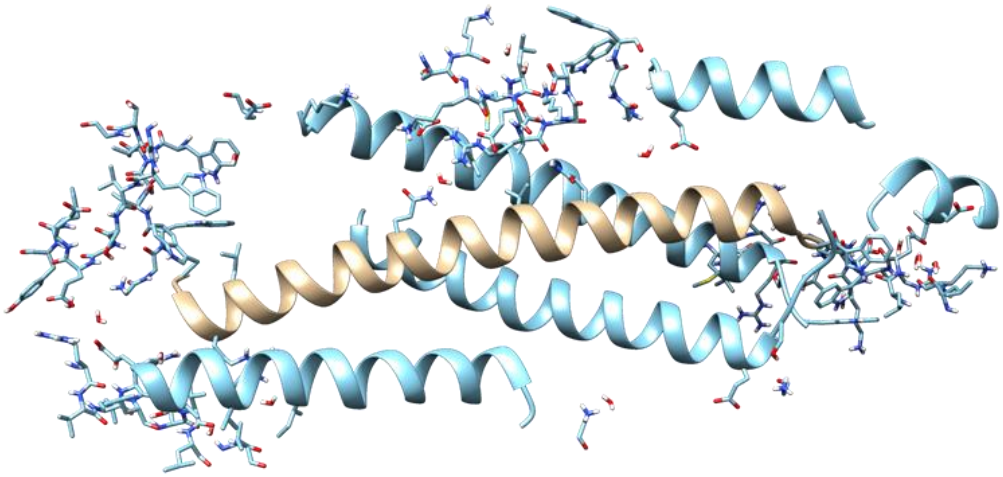
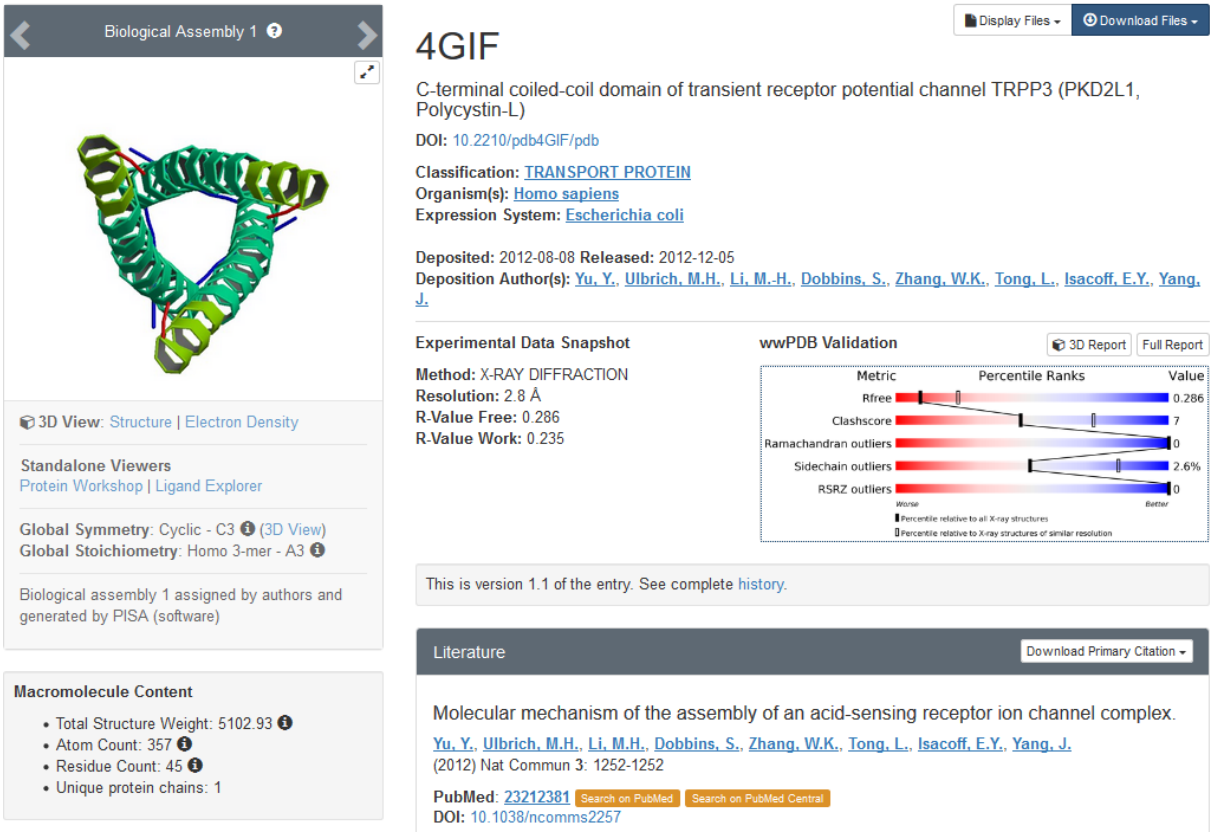
4gif for paper 3 – symmetry

