Validation

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Phenix team

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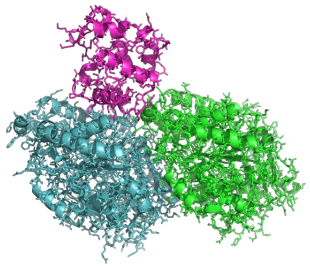
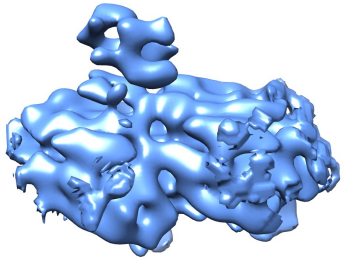
University of Nebraska, 2026

Validation

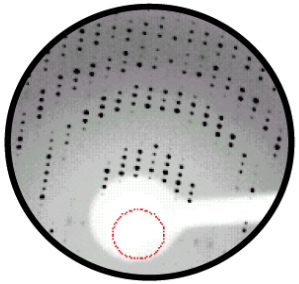
Model



Data



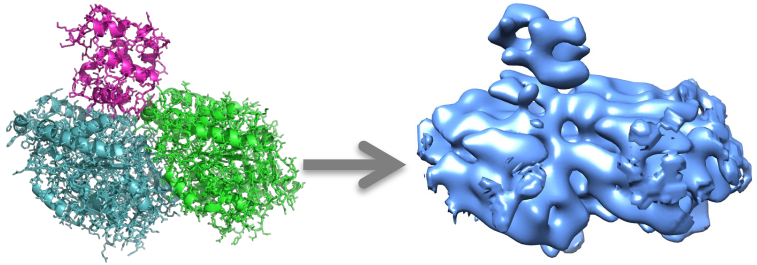
or



Cryo-EM

Diffraction

Model to data fit

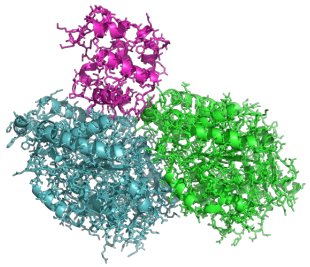


Validation = checking model, data and model-to-data fit are all make sense and obey to prior expectations

Validation : *Crystallography vs Cryo-EM*

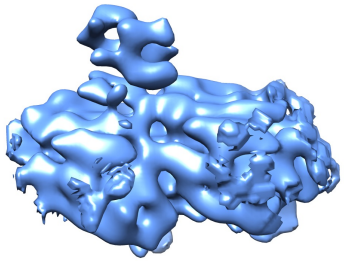
Exact same

Model

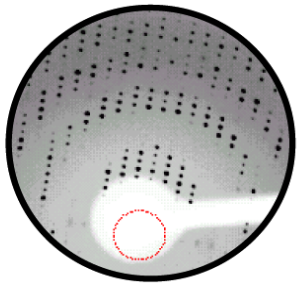


Different

Data



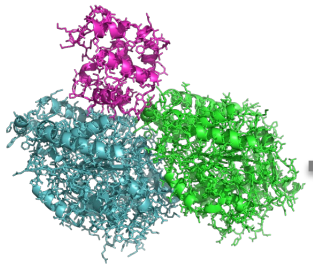
or

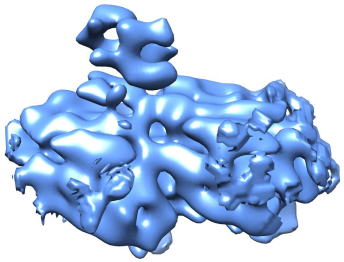


Cryo-EM

Diffraction

Model to data fit

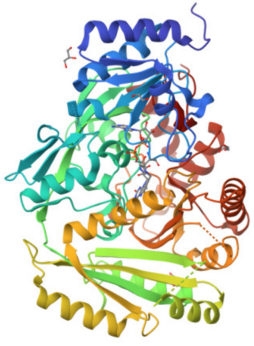




Similar

Validation

Crystallography



Explore in 3D: Structure | Sequence Annotations | Electron Density | Validation Report | Ligand Interaction (FAD)

Global Symmetry: Asymmetric - C1
Global Stoichiometry: Monomer - A1

Find Similar Assemblies

Biological assembly 1 assigned by authors.

Biological Assembly Evidence: gel filtration

8QVT | pdb_00008qvt

Crystal structure of Zea mays cytokinin oxidase/dehydrogenase 5 (ZmCKX5)

PDB DOI: https://doi.org/10.2210/pdb8QVT/pdb

Classification: FLAVOPROTEIN
Organism(s): Zea mays
Expression System: Escherichia coli
Mutation(s): No

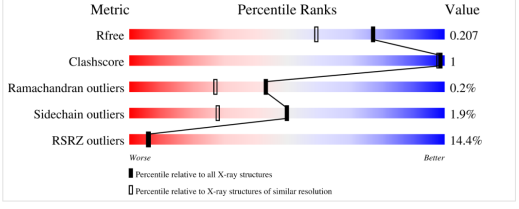
Deposited: 2023-10-18 **Released:** 2024-10-30
Deposition Author(s): Kopecny, D., Briozzo, P.
Funding Organization(s): Agence Nationale de la Recherche (ANR), Czech Science Foundation

Experimental Data Snapshot

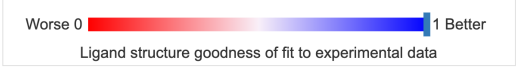
Method: X-RAY DIFFRACTION
Resolution: 1.65 Å
R-Value Free:
0.201 (Depositor), 0.207 (DCC)
R-Value Work:
0.181 (Depositor), 0.187 (DCC)
R-Value Observed:
0.182 (Depositor)

Starting Model: experimental
View more details

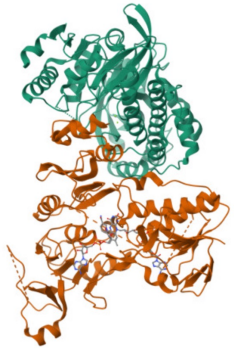
wwPDB Validation 3D Report | Full Report



Ligand Structure Quality Assessment



Cryo-EM



Explore in 3D: Structure | Sequence Annotations | Electron Density | Validation Report | Ligand Interaction (FDA)

Global Symmetry: Asymmetric - C1
Global Stoichiometry: Hetero 2-mer - A1B1

Find Similar Assemblies

Biological assembly 1 assigned by authors and generated by

8ORJ | pdb_00008orj

Cryo-EM structure of human tRNA ligase RTCB in complex with human PYROXD1.

PDB DOI: https://doi.org/10.2210/pdb8ORJ/pdb **EM Map EMD-17127:** EMDB EMDataResource

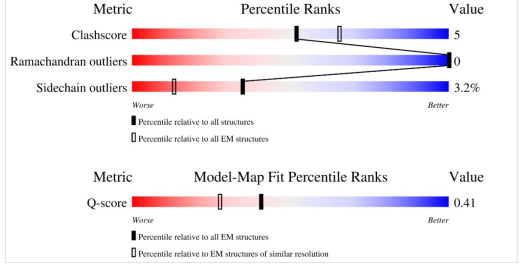
Classification: LIGASE
Organism(s): Homo sapiens
Expression System: Spodoptera frugiperda, Escherichia coli
Mutation(s): No

Deposited: 2023-04-14 **Released:** 2024-10-30
Deposition Author(s): Loeff, L., Kroupova, A., Asanovic, I., Boneberg, F., Pfleiderer, M.M., Ferdigg, A., Ackle, F., Martinez, J., Jinek, M.
Funding Organization(s): Swiss National Science Foundation

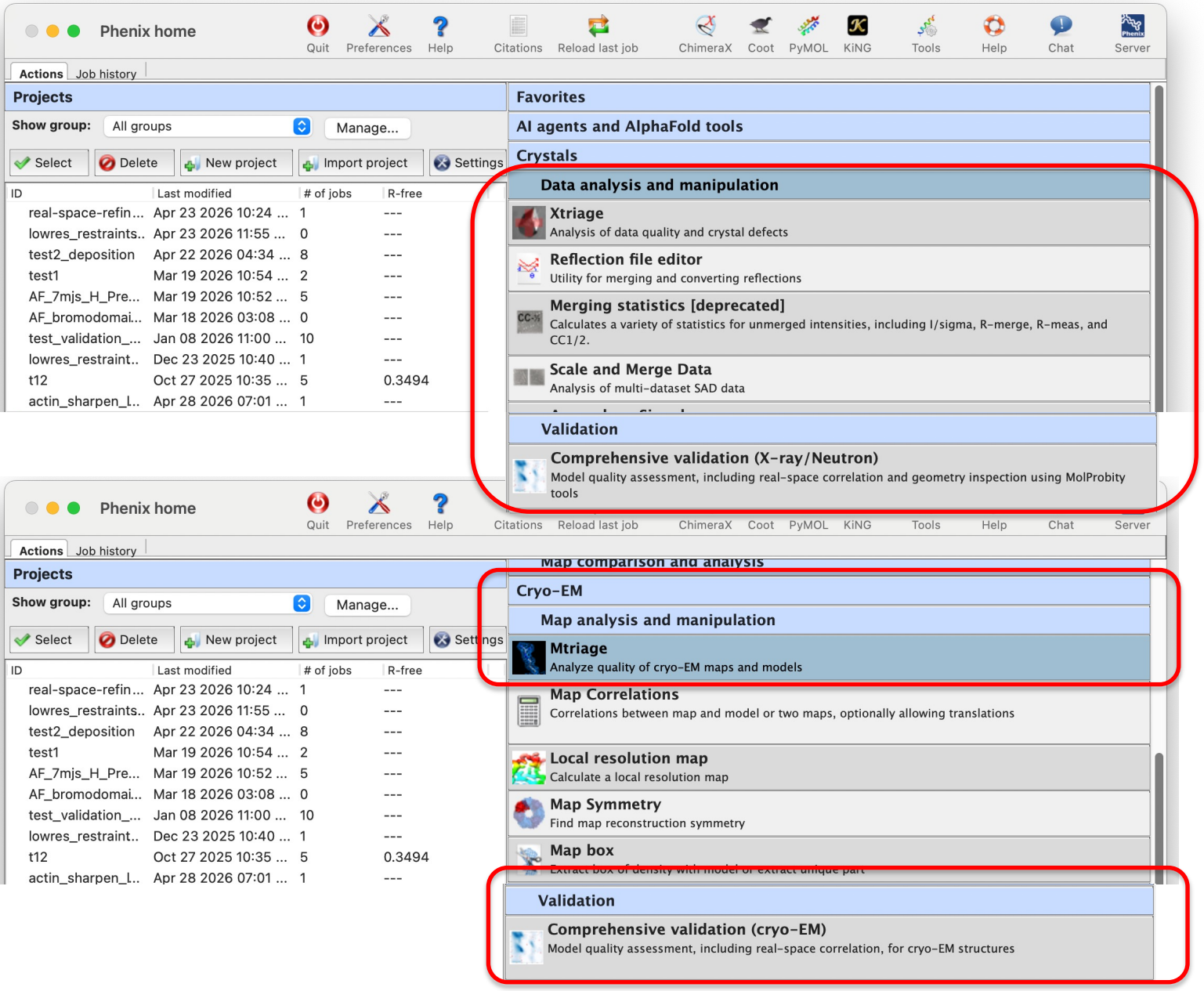
Experimental Data Snapshot

Method: ELECTRON MICROSCOPY
Resolution: 3.30 Å
Aggregation State: PARTICLE
Reconstruction Method: SINGLE PARTICLE

wwPDB Validation 3D Report | Full Report



Validation tools in Phenix



Validation: why to do?

- **Problems detected early can save a lot of time later**
- **Subjectivity**
  - Manual map interpretation: experience, skills, pressure
  - Model parameterization, target weights, starting points
  - Lack of data = multiple possibilities for interpretation
- **Human program the software**
  - Programs may contain bugs
- **Post-refinement pre-deposition manipulations**
  - Hand editing files: removing waters, hydrogens, ANISOU
- **Misusing quality metrics**
  - Choose single water or decide about twinning using R-factor
- **Fraud or honest mistakes**

Validation: why to do?

- Helps to
  - save time
  - produce better models
  - set correct expectations
- Minimize fraud or honest mistakes

Validation: why to do?

- **Quality filters:**
  - You
  - Software you use
  - Your boss
  - Reviewers (of your paper)
  - PDB deposition (software and people)
  - Community

- **Unnoticed (intentionally or not) problems**
  - Likely discovered anyway, sooner or later

Validation: why to do?

