Integrative Structure Validation Report August 07, 2024 - 03:31 PM PDT

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

| 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. |

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

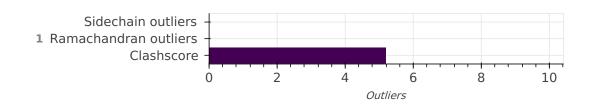
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 assessment for SAS datasets and fit to model assessments for SAS 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 unique models, with 6 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 23 rigid bodies and 3 flexible or non-rigid units.

Entry composition?

There is 1 unique type of models in this entry. This model is titled Cluster O/None.

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|-------------|-------------------|---------------|---|-------------|--------------------|-------------------|
| 1 | 1 | 1 | Intraflagellar transport protein 43 | А | А | 146 |
| 1 | 2 | 2 | Intraflagellar transport protein 121 | В | В | 1195 |
| 1 | 3 | 3 | Intraflagellar transport protein 122 | С | С | 1251 |
| 1 | 4 | 4 | Intraflagellar transport protein 139 | D | D | 1334 |
| 1 | 5 | 5 | Intraflagellar transport protein 140 | E | E | 1407 |
| 1 | 6 | 6 | Intraflagellar transport protein 144 | F | F | 1387 |

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 | ProteomeXchange | PXD032818 |
| 1 | De Novo model | File | 10.5281/zenodo.7222413 |
| 3 | 3DEM volume | EMDB | EMD-26791 |

Representation ?

This entry has only one representation and includes 23 rigid bodies and 3 flexible units.

| Chain ID | Rigid bodies | Non-rigid segments |
|-------------|--|-----------------------|
| В | 1-341, 342-655, 656-799, 800-895, 896-978, 979-1004, 1005- 1195 | - |
| С | 1-319, 320-581, 582-811, 812-1251 | - |
| D | 1-1334 | - |
| F | 1-655, 656-985, 986-1114, 1115-1387 | - |
| Е | 1-376, 377-713, 714-979, 980-1080, 1081-1407 | - |
| А | 70-80, 90-130 | 1-69, 81-89, 131-146 |

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

There are 3 software packages reported in this entry.

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

Data quality Crosslinking-MS

Validation for this section is under development.

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 do not exist or 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 the models in this entry.

| Model ID | Clash score | Number of clashes |
|----------|-------------|-------------------|
| 1 | 5.21 | 35 |

All 35 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Model ID | Atom-1 | Atom-2 | Clash overlap (Å) |
|----------|--------------|--------------|-------------------|
| 1 | A:102:PRO:CA | A:49:GLU:CA | 1.337 |
| 1 | E:51:TYR:CA | F:630:ARG:CA | 1.218 |
| 1 | A:48:GLN:CA | D:954:GLU:CA | 1.047 |
| 1 | F:290:ILE:CA | F:791:LEU:CA | 0.833 |
| 1 | C:905:LEU:CA | A:133:ASN:CA | 0.823 |
| 1 | C:710:PRO:CA | F:808:ALA:CA | 0.681 |
| 1 | C:899:MET:CA | F:806:ARG:CA | 0.632 |
| 1 | C:682:ASN:CA | F:806:ARG:CA | 0.591 |
| 1 | D:862:GLY:CA | F:631:GLY:CA | 0.510 |
| 1 | C:706:THR:CA | A:9:TRP:CA | 0.488 |
| 1 | C:901:ALA:CA | F:805:ARG:CA | 0.487 |
| 1 | F:764:GLU:CA | F:716:ASP:CA | 0.480 |
| 1 | A:132:GLY:CA | F:703:LEU:CA | 0.476 |
| 1 | C:702:ARG:CA | F:807:LEU:CA | 0.469 |
| 1 | C:902:THR:CA | F:480:PRO:CA | 0.414 |

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 | Analyzed | Favored | Allowed | Outliers |
|----------|----------|---------|---------|----------|
| 1 | 0 | 0 | 0 | 0 |

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains ?

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

| Model ID Analyzed Favored Allowed Outliers | Model ID | Analyzed | Favored | Allowed | Outliers |
|--|----------|----------|---------|---------|----------|
|--|----------|----------|---------|---------|----------|

| Model ID | Analyzed | Favored | Allowed | Outliers |
|----------|----------|---------|---------|----------|
| 1 | 0 | 0 | 0 | 0 |

Detailed list of outliers are tabulated below.

Fit of model to data used for modeling (

Crosslinking-MS

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

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