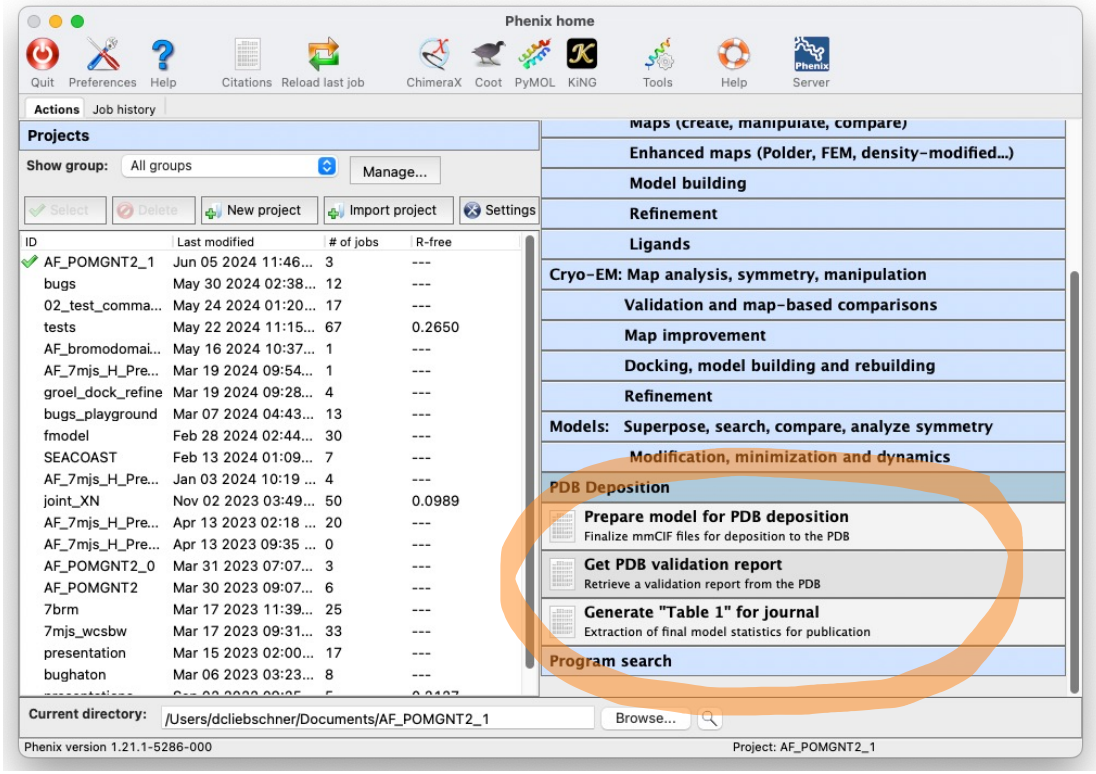
PDB deposition / publication

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



WORLDWIDE PDB
PROTEIN DATA BANK

Preliminary Full wwPDB X-ray Structure Validation Report (i)

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.

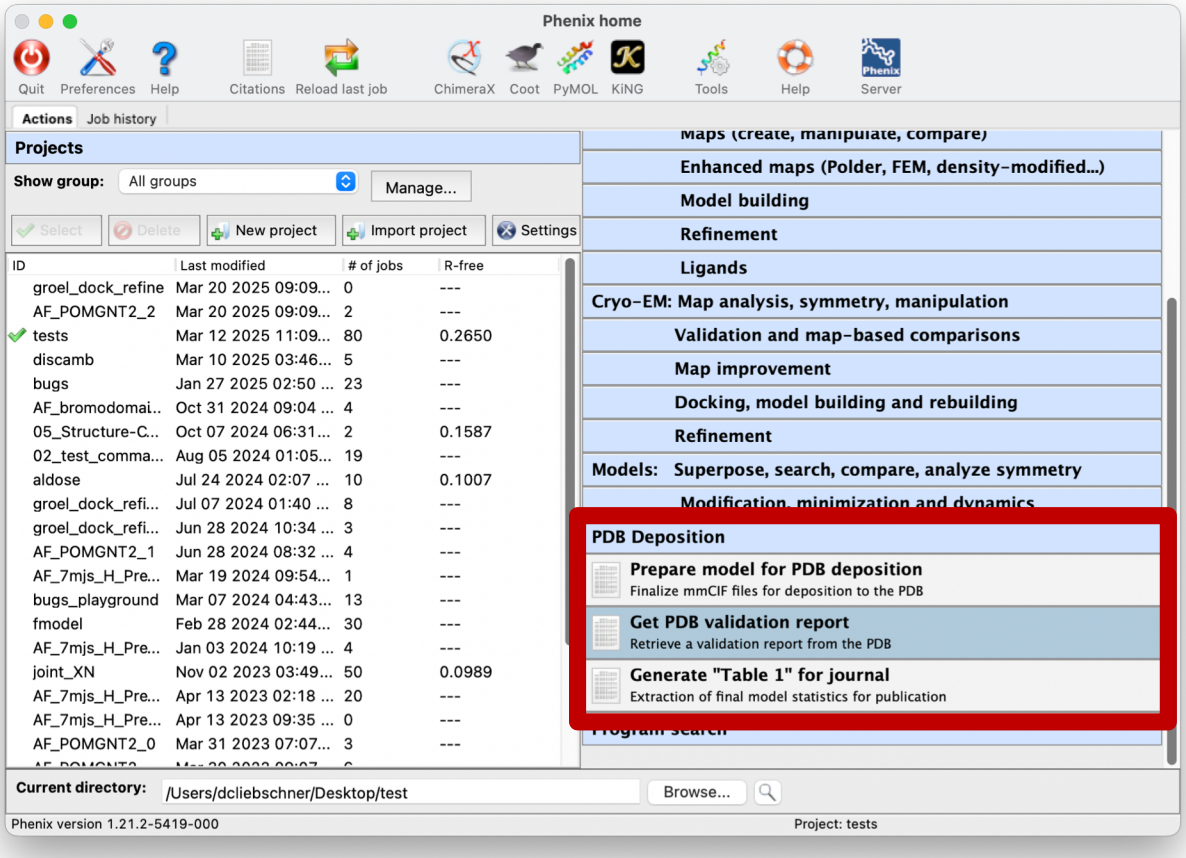
We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