Retraction: Cocrystal structure of synaptobrevin-II bound to botulinum neurotoxin type B at 2.0 Å resolution

Michael A Hanson & Raymond C Stevens

Nat. Struct. Biol. 7, 687–692 (2000); retracted 6 July 2009

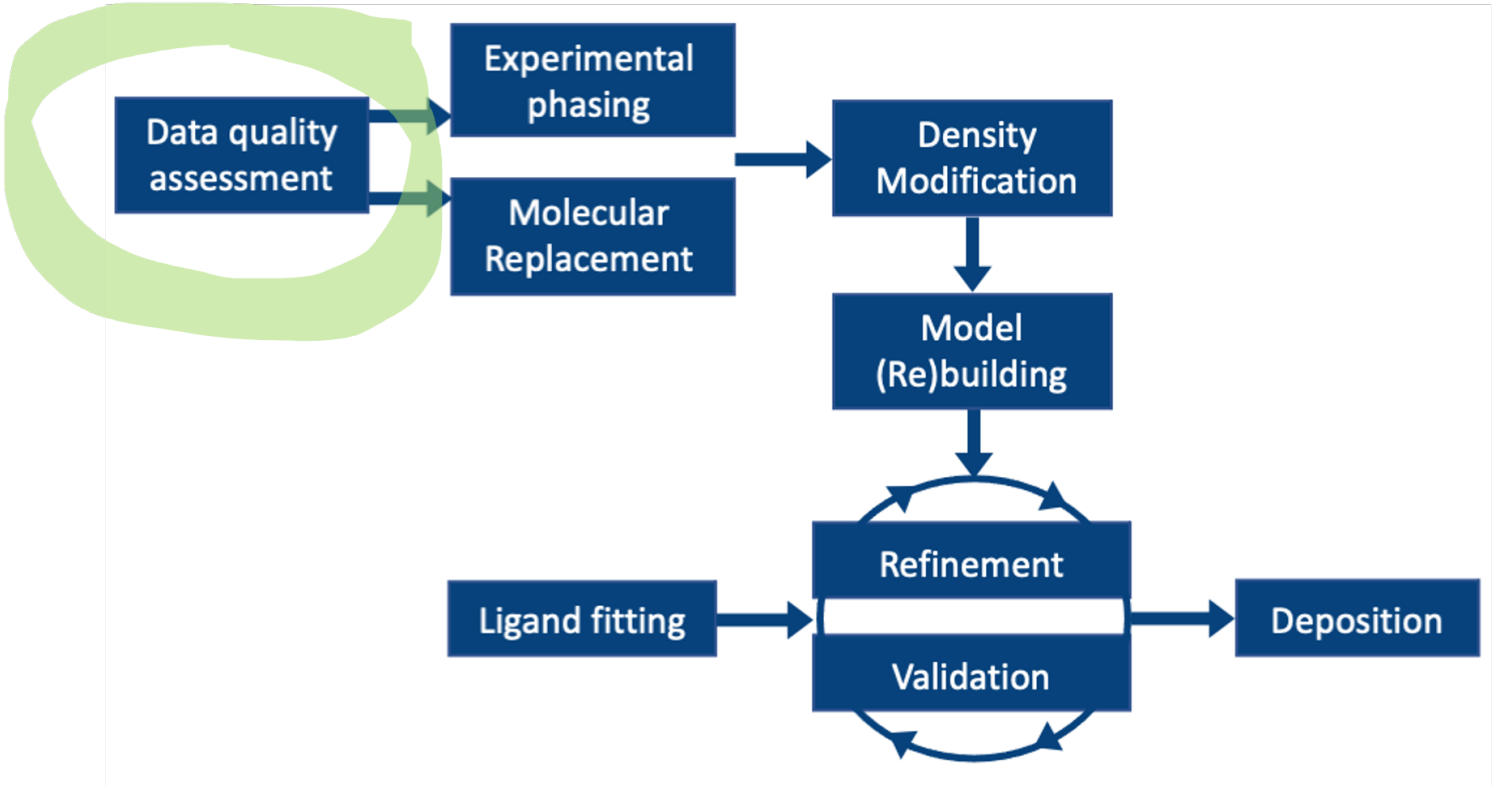
In this paper, we described both the three-dimensional crystal structure of a botulinum toxin catalytic domain separated from the holotoxin (BoNT/B-LC, PDB 1F82) and a structure of the toxin catalytic domain in complex with a peptide (Sb2–BoNT/B-LC, PDB 1F83). The complex was later refined and deposited in the Protein Data Bank (PDB 3G94). The apo structure (PDB 1F82) remains valid. However, because of the lack of clear and continuous electron density for the peptide in the complex structure, the paper is being retracted. We apologize for any confusion this may have caused.

- H.M. Krishna Murthy (University of Alabama) – Protein Fabrication scandal
  - 12 falsified structures and 10 related papers
  - 1BEF, 1CMW, 1DF9, 2QID, 1G40, 1G44, 1L6L, 2OU1, 1RID, 1Y8E, 2A01, and 2HR0
  - Murthy's falsified data ended up affecting 449 papers at that time

Data Validation

Xtriage: all about your Xtal data

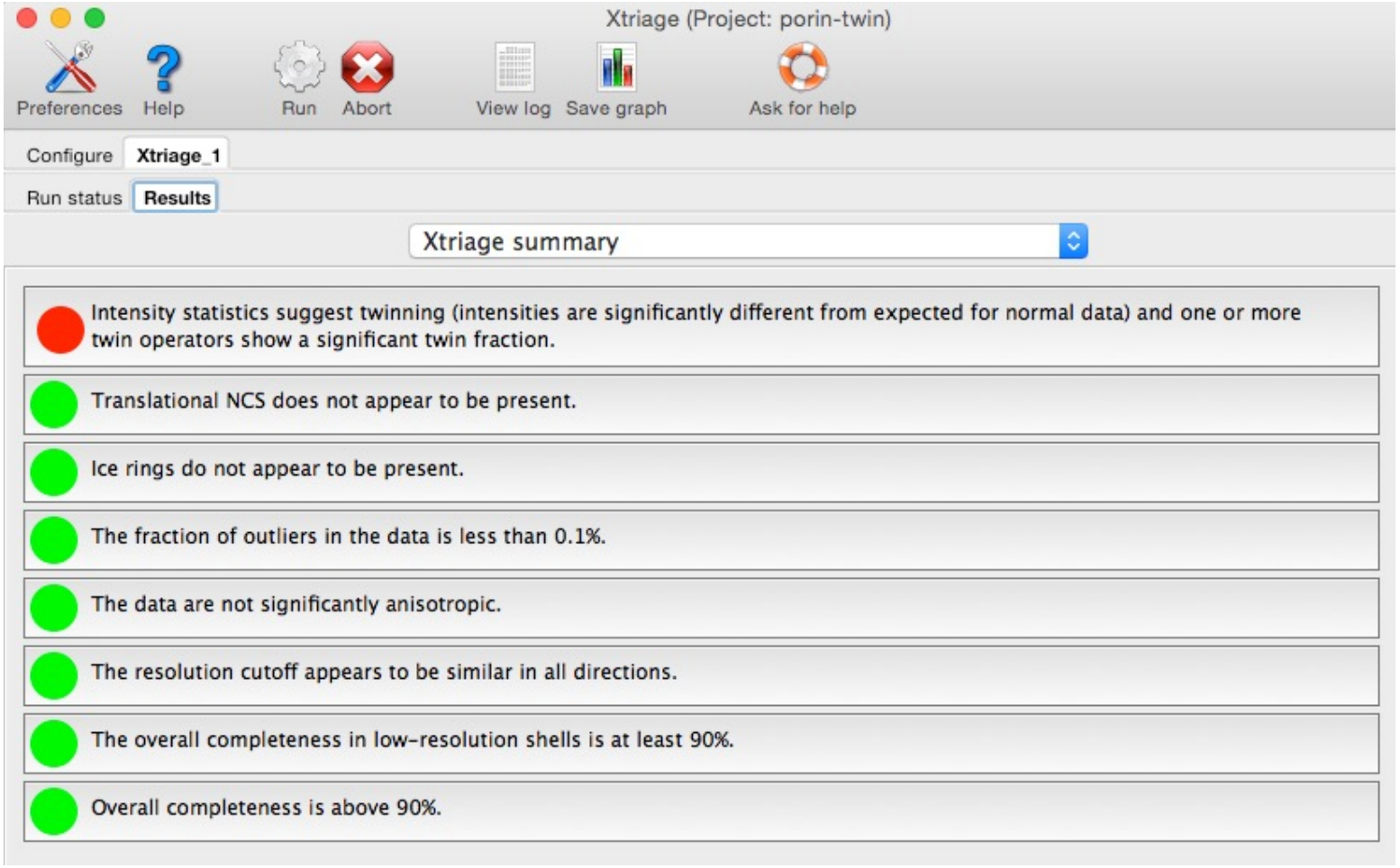
Before doing anything else, you should validate your data!



Possible experimental X-ray data problems

- Twining
- Translational NCS
- Wrong crystal
- Wrong space group
- Ice rings
- Data completeness
- Data anisotropy
- Resolution (overall, effective)
- Anomalous signal
- …

Xtriage

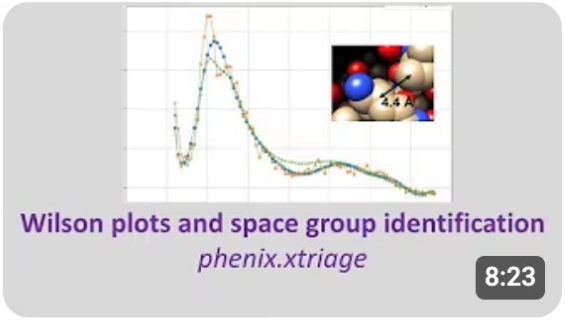


Xtriage performs diagnostics for pathologies and data properties

Several 5 minute long tutorials on YouTube

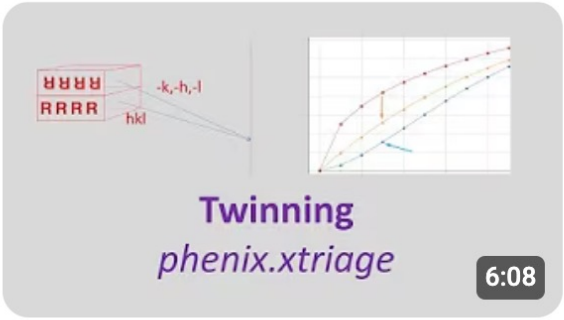
Xtriage

Several 5 minute long tutorials on ”Phenix tutorials” channel on YouTube



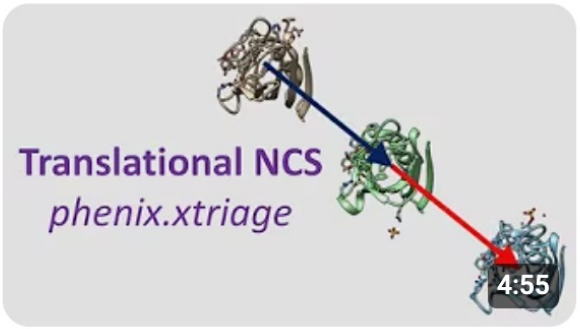
Advanced Tutorial phenix.xtriage - Space Group …

2.8K views · 8 years ago



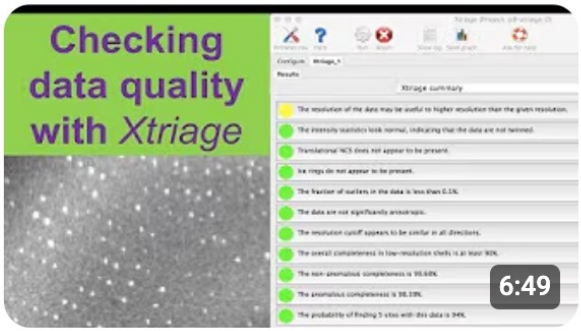
Advanced Tutorial phenix.xtriage - Checking for …

