Structure, Volume *27*

Supplemental Information

Automatically Fixing Errors

in Glycoprotein Structures with Rosetta

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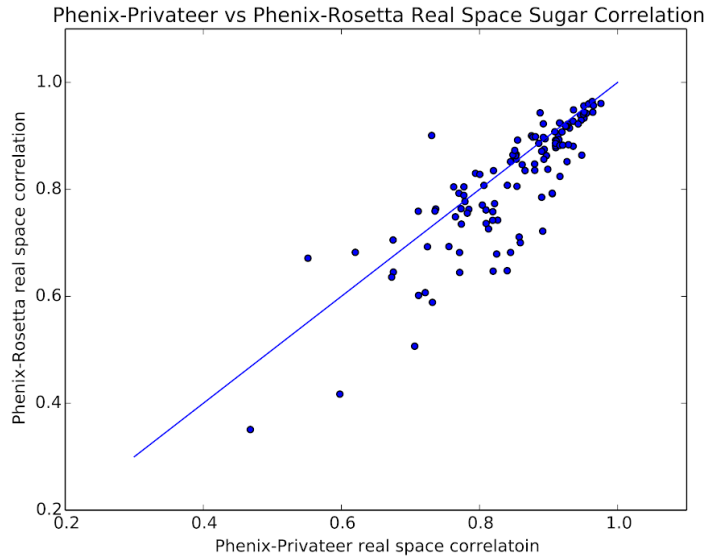
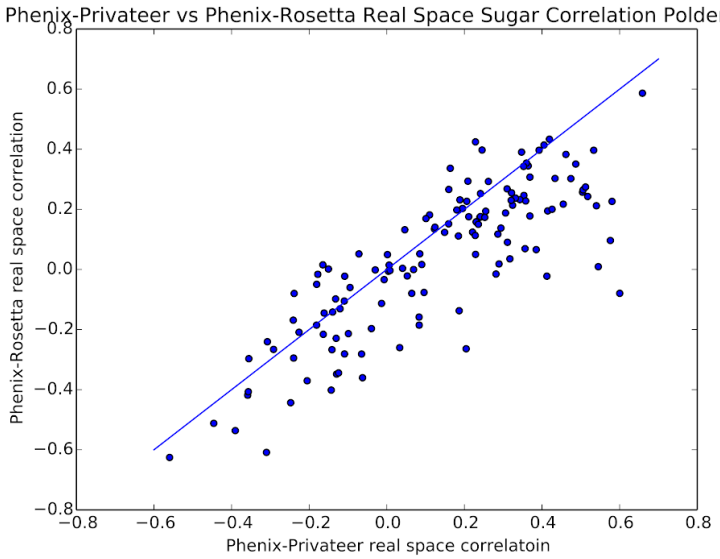
A

