

Simulation Report: sims4_kmdcm_water_k325

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

	vdw	elec	user	time	temp	tot	energy	volume	pressi
count	6781.000000	6781.000000	6781.0	6781.000000	6781.000000	6781.000000	6781.000000	6781.000000	6781.000000C
mean	2828.664630	-19846.784434	0.0	389.276508	321.388995	-14152.773274	19899.767147	58682.871258	-364.758022
std	150.851687	516.387943	0.0	275.265674	22.782964	837.657596	484.688536	6662.517117	1174.689874
min	2500.540900	-25088.512700	0.0	0.000000	60.939760	-22701.784290	19184.112920	53236.000000	-4673.544210
25%	2751.551130	-19881.610780	0.0	84.800000	322.141180	-14262.757880	19473.195450	54212.000000	-1140.743100
50%	2813.169820	-19774.718150	0.0	405.400000	324.613710	-14154.904630	19975.068560	54493.000000	-382.987180
75%	2871.745160	-19676.037550	0.0	631.400000	326.871210	-13602.424290	20068.399010	68921.000000	415.308800
max	4072.983730	-19253.468680	0.0	857.400000	336.576380	-13594.505710	24925.828760	68921.000000	3873.776910

Simulation runs

		0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT
vdw	count	2000.000000	600.000000	1500.000000	1500.000000	1181.000000
	mean	2846.734507	2824.206117	2829.542754	2812.622580	2819.588629
	std	244.618981	81.101452	84.526179	82.776622	85.370115
	min	2500.540900	2606.278640	2552.311860	2535.755250	2580.242030
	25%	2730.430975	2772.618600	2772.839207	2755.386920	2758.121060
	50%	2785.543340	2829.075540	2831.371695	2813.845745	2821.728820
	75%	2853.363680	2873.296245	2885.895462	2866.247620	2878.623240
	max	4072.983730	3064.395710	3087.228260	3072.213520	3100.553210
	elec	2000.000000	600.000000	1500.000000	1500.000000	1181.000000
elec	count	-20037.538482	-19774.032155	-19778.066006	-19759.204792	-19759.223363
	mean	892.028339	163.226544	155.108069	148.184851	156.133138
	std	-25088.512700	-20231.262550	-20304.317080	-20205.134220	-20271.961960
	25%	-19899.920200	-19878.148950	-19886.015655	-19860.803810	-19865.494670
	50%	-19793.840510	-19773.337555	-19777.534075	-19762.505385	-19758.376820
	75%	-19702.384450	-19669.070320	-19674.198120	-19658.097030	-19653.790460
	max	-19384.290650	-19334.305390	-19301.765230	-19253.468680	-19305.377530
	volume	2000.000000	600.000000	1500.000000	1500.000000	1181.000000
	mean	68921.000000	55049.860000	54316.574000	54295.351333	54308.845047
	std	0.000000	2217.555664	272.548246	308.046525	336.934685

dyna	0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT
min	68921.000000	53370.000000	53539.000000	53283.000000	53236.000000
25%	68921.000000	54156.500000	54140.000000	54095.000000	54100.000000
50%	68921.000000	54371.500000	54314.000000	54315.000000	54341.000000
75%	68921.000000	54696.250000	54492.250000	54521.000000	54540.000000
max	68921.000000	68921.000000	54998.000000	55229.000000	55089.000000
temp	count	2000.000000	600.000000	1500.000000	1500.000000
	mean	312.621960	324.761095	325.069852	325.061182
	std	40.295606	3.337162	3.509111	3.331470
	min	60.939760	314.272090	313.769610	311.533690
	25%	320.537020	322.587730	322.716835	322.909832
	50%	323.393020	324.976675	324.990320	325.065330
	75%	325.512620	327.218370	327.487467	327.314785
	max	335.085140	333.329040	336.576380	334.976480

