

Supplementary - 1

Sequences:

P_{itu}

TAATTTCTGACACAATTATGCCAATAGACCTAAAAAATAAGCAGCATCAAGGGCGTGCCTAAGTGAA
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P43

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P_{bacA}

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P_{bacA} Optimised

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P43 Optimized

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P43_{ca}

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P43_{ca} Optimized

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C

Docking Results:

Table 1. P43 Optimized + sigma A

| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| Docking Score | -204.52 | -196.27 | -195.33 | -189.22 | -188.04 | -187.96 | -186.45 | -186.07 | -183.36 | -182.8 |
| Confidence Score | 0.7485 | 0.7161 | 0.7123 | 0.6866 | 0.6815 | 0.6812 | 0.6746 | 0.6729 | 0.6609 | 0.6584 |
| Ligand rmsd (Å) | 301.14 | 253 | 347.4 | 274.38 | 289.19 | 335.12 | 284.53 | 324.15 | 254.53 | 308.5 |

Table 2. P43 Unoptimized + sigma A

| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|------------------|--------|---------|---------|--------|---------|--------|--------|---------|---------|---------|
| Docking Score | -243.3 | -197.63 | -194.77 | -191.9 | -188.94 | -188.9 | -186.9 | -185.01 | -184.58 | -183.74 |
| Confidence Score | 0.866 | 0.7216 | 0.71 | 0.698 | 0.6854 | 0.6852 | 0.6766 | 0.6682 | 0.6663 | 0.6626 |

| | | | | | | | | | | |
|------------------------|--------|--------|--------|--------|--------|-------|--------|--------|--------|--------|
| Ligand rmsd (Å) | 254.45 | 304.65 | 333.12 | 270.16 | 264.77 | 247.3 | 277.32 | 272.69 | 300.31 | 315.96 |
|------------------------|--------|--------|--------|--------|--------|-------|--------|--------|--------|--------|

Table 3. P43 Unoptimized + sigma B

| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-------------------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|-----------|
| Docking Score | -240.37 | -239.03 | -213.4 | -204.19 | -202.98 | -201.88 | -201.33 | -199.87 | -195 | -192.06 |
| Confidence Score | 0.859 | 0.8558 | 0.7804 | 0.7472 | 0.7426 | 0.7384 | 0.7363 | 0.7305 | 0.7109 | 0.6987 |
| Ligand rmsd (Å) | 84.62 | 81.51 | 55.12 | 83.81 | 114.25 | 76.66 | 114.28 | 71.45 | 109.95 | 91.42 |

Table 4. P43 Optimized + sigma B

| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-------------------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|-----------|
| Docking Score | -235.5 | -234.24 | -214.96 | -213.53 | -212.63 | -204.04 | -203.81 | -203.77 | -199.03 | -199.01 |
| Confidence Score | 0.8468 | 0.8435 | 0.7857 | 0.7808 | 0.7777 | 0.7466 | 0.7458 | 0.7456 | 0.7272 | 0.7271 |
| Ligand rmsd (Å) | 113.89 | 101.09 | 120.59 | 52.72 | 107.89 | 116.65 | 110.12 | 93.94 | 137.24 | 82.15 |

Table 5. P_{bacA} Unoptimized + sigma B

| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-------------------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|-----------|
| Docking Score | -229.9 | -227.85 | -227.35 | -225.14 | -223.5 | -217.98 | -212.95 | -210.68 | -210.45 | -208.53 |
| Confidence Score | 0.8317 | 0.8259 | 0.8245 | 0.818 | 0.8131 | 0.7957 | 0.7789 | 0.7709 | 0.7701 | 0.7633 |
| Ligand rmsd (Å) | 65.8 | 80.98 | 68.21 | 71.54 | 72.25 | 79.69 | 71.46 | 55.29 | 72.97 | 81.29 |

Table 6. P_{bacA} Optimized + sigma B

| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-------------------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|-----------|
| Docking Score | -245.43 | -225.89 | -207.36 | -204.87 | -203.11 | -200.97 | -200.26 | -199.02 | -198.85 | -197.83 |
| Confidence Score | 0.8709 | 0.8202 | 0.759 | 0.7498 | 0.7431 | 0.7349 | 0.7321 | 0.7272 | 0.7265 | 0.7224 |
| Ligand rmsd (Å) | 232.69 | 236.55 | 267.44 | 244.18 | 219.93 | 252.69 | 266.93 | 254.95 | 212.36 | 237.3 |