2.3K views · 8 years ago



Advanced Tutorial phenix.xtriage - translational …

4K views · 8 years ago

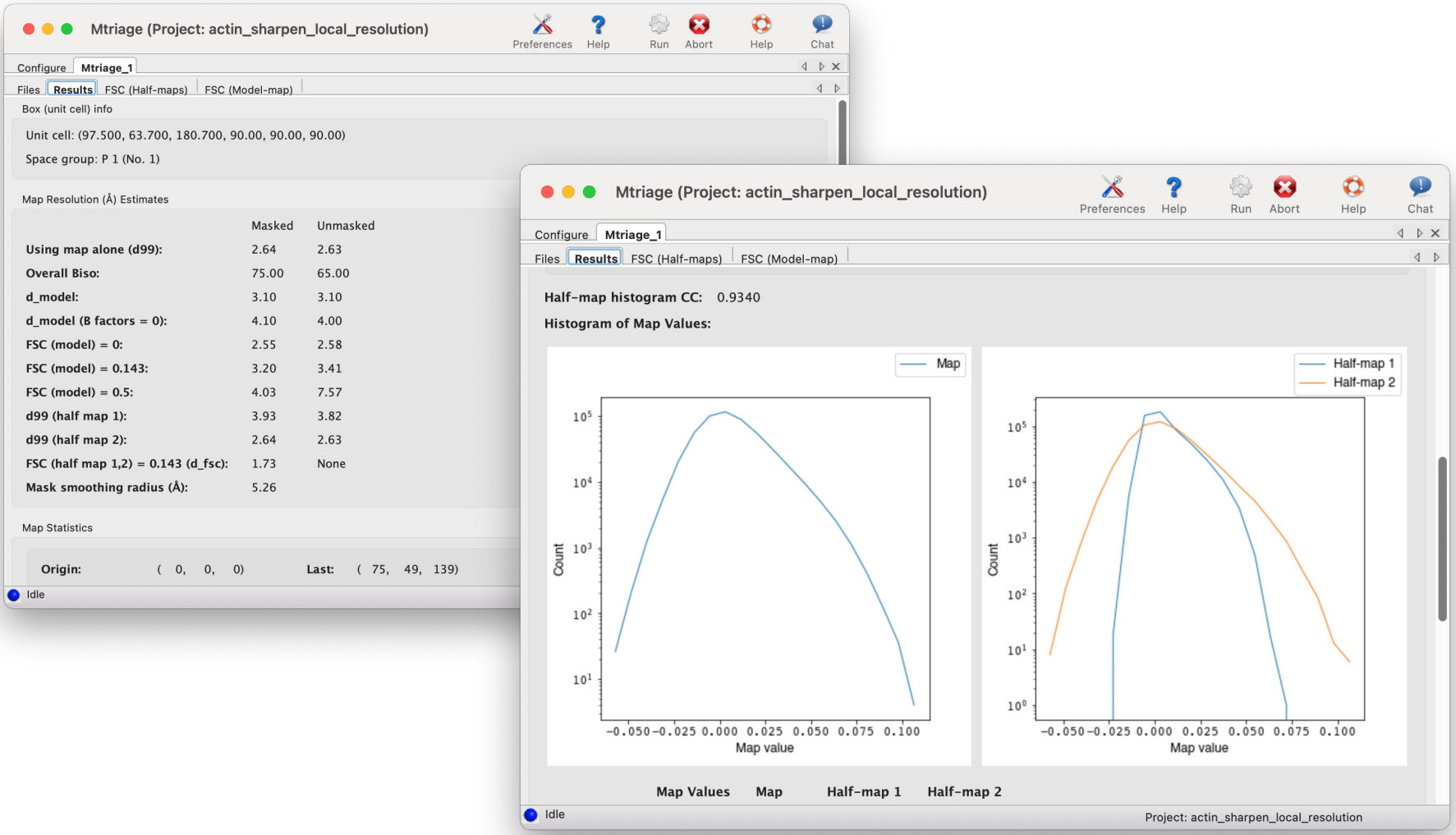


Checking data quality with phenix.xtriage

3.7K views · 8 years ago

Mtriage

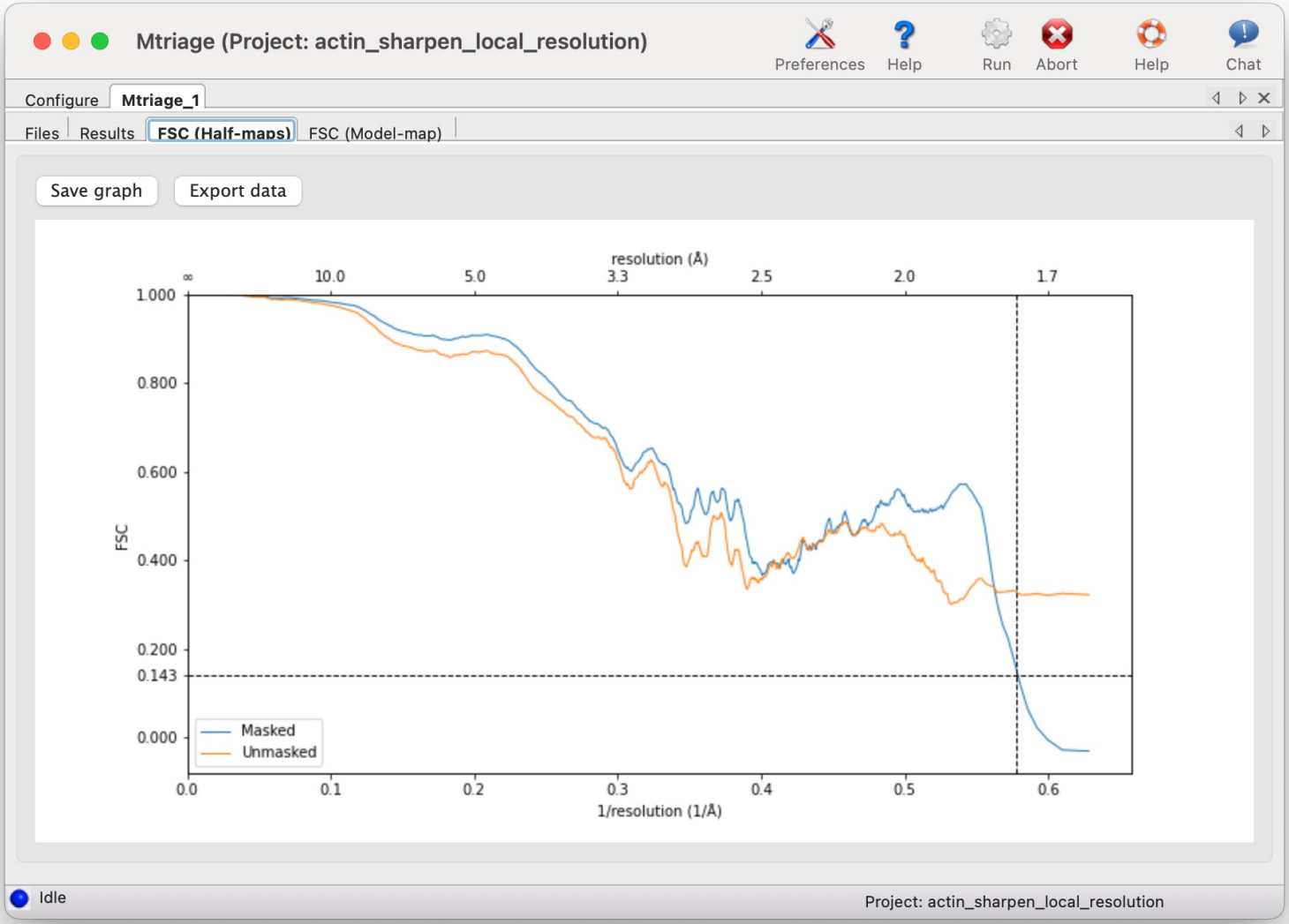
Calculates resolutions estimates and map histograms



Afonine et al. (2018). *Acta Cryst*. D**74**, 814-840

Mtriage

Calculates FSC curves



Resolution estimates

Metric	Objects used	Purpose
d_FSC	Half-maps	Highest resolution at which the experimental data are confident
d99	Map	Resolution cutoff beyond which Fourier coefficients are negligibly small
d_model	Map and model	Resolution cutoff at which the model map is the most similar to the target map
d_FSC model	Map and model	Resolution cutoff up to which the model and map Fourier coefficients are similar

Mtriage

Map Resolution (Å) Estimates

	Masked	Unmasked
Using map alone (d99):	2.64	2.63
Overall Biso:	75.00	65.00
d_model:	3.10	3.10
d_model (B factors = 0):	4.10	4.00
FSC (model) = 0:	2.55	2.58
FSC (model) = 0.143:	3.20	3.41
FSC (model) = 0.5:	4.03	7.57
d99 (half map 1):	3.93	3.82
d99 (half map 2):	2.64	2.63
FSC (half map 1,2) = 0.143 (d_fsc):	1.73	None
Mask smoothing radius (Å):	5.26	

Validation after Real-space refine

Resolution Estimates (Å)	Masked	Unmasked
d FSC (half maps; 0.143)	---	---
d 99 (full/half1/half2)	3.7/---/---	3.6/---/---
d model	3.7	3.7
d FSC model (0/0.143/0.5)	3.4/3.5/3.8	3.4/3.6/3.9
Map min/max/mean	-0.42/0.80/0.02	

Resolution estimates

Table 2 from Afonine et al. (2018). *Acta Cryst*. D**74**, 814-840

Metric	Objects used	Purpose	Values	Meaning, possible actions
d_FSC	Half-maps	Highest resolution at which the experimental data are confident	The higher the better	Resolution determined using half-maps method
d99	Map	Resolution cutoff beyond which Fourier coefficients are negligibly small	d99 ≥ d_FSC	Expected values
			d99 < d_FSC	Verify d_FSC; omit coefficients with d99 ≤ d < d_FSC
			d99 >> d_FSC	Sharpen the map
d_model	Map and model	Resolution cutoff at which the model map is the most similar to the target map	d_model ≥ d_FSC	Expected values
			d_model < d_FSC	Verify d_FSC; check ADP (too large?); validate map details
			d_model >> d_FSC	Sharpen the map
			d_model << d99	Check ADP (too large?)
			d_model >> d99	Check ADP (too small?); check the model
d_FSC_model	Map and model	Resolution cutoff up to which the model and map Fourier coefficients are similar	d_FSC_model ≥ d_FSC	Expected values
			d_FSC_model < d_FSC	Verify d_FSC; omit coefficients with d_FSC_model ≤ d < d_FSC
			d_FSC_model ≥ d_FSC	Sharpen the map
			d_FSC_model >> d_model	Omit coefficients with d_model ≤ d < d_FSC_model
			d_FSC_model << d_model	Sharpen the map

Model geometry validation

Bond Geometry

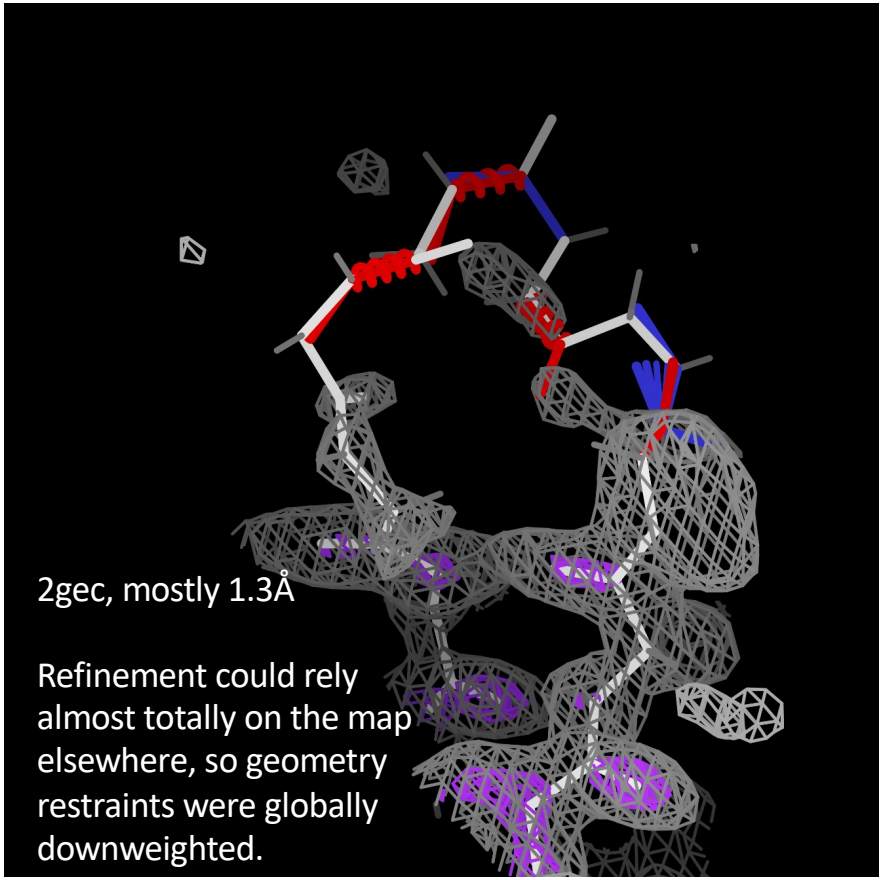
- Measure bond lengths and angles
- Check against a library of expected values
- >4σ deviation from expected = outlier

- Standard reference library has 1 value per bond or angle
- Derived from Engh and Huber
  - https://doi.org/10.1107/S0108767391001071

- Conformation-Dependent Library (CDL) has values that depend on local Ramachandran conformation
- Phenix default
- Derived from Karplus et al.
  - https://doi.org/10.1107/S2059798315022408

molprobity.mp_validate_bonds

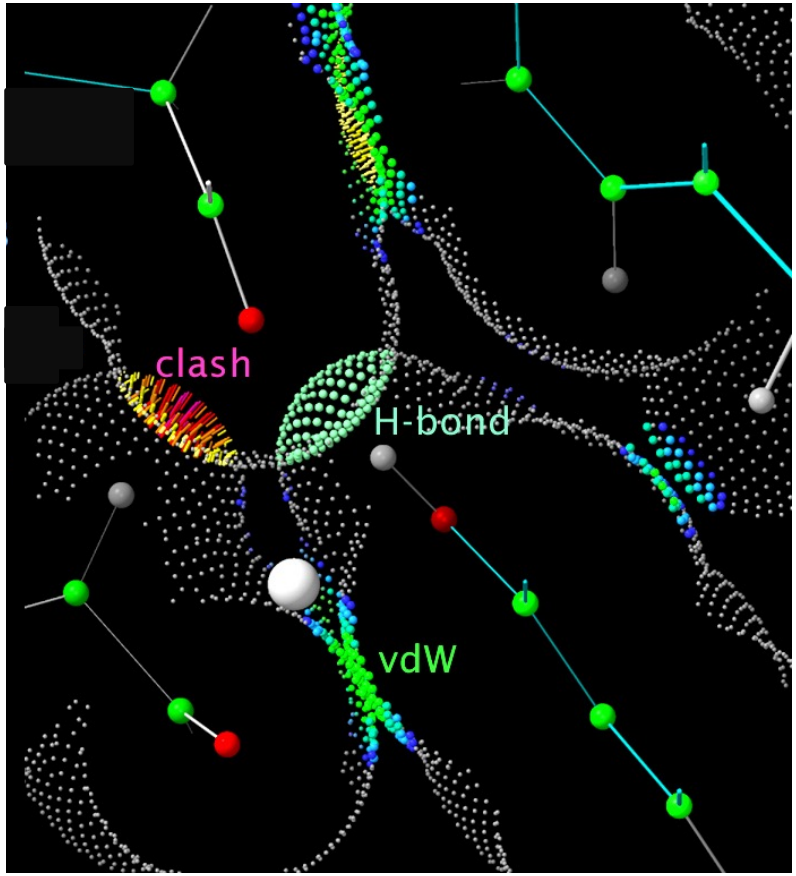
Bond Geometry: Probable causes



Localized

- Localized geometry outliers result from conformational strain and/or missing density
- Fix the source of strain
- Manually apply more restraints to low-data regions
- Leave it unmodeled if a good solution is impossible

