# Integrative Structure Validation Report

## March 27, 2025 - 10:10 AM PDT

*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 | 9A24 |
| PDB-Dev ID | PDBDEV_00000141 |
| Structure Title | PTX3 hybrid cryoEM and AlphaFold model |
| Structure Authors | Dylan P. Noone; Thomas H. Sharp |
| Deposited on | 2022-07-20 |

*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*

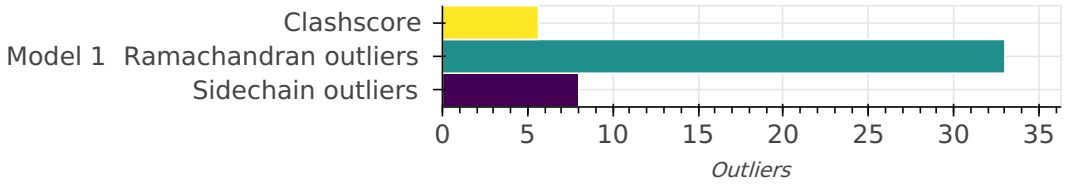
*A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the* ? symbol.

*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 6 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 | PTX3 (protein complex) | A [B] | 364 | - | 1-147, 136-364 | 100.00 / 100.00 | Atomic |
| | | | | B [A] | | | | | |
| | | | | C [D] | | | | | |
| | | | | D [C] | | | | | |
| | | | | E [F] | | | | | |
| | | | | F [E] | | | | | |
| | | | | G [H] | | | | | |
| | | | | H [G] | | | | | |
| | | 2 | N-ACETYL-D-GLUCOSAMINE | I [B] | Non-polymeric | - | - | Not available / Not available | Atomic |
| | | | | J [B] | | | | | |
| | | | | N [A] | | | | | |
| | | | | O [A] | | | | | |
| | | | | S [D] | | | | | |
| | | | | W [D] | | | | | |
| | | | | X [C] | | | | | |

| ID | Model(s) | Entity ID | Molecule name | Chain(s) [auth] | Total residues | Rigid segments | Flexible segments | Model coverage/ Starting model coverage (%) | Scale |
|---|---|---|---|---|---|---|---|---|---|
| | | | | Y [C] | | | | | |
| | | | | CA [F] | | | | | |
| | | | | DA [F] | | | | | |
| | | | | HA [E] | | | | | |
| | | | | IA [E] | | | | | |
| | | | | MA [H] | | | | | |
| | | | | NA [H] | | | | | |
| | | | | RA [G] | | | | | |
| | | | | SA [G] | | | | | |
| | | 3 | BETA-D-MANNOSE | K [B] | Non-polymeric | - | - | Not available / Not available | Atomic |
| | | | | P [A] | | | | | |
| | | | | T [D] | | | | | |
| | | | | Z [C] | | | | | |
| | | | | EA [F] | | | | | |
| | | | | JA [E] | | | | | |
| | | | | OA [H] | | | | | |
| | | | | TA [G] | | | | | |
| | | 4 | ALPHA-D-MANNOSE | L [B] | Non-polymeric | - | - | Not available / Not available | Atomic |
| | | | | M [B] | | | | | |
| | | | | Q [A] | | | | | |
| | | | | R [A] | | | | | |
| | | | | U [D] | | | | | |
| | | | | V [D] | | | | | |
| | | | | AA [C] | | | | | |
| | | | | BA [C] | | | | | |
| | | | | FA [F] | | | | | |
| | | | | GA [F] | | | | | |
| | | | | KA [E] | | | | | |
| | | | | LA [E] | | | | | |
| | | | | PA [H] | | | | | |
| | | | | QA [H] | | | | | |
| | | | | UA [G] | | | | | |

| ID | Model(s) | Entity ID | Molecule name | Chain(s) [auth] | Total residues | Rigid segments | Flexible segments | Model coverage/ Starting model coverage (%) | Scale |
|---|---|---|---|---|---|---|---|---|---|
| | | | | VA [G] | | | | | |
| | | 5 | water | WA [B] | Non-polymeric | - | - | Not available / Not available | Atomic |
| | | | | XA [F] | | | | | |
| | | | | YA [I] | | | | | |

