Supplementary information for:

# *Plasmodium falciparum* Acyl Carrier Protein Crystal Structures in Disulfide-linked and Reduced States and their Prevalence during Blood Stage Growth.

John R. Gallagher, Sean T. Prigge

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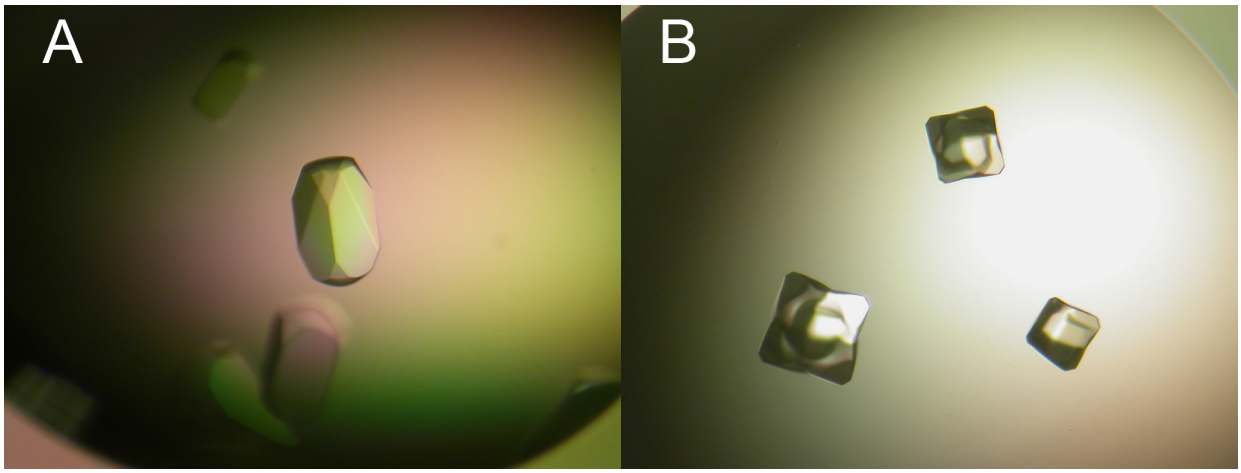



**FIGURE S1**
Crystals of (A) disulfide-linked *Pf*ACP and (B) reduced *Pf*ACP.

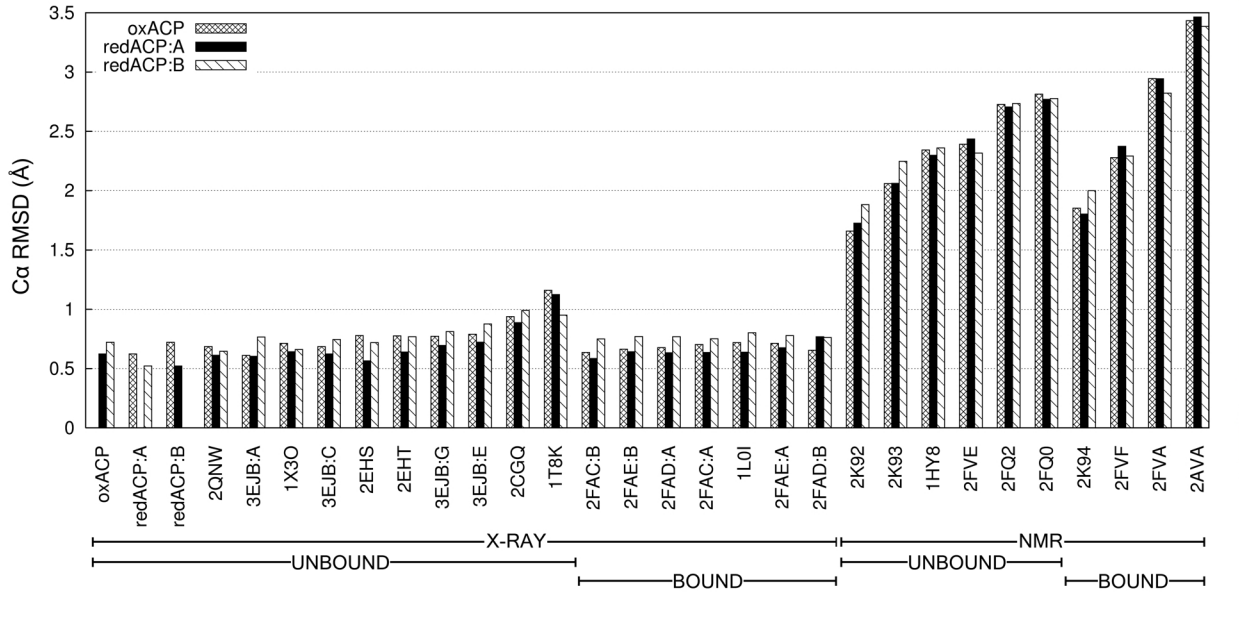



**FIGURE S2**
RMSD vales between reported *Pf*ACP structures and the existing family of ACP structures. Disulfide-linked *Pf*ACP is labeled "oxACP", and reduced *Pf*ACP is labeled "redACP." The structure determination method and liganded state are indicated below the corresponding Protein Data Bank accession codes.