MDS Results:

1) P43 optimized and sigA

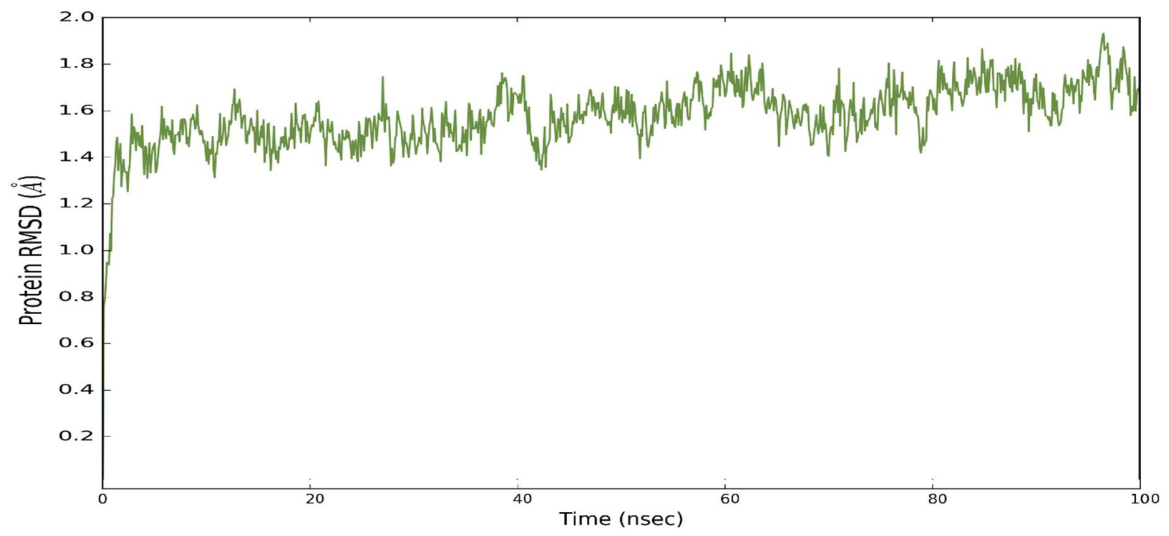


Fig: RMSD values of P43 optimized with sigA

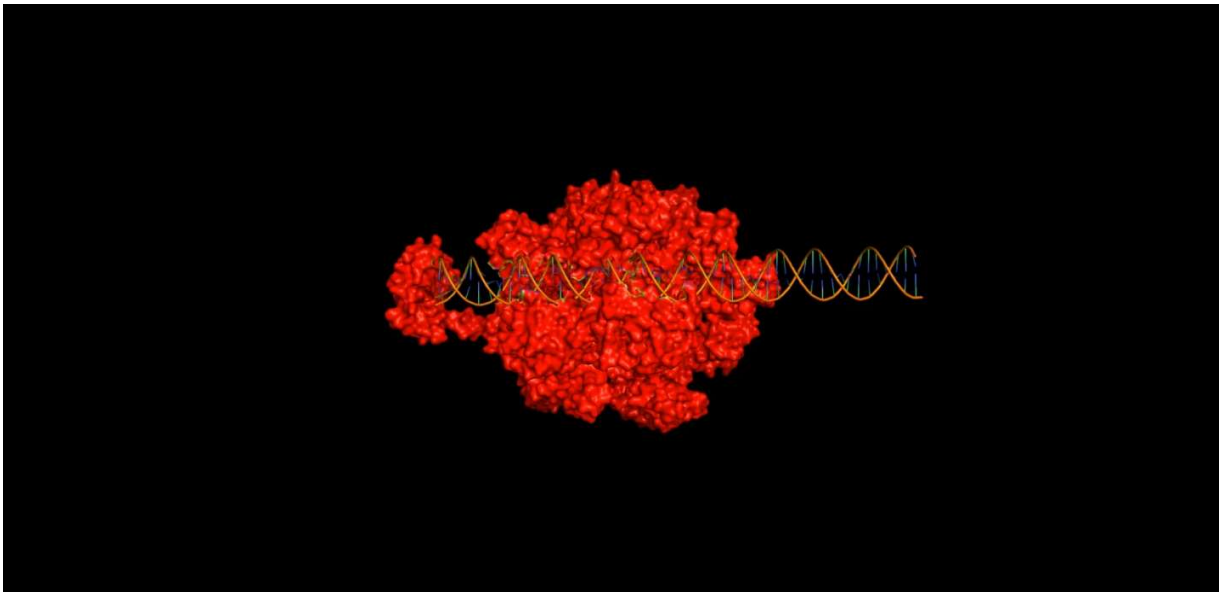


