

Simulation Report: sims4_kmdcm_water_k250

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

	vdw	elec	user	time	temp	tot	energy	volume	pressi
count	7153.000000	7153.000000	7153.0	7153.000000	7153.000000	7153.000000	7153.000000	7153.000000	7153.000000C
mean	4068.637165	-23682.159215	0.0	414.915029	254.642716	-18337.696212	22891.150589	60638.182721	-465.077914
std	313.370631	792.369381	0.0	289.524810	17.117949	1004.009200	798.303192	5380.988429	1187.155120
min	3235.485640	-25088.512700	0.0	0.000000	60.897280	-22673.641790	21085.663890	55505.000000	-5084.964790
25%	3731.066840	-24218.862120	0.0	89.400000	248.770180	-18992.996960	21721.615800	56422.000000	-1266.568270
50%	4212.641990	-24100.661660	0.0	430.200000	251.183700	-18856.056170	23330.420880	57750.000000	-347.886640
75%	4288.269790	-22640.871440	0.0	668.600000	258.633070	-16718.646880	23458.024690	68921.000000	363.977330
max	4540.375720	-21731.352280	0.0	907.000000	283.906360	-16717.818930	24925.828760	68921.000000	3015.111160

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	53.000000
	mean	3588.794704	4192.317324	4244.276010	4251.540304	4292.016072	4306.287986	
	std	115.125672	79.892145	77.816405	79.378408	77.709172	95.333261	
	min	3235.485640	3613.580440	3983.469720	3994.541390	4031.930080	4120.025820	
	25%	3519.313657	4143.190735	4191.566773	4197.280230	4243.899195	4241.139550	
	50%	3596.823605	4190.512875	4243.648505	4250.392625	4289.939030	4288.590220	
	75%	3666.007230	4238.875993	4297.194510	4307.198035	4343.457870	4390.445010	
	max	4072.983730	4439.105010	4473.063980	4540.375720	4523.431950	4526.843910	
	elec	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	53.000000
elec	mean	-22453.219898	-23953.206958	-24163.673017	-24189.881370	-24204.286533	-24214.330433	
	std	311.094124	137.036728	122.181194	117.335506	112.571769	107.468046	
	min	-25088.512700	-24368.998870	-24533.969410	-24580.066440	-24516.109620	-24480.082740	
	25%	-22549.125790	-24035.560050	-24244.625660	-24271.621615	-24281.999300	-24290.542450	
	50%	-22444.260325	-23960.954170	-24165.108930	-24187.035115	-24202.964190	-24196.063740	
	75%	-22335.677880	-23875.759950	-24081.531077	-24110.242815	-24135.735300	-24142.701060	
	max	-21731.352280	-22437.852960	-23575.105860	-23784.758630	-23890.393680	-24038.021680	
	volume	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	53.000000
	mean	68921.000000	61338.383333	57978.924667	56635.358000	56143.612667	55906.566038	
	std	0.000000	2167.649619	521.080367	324.501791	218.862396	154.125762	

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	58488.000000	56694.000000	55769.000000	55526.000000	55505.000000
25%	68921.000000	59434.000000	57607.500000	56420.000000	55991.000000	55784.000000
50%	68921.000000	60645.500000	57992.000000	56601.000000	56146.000000	55913.000000
75%	68921.000000	63023.000000	58401.000000	56886.000000	56302.000000	56041.000000
max	68921.000000	68921.000000	59366.000000	57537.000000	56817.000000	56200.000000
temp	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000
	mean	266.549244	250.023389	250.002344	250.003176	250.044436
	std	28.859485	2.862553	2.688675	2.634640	2.669812
	min	60.897280	242.460320	240.801790	240.813660	240.133680
	25%	269.481358	248.198745	248.220732	248.169885	248.294762
	50%	274.291280	250.075750	249.954820	249.914930	250.052650
	75%	276.921142	251.694500	251.848197	251.794852	251.897045
	max	283.906360	278.866630	257.148880	258.822830	258.633070

Densities

density 1: 867.0796999463153 kilogram / meter ** 3

density 2: 974.2676078572878 kilogram / meter ** 3

density 3: 1030.7193578282645 kilogram / meter ** 3

density 4: 1055.1712236020473 kilogram / meter ** 3

density 5: 1064.413156930324 kilogram / meter ** 3

density 6: 1068.9263218145636 kilogram / meter ** 3

temp. 1: 266.54924414

temp. 2: 250.0233894999995

temp. 3: 250.0023436733334

temp. 4: 250.0031755600002

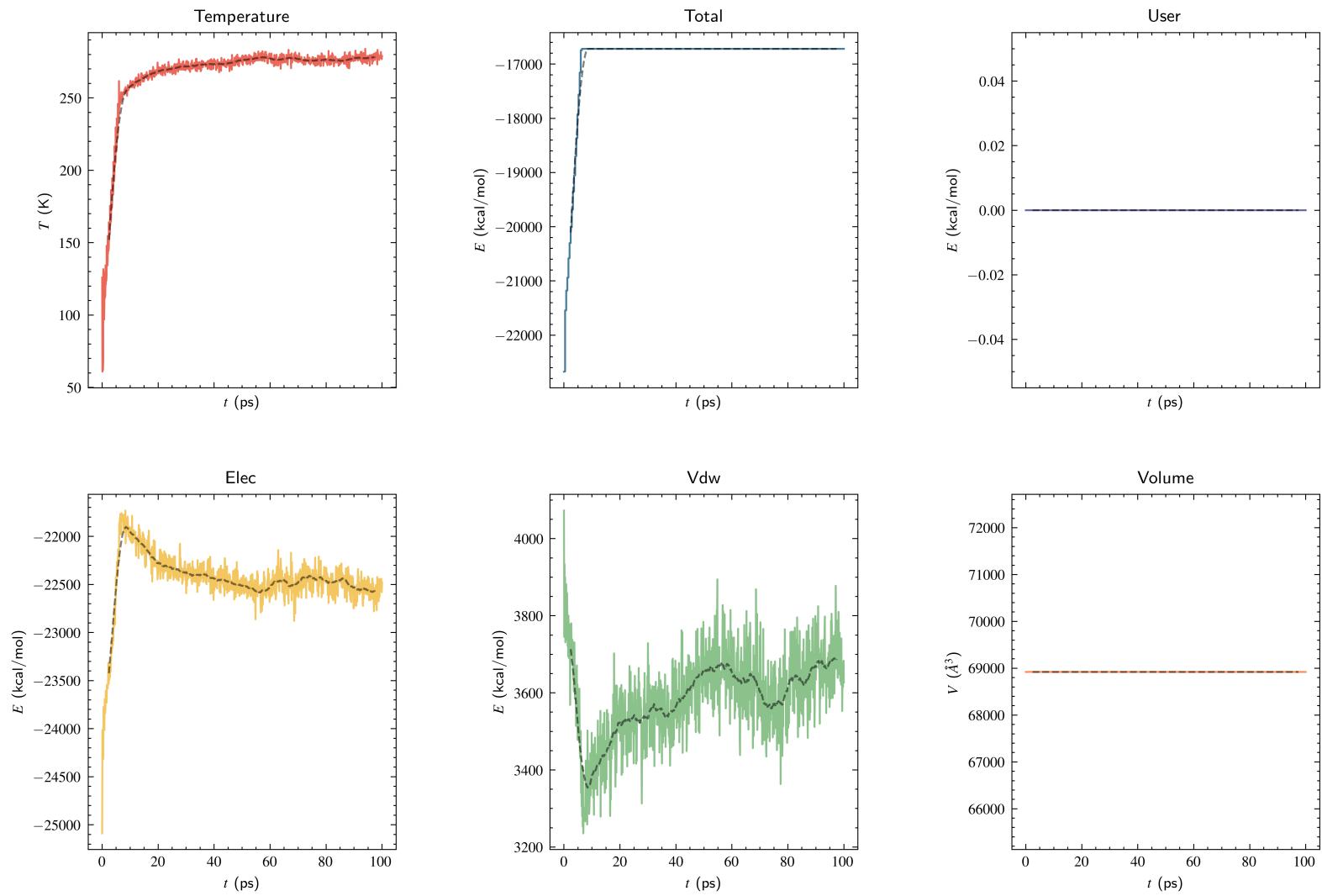
temp. 5: 250.0444360733334

temp. 6: 250.41300566037737

plotting

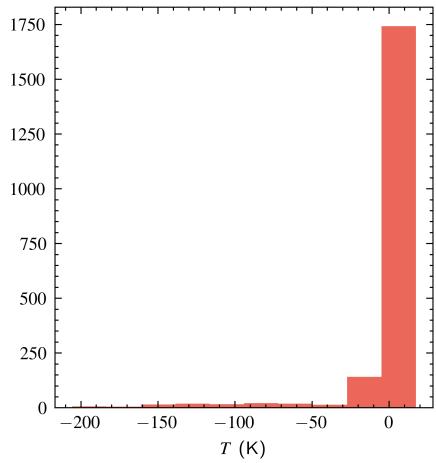
['2: DYNA RESTRT CPT', '3: DYNA RESTRT CPT', '4: DYNA RESTRT CPT', '0: DYNA STRT VERL', '1: DYNA RES
TRT CPT', '5: DYNA RESTRT CPT']

