**5-4-24 TCR- MHC**

**Checking missing residues in pymol 30xr**

python

stored.residues = []

cmd.iterate("3oxr", "stored.residues.append((chain, resi))")

for i in range(1, len(stored.residues)):

if int(stored.residues[i][1]) - int(stored.residues[i-1][1]) > 1 and stored.residues[i][0] == stored.residues[i-1][0]:

print("Missing residues between %s:%s and %s:%s" % (stored.residues[i-1][0], stored.residues[i-1][1], stored.residues[i][0], stored.residues[i][1]))

python end

Output:

Missing residues between A:275 and A:277  
Missing residues between B:110 and B:112  
Missing residues between B:121 and B:123  
Missing residues between B:127 and B:129  
Missing residues between B:129 and B:132  
Missing residues between B:132 and B:134  
Missing residues between B:134 and B:139  
Missing residues between B:139 and B:142  
Missing residues between B:143 and B:145  
Missing residues between B:145 and B:152  
Missing residues between B:152 and B:159  
Missing residues between B:160 and B:163  
Missing residues between B:163 and B:166  
Missing residues between B:166 and B:168  
Missing residues between B:168 and B:171  
Missing residues between B:171 and B:178  
Missing residues between B:178 and B:180  
Missing residues between B:180 and B:183  
Missing residues between B:183 and B:189  
Missing residues between B:189 and B:195  
Missing residues between B:195 and B:211  
Missing residues between B:211 and B:213  
Missing residues between B:213 and B:223  
Missing residues between B:225 and B:227  
Missing residues between B:227 and B:230  
Missing residues between B:230 and B:232  
Missing residues between B:232 and B:235  
Missing residues between B:235 and B:238  
Missing residues between B:238 and B:240  
Missing residues between B:240 and B:246  
Missing residues between B:246 and B:248  
Missing residues between B:248 and B:251  
Missing residues between B:256 and B:272  
Missing residues between B:272 and B:281  
Missing residues between B:281 and B:286  
Missing residues between B:286 and B:291  
Missing residues between B:293 and B:304  
Missing residues between B:304 and B:307  
Missing residues between B:307 and B:316  
Missing residues between B:316 and B:321  
Missing residues between B:322 and B:340  
Missing residues between B:340 and B:343  
Missing residues between B:343 and B:345  
Missing residues between B:345 and B:351  
Missing residues between B:351 and B:353  
Missing residues between B:353 and B:360  
Missing residues between B:362 and B:366  
Missing residues between B:366 and B:371  
Missing residues between B:372 and B:385  
Missing residues between B:387 and B:390  
Missing residues between B:390 and B:398  
Missing residues between B:398 and B:403  
Missing residues between B:404 and B:408  
Missing residues between B:409 and B:412  
Missing residues between B:413 and B:421  
Missing residues between B:421 and B:424  
Missing residues between B:446 and B:539  
Missing residues between C:10 and C:24  
Missing residues between C:24 and C:34  
Missing residues between C:34 and C:37  
Missing residues between C:37 and C:43  
Missing residues between C:43 and C:47  
Missing residues between C:47 and C:62  
Missing residues between C:62 and C:90  
Missing residues between C:90 and C:202  
Missing residues between C:202 and C:295  
Missing residues between C:295 and C:399  
Missing residues between C:399 and C:439

**Brew installed Modeler to fill missing residues**

(base) josephsteward@Josephs-MacBook-Pro ~ % brew tap salilab/salilab

==> **Auto-updating Homebrew...**

Adjust how often this is run with HOMEBREW\_AUTO\_UPDATE\_SECS or disable with

HOMEBREW\_NO\_AUTO\_UPDATE. Hide these hints with HOMEBREW\_NO\_ENV\_HINTS (see `man brew`).

==> **Auto-updated Homebrew!**

Updated 2 taps (homebrew/core and homebrew/cask).

==> **New Formulae**

ansible-creator cahute fastapi tofuenv

==> **New Casks**

msty semeru-jdk-open@11 semeru-jdk-open@17 semeru-jdk-open@8

You have **18** outdated formulae installed.

==> **Tapping salilab/salilab**

Cloning into '/opt/homebrew/Library/Taps/salilab/homebrew-salilab'...

remote: Enumerating objects: 1126, done.

remote: Counting objects: 100% (239/239), done.

remote: Compressing objects: 100% (104/104), done.

remote: Total 1126 (delta 156), reused 218 (delta 135), pack-reused 887

Receiving objects: 100% (1126/1126), 192.61 KiB | 174.00 KiB/s, done.