Densities

density 1: 867.0796999463153 kilogram / meter ** 3

density 2: 1085.5613438435628 kilogram / meter ** 3

density 3: 1100.2166668317482 kilogram / meter ** 3

density 4: 1100.6467134380946 kilogram / meter ** 3

density 5: 1100.373243967071 kilogram / meter ** 3

temp. 1: 312.62195987999996

temp. 2: 324.7610946666667

temp. 3: 325.06985202

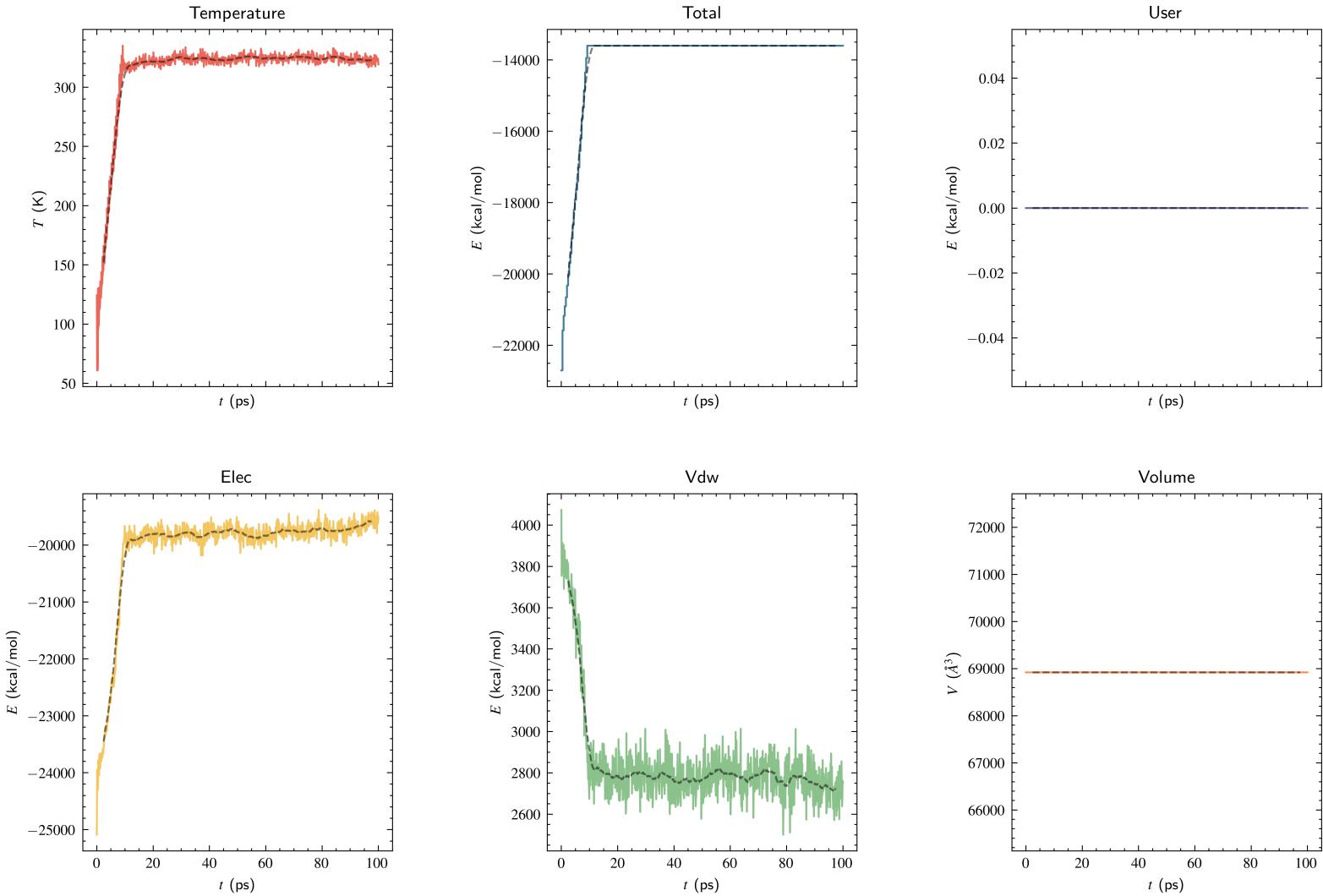
temp. 4: 325.06118238666664

temp. 5: 325.1834432514818

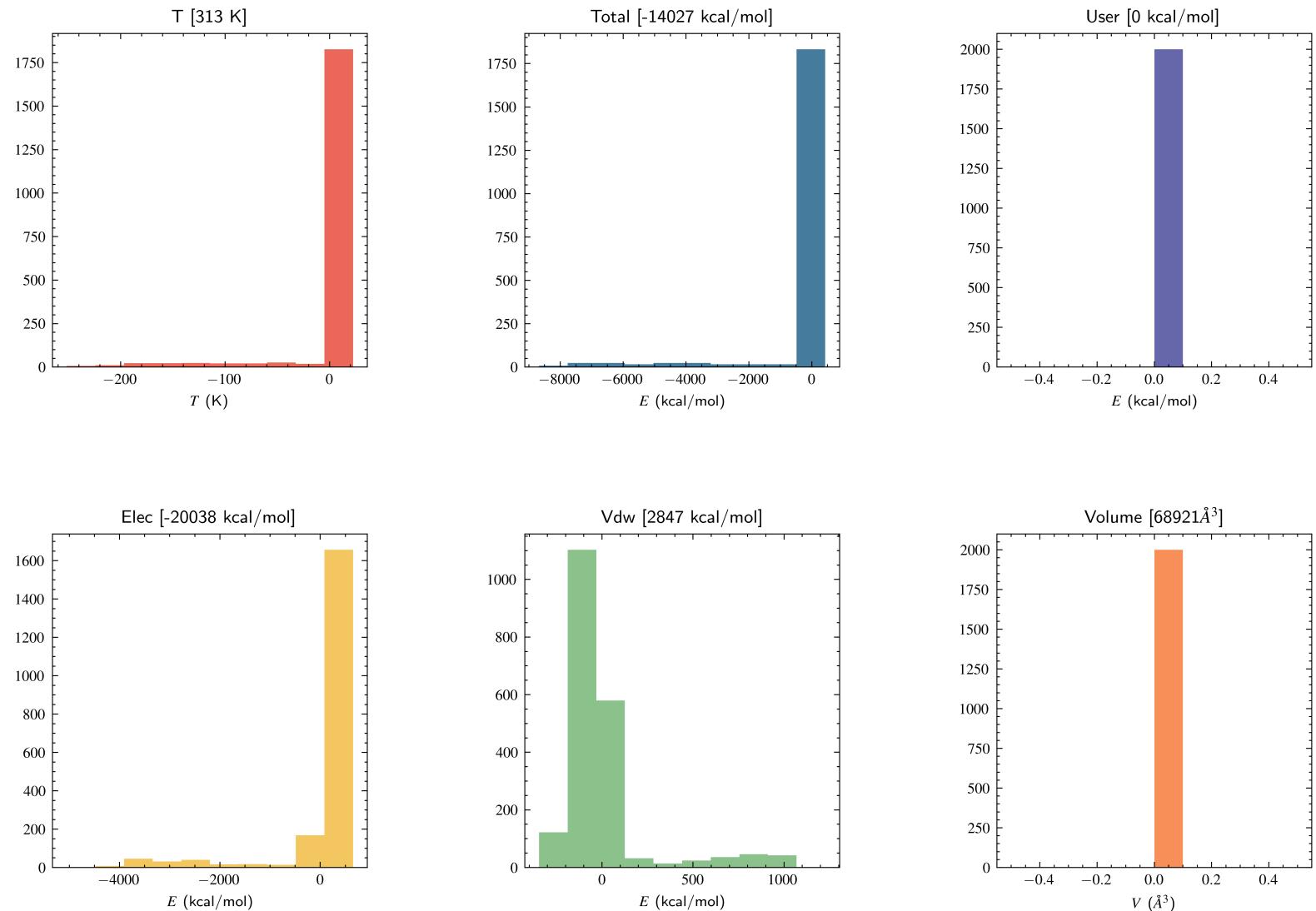
plotting