_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
0: DYNA STRT VERL [100.0 ps]

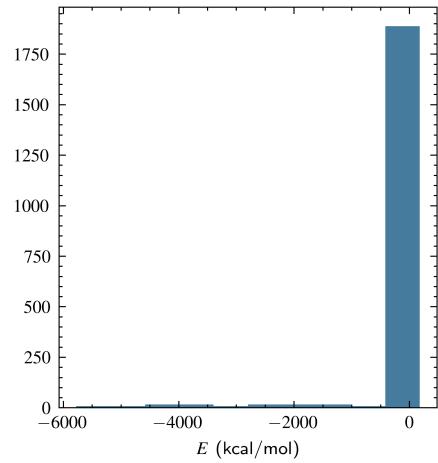


_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
0: DYNA STRT VERL [100.0 ps]

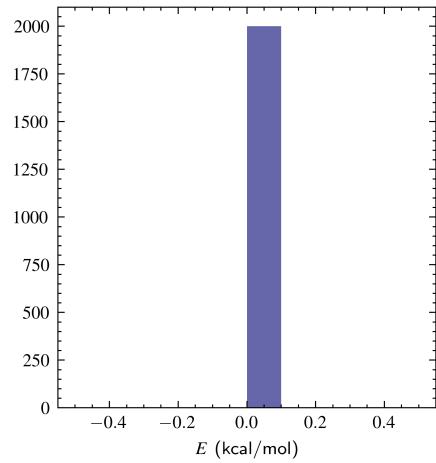
T [267 K]



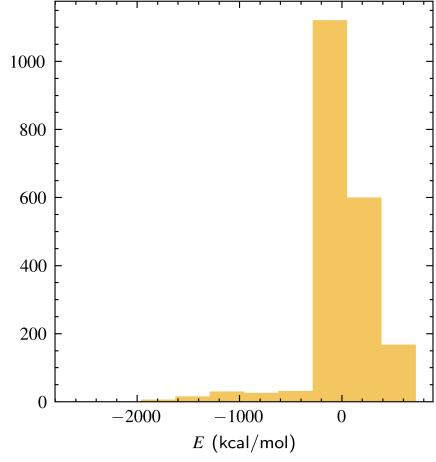
Total [-16895 kcal/mol]



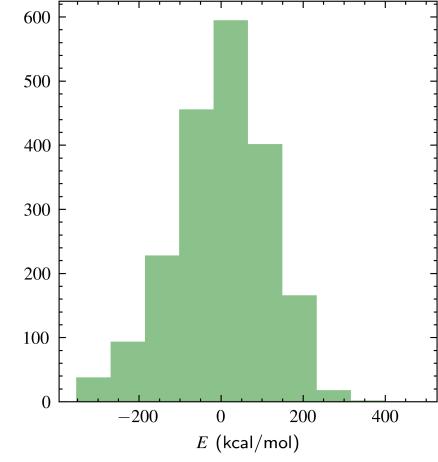
User [0 kcal/mol]



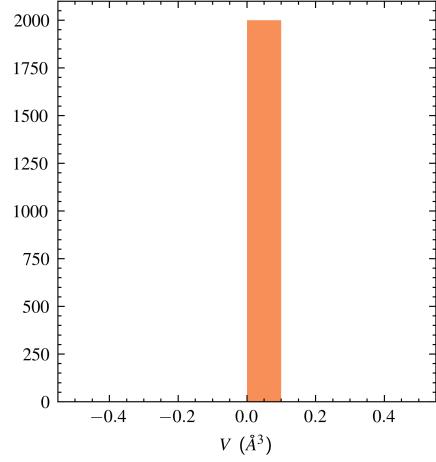
Elec [-22453 kcal/mol]



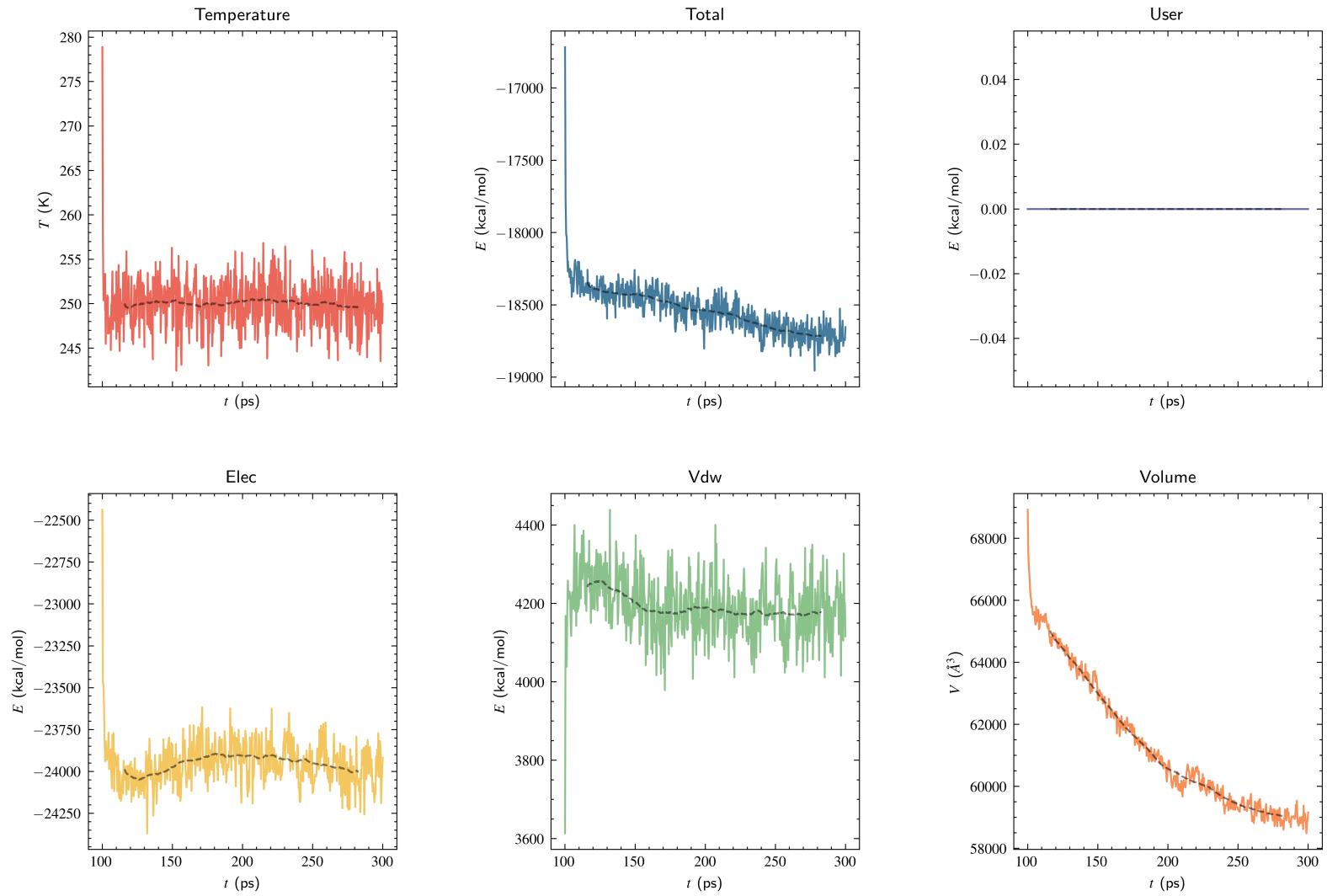
Vdw [3589 kcal/mol]



