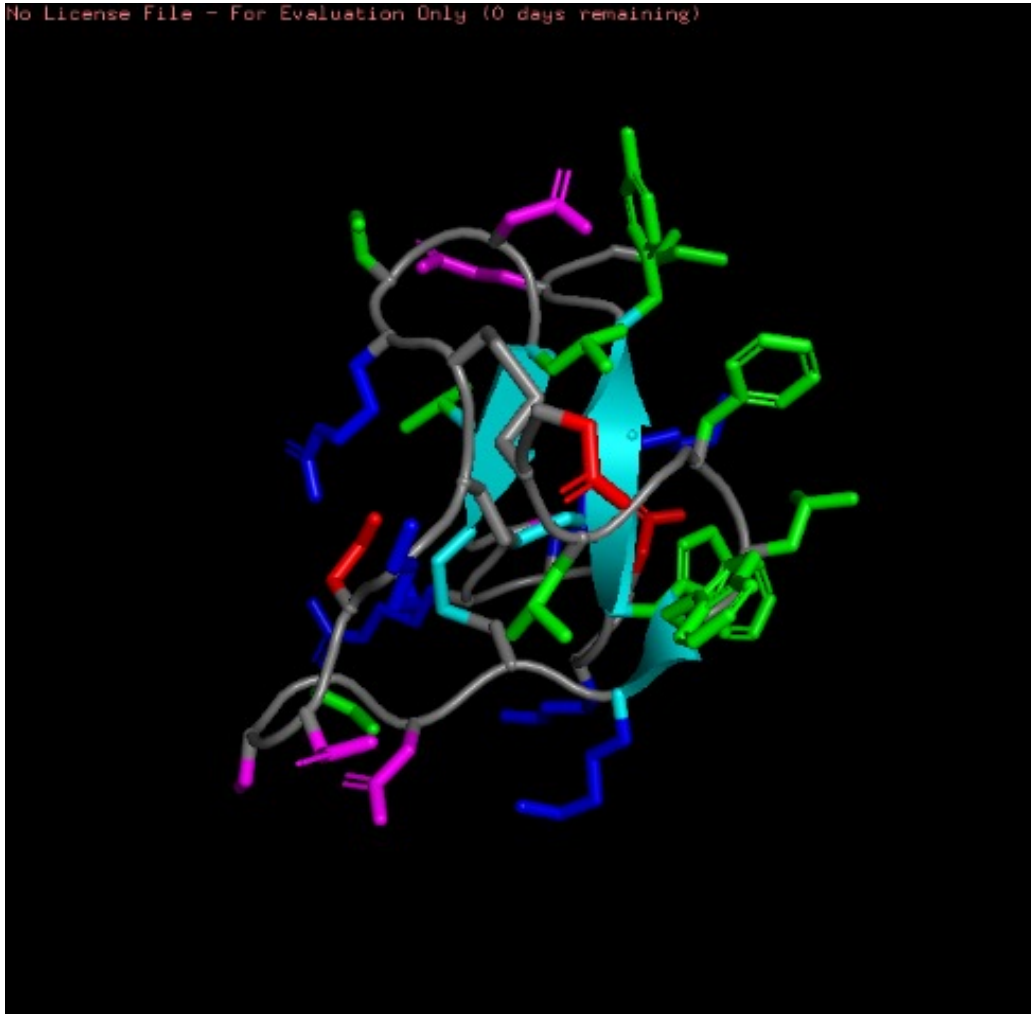
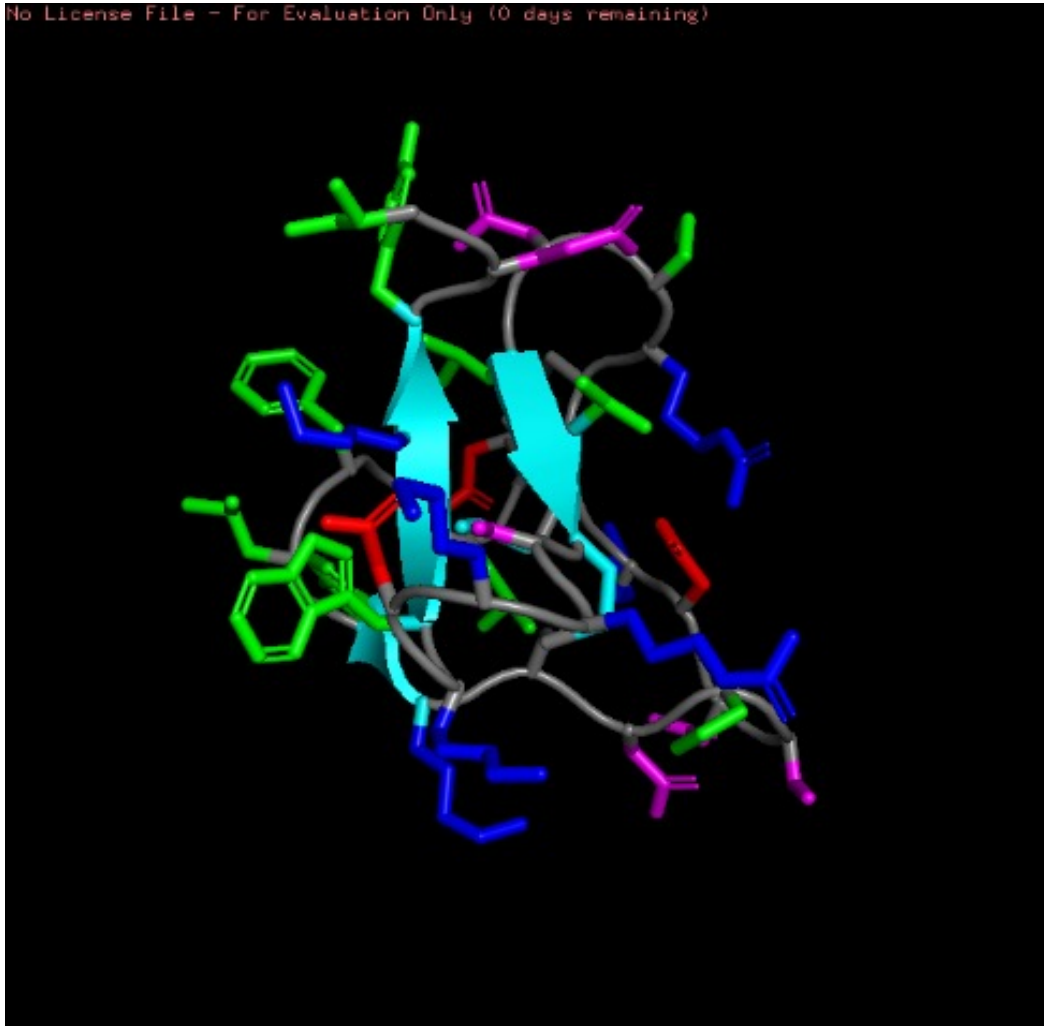
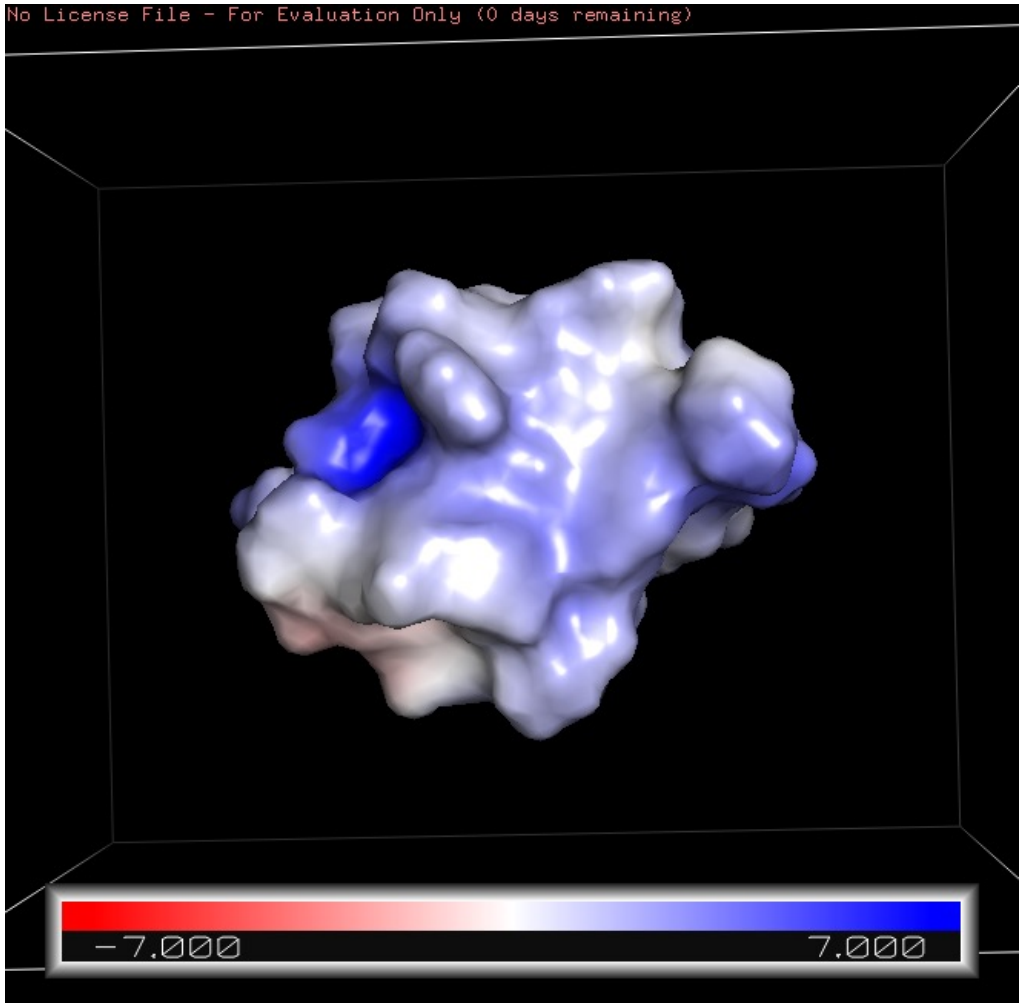
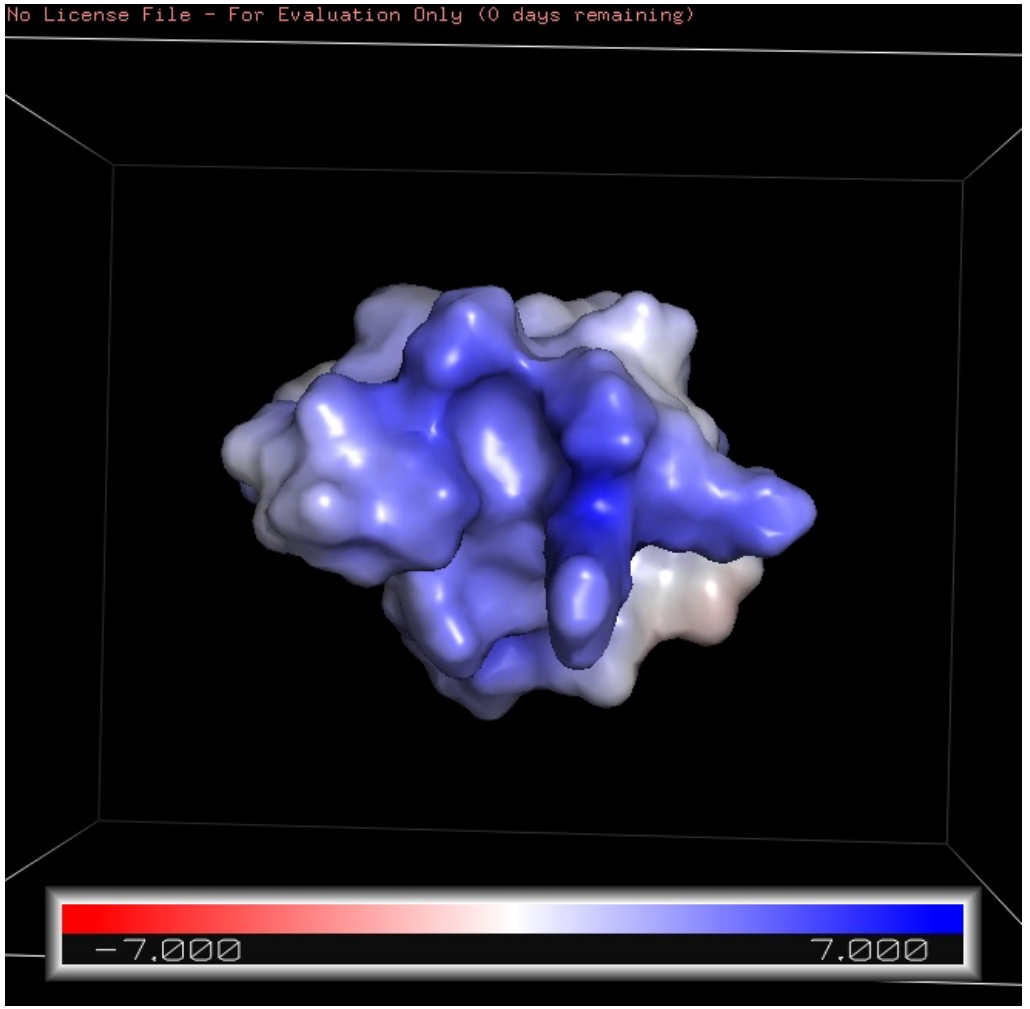
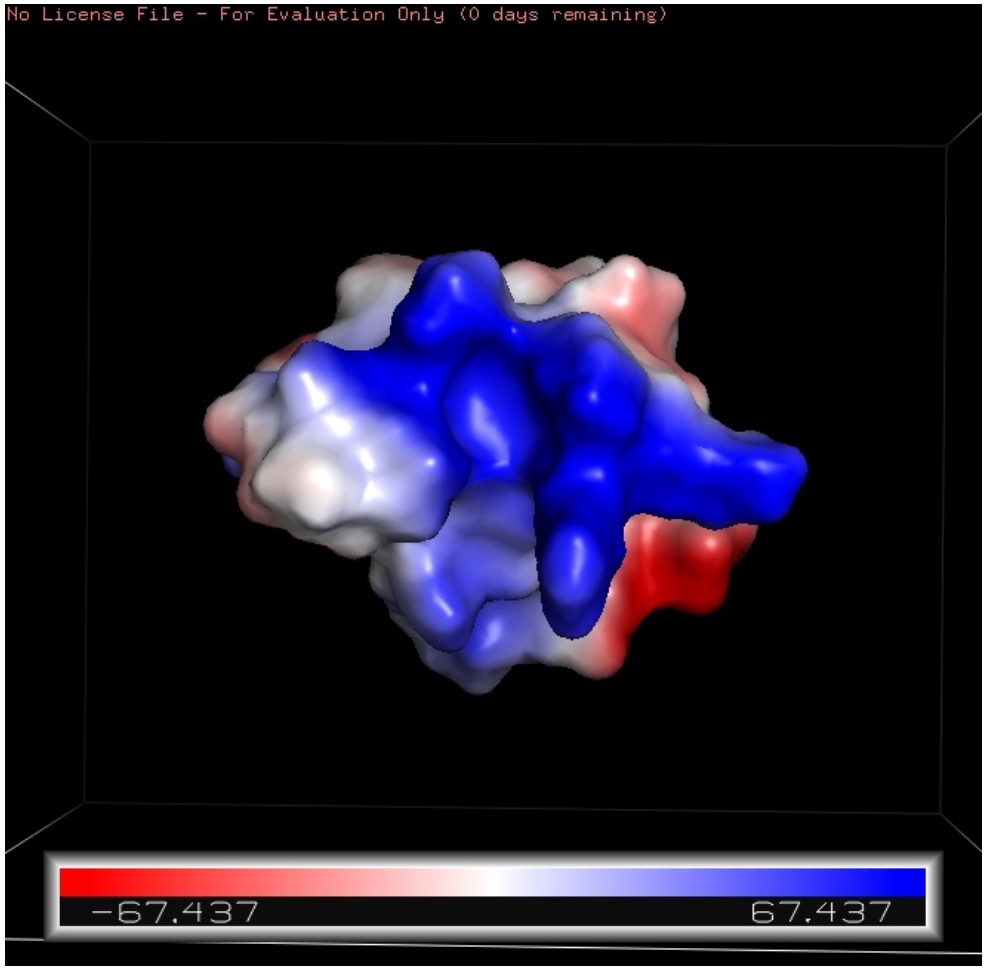
