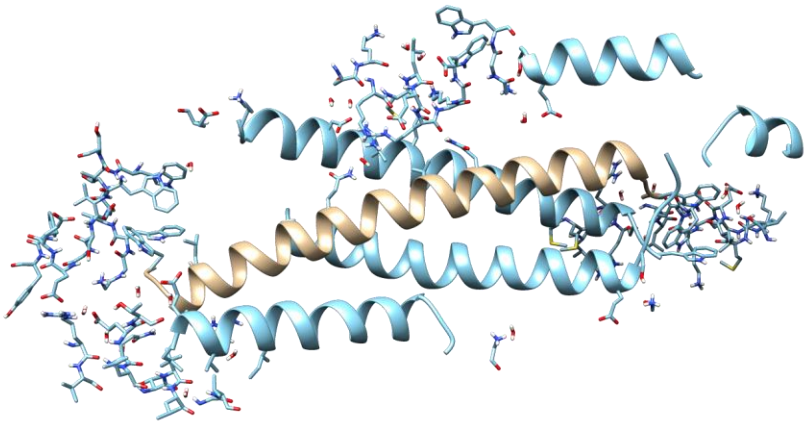
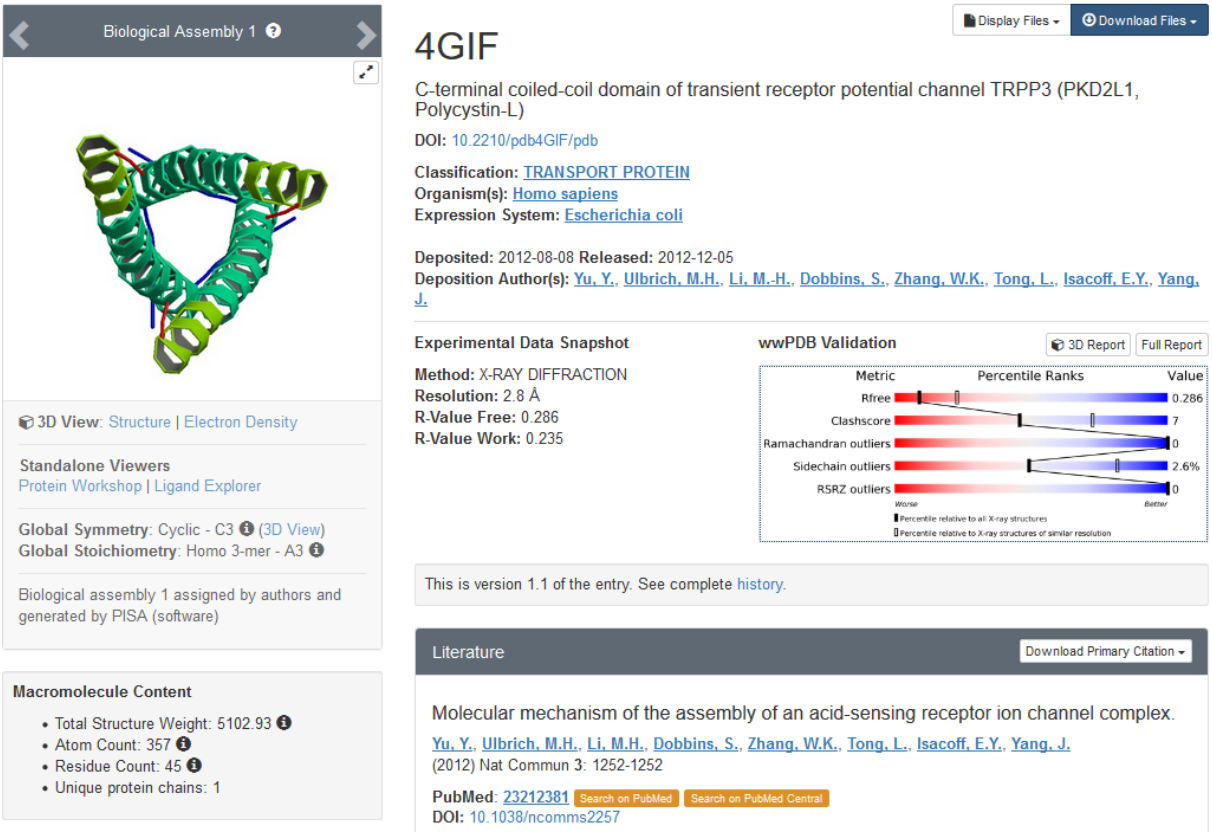
4gif for paper 3 – symmetry

I. 4gif is a simpler alternative for the non-P1 paper found by Pavel.

It is 2.8 A resolution, P_3_2_1 symmetry. Below a structure from PDB file 4gif_ready.pdb (yellow) and the expansion.pdb (blue)