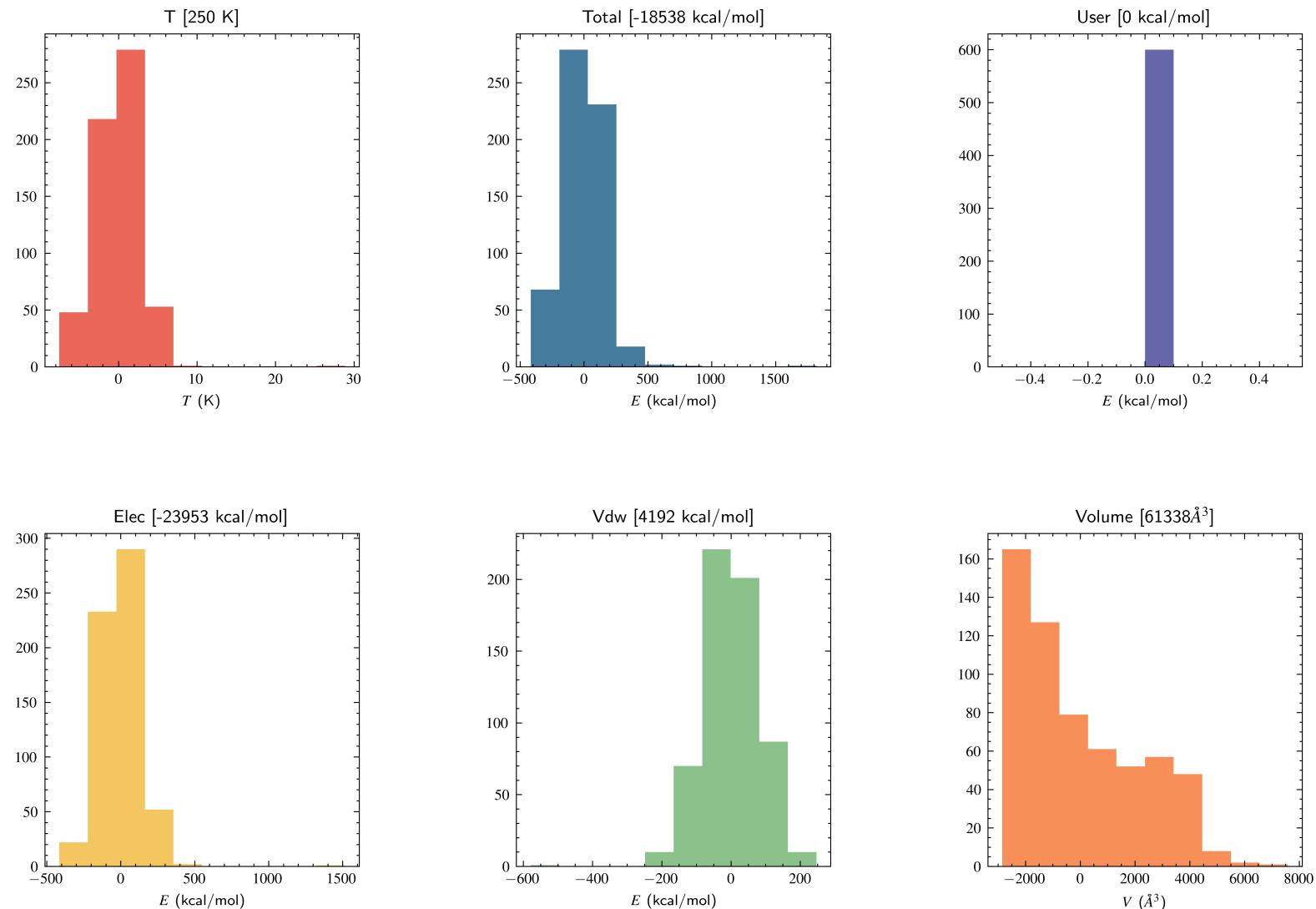
Volume [68921 Å³]



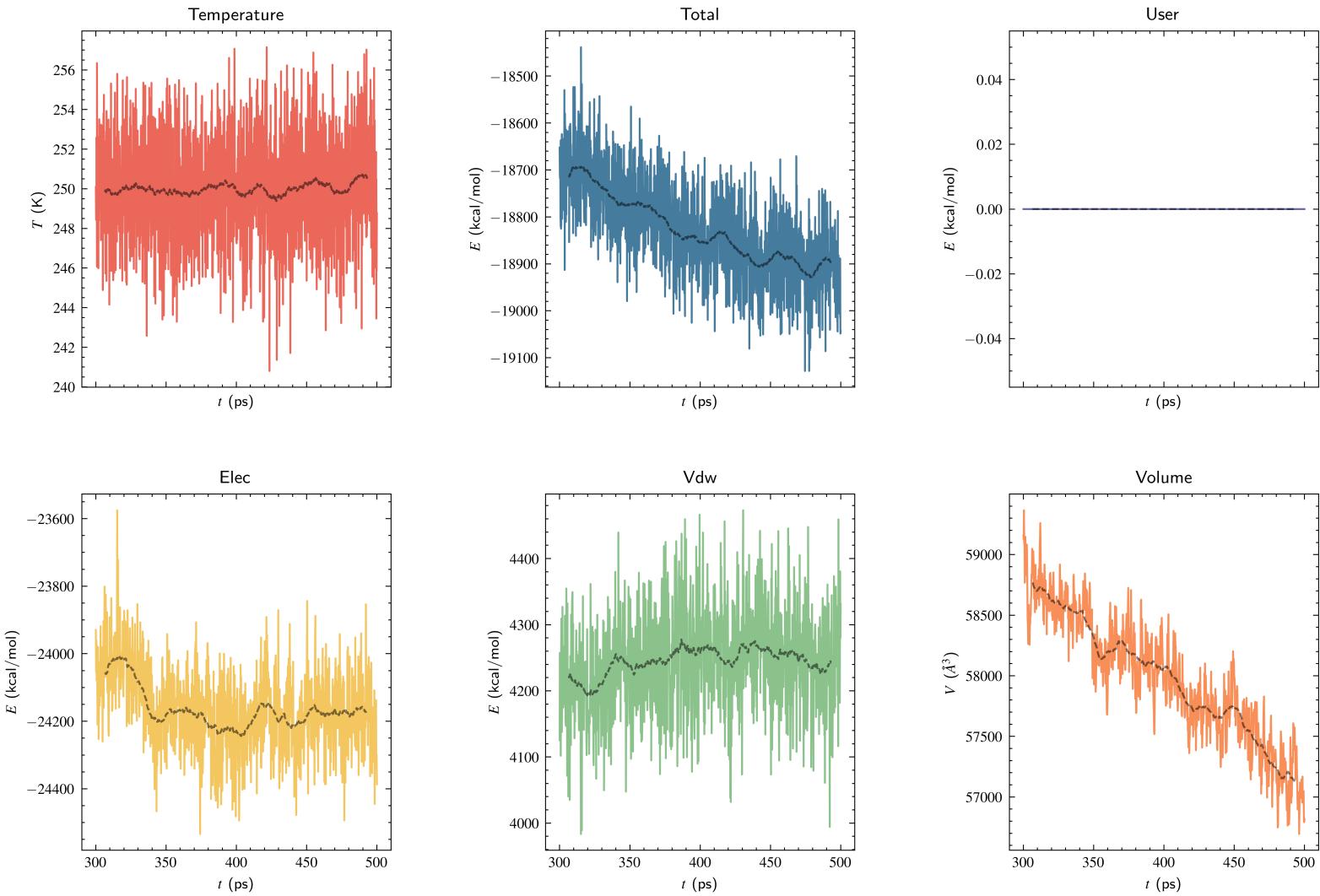
_home_boittier_pc当地_sims4_kmdcm_water_k250_dynamics.log
1: DYNA RESTRT CPT [200.0 ps]