Fig: Molecular dock of P43 optimized with sigA

2) P_{bacA} unoptimized with sigB

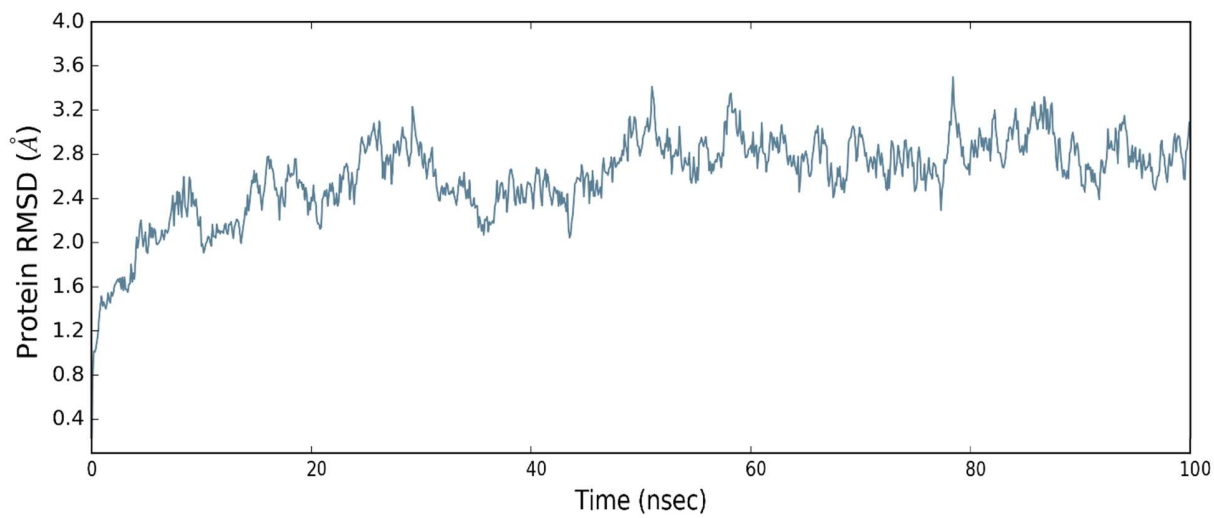


Fig: RMSD values of P_{bacA} unoptimized with sig B

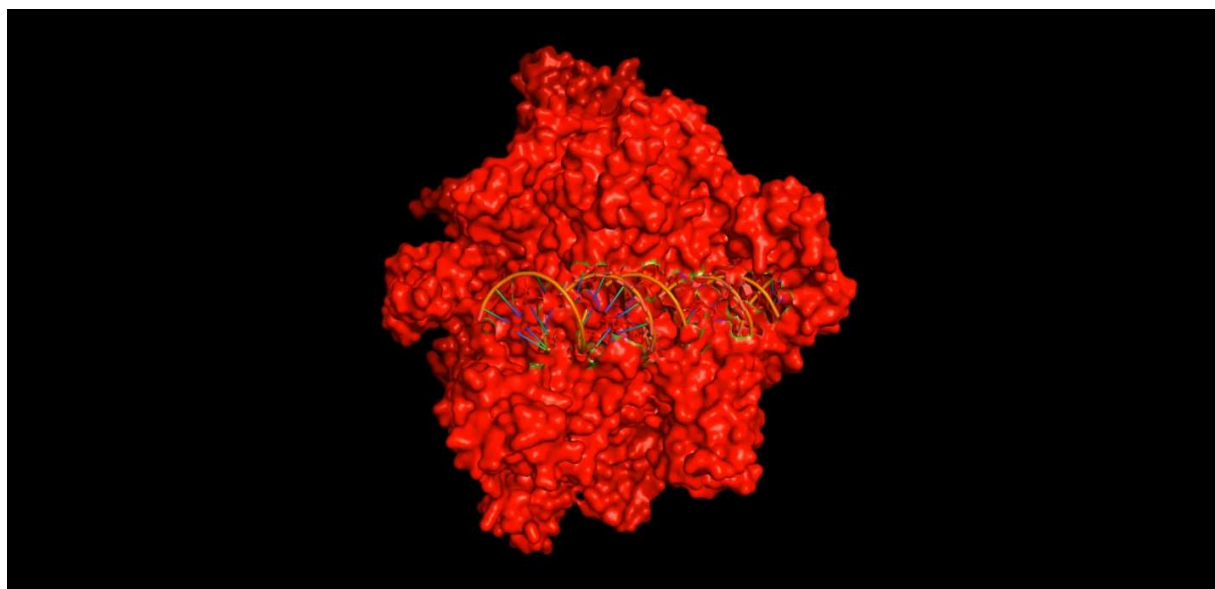