Resolving deltas: 100% (743/743), done.

Tapped 16 formulae (30 files, 295KB).

(base) josephsteward@Josephs-MacBook-Pro ~ % brew install modeller

==> **Fetching dependencies for salilab/salilab/modeller: pcre2, swig, python-setuptools, openssl@3, sqlite, xz, glib and salilab/salilab/hdf5@1.10.7**

==> **Fetching pcre2**

==> **Downloading https://ghcr.io/v2/homebrew/core/pcre2/manifests/10.43**

######################################################################### 100.0%

==> **Downloading https://ghcr.io/v2/homebrew/core/pcre2/blobs/sha256:45c605d79f32**

######################################################################### 100.0%

==> **Fetching swig**

==> **Downloading https://ghcr.io/v2/homebrew/core/swig/manifests/4.2.1**

######################################################################### 100.0%

==> **Downloading https://ghcr.io/v2/homebrew/core/swig/blobs/sha256:183268434604f**

######################################################################### 100.0%

==> **Fetching python-setuptools**

==> **Downloading https://ghcr.io/v2/homebrew/core/python-setuptools/manifests/69.**

######################################################################### 100.0%

==> **Downloading https://ghcr.io/v2/homebrew/core/python-setuptools/blobs/sha256:**

######################################################################### 100.0%

==> **Fetching openssl@3**

==> **Downloading https://ghcr.io/v2/homebrew/core/openssl/3/manifests/3.3.0-1**

######################################################################### 100.0%

==> **Downloading https://ghcr.io/v2/homebrew/core/openssl/3/blobs/sha256:ec6f9daf**

######################################################################### 100.0%

==> **Fetching sqlite**

==> **Downloading https://ghcr.io/v2/homebrew/core/sqlite/manifests/3.45.3**

######################################################################### 100.0%

==> **Downloading https://ghcr.io/v2/homebrew/core/sqlite/blobs/sha256:253a7732af3**

######################################################################### 100.0%

==> **Fetching xz**

==> **Downloading https://ghcr.io/v2/homebrew/core/xz/manifests/5.4.6**

######################################################################### 100.0%

==> **Downloading https://ghcr.io/v2/homebrew/core/xz/blobs/sha256:01ced87d92d0c11**

######################################################################### 100.0%

==> **Fetching glib**

==> **Downloading https://ghcr.io/v2/homebrew/core/glib/manifests/2.80.0\_2**

######################################################################### 100.0%

==> **Downloading https://ghcr.io/v2/homebrew/core/glib/blobs/sha256:cfb04cb6f69cc**

######################################################################### 100.0%

==> **Fetching salilab/salilab/hdf5@1.10.7**

==> **Downloading https://salilab.org/homebrew/bottles/hdf5%401.10.7-1.10.7.arm64\_**

######################################################################### 100.0%

==> **Fetching salilab/salilab/modeller**

==> **Downloading https://salilab.org/modeller/10.5/modeller-10.5-mac.pax.gz**

######################################################################### 100.0%

==> **Installing modeller from salilab/salilab**

==> **Installing dependencies for salilab/salilab/modeller: pcre2, swig, python-setuptools, openssl@3, sqlite, xz, glib and salilab/salilab/hdf5@1.10.7**

==> **Installing salilab/salilab/modeller dependency: pcre2**

==> **Downloading https://ghcr.io/v2/homebrew/core/pcre2/manifests/10.43**

Already downloaded: /Users/josephsteward/Library/Caches/Homebrew/downloads/4c12870adcfbf27eeeae4f44a420311ca3449f06a2fd8f6fcfe3d13db18087b4--pcre2-10.43.bottle\_manifest.json

==> **Pouring pcre2--10.43.arm64\_sonoma.bottle.tar.gz**

🍺 /opt/homebrew/Cellar/pcre2/10.43: 234 files, 6.3MB

==> **Installing salilab/salilab/modeller dependency: swig**

==> **Downloading https://ghcr.io/v2/homebrew/core/swig/manifests/4.2.1**

Already downloaded: /Users/josephsteward/Library/Caches/Homebrew/downloads/85c972e5ee820382598e830ab3f785897d8715c1b67f0273fea51383a7ec6b34--swig-4.2.1.bottle\_manifest.json

==> **Pouring swig--4.2.1.arm64\_sonoma.bottle.tar.gz**

🍺 /opt/homebrew/Cellar/swig/4.2.1: 829 files, 5.7MB

==> **Installing salilab/salilab/modeller dependency: python-setuptools**

==> **Downloading https://ghcr.io/v2/homebrew/core/python-setuptools/manifests/69.**

