

# PDB deposition / publication

Validation report from PDB OneDep validation (PDF, XML).

Phenix home

Quit Preferences Help Citations Reload last job ChimeraX Coot PyMOL KING Tools Help Server

Actions Job history

Projects

Show group: All groups Manage...

Select Delete New project Import project Settings

ID	Last modified	# of jobs	R-free
✓ AF_POMGNT2_1	Jun 05 2024 11:46...	3	---
bugs	May 30 2024 02:38...	12	---
02_test_comma...	May 24 2024 01:20...	17	---
tests	May 22 2024 11:15...	67	0.2650
AF_bromodomai...	May 16 2024 10:37...	1	---
AF_7mjs_H_Pre...	Mar 19 2024 09:54...	1	---
groel_dock_refine	Mar 19 2024 09:28...	4	---
bugs_playground	Mar 07 2024 04:43...	13	---
fmodel	Feb 28 2024 02:44...	30	---
SEACOAST	Feb 13 2024 01:09...	7	---
AF_7mjs_H_Pre...	Jan 03 2024 10:19 ...	4	---
joint_XN	Nov 02 2023 03:49...	50	0.0989
AF_7mjs_H_Pre...	Apr 13 2023 02:18 ...	20	---
AF_7mjs_H_Pre...	Apr 13 2023 09:35 ...	0	---
AF_POMGNT2_0	Mar 31 2023 07:07...	3	---
AF_POMGNT2	Mar 30 2023 09:07...	6	---
7brm	Mar 17 2023 11:39...	25	---
7mjs_wcsbw	Mar 17 2023 09:31...	33	---
presentation	Mar 15 2023 02:00...	17	---
bughaton	Mar 06 2023 03:23...	8	---

Current directory: /Users/dcliebschner/Documents/AF\_POMGNT2\_1 Browse...

Phenix version 1.21.1-5286-000 Project: AF\_POMGNT2\_1

maps (create, manipulate, compare)  
Enhanced maps (Polder, FEM, density-modified...)  
Model building  
Refinement  
Ligands  
Cryo-EM: Map analysis, symmetry, manipulation  
Validation and map-based comparisons  
Map improvement  
Docking, model building and rebuilding  
Refinement  
Models: Superpose, search, compare, analyze symmetry  
Modification, minimization and dynamics  
**PDB Deposition**  
Prepare model for PDB deposition  
Finalize mmCIF files for deposition to the PDB  
Get PDB validation report  
Retrieve a validation report from the PDB  
Generate "Table 1" for journal  
Extraction of final model statistics for publication  
Program search

WORLDWIDE  
wwPDB  
PROTEIN DATA BANK

Preliminary Full wwPDB X-ray Structure Validation  
Report ⓘ

Jun 6, 2024 - 12:48 PM EDT

**This wwPDB validation report is NOT for manuscript review**

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the standalone wwPDB validation server.  
The structure in question has not been deposited to the wwPDB.  
This report should not be submitted to journals.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	: 4.02b-467
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: NOT EXECUTED
EDS	: NOT EXECUTED
Percentile statistics	: 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	: Eng & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.36.2

# PDB deposition

The screenshot shows the Phenix software interface. The top menu bar includes: Quit, Preferences, Help, Citations, Reload last job, ChimeraX, Coot, PyMOL, KING, Tools, Help, and Server. The main window is divided into several sections:

- Projects:** A table listing various projects with columns for ID, Last modified, # of jobs, and R-free. The 'tests' project is selected.
- Actions:** Buttons for Select, Delete, New project, Import project, and Settings.
- Right Panel:** A list of actions categorized under 'maps (create, manipulate, compare)', 'Enhanced maps (Polder, FEM, density-modified...)', 'Model building', 'Refinement', 'Ligands', 'Cryo-EM: Map analysis, symmetry, manipulation', 'Validation and map-based comparisons', 'Map improvement', 'Docking, model building and rebuilding', 'Refinement', 'Models: Superpose, search, compare, analyze symmetry', and 'Modification, minimization and dynamics'. The 'PDB Deposition' section is highlighted with a red box and contains three items: 'Prepare model for PDB deposition', 'Get PDB validation report', and 'Generate "Table 1" for journal'.
- Bottom Bar:** Shows the current directory as '/Users/dcliebschner/Desktop/test' and the project name as 'tests'.