Fig: Molecular dock of P_{bacA} unoptimized with sig B

3) P_{bacA} optimized with sigB

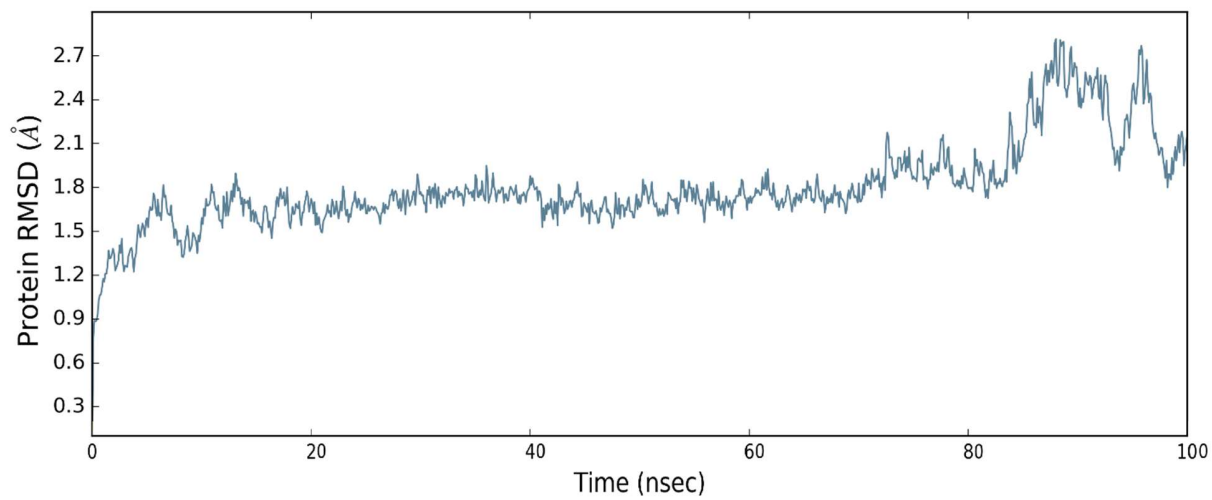


Fig: RMSD values of P_{bacA} optimized with sigB

