

Validation

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phenix-online.org



lbl.gov



qrefine.com

Hosted by the Oklahoma COBRE in Structural Biology

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Validation tools in Phenix

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Actions Job history

Projects

Show group: All groups Manage...

Select Delete New project Settings

ID	Last modified	# of jobs	R-free
✓ ChrisF	Apr 13 2020 09:42...	28	0.1944
real-space-refin...	Apr 03 2020 07:42...	2	---
zzz1	Mar 21 2020 09:10...	1	---
chris	Mar 12 2020 12:27...	11	0.1890
dan	Mar 11 2020 05:44...	1	---
3j63	Mar 11 2020 02:28...	1	---
jason	Mar 11 2020 11:36...	1	---
rt6	Mar 11 2020 10:31...	1	0.2459
mate	Mar 10 2020 01:36...	1	---
emily	Mar 09 2020 03:52...	3	---
—	Mar 05 2020 08:25...	3	0.1923
alex	Feb 27 2020 11:33...	6	---
rt20201	Feb 18 2020 12:50...	4	0.2213
1f8t	Feb 03 2020 09:00...	1	0.1977
real-space-refin...	Jan 30 2020 02:38...	2	---
real-space-refin...	Jan 29 2020 10:56...	1	---
ion_channel_den...	Jan 27 2020 07:36...	3	---
10101	Jan 27 2020 12:38...	2	---
demos	Jan 27 2020 10:57...	3	---
ion_channel_den...	Jan 27 2020 10:03...	2	---
malcolm	Jan 22 2020 10:22...	14	0.1748
real-space-refin...	Jan 16 2020 04:28...	3	---
3NIR	Dec 05 2019 10:2...	1	---
leighton	Sep 02 2019 05:1...	2	---
5pti	Aug 27 2019 03:4...	3	---

Favorites

Data analysis

- Xtrriage**
Analysis of data quality and crystal defects
- Merging statistics**
Calculates a variety of statistics for unmerged intensities, including I/sigma, R-merge, R-meas, and CC1/2.
- Mtrriage**
Analyze quality of maps in CCP4 format

Experimental phasing

Molecular replacement

Model building

Refinement

Cryo-EM

Validation

- Comprehensive validation (X-ray/Neutron)**
Model quality assessment, including real-space correlation and geometry inspection using MolProbity tools
- Comprehensive validation (cryo-EM)**
Model quality assessment, including real-space correlation, for cryo-EM structures

Structure comparison

Identify differences between multiple structures of the same protein, using multiple criteria

Calculate CC*

Comparison of unmerged data quality with refined model, as described in Karplus & Diederichs (2012)

EMRinger

Model validation for de novo electron microscopy structures

Ligands

Current directory: /Users/pafonine/Desktop/all/people/ChrisF Browse...

PHENIX version dev-svn-000 Project: ChrisF

Validation (cryo-EM)

Comprehensive validation (cryo-EM) (Project: real-space-refine-5ljv_0)

Preferences Help Run Abort Ask for help

Input/Output ValidationCryoEM_1

Run status Summary MolProbity Model vs. Data Data

Open in Coot Export Table 1

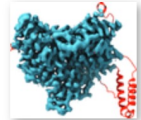
Model		Data		
Composition (#)		Box		
Chains	2	Lengths (Å)	50.92, 68.34, 83.08	
Atoms	2500 (Hydrogens: 0)	Angles (°)	90.00, 90.00, 90.00	
Residues	Protein: 325 Nucleotide: 0	Supplied Resolution (Å)	3.6	
Water	0	Resolution Estimates (Å)	Masked	Unmasked
Ligands	MG: 1 ADP: 1	d FSC (half maps; 0.143)	---	---
Bonds (RMSD)		d 99 (full/half1/half2)	3.7/---/---	3.1/---/---
Length (Å) (# > 4σ)	0.029 (146)	d model	3.7	3.7
Angles (°) (# > 4σ)	2.853 (122)	d FSC model (0/0.143/0.5)	3.4/3.5/3.6	3.4/3.6/3.9
MolProbity score	3.14	Man min/max/mean	-0.42/0.80/0.03	
Clash score	19.06	Model vs. Data		
Ramachandran plot (%)		CC (mask)	0.83	
Outliers	3.10	CC (box)	0.55	
Allowed	7.12	CC (peaks)	0.34	
Favored	89.78	CC (volume)	0.83	
Rotamer outliers (%)	11.57	Mean CC for ligands	0.86	
Cβ outliers (%)	3.68			
Peptide plane (%)				
Cis proline/general	5.6/0.0			
Twisted proline/general	11.1/0.7			
CaBLAM outliers (%)	2.18			
ADP (B-factors)				
Iso/Aniso (#)	2500/0			
min/max/mean				
Protein	30.26/493.42/109.69			
Nucleotide	---			
Ligand	57.57/99.69/75.15			
Water	---			
Occupancy				
Mean	1.00			
occ = 1 (%)	100.00			
0 < occ < 1 (%)	0.00			
occ > 1 (%)	0.00			