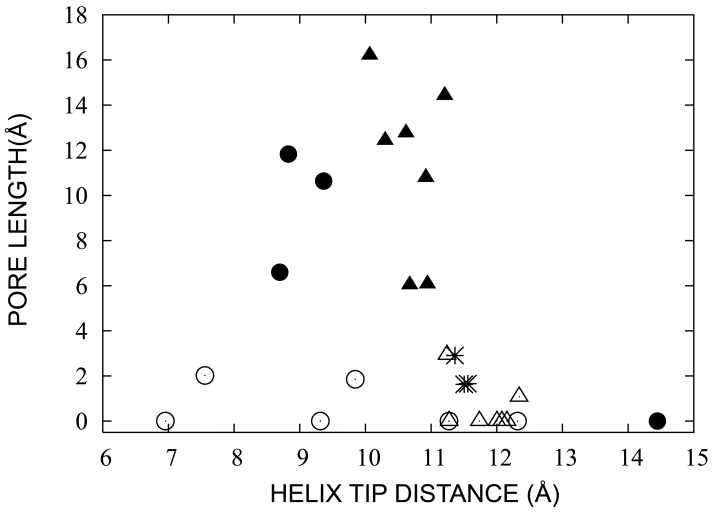



**FIGURE S3**

Test of the "helix tip distance model." Comparing the distance between N-terminal tips of helices 2 and 3 with observed pore length for representative ACP structures shows no correlation when considering both NMR and crystal structures. Circles represent NMR structures and triangles represent x-ray structures. Filled symbols represent structures with bound ligand and open symbols represent structures without ligand. Asterisks denote *Pf*ACP structures reported here.

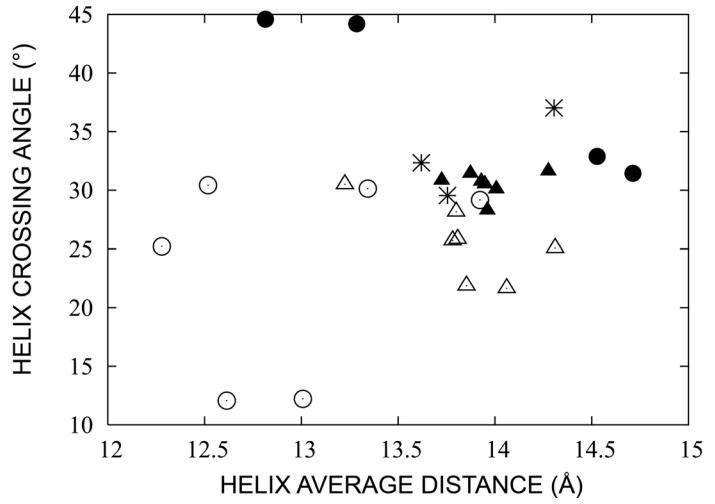



**FIGURE S4**

Comparing the crossing angle of helices 2 and 4 with the average distance between helices 2 and 4 for representative ACP structures shows no correlation. Circles represent NMR structures and triangles represent x-ray structures. Filled symbols represent structures with bound ligand and open symbols represent structures without ligand. Asterisks denote *Pf*ACP structures reported here.

