

Simulation Report: sims4_kmdcm_water_k225

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

	vdw	elec	user	time	temp	tot	energy	volume	pressi
count	7295.000000	7295.000000	7295.0	7295.000000	7295.000000	7295.000000	7295.000000	7295.000000	7295.000000C
mean	4309.962358	-24464.516063	0.0	424.679232	231.388217	-19267.894384	23405.517910	62301.035230	-491.945287
std	365.972705	909.869565	0.0	294.951727	16.736296	1024.366097	798.794605	4186.175862	1155.880168
min	3344.120500	-25413.693240	0.0	0.000000	61.112580	-22675.956070	21546.565020	58199.000000	-5796.326800
25%	3873.114840	-25068.790230	0.0	91.200000	223.935765	-19936.282970	22249.688700	59249.000000	-1295.865255
50%	4489.753630	-24955.513120	0.0	439.600000	226.081780	-19815.345370	23838.842250	59910.000000	-367.502430
75%	4558.713490	-23280.745790	0.0	682.800000	234.052560	-17575.127395	23955.208130	68921.000000	360.771770
max	4813.780700	-22220.332380	0.0	926.000000	265.808260	-17574.215120	24925.828760	68921.000000	2807.740380

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	195.000000
	mean	3731.663379	4503.176859	4493.757430	4550.117535	4546.665431	4564.779173
	std	108.468474	74.150328	73.142182	74.709898	71.021347	72.663281
	min	3344.120500	3901.263770	4301.942250	4329.851300	4354.389620	4383.394870
	25%	3662.287610	4456.946995	4440.831330	4496.700440	4499.157003	4512.042500
	50%	3736.264020	4507.062545	4492.808155	4544.992645	4545.204720	4565.829090
	75%	3809.379737	4547.670350	4544.728367	4604.207737	4593.208953	4618.658845
	max	4072.983730	4720.519070	4720.608030	4813.780700	4800.385730	4730.162630
elec	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	195.000000
	mean	-23012.282122	-24888.591535	-24944.530153	-25061.418998	-25070.525615	-25108.786476
	std	262.912422	136.273590	110.599216	101.278257	101.483560	107.360468
	min	-25088.512700	-25248.211020	-25264.019280	-25380.201190	-25413.693240	-25391.635670
	25%	-23173.862705	-24977.110993	-25021.466378	-25131.666410	-25138.127038	-25187.471250
	50%	-23034.487670	-24895.702300	-24939.917200	-25060.706500	-25071.984075	-25114.475780
	75%	-22867.412985	-24813.200830	-24875.607860	-24988.829560	-25004.523972	-25036.318570
	max	-22220.332380	-23363.146170	-24624.038780	-24706.160390	-24735.921030	-24865.928720
volume	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	195.000000
	mean	68921.000000	62413.251667	60070.538667	59546.517333	58892.077333	58627.697436
	std	0.000000	1136.821627	415.181267	291.816181	249.433371	164.827513

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	60424.000000	59219.000000	58745.000000	58312.000000	58199.000000
25%	68921.000000	61488.500000	59759.750000	59323.000000	58702.000000	58526.500000
50%	68921.000000	62241.500000	60005.000000	59552.000000	58887.000000	58621.000000
75%	68921.000000	63121.500000	60313.000000	59762.000000	59089.000000	58733.000000
max	68921.000000	68921.000000	61330.000000	60370.000000	59512.000000	59089.000000
temp	count	2000.000000	600.000000	1500.000000	1500.000000	1500.000000
	mean	248.139749	225.251123	225.061870	225.006479	225.036921
	std	24.892115	2.668894	2.445922	2.369475	2.366567
	min	61.112580	219.365250	216.326650	217.066020	217.269460
	25%	248.328847	223.451630	223.403897	223.402800	223.380632
	50%	254.885765	225.268460	225.024200	224.937330	225.047395
	75%	258.350143	226.844572	226.720225	226.579997	226.731493
	max	265.808260	257.071740	232.745080	234.012970	232.242670