Idle Project: real-space-refine-5ljv_0

RESEARCH PAPERS

Acta Cryst. (2018). D74, 814-840
<https://doi.org/10.1107/S2059798318009324>

Cited by 71 OPEN



New tools for the analysis and validation of cryo-EM maps and atomic models

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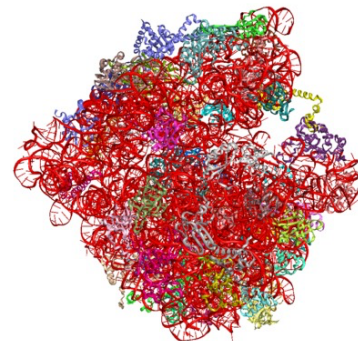
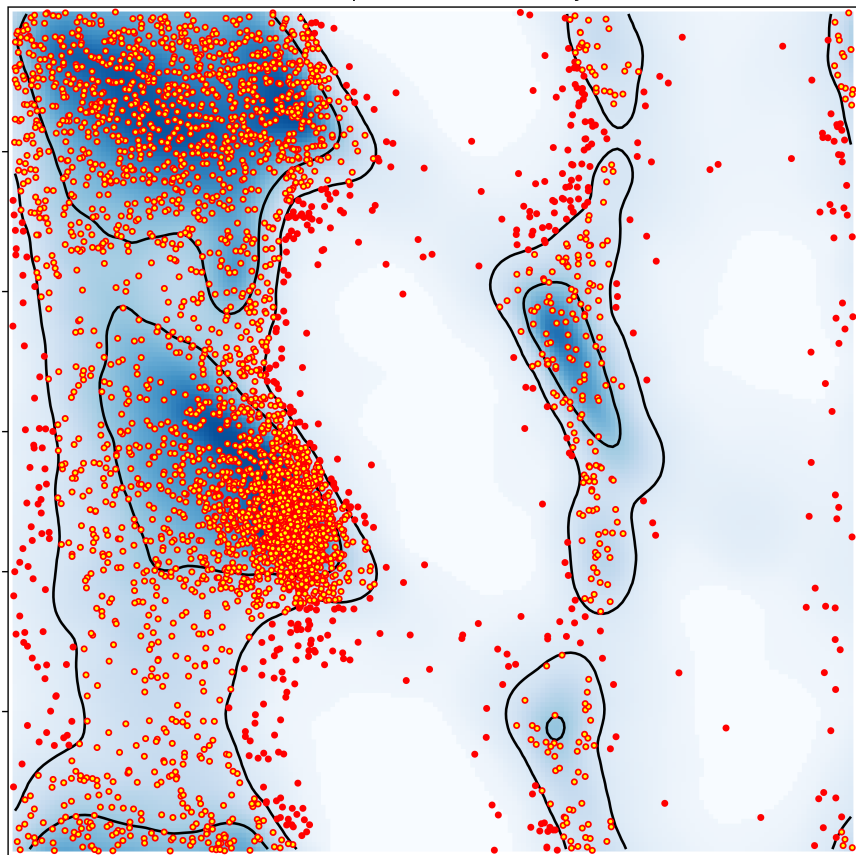
Recent advances in the field of electron cryomicroscopy (cryo-EM) have resulted in a rapidly increasing number of atomic models of biomacromolecules that have been solved using this technique and deposited in the Protein Data Bank and the Electron Microscopy Data Bank. Similar to macromolecular crystallography, validation tools for these models and maps are required. While some of these validation tools may be borrowed from crystallography, new methods specifically designed for cryo-EM validation are required. Here, new computational methods and tools implemented in PHENIX are discussed, including *d*₉₉ to estimate resolution, *phenix.auto_sharpen* to improve maps and *phenix.mtriage* to analyze cryo-EM maps. It is suggested that cryo-EM half-maps and masks should be deposited to facilitate the evaluation and validation of cryo-EM-derived atomic models and maps. The application of these tools to deposited cryo-EM atomic models and maps is also presented.