| Resolution | #Data | #Theory | %Complete | Redundancy | Mean I | Mean I/s | R(int) | Rsigma |
|---|---|---|---|---|---|---|---|---|
| Inf - 6.80 | 201 | 211 | 95.3 | 4.62 | 955.8 | 19.87 | 0.0626 | 0.0518 |
| 6.80 - 5.35 | 209 | 209 | 100.0 | 5.66 | 257.9 | 22.45 | 0.0551 | 0.0423 |
| 5.35 - 4.70 | 201 | 201 | 100.0 | 5.84 | 378.2 | 23.40 | 0.0525 | 0.0419 |
| 4.70 - 4.26 | 208 | 208 | 100.0 | 5.90 | 361.5 | 22.73 | 0.0534 | 0.0418 |
| 4.26 - 3.94 | 208 | 208 | 100.0 | 5.93 | 255.9 | 22.13 | 0.0555 | 0.0421 |
| 3.94 - 3.71 | 206 | 206 | 100.0 | 5.93 | 169.3 | 20.71 | 0.0643 | 0.0432 |
| 3.71 - 3.51 | 206 | 206 | 100.0 | 6.04 | 113.2 | 18.95 | 0.0785 | 0.0452 |
| 3.51 - 3.36 | 215 | 215 | 100.0 | 5.99 | 61.5 | 15.96 | 0.0918 | 0.0516 |
| 3.36 - 3.23 | 210 | 210 | 100.0 | 6.07 | 44.0 | 14.17 | 0.1172 | 0.0576 |
| 3.23 - 3.11 | 218 | 218 | 100.0 | 6.09 | 31.6 | 11.80 | 0.1266 | 0.0675 |
| 3.11 - 3.01 | 210 | 210 | 100.0 | 6.04 | 26.1 | 10.79 | 0.1426 | 0.0757 |
| 3.01 - 2.93 | 207 | 207 | 100.0 | 6.10 | 17.7 | 8.75 | 0.1788 | 0.0954 |
| 2.93 - 2.84 | 228 | 228 | 100.0 | 6.08 | 13.6 | 7.39 | 0.1972 | 0.1177 |
| 2.84 - 2.77 | 210 | 210 | 100.0 | 6.01 | 11.5 | 6.52 | 0.2272 | 0.1356 |
| 2.77 - 2.71 | 200 | 200 | 100.0 | 5.78 | 11.9 | 6.53 | 0.2391 | 0.1368 |
| 2.71 - 2.65 | 229 | 229 | 100.0 | 5.65 | 8.1 | 4.64 | 0.3059 | 0.1925 |
| 2.65 - 2.59 | 237 | 237 | 100.0 | 5.31 | 7.7 | 4.41 | 0.2836 | 0.2058 |
| 2.59 - 2.54 | 207 | 207 | 100.0 | 4.53 | 6.9 | 3.66 | 0.3220 | 0.2498 |
| 2.54 - 2.49 | 171 | 177 | 96.6 | 3.22 | 4.6 | 2.32 | 0.3700 | 0.4526 |
| 2.59 - 2.49 | 441 | 447 | 98.7 | 4.09 | 5.9 | 3.14 | 0.3336 | 0.3108 |
| Inf - 2.49 | 3981 | 3997 | 99.6 | 5.64 | 140.9 | 12.95 | 0.0679 | 0.0504 |

Merged [A], lowest resolution = 43.55 Angstroms, 725 outliers downweighted

3981 Reflections after merging [A], R(int) = 0.0679, R(sigma) = 0.0504

**FIGURE S5**

Diffraction data statistics for disulfide-linked *Pf*ACP collected at 296K on one crystal, as reported by XPREP.

| Resolution | #Data | #Theory | %Complete | Redundancy | Mean I | Mean I/s | R(int) | Rsigma |
|---|---|---|---|---|---|---|---|---|
| Inf - 4.49 | 1093 | 1096 | 99.7 | 89.92 | 637.4 | 95.07 | 0.1453 | 0.0107 |
| 4.49 - 3.50 | 1103 | 1103 | 100.0 | 86.12 | 701.6 | 92.00 | 0.1711 | 0.0100 |
| 3.50 - 3.03 | 1116 | 1116 | 100.0 | 81.92 | 339.0 | 77.64 | 0.2037 | 0.0120 |
| 3.03 - 2.74 | 1116 | 1116 | 100.0 | 76.92 | 196.0 | 63.37 | 0.2247 | 0.0140 |
| 2.74 - 2.53 | 1146 | 1146 | 100.0 | 67.83 | 150.0 | 55.79 | 0.2202 | 0.0157 |
| 2.53 - 2.37 | 1141 | 1141 | 100.0 | 60.88 | 117.2 | 46.23 | 0.2464 | 0.0191 |
| 2.37 - 2.25 | 1107 | 1107 | 100.0 | 55.90 | 96.6 | 39.70 | 0.2604 | 0.0224 |
| 2.25 - 2.15 | 1105 | 1105 | 100.0 | 52.32 | 72.9 | 32.08 | 0.2896 | 0.0275 |
| 2.15 - 2.06 | 1186 | 1186 | 100.0 | 48.87 | 57.5 | 26.22 | 0.3242 | 0.0340 |
| 2.06 - 1.98 | 1239 | 1239 | 100.0 | 45.33 | 41.2 | 20.02 | 0.3672 | 0.0444 |
| 1.98 - 1.91 | 1250 | 1250 | 100.0 | 42.50 | 25.3 | 13.65 | 0.4759 | 0.0684 |
| 1.91 - 1.85 | 1226 | 1226 | 100.0 | 39.11 | 17.6 | 9.89 | 0.5568 | 0.0960 |
| 1.85 - 1.80 | 1159 | 1159 | 100.0 | 36.91 | 13.1 | 7.65 | 0.6600 | 0.1276 |
| 1.80 - 1.75 | 1275 | 1275 | 100.0 | 33.30 | 10.0 | 5.77 | 0.7661 | 0.1727 |
| 1.75 - 1.71 | 1131 | 1131 | 100.0 | 28.02 | 7.4 | 4.04 | 0.8687 | 0.2518 |
| 1.71 - 1.67 | 1270 | 1270 | 100.0 | 22.62 | 6.7 | 3.20 | 0.9934 | 0.3199 |
| 1.67 - 1.63 | 1370 | 1370 | 100.0 | 12.79 | 10.6 | 3.13 | 1.0091 | 0.3152 |
| 1.63 - 1.60 | 1109 | 1120 | 99.0 | 6.15 | 22.8 | 2.93 | 0.9572 | 0.3019 |
| 1.60 - 1.55 | 681 | 1729 | 39.4 | 0.92 | 37.0 | 2.08 | 0.5786 | 0.3563 |
| 1.65 - 1.55 | 2841 | 3900 | 72.8 | 5.18 | 22.2 | 2.85 | 0.9493 | 0.3242 |
| Inf - 1.55 | 21823 | 22885 | 95.4 | 44.77 | 130.3 | 31.05 | 0.1986 | 0.0252 |

