

# Simulation Report: sims4\_kmdcm\_water\_k275

water.2000.heat.dcd  
water.2000.equi.dcd

	vdw	elec	user	time	temp	tot	energy	volume	pressi
count	7489.000000	7489.000000	7489.0	7489.000000	7489.000000	7489.000000	7489.000000	7489.000000	7489.000000C
mean	3670.564698	-22441.506399	0.0	438.000801	276.785729	-17124.361716	22073.771655	58382.313259	-373.286170
std	199.016651	462.167424	0.0	302.354334	17.057623	849.158736	660.543384	6514.479059	1171.601195
min	3027.368820	-25088.512700	0.0	0.000000	60.965490	-22690.254420	20601.565780	53038.000000	-5035.235440
25%	3529.078480	-22743.304730	0.0	93.600000	273.635420	-17592.281130	21185.163300	53985.000000	-1128.195120
50%	3738.964790	-22610.003930	0.0	452.600000	276.139850	-17497.371080	22421.053310	54328.000000	-321.070740
75%	3810.571150	-22080.826090	0.0	702.200000	280.579340	-16418.422400	22502.988820	68921.000000	421.107770
max	4092.139670	-21253.404590	0.0	951.800000	300.963800	-15785.937180	24925.828760	68921.000000	3723.326870

## Simulation runs

		dyna	0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT	5: DYNA RESTRT CPT
vdw	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	1500.000000	389.000000
	mean	3380.540786	3758.981975	3783.189306	3754.221200	3795.503996	3786.674838	
	std	120.437674	83.004697	80.015887	84.289731	81.284492	75.401609	
	min	3027.368820	3451.224340	3517.260980	3535.847270	3577.479660	3588.512900	
	25%	3301.514747	3709.579923	3731.726380	3695.624928	3738.354888	3737.440020	
	50%	3370.149435	3758.654780	3786.150350	3752.770560	3794.498700	3786.103200	
	75%	3436.845470	3820.327965	3836.004380	3809.484240	3853.594750	3828.605050	
	max	4072.983730	3975.377170	4011.914010	4034.734920	4092.139670	4005.271060	
	elec	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	389.000000
elec	mean	-21804.365670	-22779.939236	-22661.797825	-22603.340854	-22715.070250	-22666.923255	
	std	427.570429	161.513118	129.788857	150.605480	140.520180	111.020543	
	min	-25088.512700	-23177.804590	-23049.174990	-23050.202220	-23179.987970	-22932.377290	
	25%	-21850.754950	-22886.596695	-22748.736440	-22708.402165	-22817.429887	-22748.917990	
	50%	-21742.287410	-22787.683990	-22659.850760	-22605.289835	-22714.240070	-22667.681530	
	75%	-21611.735163	-22670.093380	-22581.117425	-22493.287737	-22621.338745	-22588.685370	
	max	-21253.404590	-21828.192140	-22264.364840	-22185.784610	-22331.023590	-22387.059610	
	volume	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	389.000000
	mean	68921.000000	58280.670000	54322.138667	53911.374000	54083.110667	53829.838046	
	std	0.000000	2828.326033	256.218937	285.536751	276.031973	228.541774	

dyna	0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT	5: DYNA RESTRT CPT
min	68921.000000	54246.000000	53439.000000	53038.000000	53377.000000	53194.000000
25%	68921.000000	55922.000000	54165.000000	53728.000000	53873.500000	53693.000000
50%	68921.000000	57566.000000	54318.000000	53931.000000	54070.500000	53845.000000
75%	68921.000000	60100.000000	54489.000000	54117.000000	54298.250000	53965.000000
max	68921.000000	68921.000000	55245.000000	54750.000000	54807.000000	54434.000000
temp	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000
	mean	281.702283	275.021377	274.953011	275.031843	274.985083
	std	32.154639	2.981514	2.946420	2.909245	2.783464
	min	60.965490	262.582060	265.366980	265.083230	267.364570
	25%	286.282427	273.046103	273.083962	273.125268	273.123495
	50%	290.043855	275.110645	275.046350	275.057430	275.106030
	75%	292.582783	276.888240	276.949830	277.066520	276.912555
	max	300.963800	294.390970	284.373760	283.258190	283.151600