Keywords: cryo-EM; atomic models; model quality; data quality; validation; resolution.

Read article Similar articles

Validation: **why to do?**

(2019) Nature 570: 400-404 | PDB: 6o9j | EMDB: 0661 | 3.9Å

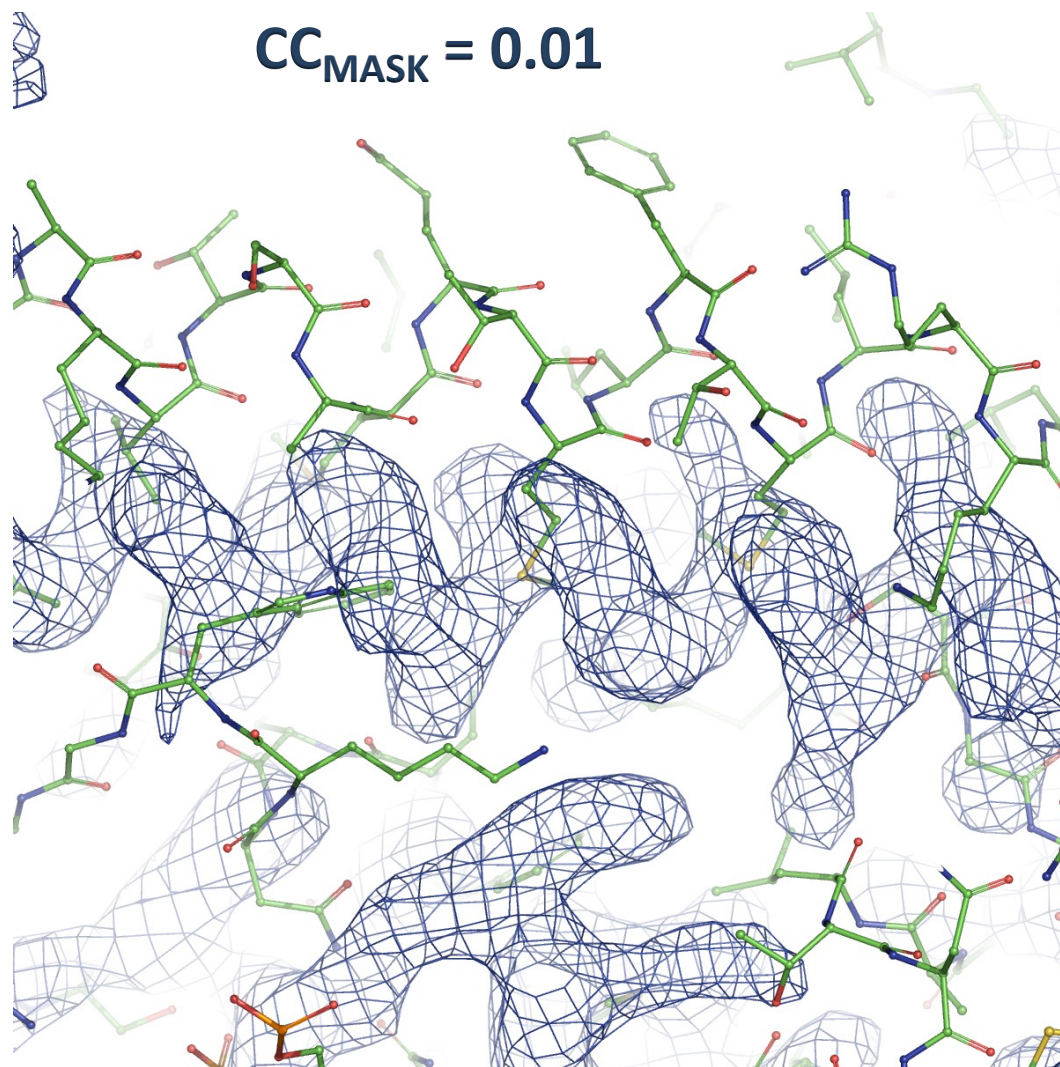


Metric	6o9j	Expected
Clashscore	70	Less than 10
Ramachandran favored, %	59	More than 98
Ramachandran outliers, %	15	0
Rotamer outliers, %	23	0
C _β deviations, %	0.5	0

