Calculation RMSD, RMSF ans SASA for the pocket
And Volume of Selected pocket along the Trajectory (with MDpocket):

Step 1: Take the first structure of the MD trajectory and calculate pockets:

(a) Remove periodic

gmx_mpi trjconv -s md_0_1.tpr -f md_0_1.xtc -o md_0_1_noPBC_Prot.xtc -pbc mol -center
Group: 1 / 1 (Prot)

(b) Take first structure of the MD trajectory

gmx_mpi trjconv -s md_0_1.tpr -f md_0_1_noPBC_Prot.xtc -o first_frame.pdb -dump 0
Group: 2 (Prot-H)

(c) Calculate Fpocket for first_frame.pdb

fpocket -f first_frame_pocket1_atm.pdb

Step 2: GROMACS Results for POCKET during MD

(a) Tell GROMACS Which Residues Form the Pocket (see file first_frame_pocket1_atm.pdb**)**

gmx_mpi make_ndx -f first_frame.pdb -o pocket_1.ndx
> r 55 | r 56 | r 57 | r 58 | r 59 | r 60 | r 61 | r 64 | r 65 | r 78 | r 79 | r 80 | r 86 | r 96 | r 99 | r 100 | r 103 | r 106 | r 107 | r 108 | r 111 | r 112 | r 113 | r 114 | r 120 | r 126 | r 129 | r 130 | r 131 | r 132 | r 133 | r 134 | r 135 | r 138 | r 165 | r 178 | r 179 | r 181 | r 182 | r 185 | r 193 | r 194 | r 195 | r 196 | r 197 | r 198 | r 201 | r 207 | r 209 | r 210 | r 338 | r 341 | r 342 | r 345 | r 346 | r 349 | r 352 | r 353 | r 356 | r 393 | r 394 | r 435 | r 442 | r 445 | r 446 | r 449
> l (This is a lowercase "L".)
>name 10 pocket_1
>q (close pocket_1.ndx)

Step-3: Calculation RMSD, RMSF ans SASA for the pocket

(a) RMSD of Pocket

gmx_mpi rms -s md_0_1.tpr -f md_0_1_noPBC_Prot.xtc -n pocket_1.ndx -o rmsd_pocket.xvg
Select the **pocket group** for both reference and fitting.
Group: 10 / 10

(b) RMSF of Pocket

gmx_mpi rmsf -s md_0_1.tpr -f md_0_1_noPBC_Prot.xtc -n pocket_1.ndx -o rmsf_pocket.xvg -res
Group: 10

(c) SASA of Pocket

gmx_mpi sasa -s md_0_1.tpr -f md_0_1_noPBC_Prot.xtc -n pocket_1.ndx -o area.xvg -tu ns

(d) Radius of Gyration:

Pocket:

gmx_mpi gyrate -s md_0_1.tpr -f md_0_1_noPBC_Prot.xtc -n pocket_1.ndx -o gyrate_pocket.xvg

Protein:

gmx_mpi gyrate -s md_0_1.tpr -f md_0_1_noPBC_Prot.xtc -o gyrate_protein.xvg

Step 4 (Volume using MDpocket):

(a) Extract Only Protein from md_0_1_noPBC.xtc

gmx_mpi trjconv -s md_0_1.tpr -f md_0_1_noPBC_Prot.xtc -o md_0_1_protein.xtc
Select a group: 2 (Protein-H)

(b) Align the Protein-Only Trajectory to first_frame.pdb

Now, align the protein-only trajectory to first_frame.pdb:

gmx_mpi trjconv -s first_frame.pdb -f md_0_1_protein.xtc -o md_0_1_aligned.xtc -fit rot+trans
Select a group for least squares fit: 3 (C-alpha)
Select a group for output: 2 (Protein-H)

(c) Command to Subsample Every 100 ns

gmx_mpi trjconv -s first_frame.pdb -f md_0_1_aligned.xtc -o md_0_1_aligned_subsampled.xtc -dt 100

(d) MDPocket:

```
mdpocket -f mdpocket_ready.pdb \
    --trajectory_file md_0_1_noPBC.xtc \
    --trajectory_format xtc \
    --selected_pocket pocket1_atm.pdb
```