## Datasets used for modeling

*There are 6 unique datasets used to build the models in this entry.*

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 1 | De Novo model | Not available | Not available |
| 2 | 3DEM volume | EMDB | EMD-14774 |
| 3 | Mass Spectrometry data | PRIDE | PXD034602 |
| 4 | 2DEM class average | Not available | Not available |
| 5 | Other | Not available | Not available |
| 6 | Experimental model | PDB | 7ZL1 |

## 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 |
|---|---|---|---|---|---|---|---|
| 4 | 1 | None | None | None | None | False | False |

*There are 4 software packages reported in this entry.*

| ID | Software name | Software version | Software classification | Software location |
|---|---|---|---|---|
| 3 | EMAN2 | Not available | Validation - 2D variability analysis | https://pubmed.ncbi.nlm.nih.gov/27572727/ |
| 4 | IMOD | Not available | validation | https://bio3d.colorado.edu/imod/ |

| ID | Software name | Software version | Software classification | Software location |
|---|---|---|---|---|
| 1 | Relion | Not available | Single particle analysis | https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3690530/ |
| 2 | AlphaFold | Not available | structural prediction | https://www.deepmind.com/research/highlighted-research/alphafold |

## Data quality

### 2DEM class average

Validation for this section is under development.

### Mass Spectrometry

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

*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 | 5.64 | 255 |

*There are 255 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) |
|---|---|---|---|---|
| H:61:ASP:OD1 | H:65:ARG:NH1 | 0.79 | 1 | 1 |
| G:61:ASP:OD1 | G:65:ARG:NH1 | 0.75 | 1 | 1 |
| A:150:GLN:NE2 | B:145:ASP:O | 0.75 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| C:150:GLN:NE2 | D:145:ASP:O | 0.73 | 1 | 1 |
| N:1:NAG:O3 | O:1:NAG:O5 | 0.73 | 1 | 1 |
| E:345:ASN:O | YA:161:HOH:O | 0.71 | 1 | 1 |
| F:179:VAL:O | YA:226:HOH:O | 0.69 | 1 | 1 |
| C:345:ASN:O | YA:167:HOH:O | 0.69 | 1 | 1 |
| MA:1:NAG:O4 | NA:1:NAG:O7 | 0.69 | 1 | 1 |
| D:226:GLN:N | D:226:GLN:OE1 | 0.69 | 1 | 1 |
| E:163:GLU:OE2 | F:315:ARG:NH1 | 0.68 | 1 | 1 |
| C:246:SER:O | YA:177:HOH:O | 0.68 | 1 | 1 |
| B:150:GLN:NE2 | C:145:ASP:O | 0.68 | 1 | 1 |
| F:171:ARG:NH2 | F:200:ASP:O | 0.67 | 1 | 1 |
| C:301:CYS:O | YA:370:HOH:O | 0.67 | 1 | 1 |
| A:85:PRO:O | A:87:ALA:N | 0.67 | 1 | 1 |
| F:121:GLU:O | G:124:ARG:NH2 | 0.66 | 1 | 1 |
| E:363:VAL:O | YA:268:HOH:O | 0.66 | 1 | 1 |
| C:85:PRO:O | C:87:ALA:N | 0.66 | 1 | 1 |
| A:363:VAL:O | YA:272:HOH:O | 0.66 | 1 | 1 |
| C:309:THR:O | YA:130:HOH:O | 0.66 | 1 | 1 |
| G:301:CYS:SG | YA:368:HOH:O | 0.66 | 1 | 1 |
| C:363:VAL:O | YA:273:HOH:O | 0.65 | 1 | 1 |
| B:121:GLU:O | C:124:ARG:NH2 | 0.65 | 1 | 1 |
| H:363:VAL:O | YA:270:HOH:O | 0.65 | 1 | 1 |
| E:206:ILE:HD13 | E:222:TYR:HB3 | 0.65 | 1 | 1 |
| C:260:GLU:N | C:260:GLU:OE1 | 0.64 | 1 | 1 |
| E:235:GLU:O | E:238:LYS:NZ | 0.64 | 1 | 1 |
| G:298:ASN:OD1 | G:299:GLY:N | 0.64 | 1 | 1 |
| C:179:VAL:O | YA:224:HOH:O | 0.64 | 1 | 1 |
| D:290:ILE:O | YA:78:HOH:O | 0.64 | 1 | 1 |
| G:260:GLU:N | G:260:GLU:OE1 | 0.64 | 1 | 1 |
| B:309:THR:O | YA:131:HOH:O | 0.64 | 1 | 1 |
| D:260:GLU:N | D:260:GLU:OE1 | 0.64 | 1 | 1 |