ID	Last modified	# of jobs	R-free
groel_dock_refine	Mar 20 2025 09:09...	0	---
AF_POMGNT2_2	Mar 20 2025 09:09...	2	---
tests	Mar 12 2025 11:09...	80	0.2650
discamb	Mar 10 2025 03:46...	5	---
bugs	Jan 27 2025 02:50 ...	23	---
AF_bromodomai..	Oct 31 2024 09:04 ...	4	---
05_Structure-C...	Oct 07 2024 06:31...	2	0.1587
02_test_comma...	Aug 05 2024 01:05...	19	---
aldose	Jul 24 2024 02:07 ...	10	0.1007
groel_dock_refi...	Jul 07 2024 01:40 ...	8	---
groel_dock_refi...	Jun 28 2024 10:34 ...	3	---
AF_POMGNT2_1	Jun 28 2024 08:32 ...	4	---
AF_7mjs_H_Pre...	Mar 19 2024 09:54...	1	---
bugs_playground	Mar 07 2024 04:43...	13	---
fmodel	Feb 28 2024 02:44...	30	---
AF_7mjs_H_Pre...	Jan 03 2024 10:19 ...	4	---
joint_XN	Nov 02 2023 03:49...	50	0.0989
AF_7mjs_H_Pre...	Apr 13 2023 02:18 ...	20	---
AF_7mjs_H_Pre...	Apr 13 2023 09:35 ...	0	---
AF_POMGNT2_0	Mar 31 2023 07:07...	3	---
AF_POMGNT2_0	Mar 31 2023 07:07...	3	---

# PDB deposition

The screenshot displays the Phenix software interface. The top menu bar includes 'Quit', 'Preferences', 'Help', 'Citations', 'Reload last job', 'ChimeraX', 'Coot', 'PyMOL', 'KING', 'Tools', 'Help', and 'Server'. The 'Actions' menu is open, showing a list of tasks. A red box highlights the 'PDB Deposition' section of this menu, which contains three items: 'Prepare model for PDB deposition', 'Get PDB validation report', and 'Generate "Table 1" for journal'. A red arrow points from this menu to a larger, detailed view of the same 'PDB Deposition' menu on the right side of the image. This detailed view shows the same three items with their descriptions: 'Finalize mmCIF files for deposition to the PDB', 'Retrieve a validation report from the PDB', and 'Extraction of final model statistics for publication'. The background interface shows a 'Projects' table with columns for ID, Last modified, # of jobs, and R-free. The 'Current directory' is set to '/Users/dcliebschner/Desktop/test' and the project is named 'tests'.

ID	Last modified	# of jobs	R-free
groel_dock_refine	Mar 20 2025 09:09...	0	---
AF_POMGNT2_2	Mar 20 2025 09:09...	2	---
tests	Mar 12 2025 11:09...	80	0.2650
discamb	Mar 10 2025 03:46...	5	---
bugs	Jan 27 2025 02:50 ...	23	---
AF_bromodomai..	Oct 31 2024 09:04 ...	4	---
05_Structure-C...	Oct 07 2024 06:31...	2	0.1587
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aldose	Jul 24 2024 02:07 ...	10	0.1007
groel_dock_refi...	Jul 07 2024 01:40 ...	8	---
groel_dock_refi...	Jun 28 2024 10:34 ...	3	---
AF_POMGNT2_1	Jun 28 2024 08:32 ...	4	---
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AF_POMGNT2_0	Mar 31 2023 07:07...	3	---
AF_POMGNT2_0	Mar 31 2023 07:07...	0	---




**PDB Deposition**

- Prepare model for PDB deposition**  
Finalize mmCIF files for deposition to the PDB
- Get PDB validation report**  
Retrieve a validation report from the PDB
- Generate "Table 1" for journal**  
Extraction of final model statistics for publication

Current directory: /Users/dcliebschner/Desktop/test  
Project: tests  
Phenix version 1.21.2-5419-000

# Prepare PDB deposition

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PDB Deposition	
	<b>Prepare model for PDB deposition</b> Finalize mmCIF files for deposition to the PDB
	<b>Get PDB validation report</b> Retrieve a validation report from the PDB
	<b>Generate "Table 1" for journal</b> Extraction of final model statistics for publication

Add sequence information to the mmCIF file.


