

# Supplementary material 4 - Complete Molecular Dynamics Results

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Daniel Ferreira de Lima Neto<sup>2</sup>

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## Contents

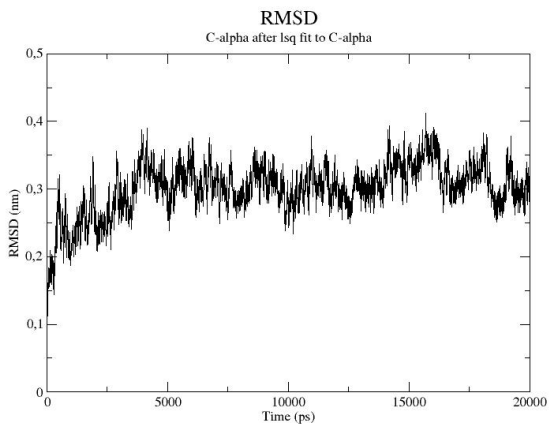
<b>A Complete results</b>	<b>1</b>
RMSD . . . . .	1
HHP . . . . .	1
HHP and low temperature . . . . .	1
RMSF . . . . .	10
HHP . . . . .	10
HHP and low temperature . . . . .	14
Rg . . . . .	19
HHP . . . . .	19
HHP and low temperature . . . . .	23
SASA . . . . .	28
HHP . . . . .	28
HHP and low temperature . . . . .	32
Hbonds . . . . .	37
HHP . . . . .	37
HHP and low temperature . . . . .	41
Hierarchical Clustering . . . . .	46
HHP . . . . .	46
HHP and low temperature . . . . .	47
PCA . . . . .	55
HHP . . . . .	55
HHP and low temperature . . . . .	58

