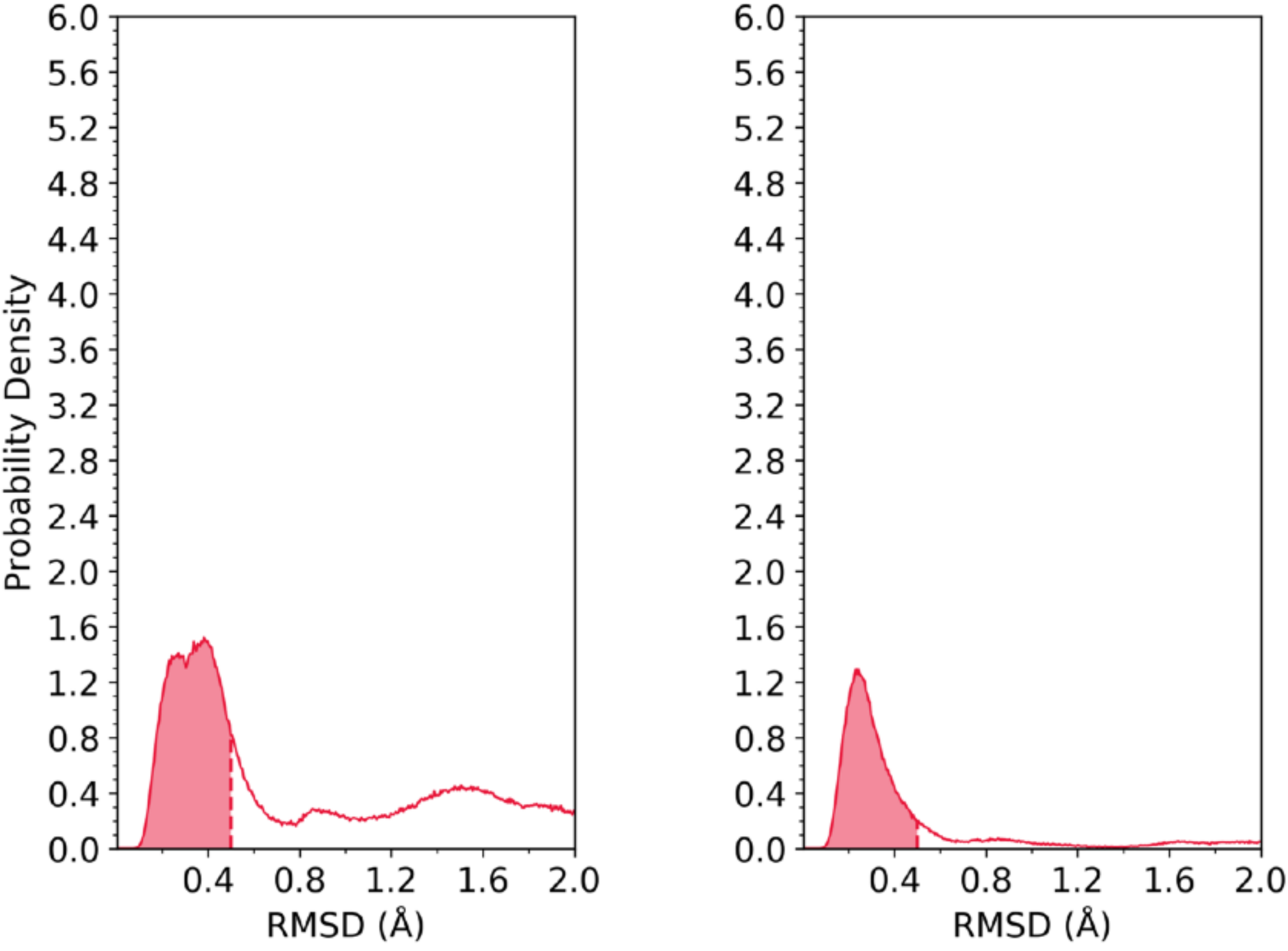
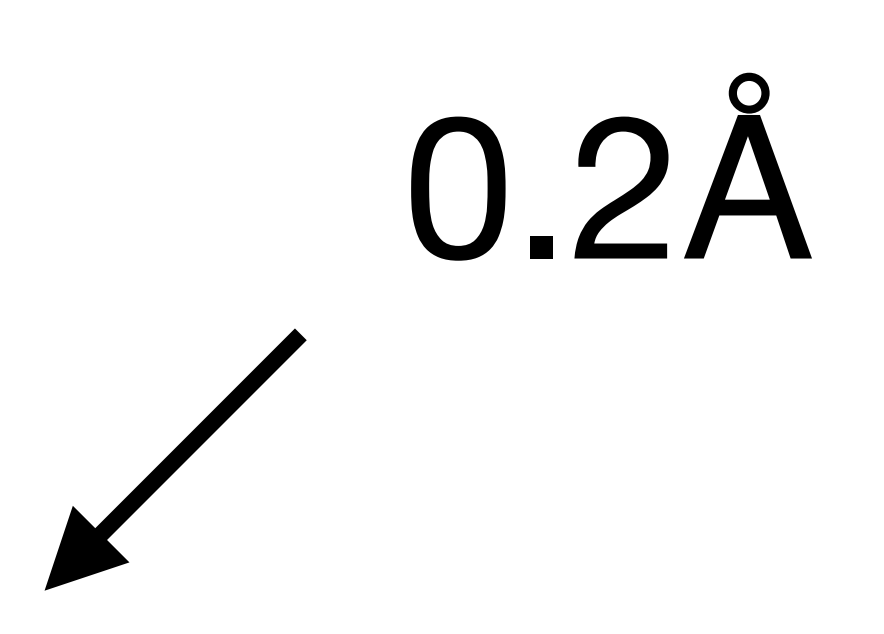
cyclo-(SESEGGGG) as the starting point