Examples of **very poor** model-to-map fit

PDB: 8gwb | EMDB: 34308 | 2.8 Å | Cell (2022) 185: 4347-4360

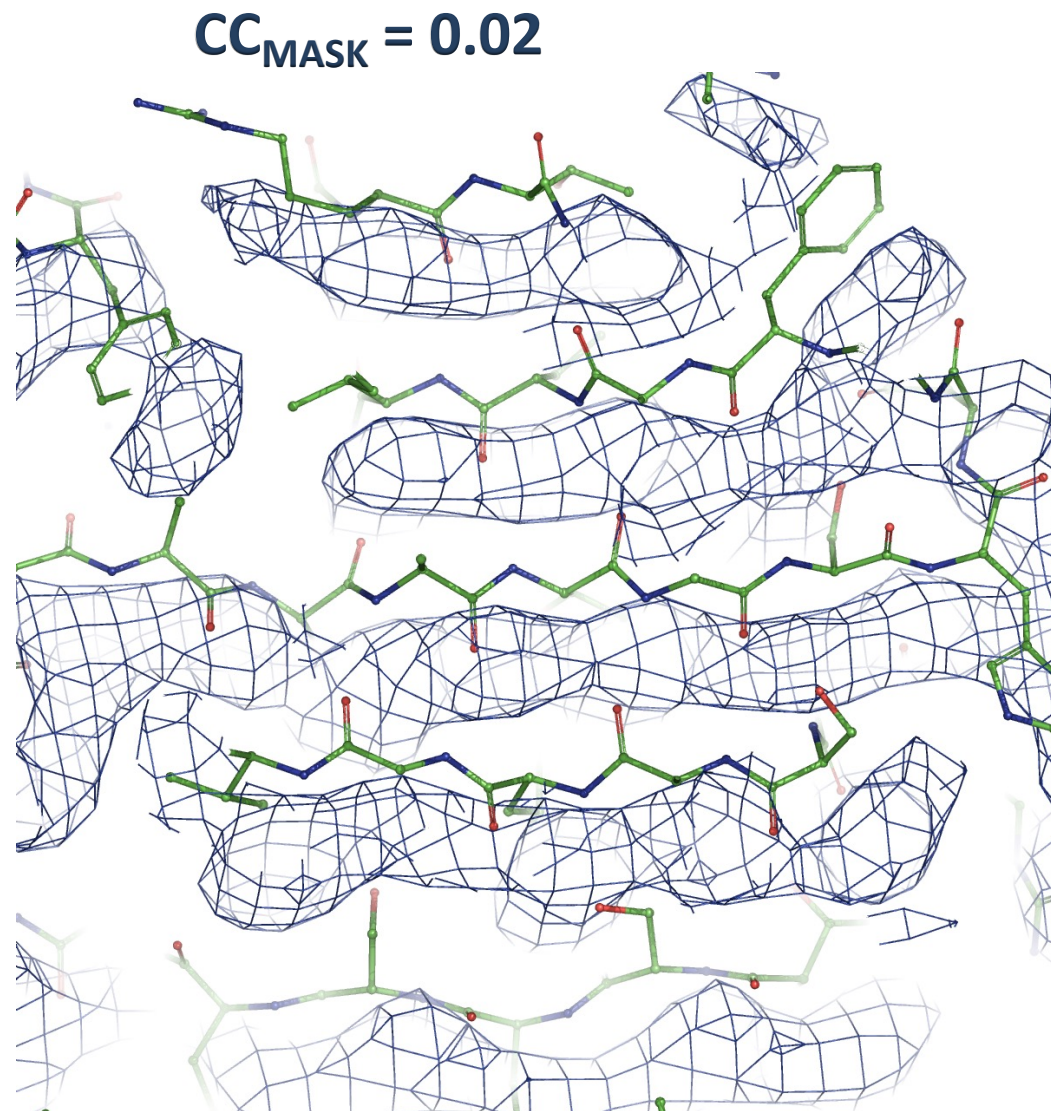
Chain	CC _{MASK}
A	0.01
B	0.02
C	0
D	0.01
I	0.04
J	0
F	0.12
E	0.08
G	0.1
M	0.16
A	0
F	-0.13
E	0.16
A	0.1
G	0.15
M	0.19