Already downloaded: /Users/josephsteward/Library/Caches/Homebrew/downloads/f7a54d89eac25d9069fa653fbe99f04c826264b2faa00483e74c9cfb35768bcf--python-setuptools-69.5.1.bottle\_manifest.json

==> **Pouring python-setuptools--69.5.1.arm64\_sonoma.bottle.tar.gz**

🍺 /opt/homebrew/Cellar/python-setuptools/69.5.1: 274 files, 3.2MB

==> **Installing salilab/salilab/modeller dependency: openssl@3**

==> **Downloading https://ghcr.io/v2/homebrew/core/openssl/3/manifests/3.3.0-1**

Already downloaded: /Users/josephsteward/Library/Caches/Homebrew/downloads/cd7e4cb72da375d51619d8c60fb91a70696e352edb515631b5751d05342e471d--openssl@3-3.3.0-1.bottle\_manifest.json

==> **Pouring openssl@3--3.3.0.arm64\_sonoma.bottle.1.tar.gz**

==> **Downloading https://formulae.brew.sh/api/formula.jws.json**

🍺 /opt/homebrew/Cellar/openssl@3/3.3.0: 6,976 files, 32.4MB

==> **Installing salilab/salilab/modeller dependency: sqlite**

==> **Downloading https://ghcr.io/v2/homebrew/core/sqlite/manifests/3.45.3**

Already downloaded: /Users/josephsteward/Library/Caches/Homebrew/downloads/9eebda014aefbd585433274db989aa060c29200f656e6e106b4c1956438a2401--sqlite-3.45.3.bottle\_manifest.json

==> **Pouring sqlite--3.45.3.arm64\_sonoma.bottle.tar.gz**

🍺 /opt/homebrew/Cellar/sqlite/3.45.3: 11 files, 4.8MB

==> **Installing salilab/salilab/modeller dependency: xz**

==> **Downloading https://ghcr.io/v2/homebrew/core/xz/manifests/5.4.6**

Already downloaded: /Users/josephsteward/Library/Caches/Homebrew/downloads/b2cc4077807c100af6e0253f51d186f187ff55165638cbe3a4aa16d1c4762660--xz-5.4.6.bottle\_manifest.json

==> **Pouring xz--5.4.6.arm64\_sonoma.bottle.tar.gz**

🍺 /opt/homebrew/Cellar/xz/5.4.6: 163 files, 2.6MB

==> **Installing salilab/salilab/modeller dependency: glib**

==> **Downloading https://ghcr.io/v2/homebrew/core/glib/manifests/2.80.0\_2**

Already downloaded: /Users/josephsteward/Library/Caches/Homebrew/downloads/bad07197fbf4d9c1af0f49bb79d89a3b369de9b90872243c8bbcfea7d4385475--glib-2.80.0\_2.bottle\_manifest.json

==> **Pouring glib--2.80.0\_2.arm64\_sonoma.bottle.tar.gz**

🍺 /opt/homebrew/Cellar/glib/2.80.0\_2: 524 files, 36MB

==> **Installing salilab/salilab/modeller dependency: salilab/salilab/hdf5@1.**

==> **Pouring hdf5@1.10.7-1.10.7.arm64\_big\_sur.bottle.tar.gz**

🍺 /opt/homebrew/Cellar/hdf5@1.10.7/1.10.7: 142 files, 15.2MB

==> **Installing salilab/salilab/modeller**

==> **install\_name\_tool -id /opt/homebrew/Cellar/modeller/10.5\_1/lib/libmodeller.1**

==> **lipo -extract arm64 -output /opt/homebrew/Cellar/modeller/10.5\_1/lib/libmode**

==> **lipo -extract arm64 -output /opt/homebrew/Cellar/modeller/10.5\_1/lib/libsaxs**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libhdf5.103.dyl**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libhdf5\_hl.100.**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libintl.8.dylib**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libglib-2.0.0.d**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libmodeller.13.**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libsaxs.dylib /**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libquadmath.0.d**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libhdf5.103.dyl**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libhdf5\_hl.100.**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libintl.8.dylib**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libglib-2.0.0.d**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libmodeller.13.**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libsaxs.dylib /**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libquadmath.0.d**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libhdf5.103.dyl**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libhdf5\_hl.100.**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libintl.8.dylib**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libglib-2.0.0.d**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libmodeller.13.**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libsaxs.dylib /**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libquadmath.0.d**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libhdf5.103.dyl**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libhdf5\_hl.100.**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libintl.8.dylib**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libglib-2.0.0.d**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libmodeller.13.**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libsaxs.dylib /**