## A Complete results

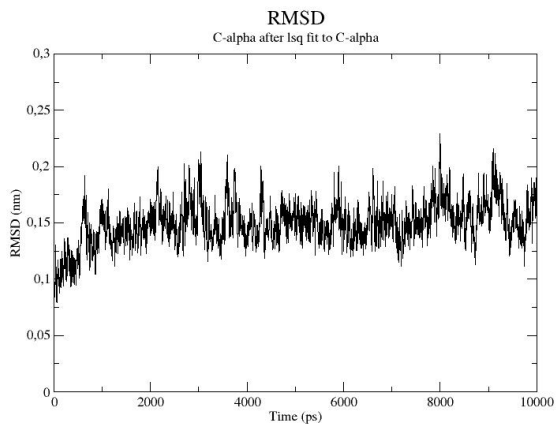
**RMSD**

**HHP**

**HHP and low temperature**

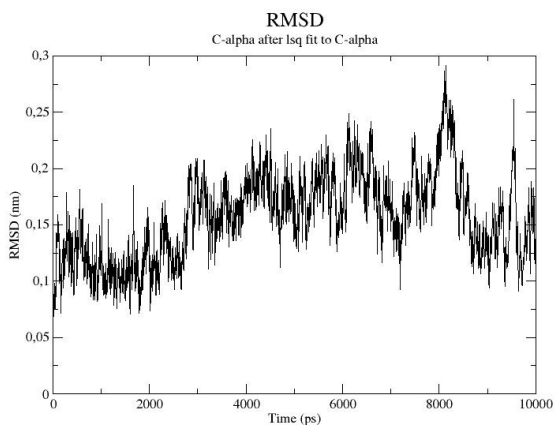


A) 1 bar

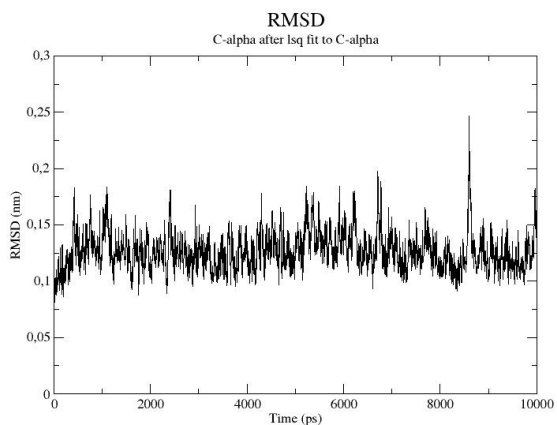


B) 250 bar

Figure 1: RMSD side-by-side - High Hydrostatic Pressure

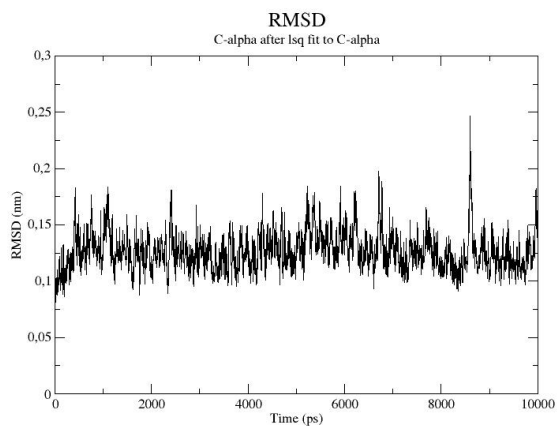


A) 500 bar

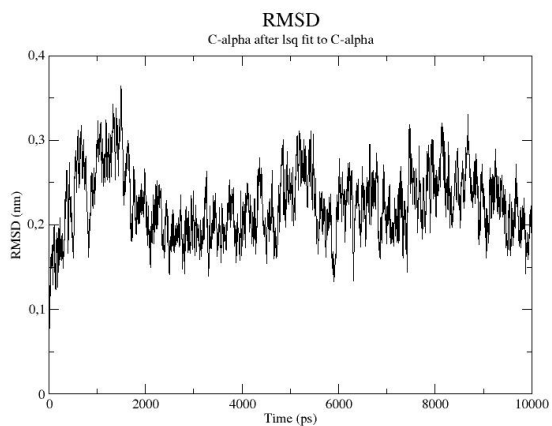


B) 750 bar

Figure 2: RMSD side-by-side - High Hydrostatic Pressure

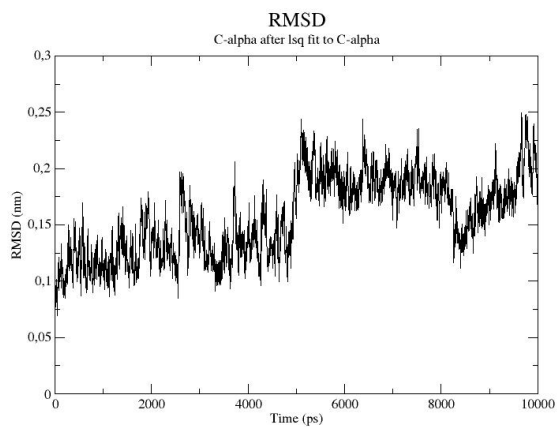


A) 1000 bar

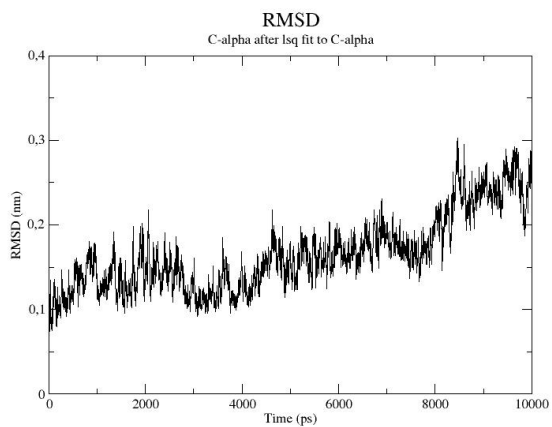


B) 1250 bar

Figure 3: RMSD side-by-side - High Hydrostatic Pressure

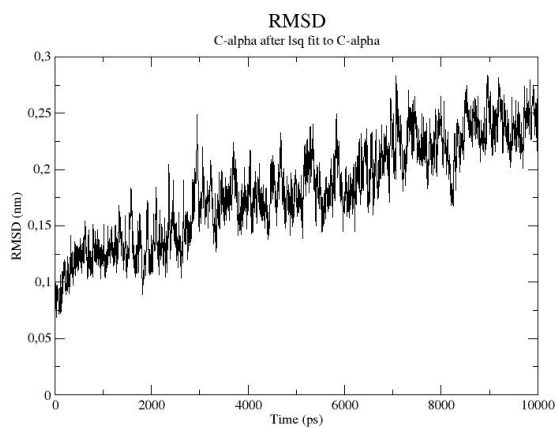


A) 1500 bar

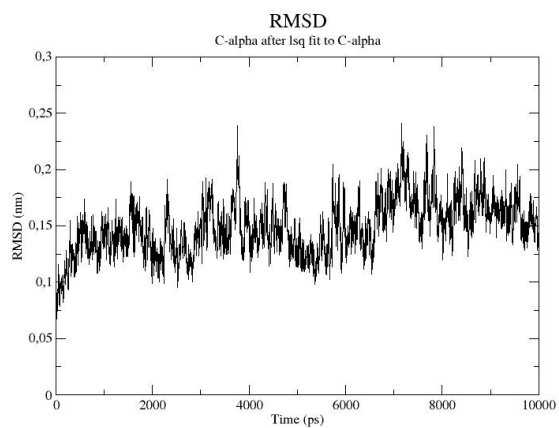


B) 1750 bar

Figure 4: RMSD side-by-side - High Hydrostatic Pressure

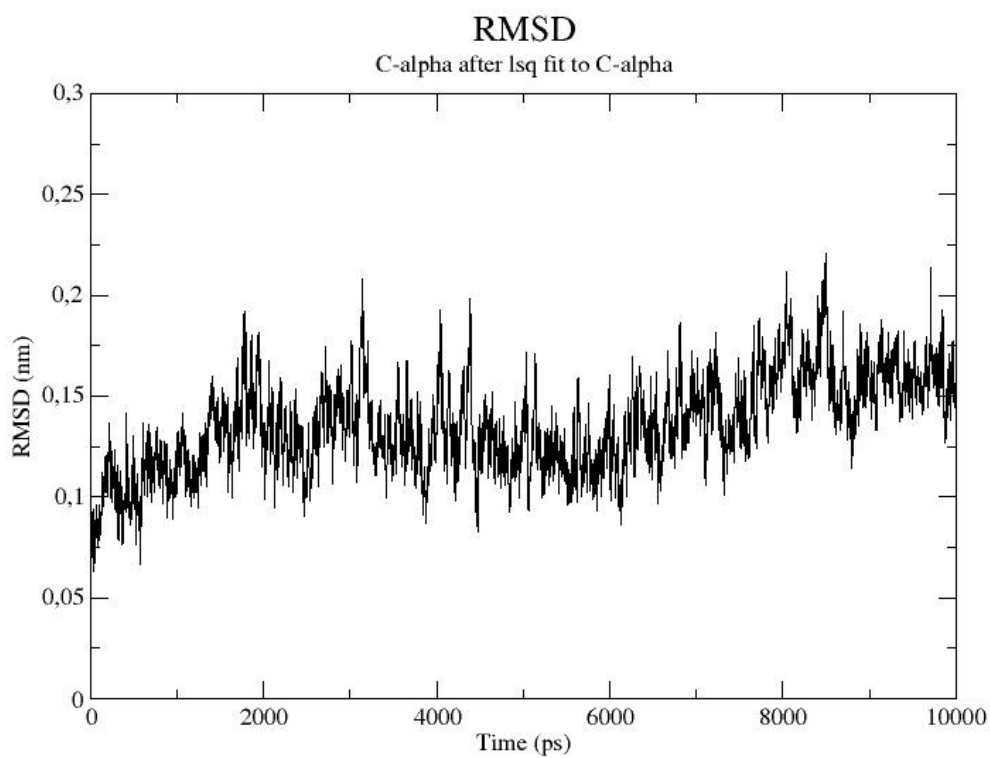


A) 2000 bar



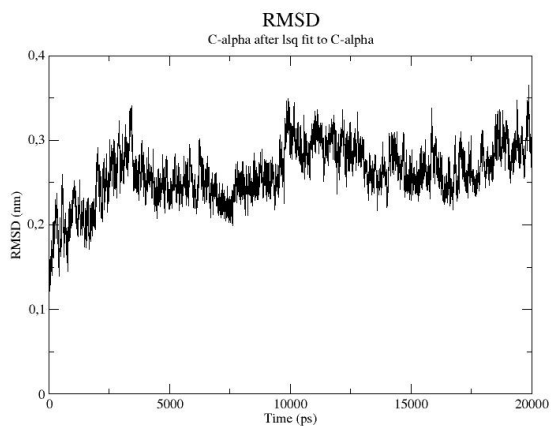
B) 2250 bar

Figure 5: RMSD side-by-side - High Hydrostatic Pressure

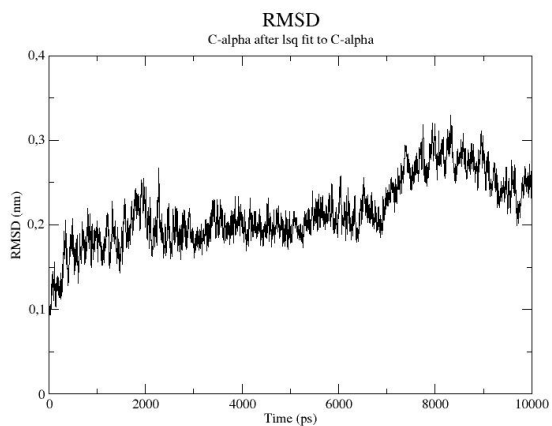


A) 2500 bar

Figure 6: RMSD side-by-side - High Hydrostatic Pressure

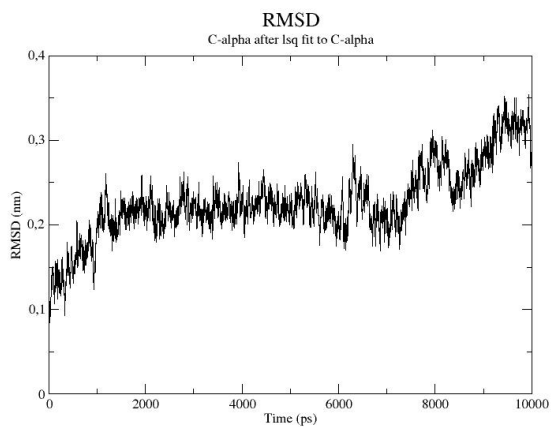


A) 1 bar

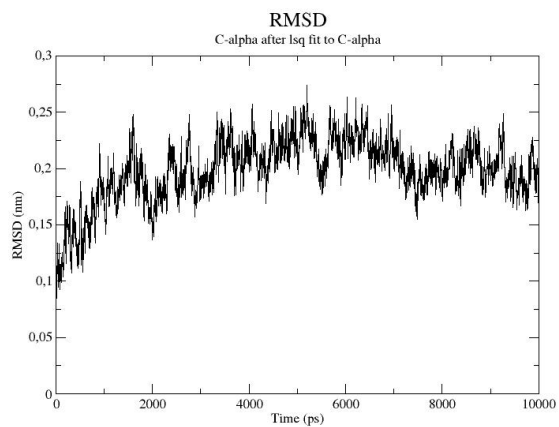


B) 250 bar

Figure 7: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

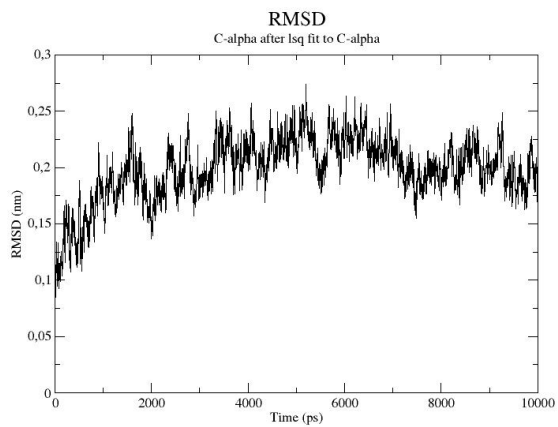


A) 500 bar

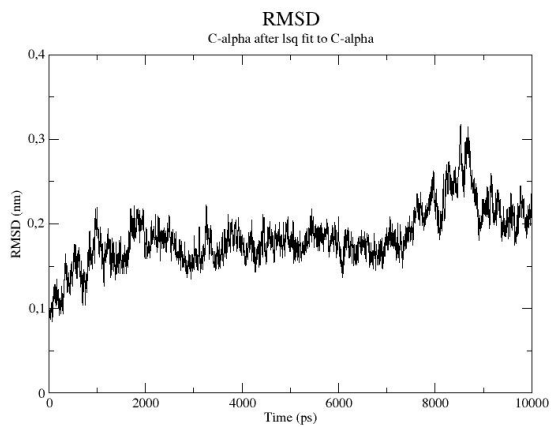


B) 750 bar

Figure 8: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

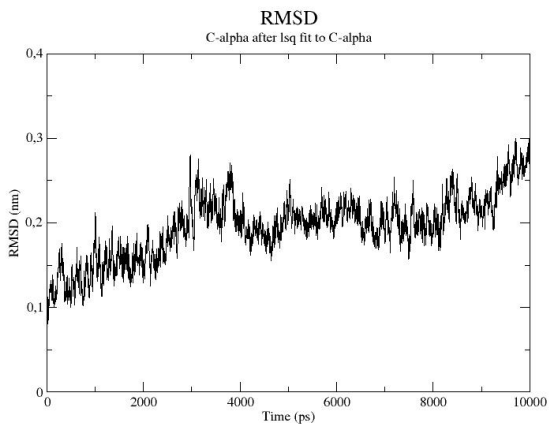


A) 1000 bar

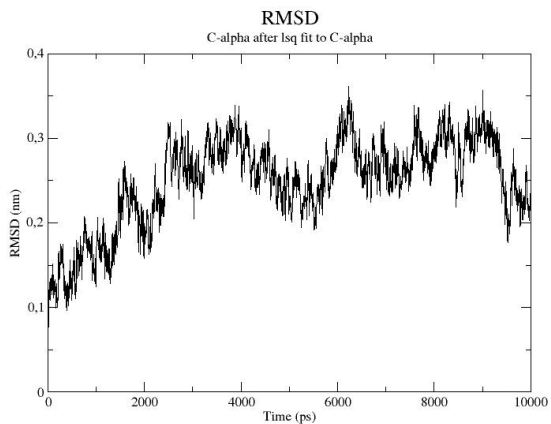


B) 1250 bar

Figure 9: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

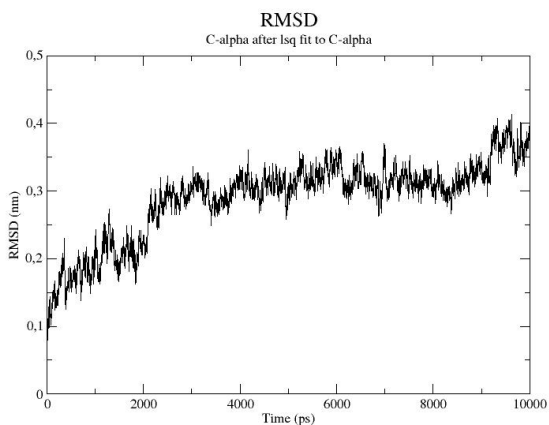


A) 1500 bar

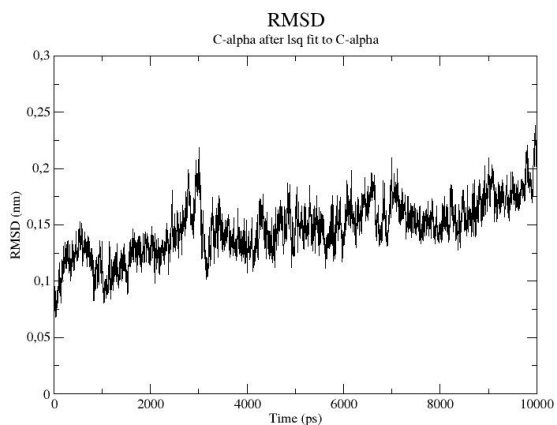


B) 1750 bar

Figure 10: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

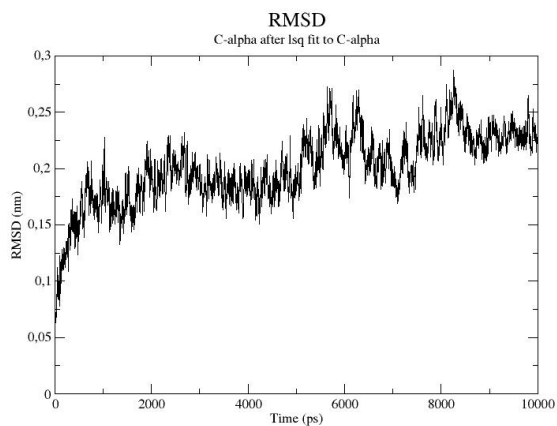


A) 2000 bar

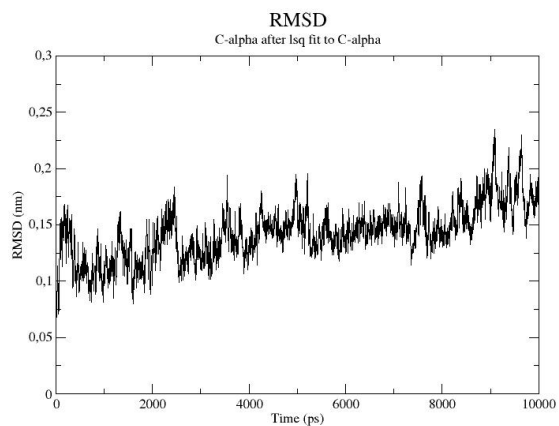


B) 2250 bar

Figure 11: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

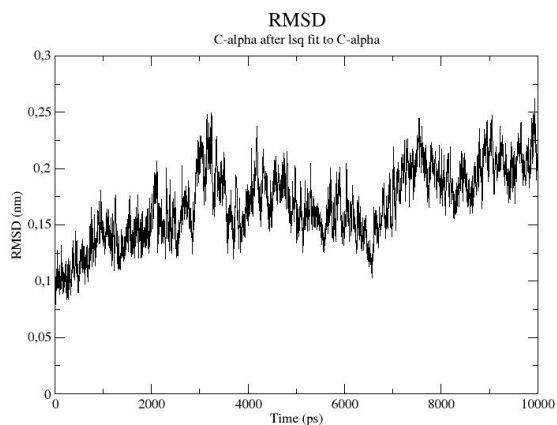


A) 2500 bar @ 300 K

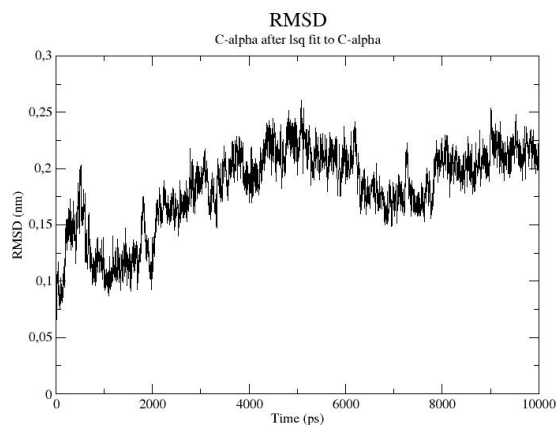


B) 2500 bar @ 295 K

Figure 12: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

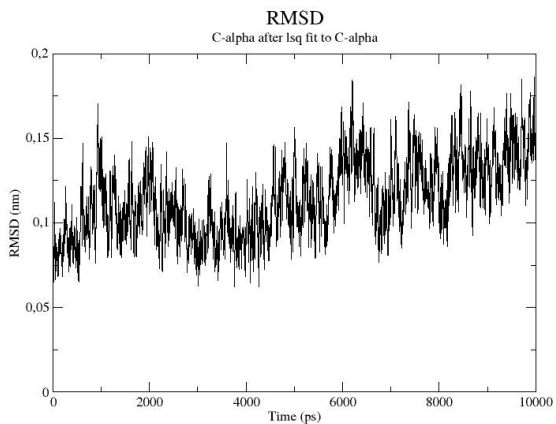


A) 2500 bar @ 290 K

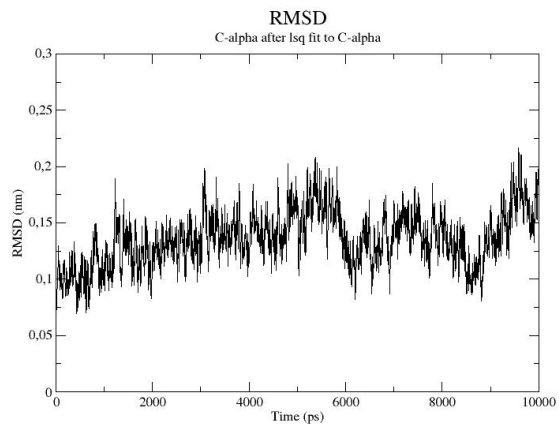


B) 2500 bar @ 285 K

Figure 13: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

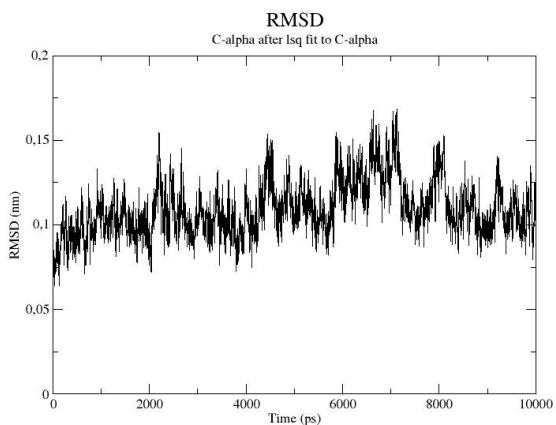


A) 2500 bar @ 280 K

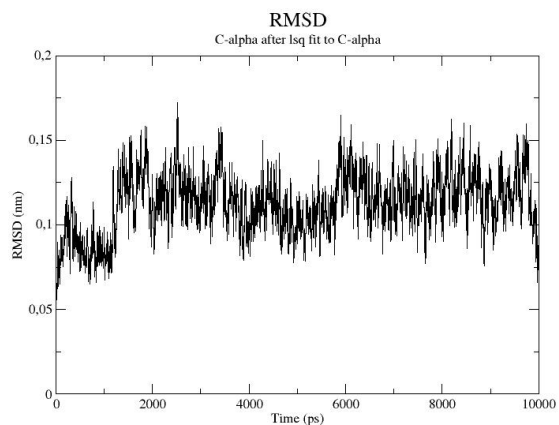


B) 2500 bar @ 275 K

Figure 14: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

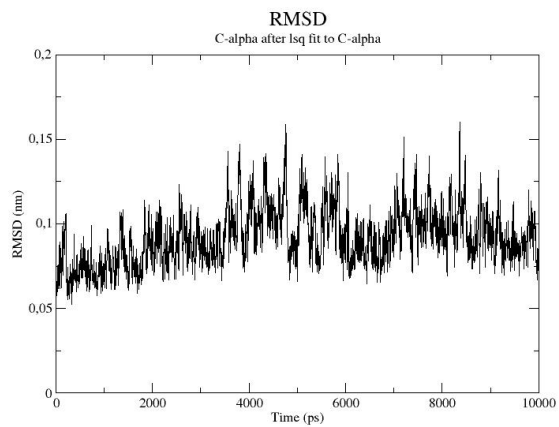
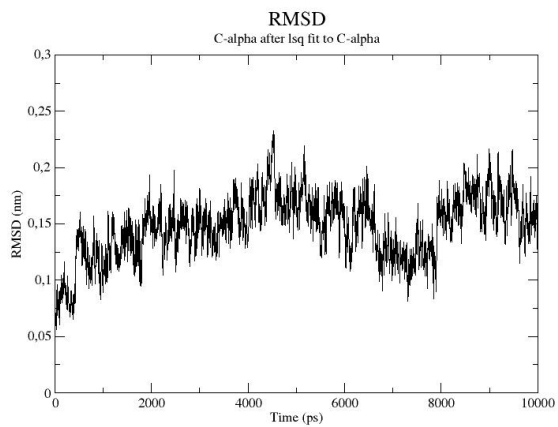


A) 2500 bar @ 270 K



B) 2500 bar @ 265 K

Figure 15: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature



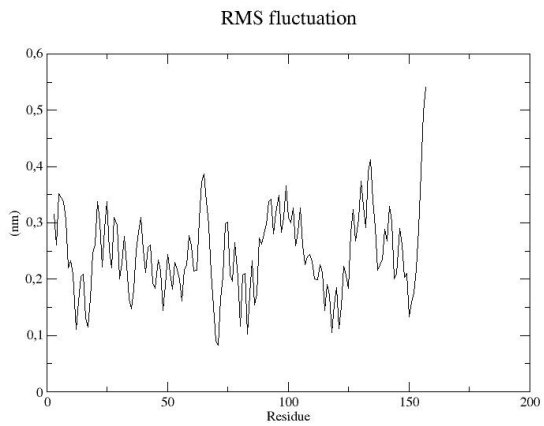
A) 2500 bar @ 260 K

B) 2500 bar @ 255 K

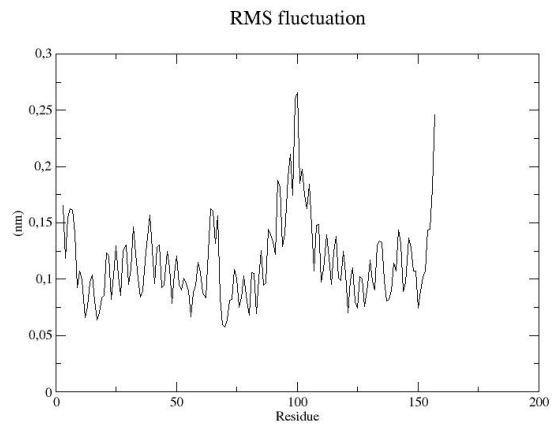
Figure 16: RMSD side-by-side - High Hydrostatic Pressure and Low Temperature

**RMSF**

**HHP**

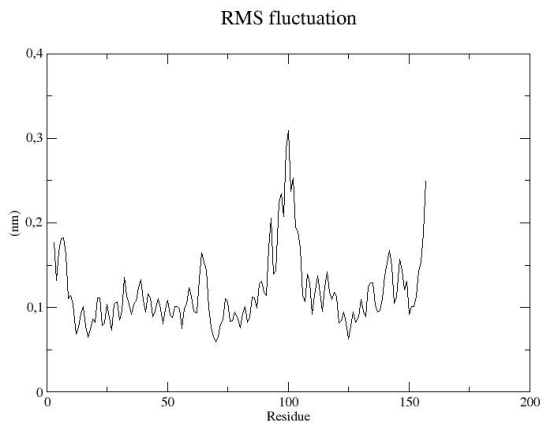


A) 1 bar

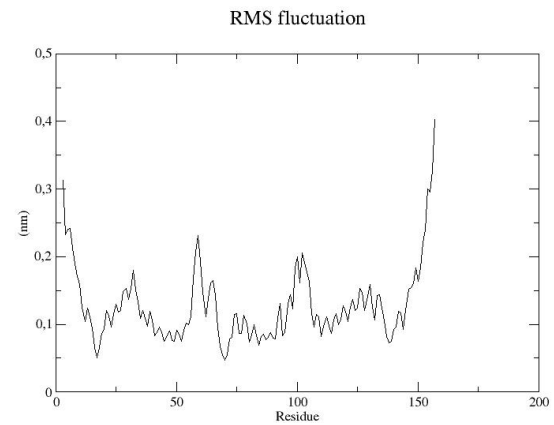


B) 250 bar

Figure 17: RMSF side-by-side - High Hydrostatic Pressure

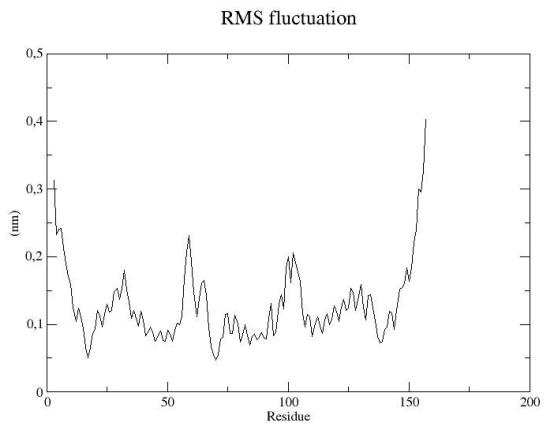


A) 500 bar

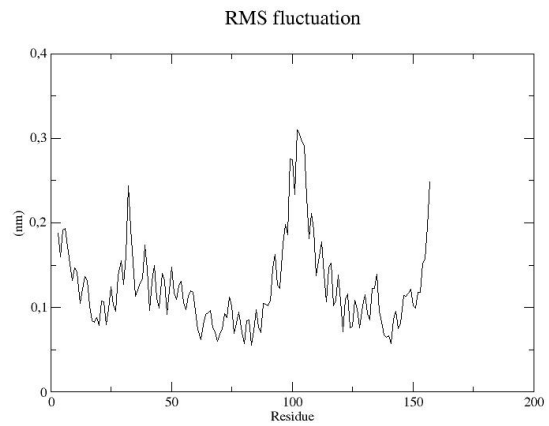


B) 750 bar

Figure 18: RMSF side-by-side - High Hydrostatic Pressure

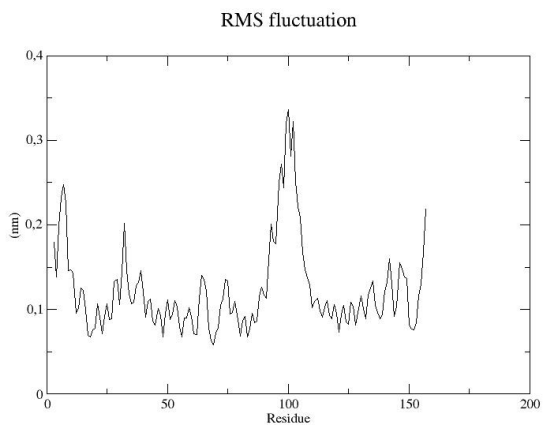


A) 1000 bar

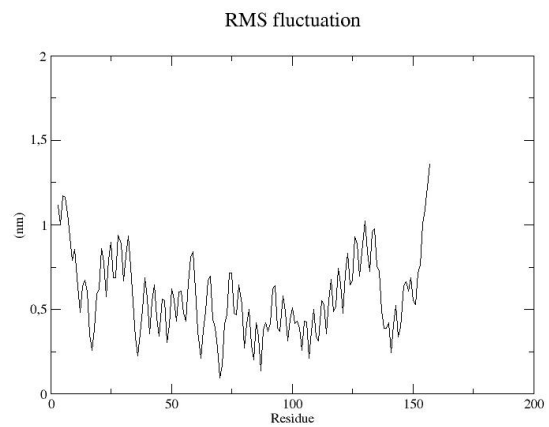


B) 1250 bar

Figure 19: RMSF side-by-side - High Hydrostatic Pressure

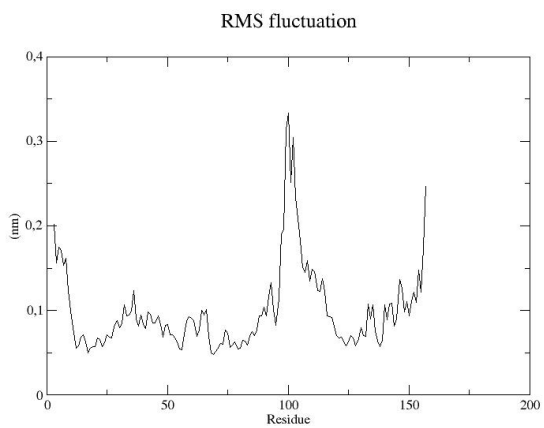


A) 1500 bar

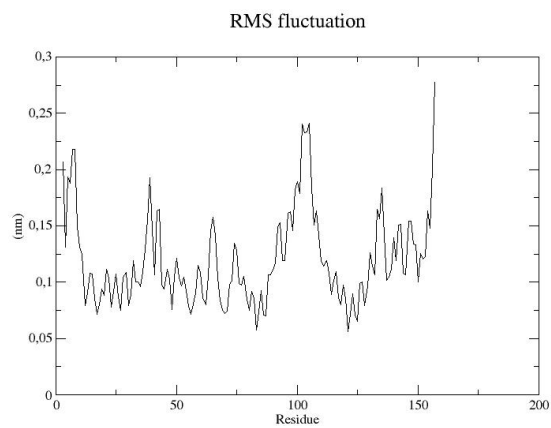


B) 1750 bar

Figure 20: RMSF side-by-side - High Hydrostatic Pressure

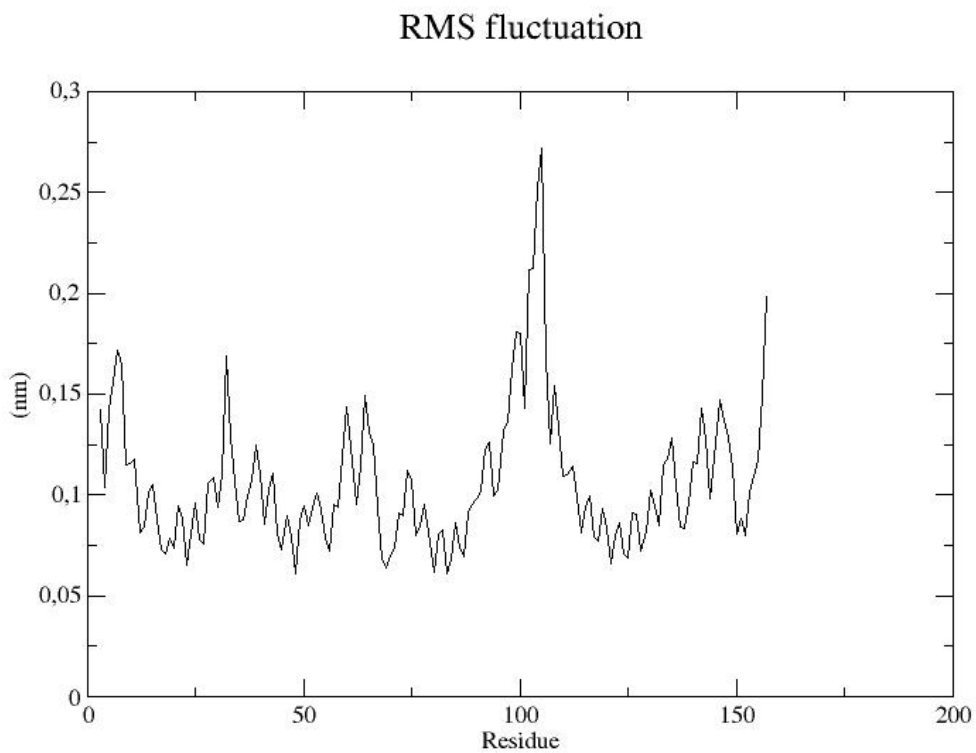


A) 2000 bar



B) 2250 bar

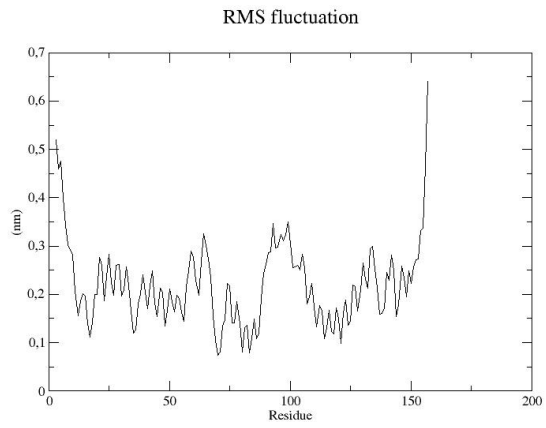
Figure 21: RMSF side-by-side - High Hydrostatic Pressure