## Densities

density 1: 867.0796999463153 kilogram / meter \*\* 3

density 2: 1025.3828585017982 kilogram / meter \*\* 3

density 3: 1100.1039625244011 kilogram / meter \*\* 3

density 4: 1108.4859384218253 kilogram / meter \*\* 3

density 5: 1104.9660284579784 kilogram / meter \*\* 3

density 6: 1110.1649599731268 kilogram / meter \*\* 3

temp. 1: 281.702283425

temp. 2: 275.02137695

temp. 3: 274.95301112

temp. 4: 275.0318432533333

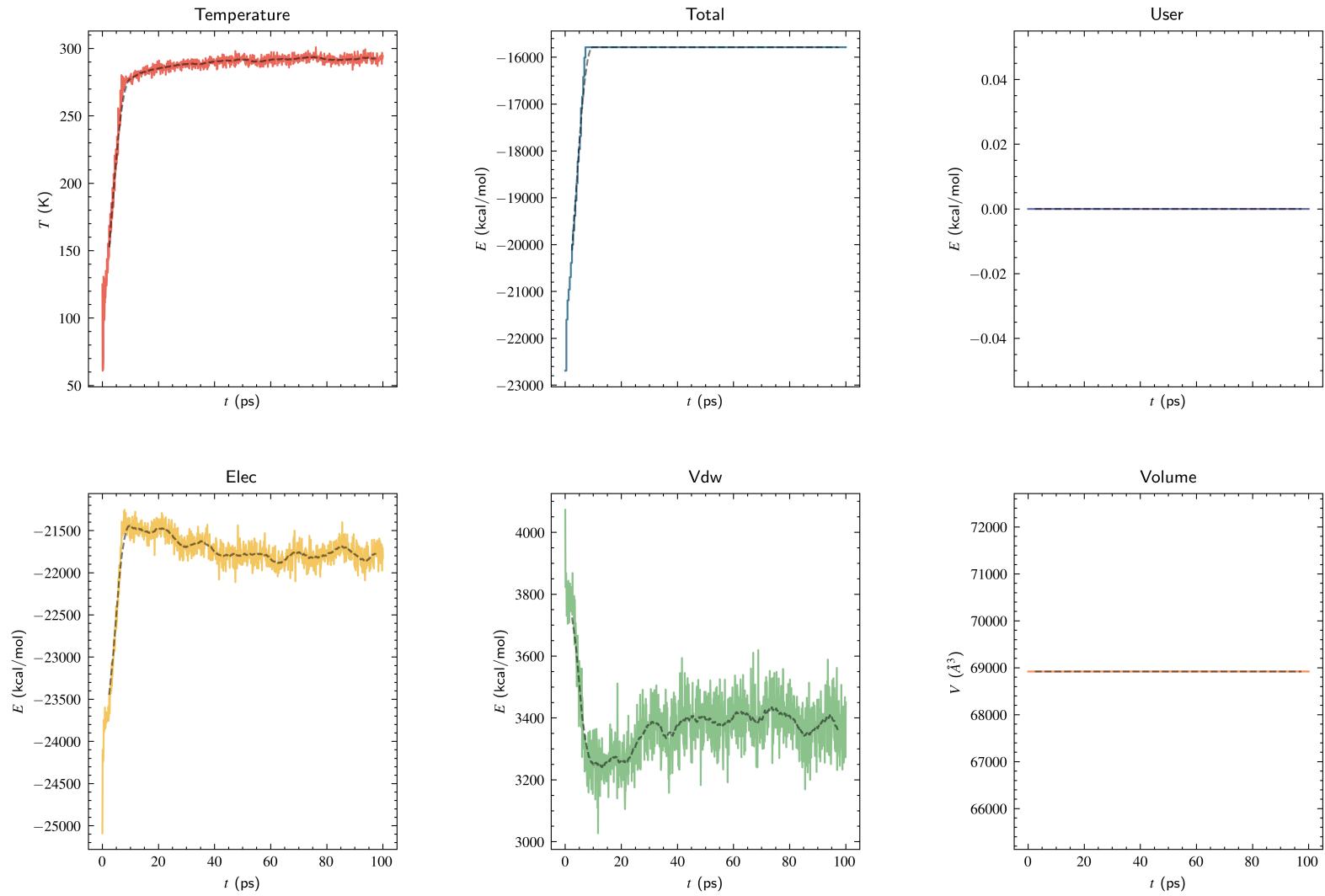
temp. 5: 274.9850828866667

temp. 6: 275.00262714652956

plotting

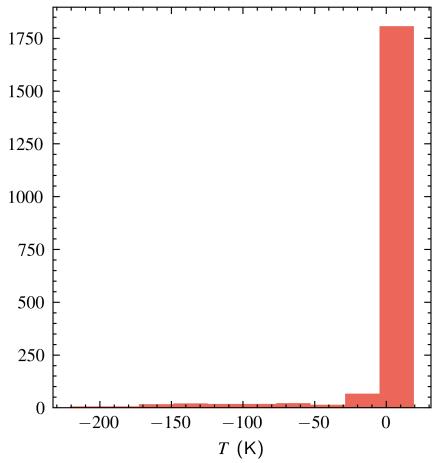
['3: DYNA RESTRT CPT', '5: DYNA RESTRT CPT', '1: DYNA RESTRT CPT', '2: DYNA RESTRT CPT', '4: DYNA RESTRT CPT', '0: DYNA STRT VERL']

\_home\_boittier\_pc当地\_sims4\_kmdcm\_water\_k275\_dynamics.log  
0: DYNA STRT VERL [100.0 ps]

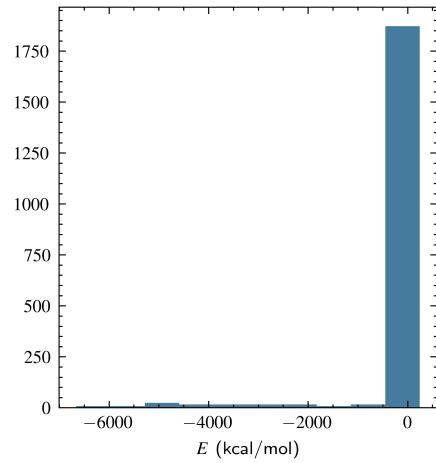


\_home\_boittier\_pc当地\_sims4\_kmdcm\_water\_k275\_dynamics.log  
0: DYNA STRT VERL [100.0 ps]

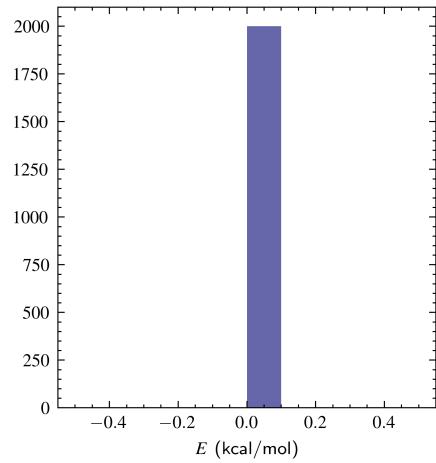
T [282 K]



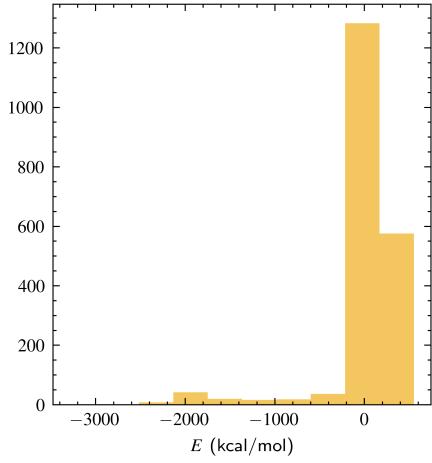
Total [-16028 kcal/mol]



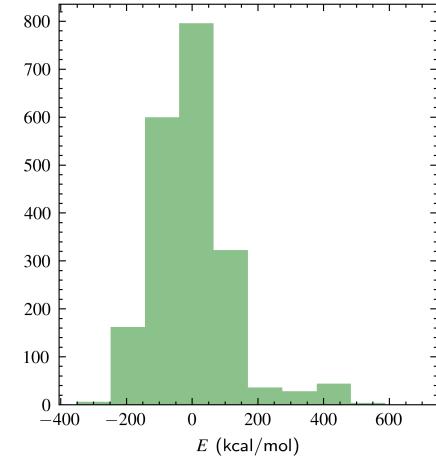
User [0 kcal/mol]



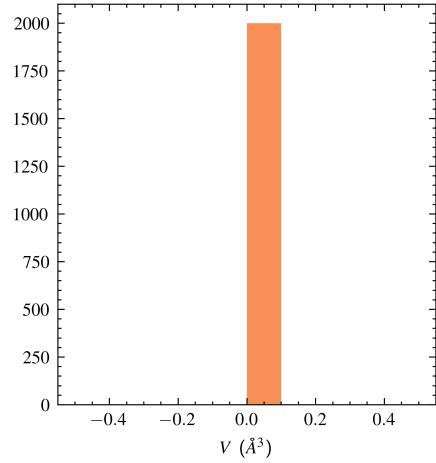
Elec [-21804 kcal/mol]



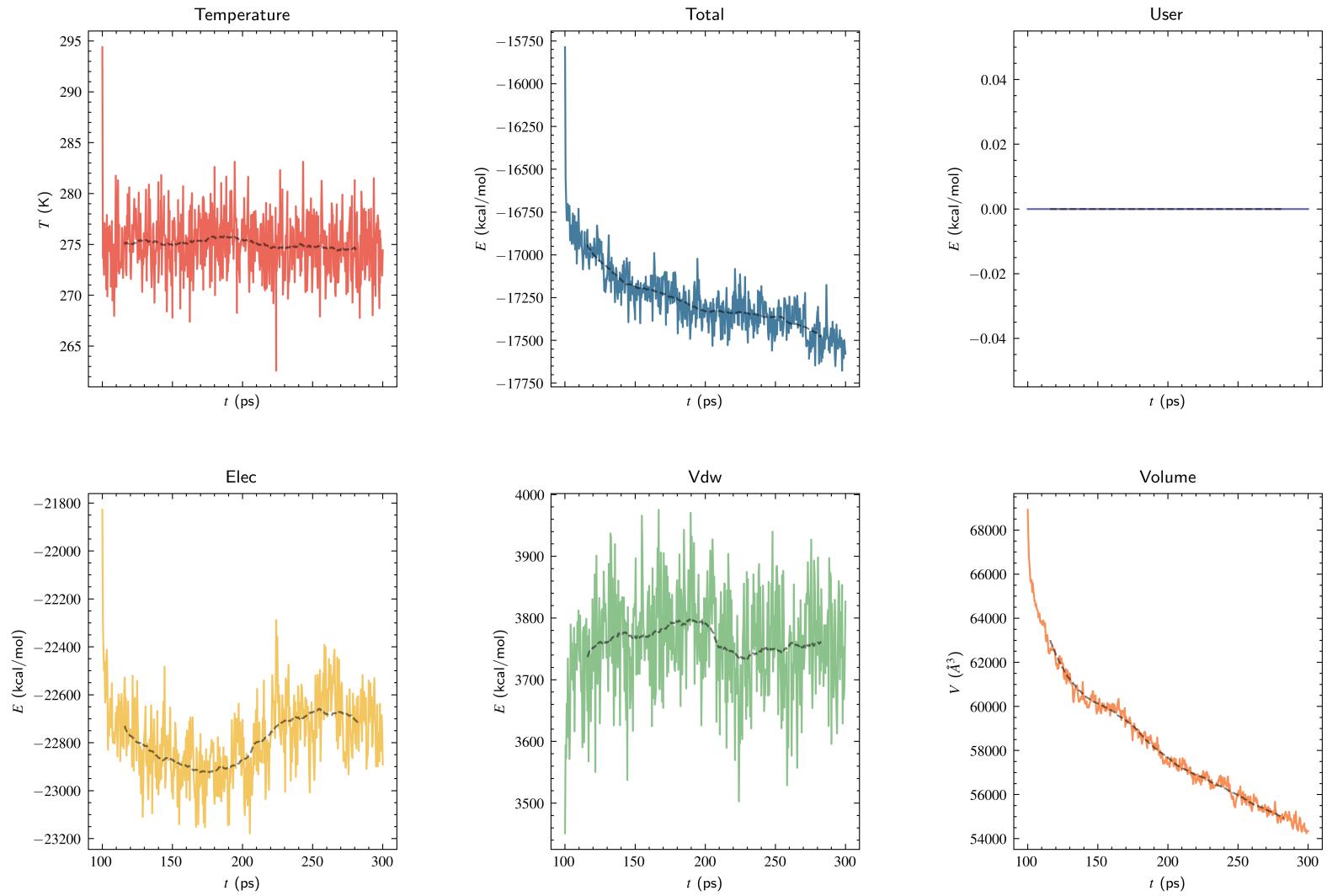
Vdw [3381 kcal/mol]