Minimum inputs: the model from phenix.refine and a sequence file.

# Get PDB validation report

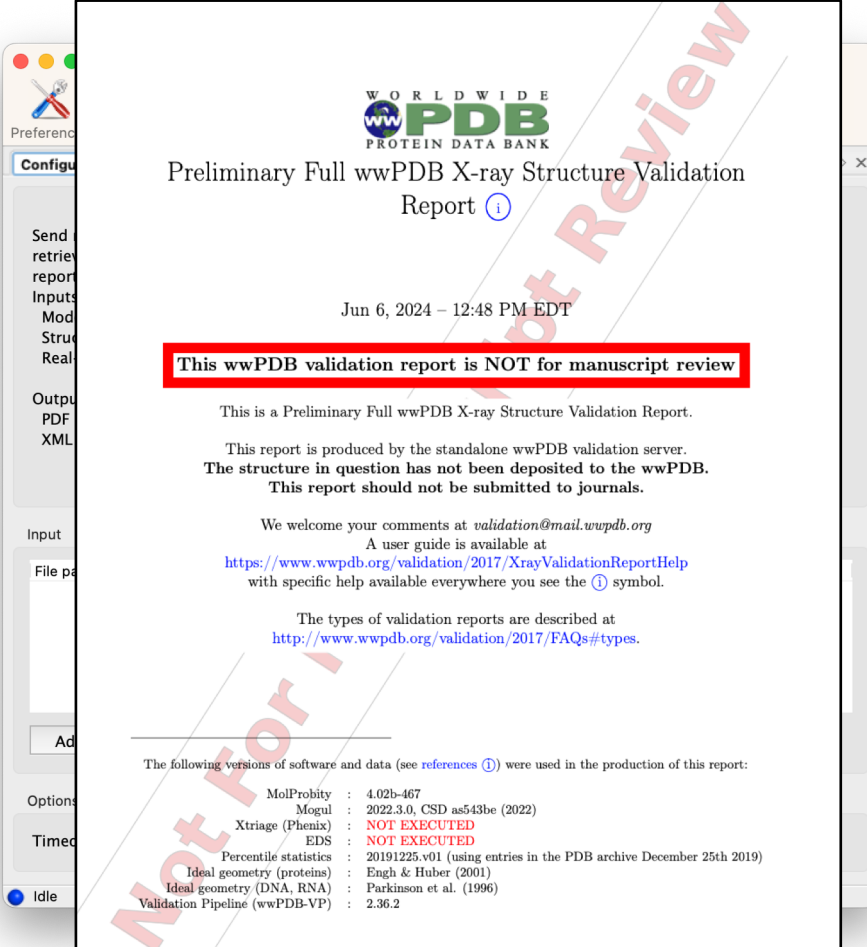
## PDB Deposition

 **Prepare model for PDB deposition**  
Finalize mmCIF files for deposition to the PDB

 **Get PDB validation report**  
Retrieve a validation report from the PDB

 **Generate "Table 1" for journal**  
Extraction of final model statistics for publication

Takes model and X-ray data files in mmCIF format and retrieves PDB validation report in PDF and XML format.



**WORLDWIDE PDB**  
PROTEIN DATA BANK

### Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2024 – 12:48 PM EDT

**This wwPDB validation report is NOT for manuscript review**

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the standalone wwPDB validation server. The structure in question has not been deposited to the wwPDB. This report should not be submitted to journals.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <https://www.wwpdb.org/validation/2017/XrayValidationReportHelp> with specific help available everywhere you see the ⓘ symbol.