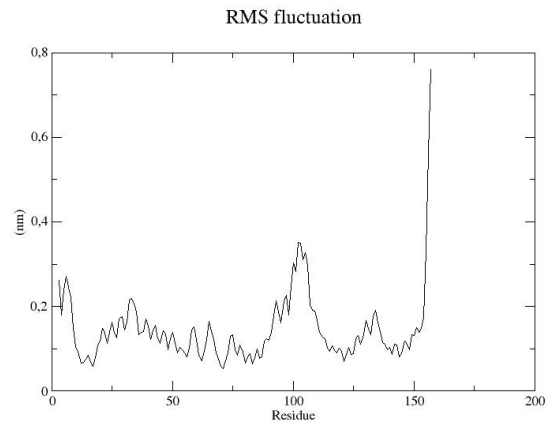
A) 2500 bar

Figure 22: RMSF side-by-side - High Hydrostatic Pressure

## HHP and low temperature

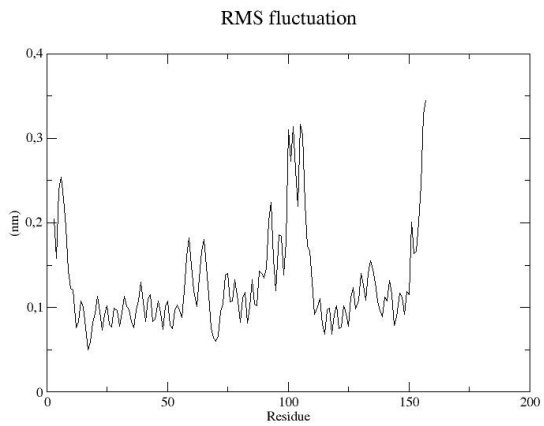


A) 1 bar

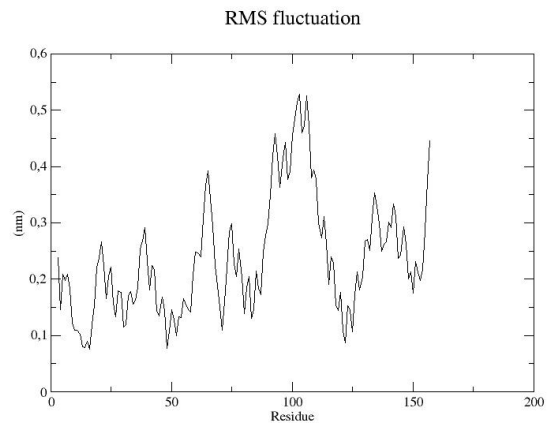


B) 250 bar

Figure 23: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

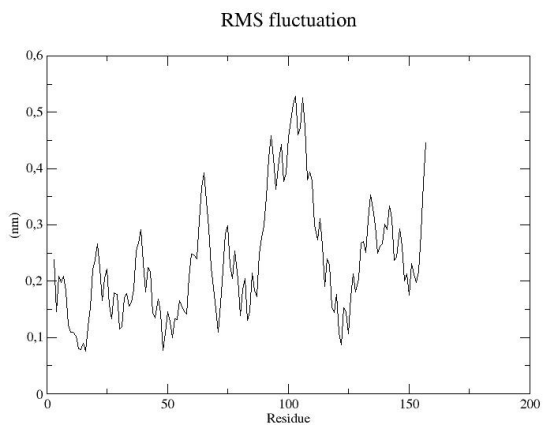


**A) 500 bar**

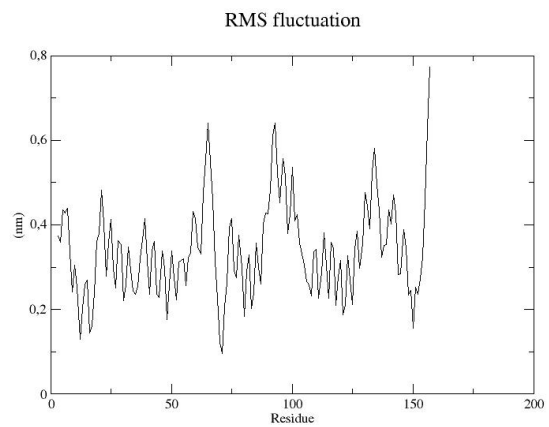


**B) 750 bar**

Figure 24: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

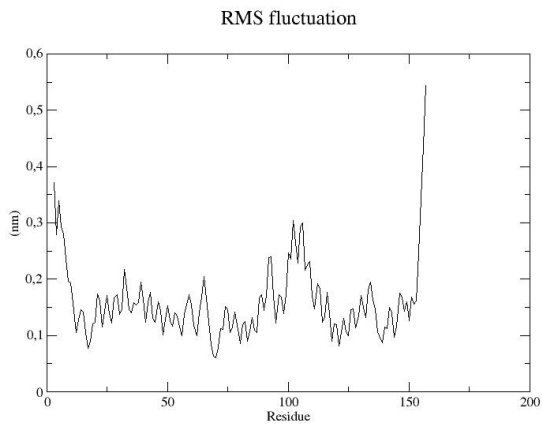


**A) 1000 bar**

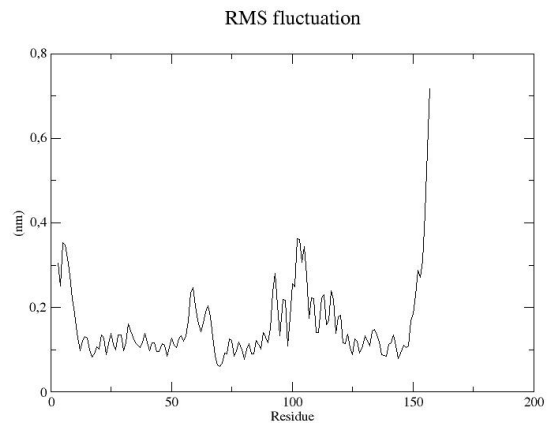


**B) 1250 bar**

Figure 25: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

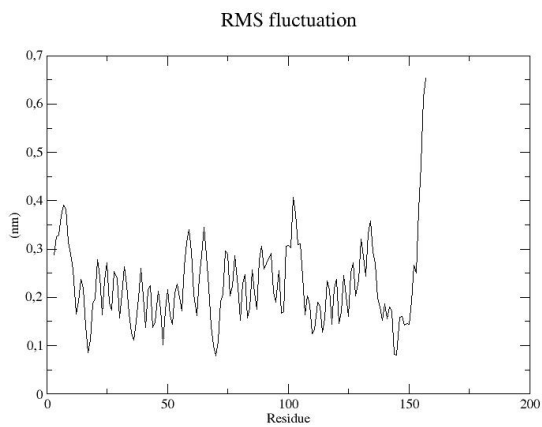


A) 1500 bar

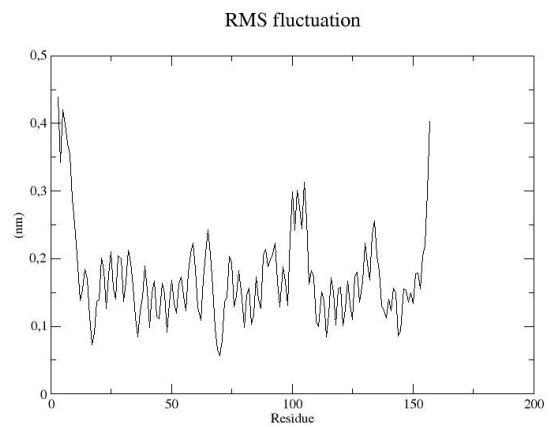


B) 1750 bar

Figure 26: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

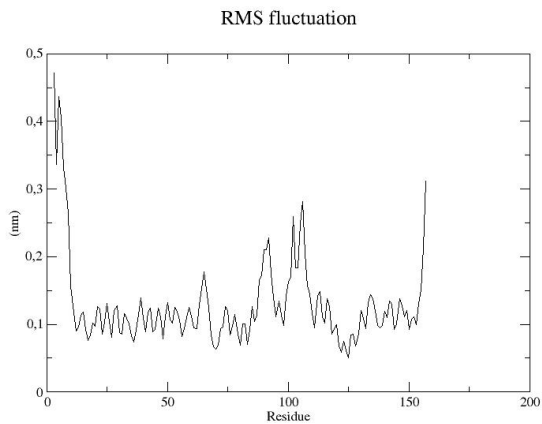


A) 2000 bar

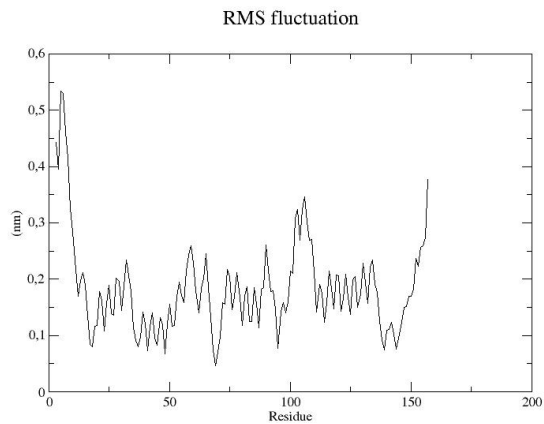


B) 2250 bar

Figure 27: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

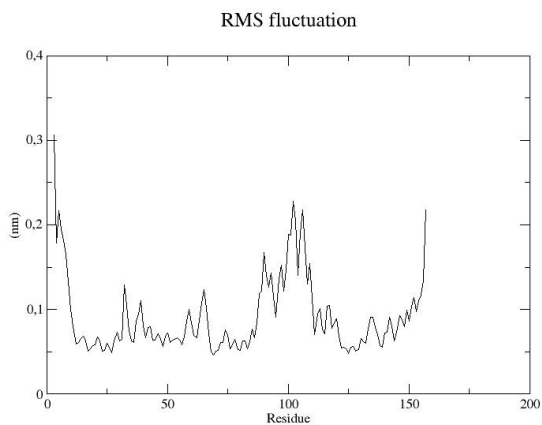


A) 2500 bar @ 300 K

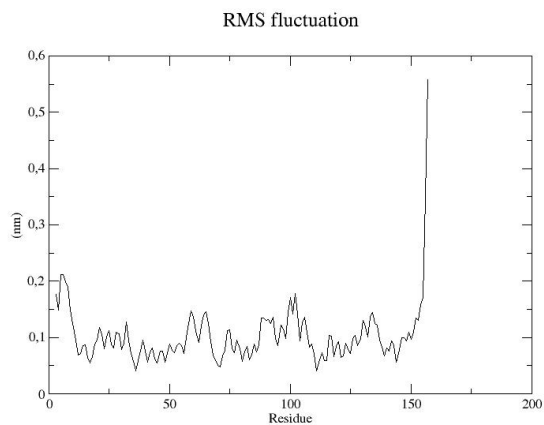


B) 2500 bar @ 295 K

Figure 28: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

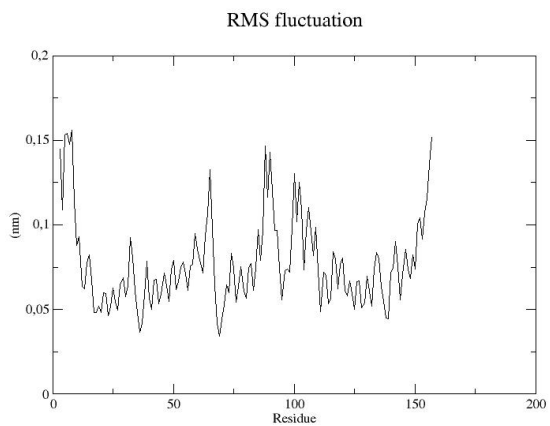


A) 2500 bar @ 290 K

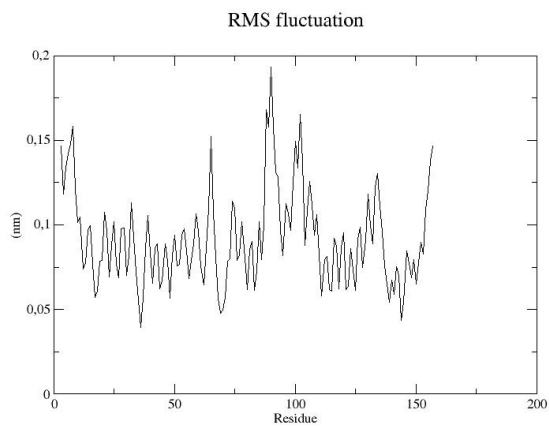


B) 2500 bar @ 285 K

Figure 29: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

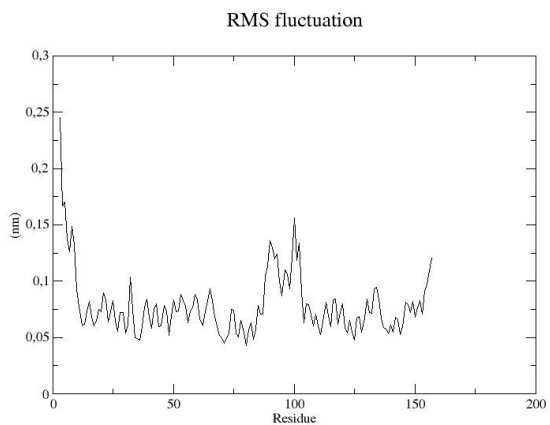


A) 2500 bar @ 280 K

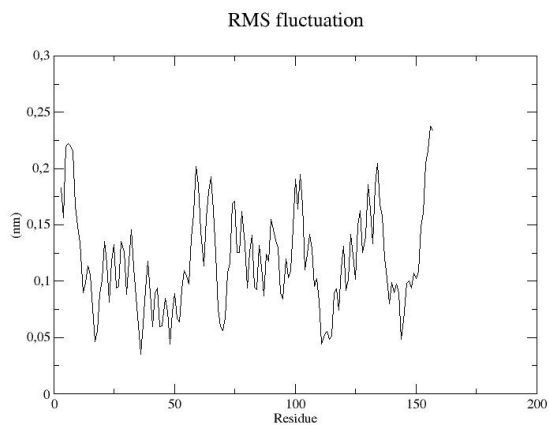


B) 2500 bar @ 275 K

Figure 30: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

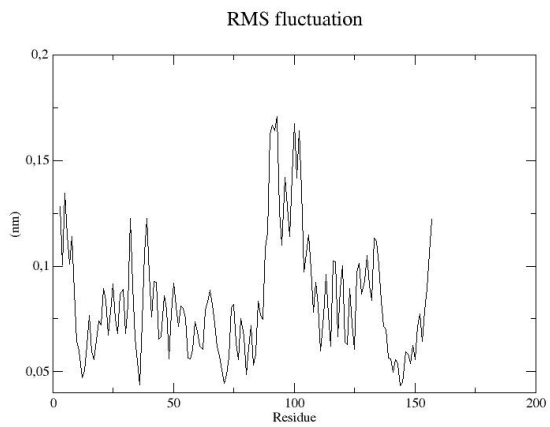


A) 2500 bar @ 270 K

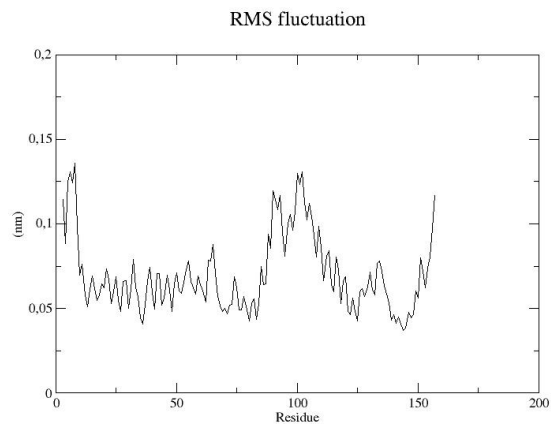


B) 2500 bar @ 265 K

Figure 31: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature



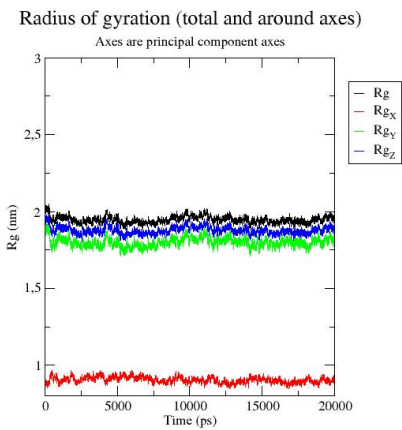
A) 2500 bar @ 260 K



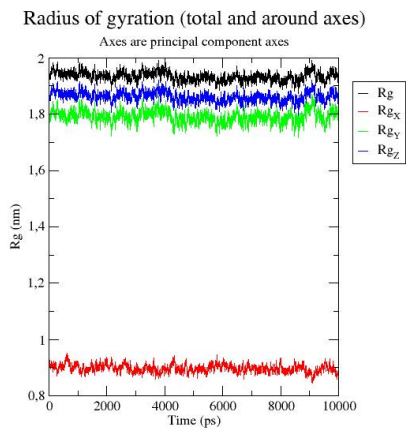
B) 2500 bar @ 255 K

Figure 32: RMSF side-by-side - High Hydrostatic Pressure and Low Temperature

**Rg**  
**HHP**

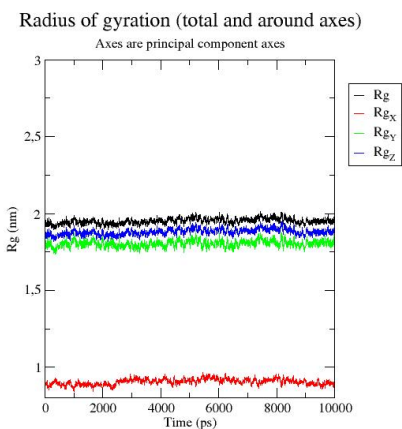


A) 1 bar

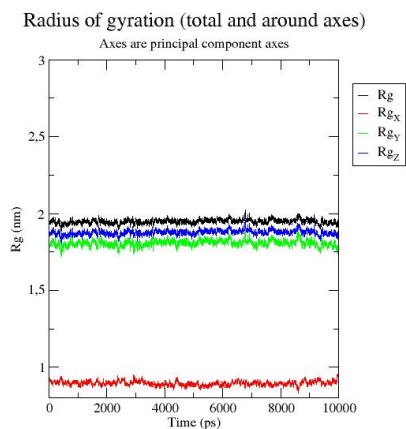


B) 250 bar

Figure 33: Rg side-by-side - High Hydrostatic Pressure

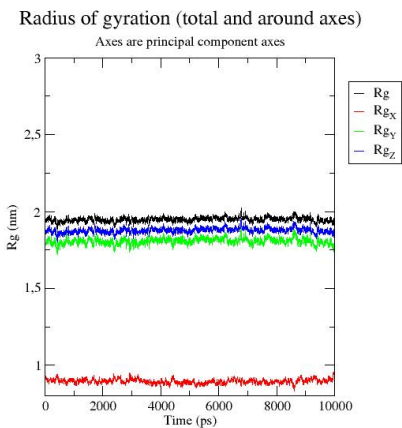


A) 500 bar

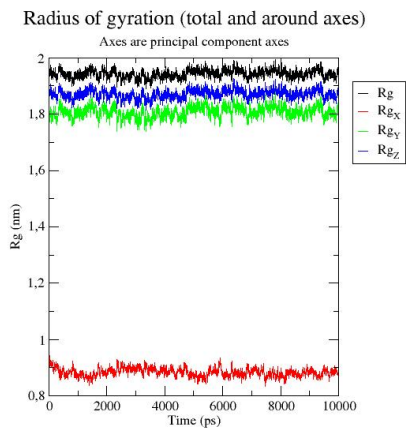


B) 750 bar

Figure 34: Rg side-by-side - High Hydrostatic Pressure

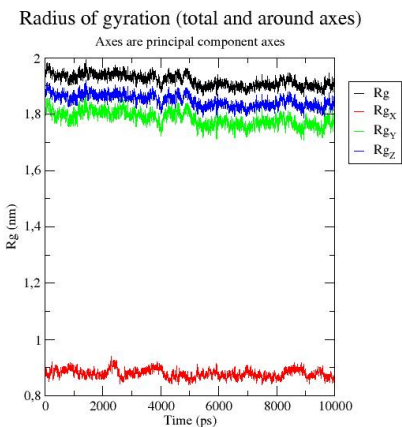


A) 1000 bar

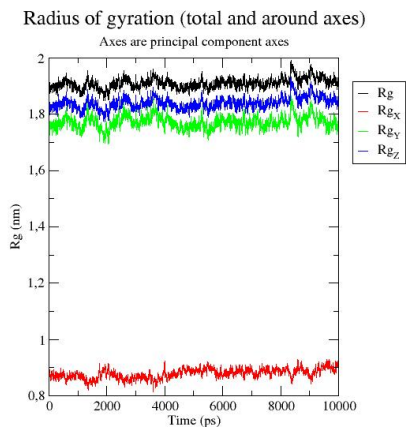


B) 1250 bar

Figure 35: Rg side-by-side - High Hydrostatic Pressure



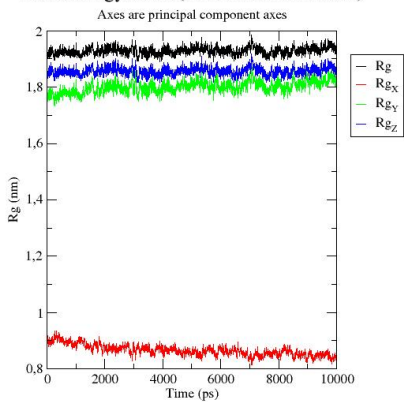
A) 1500 bar



B) 1750 bar

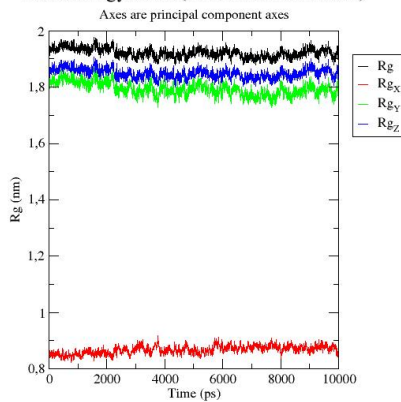
Figure 36: Rg side-by-side - High Hydrostatic Pressure

Radius of gyration (total and around axes)



A) 2000 bar

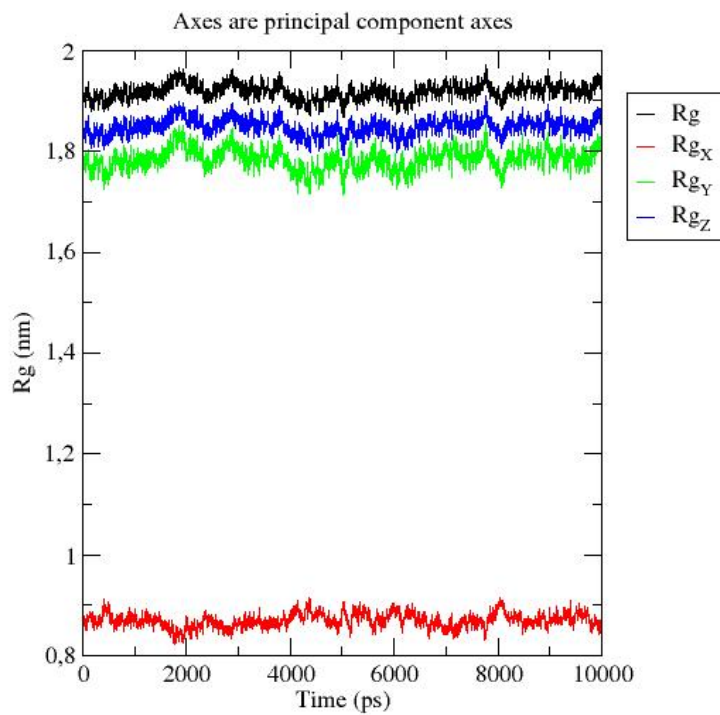
Radius of gyration (total and around axes)



B) 2250 bar

Figure 37: Rg side-by-side - High Hydrostatic Pressure

Radius of gyration (total and around axes)