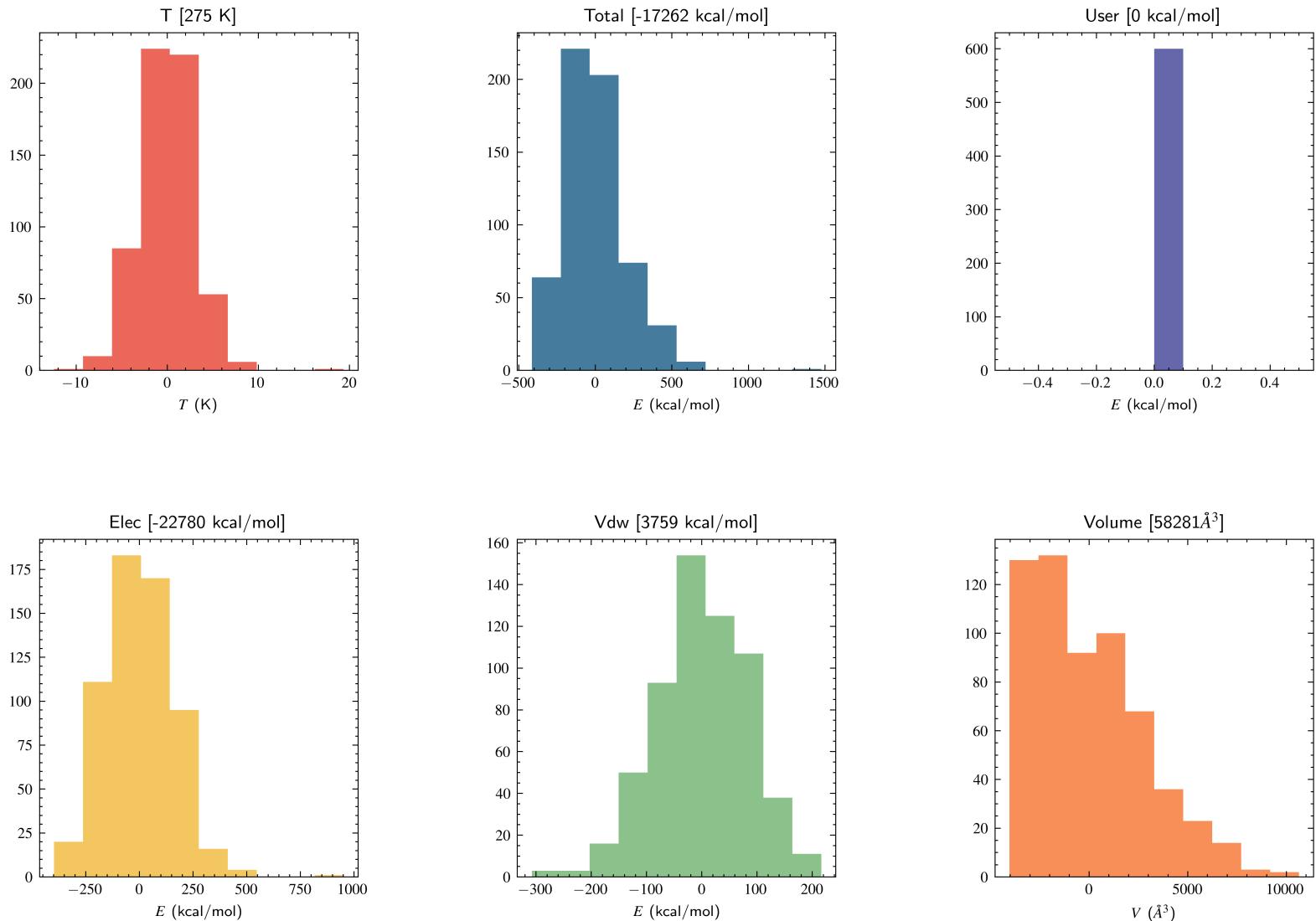
Volume [68921 Å³]



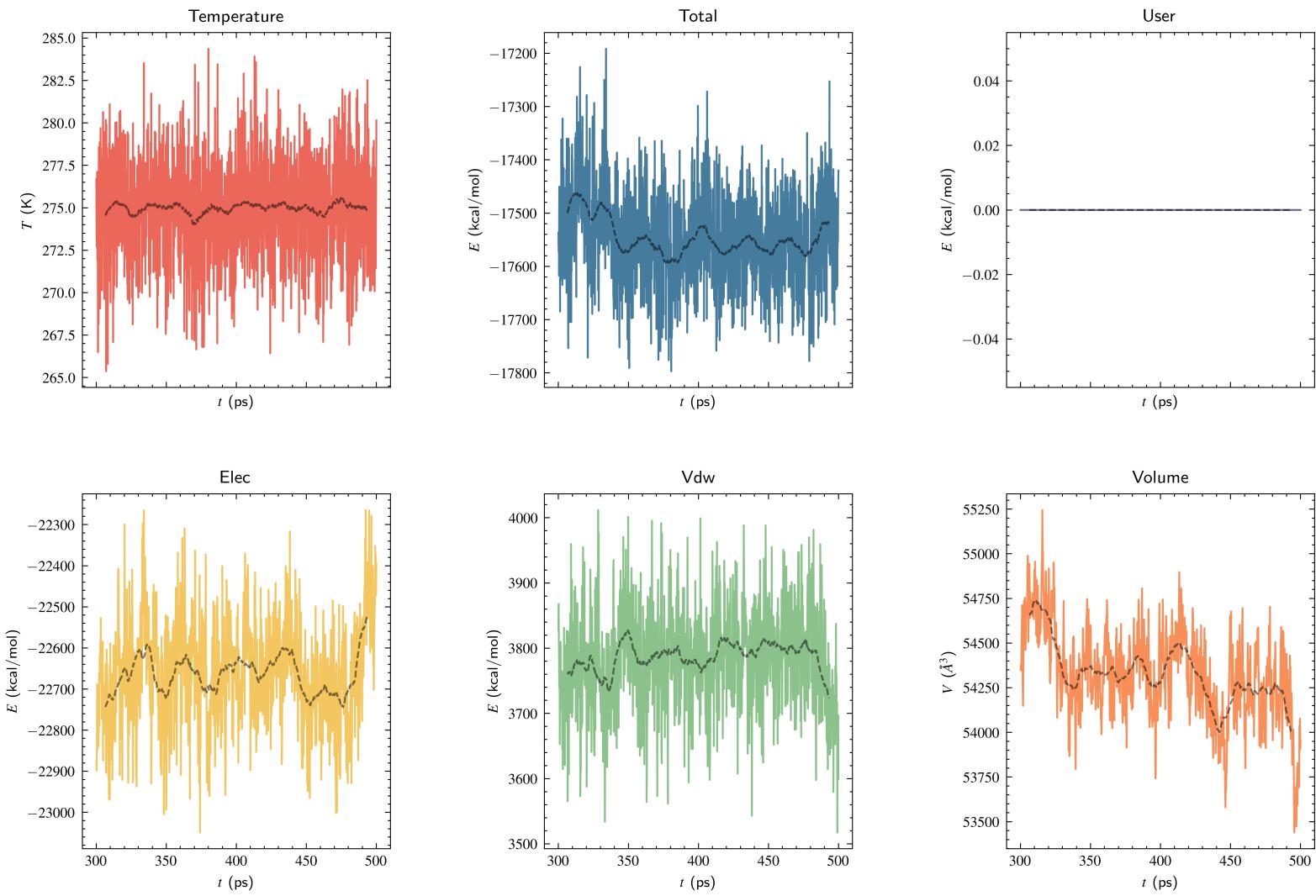
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
1: DYNA RESTRT CPT [200.0 ps]