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 4gif_refine_001_complete.pdb_modified_Pavel16March.pdb PDB file (yellow) and the expansion.pdb (blue)





II. Model preparation (Pavel 16March, redone by Goska)

1. phenix.fetch_pdb --mtz 4gif
    a. 4gif.mtz
    b. 4gif.pdb
2. phenix.refine 4gif.{pdb,mtz} ordered_solvent=true ordered_solvent.low_res=3
    a. 4gif_refine_001.pdb
    b. 4gif_refine_001.mtz
3. qr.finalise 4gif_refine_001.pdb
    a. 4gif_refine_001_complete.pdb
4. phenix.pdbtools 4gif_refine_001_complete.pdb occupancies.set=0 modify.selection="element H"
    a. 4gif_refine_001_complete.pdb_modified.pdb

III. Refinements have been done with

1. **Xtb** : xtb.6.0 gfn2+water solvent (--gfn 2 --etemp 500 --acc 0.1 --gbsa h2o)

    qr@cu38

    nohup qr.refine 4gif_refine_001_complete.pdb_modified_Pavel16March.pdb 4gif_fresh_ready_again_refine_001.mtz mode=refine quantum.nproc=1 parallel.nproc=14 max_bond_rmsd=0.02 stpmax=0.2 gradient_only=true clustering=true use_convergence_test=true opt_log=1 restraints=qm engine_name=xtb > 4gif_refine_001_complete.pdb_modified_Pavel16March_xtb_stpmax02_dev-3407_MaxItRef100.log 2>&1 &

    second refinement with max_iterations_refine=100

2. **TeraChem** : TeraChem v1.93P , HF-D3/6-31G plus water solvent with COSMO model

    [qr@mu 4gif]

    #!/bin/bash

    nohup qr.refine 4gif_refine_001_complete.pdb_modified_Pavel16March.pdb 4gif_fresh_ready_again_refine_001.mtz mode=refine max_bond_rmsd=0.02 stpmax=0.2 clustering=true restraints=qm parallel.method=lsf parallel.qsub_command="bsub -n 4 -q gpu" engine_name=terachem basis=6-31g opt_log=1 gradient_only=true use_convergence_test=true > 4gif_refine_001_complete.pdb_modified_Pavel16March_HF3D_631G_h2o_dev-3407.log &

    For xtb and TeraChem the same qr.refine options have been used (*described below*)

3. **Cctbx** and **Phenix** – 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= default=15, 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

IV. Results/comparison

		Re-refinement			
Metric	4gif.pdb	phenix	xtb50MaxItRef	xtb100MaxItRef	TeraChem
R factors					
R work	0.235	0.2373	0.2557	0.2561	0.2466
R free	0.286	0.3025	0.2902	0.2920	0.2890
R free – R w	0.051	0.0652	0.0345	0.0359	0.0424
Ramachandran plot					
Favoured	43	43	43	43	43
Allowed					
Outliers	0	0	0	0	0
Rotamers					
Poor	2	0	1	1	0
Favoured	31	28	35	35	34
Clashscore		8.38	0	0	0
Cbeta devia	0				

Below are OLD results and comments

	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.