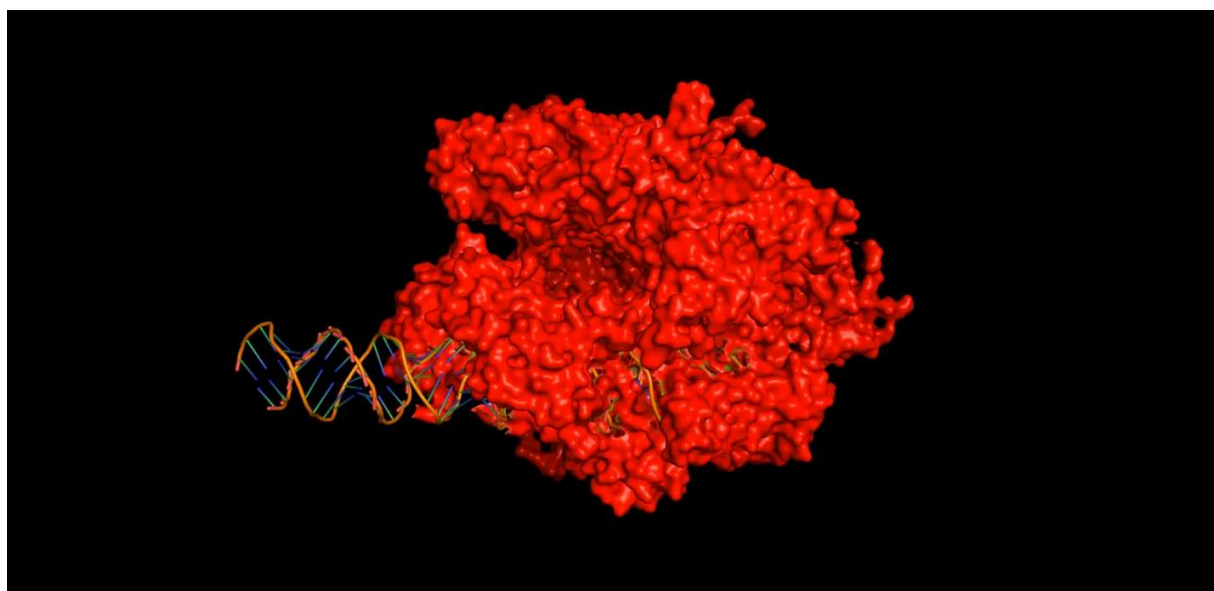


Fig: Molecular dock of P_{bacA} optimized with sigB

4) P43 unoptimized with sigB

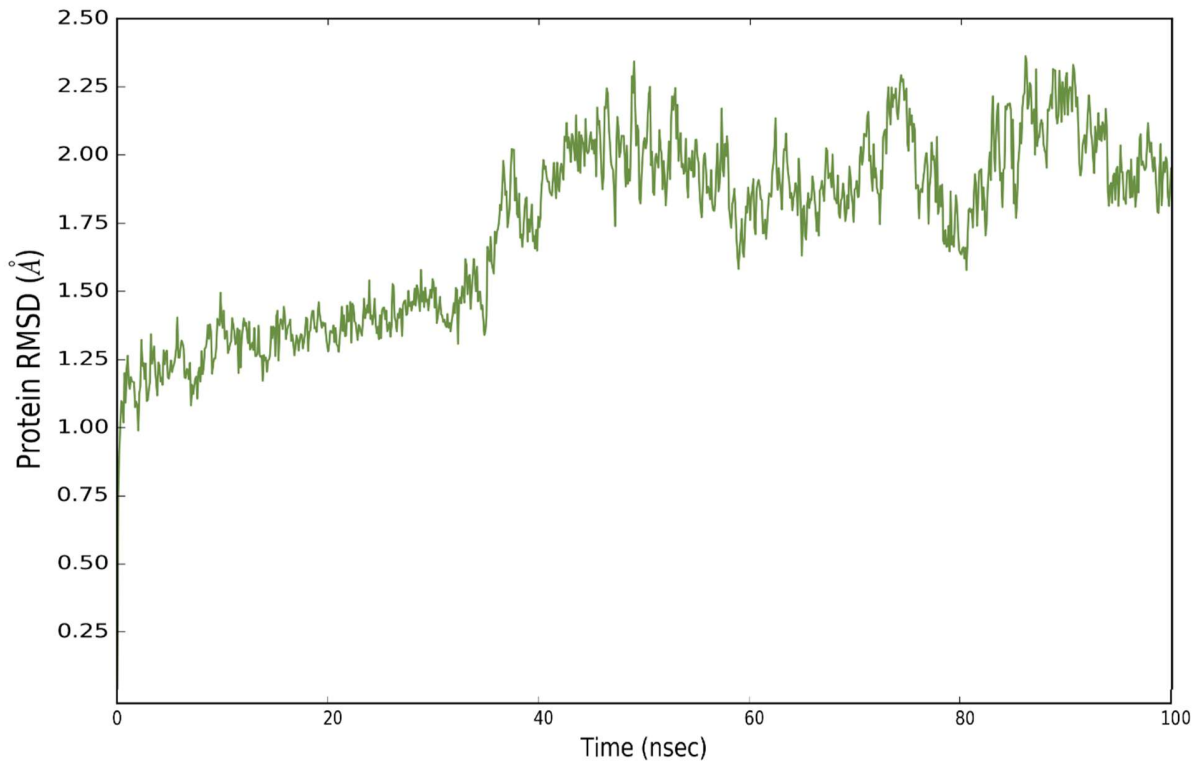