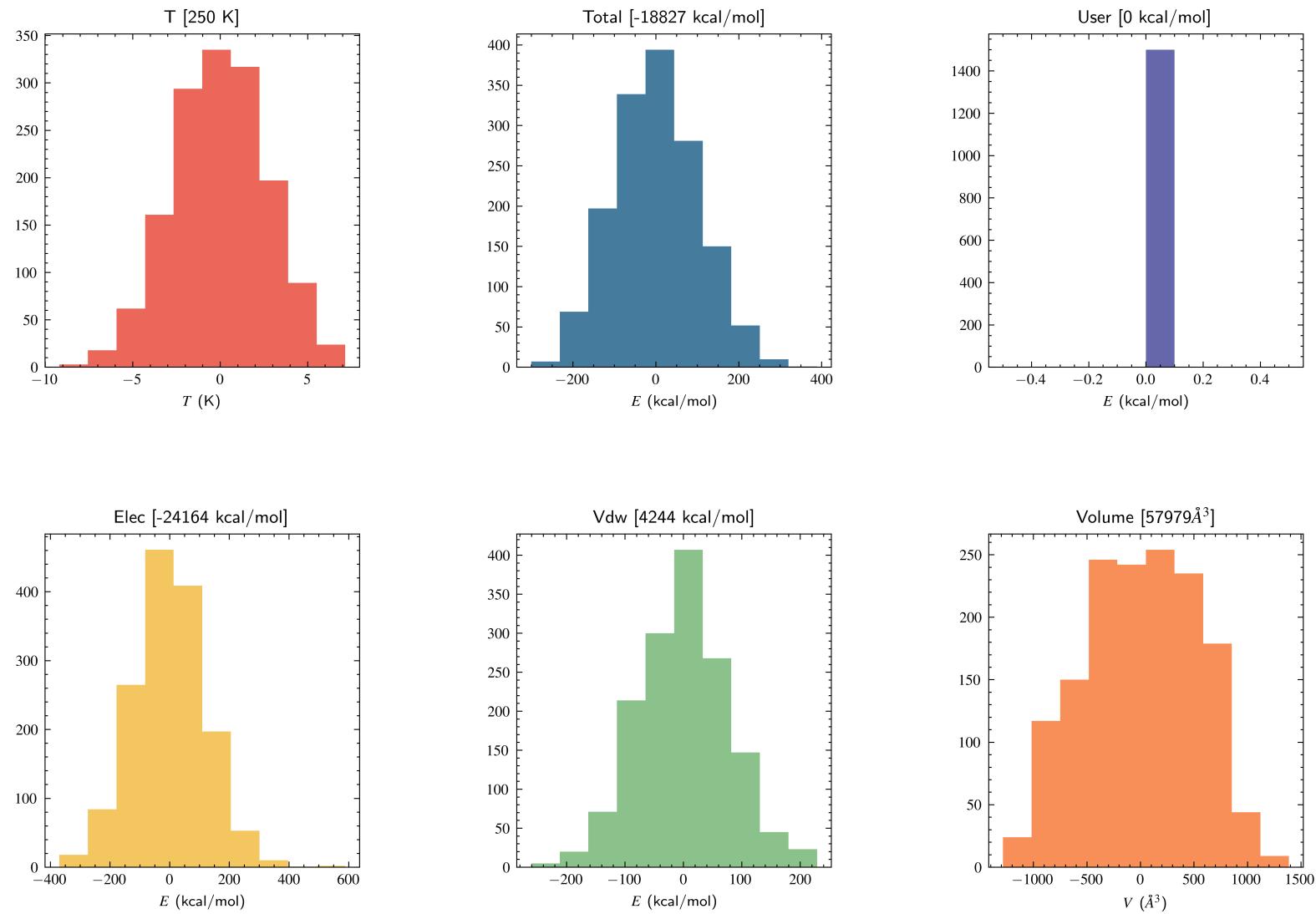
_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
1: DYNA RESTRT CPT [200.0 ps]



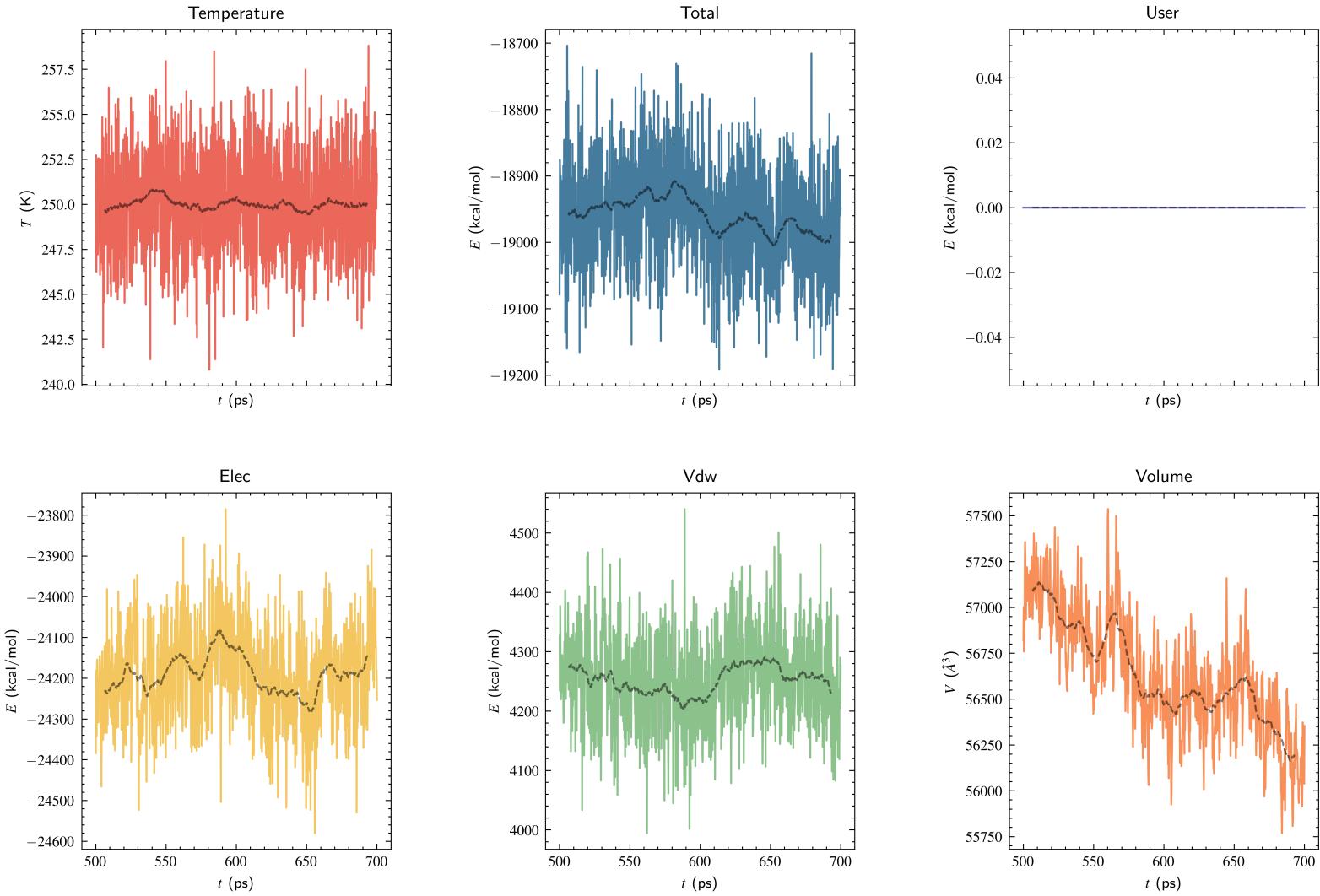
_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
2: DYNA RESTRT CPT [200.0 ps]