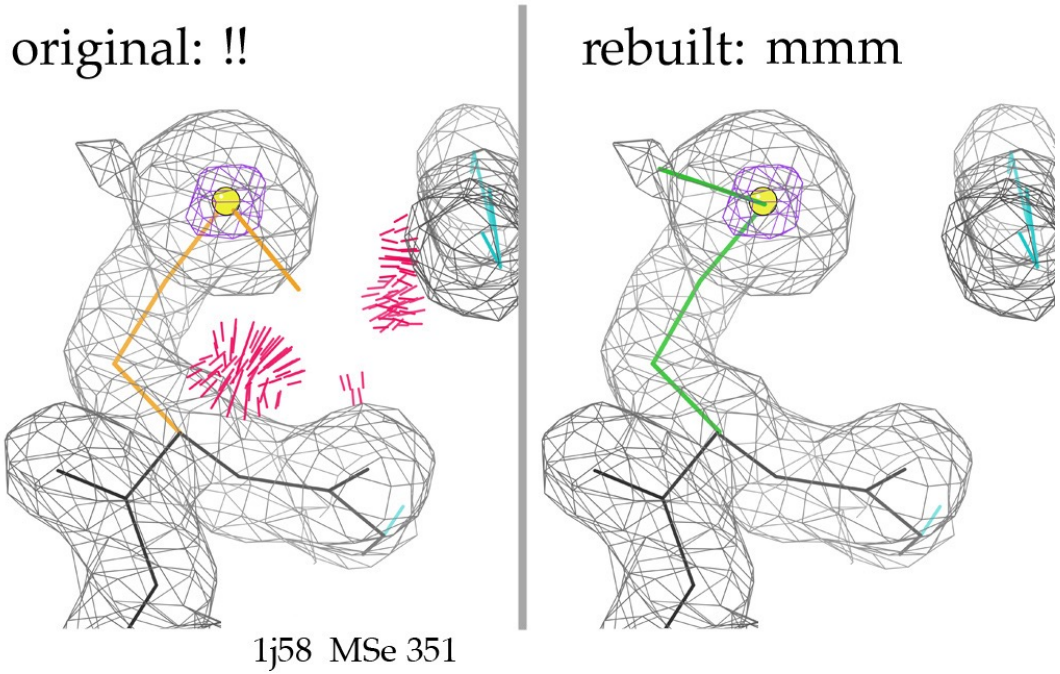
All-Atom Contacts and Clashes



- Roll a 0.25Å radius “Probe” sphere over the van der Waals surface of each atom
- Mark where the probe touches or overlaps with another van der Waals surface
- Note that hydrogen atom surfaces can shield heavy atom surfaces

molprobity.clashscore

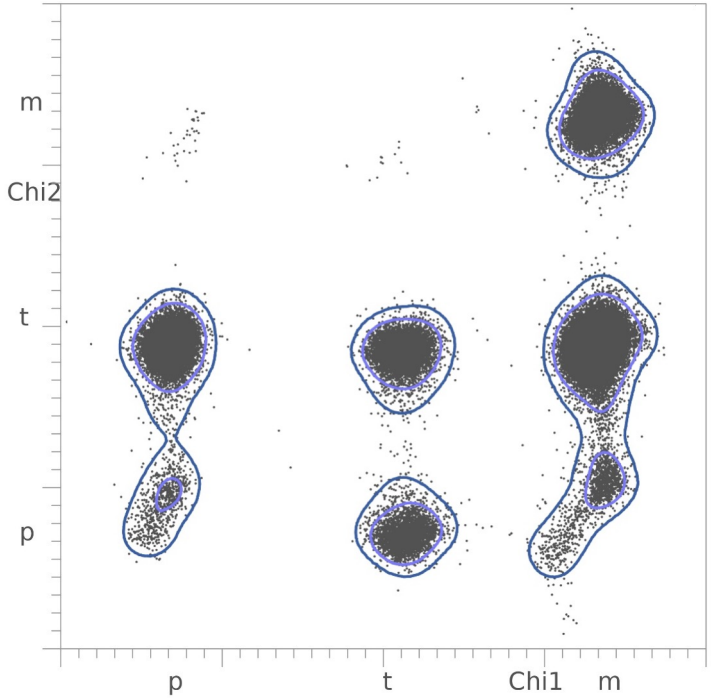
All-Atom Contacts and Clashes: Probable causes



Other outliers

- Clashes usually occur alongside other outliers
- Emphasize modeling errors
  - *Real* rare features are less likely to have clashes
- Can imply direction for fixups

Sidechain Rotamers

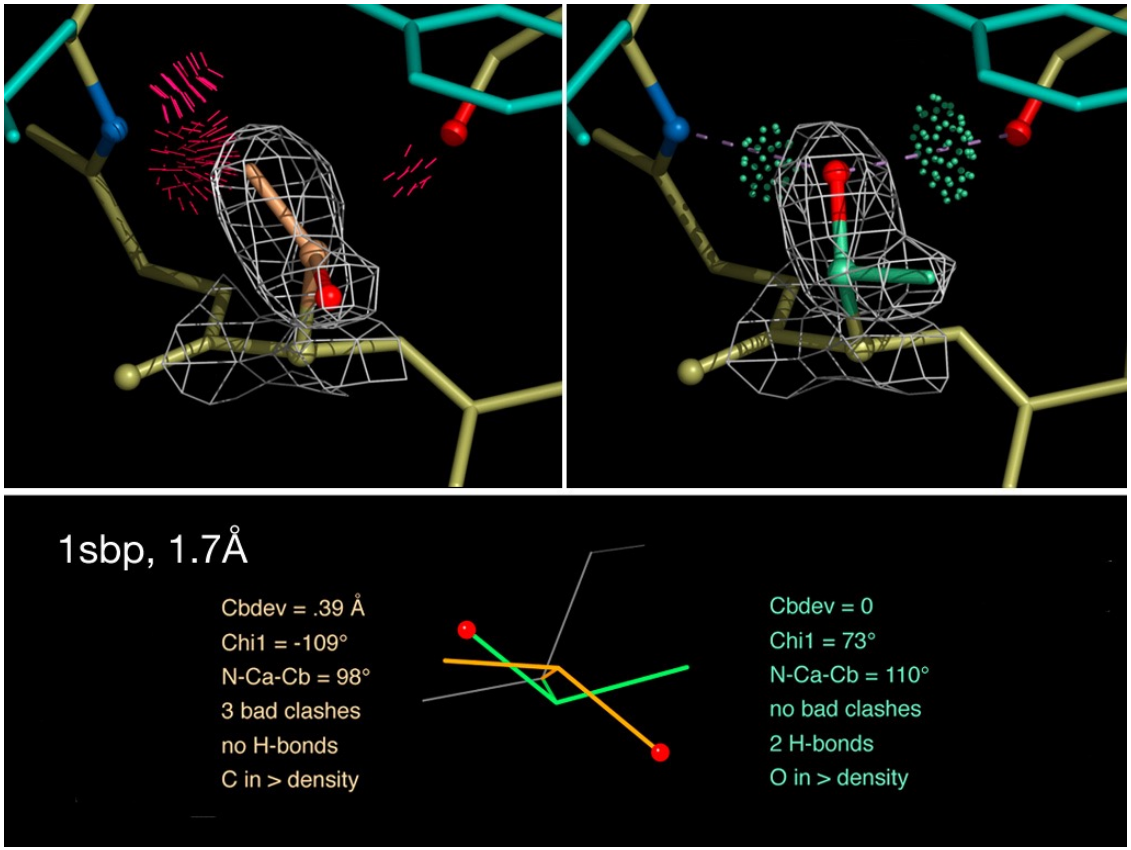


Rotamer distribution for
Isoleucine in χ1/ χ2 space

- Sidechain conformations are described by a series of χ (Chi) torsions
- Rotamers are statistically expected combinations of χ values
- For tetrahedral atom centers, this means staggered
  - p +60°
  - t 180°
  - m -60°
- For planar atom centers, rotamers are much more continuous
  - Rotamers are named with a central value
  - e.g m90 or p-80 for Histidine
- Updated in 2016:
  - Favored (98% of data) Allowed (99.7% of data)

molprobity.rotalyze

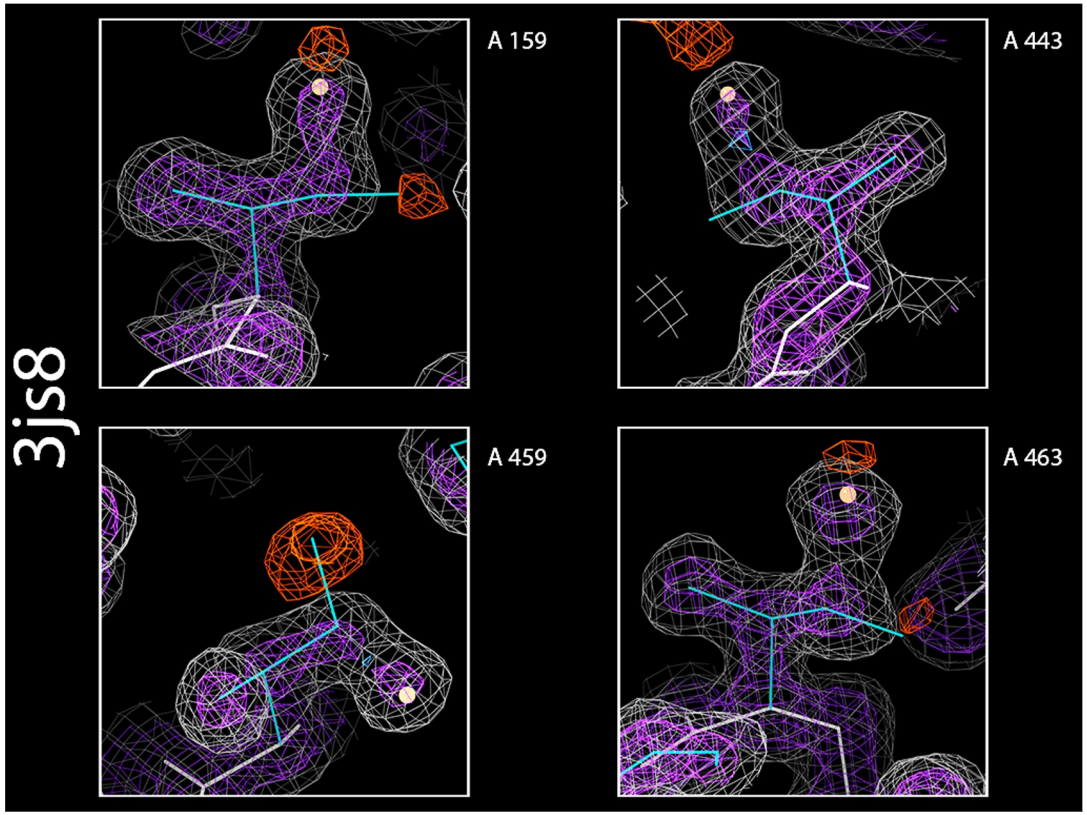
Sidechain Rotamers: Probable causes



<u>Backwards Valine, Leucine, Threonine</u>

- May find terminal atoms fit into density at the expense of the branch atom
- Simple to fix with a flip (then re-refinement)

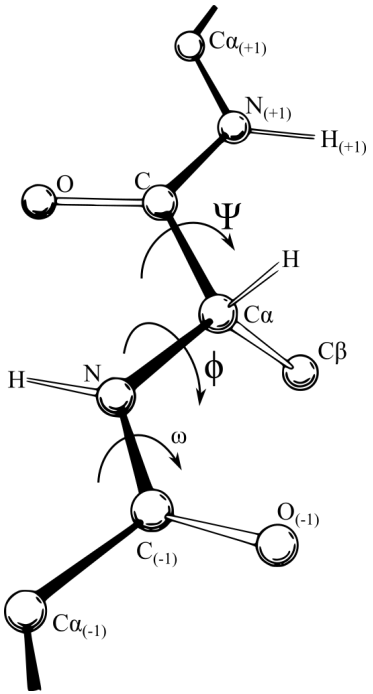
Sidechain Rotamers: Probable causes



Water problems

- Modeled water may co-opt sidechain density and create a rotamer outlier
- Isoleucine CD1 is especially vulnerable
- Delete water, rebuild sidechain