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

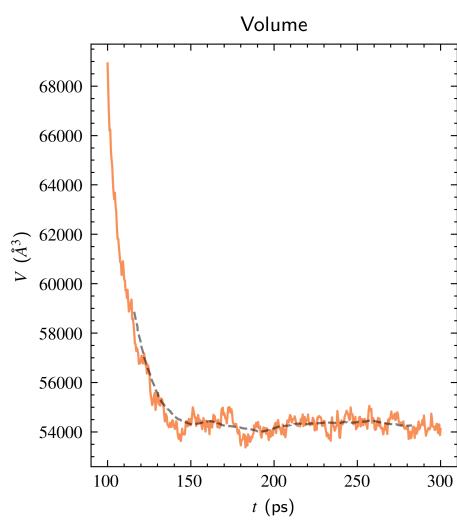
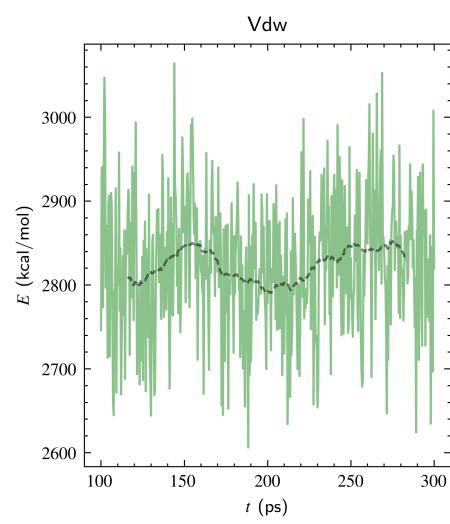
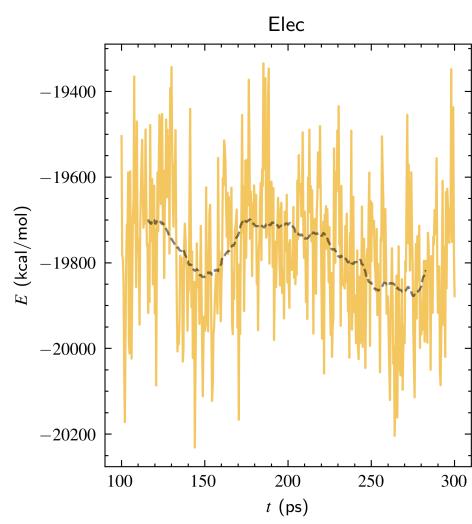
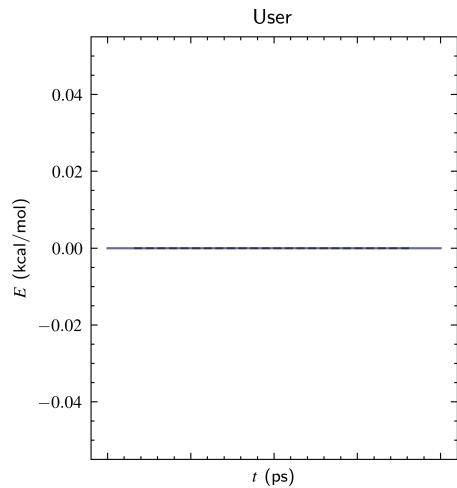
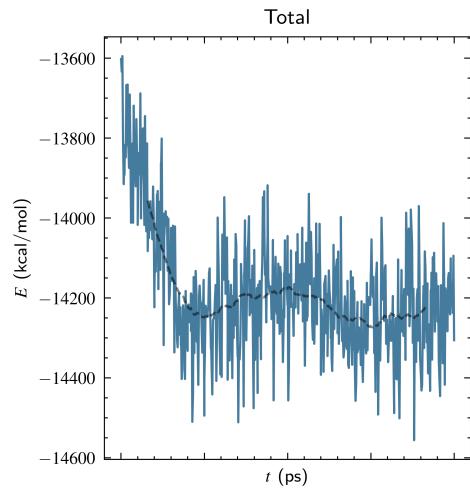
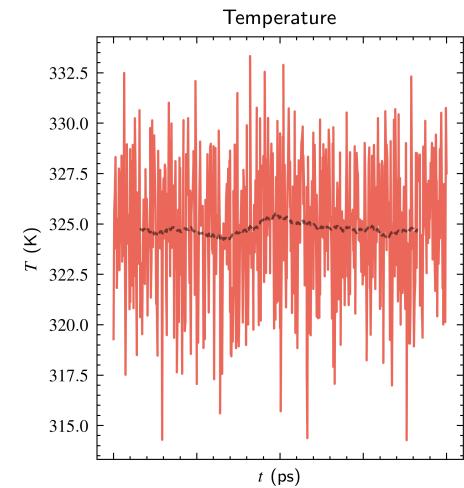
_home_boittier_pc当地_sims4_kmdcm_water_k325_dynamics.log
0: DYNA STRT VERL [100.0 ps]



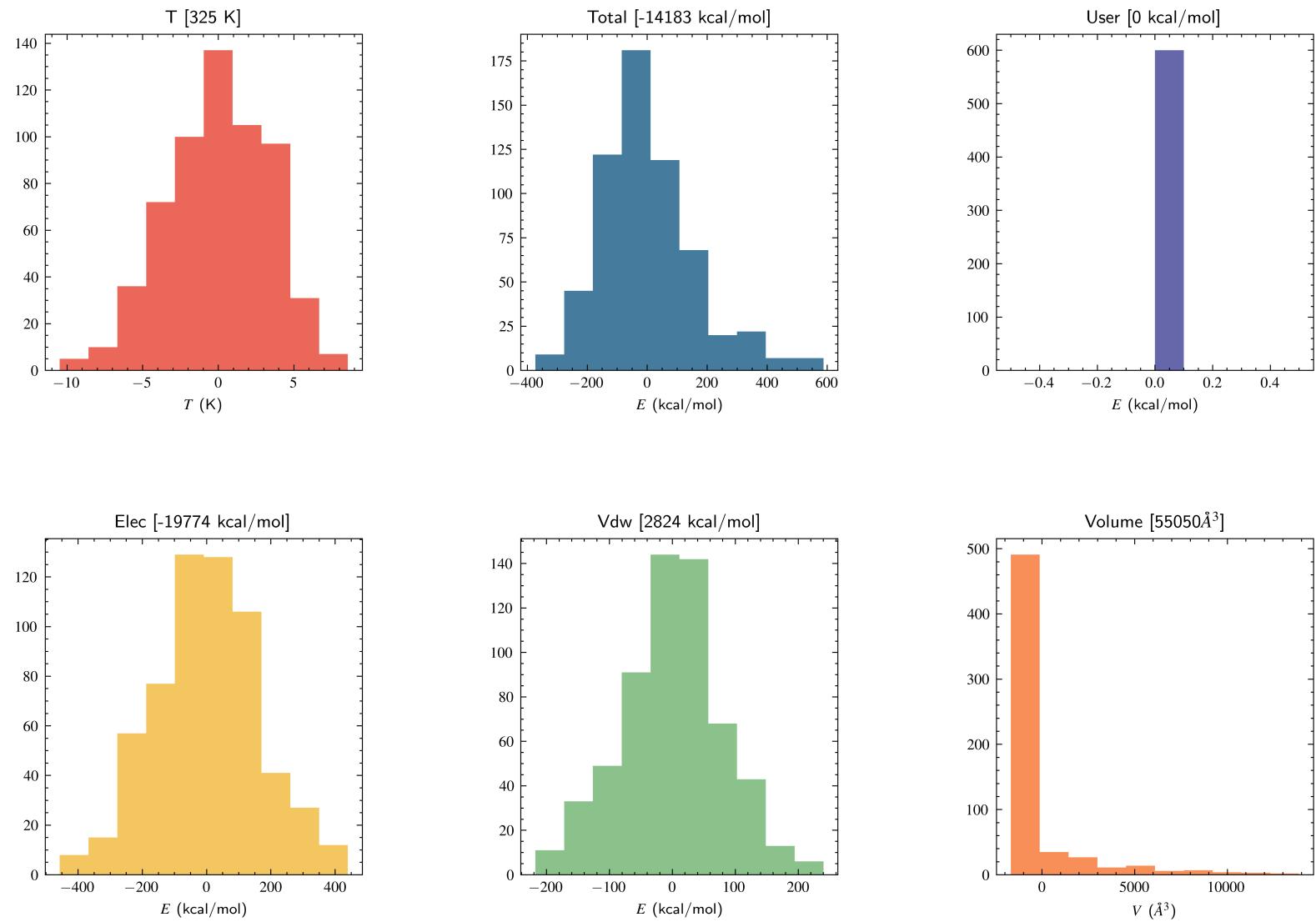
_home_boittier_pcbach_sims4_kmdcm_water_k325_dynamics.log
0: DYNA STRT VERL [100.0 ps]