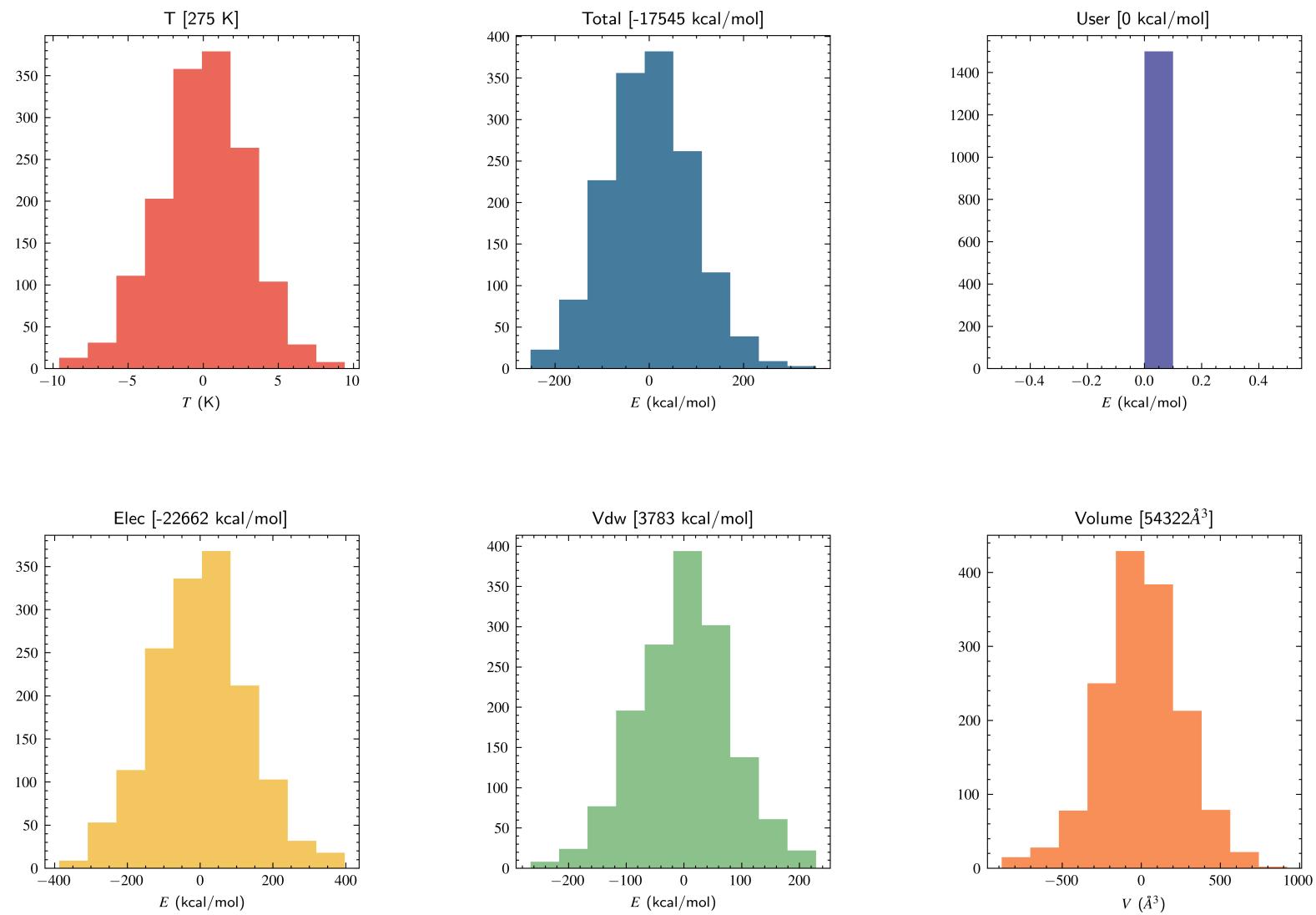
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
1: DYNA RESTRT CPT [200.0 ps]



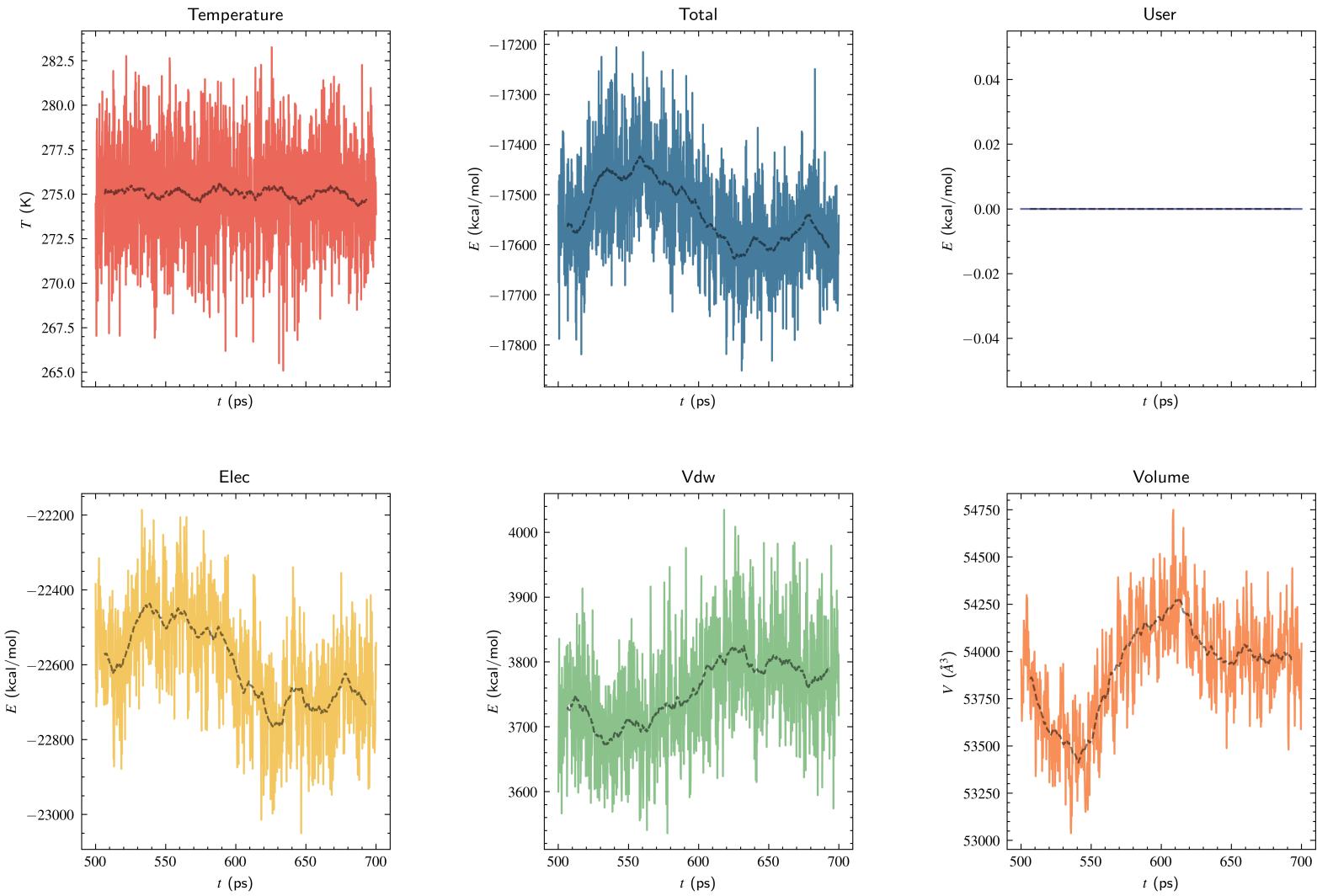
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
2: DYNA RESTRT CPT [200.0 ps]