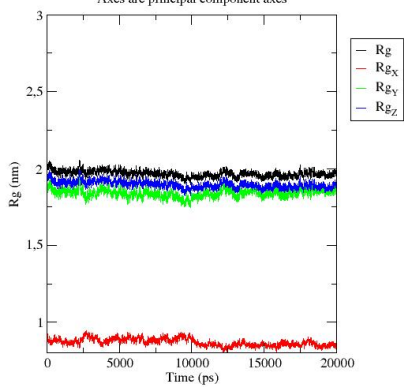


A) 2500 bar

Figure 38: Rg side-by-side - High Hydrostatic Pressure

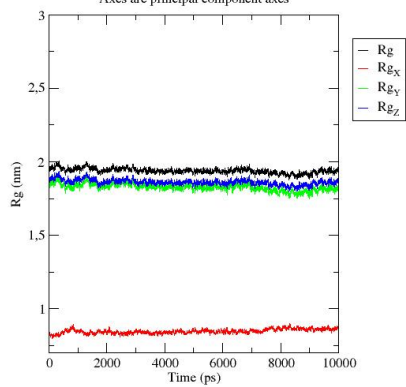
## HHP and low temperature

Radius of gyration (total and around axes)  
Axes are principal component axes



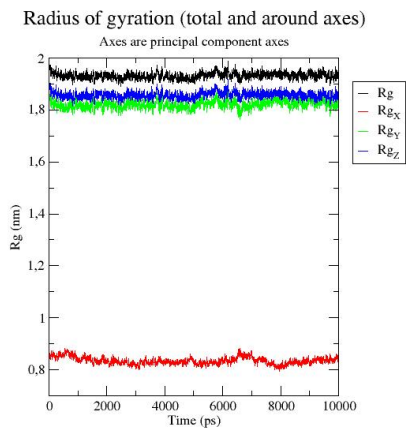
A) 1 bar

Radius of gyration (total and around axes)  
Axes are principal component axes

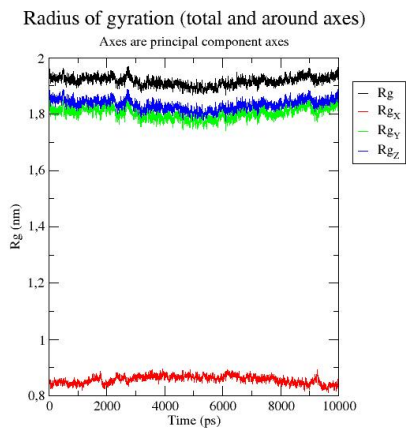


B) 250 bar

Figure 39: Rg side-by-side - High Hydrostatic Pressure and Low Temperature

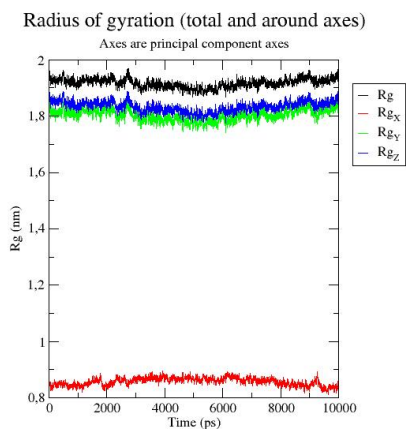


A) 500 bar

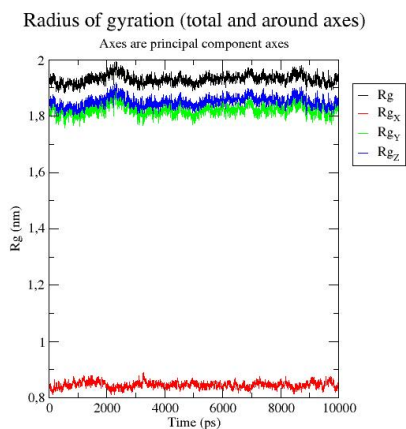


B) 750 bar

Figure 40: Rg side-by-side - High Hydrostatic Pressure and Low Temperature

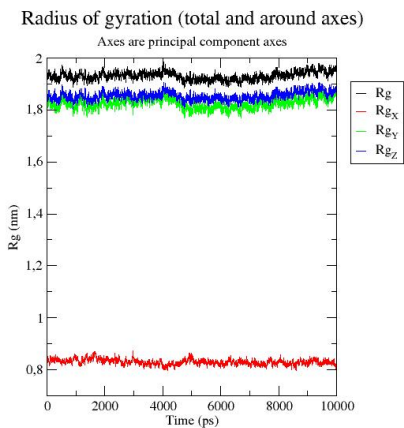


A) 1000 bar

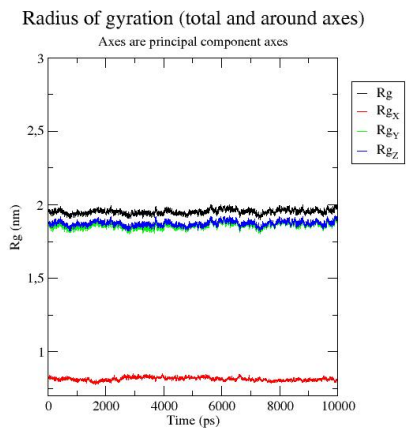


B) 1250 bar

Figure 41: Rg side-by-side - High Hydrostatic Pressure and Low Temperature

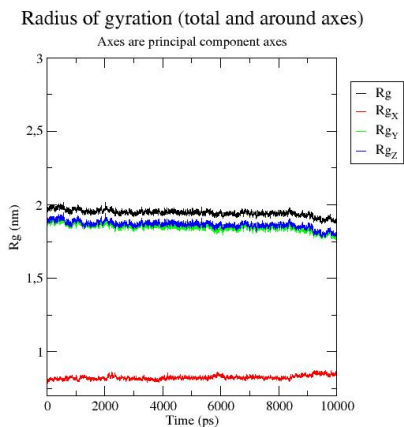


A) 1500 bar

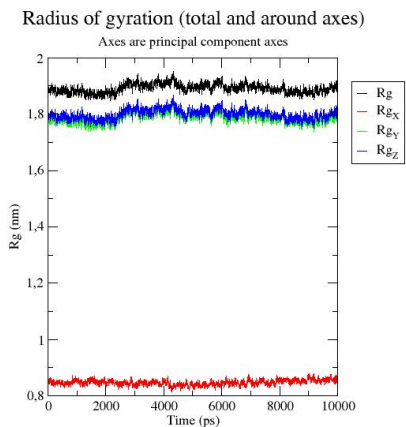


B) 1750 bar

Figure 42: Rg side-by-side - High Hydrostatic Pressure and Low Temperature



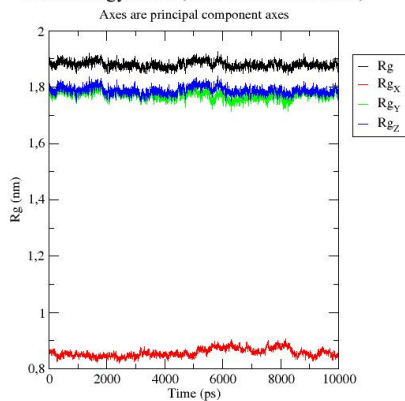
A) 2000 bar



B) 2250 bar

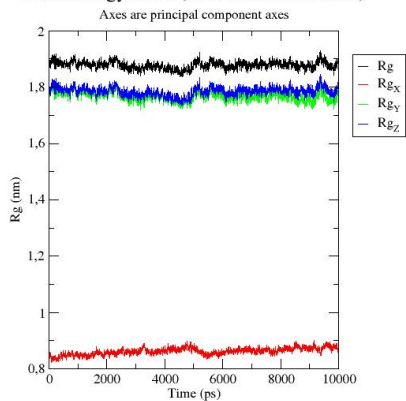
Figure 43: Rg side-by-side - High Hydrostatic Pressure and Low Temperature

Radius of gyration (total and around axes)



A) 2500 bar @ 300 K

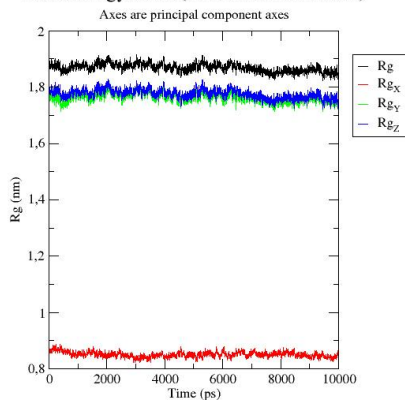
Radius of gyration (total and around axes)



B) 2500 bar @ 295 K

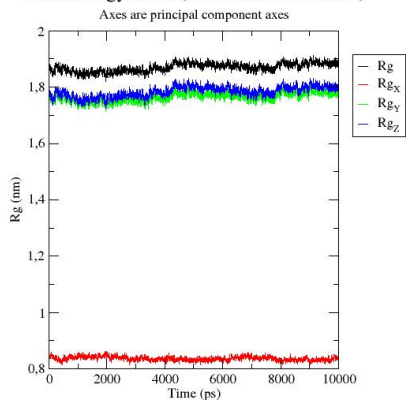
Figure 44: Rg side-by-side - High Hydrostatic Pressure and Low Temperature

Radius of gyration (total and around axes)



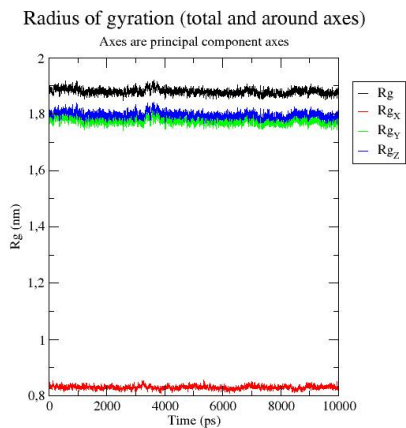
A) 2500 bar @ 290 K

Radius of gyration (total and around axes)

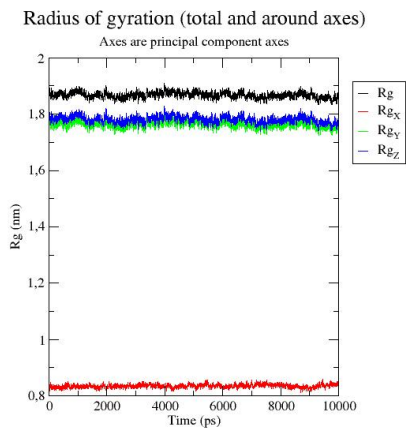


B) 2500 bar @ 285 K

Figure 45: Rg side-by-side - High Hydrostatic Pressure and Low Temperature

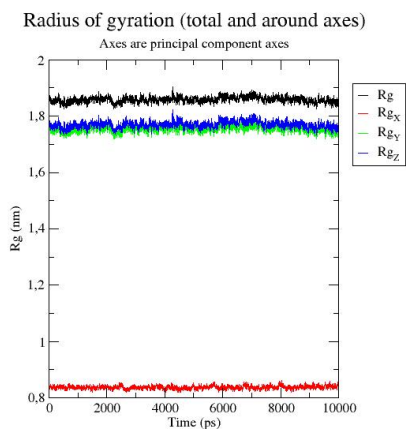


A) 2500 bar @ 280 K

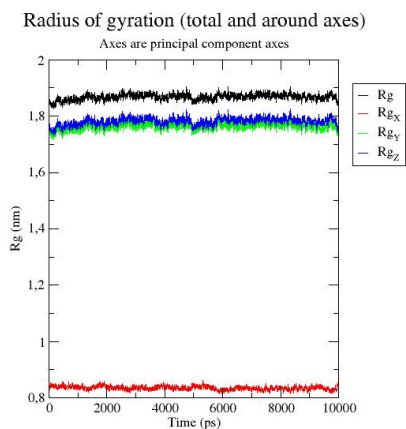


B) 2500 bar @ 275 K

Figure 46: Rg side-by-side - High Hydrostatic Pressure and Low Temperature

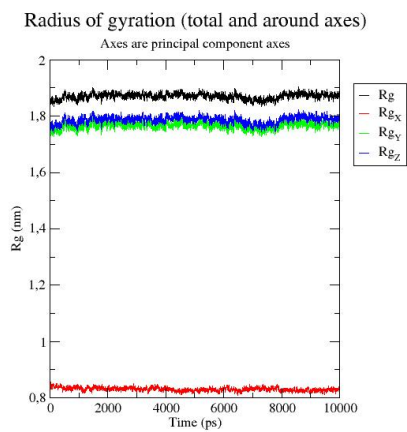


A) 2500 bar @ 270 K

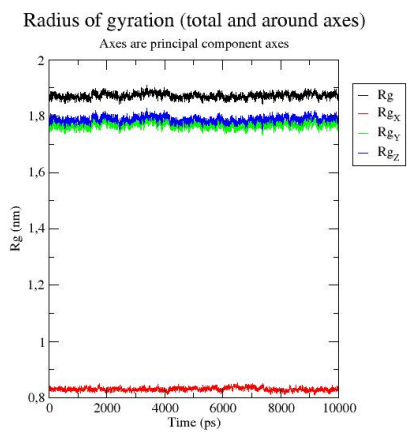


B) 2500 bar @ 265 K

Figure 47: Rg side-by-side - High Hydrostatic Pressure and Low Temperature



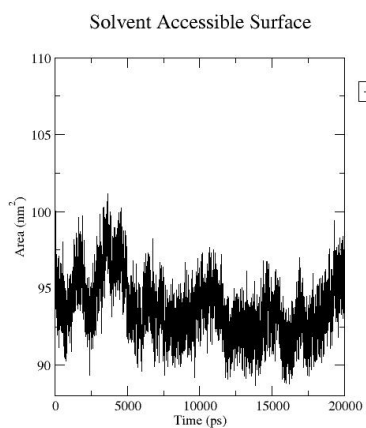
A) 2500 bar @ 260 K



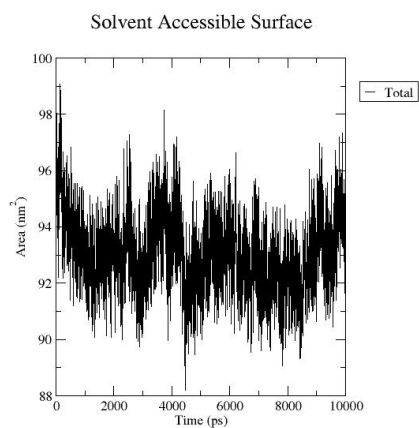
B) 2500 bar @ 255 K

Figure 48: Rg side-by-side - High Hydrostatic Pressure and Low Temperature

SASA  
HHP

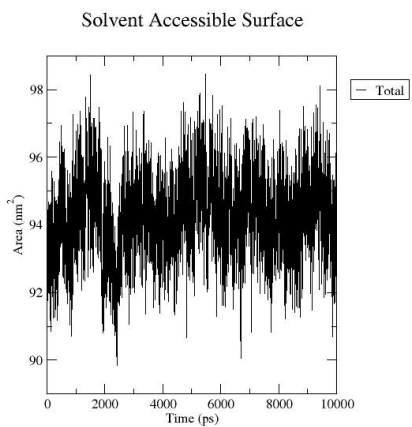


A) 1 bar

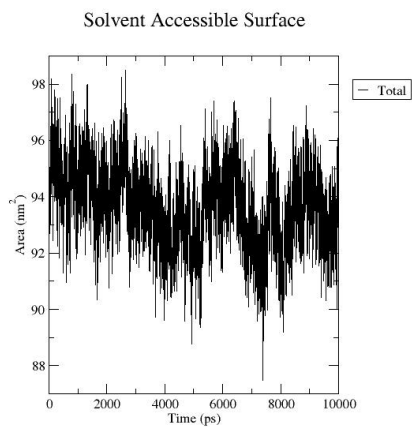


B) 250 bar

Figure 49: SASA side-by-side - High Hydrostatic Pressure

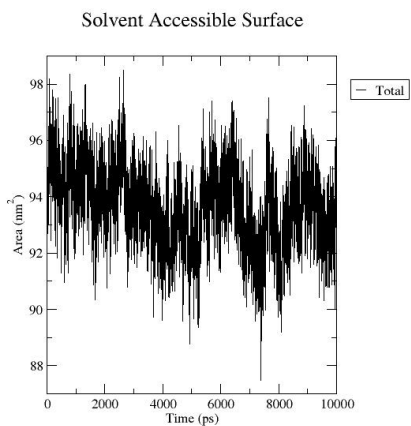


A) 500 bar

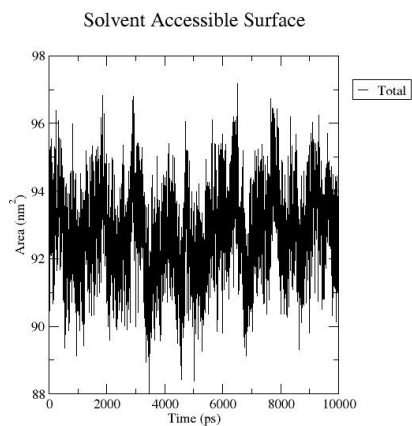


B) 750 bar

Figure 50: SASA side-by-side - High Hydrostatic Pressure

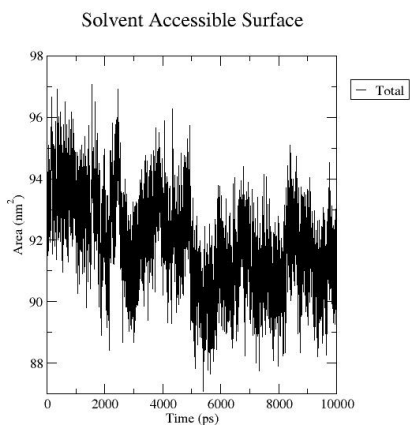


A) 1000 bar

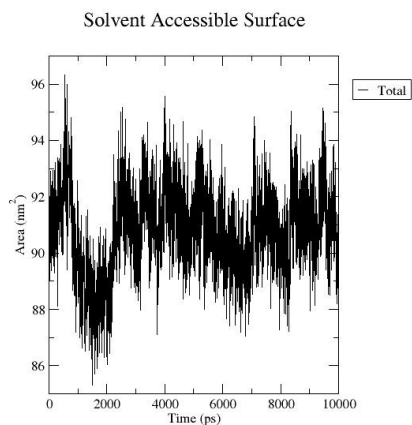


B) 1250 bar

Figure 51: SASA side-by-side - High Hydrostatic Pressure

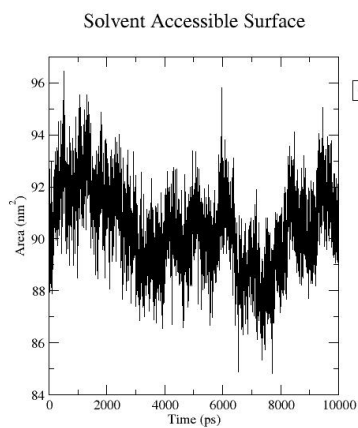


A) 1500 bar

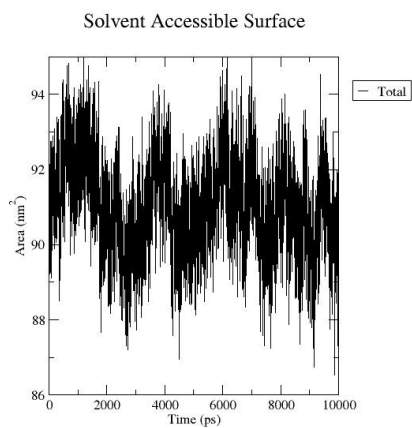


B) 1750 bar

Figure 52: SASA side-by-side - High Hydrostatic Pressure

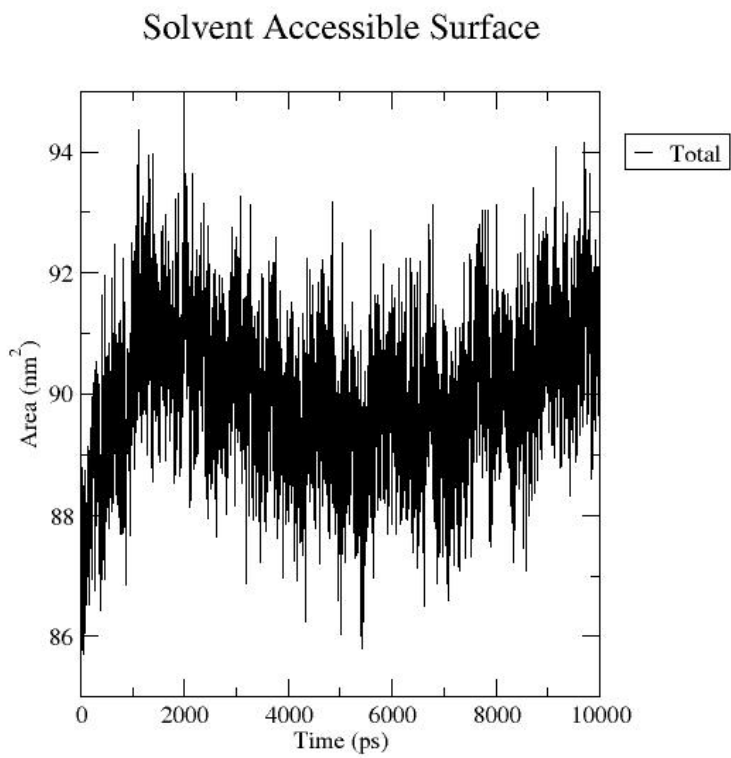


A) 2000 bar



B) 2250 bar

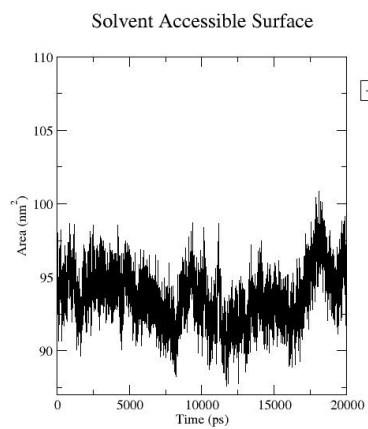
Figure 53: SASA side-by-side - High Hydrostatic Pressure



