA	E:1084:ASP:CA	0.47	1	1
F:787:THR:CA	F:807:LEU:CA	0.47	1	1
F:479:PHE:CA	F:480:PRO:CA	0.41	1	1
E:52:GLU:CA	F:1068:LYS:CA	0.41	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
C:1192:THR:CA	E:1084:ASP:CA	0.41	1	1
C:705:ASP:CA	E:1394:LYS: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	0	0	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	0	0	0	0

## 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 100 crosslinking restraints combined in 100 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	CA	LYS	CA	upper bound	21.0	96
DSSO	GLU	CA	GLU	CA	upper bound	21.0	2
DSSO	ASP	CA	GLU	CA	upper bound	21.0	1
DSSO	LYS	CA	TYR	CA	upper bound	21.0	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=100)
1	1	1	1/1	All	Not available	Not available	0

#### 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.

#### 3DEM volume

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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