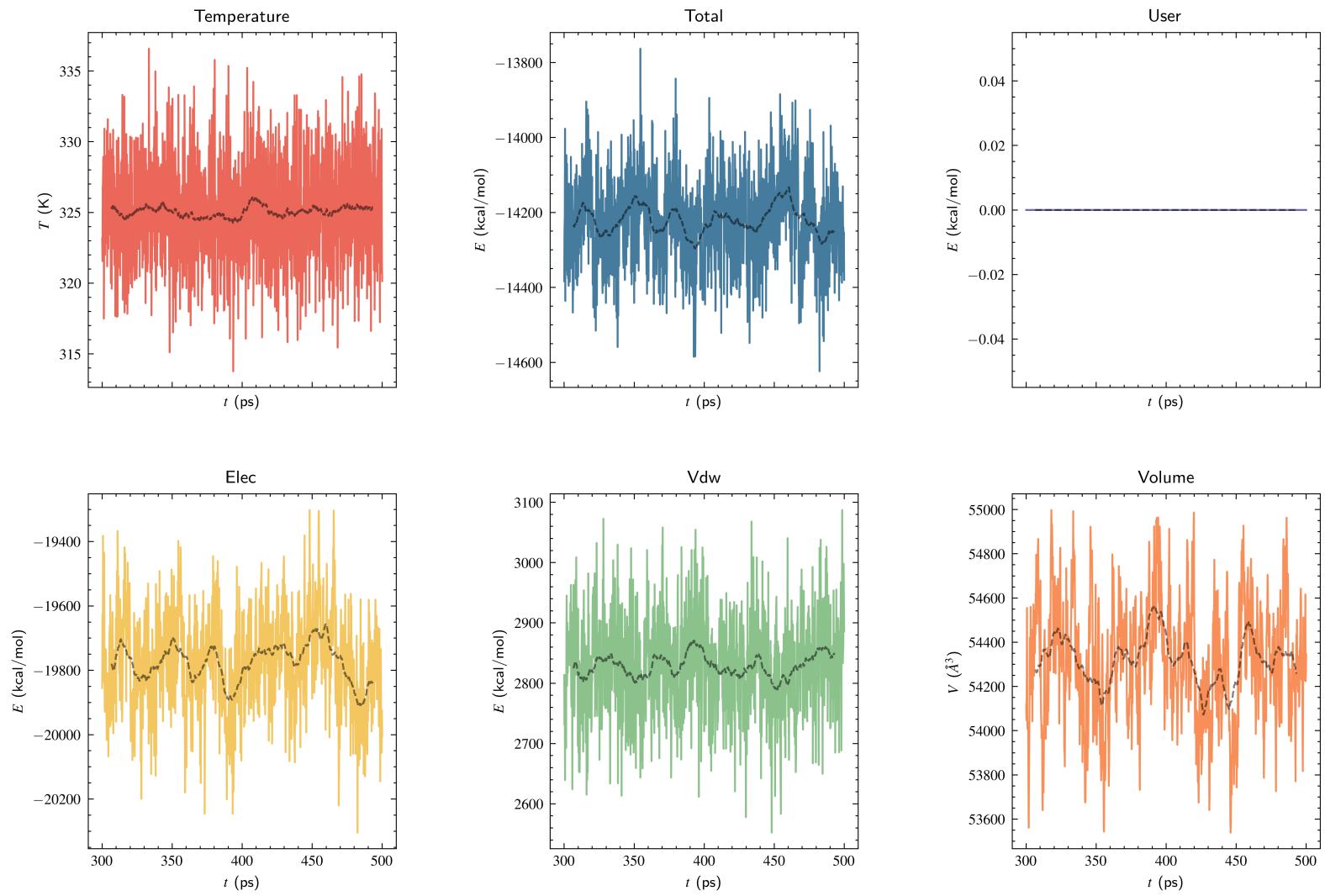
_home_boittier_pcbach_sims4_kmdcm_water_k325_dynamics.log
1: DYNA RESTRT CPT [200.0 ps]



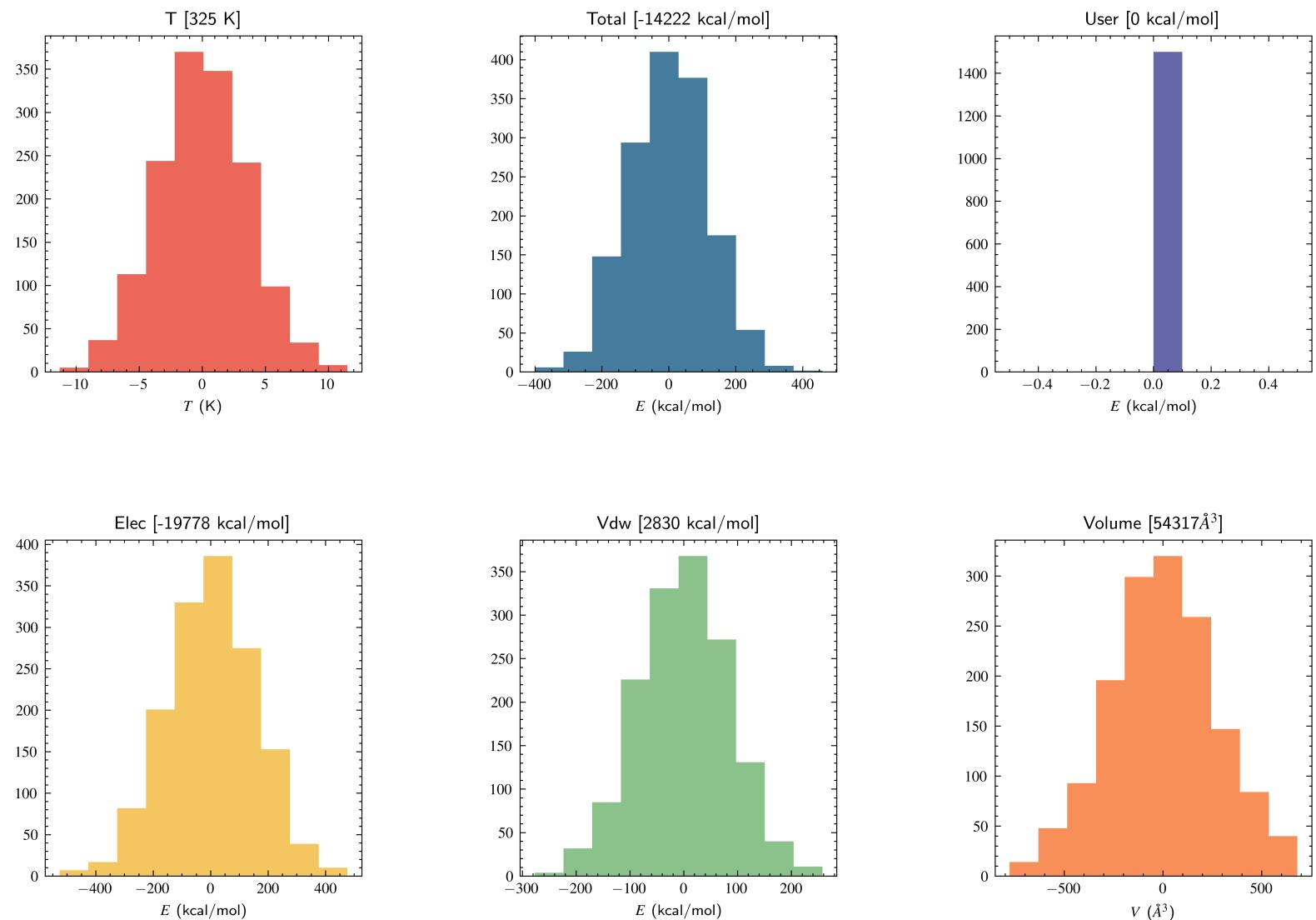
_home_boittier_pcbach_sims4_kmdcm_water_k325_dynamics.log
1: DYNA RESTRT CPT [200.0 ps]