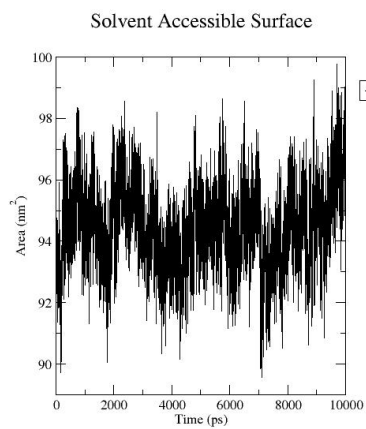
A) 2500 bar

Figure 54: SASA side-by-side - High Hydrostatic Pressure

## HHP and low temperature

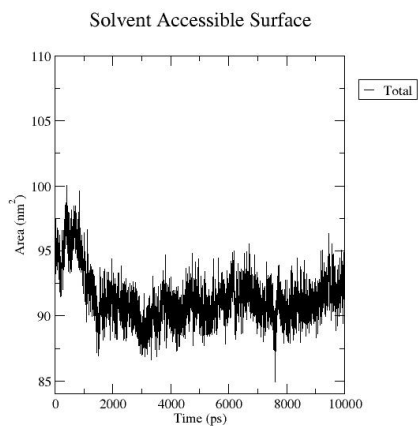


A) 1 bar

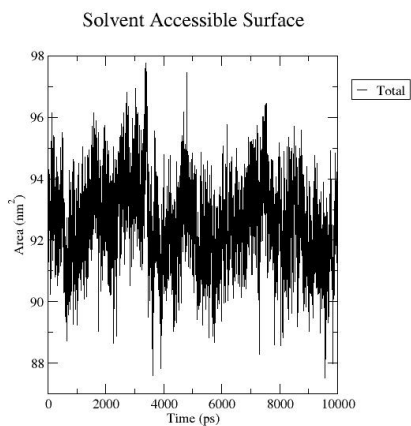


B) 250 bar

Figure 55: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

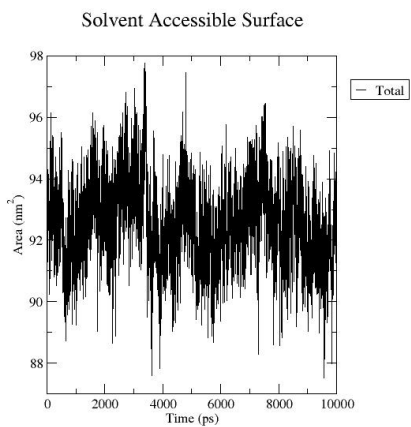


A) 500 bar

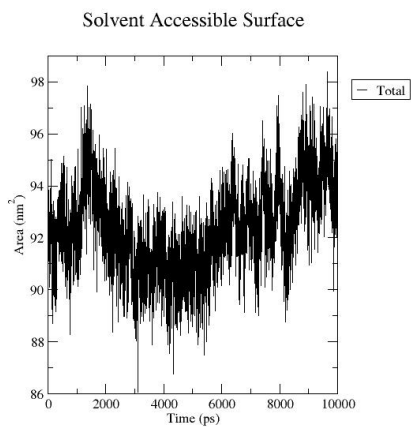


B) 750 bar

Figure 56: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

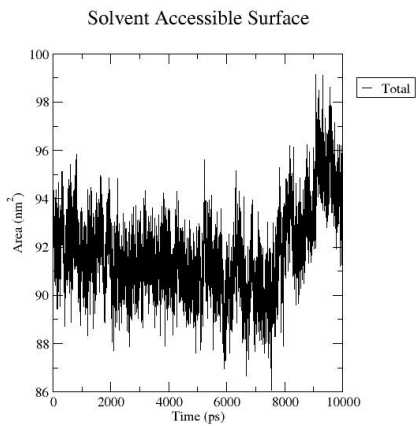


A) 1000 bar

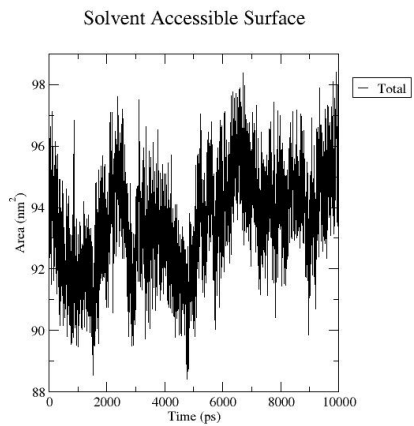


B) 1250 bar

Figure 57: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

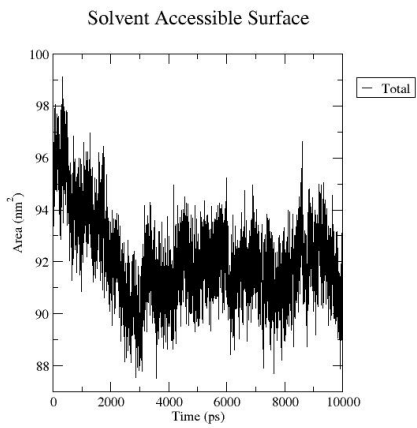


A) 1500 bar

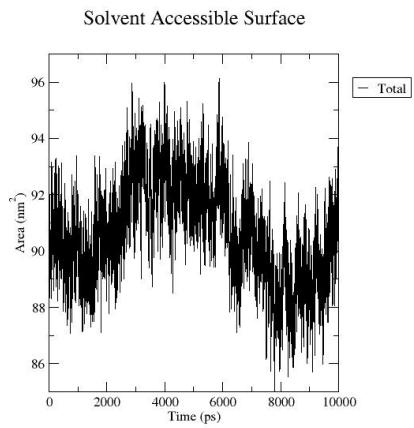


B) 1750 bar

Figure 58: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

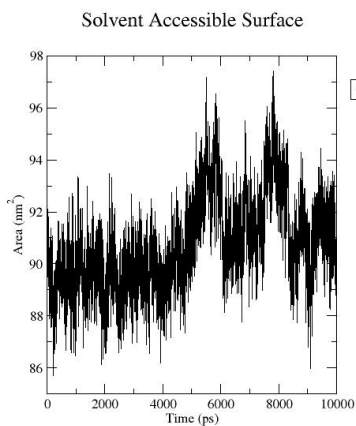


A) 2000 bar

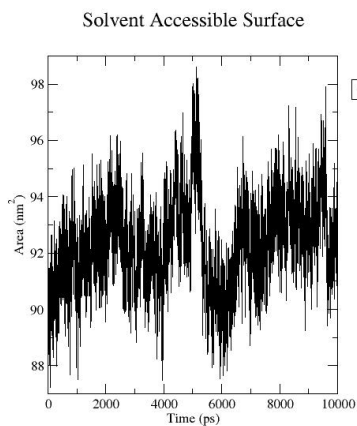


B) 2250 bar

Figure 59: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

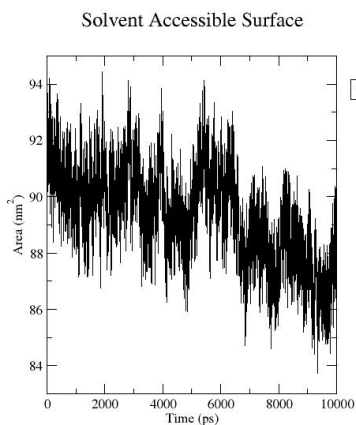


A) 2500 bar @ 300 K

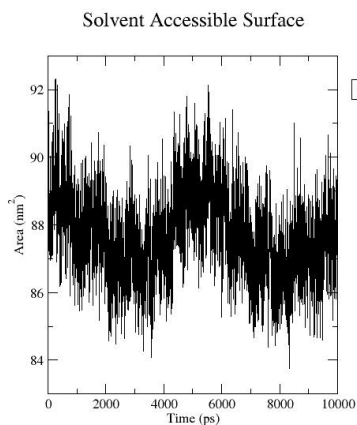


B) 2500 bar @ 295 K

Figure 60: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

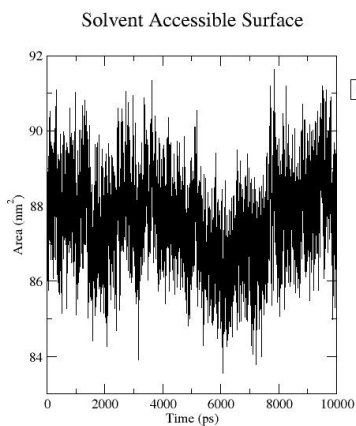


A) 2500 bar @ 290 K

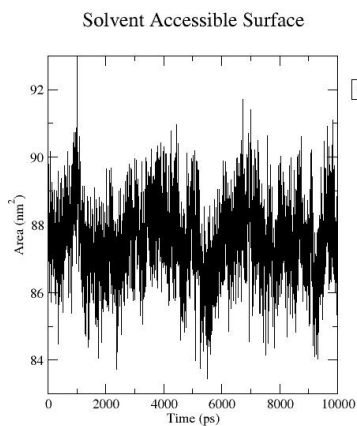


B) 2500 bar @ 285 K

Figure 61: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

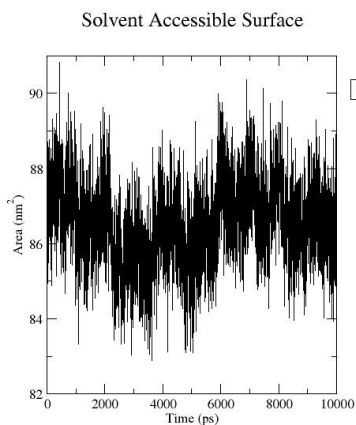


A) 2500 bar @ 280 K

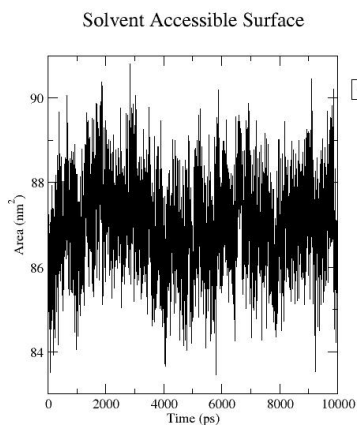


B) 2500 bar @ 275 K

Figure 62: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

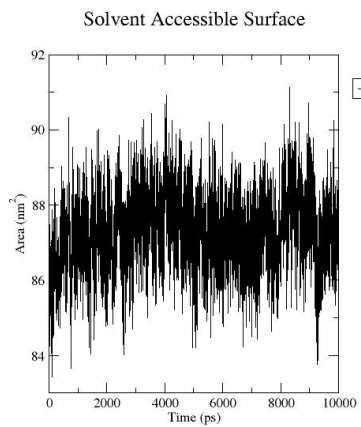


A) 2500 bar @ 270 K

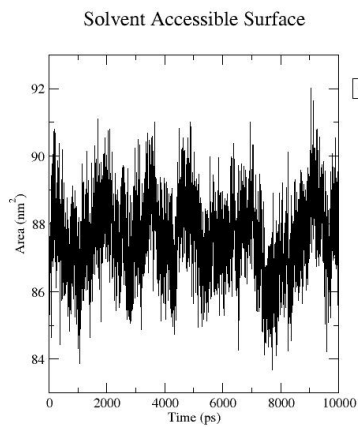


B) 2500 bar @ 265 K

Figure 63: SASA side-by-side - High Hydrostatic Pressure and Low Temperature



A) 2500 bar @ 260 K

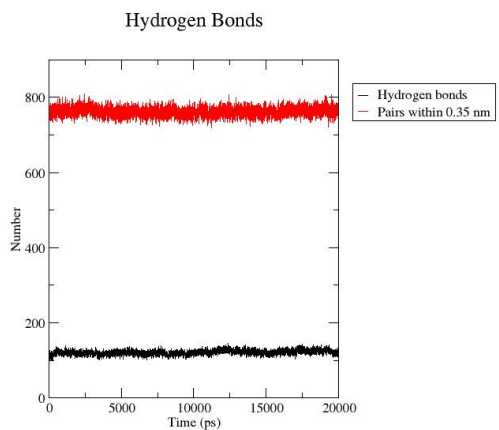


B) 2500 bar @ 255 K

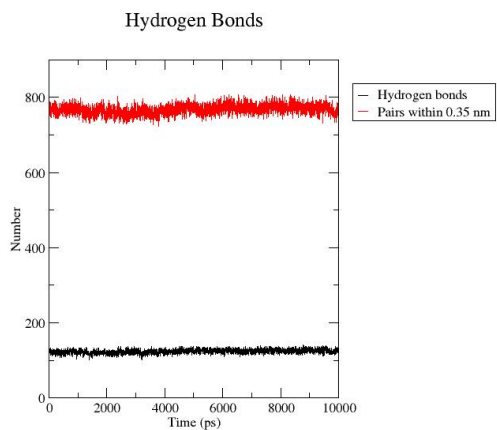
Figure 64: SASA side-by-side - High Hydrostatic Pressure and Low Temperature

**Hbonds**

**HHP**

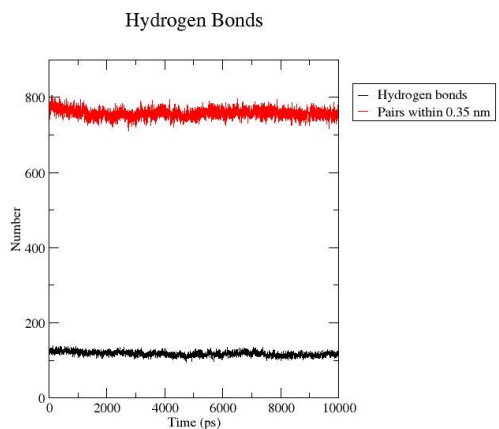


A) 1 bar

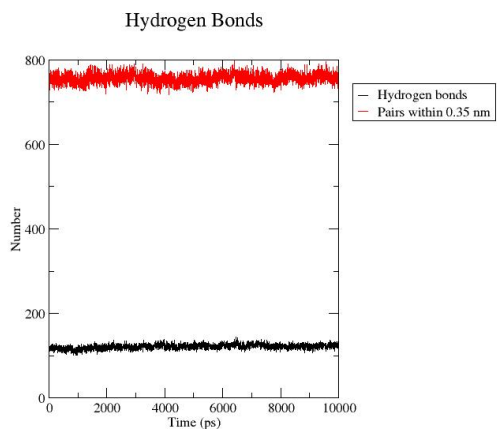


B) 250 bar

Figure 65: Hbond side-by-side - High Hydrostatic Pressure

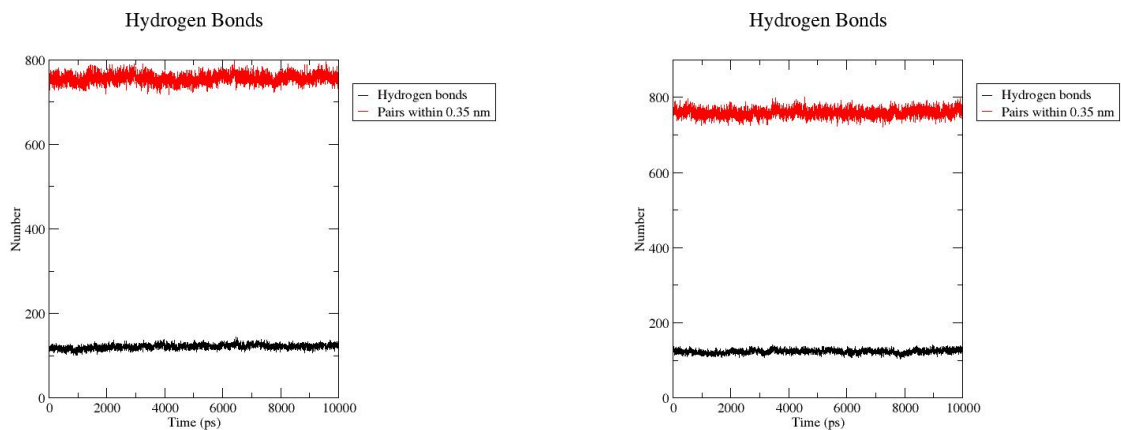


A) 500 bar



B) 750 bar

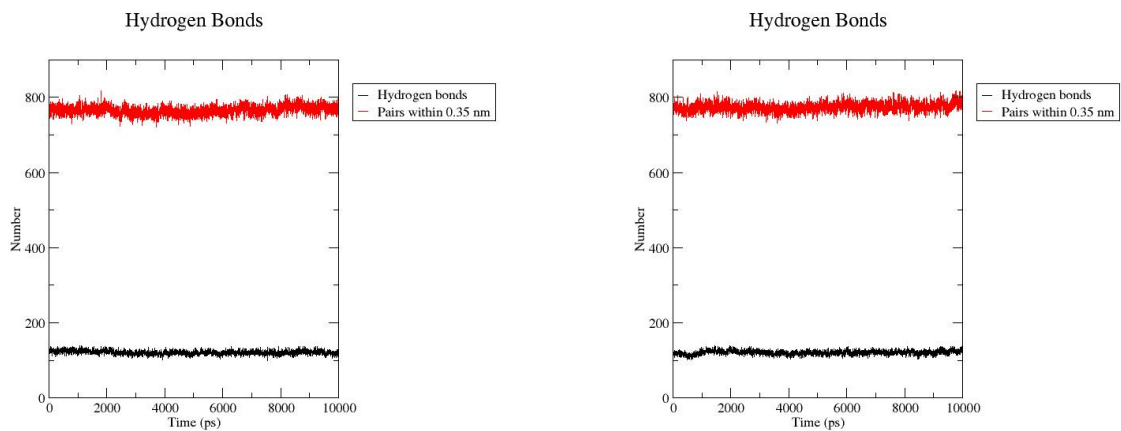
Figure 66: Hbond side-by-side - High Hydrostatic Pressure



A) 1000 bar

B) 1250 bar

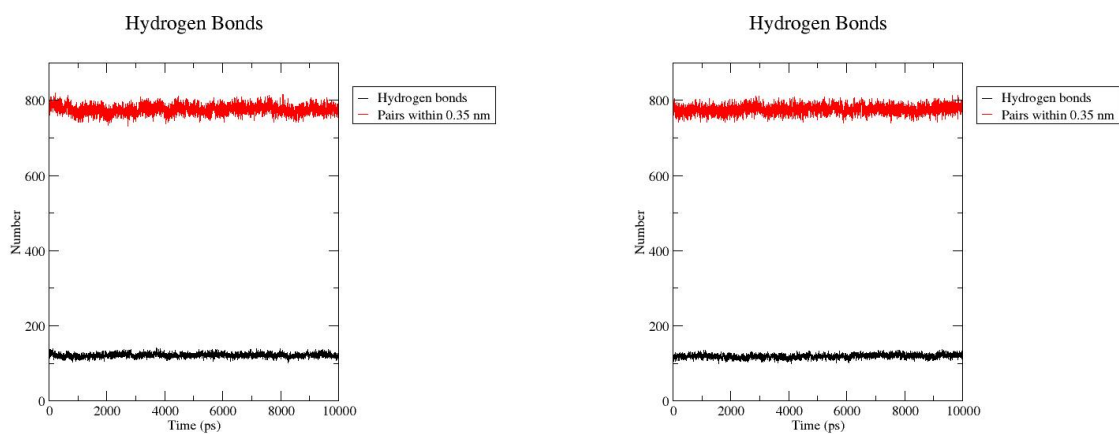
Figure 67: Hbond side-by-side - High Hydrostatic Pressure



A) 1500 bar

B) 1750 bar

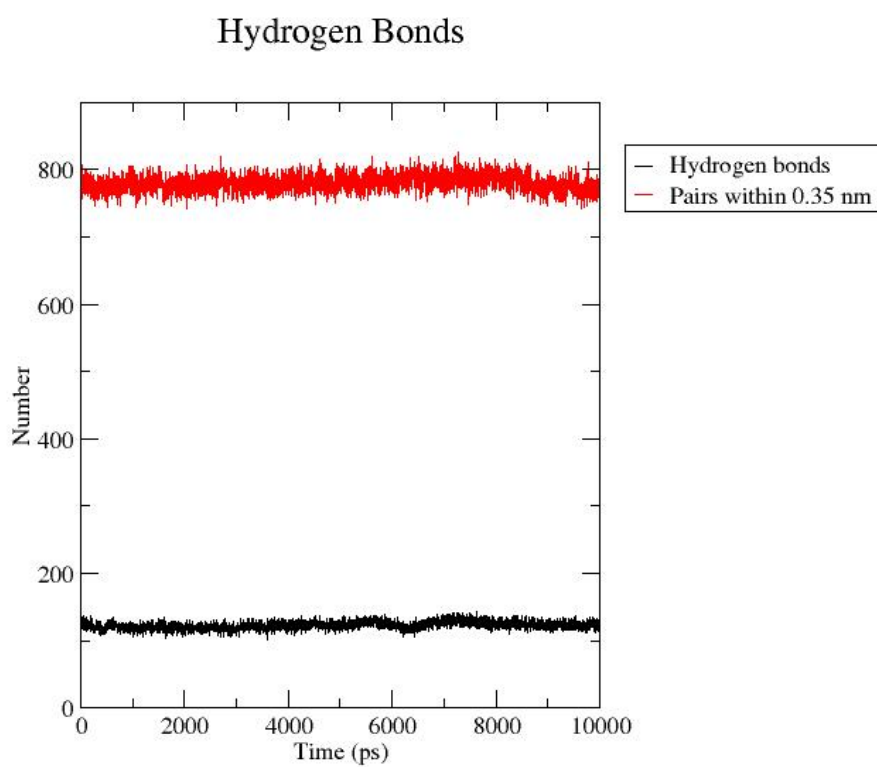
Figure 68: Hbond side-by-side - High Hydrostatic Pressure



