

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 ALL DSR	Rosetta Coo All All	de	<pre>Default HETNAM PA ->?)-beta-D-Allp ->?)-beta-D-Allp</pre>	TCHES
	DOR				
	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		<pre>->?)-beta-D-Glcp</pre>	
	GDA	Glc		->?)-alpha-D-Glcp	
	GFP	Glc		->?)-alpha-D-Glcp	
	GLF	Glc		->?)-alpha-D-Glcp	
	GL0	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.