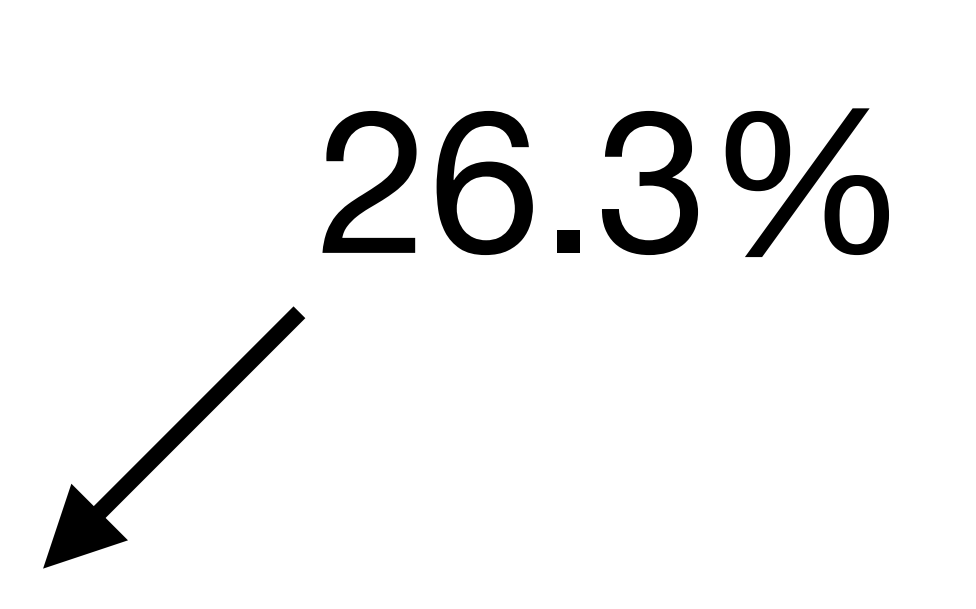

Probability Density
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
0.4
0.8
1.2
1.6
2.0
RMSD (Å)
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
0.4
0.8
1.2
1.6
2.0
RMSD (Å)

cyclo-(SESEGGGG)