II. Refinement and Optimisations have been done with

1. **Xtb** : xtb.6.0 gfn2+water solvent (--gfn 2 --etemp 500 --acc 0.1 --gbsa h2o)
2. **TeraChem** : TeraChem v1.93P , HF-D3/6-31G plus water solvent with COSMO model
   For xtb and TeraChem the same qr.refine options have been used (*described below*)
   Timing: xtb takes about 8 h, TeraChem 60 h
   xtb: 8 weigth cycles 5 refinement, TeraChem: 7 weight cycles, 5 refinement (so essentially the same)
3. **Cctbx** – all default parameters

In all cases phenix-dev-3407 and Q|R v1.0-39 have been used

qr.refine options:

mode=refine

maxnum_residues_in_cluster=50 (or default=15, in both cases the same 9 clusters are created)

~ # clusters : 9
~ list of atoms per cluster:
~ [198, 166, 148, 108, 78, 56, 6, 3, 3]
~ list of atoms per fragment:
~ [890, 1347, 1458, 1091, 1088, 828, 339, 267, 449]

max_bond_rmsd=0.02 (preliminary run with larger max_bond_rmsd was not satisfactory, see /home/qr/paper4_refine on cu39)

stpmax=0.2 (larger steps create problems for quantum computations – atoms can move too far)

gradient_only=true

clustering=true

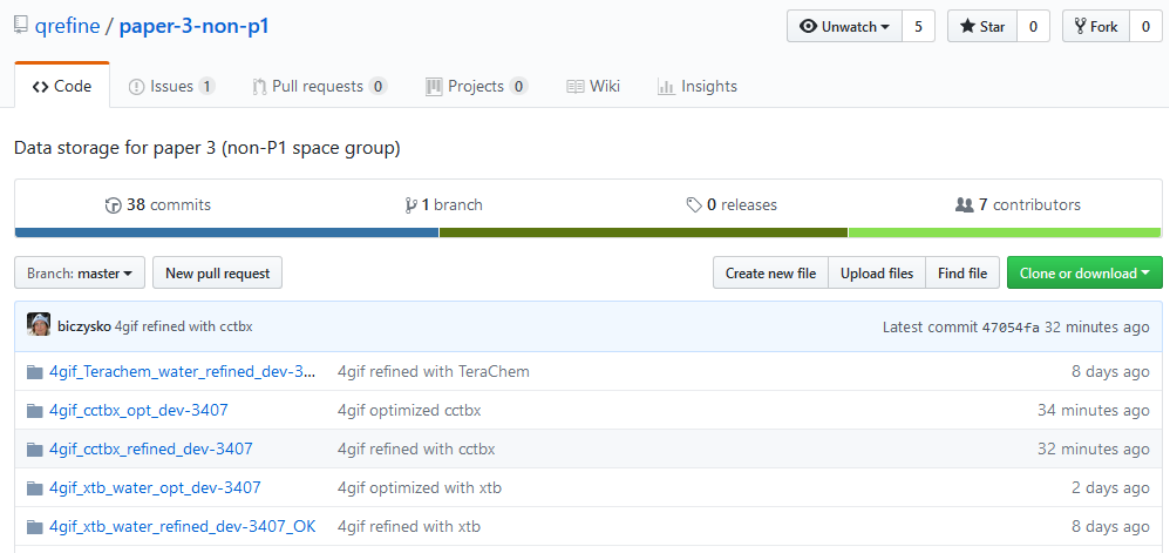
use_convergence_test=true

opt_log=1

restraints=qm

III. Results/comparison

1. All files are uploaded on github in



Note: TeraChem optimization is still running

2. Starting PDB is showing several clash-scores which are removed fully by both xtb and Terachem qr.refine

		Re-refinement			Optimization		
Metric	4gif.pdb	cctbx	xtb	TeraChem	cctbx	xtb	TeraChem
R factors							running
R work	0.235	0.2331	0.2393	0.2302			
R free	0.286	0.2799	0.2885	0.2789			
R free – R work	0.051	0.0468	0.0492	0.0487			
Ramachandran plot							
Favoured	43	43	43	43	43	42	
Allowed							
Outliers	0	0	0	0	0	0	
Rotamers							
Poor	2	1	3	0	1	1	
Favoured	31	29	33	32	43	35	
Clashscore		2.8	0	0	8.4	0	
Cbeta deviations	0	0	0	0	0	0	

Comments (for xtb refinement file)

Nigel: My validation shows that this is a fine model. There are two ARG that are not planar which is fine in my opinion. The three rotamer outliers seem to be due to a lack of density.

Pavel: What's also remarkable is the clashscore being zero as well as cross-symmetry interactions of some side chains.