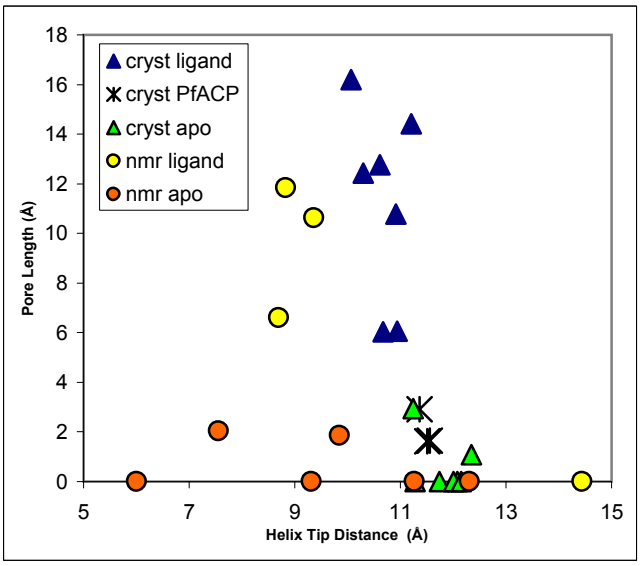
Merged [A], lowest resolution = 54.18 Angstroms, 309907 outliers downweighted

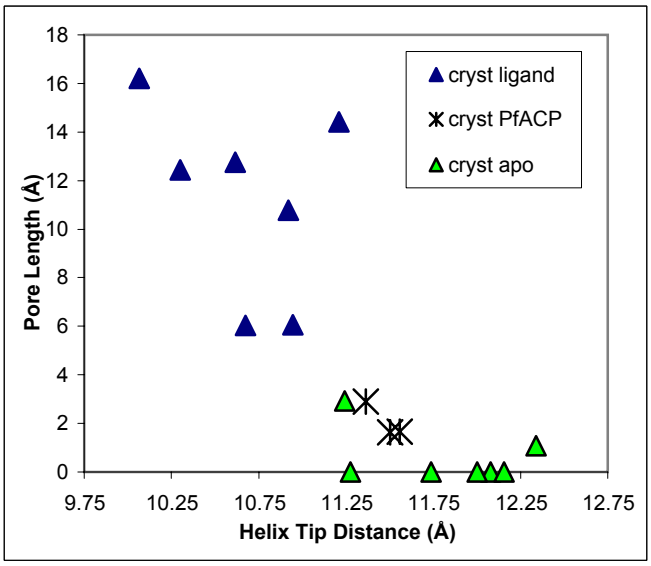
21823 Reflections after merging [A], R(int) = 0.1986, R(sigma) = 0.0252

**FIGURE S6**

Diffraction data statistics for reduced *Pf*ACP collected at 100K on 4 crystals, as reported by XPREP.

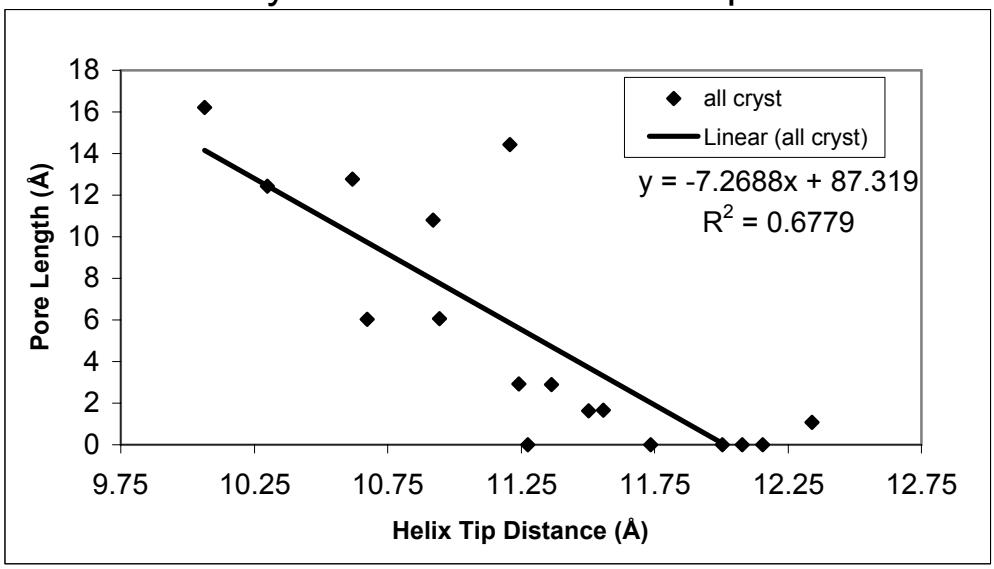
# Pore Length vs. "Helix Tip Distance"