A) 2000 bar

B) 2250 bar

Figure 69: Hbond side-by-side - High Hydrostatic Pressure



A) 2500 bar

Figure 70: Hbond side-by-side - High Hydrostatic Pressure

## HHP and low temperature

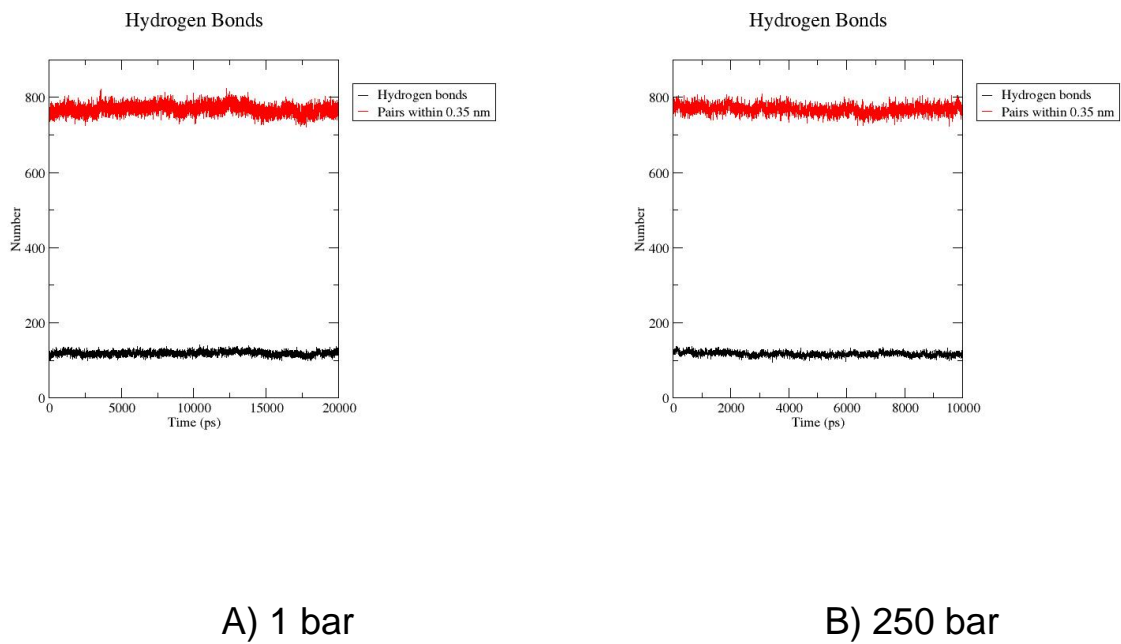
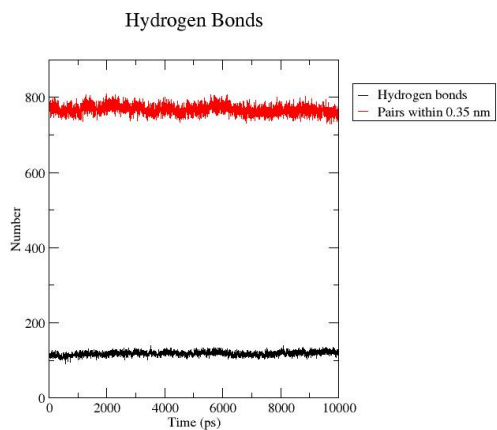
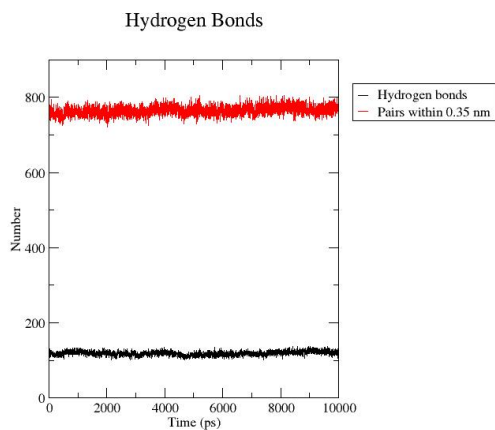


Figure 71: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

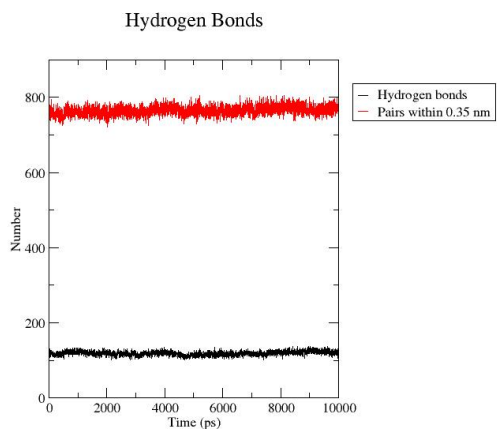


A) 500 bar

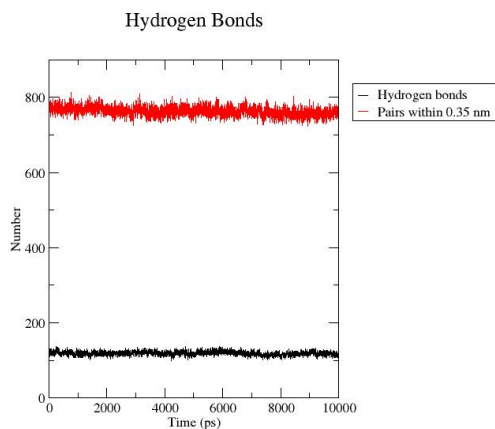


B) 750 bar

Figure 72: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

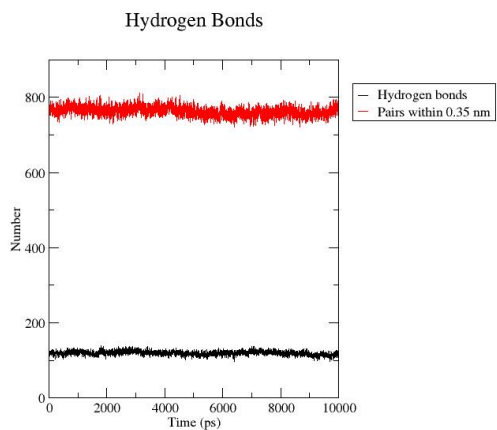


A) 1000 bar

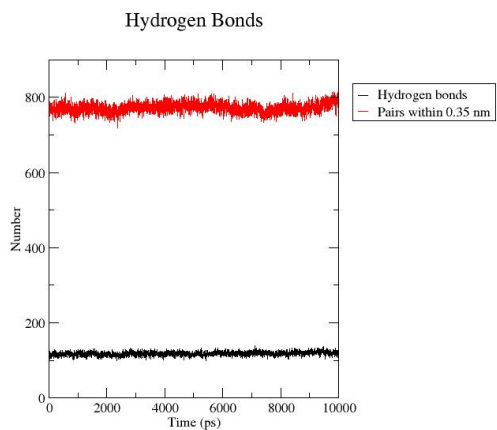


B) 1250 bar

Figure 73: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

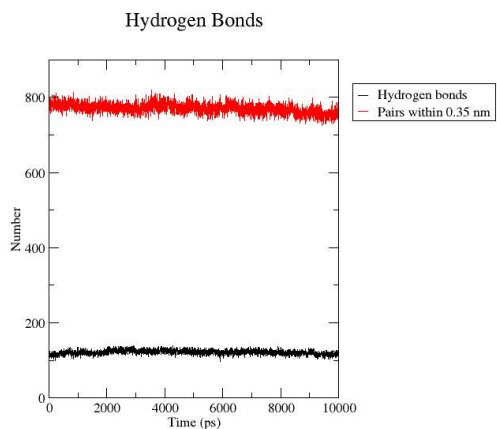


A) 1500 bar

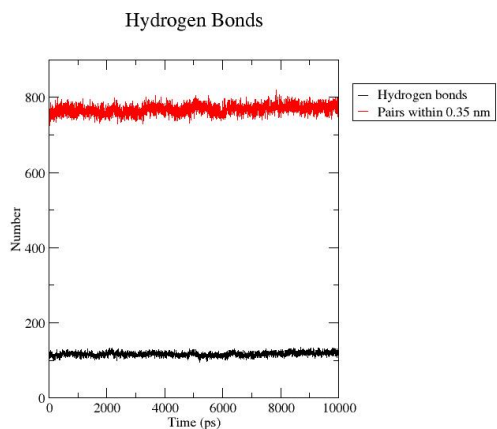


B) 1750 bar

Figure 74: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

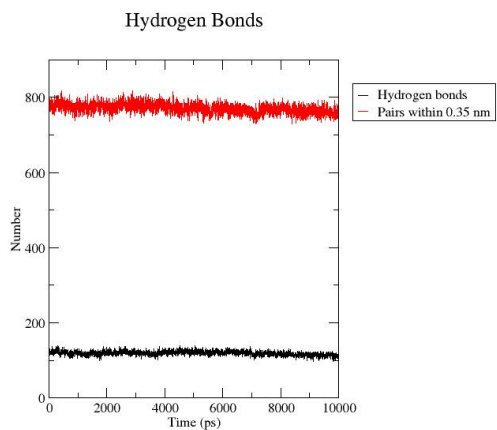


A) 2000 bar

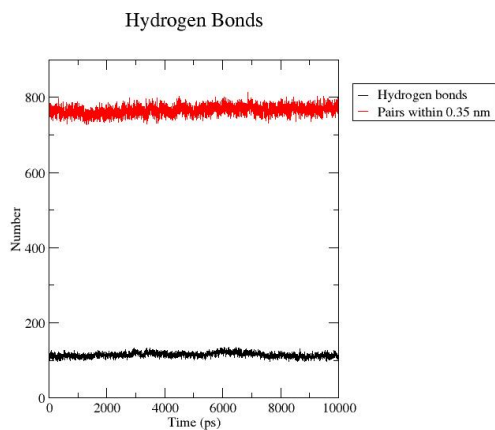


B) 2250 bar

Figure 75: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

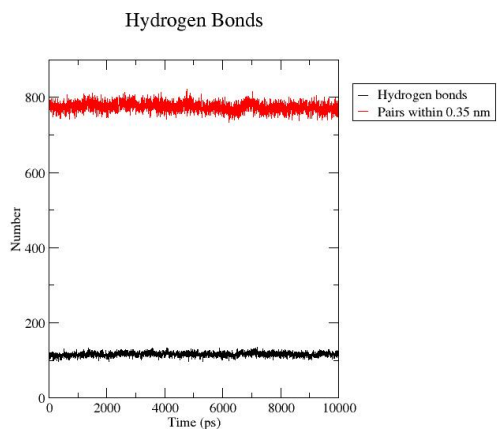


A) 2500 bar @ 300 K

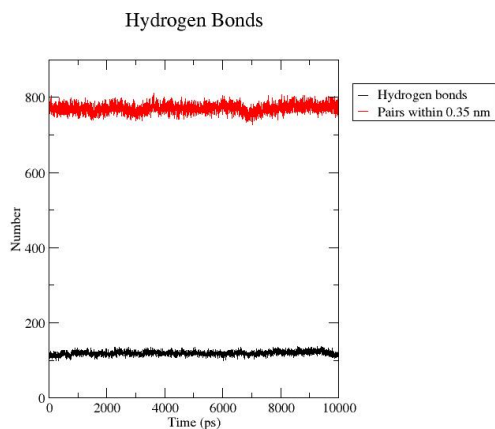


B) 2500 bar @ 295 K

Figure 76: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

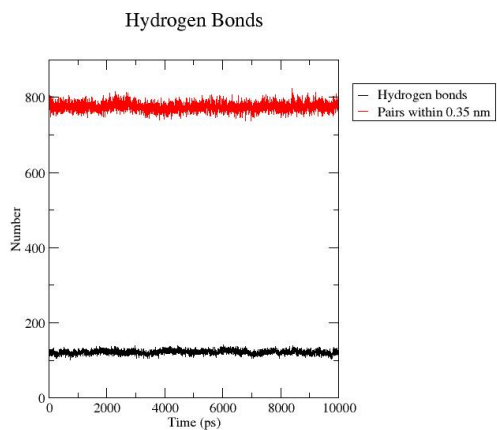


A) 2500 bar @ 290 K

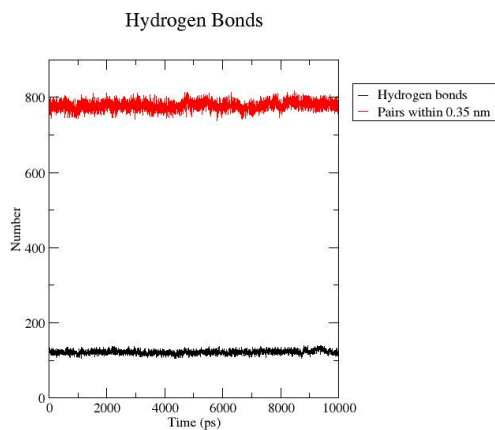


B) 2500 bar @ 285 K

Figure 77: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

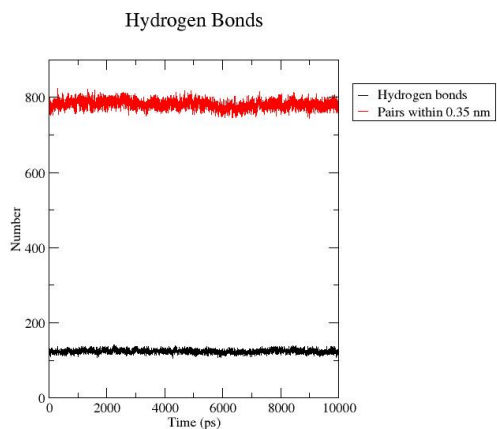


A) 2500 bar @ 280 K

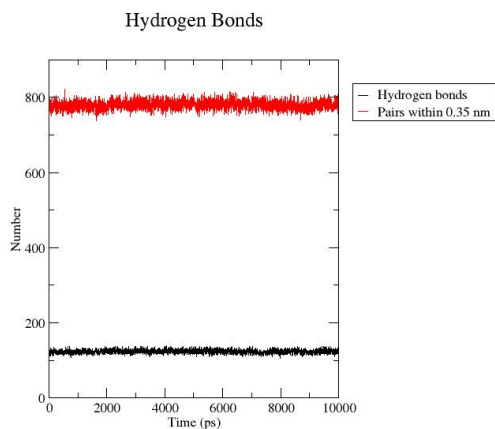


B) 2500 bar @ 275 K

Figure 78: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

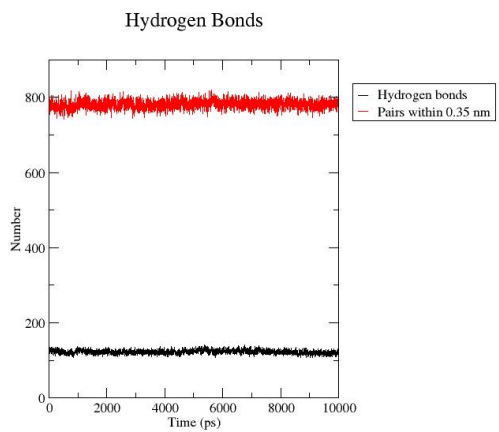


A) 2500 bar @ 270 K

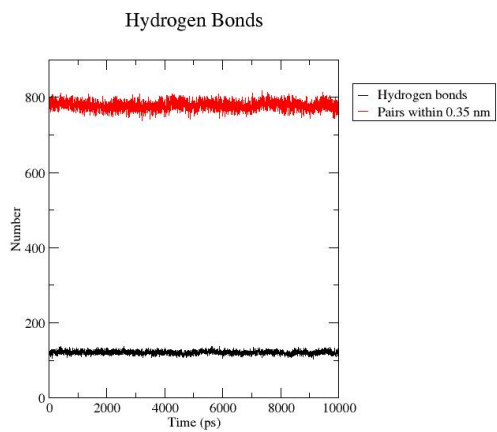


B) 2500 bar @ 265 K

Figure 79: HBond side-by-side - High Hydrostatic Pressure and Low Temperature



A) 2500 bar @ 260 K

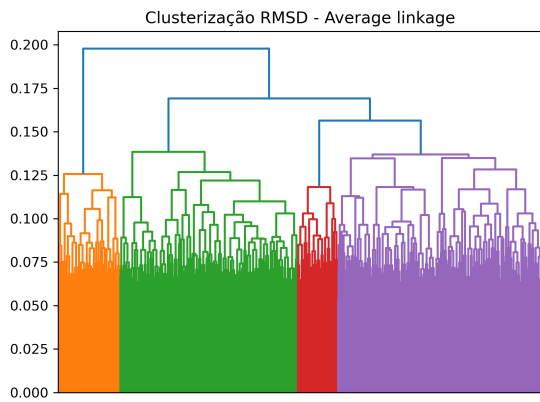


B) 2500 bar @ 255 K

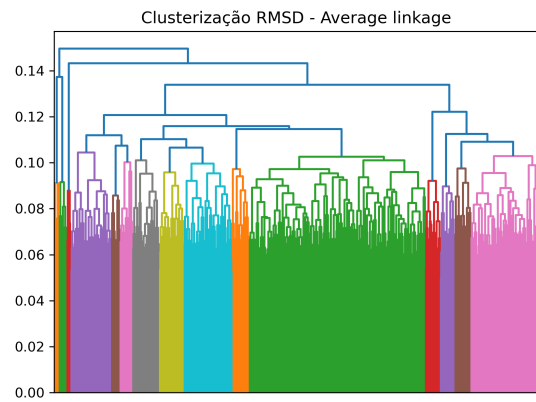
Figure 80: HBond side-by-side - High Hydrostatic Pressure and Low Temperature

## Hierarchical Clustering

### HHP



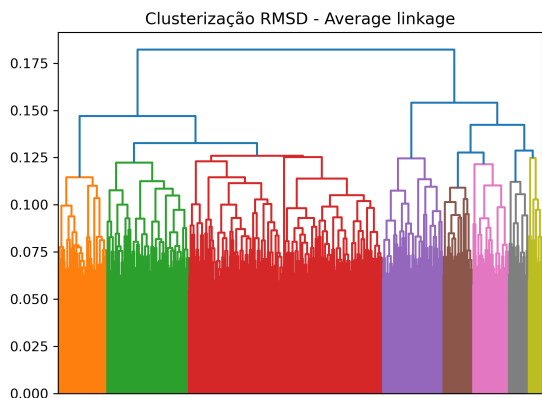
A) 1 bar



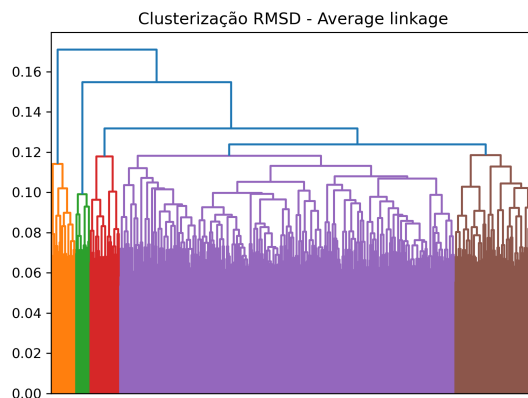
B) 250 bar

Figure 81: Hierarchical Clustering side-by-side - High Hydrostatic Pressure

**HHP and low temperature**

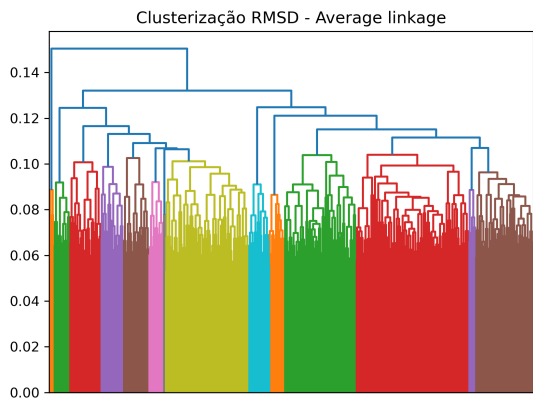


C) 500 bar

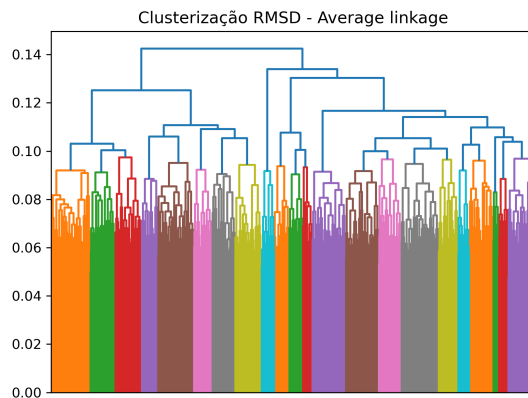


D) 750 bar

Figure 82: Hierarchical Clustering side-by-side - High Hydrostatic Pressure

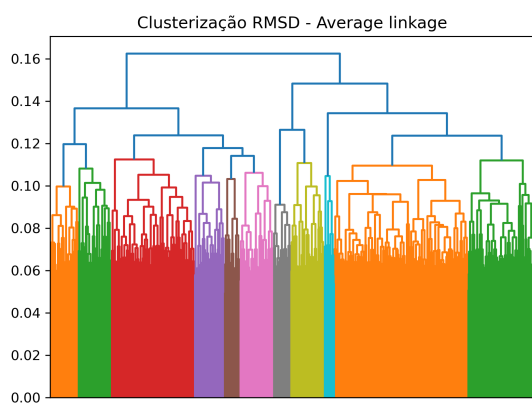


E) 1000 bar

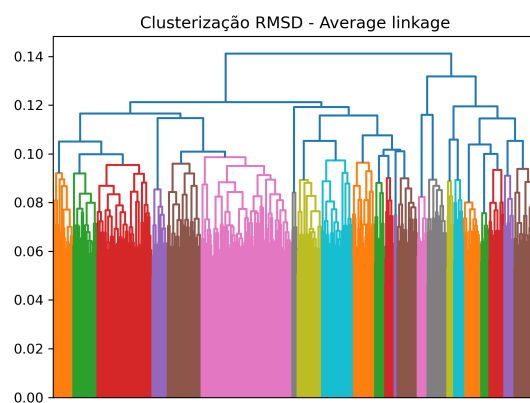


F) 1250 bar

Figure 83: Hierarchical Clustering side-by-side - High Hydrostatic Pressure

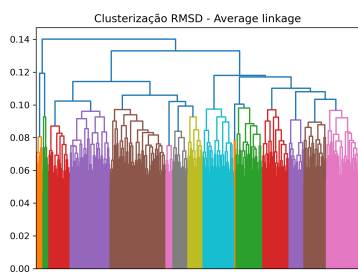


G) 1500 bar

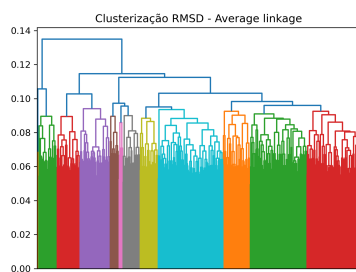


H) 1750 bar

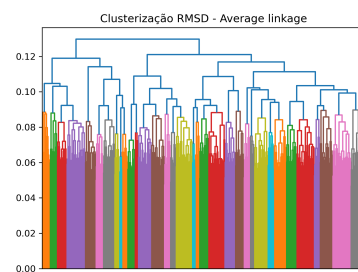
Figure 84: Hierarchical Clustering side-by-side - High Hydrostatic Pressure