Fig: RMSD values of P43 unoptimized with sigB

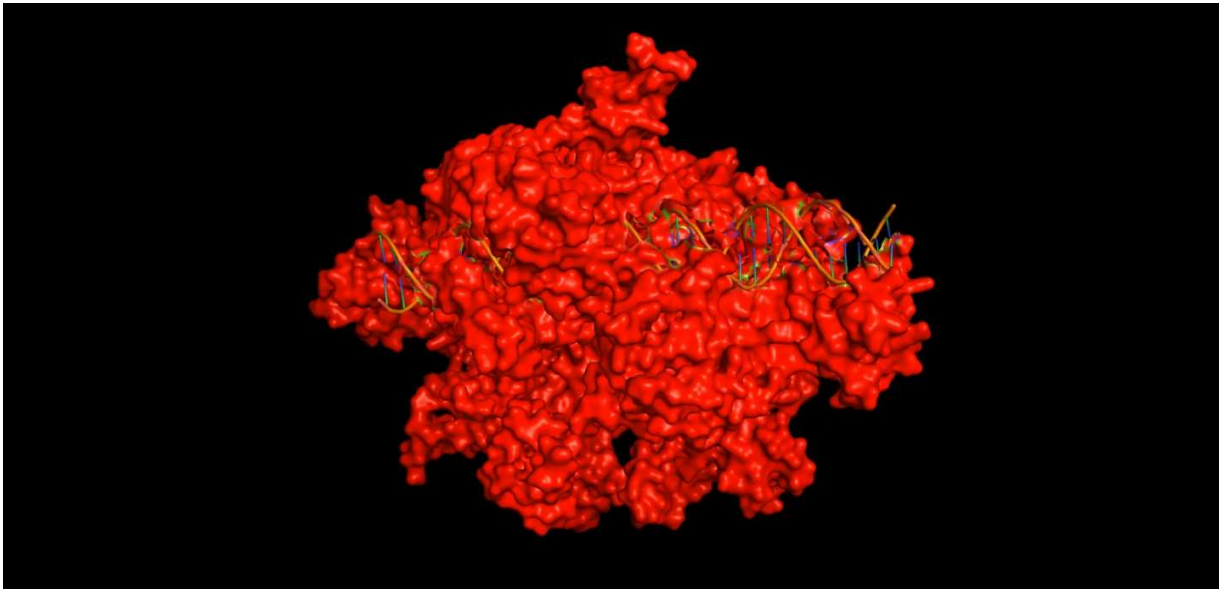


Fig: Molecular dock of P43 unoptimized with sigB

5) P43 unoptimized with sigA