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Percentile statistics	: 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinsson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.36.2




# Generate Table 1

## PDB Deposition

 **Prepare model for PDB deposition**  
Finalize mmCIF files for deposition to the PDB

 **Get PDB validation report**  
Retrieve a validation report from the PDB

 **Generate "Table 1" for journal**  
Extraction of final model statistics for publication

Generate the standard table of crystallographic statistics required by most scientific journals.

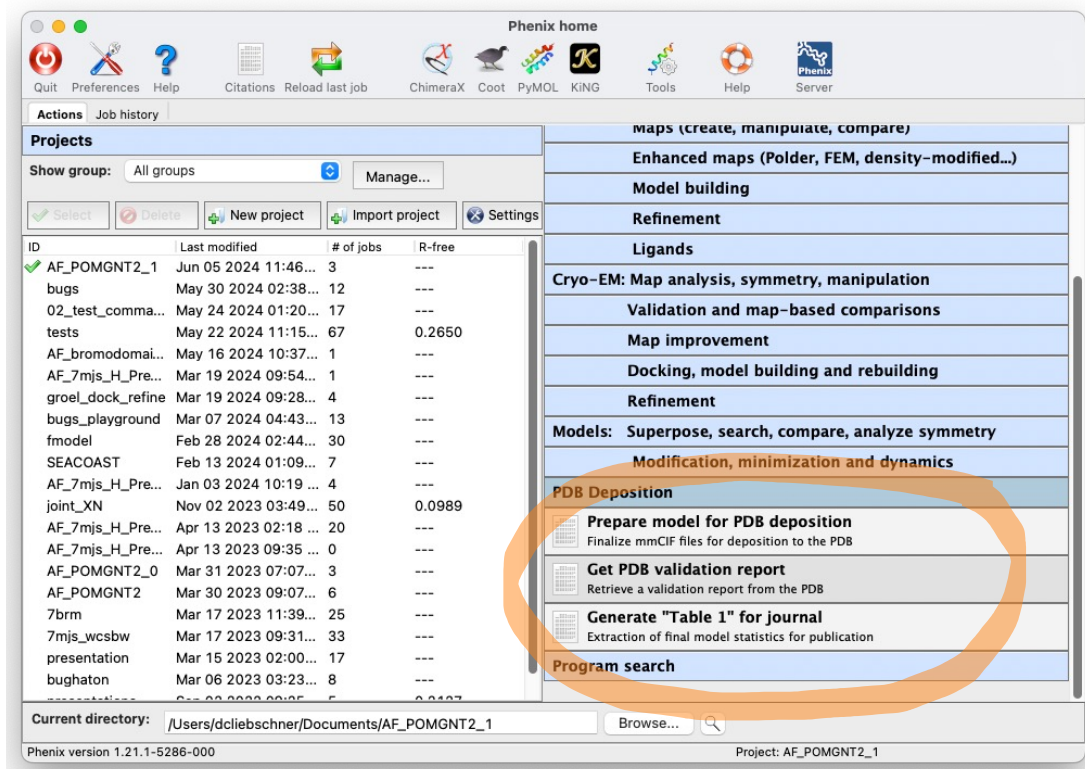
If you provide unmerged data, the table will include merging statistics.

Table 1. Data collection and refinement statistics.

	1aba
<b>Wavelength</b>	
<b>Resolution range</b>	37.69 - 1.447 (1.46 - 1.45)
<b>Space group</b>	P 21 21 21
<b>Unit cell</b>	30.2 47.8 61.3 90 90 90
<b>Total reflections</b>	
<b>Unique reflections</b>	15730 (452)
<b>Multiplicity</b>	
<b>Completeness (%)</b>	95.66 (84.80)
<b>Mean I/sigma(I)</b>	
<b>Wilson B-factor</b>	14.51
<b>R-merge</b>	
<b>R-meas</b>	
<b>R-pim</b>	
<b>CC1/2</b>	
<b>Reflections used in refinement</b>	15730 (452)
<b>Reflections used for R-free</b>	0 (0)
<b>R-work</b>	0.2075 (0.2842)