| pdbFile | helix Tip Dist (Å) | CAVER Pore Length (Å) | crystal | ligand | PfACP crystal |
|---|---|---|---|---|---|
| 2FQ2 | 11.272 | 0 | 0 | 0 | 0 |
| 2FVE | 9.314 | 0 | 0 | 0 | 0 |
| 1HY8 | 9.844 | 1.8575 | 0 | 0 | 0 |
| 2K93 | 7.557 | 2.0252 | 0 | 0 | 0 |
| 2FQ0 | 12.315 | 0 | 0 | 0 | 0 |
| 2K92 | 6.954 | 0 | 0 | 0 | 0 |
| 2AVA | 8.696 | 6.5995 | 0 | 1 | 0 |
| 2K94 | 14.446 | 0 | 0 | 1 | 0 |
| 2FVF | 9.364 | 10.6338 | 0 | 1 | 0 |
| 2FVA | 8.825 | 11.835 | 0 | 1 | 0 |
| 2CGQ | 11.736 | 0 | 1 | 0 | 0 |
| 2EHS | 12.078 | 0 | 1 | 0 | 0 |
| 2EHT | 12.003 | 0 | 1 | 0 | 0 |
| 2QNW | 11.241 | 2.9297 | 1 | 0 | 0 |
| 1X3O | 11.275 | 0 | 1 | 0 | 0 |
| 1T8K | 12.34 | 1.0769 | 1 | 0 | 0 |
| 1L0H | 12.156 | 0 | 1 | 0 | 0 |
| redPfACP:A | 11.364 | 2.9057 | 1 | 0 | 1 |
| redPfACP:B | 11.504 | 1.6284 | 1 | 0 | 1 |
| oxPfACP | 11.558 | 1.6594 | 1 | 0 | 1 |
| 2FAD:A | 10.617 | 12.7641 | 1 | 1 | 0 |
| 2FAC:B | 10.921 | 10.7897 | 1 | 1 | 0 |
| 2FAE:A | 10.3 | 12.4318 | 1 | 1 | 0 |
| 2FAE:B | 11.208 | 14.4232 | 1 | 1 | 0 |
| 2FAD:B | 10.945 | 6.0697 | 1 | 1 | 0 |
| 1L0I | 10.674 | 6.0335 | 1 | 1 | 0 |
| 2FAC:A | 10.065 | 16.2071 | 1 | 1 | 0 |

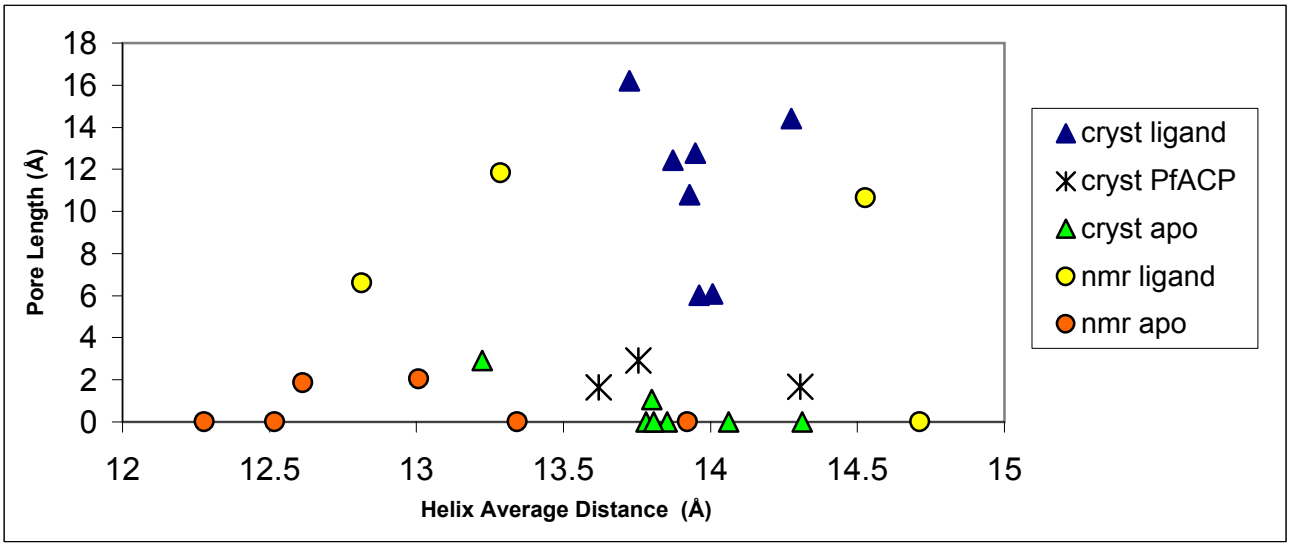
# Linear Fit of X-Ray Structures for "Helix Tip Distance"