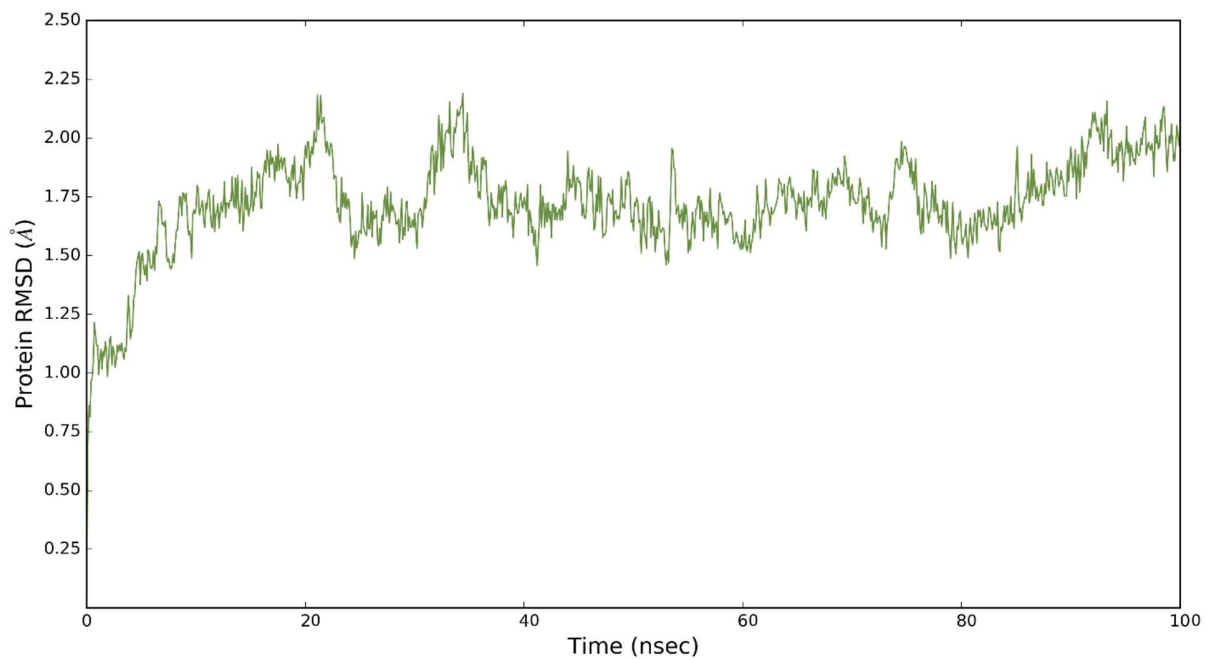


Fig: RMSD values of P43 Unoptimized with sigA

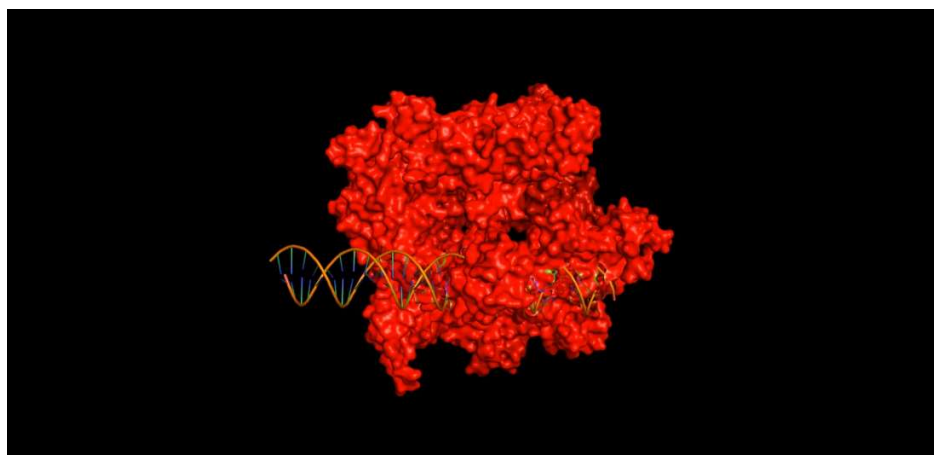


Fig: Molecular dock of P43 Unoptimized with sigA

6) P43 optimized with sigB