Ramachandran



- Phi and Psi torsions describe local protein backbone conformation
- Phi **ϕ** = C_{i-1}-N-CA-C
- Psi **ψ** = N-CA-C-N_{i+1}
- Each residue's ϕ/ψ pair is converted into cartesian coordinates and checked against contours of expected behavior

molprobity.ramalyze

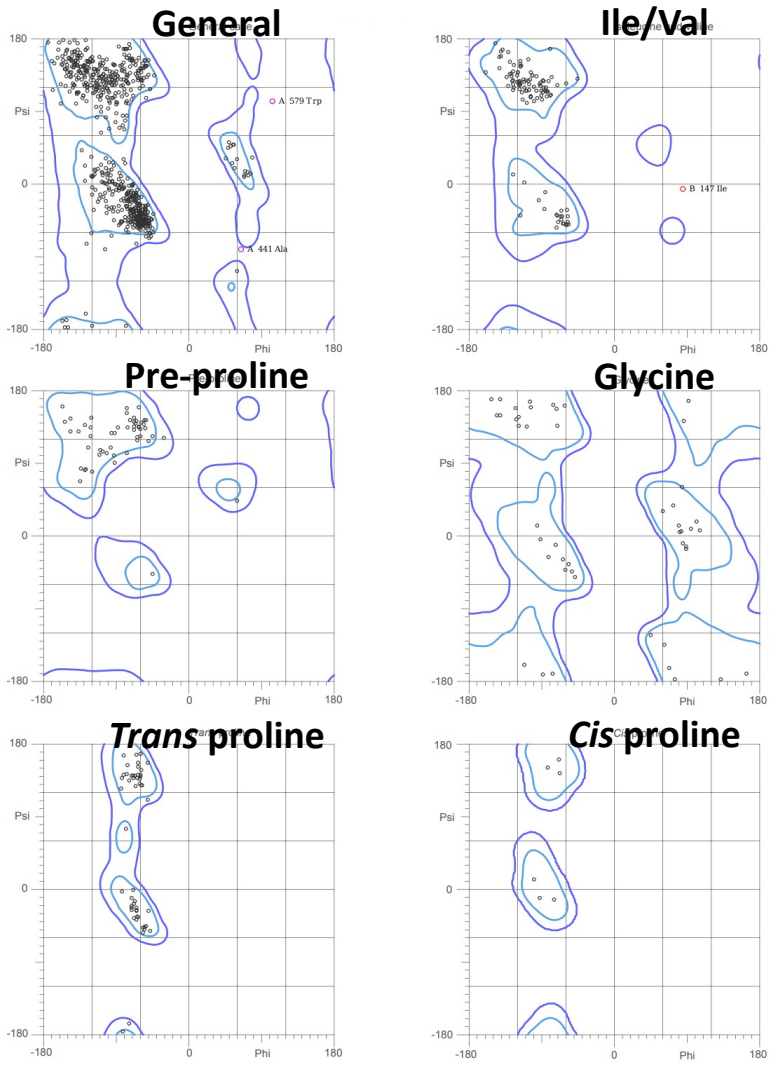
Ramachandran: Visualization

Ramachandran plots shows location of each residue relative to contours of expected behavior

Different residue categories have very different expectations!

Glycine is permissive and symmetrical
Proline is restrictive
Branched C-Beta sidechain (Ile,Val) affect distribution

Favored (98% of data) Allowed (99.5% of data)



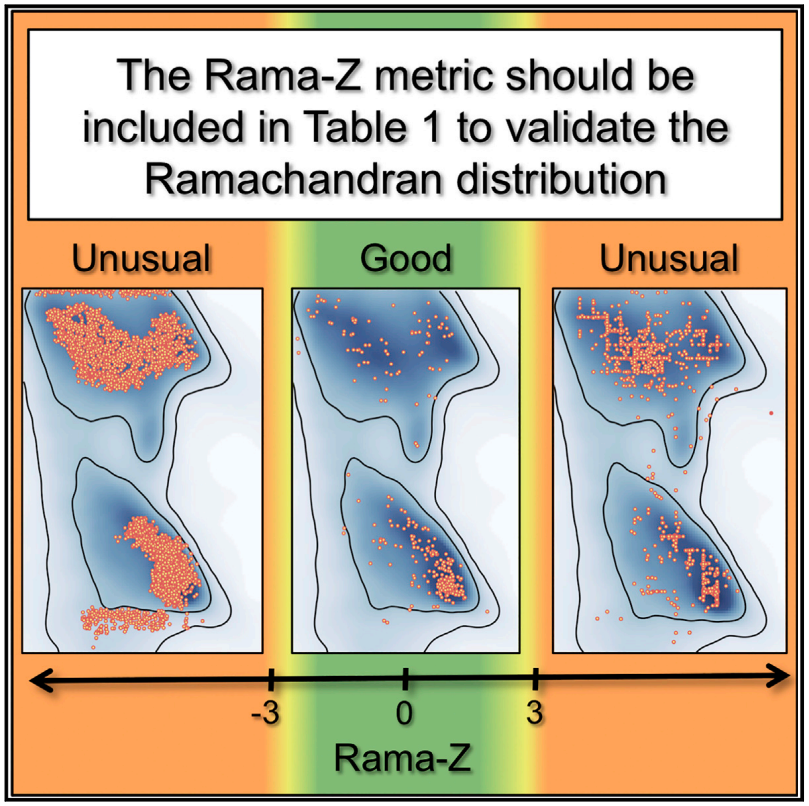
Rama-Z updated study

Resource

Structure

A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry

Graphical Abstract



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Correspondence

osobolev@lbl.gov (O.V.S.), r.joosten@nki.nl (R.P.J.)

In Brief

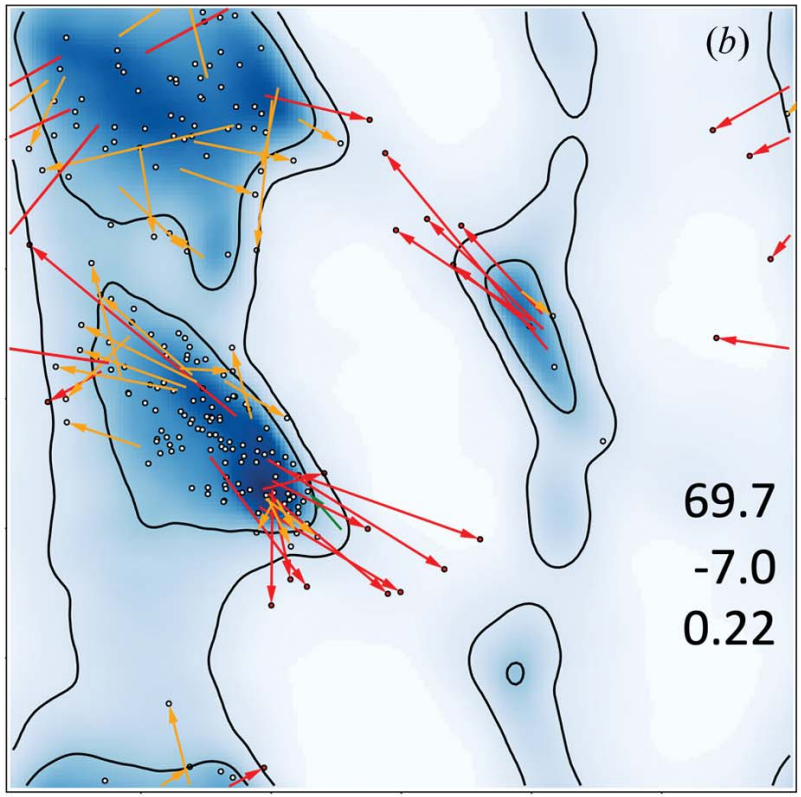
Counting the number of Ramachandran outliers is not sufficient for protein backbone validation. Sobolev et al. revisited the underutilized Ramachandran *Z* score. The authors describe its reimplementation in Phenix and PDB-REDO and showcase its utility. They advocate including it in the validation reports provided by the Protein Data Bank.

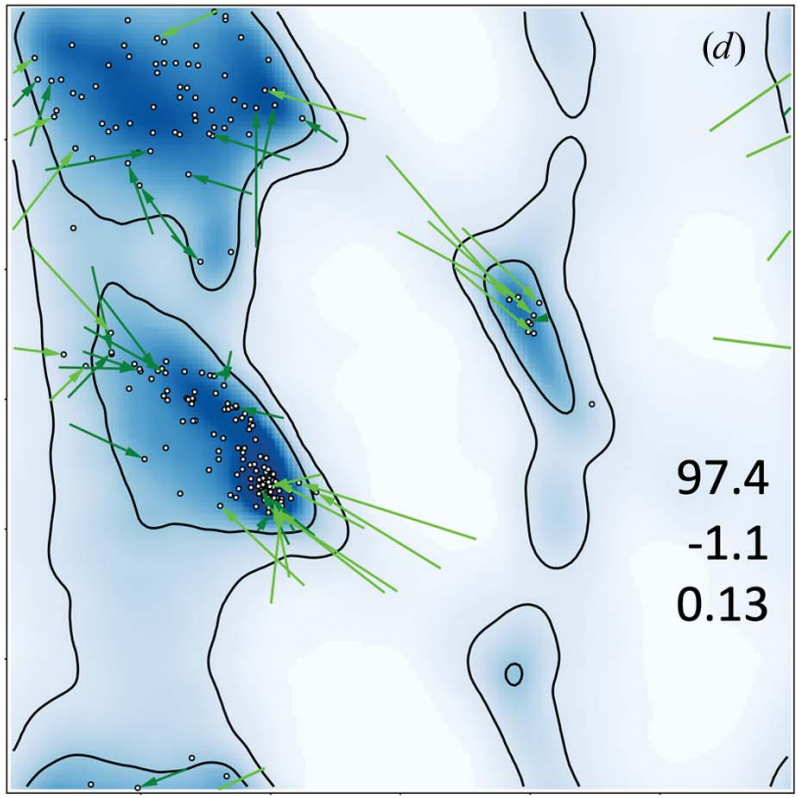
Structure, **28**. 1249-1258.

How to improve Rama-Z

- Analyze the refinement strategy and restraints applied.
- Don’t abuse restraints to get rid of Ramachandran outliers in poor starting model.
- Careful manual model rebuilding and refining.
- Analyze separate Rama-Z scores for helices, sheets and loops. If they vary greatly that may hint on particular class of residues worth checking.