# PDB deposition / publication

Table 1 for publication



## Data collection

Space group	P3 <sub>1</sub> 2 1
Unit cell dimensions	
a, b, c (Å)	77.03, 77.03, 108.17
α, β, γ (°)	90.00, 90.00, 120.00
Wavelength	0.9537
Resolution (Å)	1.8
R <sub>merge</sub> (%)	6.0 (43.3)
I/σI	14.7 (2.2)
Completeness (%)	93.8 (65.1)
Redundancy	4.1 (1.8)
CC 1/2	0.997 (0.727)

## Refinement

Resolution (Å)	66.71-1.80
No. reflections	31205
R <sub>work</sub> /R <sub>free</sub>	15.15/18.88
No. Atoms	2415
Protein	2168
Water	229
Ligand	18
Wilson B (Å <sup>2</sup> )	15.7
Average refined B-factor (Å <sup>2</sup> )	
Protein only (Å <sup>2</sup> )	22.2
Water (Å <sup>2</sup> )	35.0
Ligand (Å <sup>2</sup> )	41.1
r.m.s deviations:	
Bond lengths (Å)	0.018
Bond angles (°)	1.84

## Ramachandran analysis

Favored (%)	98.84
Allowed (%)	1.16
Outliers (%)	0

# PDB deposition

mmCIF format is mandatory for deposition as of 2019



ISSN 2059-7983

## Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB)

**Paul D. Adams,<sup>a,b</sup> Pavel V. Afonine,<sup>a</sup> Kumaran Baskaran,<sup>c</sup> Helen M. Berman,<sup>d</sup> John Berrisford,<sup>e</sup> Gerard Bricogne,<sup>f</sup> David G. Brown,<sup>g</sup> Stephen K. Burley,<sup>d,h,i,\*</sup> Minyu Chen,<sup>j</sup> Zukang Feng,<sup>d</sup> Claus Flensburg,<sup>f</sup> Aleksandras Gutmanas,<sup>e</sup> Jeffrey C. Hoch,<sup>k,\*</sup> Yasuyo Ikegawa,<sup>j</sup> Yumiko Kengaku,<sup>j</sup> Eugene Krissinel,<sup>l</sup> Genji Kurisu,<sup>j,\*</sup> Yuhe Liang,<sup>d</sup> Dorothee Liebschner,<sup>a</sup> Lora Mak,<sup>e</sup> John L. Markley,<sup>c,\*</sup> Nigel W. Moriarty,<sup>a</sup> Garib N. Murshudov,<sup>m</sup> Martin Noble,<sup>n</sup> Ezra Peisach,<sup>d</sup> Irina Persikova,<sup>d</sup> Billy K. Poon,<sup>a</sup> Oleg V. Sobolev,<sup>a</sup> Eldon L. Ulrich,<sup>c</sup> Sameer Velankar,<sup>e,\*</sup> Clemens Vornrhein,<sup>f</sup> John Westbrook,<sup>d</sup> Marcin Wojdyr,<sup>f,l</sup> Masashi Yokochi<sup>j</sup> and Jasmine Y. Young<sup>d</sup>**

Received 21 February 2019  
Accepted 3 April 2019

Edited by R. J. Read, University of Cambridge,  
England



# PDB deposition: mmCIF file

- Contains a lot more information than PDB
- Not intended to be human editable
  - You can read it but it is (much) harder than PDB
- Phenix tools generally produce output in mmCIF format
- Avoid editing by hand
  - Easy to make hard-to-recover mistakes

# CIF file confusion

- CIF is a file format
- CIF file can contain:
  - Ligand information
  - Atomic model
  - Reflection data
  - Any mixture of three above

# PDB deposition: dos and don'ts

- Do not change file content from refinement for any reason:
  - Add/remove atoms (hydrogens, water, remove ANISOU)
  - Edit labels, header information
- Use Comprehensive validation (Phenix GUI) to address all outstanding issues before deposition
- Don't panic if validation statistics reported by Phenix does not match PDB validation report or Coot
  - If that happens and presents a problem – start conversation with PDB staff and involve Phenix developers
  - Different (versions) of geometry libraries
- Once all is deposited and up on the web – check everything: mistakes at PDB end happen