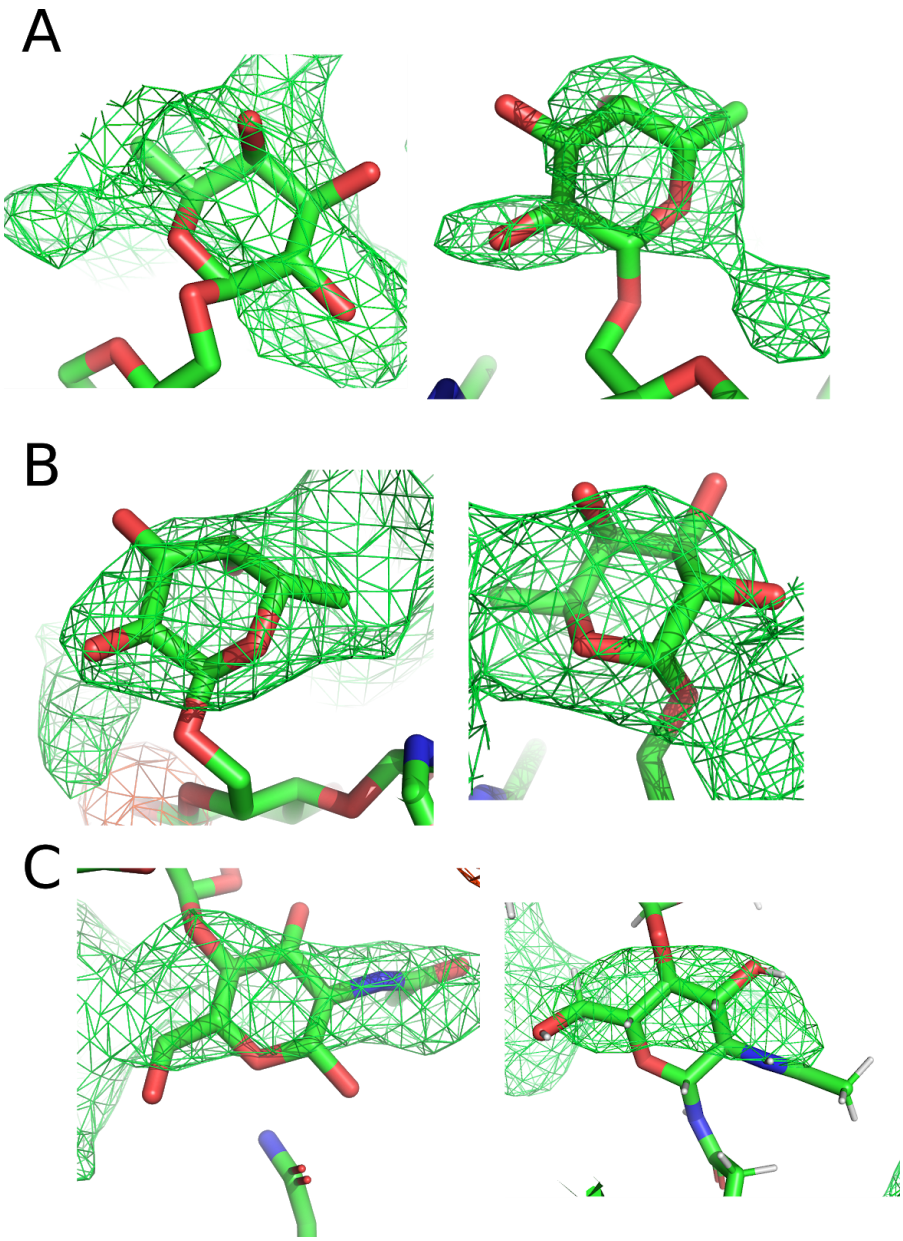


B



Supplemental Figure 1. Related to Table 1. The real space correlation of the models when refined with Phenix and Privateer or Phenix Rosetta in the raw data and in the Polder Map.

This figure shows the per-glycan real-space correlation for each of 133 glycans in the crystal structure benchmark set. Axis indicate the correlation following: refinement with Phenix using Privateer-produced constraints on high-energy ring conformations (x-axis); and Phenix-Rosetta (y-axis). **A.** shows the correlation to the 2mFo-dFc density map. **B.** shows the correlation to the polder map. Correlations tend to decrease in the Rosetta refined models, likely due to the increased constraints on the geometry preventing the structure from over fitting to the data.



Supplemental Figure 2. Related To Figure 1. Polder Omit Map of Problem Glycans.
A. Fucose 507 of 5nsc of the input model left and the refined model right. Poor geometry of the glycosidic bond is resolved while fit to density is maintained. **B.** Fucose 507 of 5k65 input (left) and refined (right). Both models agree with the data but in the refined model the high energy ring conformation is resolved while maintaining good fit. **C.** The glycosidic bond between asparagine 297 and NAG 501 is missing from the input model (right) and formed in the refined model (left).

```
# Aldohexoses

# Code  Rosetta Code  Default HETNAM  PATCHES
  ALL   All           ->?)-beta-D-Allp
  DSR   All           ->?)-beta-D-Allp

  GLC   Glc           ->?)-alpha-D-Glcp default
  AGL   Glc           ->?)-alpha-D-Glcp
  BG6   Glc           ->?)-beta-D-Glcp
  BGC   Glc           ->?)-beta-D-Glcp
  DDA   Glc           ->?)-beta-D-Glcp
  DRI   Glc           ->?)-beta-D-Glcp
  G16   Glc           ->?)-alpha-D-Glcp
  G1P   Glc           ->?)-alpha-D-Glcp
  G4D   Glc           ->?)-alpha-D-Glcp
  G6P   Glc           ->?)-alpha-D-Glcp
  G6Q   Glc           ->?)-D-Glc
  GCS   Glc           ->?)-beta-D-Glcp
  GDA   Glc           ->?)-alpha-D-Glcp
  GFP   Glc           ->?)-alpha-D-Glcp
  GLF   Glc           ->?)-alpha-D-Glcp
  GLO   Glc           ->?)-alpha-D-Glc
  GLT   Glc           ->?)-alpha-D-Glcp
  GTM   Glc           ->?)-beta-D-Glcp
  KBG   Glc           ->?)-beta-D-Glcp
  MA3   Glc           ->?)-alpha-D-Glcp
  MGL   Glc           ->?)-beta-D-Glcp
  NDG   Glc           ->?)-alpha-D-Glcp 2-AcNH
  TOA   Glc           ->?)-alpha-D-Glcp
  TOC   Glc           ->?)-alpha-D-Glcp
  NAG   Glc           ->?)-beta-D-Glcp  2-AcNH
  MUR   Mur           ->?)-beta-D-Murp
  G6D   Qui           ->?)-alpha-D-Quip
```

Supplemental Figure 3. Related To STAR Methods Writing Glycans In Standard Format. An example of additional patch names added to the glycan naming database

A new column for a list of patch names has been added to the database that maps PDB codes to Rosetta names. Patch names are added to eliminate redundancy when returning from Rosetta name to PDB code. The “default” keyword signals that this is the base, unmodified, code name.