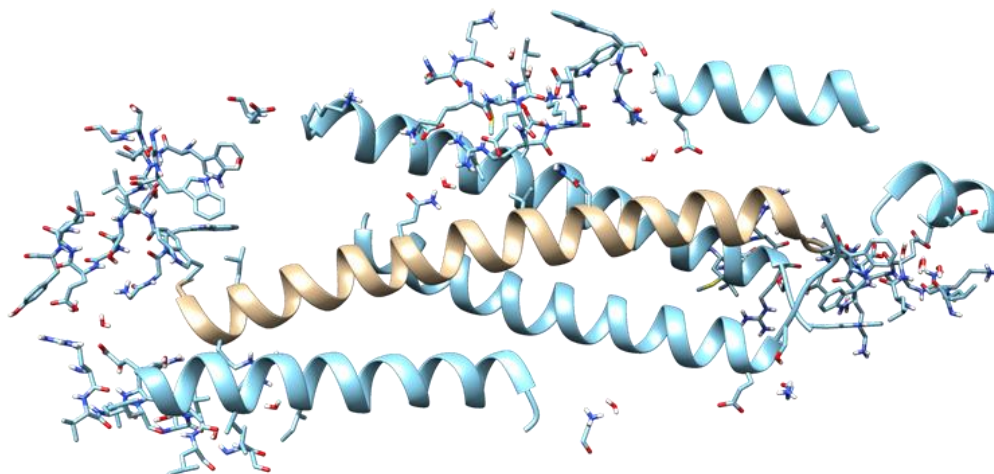


4gif for paper 3 – symmetry

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 4gif_refine_001_complete.pdb_modified_Pavel16March.pdb PDB file (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

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. 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

maximum_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

Metric	Re-refinement				
	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

Metric	Re-refinement				Optimization		
	4gif.pdb	cctbx	xtb	TeraChem	cctbx	xtb	TeraChem running
R factors							
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.