I) 2000 bar

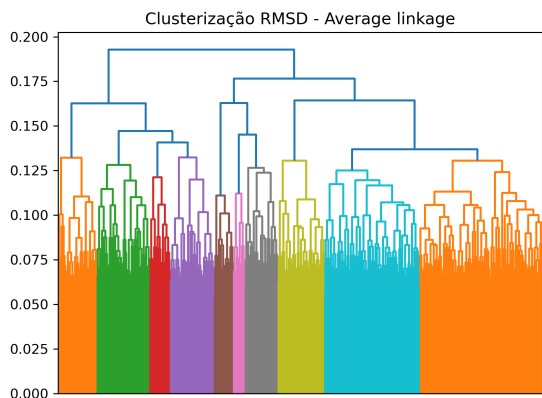


J) 2250 bar

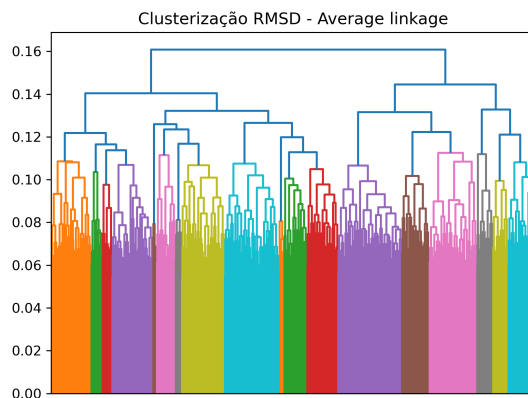


K) 2500 bar

Figure 85: Hierarchical Clustering side-by-side - High Hydrostatic Pressure

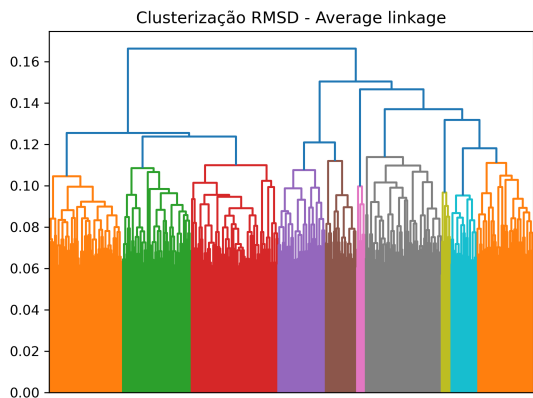


A) 1 bar

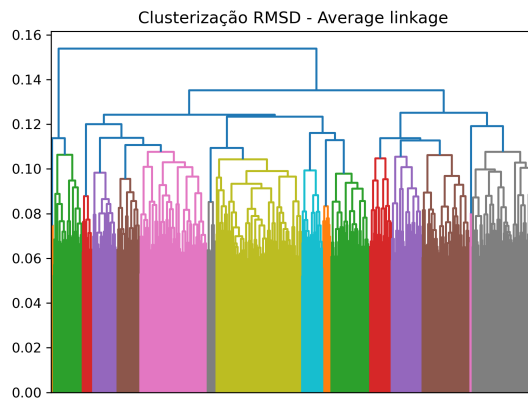


B) 250 bar

Figure 86: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature

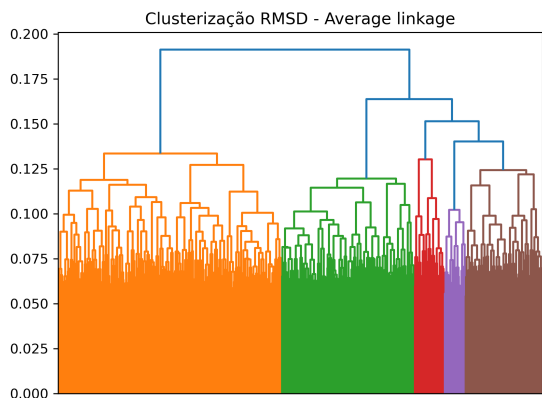


C) 500 bar

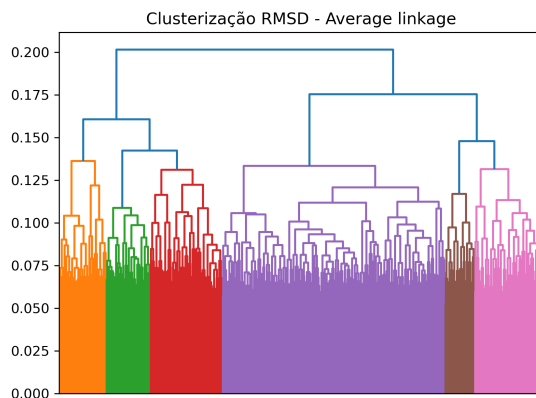


D) 750 bar

Figure 87: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature

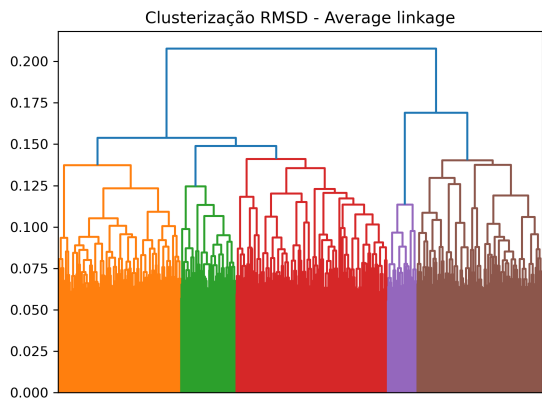


E) 1000 bar

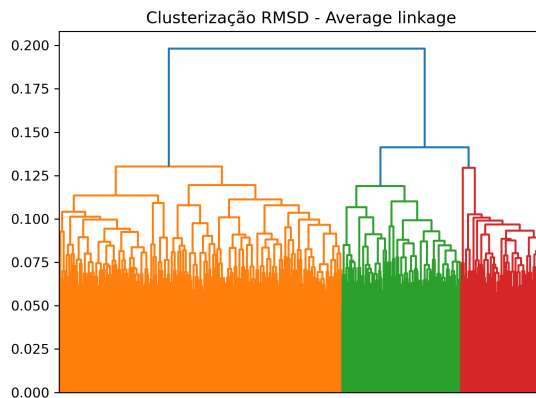


F) 1250 bar

Figure 88: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature

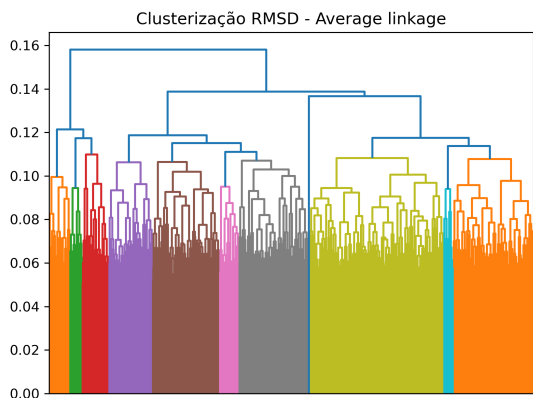


G) 1500 bar

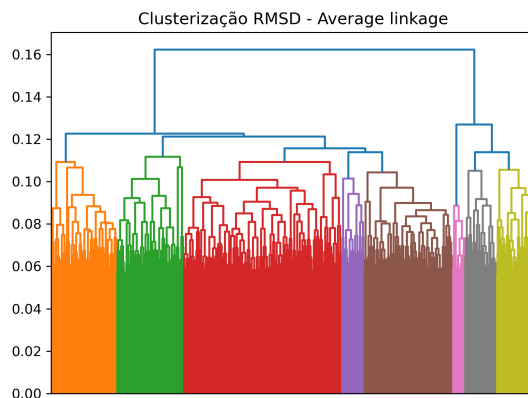


H) 1750 bar

Figure 89: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature

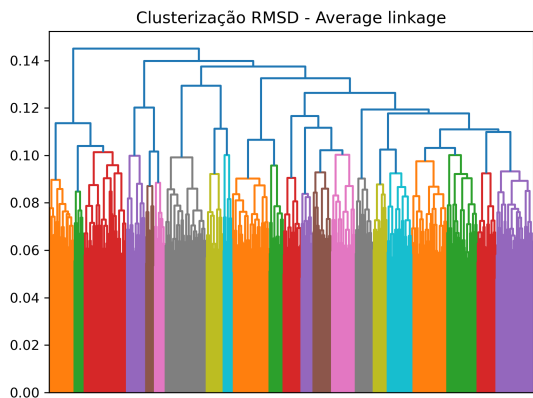


I) 2000 bar

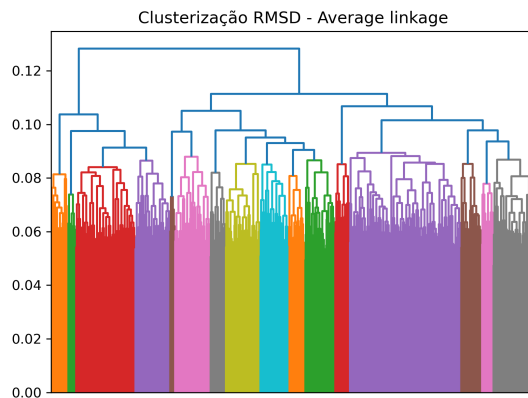


J) 2250 bar

Figure 90: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature

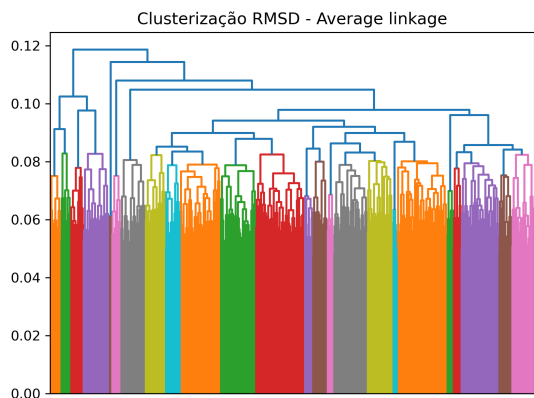


K) 2500 bar

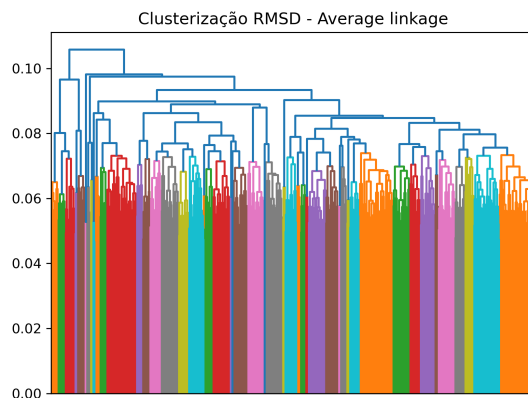


L) 2500 bar @ 300 k

Figure 91: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature

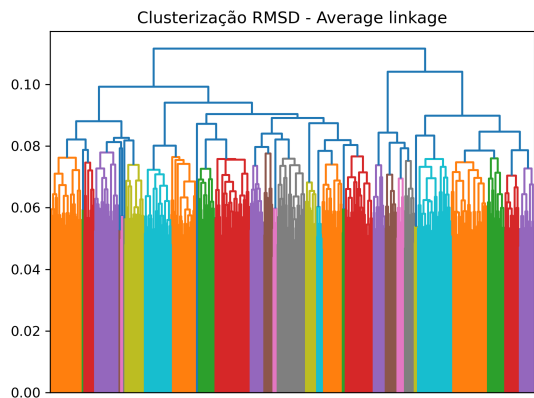


M) 2500 bar @ 295 k

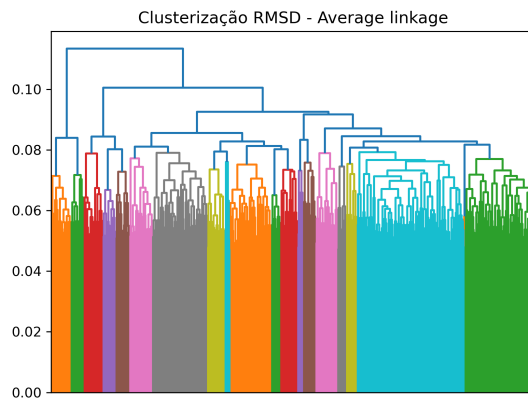


N) 2500 bar @ 290 k

Figure 92: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature

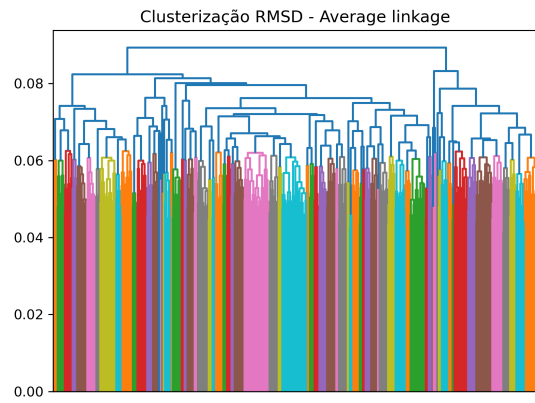
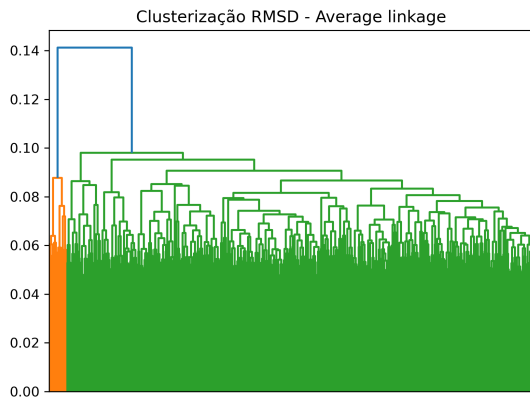


O) 2500 bar @ 285 k



P) 2500 bar @ 280 k

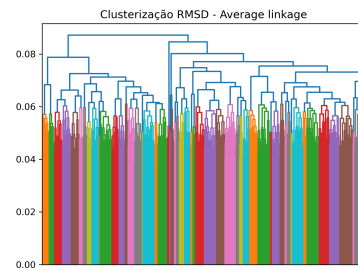
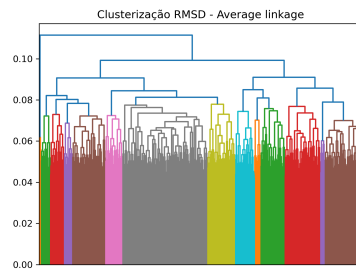
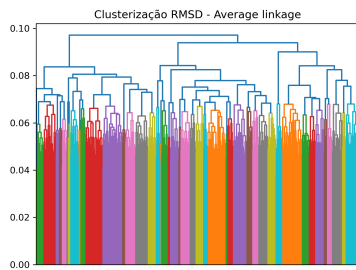
Figure 93: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature



Q) 2500 bar @ 275 k

R) 2500 bar @ 270 k

Figure 94: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature



S) 2500 bar @ 265 k

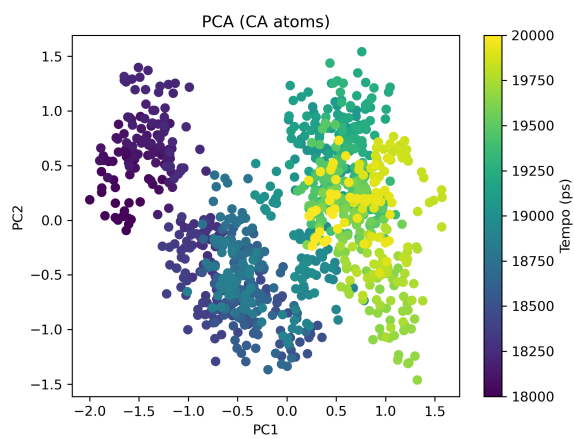
T) 2500 bar @ 260 k

U) 2500 bar @ 255 k

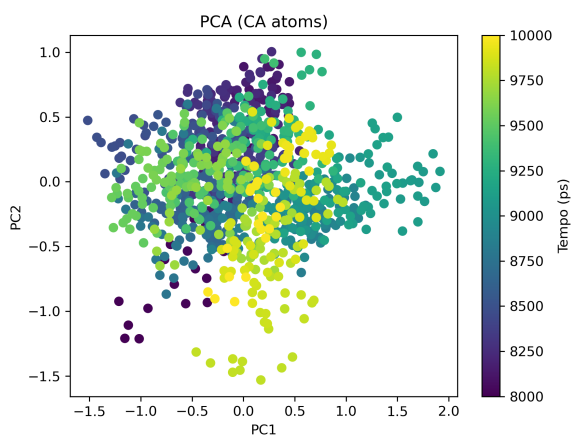
Figure 95: Hierarchical Clustering side-by-side - High Hydrostatic Pressure and Low Temperature