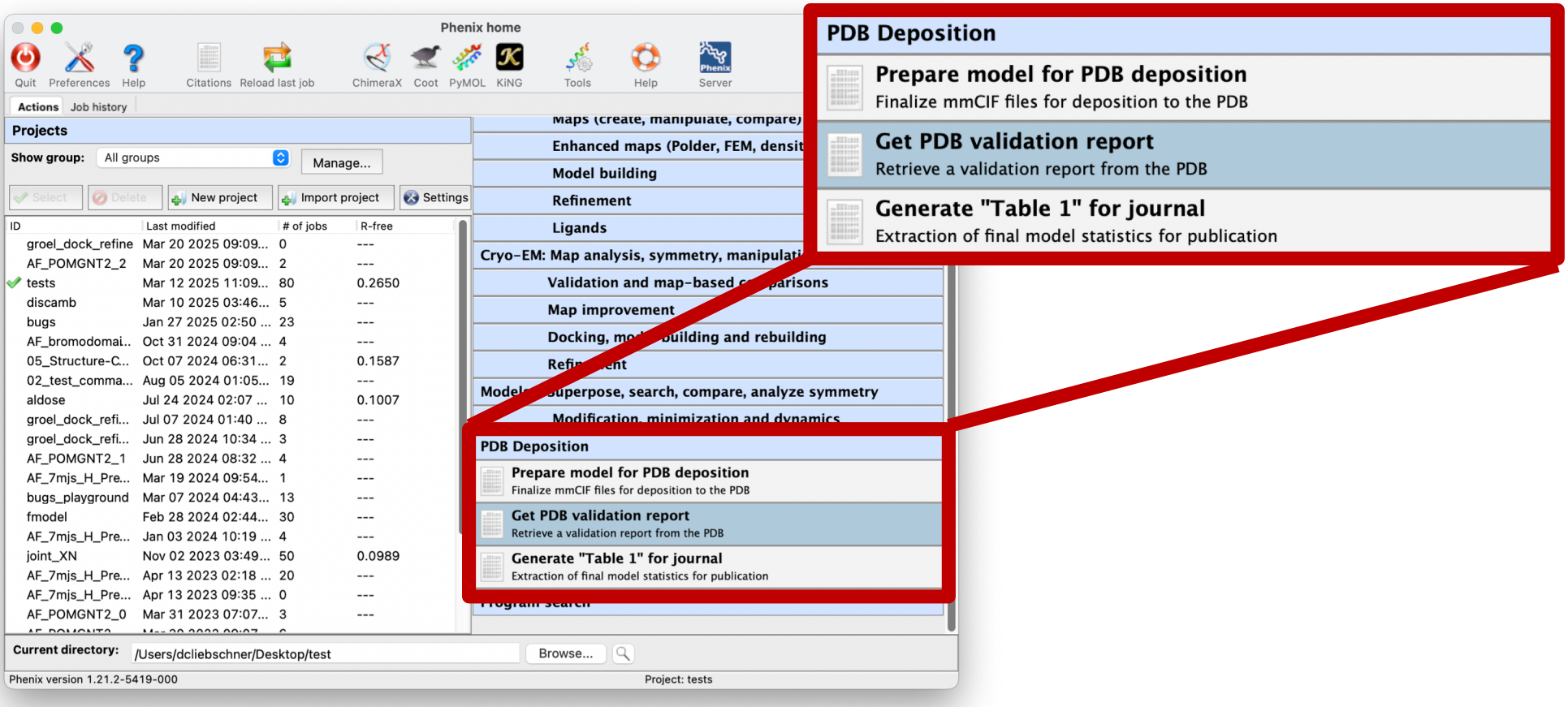
The following versions of software and data (see references (i)) were used in the production of this report:

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)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

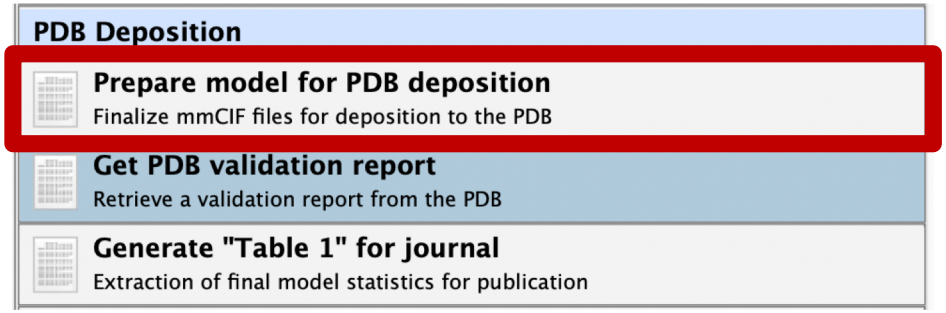
PDB deposition



PDB deposition



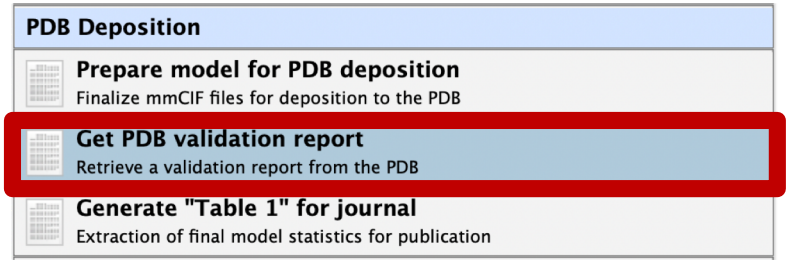
Prepare PDB deposition



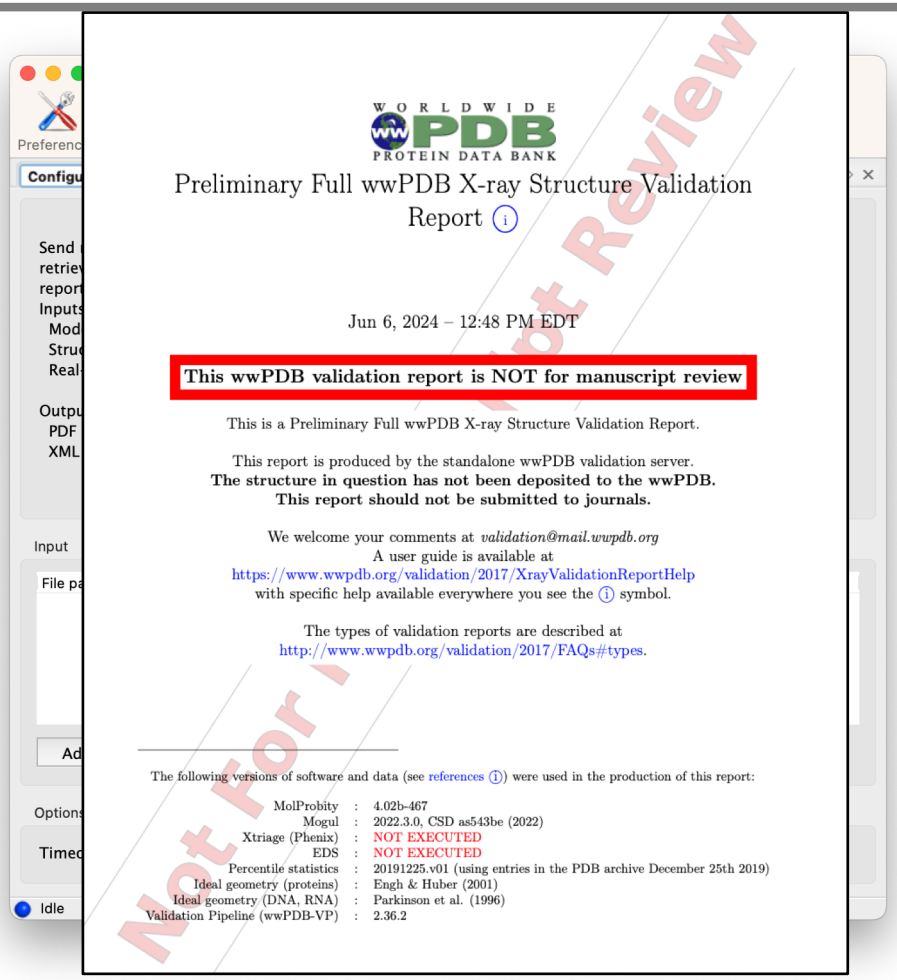
Add sequence information to the mmCIF file.