Densities

density 1: 867.0796999463153 kilogram / meter ** 3

density 2: 957.4889691561496 kilogram / meter ** 3

density 3: 994.8304331281284 kilogram / meter ** 3

density 4: 1003.5851411002194 kilogram / meter ** 3

density 5: 1014.737511495038 kilogram / meter ** 3

density 6: 1019.3134408074035 kilogram / meter ** 3

temp. 1: 248.139748995

temp. 2: 225.2511229833335

temp. 3: 225.061870233333

temp. 4: 225.0064788133336

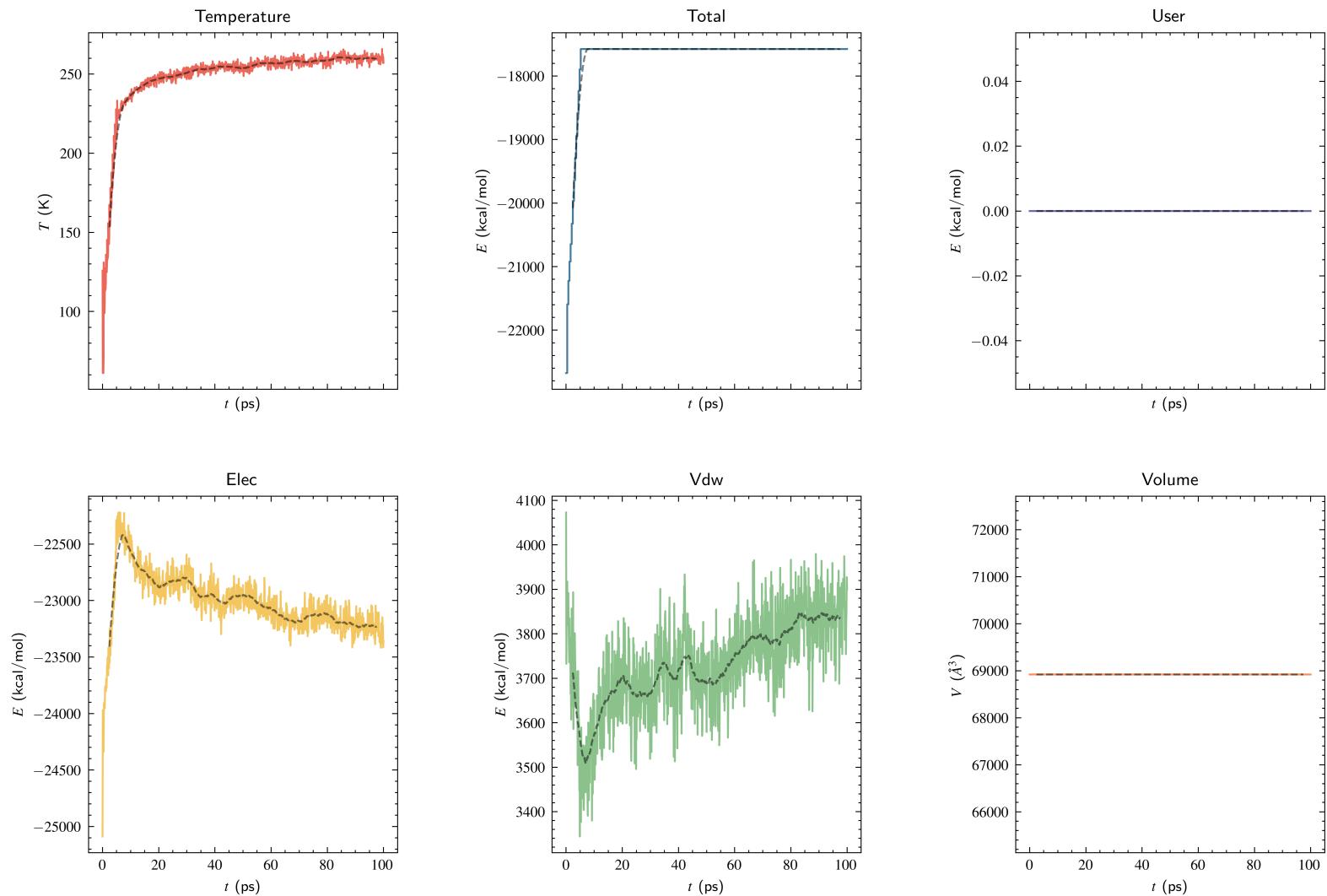
temp. 5: 225.03692102666665

temp. 6: 225.07162984615383

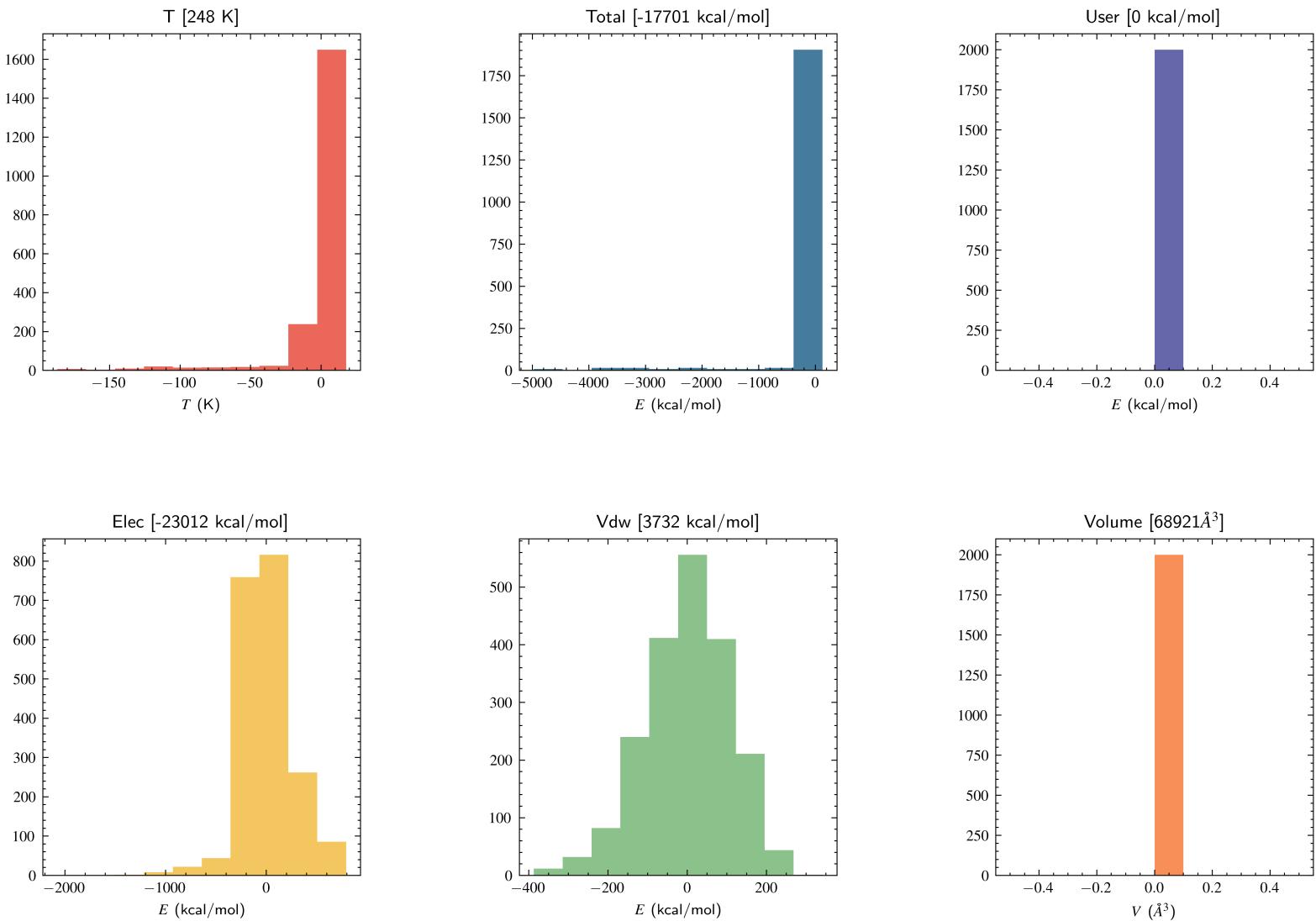
plotting

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

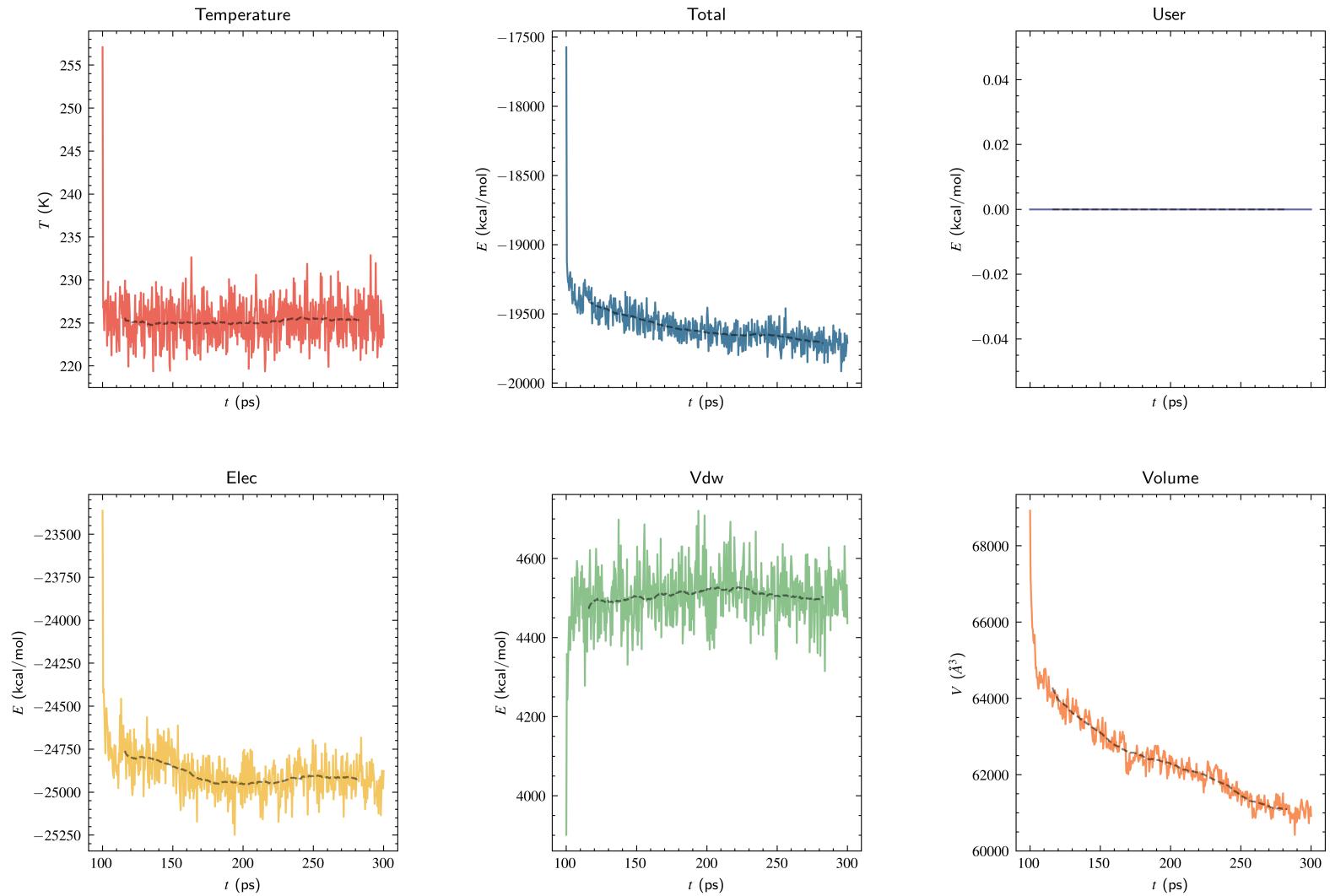
_home_boittier_pc当地_sims4_kmdcm_water_k225_dynamics.log
0: DYNA STRT VERL [100.0 ps]