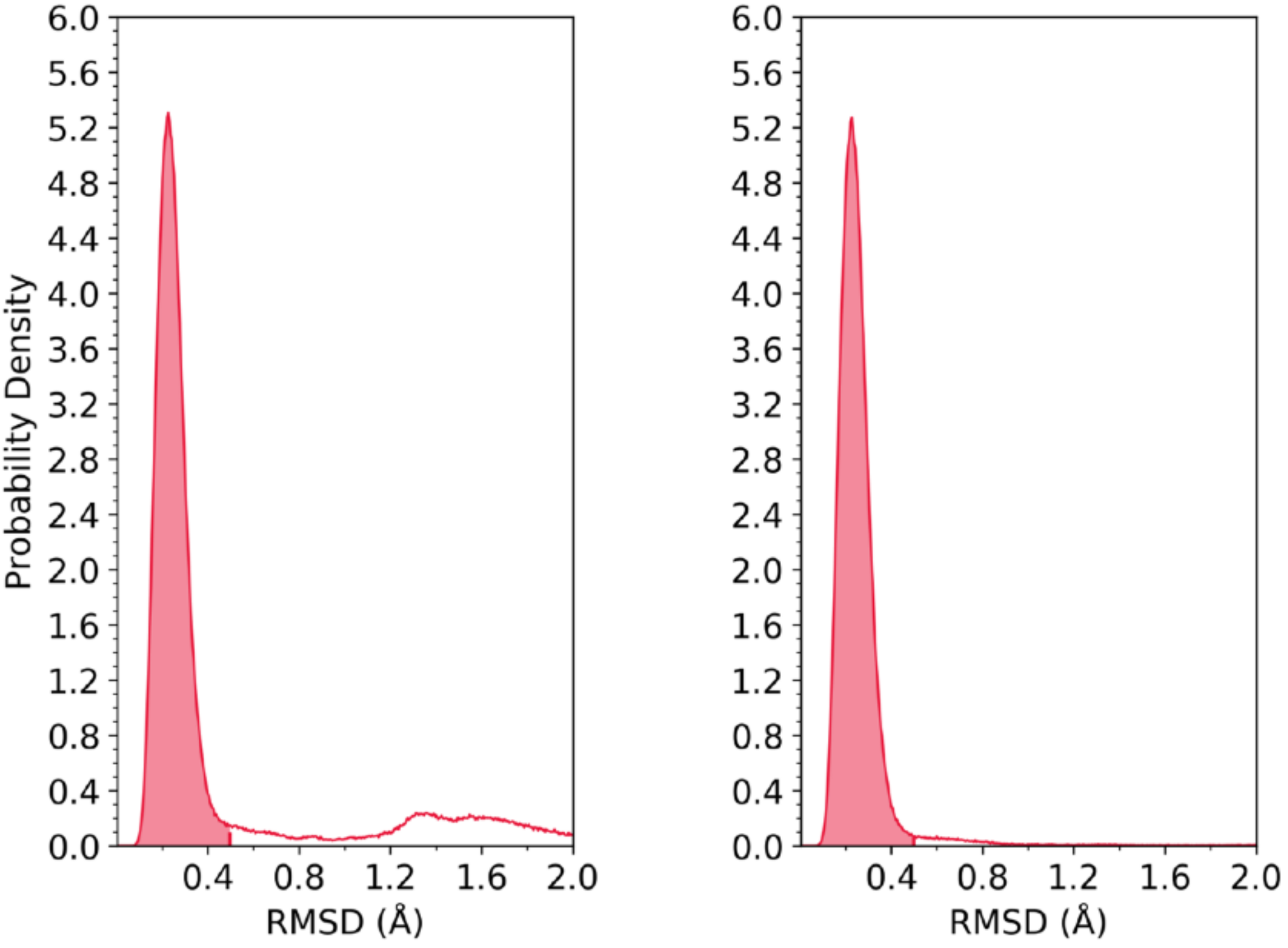
all conformations

conformations without clash


0.2Å


26.3%

Cyclo-(SESEavTG) greatly stabilizes target conformation


Probability Density
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
0.4
0.8
1.2
1.6
2.0
RMSD (Å)
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
0.4
0.8
1.2
1.6
2.0
RMSD (Å)

cyclo-(SESEavTG)