PCA

HHP

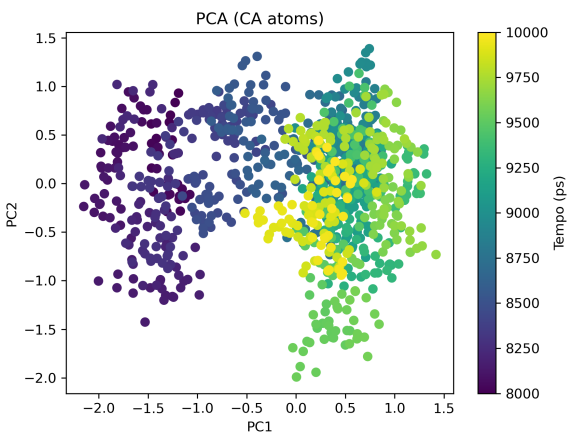


A) 1 bar

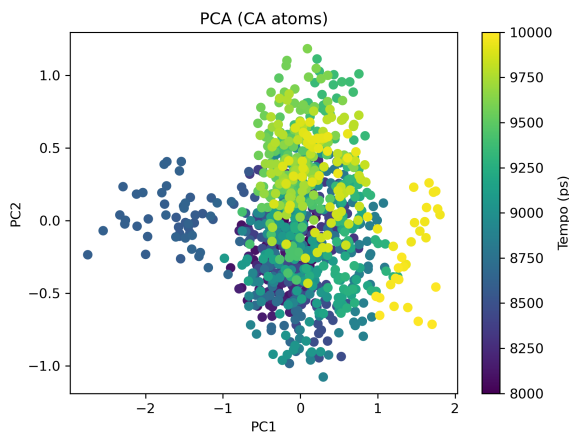


B) 250 bar

Figure 96: Principal Component Analysis side-by-side - High Hydrostatic Pressure

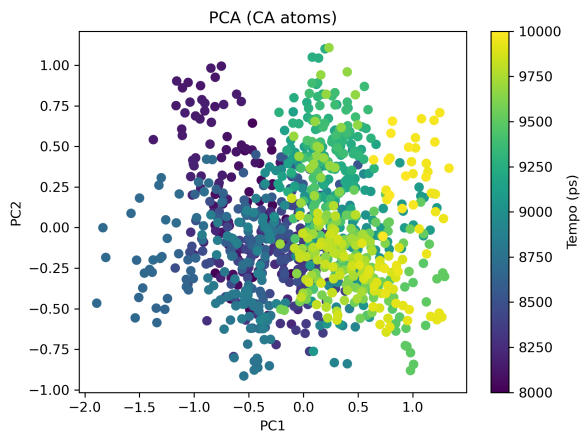


C) 500 bar

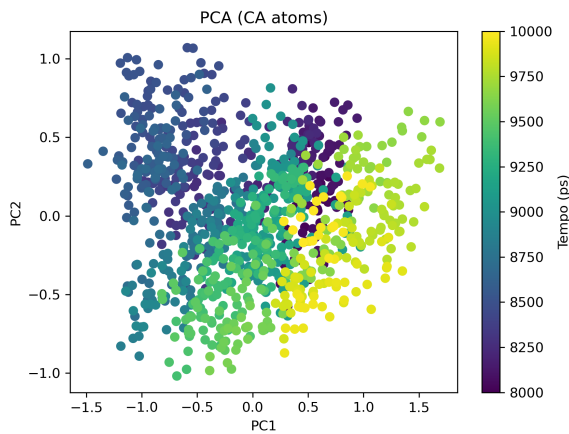


D) 750 bar

Figure 97: Principal Component Analysis side-by-side - High Hydrostatic Pressure

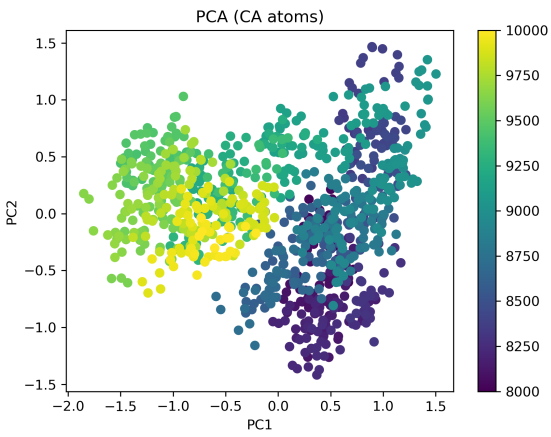


E) 1000 bar

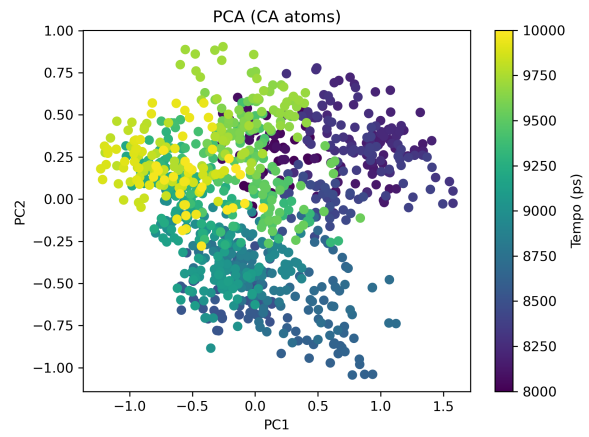


F) 1250 bar

Figure 98: Principal Component Analysis side-by-side - High Hydrostatic Pressure

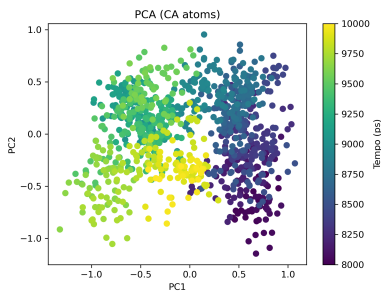


G) 1500 bar

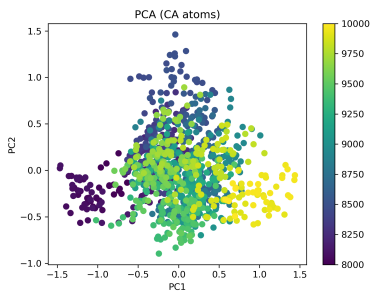


H) 1750 bar

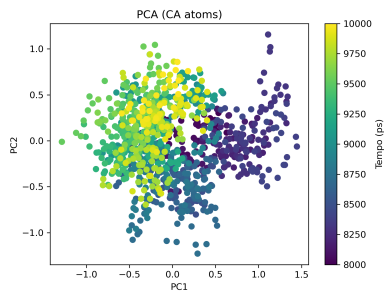
Figure 99: Principal Component Analysis side-by-side - High Hydrostatic Pressure



I) 2000 bar



J) 2250 bar



K) 2500 bar

Figure 100: Principal Component Analysis side-by-side - High Hydrostatic Pressure

## HHP and low temperature

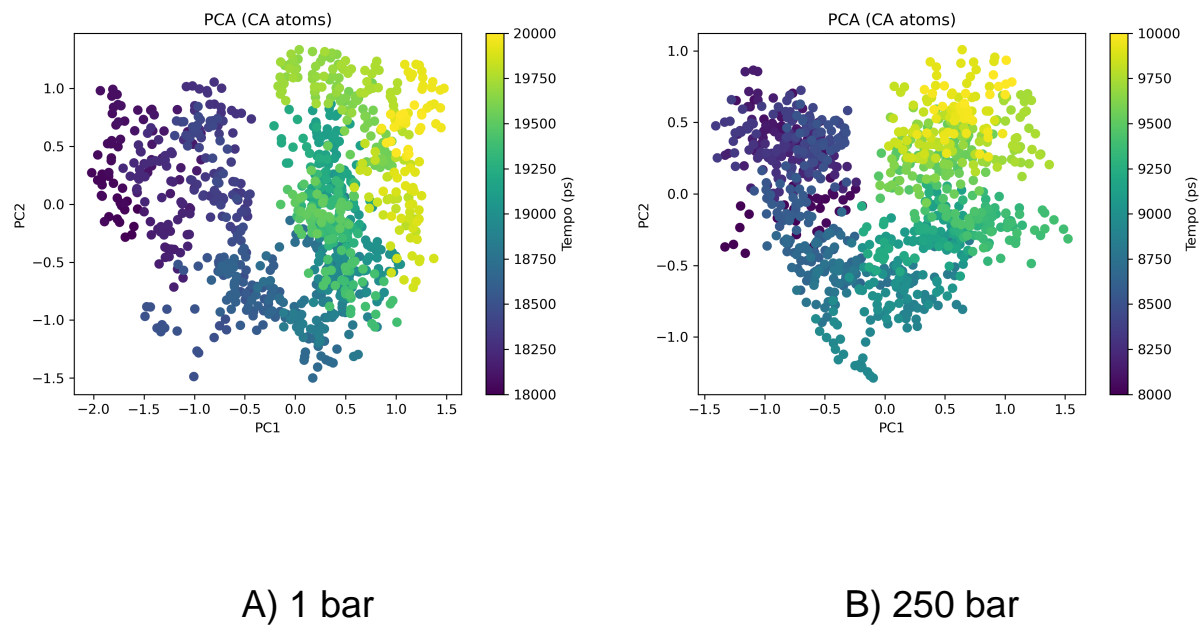
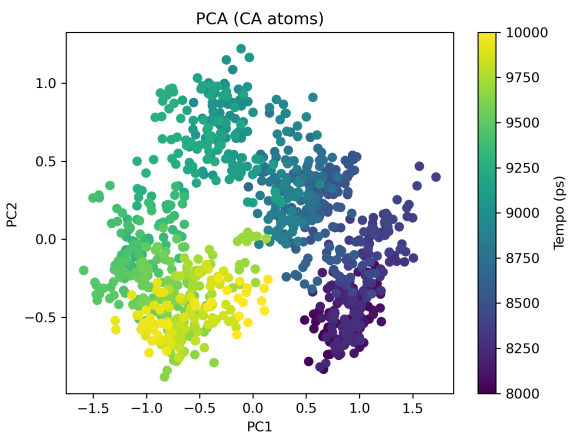
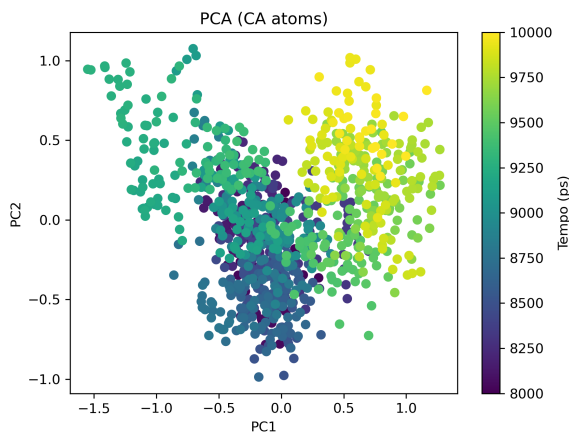


Figure 101: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature

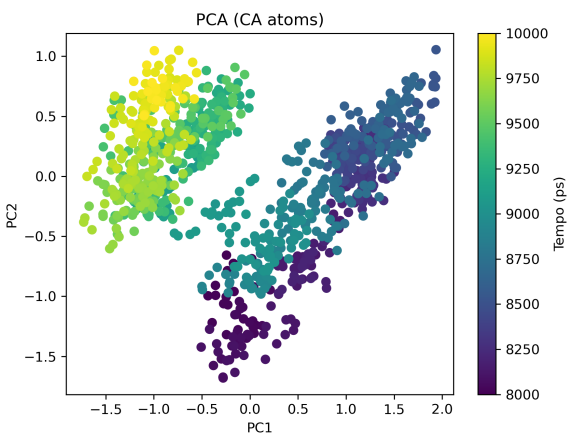


C) 500 bar

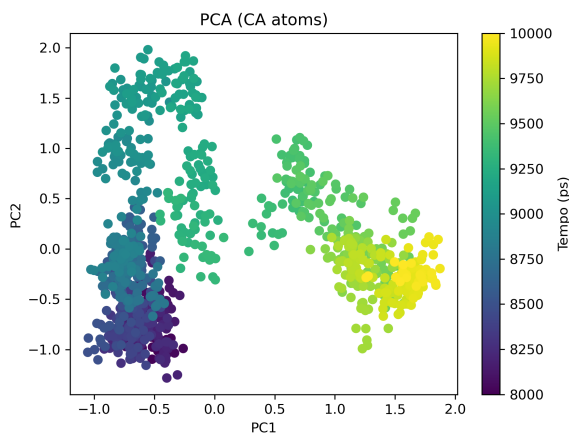


D) 750 bar

Figure 102: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature

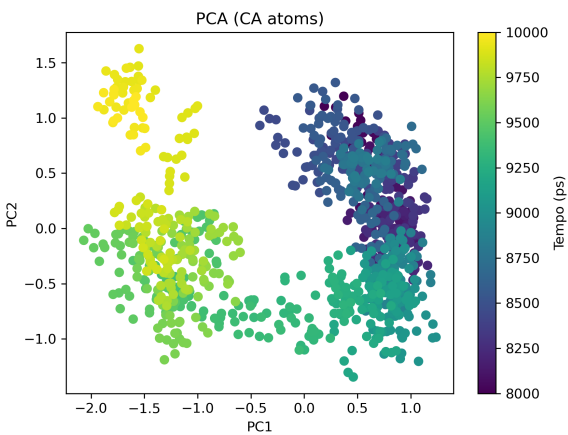


E) 1000 bar

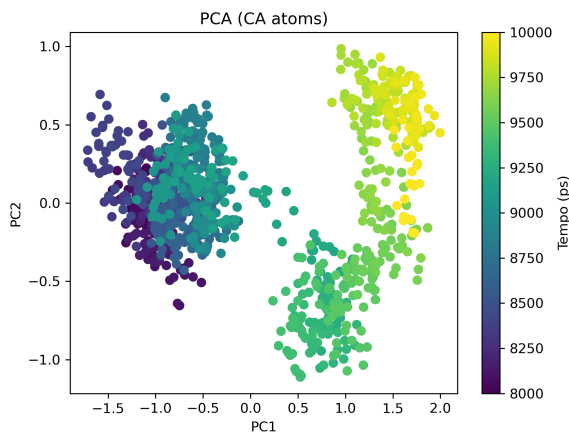


F) 1250 bar

Figure 103: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature

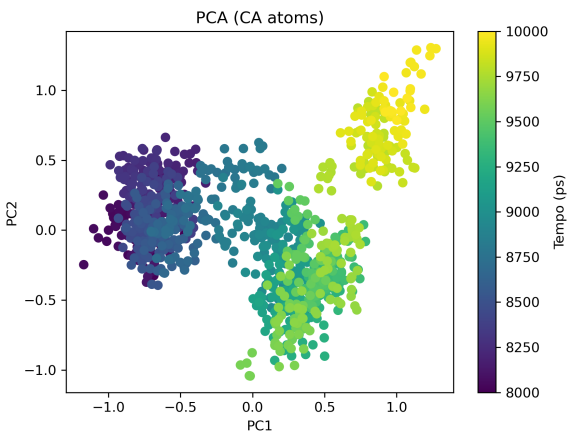


G) 1500 bar

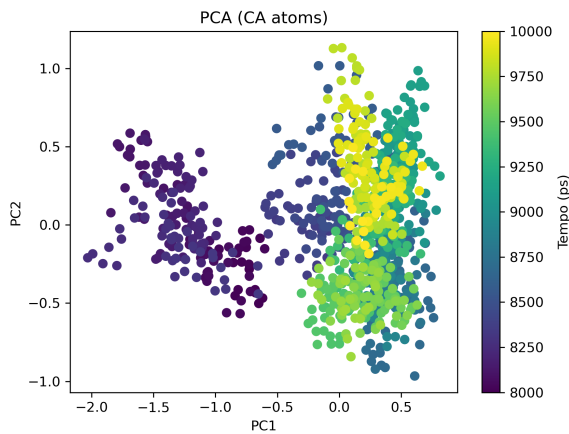


H) 1750 bar

Figure 104: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature

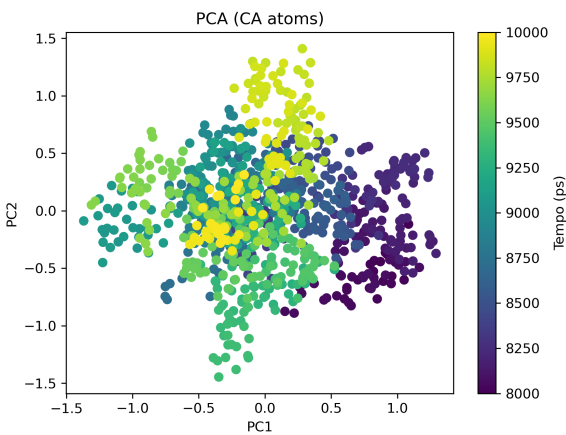


I) 2000 bar

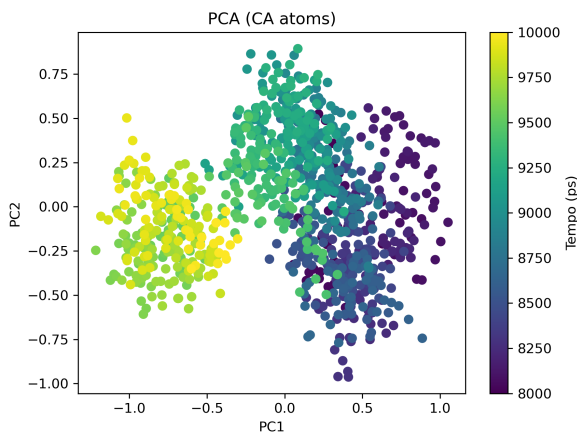


J) 2250 bar

Figure 105: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature

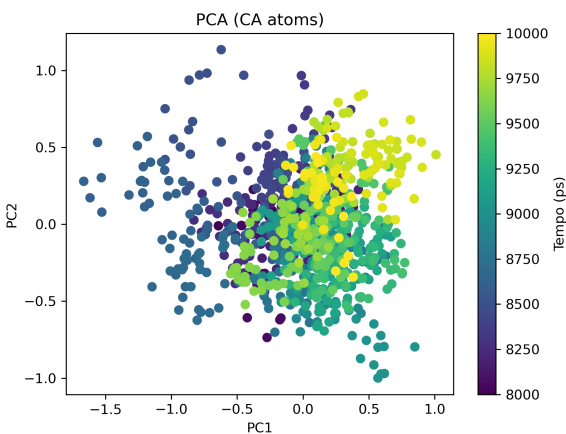


K) 2500 bar

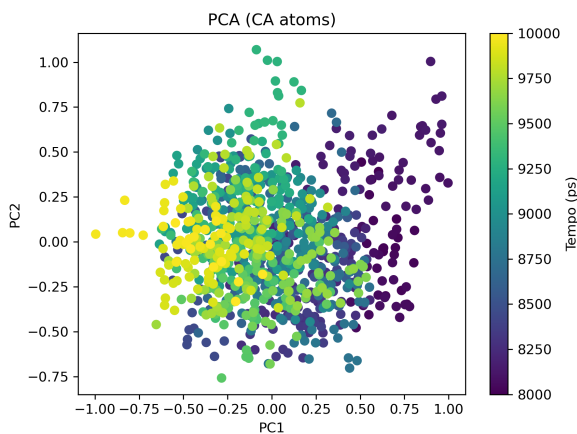


L) 2500 bar @ 300 k

Figure 106: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature

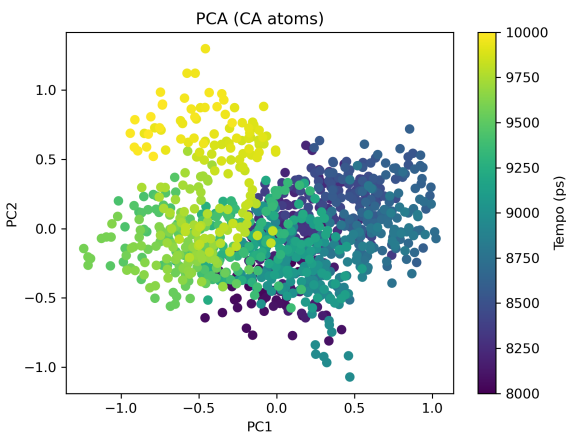


M) 2500 bar @ 295 k

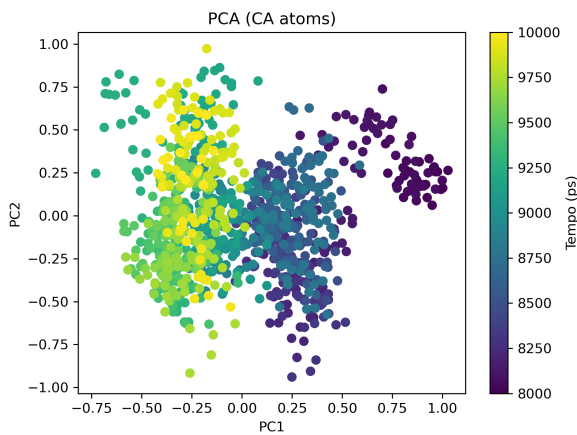


N) 2500 bar @ 290 k

Figure 107: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature

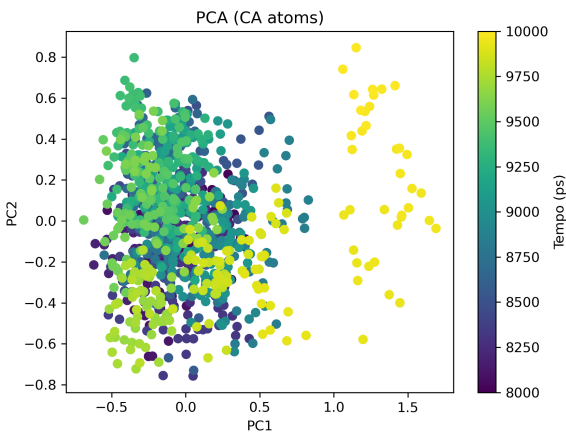


O) 2500 bar @ 285 k

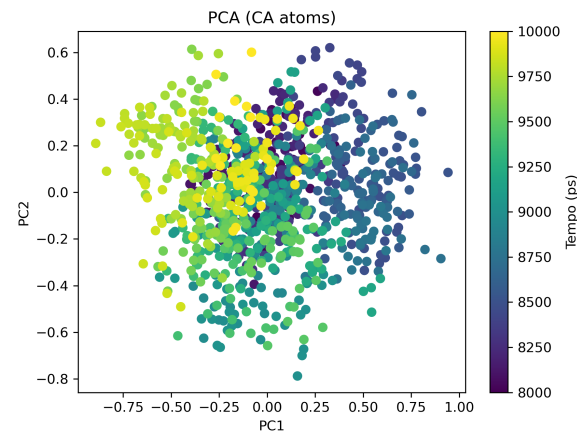


P) 2500 bar @ 280 k

Figure 108: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature

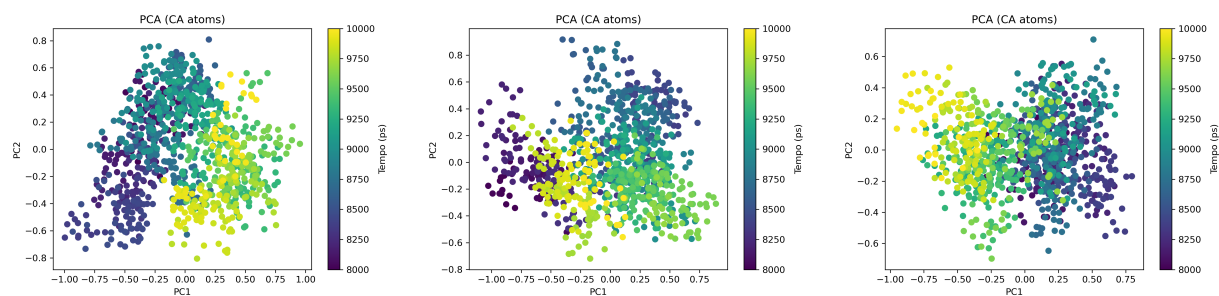


Q) 2500 bar @ 275 k



R) 2500 bar @ 270 k

Figure 109: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature



S) 2500 bar @ 265 k      T) 2500 bar @ 260 k      U) 2500 bar @ 255 k

Figure 110: Principal Component Analysis side-by-side - High Hydrostatic Pressure and Low Temperature