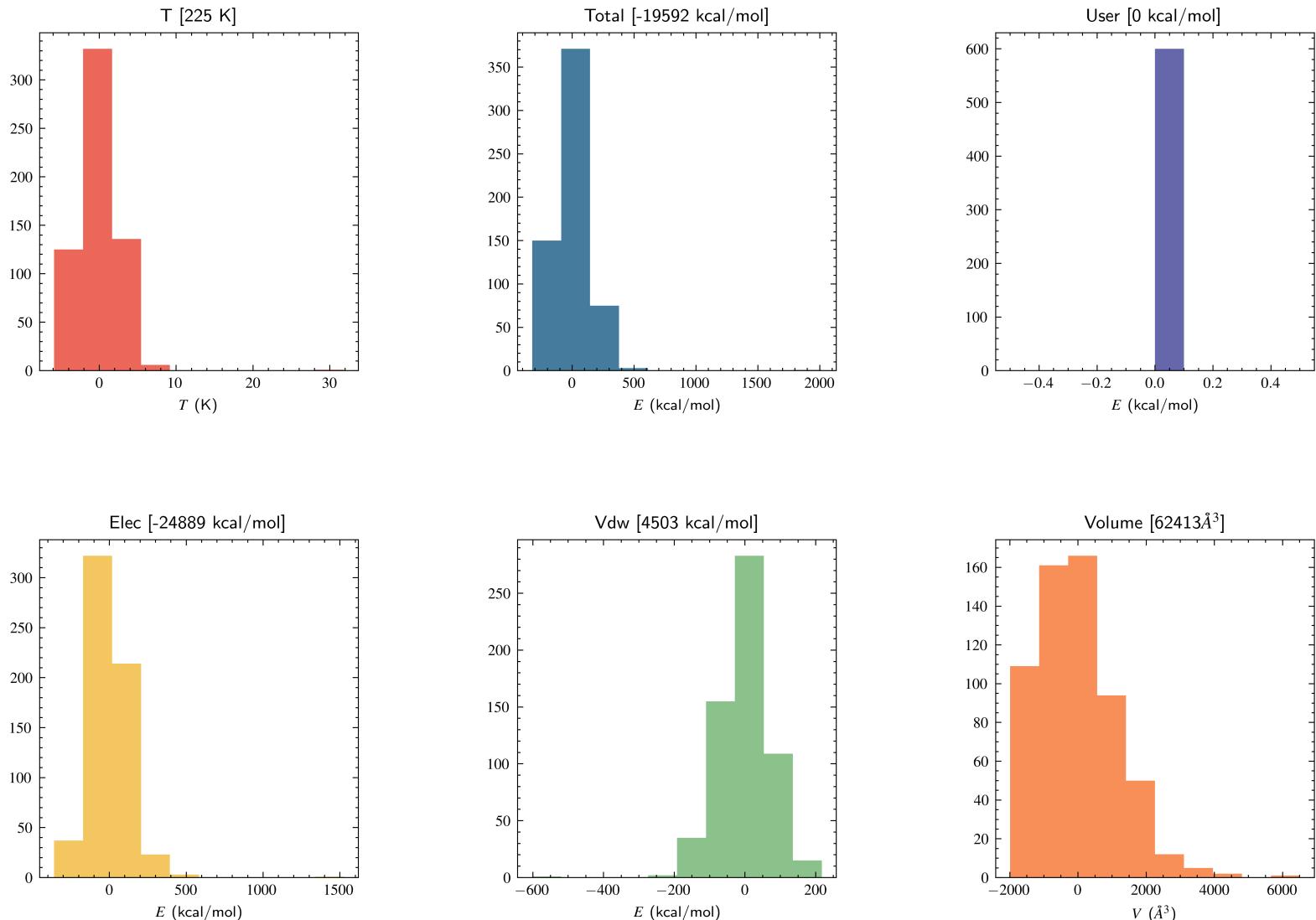
_home_boittier_pc当地_sims4_kmdcm_water_k225_dynamics.log
0: DYNA STRT VERL [100.0 ps]



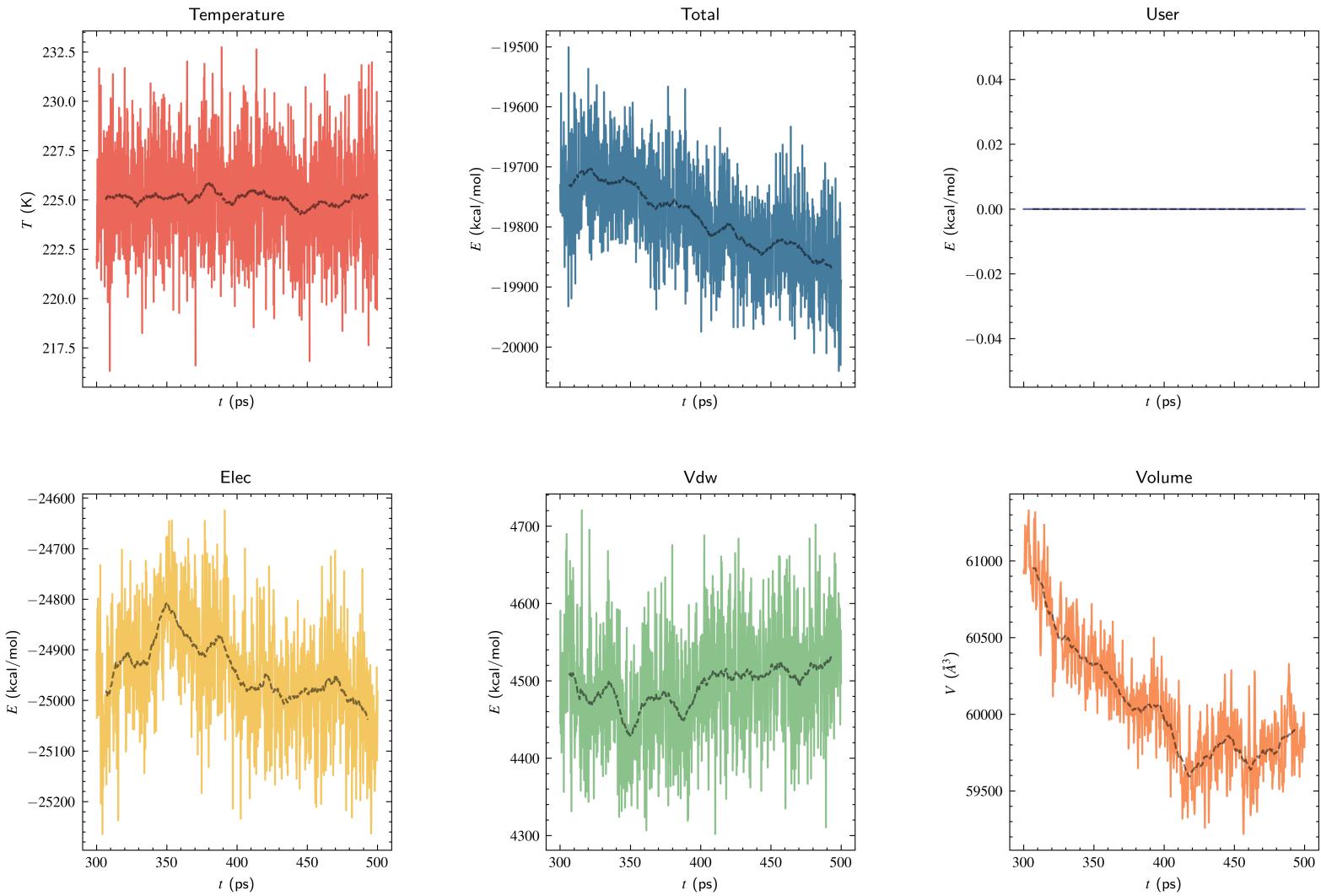
_home_boittier_pcbach_sims4_kmdcm_water_k225_dynamics.log
1: DYNA RESTRT CPT [200.0 ps]