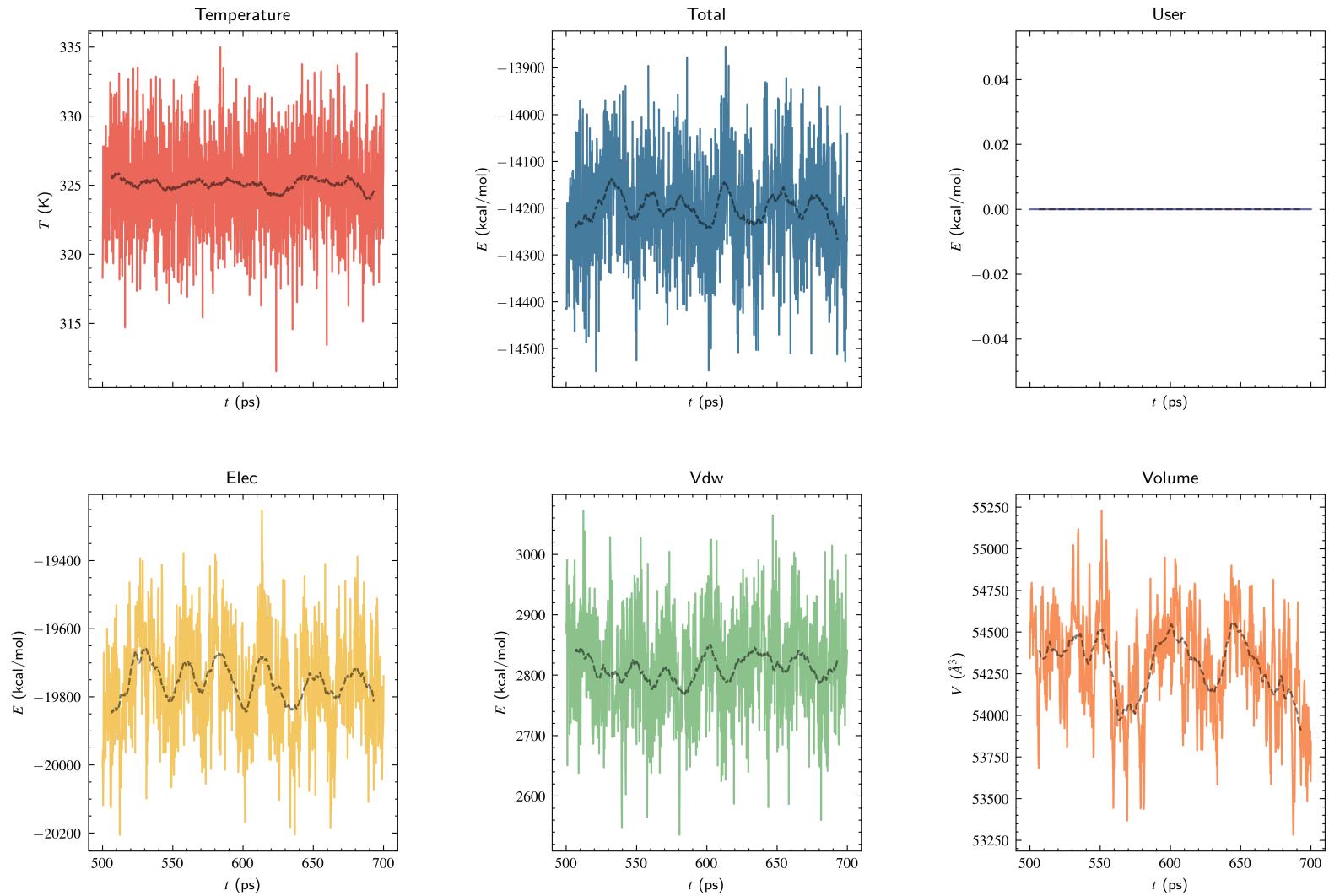
_home_boittier_pcbach_sims4_kmdcm_water_k325_dynamics.log
2: DYNA RESTRT CPT [200.0 ps]