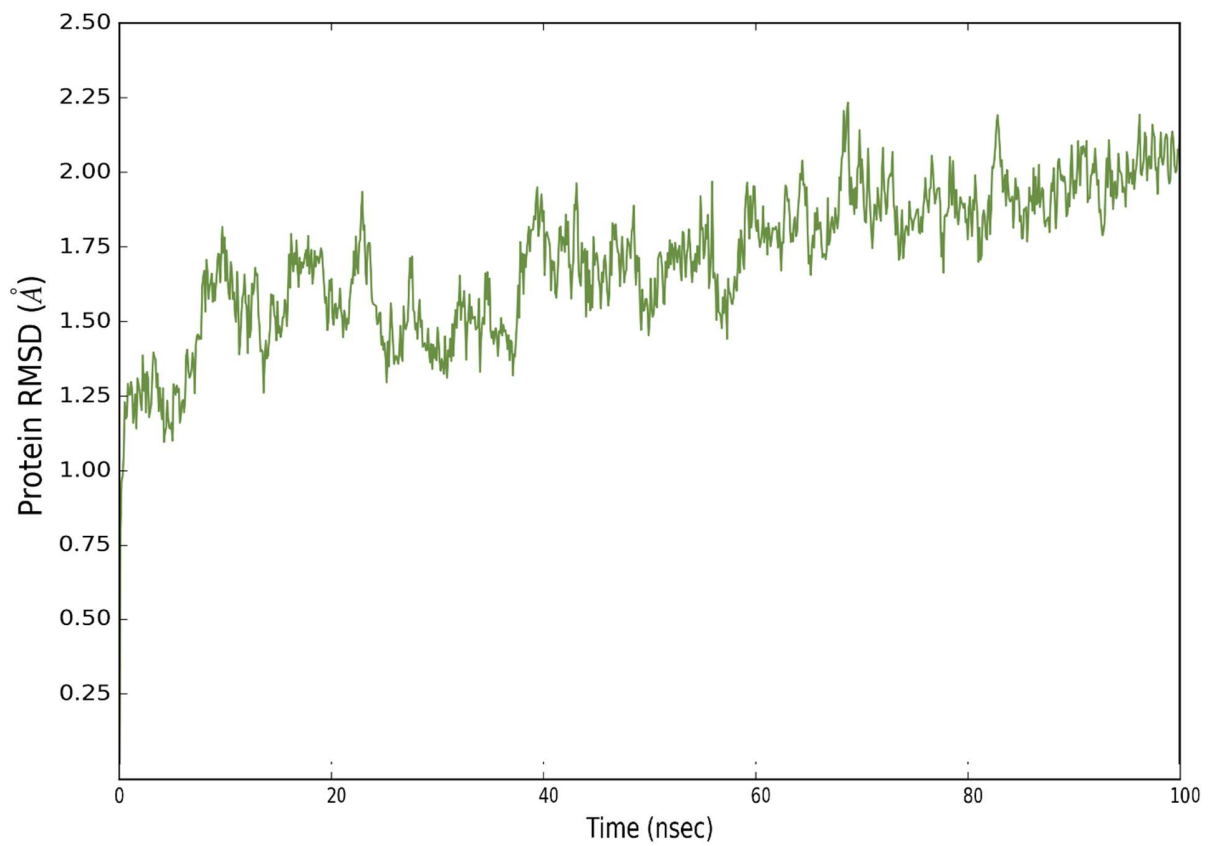


Fig: RMSD values for P43 optimized with sigB

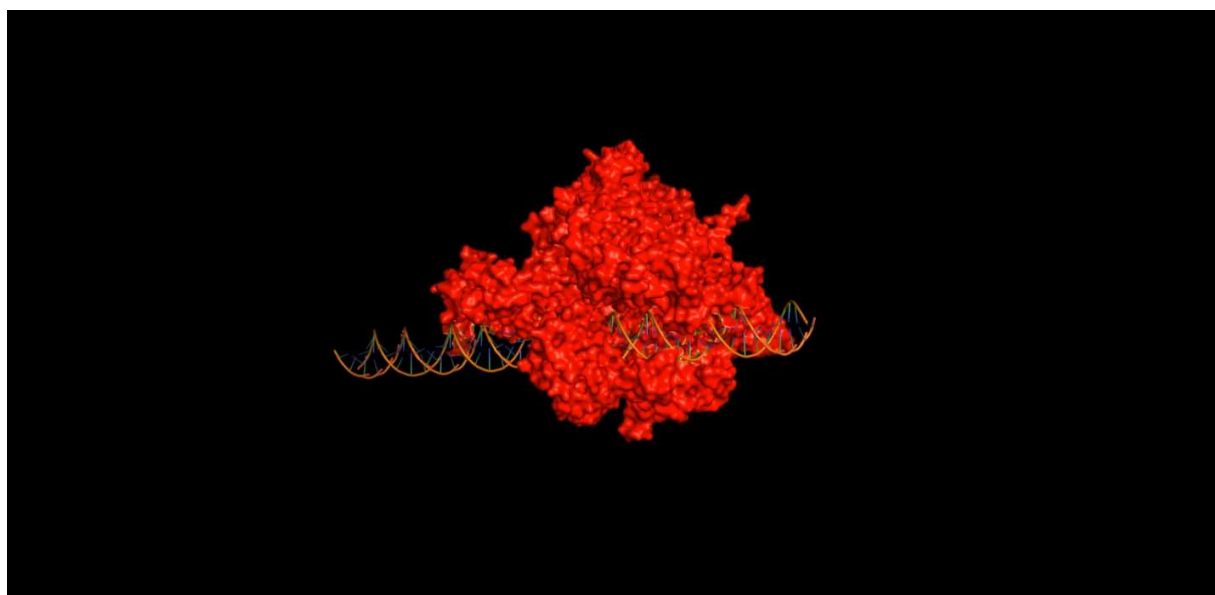


Fig: Molecular dock of P43 optimized with sigB