_home_boittier_pcbach_sims4_kmdcm_water_k225_dynamics.log
1: DYNA RESTRT CPT [200.0 ps]

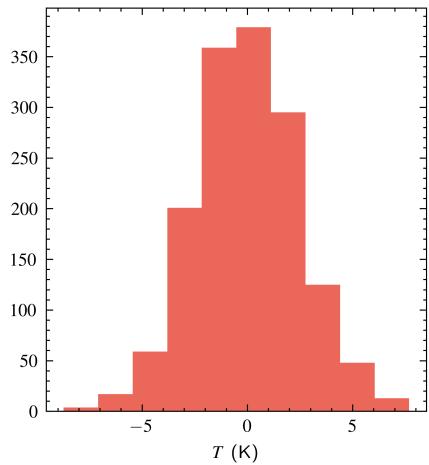


_home_boittier_pcbach_sims4_kmdcm_water_k225_dynamics.log
2: DYNA RESTRT CPT [200.0 ps]

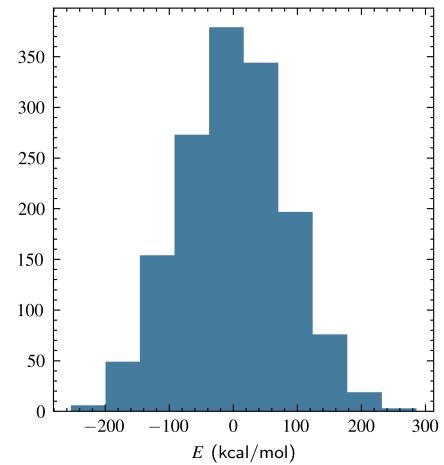


_home_boittier_pcbach_sims4_kmdcm_water_k225_dynamics.log
2: DYNA RESTRT CPT [200.0 ps]

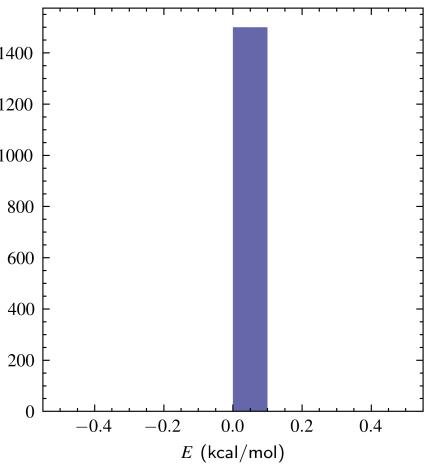
T [225 K]



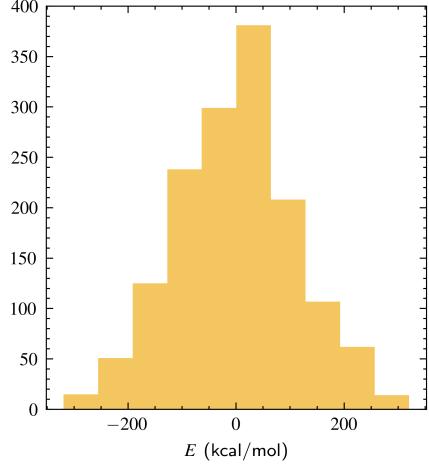
Total [-19786 kcal/mol]



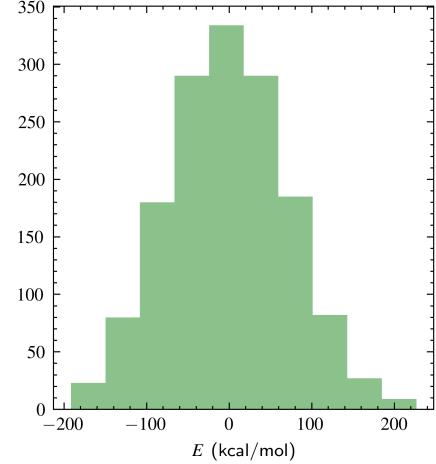
User [0 kcal/mol]



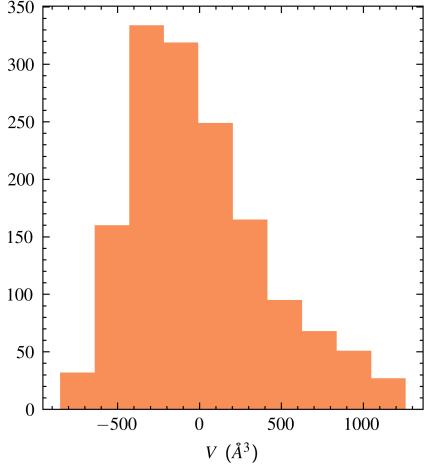
Elec [-24945 kcal/mol]



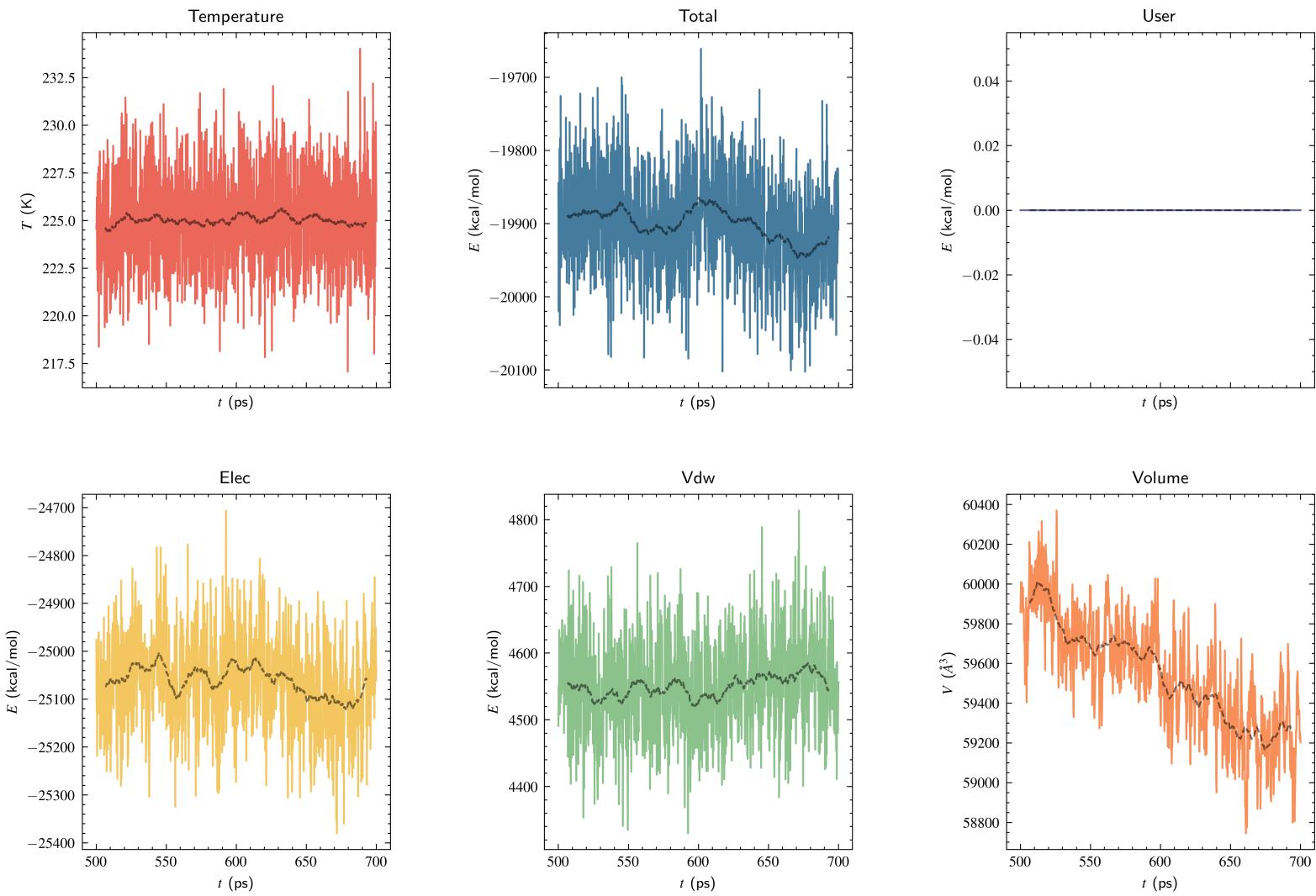
Vdw [4494 kcal/mol]