| F:260:GLU:N | F:260:GLU:OE1 | 0.64 | 1 | 1 |
| B:160:ALA:O | YA:172:HOH:O | 0.64 | 1 | 1 |
| A:242:GLU:N | A:242:GLU:OE1 | 0.63 | 1 | 1 |
| H:260:GLU:N | H:260:GLU:OE1 | 0.63 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| E:260:GLU:N | E:260:GLU:OE1 | 0.63 | 1 | 1 |
| DA:1:NAG:O3 | EA:1:BMA:O5 | 0.63 | 1 | 1 |
| T:1:BMA:O4 | U:1:MAN:O5 | 0.63 | 1 | 1 |
| E:179:VAL:O | YA:227:HOH:O | 0.63 | 1 | 1 |
| H:242:GLU:N | H:242:GLU:OE1 | 0.63 | 1 | 1 |
| D:61:ASP:OD1 | D:65:ARG:NH1 | 0.62 | 1 | 1 |
| E:242:GLU:N | E:242:GLU:OE1 | 0.62 | 1 | 1 |
| F:242:GLU:N | F:242:GLU:OE1 | 0.62 | 1 | 1 |
| C:329:GLU:N | C:329:GLU:OE1 | 0.62 | 1 | 1 |
| F:199:THR:OG1 | YA:69:HOH:O | 0.62 | 1 | 1 |
| G:179:VAL:O | YA:230:HOH:O | 0.62 | 1 | 1 |
| A:329:GLU:N | A:329:GLU:OE1 | 0.62 | 1 | 1 |
| B:260:GLU:N | B:260:GLU:OE1 | 0.62 | 1 | 1 |
| A:297:LYS:O | H:213:LYS:NZ | 0.62 | 1 | 1 |
| C:258:ASN:OD1 | C:259:SER:N | 0.62 | 1 | 1 |
| E:204:LYS:HE2 | E:206:ILE:HD11 | 0.62 | 1 | 1 |
| C:242:GLU:N | C:242:GLU:OE1 | 0.62 | 1 | 1 |
| C:109:ASP:OD1 | C:112:ARG:NH2 | 0.61 | 1 | 1 |
| E:315:ARG:NH1 | H:163:GLU:OE2 | 0.61 | 1 | 1 |
| F:329:GLU:N | F:329:GLU:OE1 | 0.61 | 1 | 1 |
| H:329:GLU:N | H:329:GLU:OE1 | 0.61 | 1 | 1 |
| B:242:GLU:N | B:242:GLU:OE1 | 0.61 | 1 | 1 |
| A:109:ASP:OD1 | A:112:ARG:NH2 | 0.61 | 1 | 1 |
| D:242:GLU:N | D:242:GLU:OE1 | 0.61 | 1 | 1 |
| B:4:ASP:OD2 | B:70:ARG:NH2 | 0.61 | 1 | 1 |
| G:329:GLU:N | G:329:GLU:OE1 | 0.61 | 1 | 1 |
| E:329:GLU:N | E:329:GLU:OE1 | 0.61 | 1 | 1 |
| F:258:ASN:OD1 | F:259:SER:N | 0.61 | 1 | 1 |
| G:347:VAL:HG13 | G:352:THR:HG21 | 0.60 | 1 | 1 |
| A:12:ASN:OD1 | A:13:LEU:N | 0.60 | 1 | 1 |
| C:61:ASP:OD1 | C:65:ARG:NH1 | 0.60 | 1 | 1 |
| A:347:VAL:HG13 | A:352:THR:HG21 | 0.60 | 1 | 1 |
| G:38:GLU:N | G:38:GLU:OE1 | 0.60 | 1 | 1 |
| F:170:MET:N | F:170:MET:SD | 0.59 | 1 | 1 |
| H:170:MET:N | H:170:MET:SD | 0.59 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| G:258:ASN:OD1 | G:259:SER:N | 0.59 | 1 | 1 |
| G:163:GLU:OE2 | H:315:ARG:NH1 | 0.59 | 1 | 1 |
| D:258:ASN:OD1 | D:259:SER:N | 0.59 | 1 | 1 |
| H:38:GLU:N | H:38:GLU:OE1 | 0.59 | 1 | 1 |
| F:347:VAL:HG13 | F:352:THR:HG21 | 0.59 | 1 | 1 |
| B:258:ASN:OD1 | B:259:SER:N | 0.59 | 1 | 1 |
| E:258:ASN:OD1 | E:259:SER:N | 0.58 | 1 | 1 |
| A:246:SER:O | YA:183:HOH:O | 0.58 | 1 | 1 |
| D:38:GLU:N | D:38:GLU:OE1 | 0.58 | 1 | 1 |
| H:347:VAL:HG13 | H:352:THR:HG21 | 0.58 | 1 | 1 |
| A:315:ARG:NH1 | D:163:GLU:OE2 | 0.57 | 1 | 1 |
| B:215:ASN:ND2 | B:218:GLU:OE2 | 0.57 | 1 | 1 |
| C:38:GLU:N | C:38:GLU:OE1 | 0.57 | 1 | 1 |
| F:319:PHE:CE2 | F:347:VAL:HG11 | 0.57 | 1 | 1 |
| H:79:ALA:O | H:83:ALA:N | 0.57 | 1 | 1 |
| A:319:PHE:CE2 | A:347:VAL:HG11 | 0.57 | 1 | 1 |
| C:213:LYS:NZ | F:297:LYS:O | 0.57 | 1 | 1 |
| E:145:ASP:O | H:150:GLN:NE2 | 0.56 | 1 | 1 |
| H:319:PHE:CE2 | H:347:VAL:HG11 | 0.56 | 1 | 1 |
| C:347:VAL:HG13 | C:352:THR:HG21 | 0.56 | 1 | 1 |
| E:121:GLU:O | F:124:ARG:NH2 | 0.56 | 1 | 1 |
| A:236:GLU:N | A:236:GLU:OE1 | 0.56 | 1 | 1 |
| G:215:ASN:ND2 | G:218:GLU:OE2 | 0.55 | 1 | 1 |
| B:231:VAL:HG13 | B:237:ASN:O | 0.55 | 1 | 1 |
| B:297:LYS:O | G:213:LYS:NZ | 0.55 | 1 | 1 |
| H:244:MET:N | H:244:MET:SD | 0.55 | 1 | 1 |
| A:231:VAL:HG13 | A:237:ASN:O | 0.55 | 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 | 2896 | 2542 | 321 | 33 |