Comparama: `phenix.comparama`

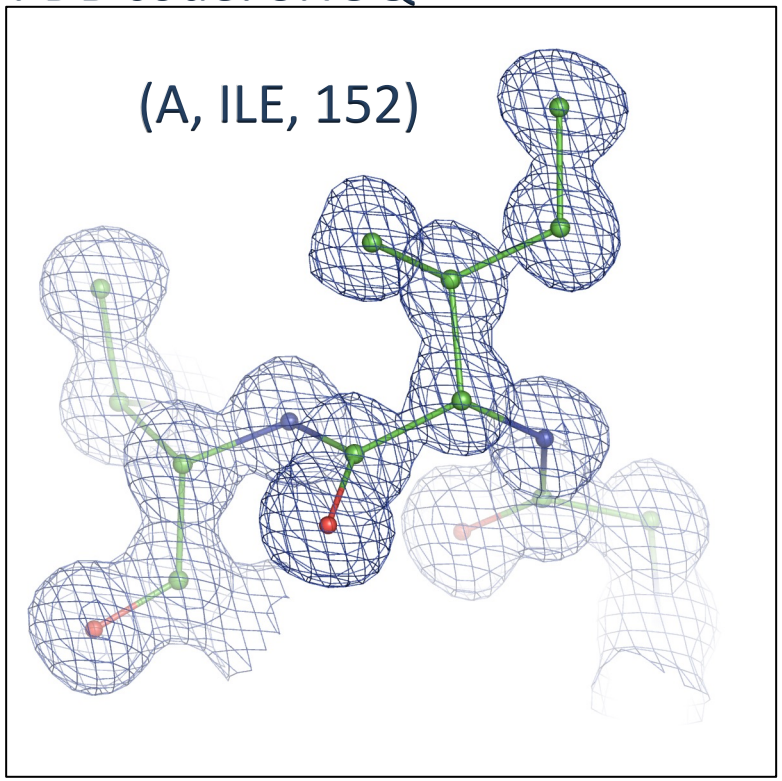


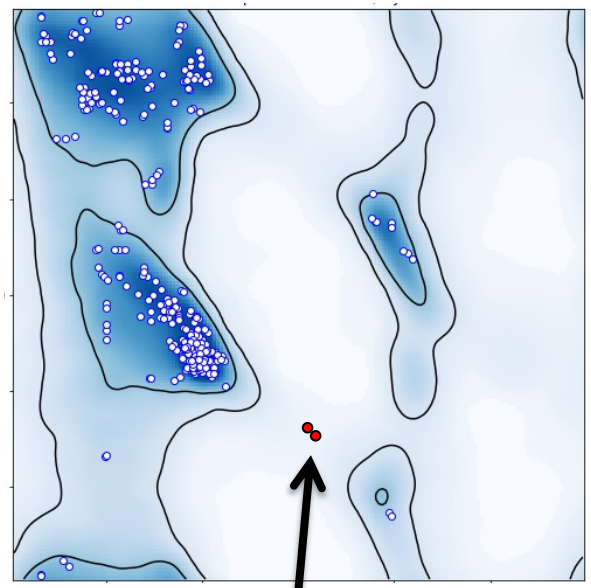


Validation: *outliers are not always wrong*

- A Ramachandran plot outlier ≠ wrong

PDB code: 3NOQ





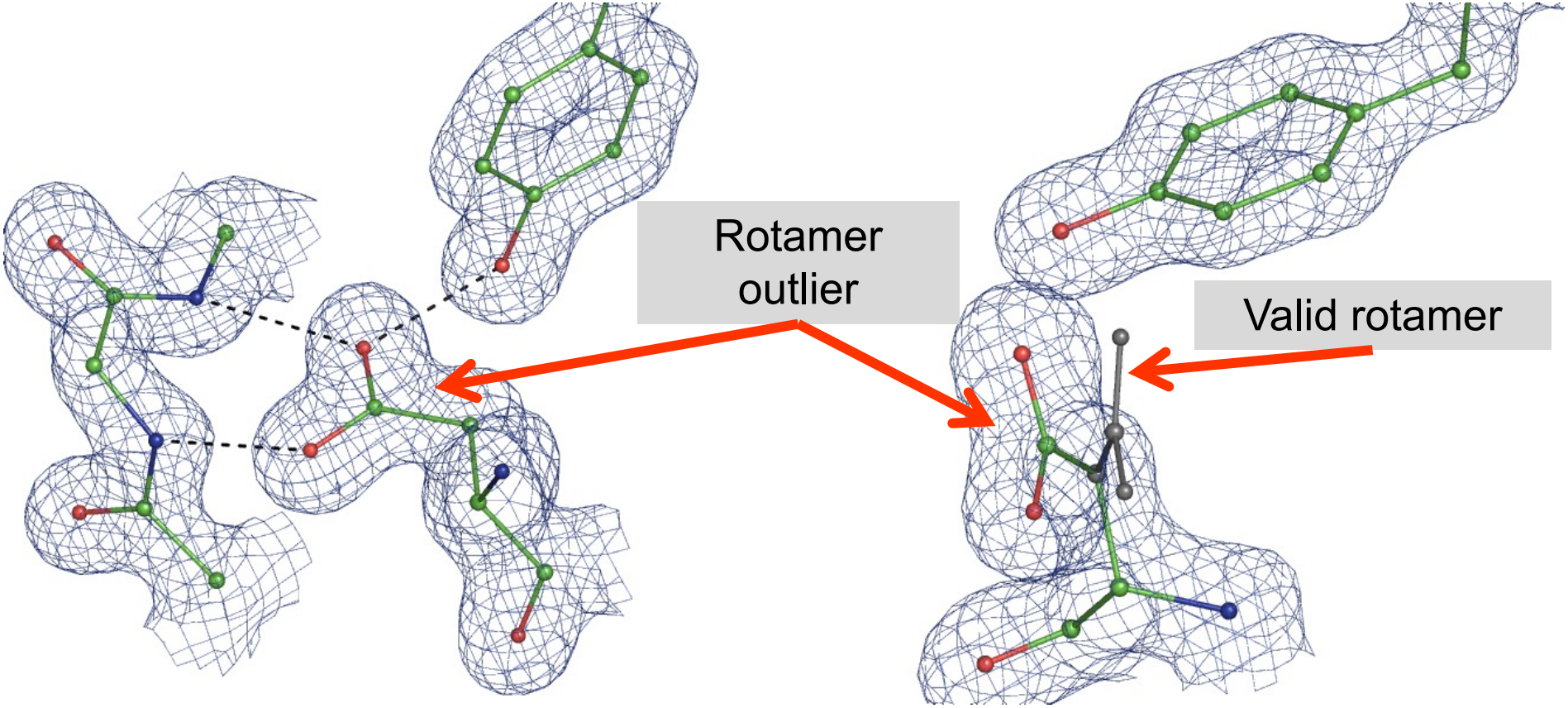
Outliers:

(A, ILE, 152), (B, ILE, 154)

- All outliers need to be explained (supported by the data)

Validation: *outliers are not always wrong*

- An outlier ≠ wrong
  - However, each outlier has to be explained



MolProbity Score

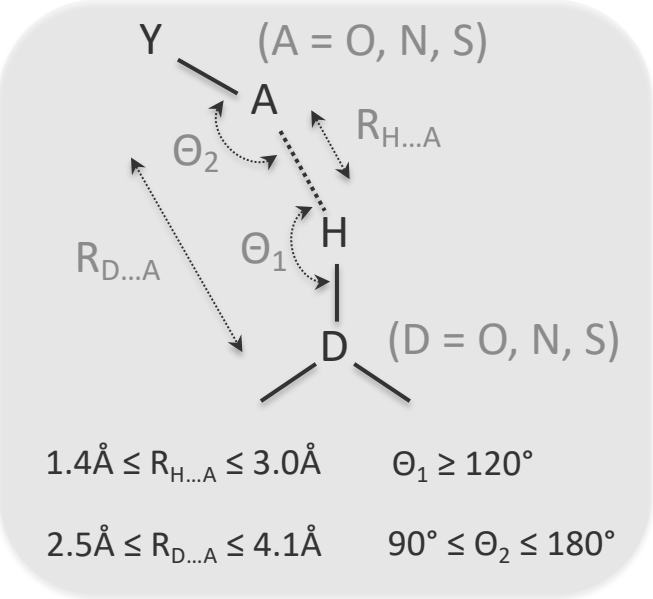
- The MolProbity Score combines validations and scales the result to look like a resolution
  - Clashscore
  - Ramachandran
  - Rotamers

- MolProbity better than model resolution is good
- MolProbity worse than model resolution is bad

molprobity.molprobity

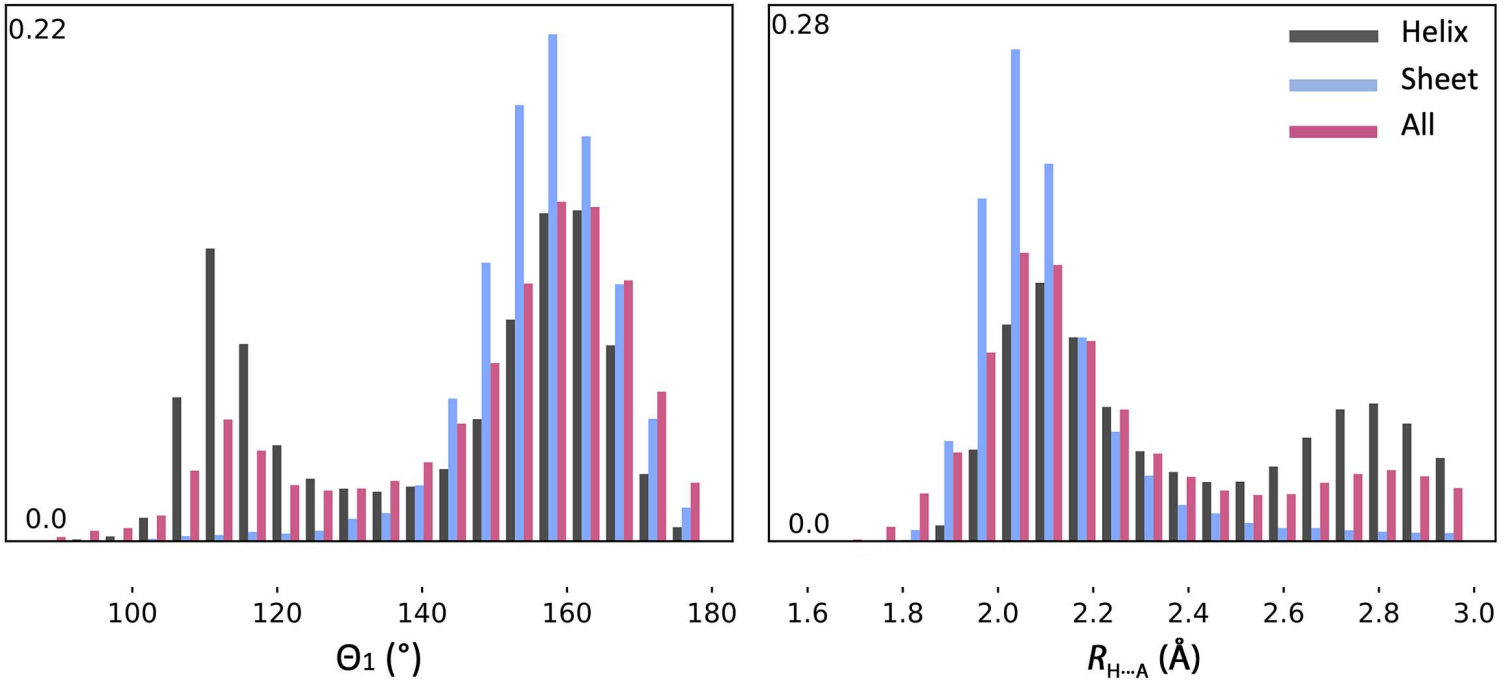
Hydrogen bond validation

- There are many definitions and rules exist. Here is what we use:
  - Voth & Ho Shing. Current Topics in Medicinal Chemistry, 2007, pp. 1336-1348
  - McDonald & Thornton. J. Mol. Biol., 1994, 777-793



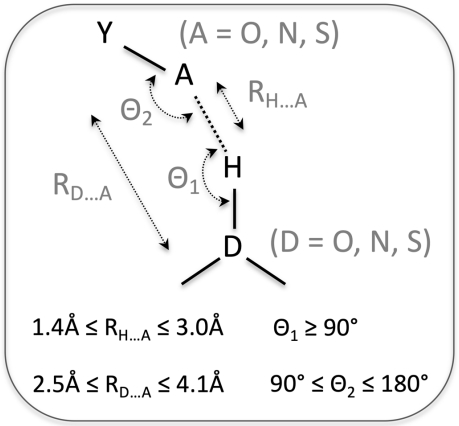
- We focus on R_{HA} distance and Θ_1 angle in *proteins*
  - Break down by resolution (high *vs* low) and secondary structure (helices, sheets, all atoms)
  - Use `phenix.find_ss_from_ca` to annotate secondary structure because it does not use any of the parameters above explicitly

H bond distributions

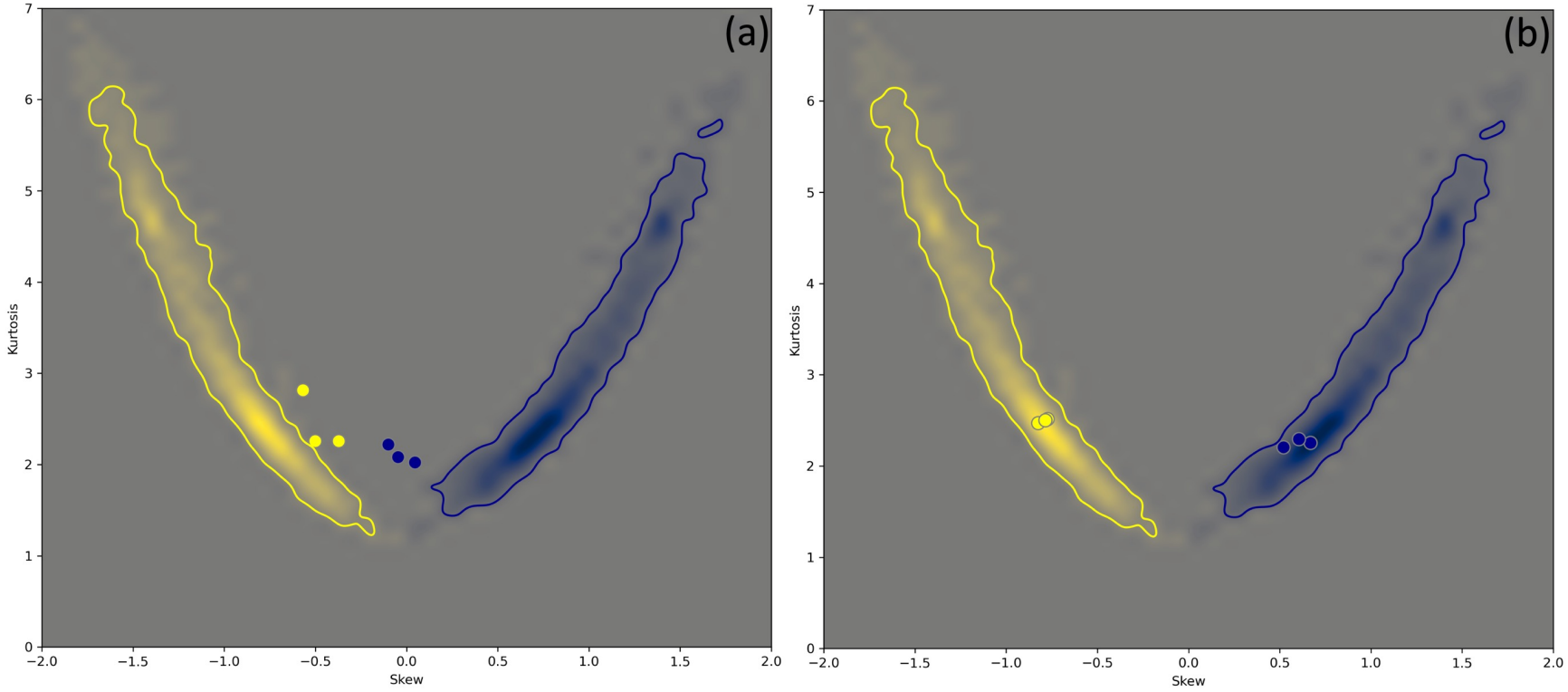


Skew or skewness is a way we can measure the shape of a distribution: in particular, skew refers to the asymmetry a distribution may experience

Kurtosis is a measurement of tailedness of a distribution - that is, what the ends of a distribution curve look like.



Overall kurtosis and skewness of Θ1 angle (yellow) and RHA distance (blue) distributions



Low resolution models	High-resolution homologues
1JKT (3.5 Å)	4PF4 (1.1 Å)
1Z8L (3.5 Å)	5o5T (1.4 Å)
4YJ3 (3.8 Å	5iyz (1.8 Å)

Afonine et al. (2023). *Acta Cryst*. D**79**, 648-693.