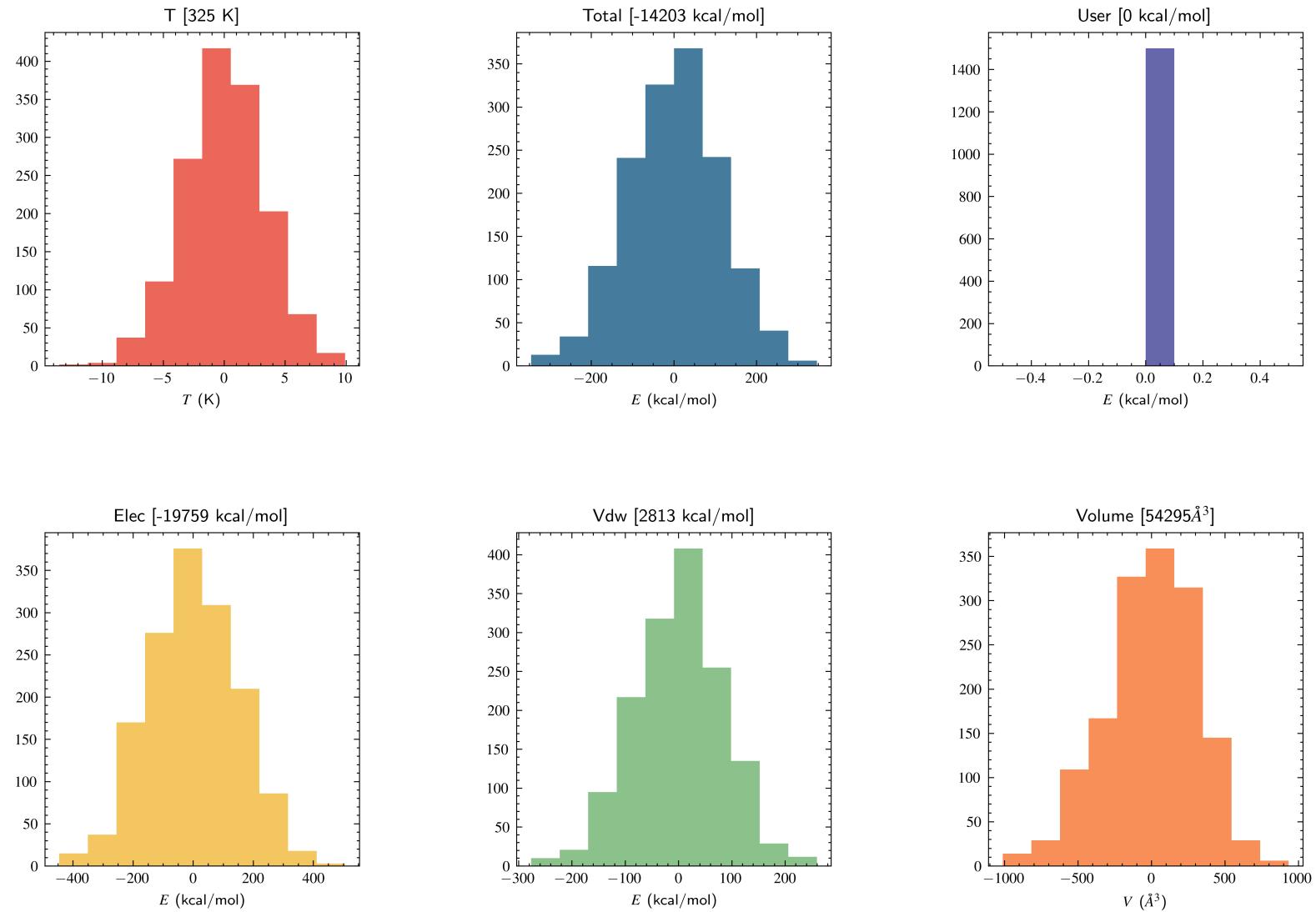
_home_boittier_pcbach_sims4_kmdcm_water_k325_dynamics.log
2: DYNA RESTRT CPT [200.0 ps]



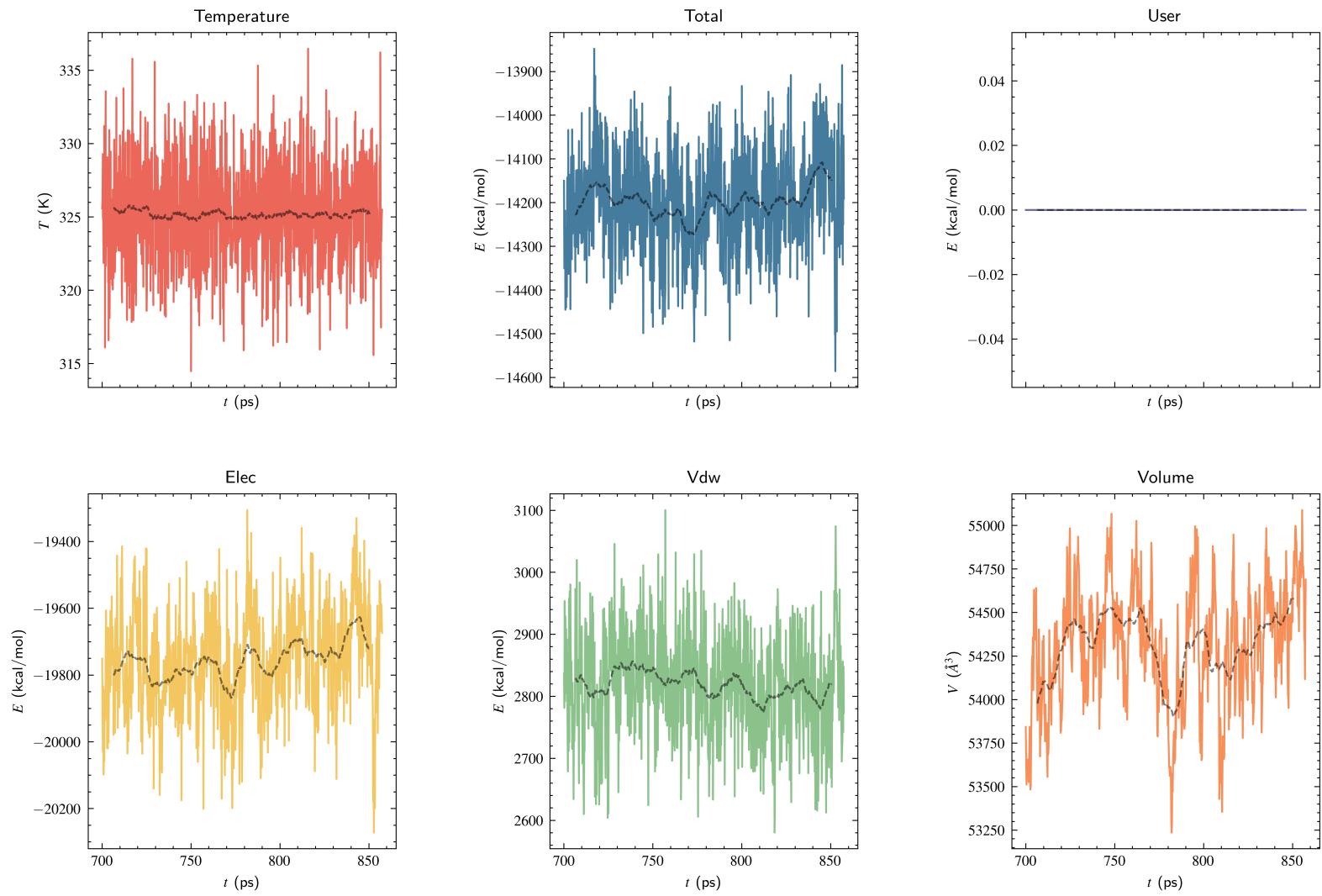
_home_boittier_pcbach_sims4_kmdcm_water_k325_dynamics.log
3: DYNA RESTRT CPT [200.0 ps]