Examples of **very poor** model-to-map fit

PDB: 7xov | EMDB: 33360 | 3 Å | Cell Discov (2022) 8: 55-55

Chain	CC_{MASK}
A	0.04
B	-0.01
G	0.18
N	0.06
R	0.03
R	-0.02

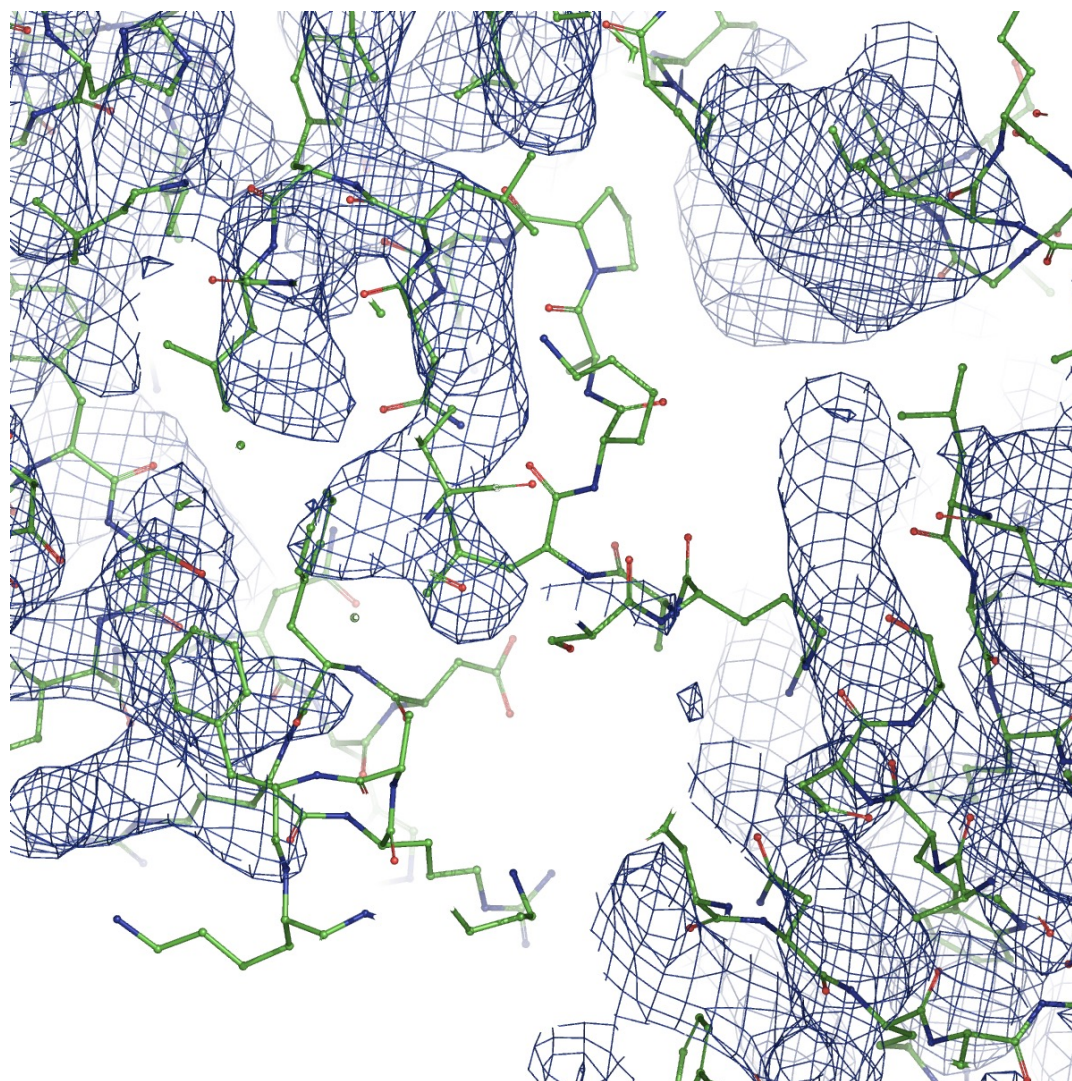


Examples of **very poor** model-to-map fit

PDB: 7w6p | EMDB: 32331 | 3.5 Å | Science (2022) 377: 7065-7065

Chain	CC_{MASK}
A	0.09
B	0.11
G	0.12
H	0.07
R	0.16
R	-0.08

$CC_{\text{MASK}} = 0.1$

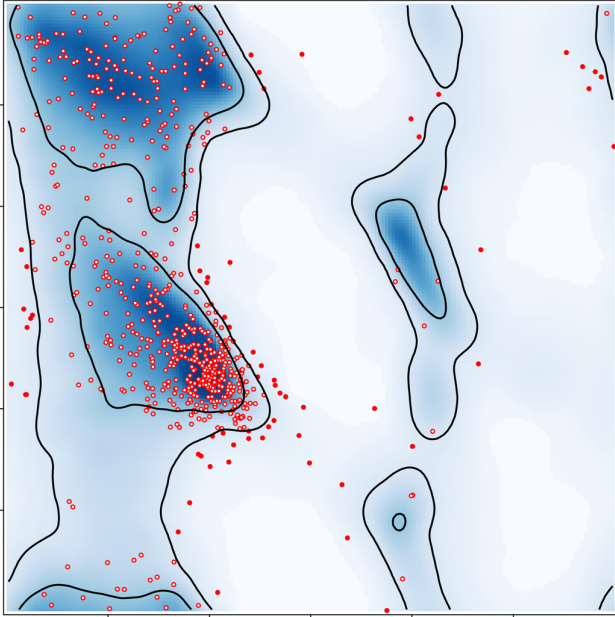