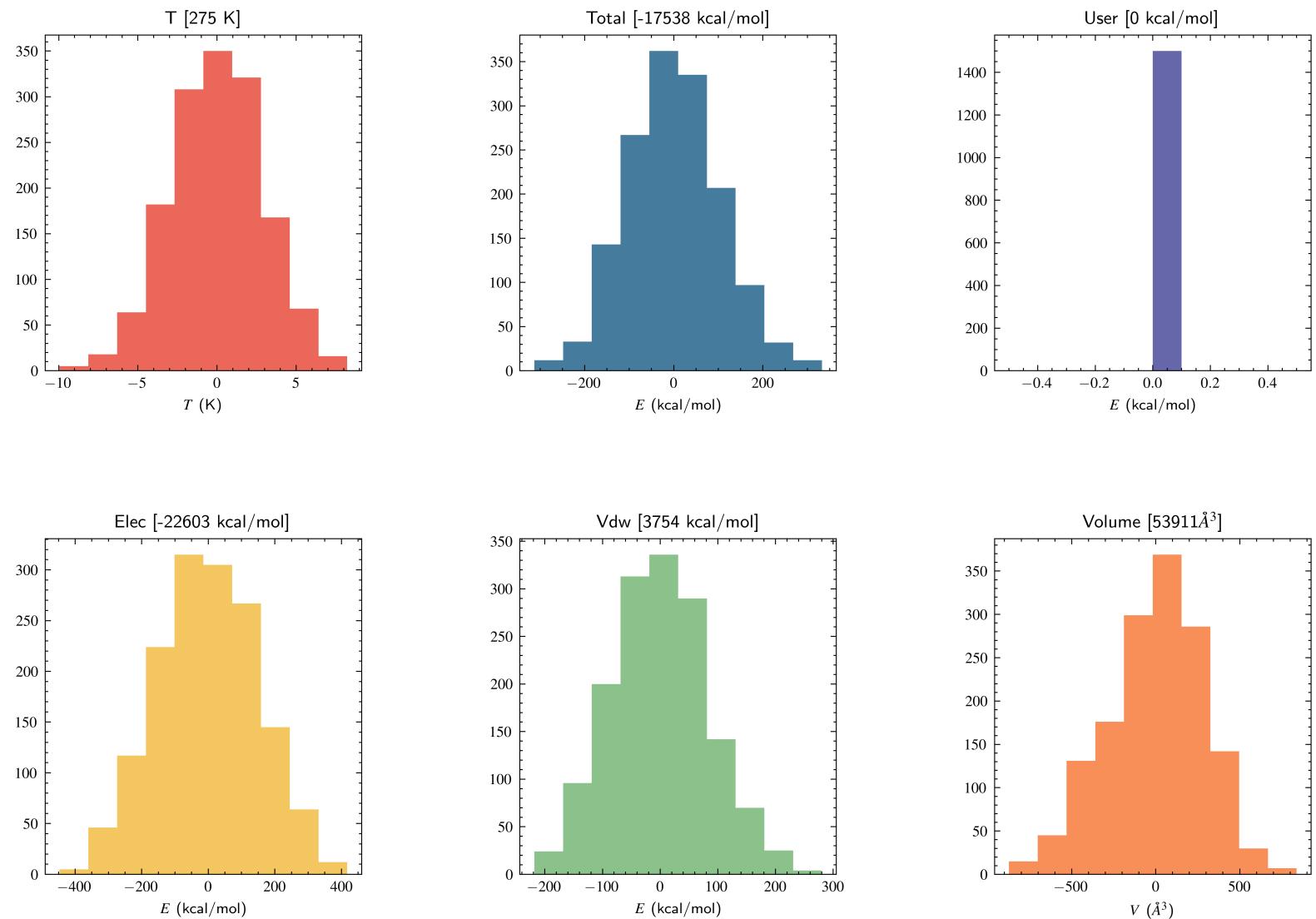
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
2: DYNA RESTRT CPT [200.0 ps]



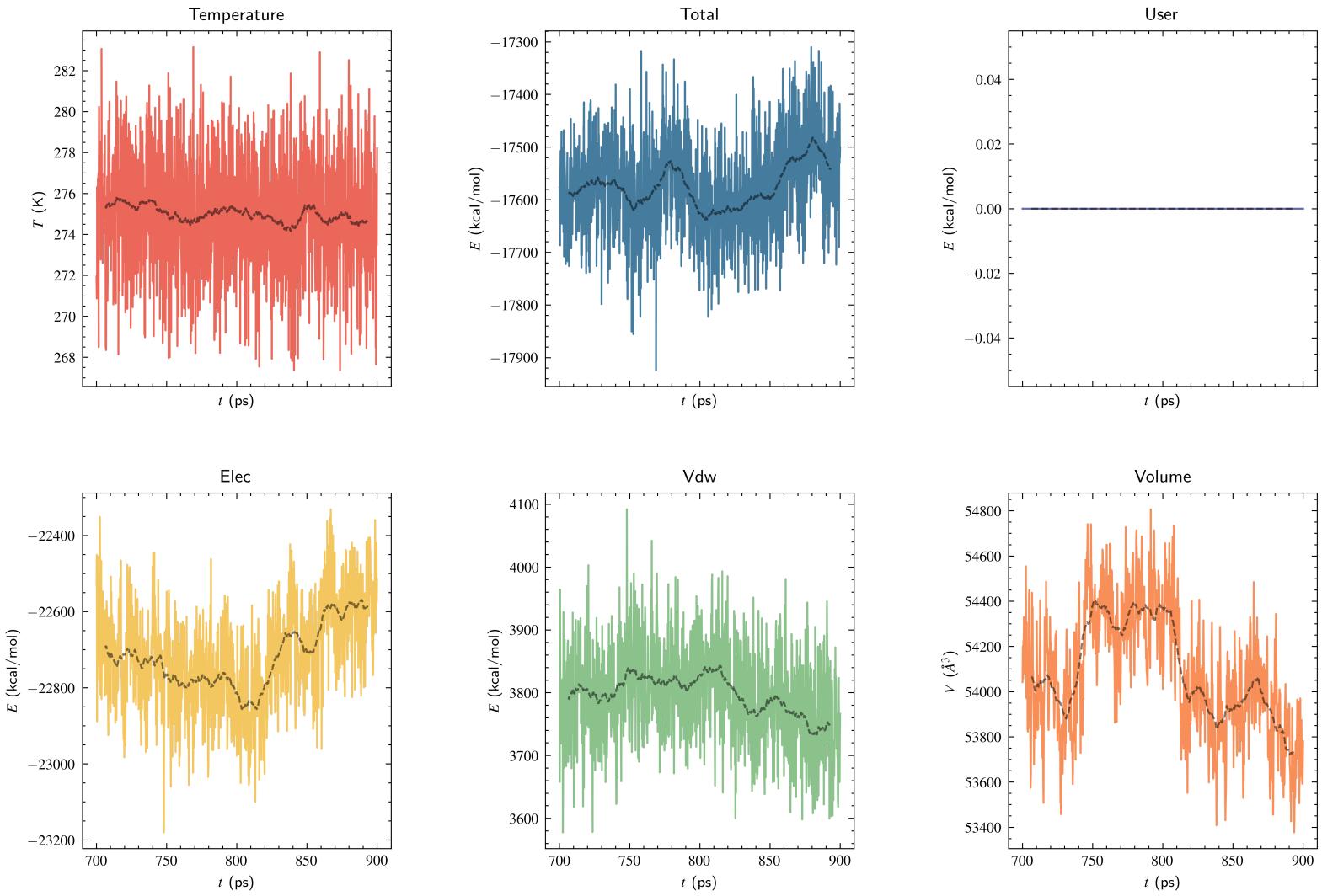
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
3: DYNA RESTRT CPT [200.0 ps]