5WE3 (PaurTx-3)

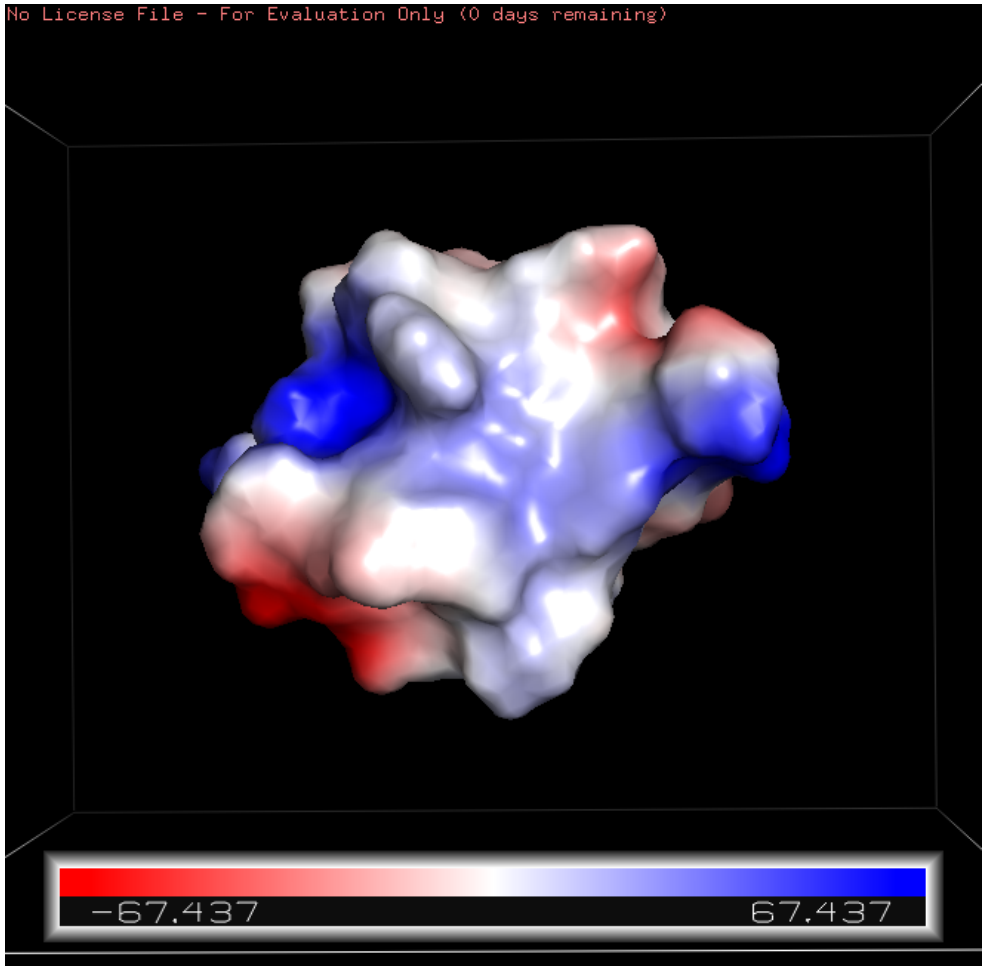


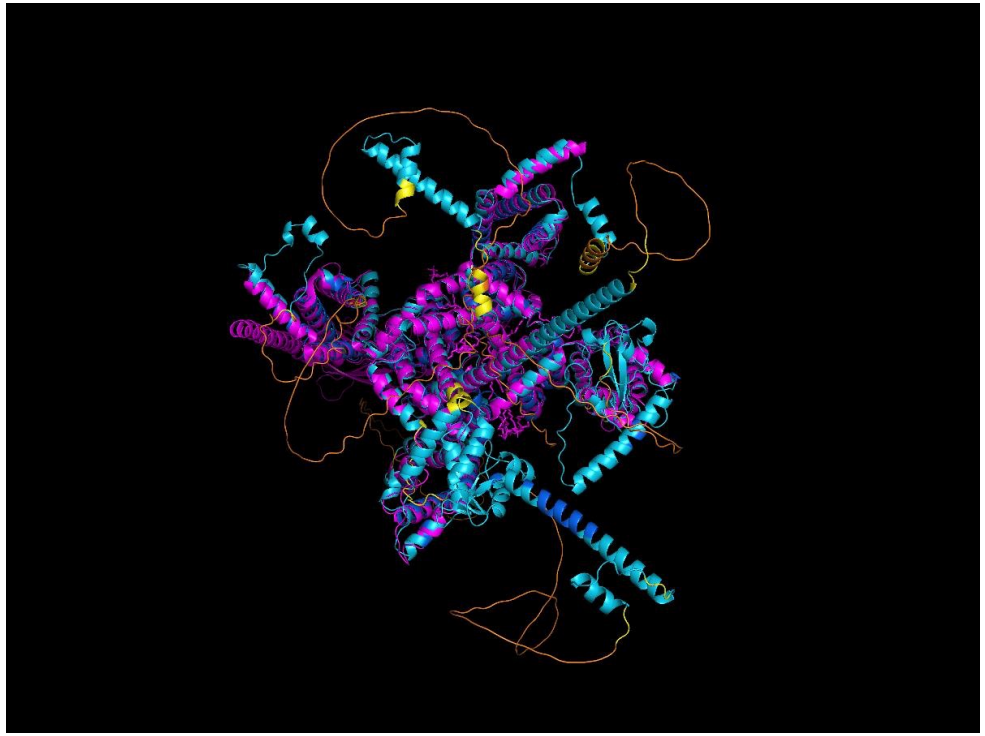


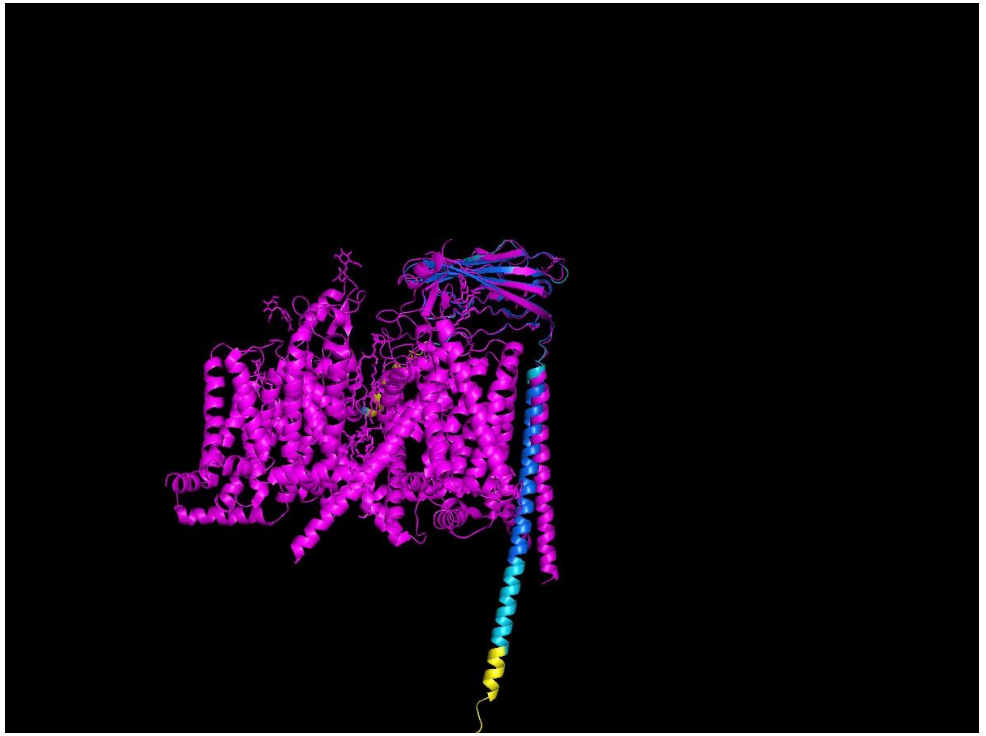

No License File - For Evaluation Only (0 days remaining)
−7.000
7.000


No License File - For Evaluation Only (0 days remaining)
−7.000
7.000


No License File - For Evaluation Only (0 days remaining)
-67.437
67.437


No License File - For Evaluation Only (0 days remaining)
-67.437
67.437





```
PyMOL>super chainA_obj, af3_model_a
 MatchAlign: aligning residues (1879 vs 1879)...
 MatchAlign: score 4006.245
 ExecutiveAlign: 8896 atoms aligned.
 ExecutiveRMS: 340 atoms rejected during cycle 1 (RMSD=7.92).
 ExecutiveRMS: 475 atoms rejected during cycle 2 (RMSD=2.05).
 ExecutiveRMS: 470 atoms rejected during cycle 3 (RMSD=1.38).
 ExecutiveRMS: 317 atoms rejected during cycle 4 (RMSD=1.16).
 ExecutiveRMS: 220 atoms rejected during cycle 5 (RMSD=1.06).