Positions Homlogous to EcACP T39-D56

| | | | | |
|---|---|---|---|---|
| VAL | 39 | ASP | 56 | 1HY8.pdb |
| THR | 39 | ASP | 56 | 1L0H.pdb |
| THR | 39 | ASP | 56 | 1L0I.pdb |
| THR | 39 | ASP | 56 | 1T8K.pdb |
| THR | 42 | ASP | 59 | 1X3O.pdb |
| THR | 41 | GLU | 58 | 2AVA.pdb |
| LEU | 36 | PHE | 53 | 2CGQ.pdb |
| VAL | 38 | ASP | 55 | 2EHS.pdb |
| VAL | 38 | ASP | 55 | 2EHT.pdb |
| THR | 39 | ASP | 56 | 2FAC:A.pdb |
| THR | 39 | ASP | 56 | 2FAC:B.pdb |
| THR | 39 | ASP | 56 | 2FAD:A.pdb |
| THR | 39 | ASP | 56 | 2FAD:B.pdb |
| THR | 39 | ASP | 56 | 2FAE:A.pdb |
| THR | 39 | ASP | 56 | 2FAE:B.pdb |
| LEU | 40 | ASP | 57 | 2FQ0.pdb |
| LEU | 40 | ASP | 57 | 2FQ2.pdb |
| THR | 41 | GLU | 58 | 2FVA.pdb |
| THR | 41 | GLU | 58 | 2FVE.pdb |
| THR | 41 | GLU | 58 | 2FVF.pdb |
| THR | 39 | ASP | 56 | 2K92.pdb |
| THR | 39 | ASP | 56 | 2K93.pdb |
| THR | 39 | ASP | 56 | 2K94.pdb |
| SER | 44 | ASP | 61 | 2QNW.pdb |
| LEU | 42 | ASP | 59 | redPfACP:A.pdb |
| LEU | 42 | ASP | 59 | redPfACP:B.pdb |
| LEU | 42 | ASP | 59 | oxPfACP.pdb |