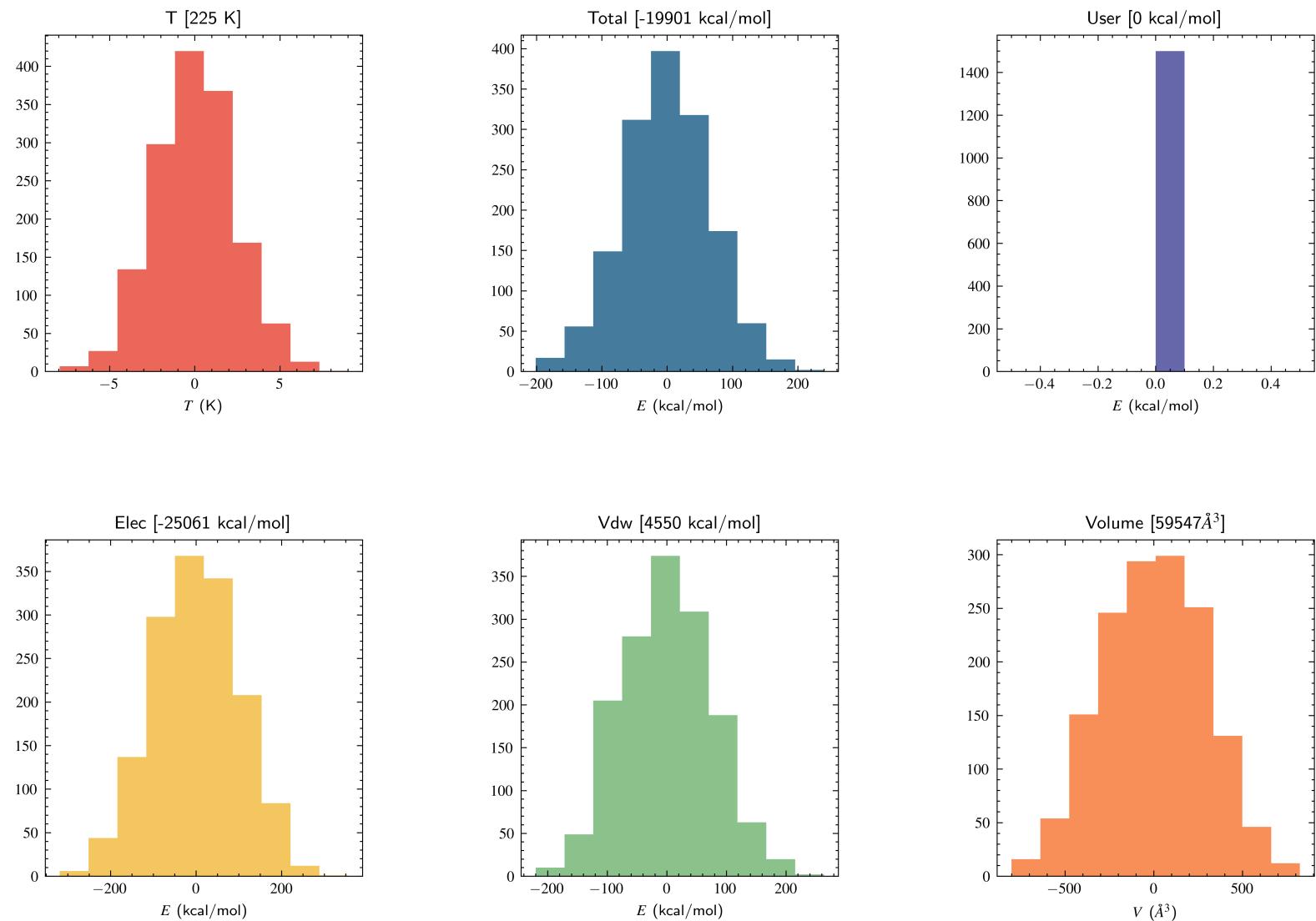
Volume [60071 Å³]



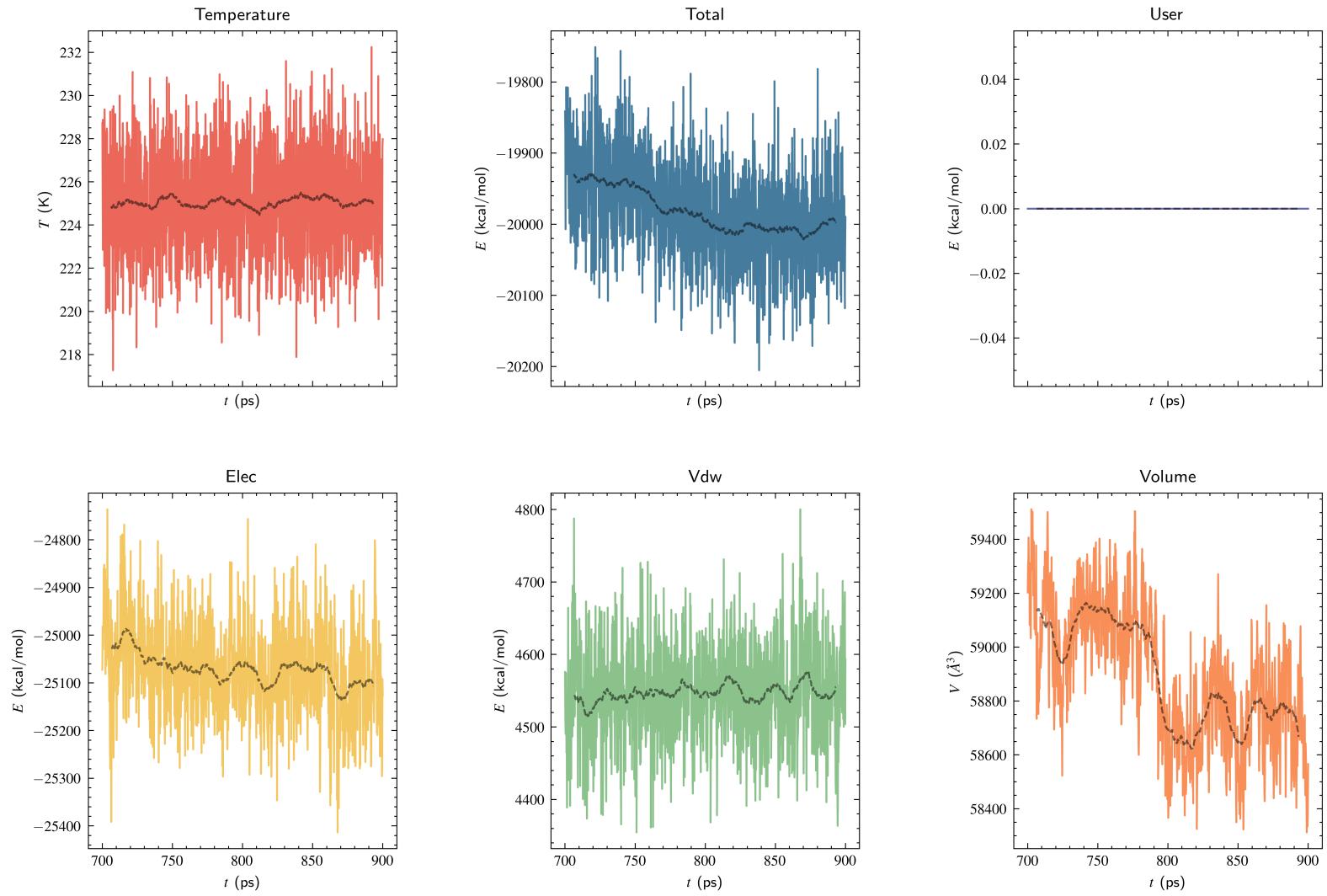
_home_boittier_pcbach_sims4_kmdcm_water_k225_dynamics.log
3: DYNA RESTRT CPT [200.0 ps]