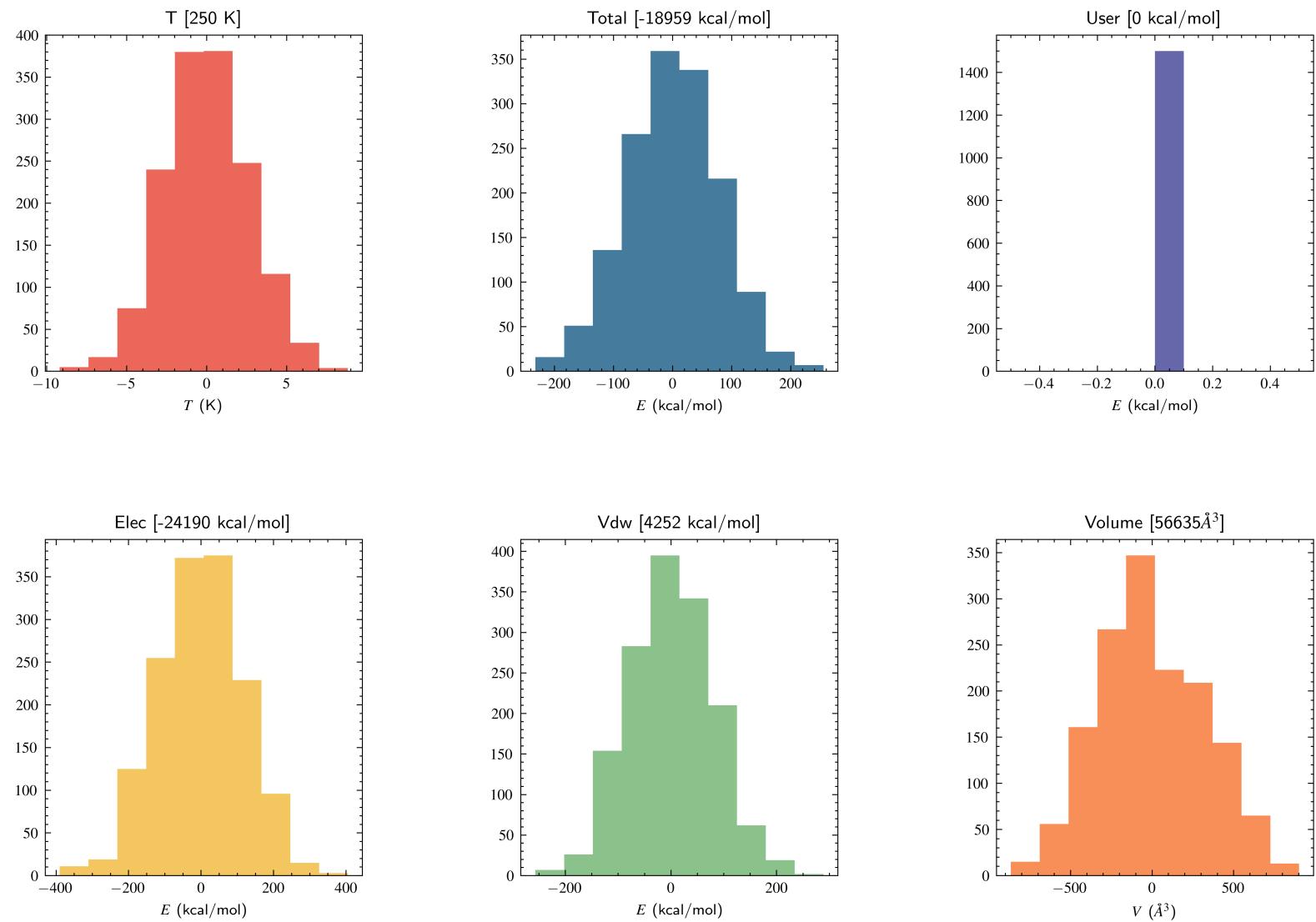
_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
2: DYNA RESTRT CPT [200.0 ps]



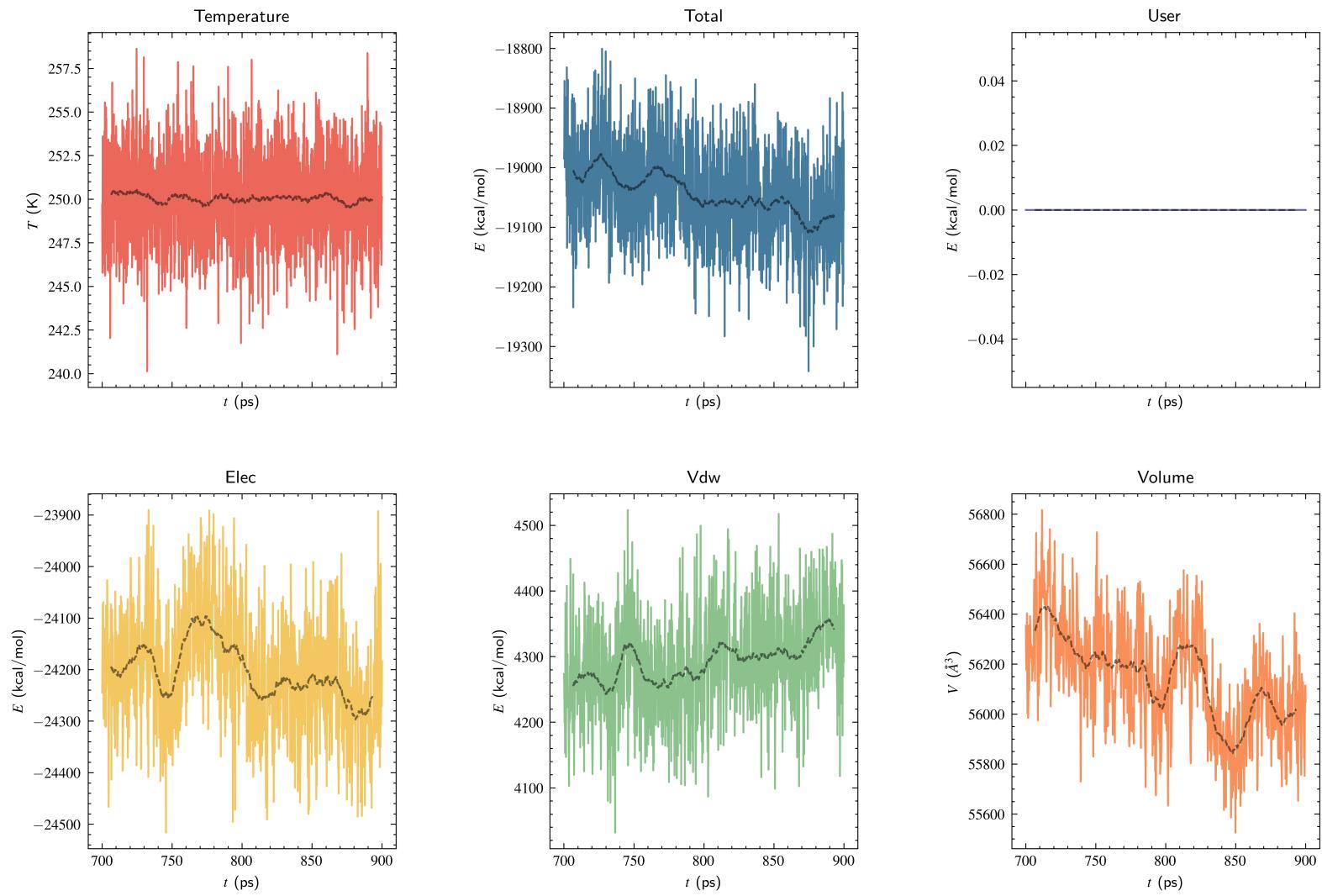
_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
3: DYNA RESTRT CPT [200.0 ps]