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

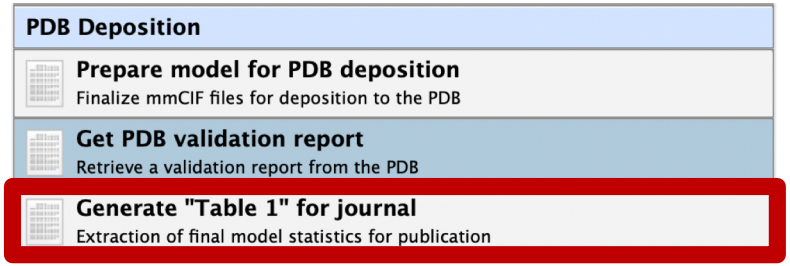
Get PDB validation report



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



Generate Table 1



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

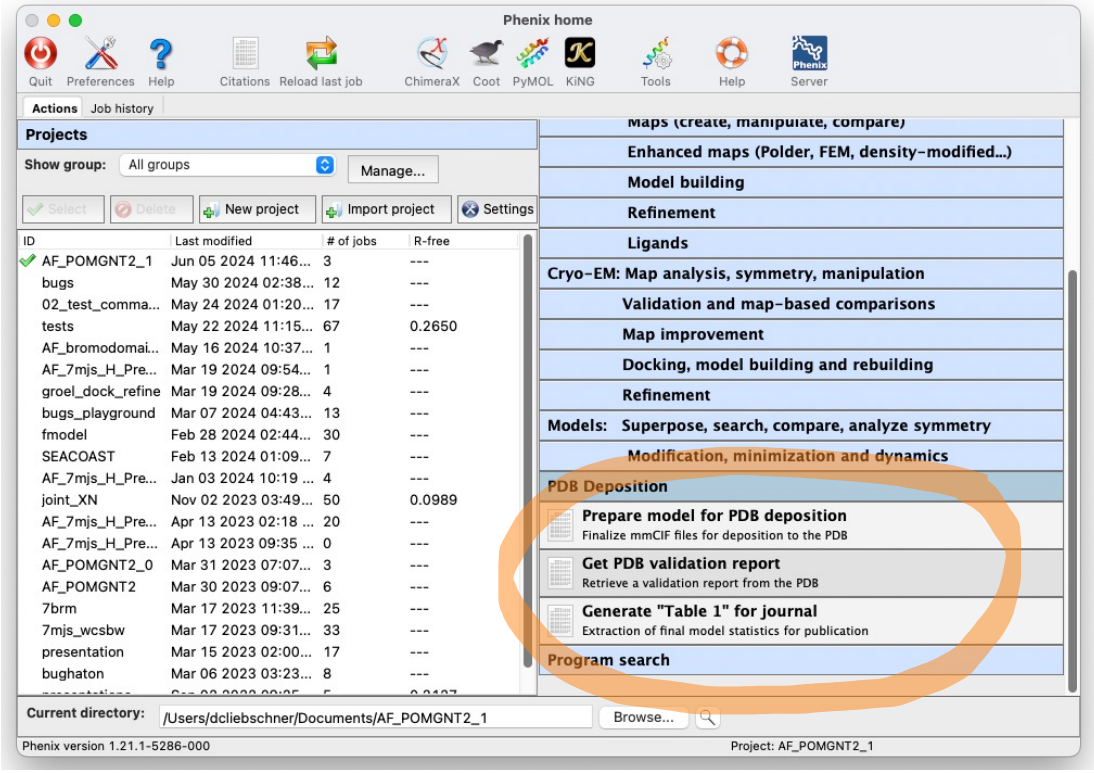
If you provide unmerged data, the table will include merging statistics.

Table 1. Data collection and refinement statistics.

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

PDB deposition / publication

Table 1 for publication



Data collection	
Space group	$P3_1\ 2\ 1$
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_{merge} (%)	6.0 (43.3)
$I/\sigma I$	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_{work}/R_{free}	15.15/18.88
No. Atoms	2415
Protein	2168
Water	229
Ligand	18
Wilson B (Å^2)	15.7
Average refined B-factor (Å^2)	
Protein only (Å^2)	22.2
Water (Å^2)	35.0
Ligand (Å^2)	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

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

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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