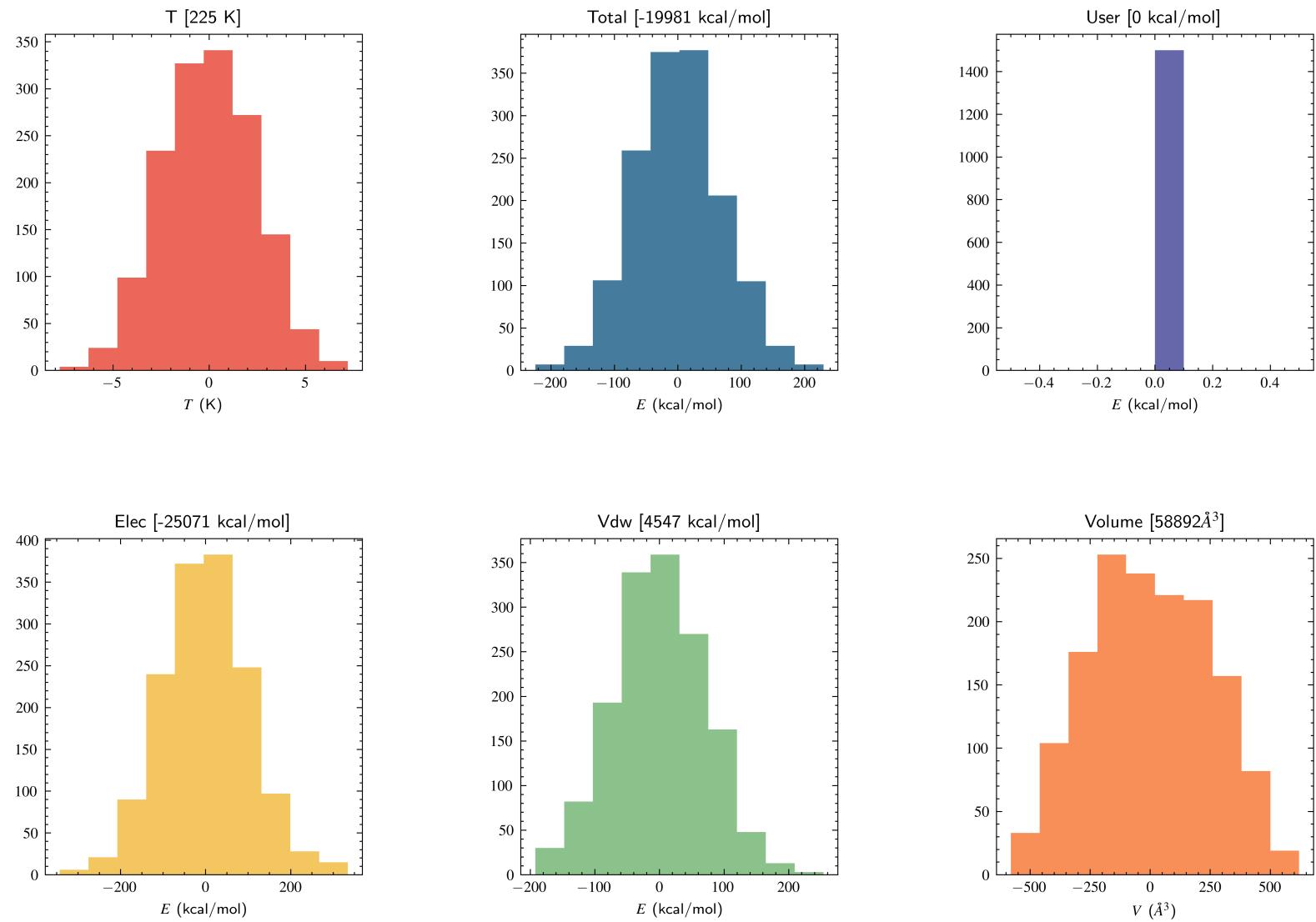
_home_boittier_pcbach_sims4_kmdcm_water_k225_dynamics.log
3: DYNA RESTRT CPT [200.0 ps]



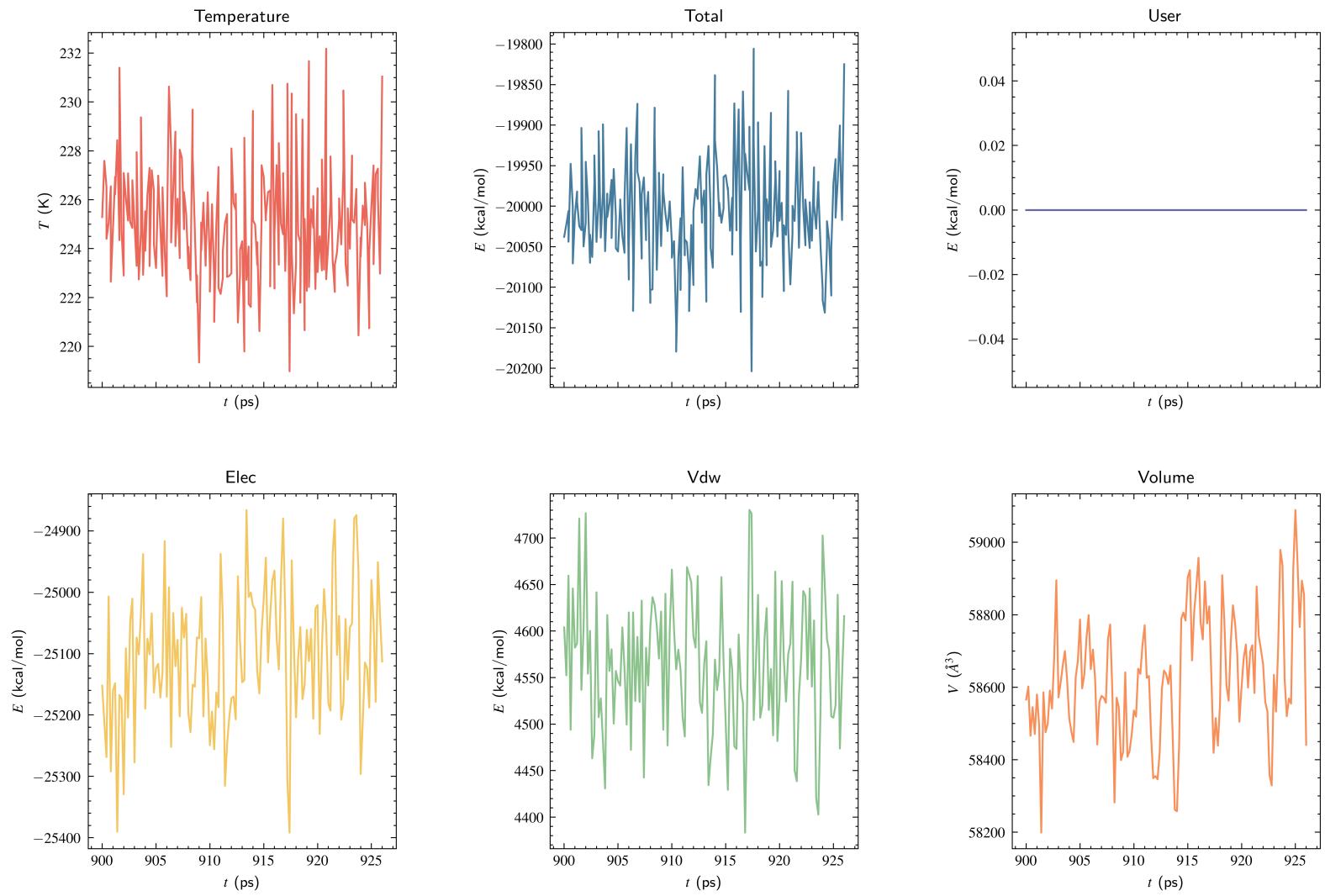
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4: DYNA RESTRT CPT [200.0 ps]