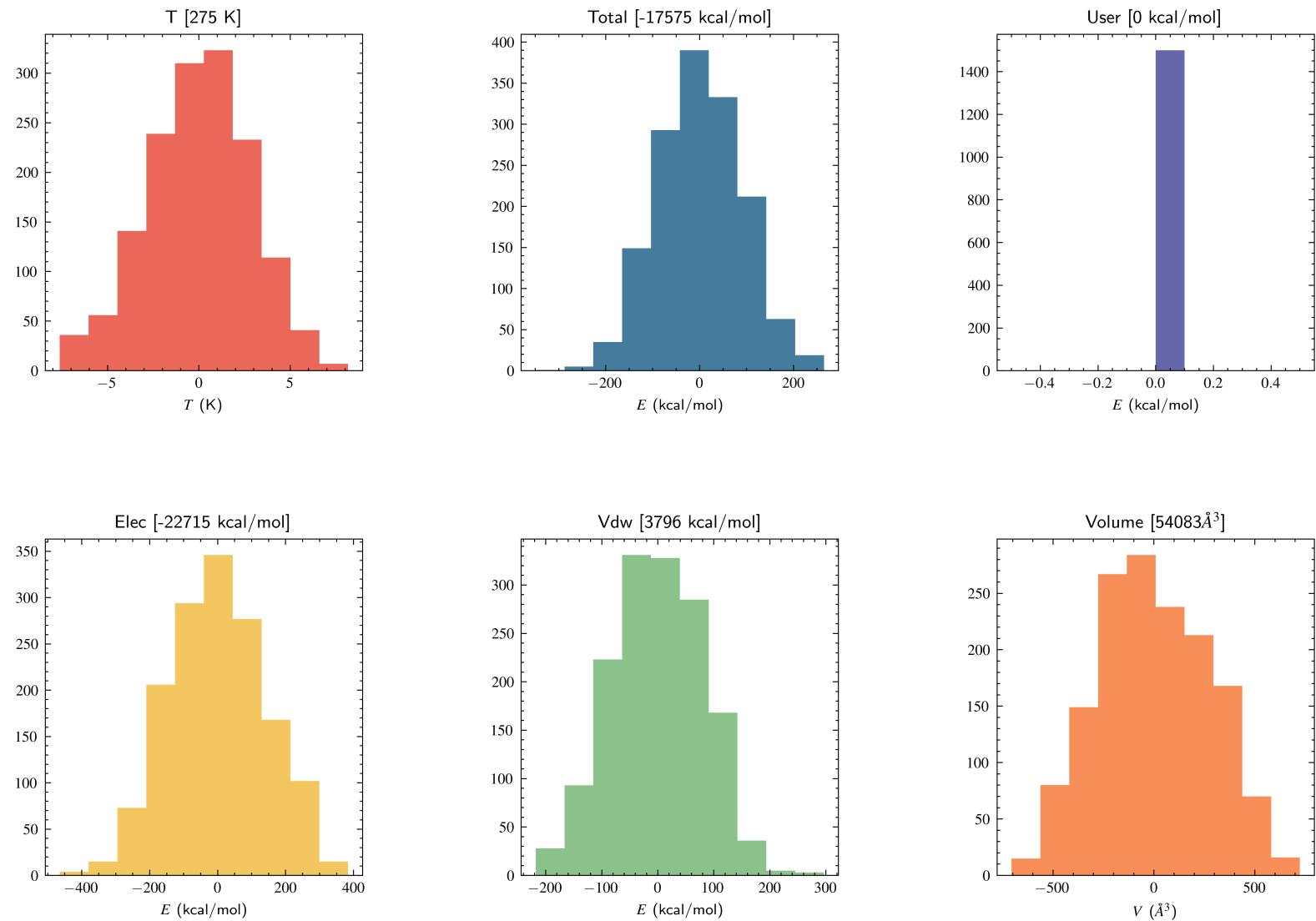
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
3: DYNA RESTRT CPT [200.0 ps]



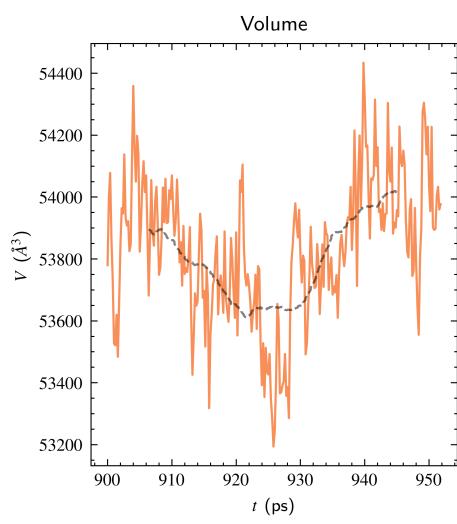
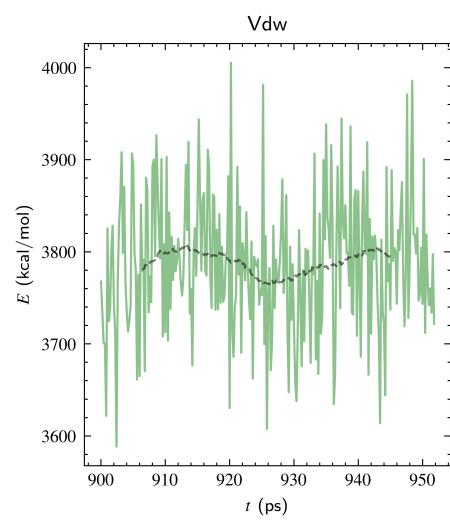
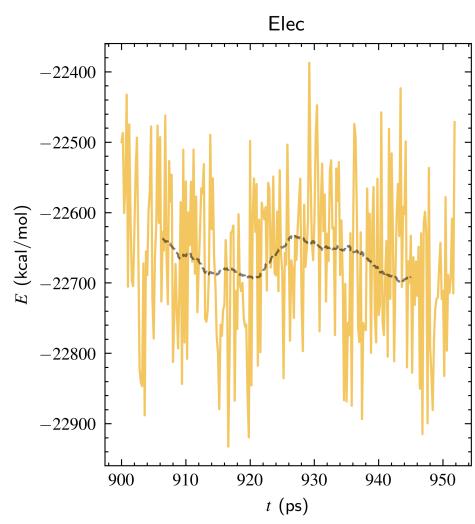
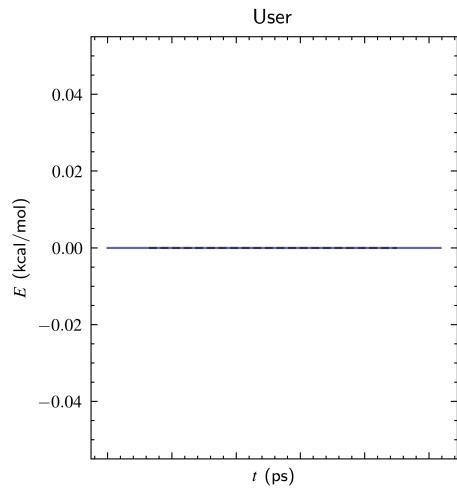
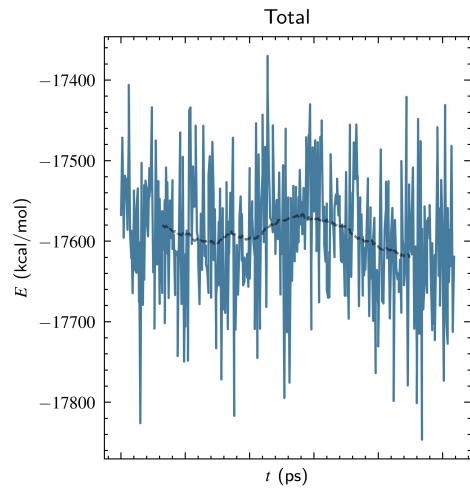
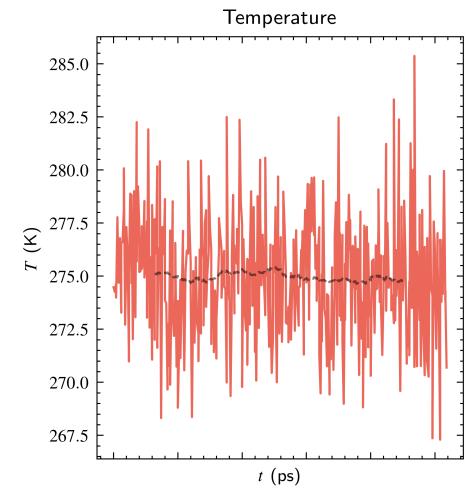
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
4: DYNA RESTRT CPT [200.0 ps]