When do you stop?

- Realistically? Do as much as you can.
  - Ideally stop when you – and refinement – can't make the structure better
- Zero outliers is not the goal!
  - Some outliers are justified
  - Some outliers are not justified, but can't be fixed
- If you can't obtain a physically-reasonable solution, consider deleting the region.

Model vs Map Validation

Despite all efforts to popularize (and enforce) the validation in recent years, poorly scoring models are still getting into databases now

Examples (recent years)!

Model does not fit the map

PDB: 9c91 | EMDB: 45359 | 2.78 Å | Nat Commun (2025) 16: 2955

nature communications

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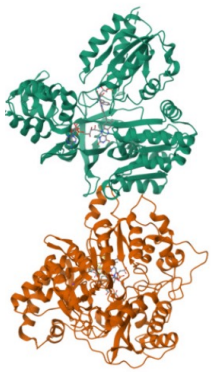
Article | Open access | Published: 26 March 2025

Structure of dimerized assimilatory NADPH-dependent sulfite reductase reveals the minimal interface for diflavin reductase binding

Behrouz Ghazi Esfahani, Nidhi Walia, Kasahun Neselu, Yashika Garg, Mahira Aragon, Isabel Askenasy, Hui Alex Wei, Joshua H. Mendez & M. Elizabeth Stroupe

Nature Communications **16**, Article number: 2955 (2025) | Cite this article

1343 Accesses | **1** Altmetric | Metrics



in 3D: Structure | Sequence
s | Electron Density |
Report |
raction (SRM)

metry: Asymmetric - C1
chiometry: Hetero 2-mer -

9C91 | pdb_00

Assimilatory NADPH-dependent sulf

PDB DOI: https://doi.org/10.2210/pdb9C91/pdb

Classification: FLAVOPROTEIN
Organism(s): Escherichia coli
Expression System: Escherichia coli
Mutation(s): No

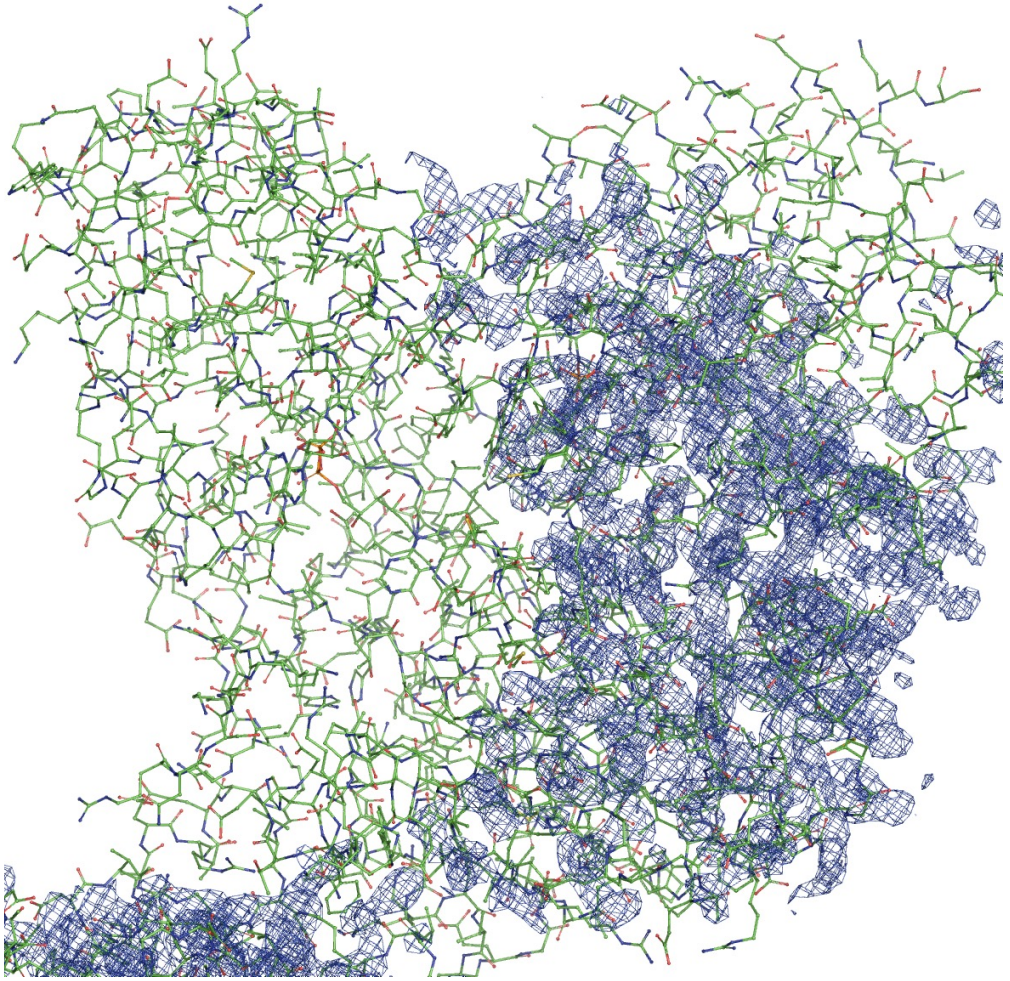
Deposited: 2024-06-13 **Released:** 2025-02-12
Deposition Author(s): Ghazi Esfahani, B., Walia
Mendez, J.H., Stroupe, M.E.
Funding Organization(s): National Science Fou

Experimental Data Snapshot ww

Method: ELECTRON MICROSCOPY
Resolution: 2.78 Å
Aggregation State: PARTICLE
Reconstruction Method: SINGLE PARTICLE

Ran

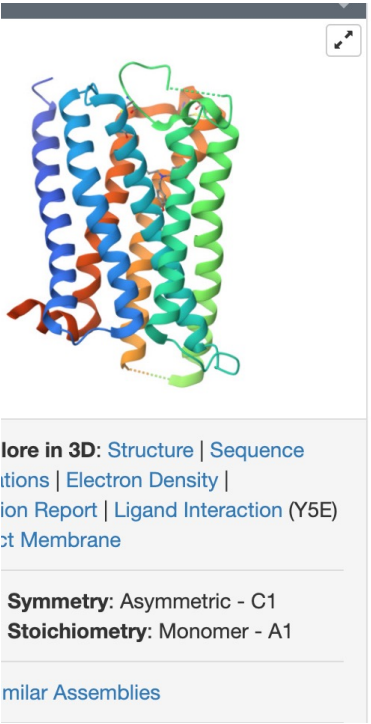
CC_{MASK} = 0.0



Model does not fit the map

PDB: 8x63 | EMDB: 38078 | 3.2 Å | Nat Commun (2024) 15: 84-84

CC_{MASK} = 0.13



lore in 3D: Structure | Sequence
tions | Electron Density |
ion Report | Ligand Interaction (Y5E)
ct Membrane

Symmetry: Asymmetric - C1
Stoichiometry: Monomer - A1

milar Assemblies

8X63 | pdb_00008x

CryoEM structure of the histamine H1 recep
with mepyramine

PDB DOI: https://doi.org/10.2210/pdb8X63/pdb **EM Ma**

Classification: MEMBRANE PROTEIN
Organism(s): Homo sapiens, Escherichia coli
Expression System: Spodoptera frugiperda
Mutation(s): Yes
Membrane Protein: Yes PDBTM MemProtMD mpstruc

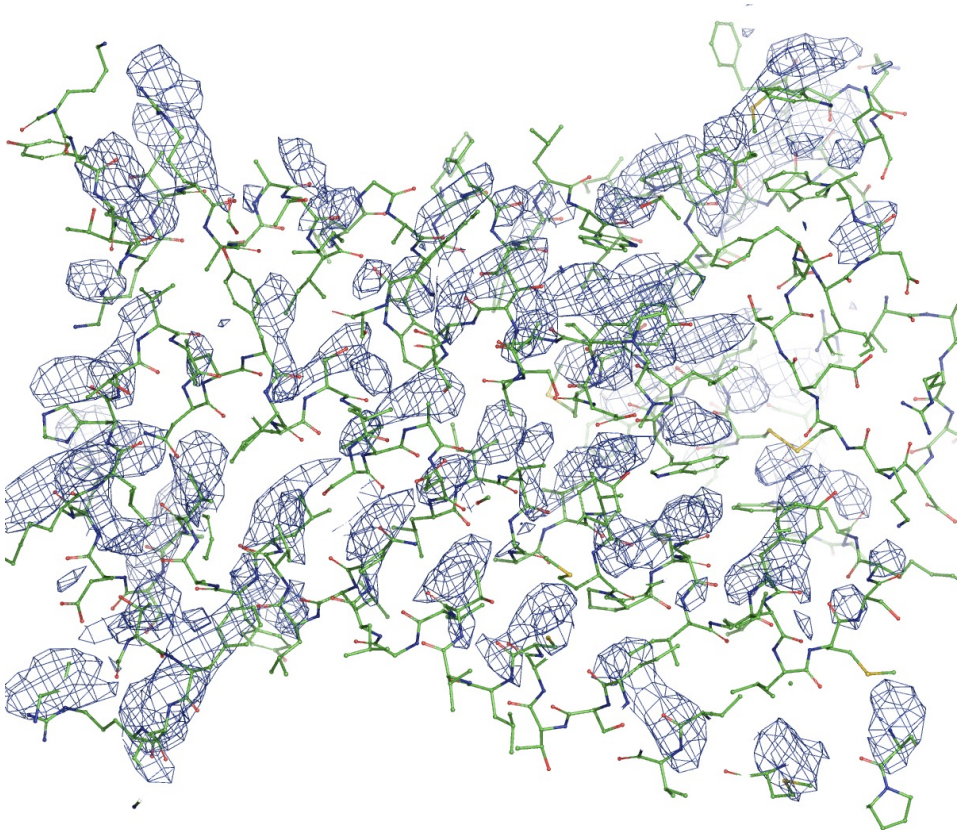
Deposited: 2023-11-20 **Released:** 2024-01-17
Deposition Author(s): Wang, D.D., Guo, Q.
Funding Organization(s): National Natural Science Found

Experimental Data Snapshot

Method: ELECTRON MICROSCOPY
Resolution: 3.20 Å
Aggregation State: PARTICLE
Reconstruction Method: SINGLE PARTICLE

wwPDB Vali

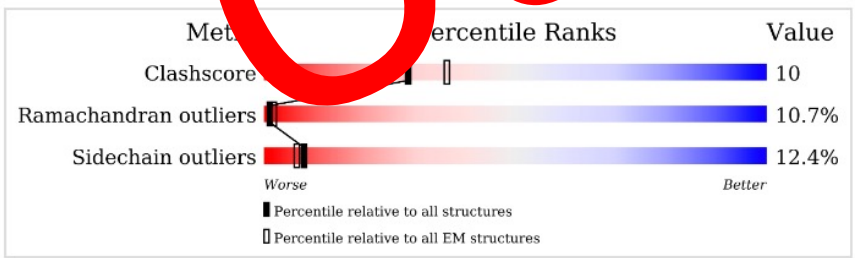
Clash
Ramachandran ou
Sidechain ou



Validation reports (RCSB)

Outdated!

wwPDB Valid tion | 3D eport | Full Report



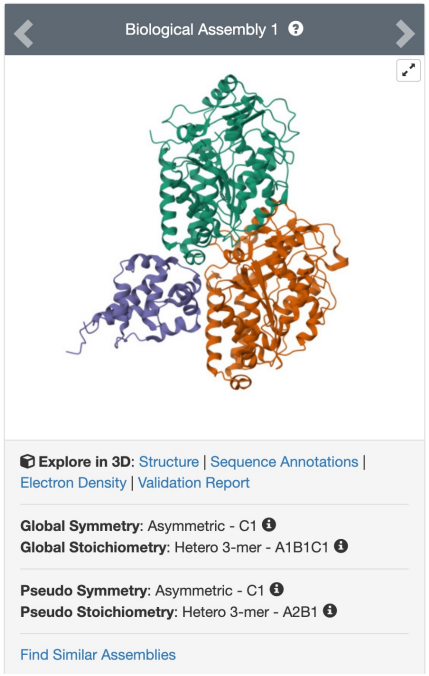
9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.125) a for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9062	0.4550
M	0.5810	0.3210
a	0.9659	0.4790
b	0.9656	0.4730

Lack of (useful) model-to-map fit statistics!