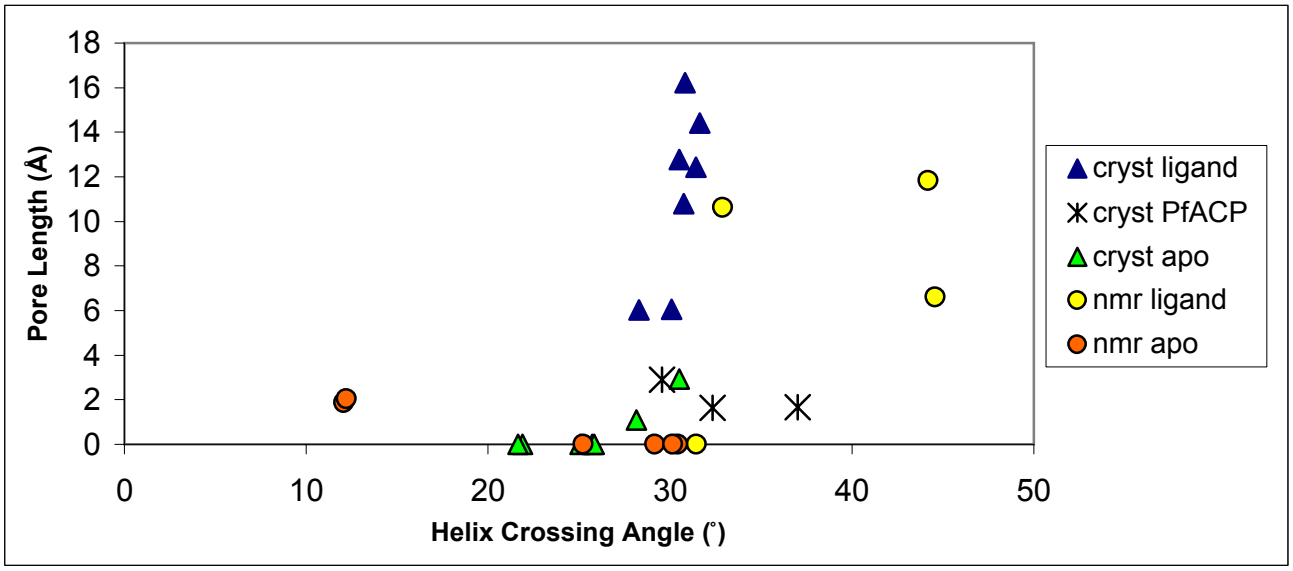
# Pore Length vs. Helix Distance




Data for helices 2 and 3

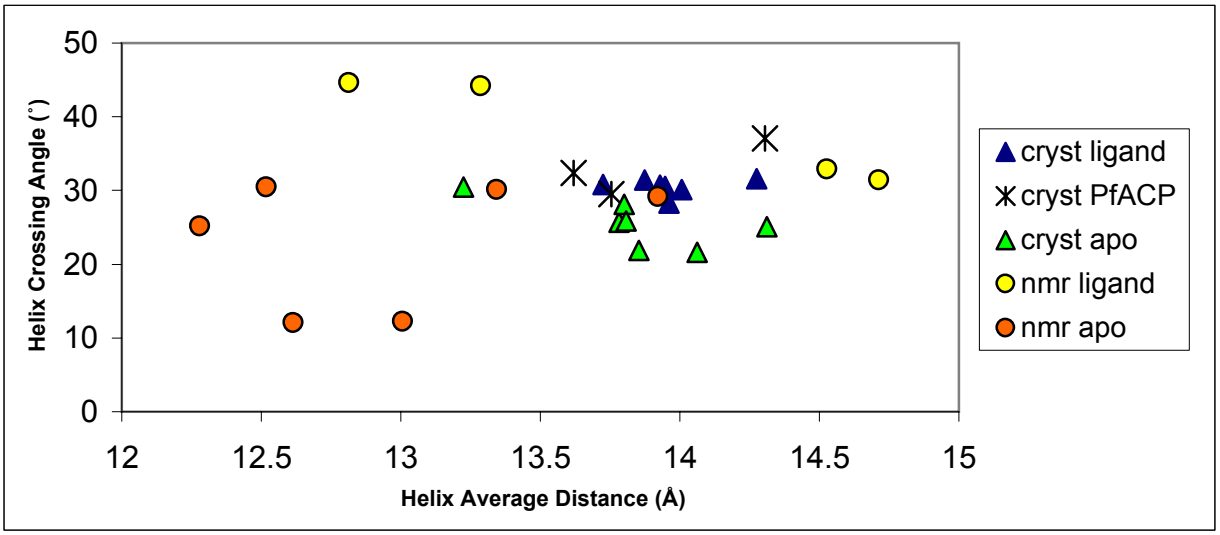
| pdbFile | Helix Dist (Å) | CAVER Pore Length (Å) | cryst | ligand | PfACP crystal |
|---|---|---|---|---|---|
| 2FQ2 | 12.5185 | 0 | 0 | 0 | 0 |
| 2FVE | 13.923 | 0 | 0 | 0 | 0 |
| 1HY8 | 12.614 | 1.8575 | 0 | 0 | 0 |
| 2K93 | 13.008 | 2.0252 | 0 | 0 | 0 |
| 2FQ0 | 12.2795 | 0 | 0 | 0 | 0 |
| 2K92 | 13.343 | 0 | 0 | 0 | 0 |
| 2AVA | 12.8145 | 6.5995 | 0 | 1 | 0 |
| 2K94 | 14.713 | 0 | 0 | 1 | 0 |
| 2FVF | 14.528 | 10.6338 | 0 | 1 | 0 |
| 2FVA | 13.286 | 11.835 | 0 | 1 | 0 |
| 2CGQ | 14.311 | 0 | 1 | 0 | 0 |
| 2EHS | 13.853 | 0 | 1 | 0 | 0 |
| 2EHT | 14.061 | 0 | 1 | 0 | 0 |
| 2QNW | 13.2245 | 2.9297 | 1 | 0 | 0 |
| 1X3O | 13.7815 | 0 | 1 | 0 | 0 |
| 1T8K | 13.8 | 1.0769 | 1 | 0 | 0 |
| 1L0H | 13.8075 | 0 | 1 | 0 | 0 |
| redPfACP:A | 13.755 | 2.9057 | 1 | 0 | 1 |
| redPfACP:B | 13.62 | 1.6284 | 1 | 0 | 1 |
| oxPfACP | 14.305 | 1.6594 | 1 | 0 | 1 |
| 2FAD:A | 13.948 | 12.7641 | 1 | 1 | 0 |
| 2FAC:B | 13.929 | 10.7897 | 1 | 1 | 0 |
| 2FAE:A | 13.873 | 12.4318 | 1 | 1 | 0 |
| 2FAE:B | 14.276 | 14.4232 | 1 | 1 | 0 |
| 2FAD:B | 14.007 | 6.0697 | 1 | 1 | 0 |
| 1L0I | 13.961 | 6.0335 | 1 | 1 | 0 |
| 2FAC:A | 13.7245 | 16.2071 | 1 | 1 | 0 |