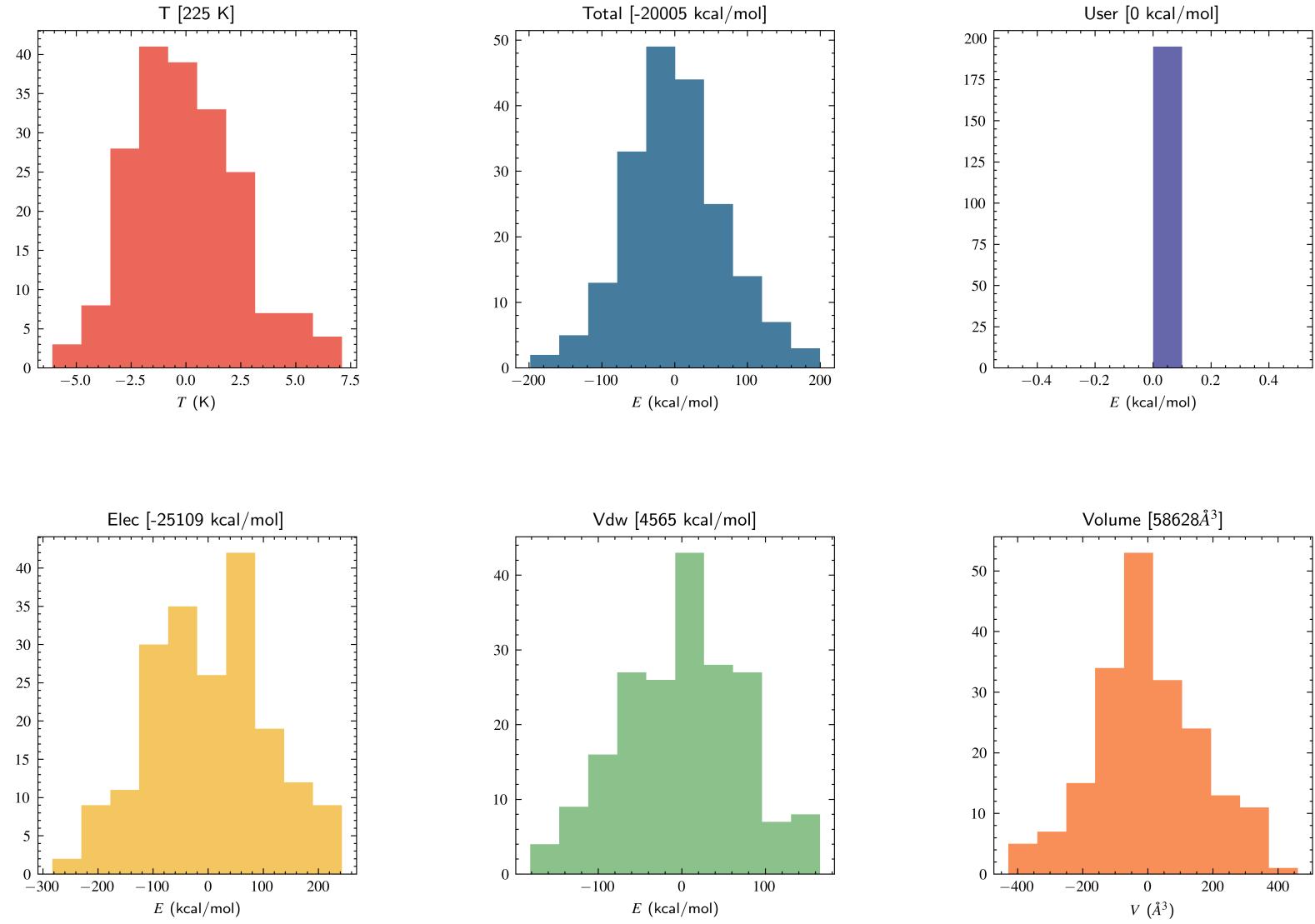
_home_boittier_pcbach_sims4_kmdcm_water_k225_dynamics.log
4: DYNA RESTRT CPT [200.0 ps]



_home_boittier_pc当地_sims4_kmdcm_water_k225_dynamics.log
5: DYNA RESTRT CPT [26.0 ps]



_home_boittier_pcbach_sims4_kmdcm_water_k225_dynamics.log
 5: DYNA RESTRT CPT [26.0 ps]



Trajectory info.

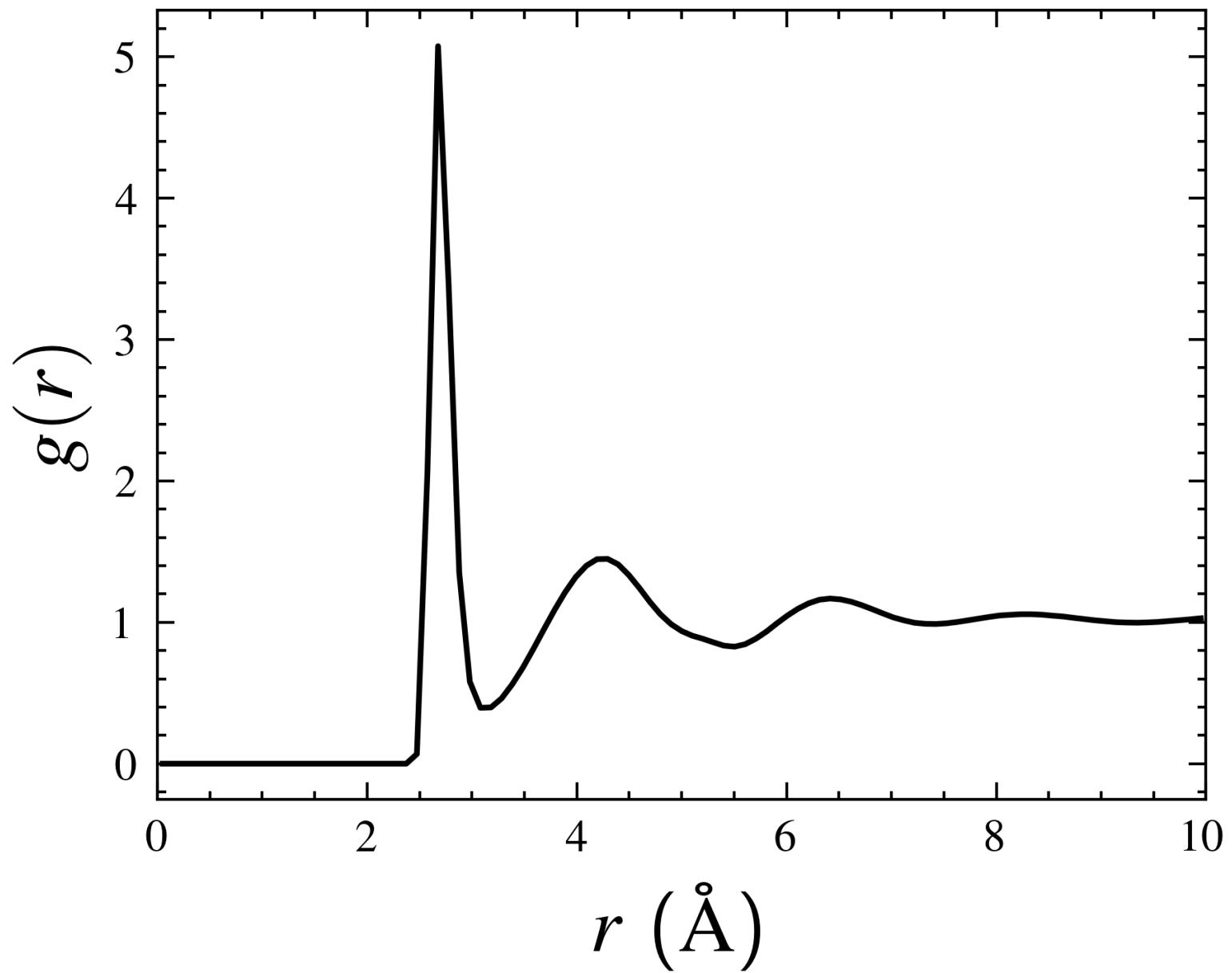
```
<Universe with 6000 atoms>
<ChainReader containing water.2000.dyna.0.dcd, water.2000.dyna.1.dcd with 2000 frames of 6000 atoms>
/home/boittier/miniconda3/envs/pycharmm/lib/python3.8/site-packages/MDAnalysis/coordinates/DCD.py:16
5: DeprecationWarning: DCDReader currently makes independent timesteps by copying self.ts while othe
r readers update self.ts inplace. This behavior will be changed in 3.0 to be the same as other reade
rs. Read more at https://github.com/MDAnalysis/mdanalysis/issues/3889 to learn if this change in beh
avior 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, resi
d 2000 and segid WAT>]>
[2.75626263 4.45242424 6.67863636 8.69282828] [5.0747333 1.44847011 1.16800797 1.05698898]
```