Validation reports (RCSB) on 4/28/2026



Display Files | Download Files | Data API

6KIQ | pdb_00006kiq

Complex of yeast cytoplasmic dynein MTBD-High and MT with DTT

PDB DOI: https://doi.org/10.2210/pdb6KIQ/pdb **EM Map EMD-9997:** EMDB EMDataResource

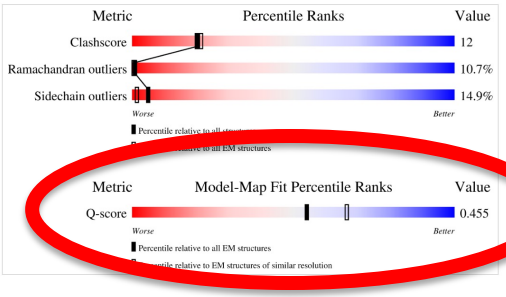
Classification: MOTOR PROTEIN/STRUCTURAL PROTEIN
Organism(s): Sus scrofa, Saccharomyces cerevisiae S288C
Expression System: Escherichia coli
Mutation(s): Yes

Deposited: 2019-07-19 **Released:** 2020-03-04
Deposition Author(s): Komori, Y., Nishida, N., Shimada, I., Kikkawa, M.
Funding Organization(s): Japan Science and Technology, Japan Agency for Medical Research and Development (AMED)

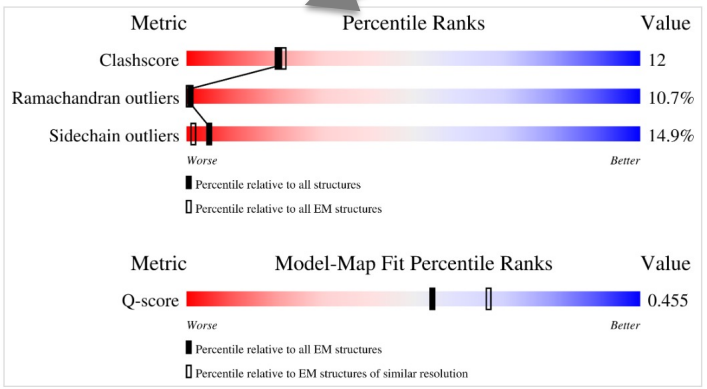
Experimental Data Snapshot

Method: ELECTRON MICROSCOPY
Resolution: 3.62 Å
Aggregation State: FILAMENT
Reconstruction Method: HELICAL

wwPDB Validation 3D Report | Full Report



wwPDB Validation 3D Report | Full Report



Page 57 Full wwPDB EM Validation Report

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour lev
for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.4550
M	0.5810	0.3210
a	0.9660	0.4790
b	0.9660	0.4730

Lack of (useful) model-to-map fit statistics!

Q-Score

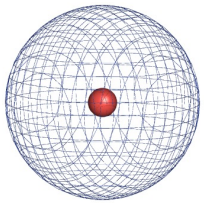
- **Q-score**: measure the resolvability of individual atoms in a cryo-EM map, using an atomic model fitted to or built into the map
  - No use of atomic model parameters such as ADP, occupancy, atom type, …
  - Shape of density is not used:
    - How SER placed into PHE density is going to score?
    - How water O placed into Mg peak will score?
  - Does not account for missing atoms (it shouldn't given the definition)
  - Alternative conformations are ***not*** handled
  - Anisotropic atoms are ***not*** handled

Atom inclusion

- **Atom inclusion**: fraction of atoms inside molecular envelope contoured at a given level
  - Contouring threshold: Arbitrarily? What is optimal level?
  - No use of atomic model parameters such as ADP, occupancy, atom type, …
  - Does not compare shape of density:
    - How SER placed into PHE density is going to score?
    - How water O placed into Mg peak will score?
  - Does not account for missing atoms
  - Partially occupied atoms (alternative conformations):
    - Chosen level for fully occupied atoms needs to be scaled by occupancy for partially occupied atoms

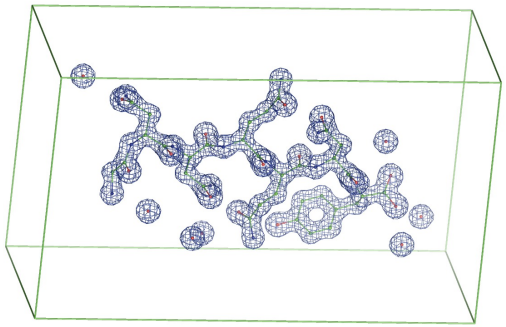
Model-to-map fit validation: CC_{MASK}

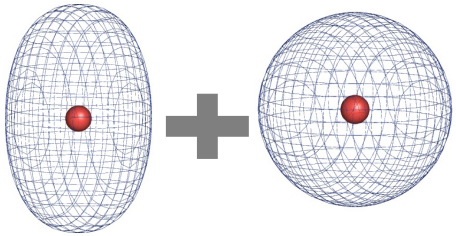
- Gaussian IAM (Independent Atom Model)



$$\rho_{atom}(\mathbf{r},\mathbf{r}_0,B,q) = q\sum_{k=1}^{5} a_k \left(\frac{4\pi}{b_k+B}\right)^{3/2} \exp\left(-\frac{4\pi^2|\mathbf{r}-\mathbf{r}_0|^2}{b_k+B}\right)$$

```
ATOM     25  CA  PRO A   4      31.309  29.489  26.044  1.00 57.79           C
```

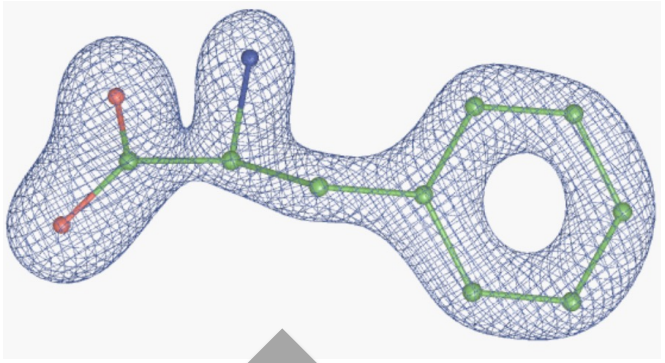




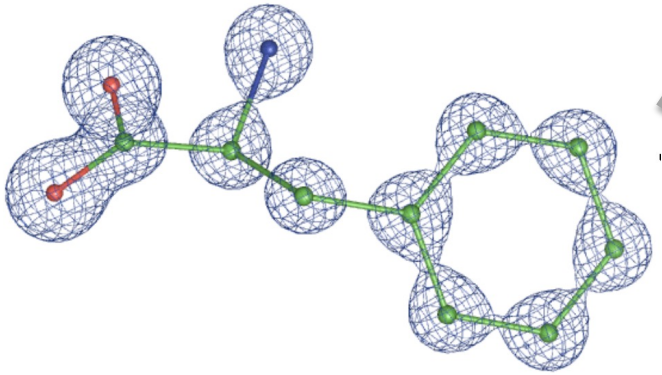
$$\rho_{MODEL}(\mathbf{r}) = \sum_{i=1}^{Natoms} \rho_{atoms}(\mathbf{r})$$

Model-to-map fit validation: CC_{MASK}

3Å model-calculated map



Exact model map

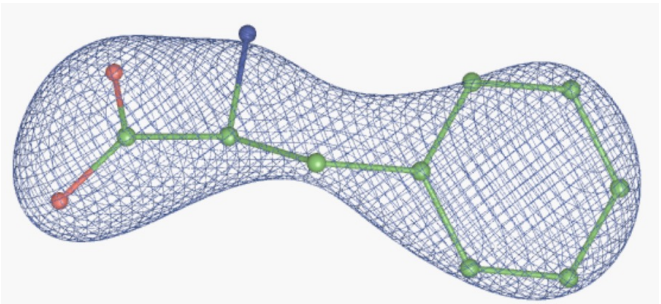


FT

CC_{MASK}

CC_{MASK}

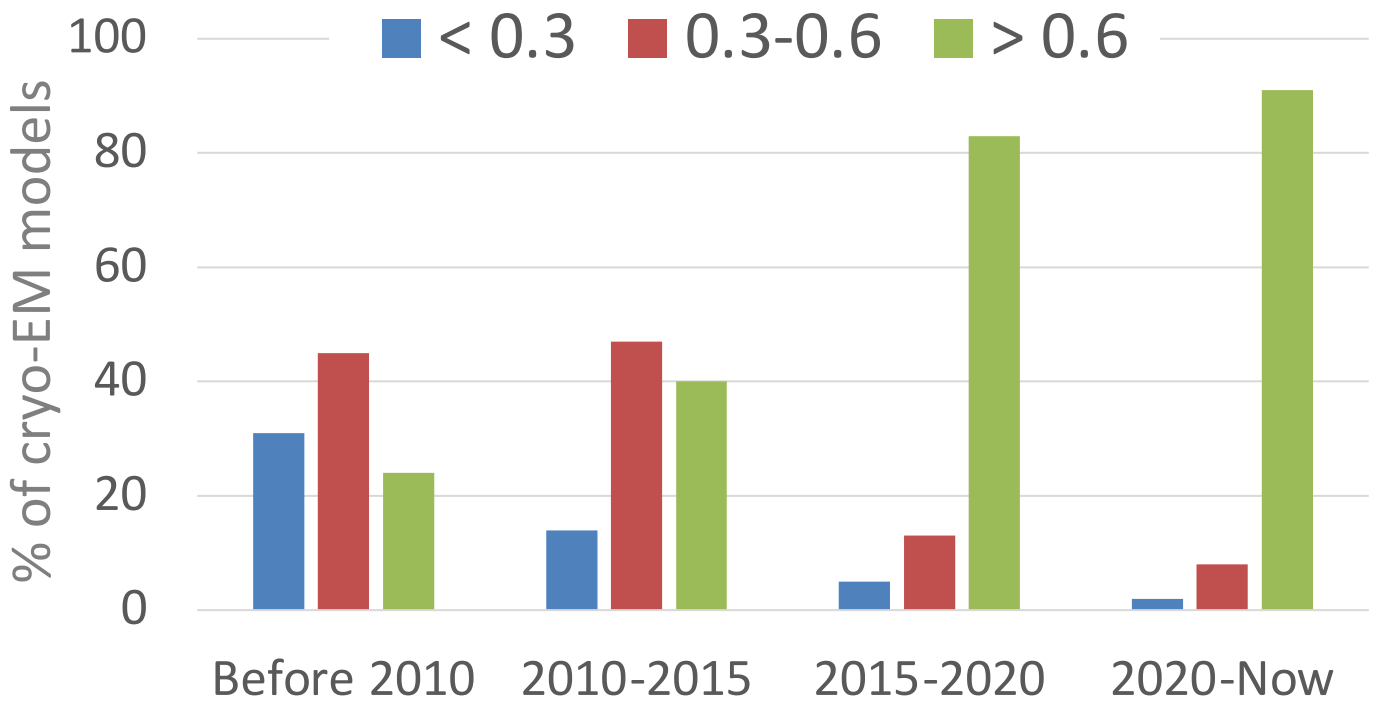
3Å experimental map



$$\rho_{MODEL}(\mathbf{r}) = \sum_{i=1}^{Natoms} \rho_{atoms}(\mathbf{r})$$

- FT exact model map
- Remove terms up to specified resolution
- FT back to real space to get a Fourier image = “Model map”

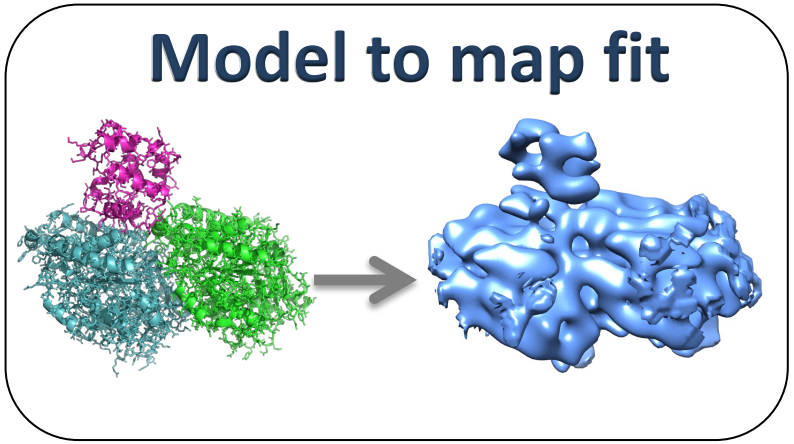
CC_{MASK} for all cryo-EM entries by year



Real-space refinement in Phenix

■ < 0.3 = No correlation between model and experimental map!

Model-to-map fit validation: CC_{MASK}



$$CC_{MASK} = \frac{\sum \rho_{obs}\, \rho_{calc}}{(\sum \rho_{obs}^{2}\ \sum \rho_{calc}^{2})^{1/2}}$$

ρ_{obs} = experimental map
ρ_{calc} = model calculated map

- Easy interpretation: -1: anticorrelation, 0: no correlation, 1: perfect correlation
- Uses all atomic model parameters (XYZ, B-factors, occ, atom type)
- Not specific to map type (any map: x-ray, neutron, electron, cryo-EM, …)
- Can be calculated locally (per atom, residue, chain, molecule, whole box, …)
  - Local resolution can be trivially taken into account

Metric	Expected value
CC_{MASK}	Poor: < 0.3 So-so: 0.3-0.6 Good: > 0.6

Model-to-map fit validation: CC flavors

Metric	Region of map used	Purpose
CC box	Whole map	Similarity of maps
CC mask	Jiang & Brunger (1994) mask with a fixed radius	Fit of the atomic centers
CC volume	Mask of points with the highest values in the model map	Fit of the molecular envelope defined by the model map
CC peaks	Mask of points with the highest values in the model and in the target maps	Fit of the strongest peaks in the model and target maps

Metric	Expected value
CC_{MASK}	Poor: < 0.3 So-so: 0.3-0.6 Good: > 0.6

From validation after RSR:

Model vs. Data	
CC (mask)	0.80
CC (box)	0.61
CC (peaks)	0.45
CC (volume)	0.77
Mean CC for ligands	0.69

Afonine et al. (2018). *Acta Cryst*. D**74**, 814-840

Questions?