# Helix Crossing Angle vs. Pore Length




| pdbFile | Helix Angle (° | CAVER Pore Length (Á) | cryst | ligand | PfACP Crystal |
|---|---|---|---|---|---|
| 2FQ2 | 30.4266 | 0 | 0 | 0 | 0 |
| 2FVE | 29.1612 | 0 | 0 | 0 | 0 |
| 1HY8 | 12.0675 | 1.8575 | 0 | 0 | 0 |
| 2K93 | 12.2236 | 2.0252 | 0 | 0 | 0 |
| 2FQ0 | 25.2164 | 0 | 0 | 0 | 0 |
| 2K92 | 30.1441 | 0 | 0 | 0 | 0 |
| 2AVA | 44.5943 | 6.5995 | 0 | 1 | 0 |
| 2K94 | 31.4511 | 0 | 0 | 1 | 0 |
| 2FVF | 32.8832 | 10.6338 | 0 | 1 | 0 |
| 2FVA | 44.2044 | 11.835 | 0 | 1 | 0 |
| 2CGQ | 25.0653 | 0 | 1 | 0 | 0 |
| 2EHS | 21.8701 | 0 | 1 | 0 | 0 |
| 2EHT | 21.6547 | 0 | 1 | 0 | 0 |
| 2QNW | 30.4957 | 2.9297 | 1 | 0 | 0 |
| 1X3O | 25.7073 | 0 | 1 | 0 | 0 |
| 1T8K | 28.1617 | 1.0769 | 1 | 0 | 0 |
| 1L0H | 25.8288 | 0 | 1 | 0 | 0 |
| redPfACP:A | 29.5488 | 2.9057 | 1 | 0 | 1 |
| redPfACP:B | 32.3367 | 1.6284 | 1 | 0 | 1 |
| oxPfACP | 37.0286 | 1.6594 | 1 | 0 | 1 |
| 2FAD:A | 30.5179 | 12.7641 | 1 | 1 | 0 |
| 2FAC:B | 30.7428 | 10.7897 | 1 | 1 | 0 |
| 2FAE:A | 31.4234 | 12.4318 | 1 | 1 | 0 |
| 2FAE:B | 31.6199 | 14.4232 | 1 | 1 | 0 |
| 2FAD:B | 30.0963 | 6.0697 | 1 | 1 | 0 |
| 1L0I | 28.2864 | 6.0335 | 1 | 1 | 0 |
| 2FAC:A | 30.8338 | 16.2071 | 1 | 1 | 0 |

# Helix Crossing Angle vs. Helix Distance




| | Data for helices 2 and 4 | Data for helices 2 and 3 | | | |
|---|---|---|---|---|---|
| pdbFile | Helix Angle (°) | Helix Dist (Á) | cryst | ligand | PfACP Crystal |
| 2FQ2 | 30.4266 | 12.5185 | 0 | 0 | 0 |
| 2FVE | 29.1612 | 13.923 | 0 | 0 | 0 |
| 1HY8 | 12.0675 | 12.614 | 0 | 0 | 0 |
| 2K93 | 12.2236 | 13.008 | 0 | 0 | 0 |
| 2FQ0 | 25.2164 | 12.2795 | 0 | 0 | 0 |
| 2K92 | 30.1441 | 13.343 | 0 | 0 | 0 |
| 2AVA | 44.5943 | 12.8145 | 0 | 1 | 0 |
| 2K94 | 31.4511 | 14.713 | 0 | 1 | 0 |
| 2FVF | 32.8832 | 14.528 | 0 | 1 | 0 |
| 2FVA | 44.2044 | 13.286 | 0 | 1 | 0 |
| 2CGQ | 25.0653 | 14.311 | 1 | 0 | 0 |
| 2EHS | 21.8701 | 13.853 | 1 | 0 | 0 |
| 2EHT | 21.6547 | 14.061 | 1 | 0 | 0 |
| 2QNW | 30.4957 | 13.2245 | 1 | 0 | 0 |
| 1X3O | 25.7073 | 13.7815 | 1 | 0 | 0 |
| 1T8K | 28.1617 | 13.8 | 1 | 0 | 0 |
| 1L0H | 25.8288 | 13.8075 | 1 | 0 | 0 |
| redPfACP:A | 29.5488 | 13.755 | 1 | 0 | 1 |
| redPfACP:B | 32.3367 | 13.62 | 1 | 0 | 1 |
| oxPfACP | 37.0286 | 14.305 | 1 | 0 | 1 |
| 2FAD:A | 30.5179 | 13.948 | 1 | 1 | 0 |
| 2FAC:B | 30.7428 | 13.929 | 1 | 1 | 0 |
| 2FAE:A | 31.4234 | 13.873 | 1 | 1 | 0 |
| 2FAE:B | 31.6199 | 14.276 | 1 | 1 | 0 |
| 2FAD:B | 30.0963 | 14.007 | 1 | 1 | 0 |
| 1L0I | 28.2864 | 13.961 | 1 | 1 | 0 |
| 2FAC:A | 30.8338 | 13.7245 | 1 | 1 | 0 |