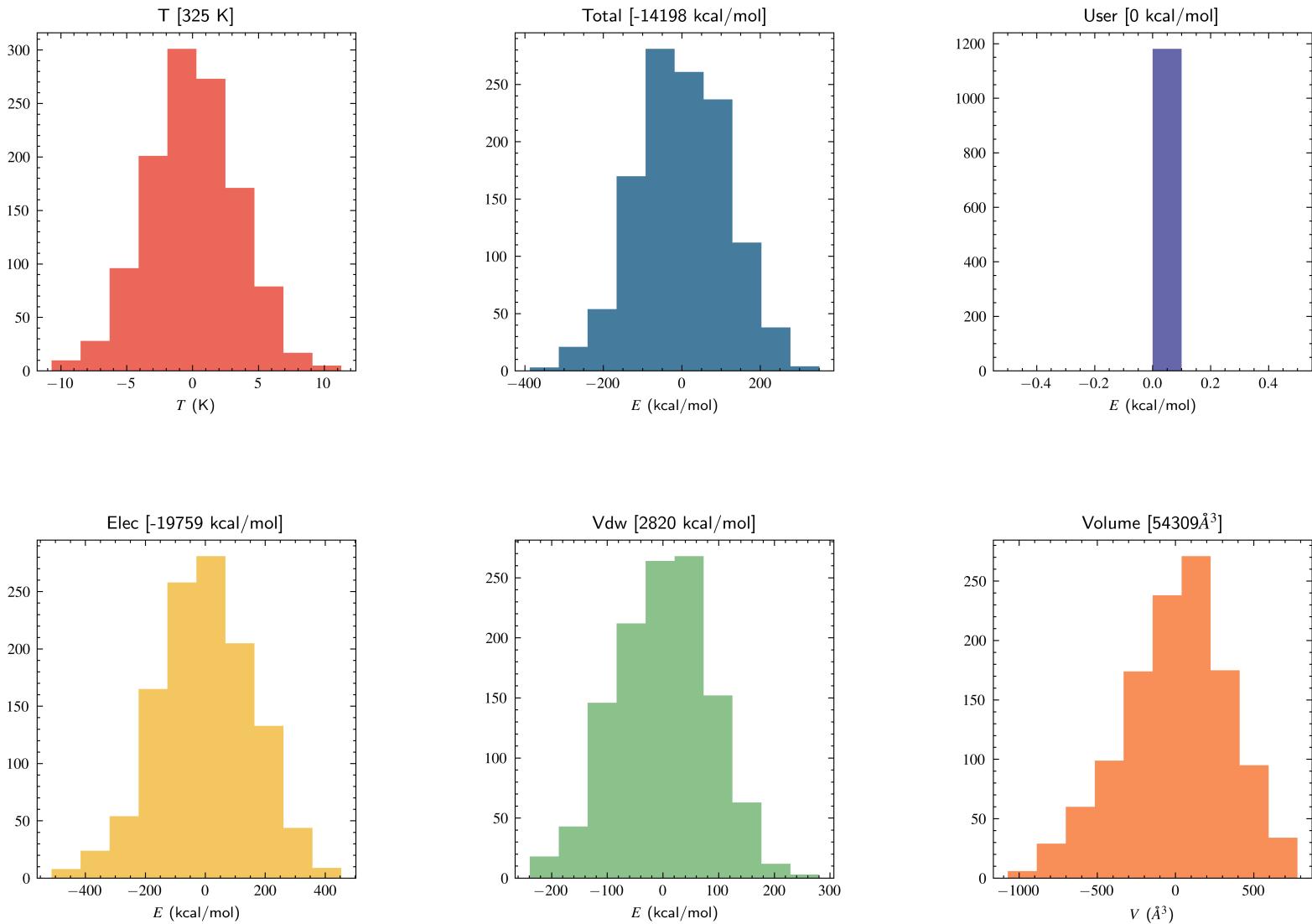
_home_boittier_pcbach_sims4_kmdcm_water_k325_dynamics.log
3: DYNA RESTRT CPT [200.0 ps]



_home_boittier_pc当地_sims4_kmdcm_water_k325_dynamics.log
4: DYNA RESTRT CPT [157.0 ps]



_home_boittier_pcbach_sims4_kmdcm_water_k325_dynamics.log
 4: DYNA RESTRT CPT [157.0 ps]



Trajectory info.

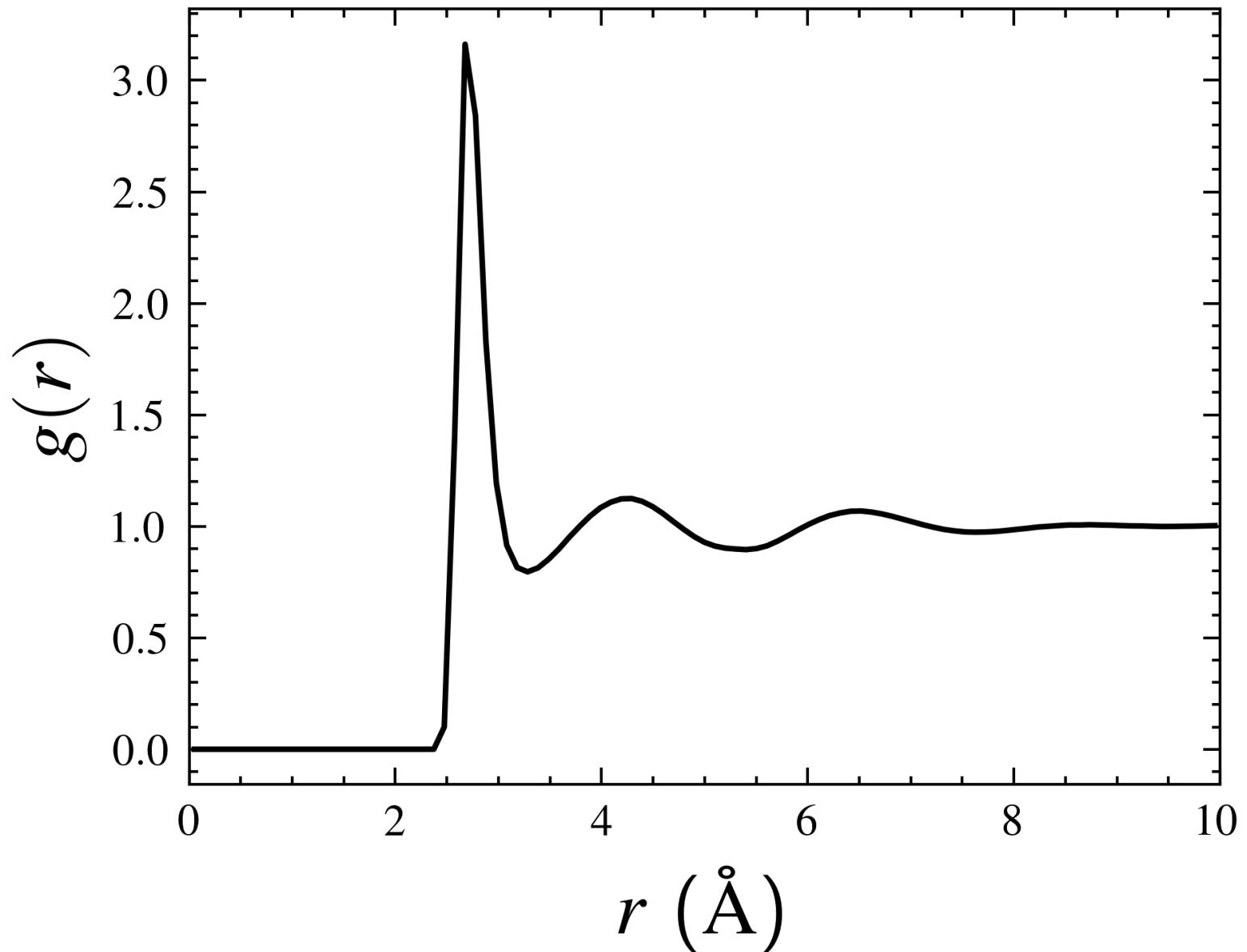
```
<Universe with 6000 atoms>
<ChainReader containing water.2000.dyna.0.dcd, water.2000.dyna.1.dcd with 2000 frames of 6000 atoms>
/home/boittier/miniconda3/envs/pycharmm/lib/python3.8/site-packages/MDAnalysis/coordinates/DCD.py:16
5: DeprecationWarning: DCDReader currently makes independent timesteps 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 6.78464646 8.90484848 9.11686869] [3.16184813 1.12439877 1.06854779 1.0057317
5 1.0069232 ]
```