 Executive: RMSD =    0.999 (7065 to 7065 atoms)
```

```
PyMOL>align chainA_obj and name N+CA+C+O, af3_model_a and name N+CA+C+O
 Match: read scoring matrix.
 Match: assigning 1879 x 1879 pairwise scores.
 MatchAlign: aligning residues (1879 vs 1879)...
 MatchAlign: score 9933.000
 ExecutiveAlign: 5293 atoms aligned.
 ExecutiveRMS: 176 atoms rejected during cycle 1 (RMSD=1.32).
 ExecutiveRMS: 158 atoms rejected during cycle 2 (RMSD=0.98).
 ExecutiveRMS: 83 atoms rejected during cycle 3 (RMSD=0.89).
 ExecutiveRMS: 41 atoms rejected during cycle 4 (RMSD=0.86).
 ExecutiveRMS: 21 atoms rejected during cycle 5 (RMSD=0.85).
 Executive: RMSD =    0.842 (4073 to 4073 atoms)
```

```
PyMOL>align chainA_obj, af3_model_a
 Match: read scoring matrix.
 Match: assigning 1886 x 1879 pairwise scores.
 MatchAlign: aligning residues (1886 vs 1879)...
 MatchAlign: score 9933.000
 ExecutiveAlign: 9904 atoms aligned.
 ExecutiveRMS: 413 atoms rejected during cycle 1 (RMSD=1.87).
 ExecutiveRMS: 505 atoms rejected during cycle 2 (RMSD=1.32).
 ExecutiveRMS: 366 atoms rejected during cycle 3 (RMSD=1.12).
 ExecutiveRMS: 232 atoms rejected during cycle 4 (RMSD=1.02).
 ExecutiveRMS: 134 atoms rejected during cycle 5 (RMSD=0.97).
 Executive: RMSD =    0.940 (7513 to 7513 atoms)
```

```
PyMOL>super chainB_obj, af3_model_b
 MatchAlign: aligning residues (218 vs 218)...
 MatchAlign: score 773.929
 ExecutiveAlign: 1382 atoms aligned.
 ExecutiveRMS: 71 atoms rejected during cycle 1 (RMSD=2.86).
 ExecutiveRMS: 64 atoms rejected during cycle 2 (RMSD=2.36).
 ExecutiveRMS: 56 atoms rejected during cycle 3 (RMSD=1.97).
 ExecutiveRMS: 68 atoms rejected during cycle 4 (RMSD=1.67).
 ExecutiveRMS: 70 atoms rejected during cycle 5 (RMSD=1.40).
 Executive: RMSD =    1.174 (1053 to 1053 atoms)
```

```
PyMOL>align chainB_obj, af3_model_b
 Match: read scoring matrix.
 Match: assigning 220 x 218 pairwise scores.
 MatchAlign: aligning residues (220 vs 218)...
 MatchAlign: score 1120.000
 ExecutiveAlign: 1461 atoms aligned.
 ExecutiveRMS: 77 atoms rejected during cycle 1 (RMSD=2.87).
 ExecutiveRMS: 67 atoms rejected during cycle 2 (RMSD=2.38).
 ExecutiveRMS: 56 atoms rejected during cycle 3 (RMSD=2.02).
 ExecutiveRMS: 72 atoms rejected during cycle 4 (RMSD=1.72).
 ExecutiveRMS: 69 atoms rejected during cycle 5 (RMSD=1.44).
 Executive: RMSD =    1.219 (1075 to 1075 atoms)
```

```
PyMOL>align chainB_obj and name N+CA+C+O, af3_model_b and name N+CA+C+O
 Match: read scoring matrix.
 Match: assigning 218 x 218 pairwise scores.
 MatchAlign: aligning residues (218 vs 218)...
 MatchAlign: score 1120.000
 ExecutiveAlign: 737 atoms aligned.
 ExecutiveRMS: 28 atoms rejected during cycle 1 (RMSD=2.48).
 ExecutiveRMS: 28 atoms rejected during cycle 2 (RMSD=2.19).
 ExecutiveRMS: 28 atoms rejected during cycle 3 (RMSD=1.86).
 ExecutiveRMS: 41 atoms rejected during cycle 4 (RMSD=1.56).
 ExecutiveRMS: 36 atoms rejected during cycle 5 (RMSD=1.26).
 Executive: RMSD =    0.980 (531 to 531 atoms)
```