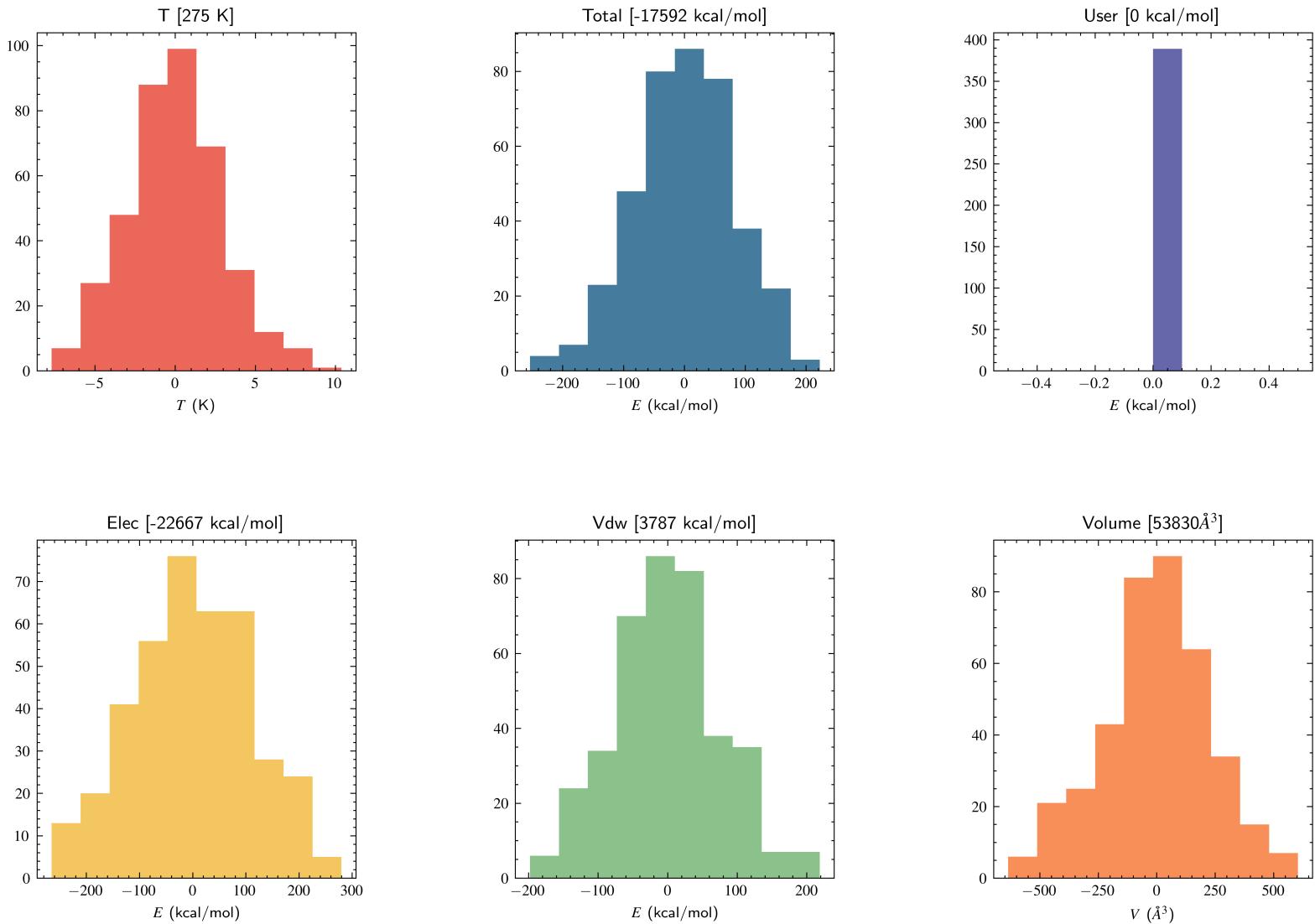
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
4: DYNA RESTRT CPT [200.0 ps]



\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
5: DYNA RESTRT CPT [51.0 ps]



\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k275\_dynamics.log  
 5: DYNA RESTRT CPT [51.0 ps]



## Trajectory info.

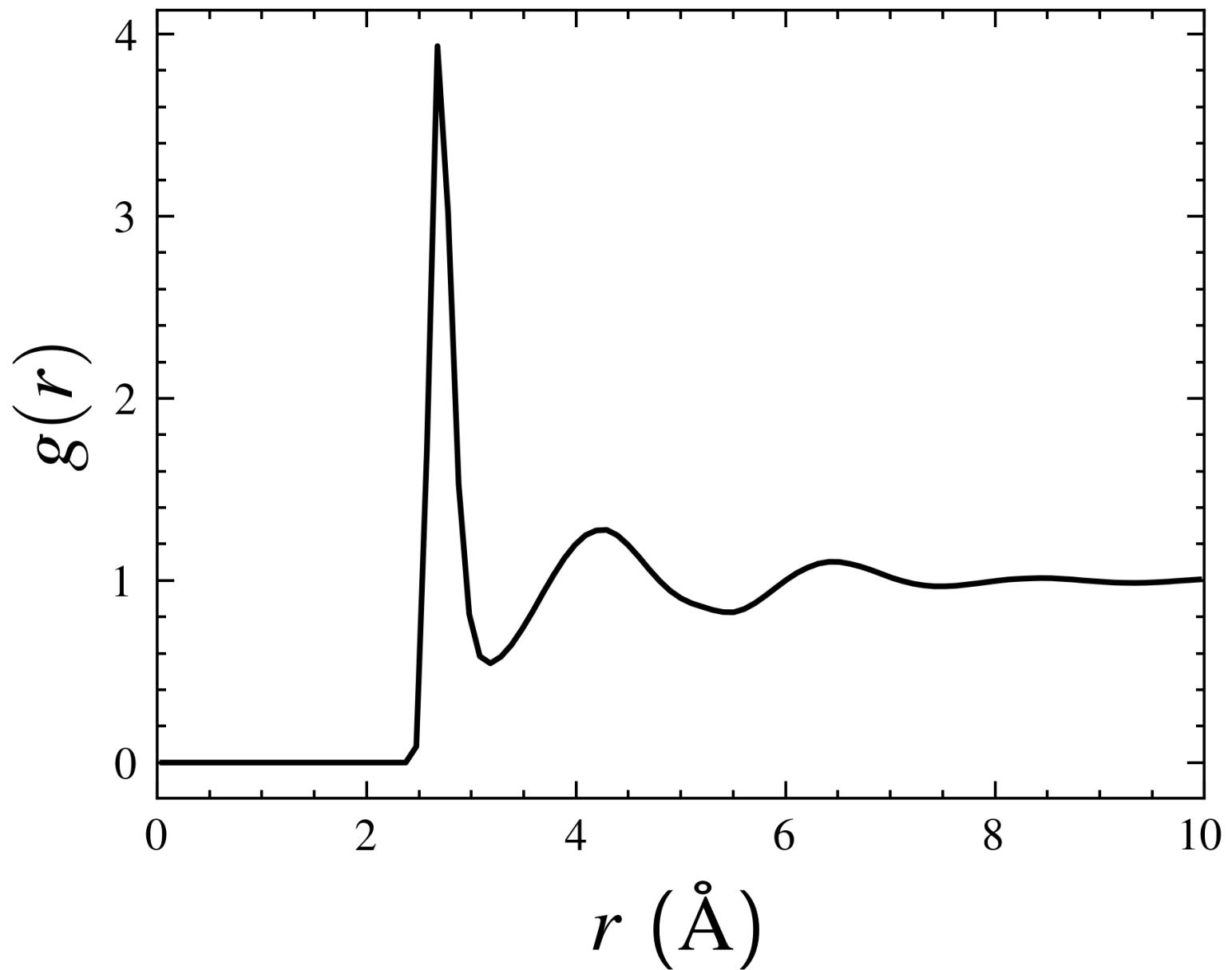
```
<Universe with 6000 atoms>
<ChainReader containing water.2000.dyna.0.dcd, water.2000.dyna.1.dcd with 2000 frames of 6000 atoms>
/home/boittier/miniconda3/envs/pycharmm/lib/python3.8/site-packages/MDAnalysis/coordinates/DCD.py:16
5: DeprecationWarning: DCDReader currently makes independent timesteps by copying self.ts while other readers update self.ts inplace. This behavior will be changed in 3.0 to be the same as other readers. Read more at https://github.com/MDAnalysis/mdanalysis/issues/3889 to learn if this change in behavior might affect you.
```

```
warnings.warn("DCDReader currently makes independent timesteps")
```