RDF



MSD and D

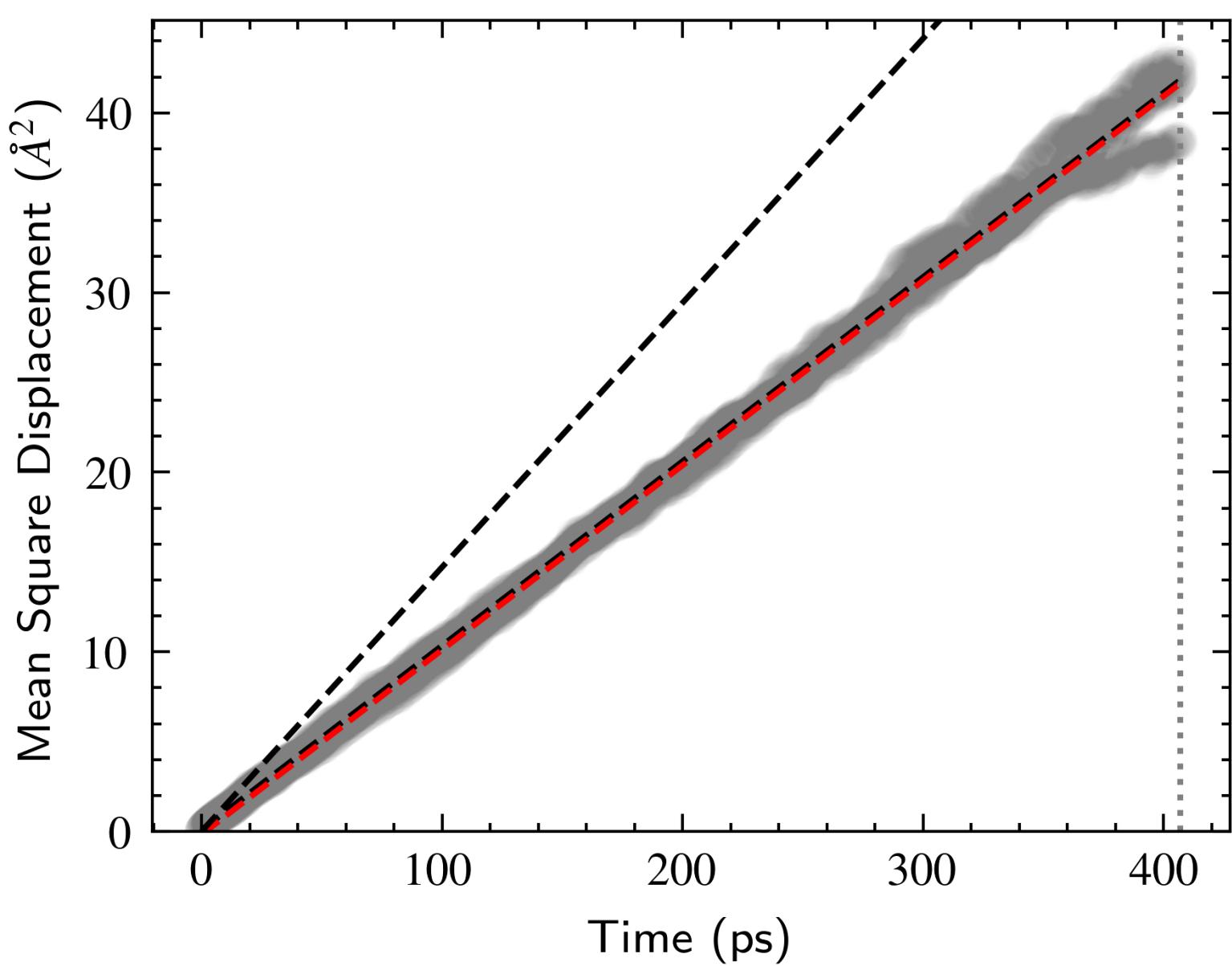
true ρ : 987

true D : 4.12e-05

0.0002

407.0166167328458

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

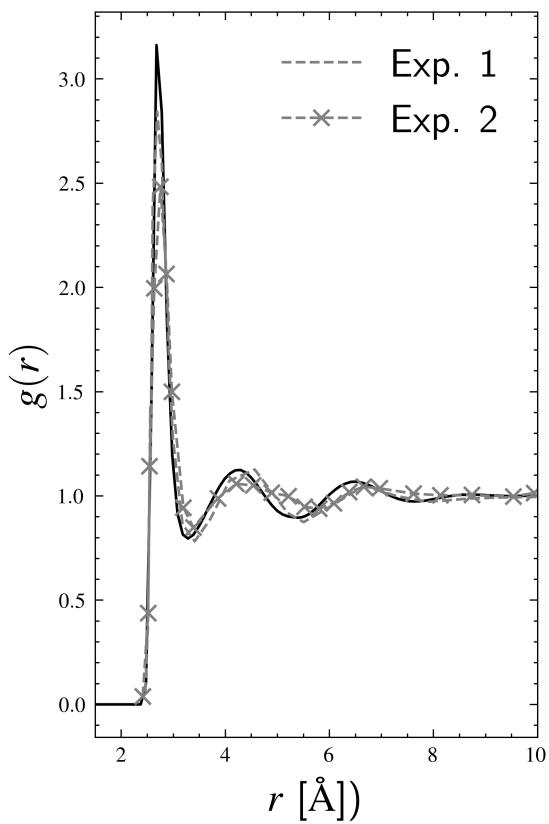


Structure and Transport

407.0166167328458

$\rho = 1097 \text{ [kg/m}^3\text{]} \text{ (error} = 11.1\%\text{)}$

RDF



$D = 1.0 \text{ [10}^{-5} \text{ cm s}^{-1}\text{]} \text{ (error} = -74.6\%\text{)}$

MSD