==> **install\_name\_tool -change /Library/modeller-10.5/lib/mac10v4/libquadmath.0.d**

==> **install\_name\_tool -change /System/Library/Frameworks/Python.framework/Versio**

==> **install\_name\_tool -change /System/Library/Frameworks/Python.framework/Versio**

==> **codesign -f -s - /opt/homebrew/Cellar/modeller/10.5\_1/modbin/mod10.5\_mac10v4**

==> **codesign -f -s - Library/modeller-10.5/lib/mac10v4/\_modeller.so**

==> **codesign -f -s - /opt/homebrew/Cellar/modeller/10.5\_1/lib/libmodeller.13.dyl**

==> **codesign -f -s - /opt/homebrew/Cellar/modeller/10.5\_1/lib/libsaxs.dylib**

==> **codesign -f -s - /opt/homebrew/Cellar/modeller/10.5\_1/py2\_compat/mod10.5\_mac**

==> **swig -python -keyword -nodefaultctor -nodefaultdtor -noproxy modeller.i**

==> **/opt/homebrew/opt/python@3.12/bin/python3.12 setup.py build**

==> **Caveats**

Edit /opt/homebrew/opt/modeller/modlib/modeller/config.py

and replace XXXX with your Modeller license key

(or write your license key into /opt/homebrew/etc/modeller/license before

running "brew install").

==> **Summary**

🍺 /opt/homebrew/Cellar/modeller/10.5\_1: 1,503 files, 61.2MB, built in 9 seconds

==> **Running `brew cleanup modeller`...**

Disable this behaviour by setting HOMEBREW\_NO\_INSTALL\_CLEANUP.

Hide these hints with HOMEBREW\_NO\_ENV\_HINTS (see `man brew`).

Removing: /Users/josephsteward/Library/Caches/Homebrew/modeller--10.5.pax.gz... (37.6MB)

==> **Upgrading 2 dependents of upgraded formulae:**

Disable this behaviour by setting HOMEBREW\_NO\_INSTALLED\_DEPENDENTS\_CHECK.

Hide these hints with HOMEBREW\_NO\_ENV\_HINTS (see `man brew`).

boost 1.84.0\_1 -> 1.85.0, open-mpi 5.0.2\_1 -> 5.0.3

==> **Downloading https://ghcr.io/v2/homebrew/core/boost/manifests/1.85.0**

######################################################################### 100.0%

==> **Downloading https://ghcr.io/v2/homebrew/core/open-mpi/manifests/5.0.3**

######################################################################### 100.0%

==> **Checking for dependents of upgraded formulae...**

==> **No broken dependents found!**

==> **Caveats**

==> **modeller**

Edit /opt/homebrew/opt/modeller/modlib/modeller/config.py

and replace XXXX with your Modeller license key

(or write your license key into /opt/homebrew/etc/modeller/license before

running "brew install").

**Path to biopython**

base) josephsteward@Josephs-MacBook-Pro ~ % pip show biopython

Name: biopython

Version: 1.83

Summary: Freely available tools for computational molecular biology.

Home-page: https://biopython.org/

Author: The Biopython Contributors

Author-email: biopython@biopython.org

License:

Location: /opt/anaconda3/lib/python3.11/site-packages

Requires: numpy

Required-by:

**Ran Biopython script below to create cleaned PDB file:**

from Bio import PDB

input\_pdb = "/Users/josephsteward/Biopython /5ni9.pdb"

# Define the input and output PDB file paths

input\_pdb = "/Users/josephsteward/Biopython /5ni9.pdb"

output\_pdb = "/Users/josephsteward/Biopython /5ni9-output.pdb"

# Create a PDB parser

parser = PDB.PDBParser()

# Parse the input PDB file

structure = parser.get\_structure("structure", "/Users/josephsteward/Biopython /5ni9.pdb")

# Create a list to store the residues to be removed

residues\_to\_remove = ["MRD", "MPD", "URE", "HOH"]

# Iterate over each model, chain, and residue in the structure

for model in structure:

for chain in model:

residues\_to\_delete = []

for residue in chain:

if residue.get\_resname() in residues\_to\_remove:

residues\_to\_delete.append(residue)

# Remove the unwanted residues from the chain

for residue in residues\_to\_delete:

chain.detach\_child(residue.get\_id())

# Create a PDB writer

io = PDB.PDBIO()

# Set the structure to be written

io.set\_structure(structure)

# Write the modified structure to the output PDB file

io.save(output\_pdb)