RDF



MSD and D

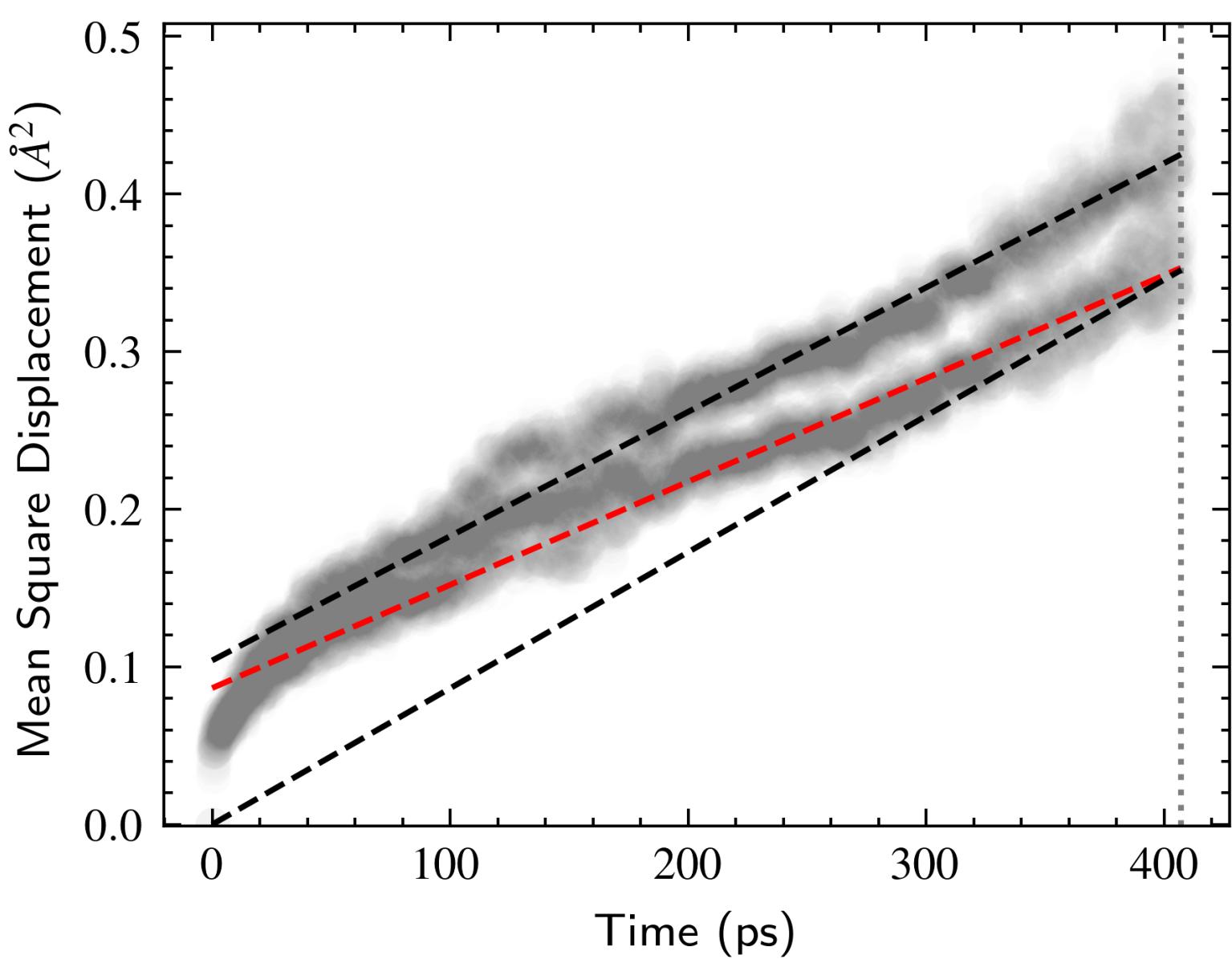
true ρ : 996

true D : -1.82e-07

0.0002

407.0166167328458

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

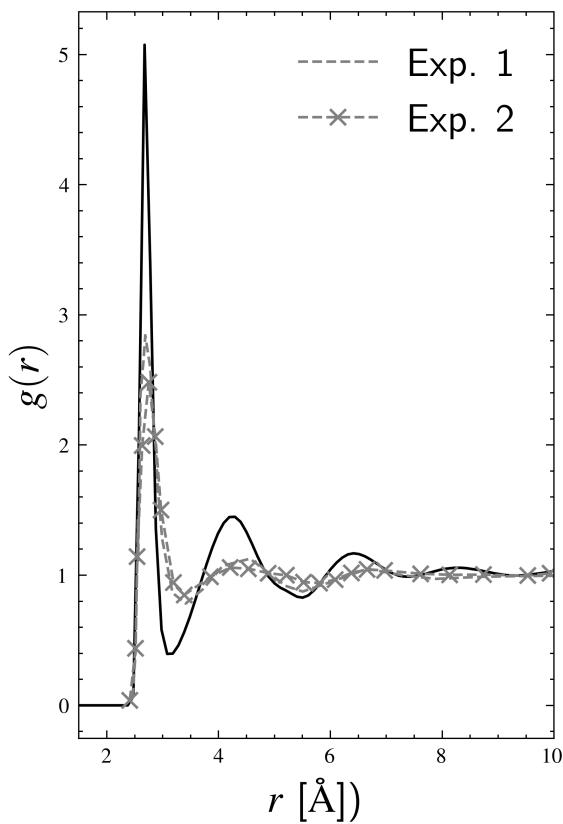


Structure and Transport

407.0166167328458

$$\rho = 998 \text{ [kg/m}^3\text{]} \text{ (error} = 0.2\%\text{)}$$

RDF



$$D = 0.0 [10^{-5} \text{ cm s}^{-1}] \text{ (error} = -144.1\%\text{)}$$

MSD