*There are 33 unique backbone outliers. Detailed list of outliers are tabulated below.*

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 86 | CYS | 1 |
| A | 89 | GLY | 1 |
| A | 159 | PRO | 1 |
| A | 182 | VAL | 1 |
| A | 302 | VAL | 1 |
| B | 86 | CYS | 1 |
| B | 89 | GLY | 1 |
| B | 182 | VAL | 1 |
| B | 226 | GLN | 1 |
| B | 303 | GLY | 1 |
| C | 86 | CYS | 1 |
| C | 89 | GLY | 1 |
| C | 159 | PRO | 1 |
| C | 300 | CYS | 1 |
| D | 86 | CYS | 1 |
| D | 89 | GLY | 1 |
| D | 159 | PRO | 1 |
| D | 182 | VAL | 1 |
| D | 298 | ASN | 1 |
| D | 300 | CYS | 1 |
| E | 86 | CYS | 1 |
| E | 89 | GLY | 1 |
| E | 159 | PRO | 1 |
| E | 297 | LYS | 1 |
| E | 300 | CYS | 1 |
| F | 297 | LYS | 1 |
| F | 304 | GLY | 1 |
| G | 86 | CYS | 1 |
| G | 159 | PRO | 1 |
| G | 303 | GLY | 1 |
| H | 86 | CYS | 1 |
| H | 159 | PRO | 1 |
| H | 300 | CYS | 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 | 2360 | 2336 | 16 | 8 |

*There are 8 unique sidechain outliers. Detailed list of outliers are tabulated below.*

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 203 | ASN | 1 |
| B | 213 | LYS | 1 |
| C | 203 | ASN | 1 |
| D | 213 | LYS | 1 |
| F | 86 | CYS | 1 |
| F | 170 | MET | 1 |
| H | 170 | MET | 1 |
| H | 301 | CYS | 1 |

## Fit of model to data used for modeling

### 2DEM class average

Validation for this section is under development.

### Mass Spectrometry

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.

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