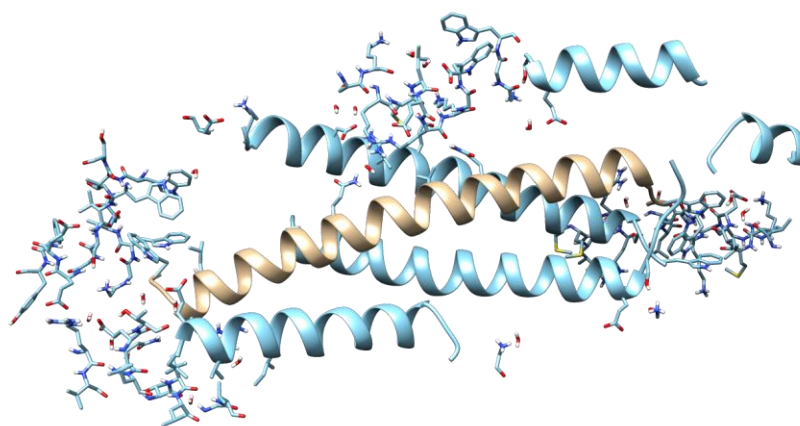


4gif for paper 3 – symmetry

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

It is 2.8 Å resolution, P₃₂₁ symmetry. Below a structure from PDB file 4gif_ready.pdb (yellow) and the expansion.pdb (blue)



Biological Assembly 1

3D View: [Structure](#) | [Electron Density](#)

Standalone Viewers
[Protein Workshop](#) | [Ligand Explorer](#)

Global Symmetry: Cyclic - C3 (3D View)
Global Stoichiometry: Homo 3-mer - A3

Biological assembly 1 assigned by authors and generated by PISA (software)

Macromolecule Content

- Total Structure Weight: 5102.93
- Atom Count: 357
- Residue Count: 45
- Unique protein chains: 1

4GIF

C-terminal coiled-coil domain of transient receptor potential channel TRPP3 (PKD2L1, Polycystin-L)

DOI: [10.2210/pdb4GIF/pdb](https://doi.org/10.2210/pdb4GIF/pdb)

Classification: [TRANSPORT PROTEIN](#)
Organism(s): [Homo sapiens](#)
Expression System: [Escherichia coli](#)

Deposited: 2012-08-08 Released: 2012-12-05
Deposition Author(s): [Yu, Y.](#), [Ulbrich, M.H.](#), [Li, M.-H.](#), [Dobbins, S.](#), [Zhang, W.K.](#), [Tong, L.](#), [Isacoff, E.Y.](#), [Yang, J.](#)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.8 Å
R-Value Free: 0.286
R-Value Work: 0.235

wwPDB Validation

Metric	Percentile Ranks	Value
Rfree		0.286
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		2.6%
RSRZ outliers		0

Worse | Better
■ Percentile relative to all X-ray structures
■ Percentile relative to X-ray structures of similar resolution

This is version 1.1 of the entry. See complete [history](#).

Literature

[Download Primary Citation](#)

Molecular mechanism of the assembly of an acid-sensing receptor ion channel complex.

[Yu, Y.](#), [Ulbrich, M.H.](#), [Li, M.H.](#), [Dobbins, S.](#), [Zhang, W.K.](#), [Tong, L.](#), [Isacoff, E.Y.](#), [Yang, J.](#)
(2012) Nat Commun 3: 1252-1252

PubMed: [23212381](#) [Search on PubMed](#) [Search on PubMed Central](#)
DOI: [10.1038/ncomms2257](https://doi.org/10.1038/ncomms2257)

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 weight 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

maxum_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

qrefine / paper-3-non-p1

Unwatch 5 Star 0 Fork 0

Code Issues 1 Pull requests 0 Projects 0 Wiki Insights

Data storage for paper 3 (non-P1 space group)

38 commits 1 branch 0 releases 7 contributors

Branch: master New pull request Create new file Upload files Find file Clone or download

biczysko 4gif refined with cctbx Latest commit 47054fa 32 minutes ago

- 4gif_TeraChem_water_refined_dev-3... 4gif refined with TeraChem 8 days ago
- 4gif_cctbx_opt_dev-3407 4gif optimized cctbx 34 minutes ago
- 4gif_cctbx_refined_dev-3407 4gif refined with cctbx 32 minutes ago
- 4gif_xtb_water_opt_dev-3407 4gif optimized with xtb 2 days ago
- 4gif_xtb_water_refined_dev-3407_OK 4gif refined with xtb 8 days ago

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

Metric	Re-refinement				Optimization		
	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.