Model

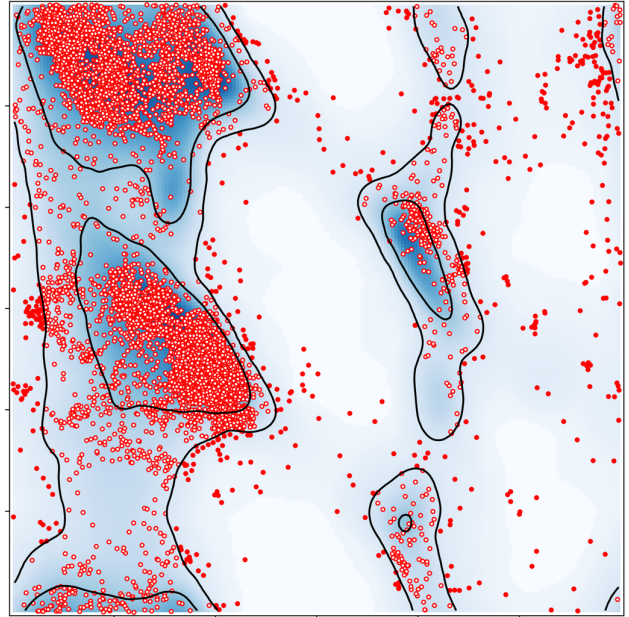
	6kio	6kiq	6o9j	7ase
Bond/angle	0.04/3.4	0.04/3.7	0.01/1.3	0.02/2.2
Clashscore	11	12	55	9
Rotamer outl., %	8	15	23	3
Cb deviations, %	5	16	0.5	1.4
Ramachandran, % favored	74	70	59	79
outliers	7	11	15	7
Resolution (Å)	3.9	3.6	3.9	3.3
Published in	Nature Comm.	Nature Comm.	Nature	Cell
Year	2020	2020	2019	2020

Model

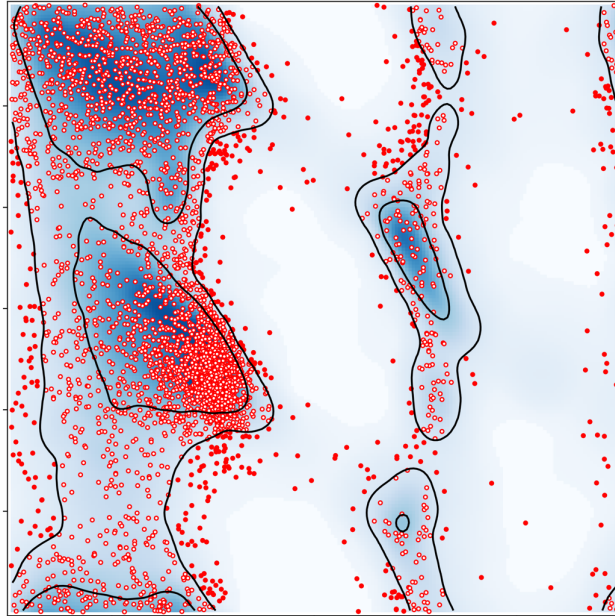
6kiq



7ase



6o9j



6kio