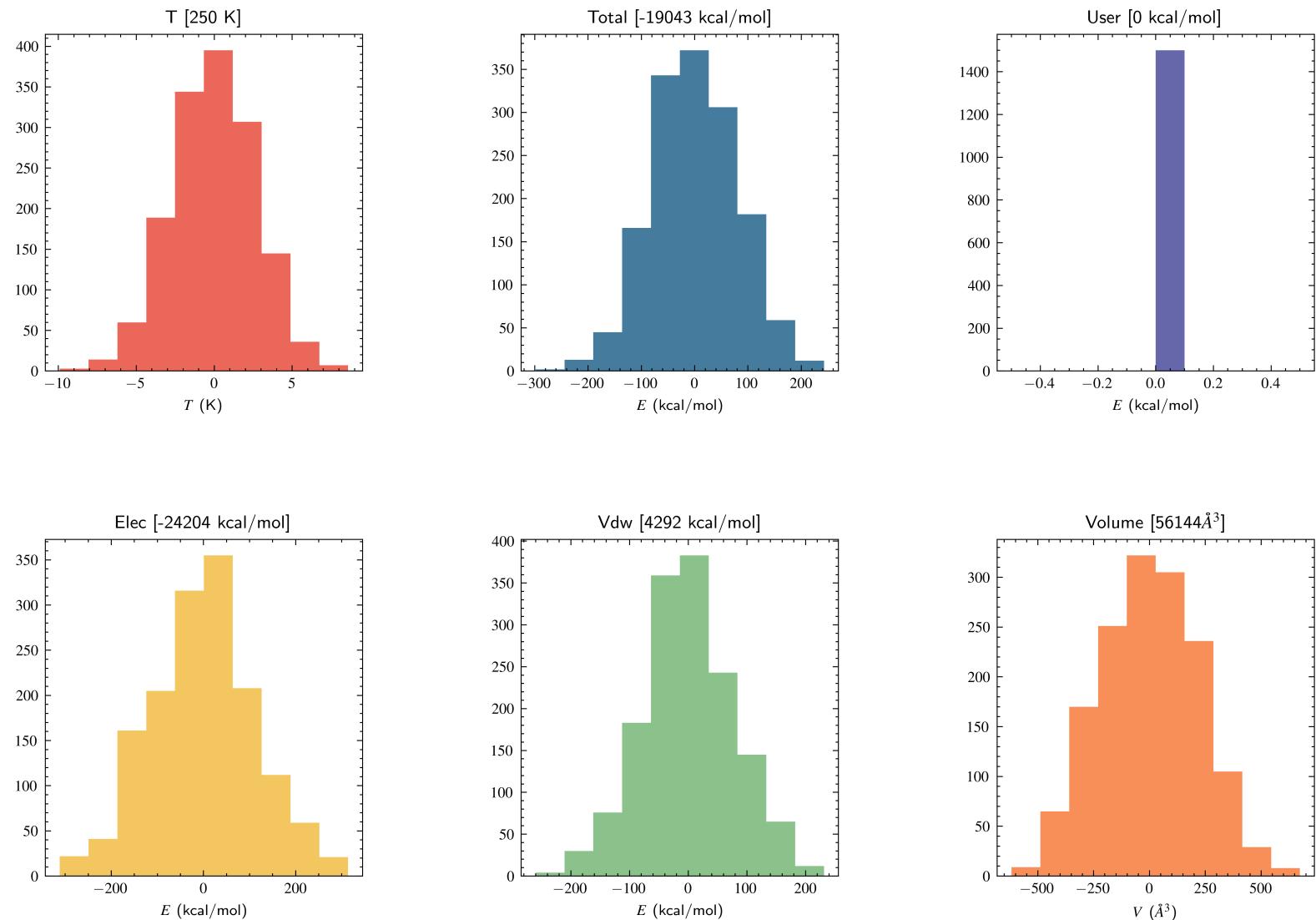
_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
3: DYNA RESTRT CPT [200.0 ps]



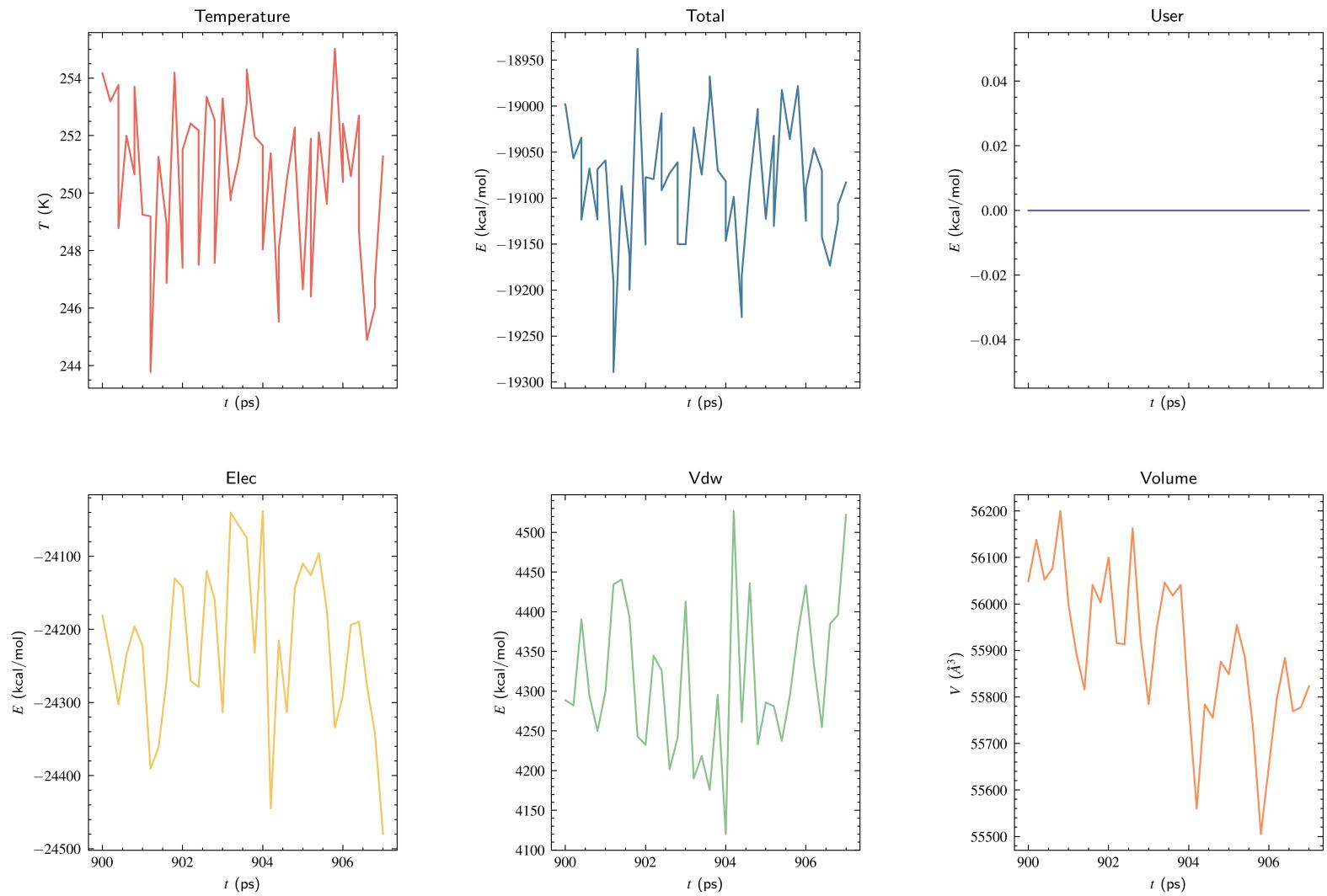
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4: DYNA RESTRT CPT [200.0 ps]