sim. time : 400 (ps)

```
<AtomGroup [<Atom 1: OH2 of type OT of resname TIP3, resid 1 and segid WAT>, <Atom 4: OH2 of type OT of resname TIP3, resid 2 and segid WAT>, <Atom 7: OH2 of type OT of resname TIP3, resid 3 and segid WAT>, ..., <Atom 5992: OH2 of type OT of resname TIP3, resid 1998 and segid WAT>, <Atom 5995: OH2 of type OT of resname TIP3, resid 1999 and segid WAT>, <Atom 5998: OH2 of type OT of resname TIP3, resid 2000 and segid WAT>]>
[2.75626263 4.45242424 6.67863636 8.79883838] [3.93392432 1.27738323 1.10232535 1.01301082]
```

# RDF



$MSD$  and  $D$

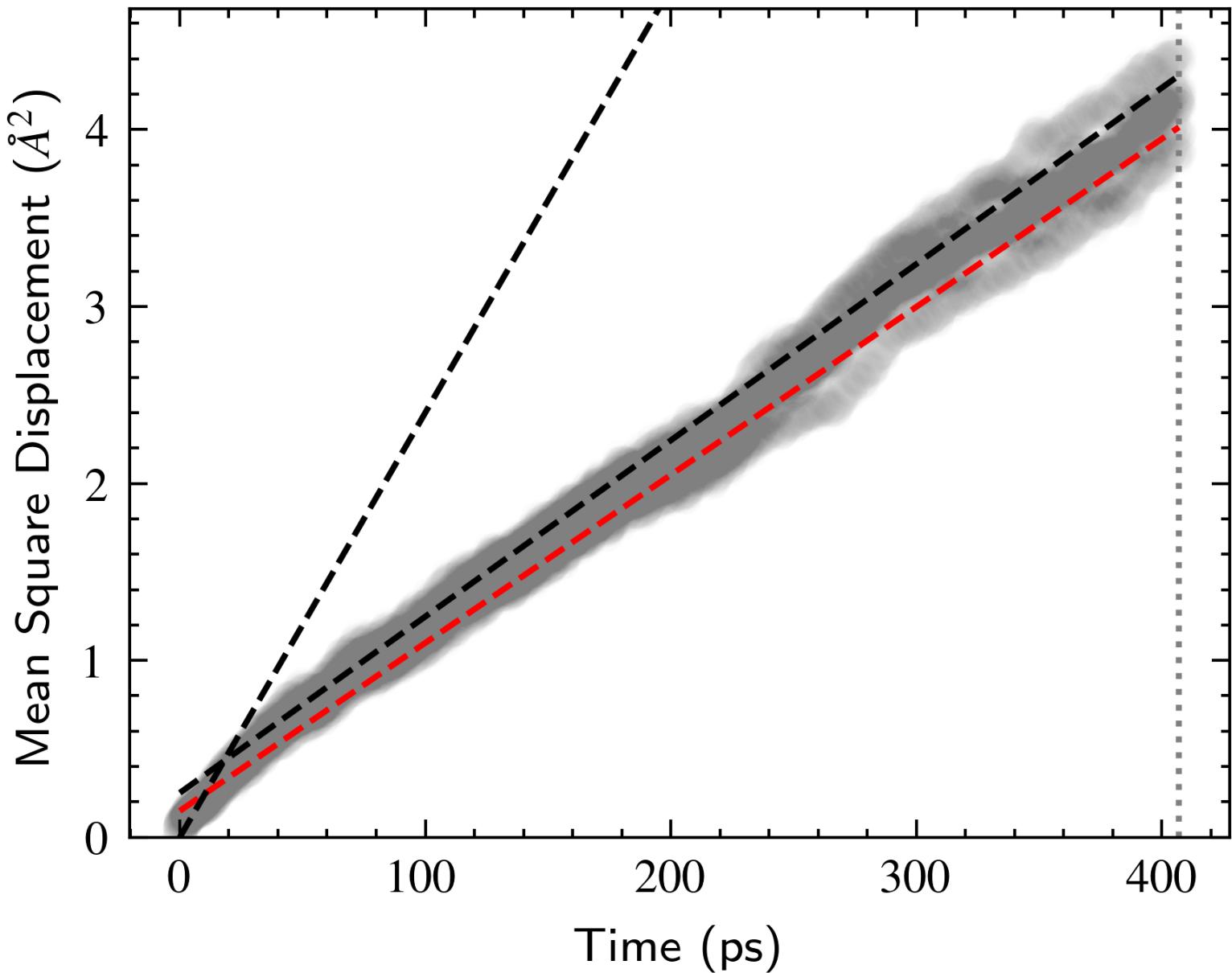
true  $\rho$ : 1001

true  $D$ : 1.15e-05

0.0002

407.0166167328458

<Axes: xlabel='Time (ps)', ylabel='Mean Square Displacement (\$\AA^2\$)'>

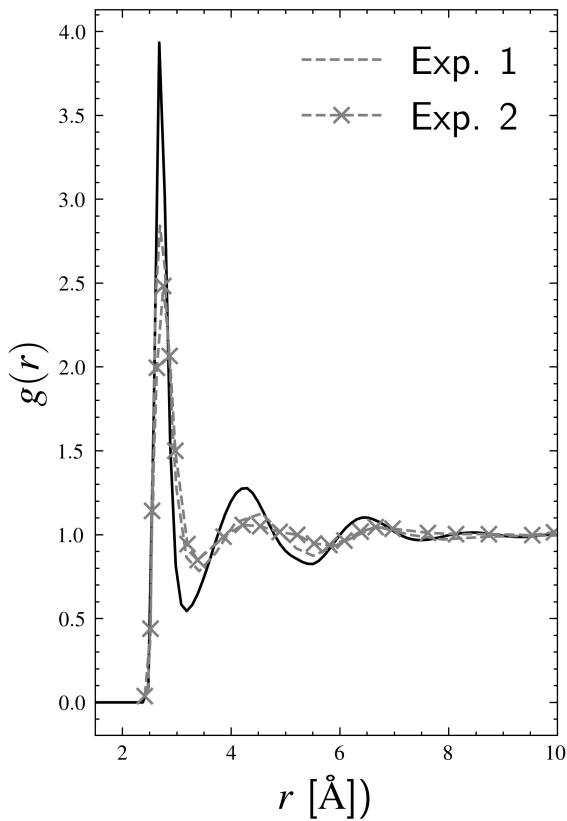


## Structure and Transport

407.0166167328458

$$\rho = 1090 \text{ [kg/m}^3\text{]} \text{ (error} = 8.9\%\text{)}$$

RDF



$$D = 0.1 \text{ [10}^{-5} \text{ cm s}^{-1}\text{]} \text{ (error} = -91.2\%\text{)}$$

MSD