all structures

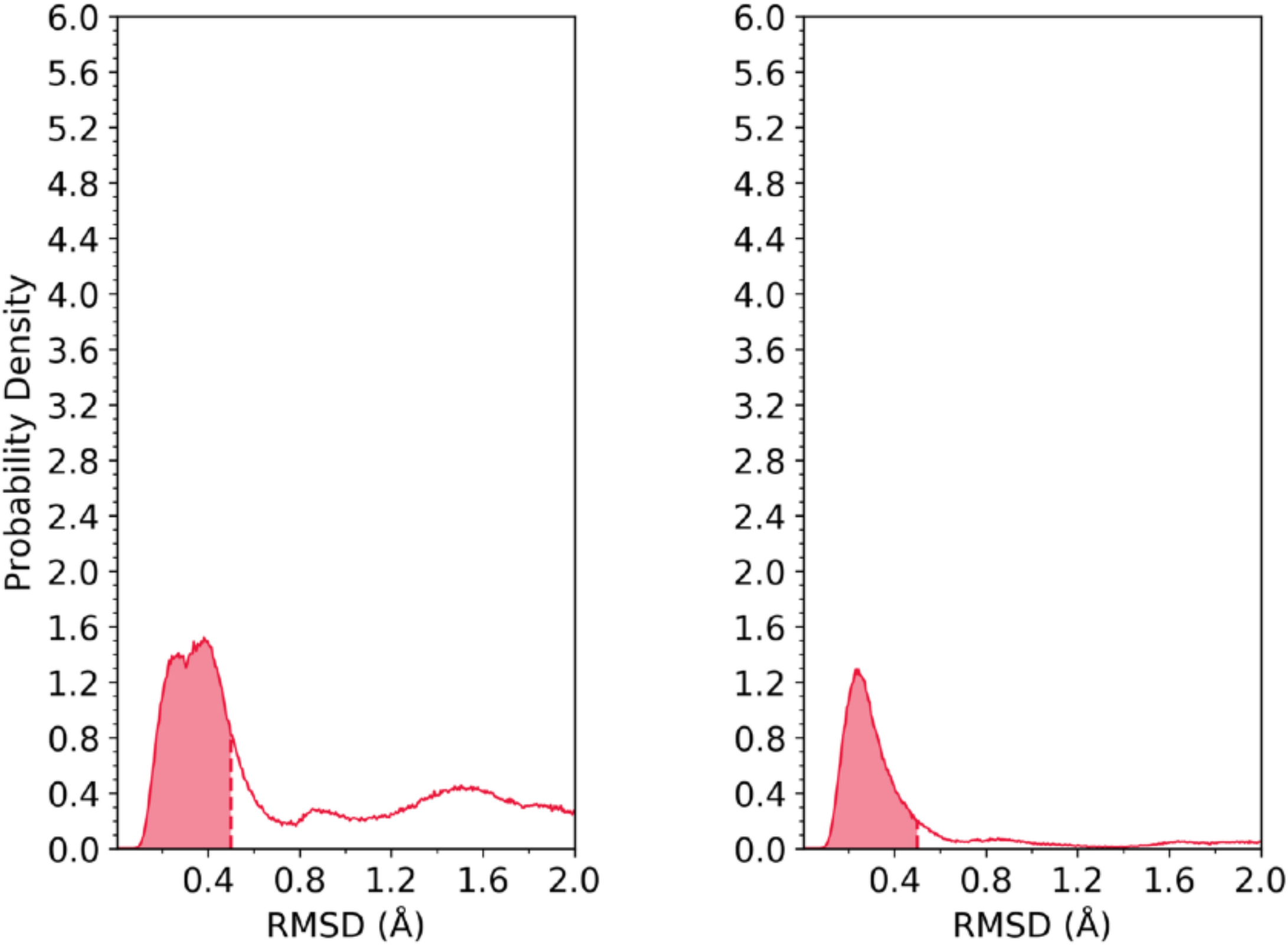
structures without clash

0.2Å

26.3%

all structures

structures without clash


Probability Density
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
0.4
0.8
1.2
1.6
2.0
RMSD (Å)
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
0.4
0.8
1.2
1.6
2.0
RMSD (Å)

cyclo-(SESEGGGG)