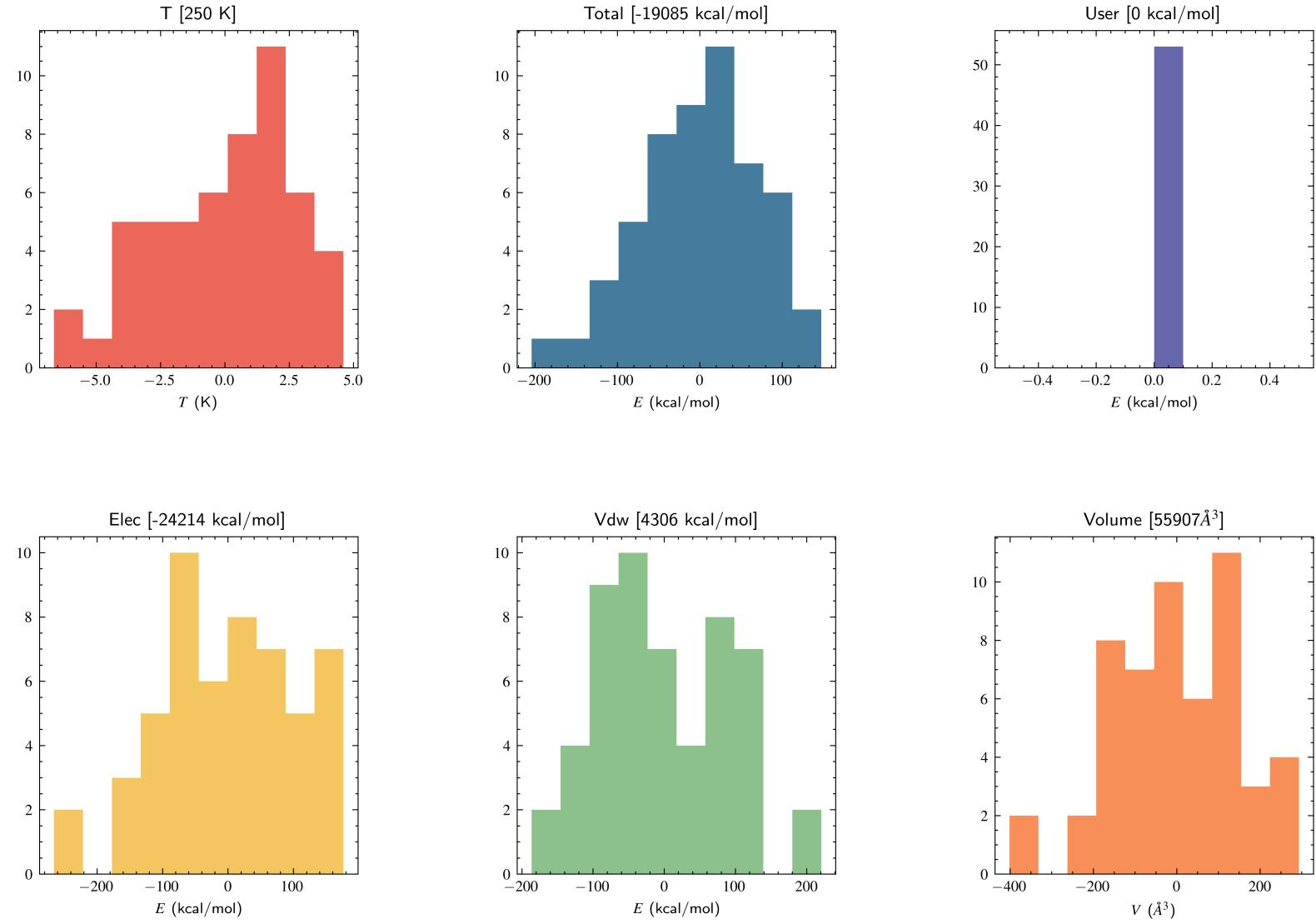
_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
4: DYNA RESTRT CPT [200.0 ps]



_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
5: DYNA RESTRT CPT [7.0 ps]



_home_boittier_pcbach_sims4_kmdcm_water_k250_dynamics.log
 5: DYNA RESTRT CPT [7.0 ps]



Trajectory info.

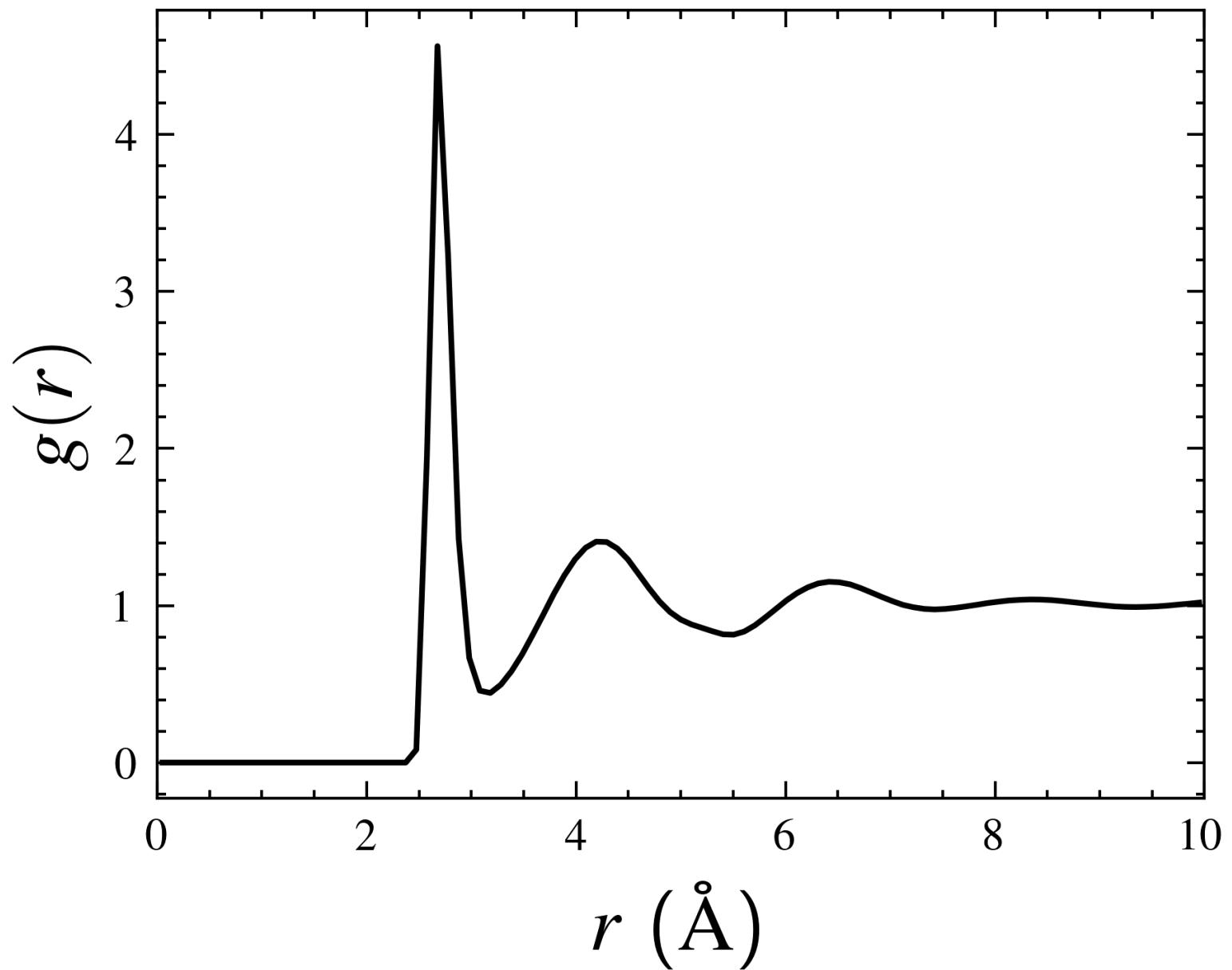
```
<Universe with 6000 atoms>
<ChainReader containing water.2000.dyna.0.dcd, water.2000.dyna.1.dcd with 2000 frames of 6000 atoms>
/home/boittier/miniconda3/envs/pycharmm/lib/python3.8/site-packages/MDAnalysis/coordinates/DCD.py:16
5: DeprecationWarning: DCDReader currently makes independent timesteps 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 4.34641414 6.67863636 8.69282828] [4.56290477 1.40703739 1.15155643 1.03862413]
```

RDF



MSD and D

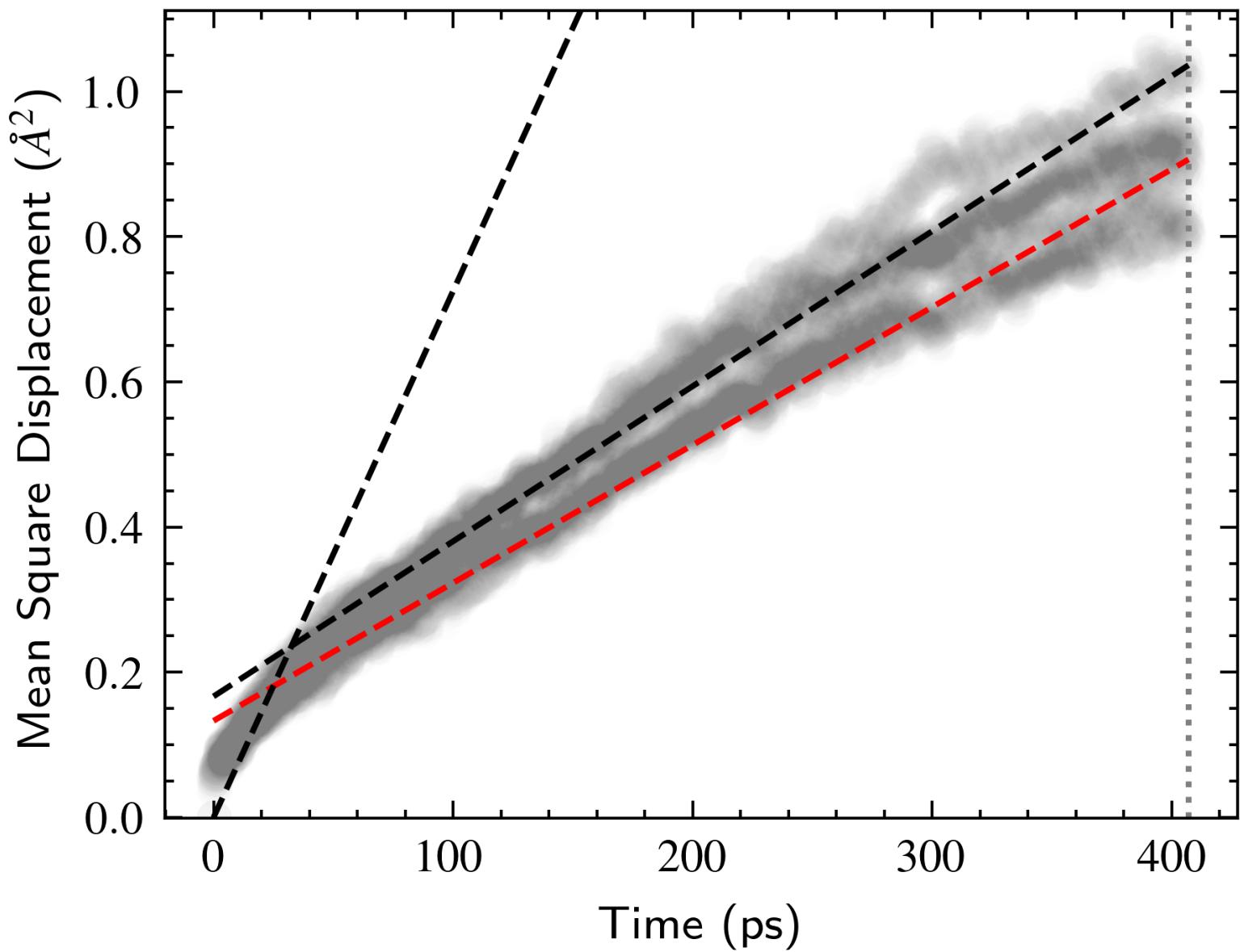
true ρ : 1001

true D : 3.46e-06

0.0002

407.0166167328458

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

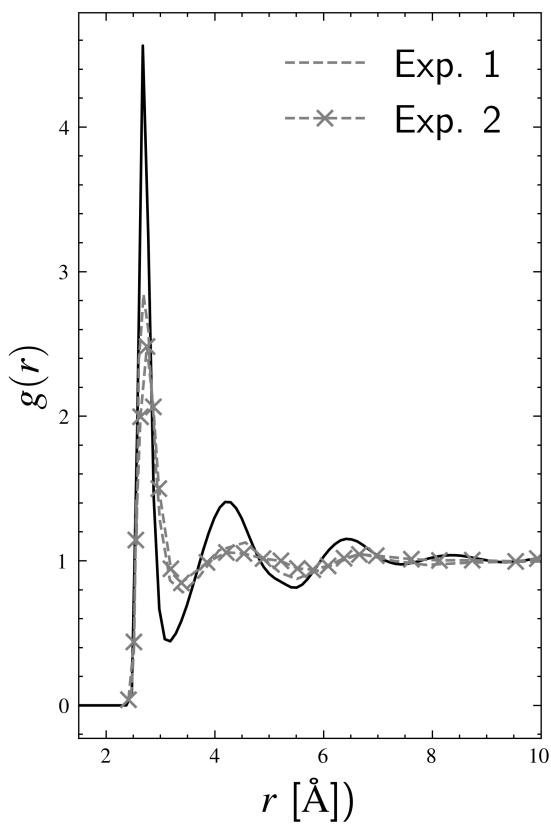


Structure and Transport

407.0166167328458

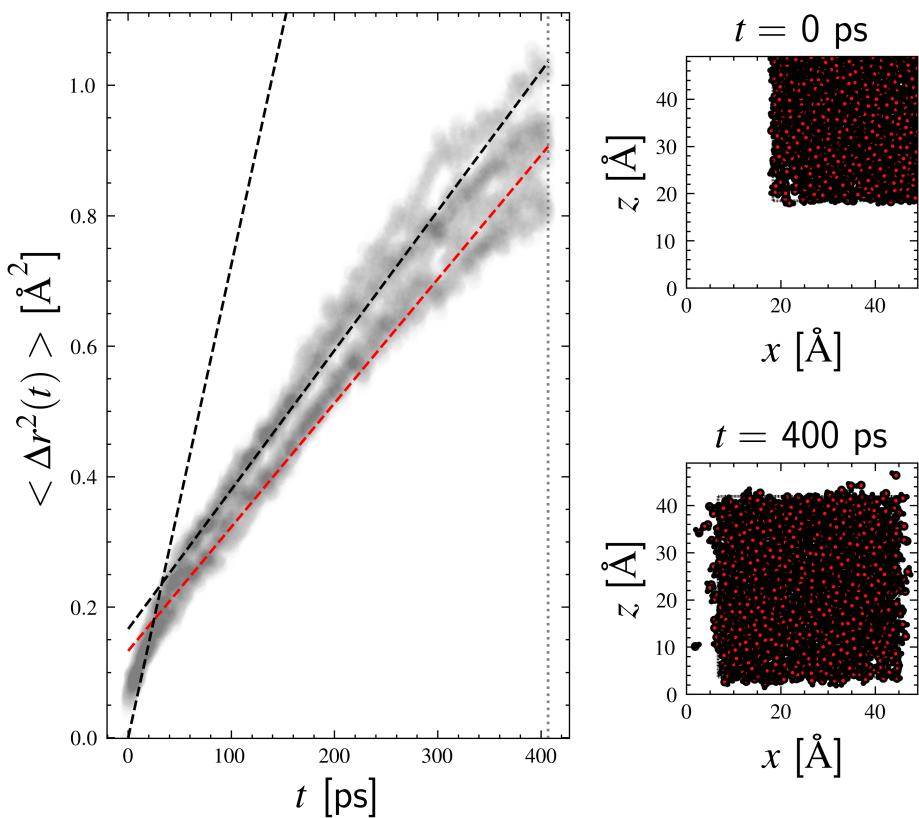
$\rho = 1039 \text{ [kg/m}^3\text{]} \text{ (error} = 3.8\%\text{)}$

RDF

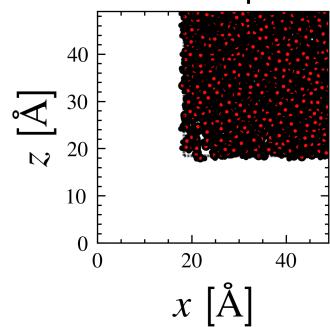


$D = 0.0 \text{ [10}^{-5} \text{ cm s}^{-1}\text{]} \text{ (error} = -93.7\%\text{)}$

MSD



$t = 0 \text{ ps}$



$t = 400 \text{ ps}$

