Simulation Report: sims4_kmdcm_water_k350

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

	vdw	elec	user	time	temp	tot	energy	volume	pressi
count	6958.000000	6958.000000	6958.0	6958.000000	6958.000000	6958.000000	6958.000000	6958.000000	6958.000000
mean	2489.205261	-18703.224838	0.0	401.486663	344.150620	-12690.515285	18844.526585	59105.706956	-293.854333
std	199.082111	708.588719	0.0	282.058661	25.875253	995.541903	556.462333	6278.449999	1132.949354
min	2121.180810	-25088.512700	0.0	0.000000	60.855870	-22697.105620	18232.947790	53984.000000	-4790.353320
25%	2402.508295	-18786.302520	0.0	87.000000	343.925198	-12637.552532	18624.394735	54943.000000	-1080.331283
50%	2463.936100	-18570.919540	0.0	417.200000	348.095595	-12525.137045	18790.842180	55239.000000	-304.084745
75%	2524.502092	-18416.238240	0.0	649.150000	351.384667	-12438.992260	18886.982980	68921.000000	457.954870
max	4072.983730	-17909.935700	0.0	881.000000	363.652640	-11844.100190	24925.828760	68921.000000	3882.564850

Simulation runs

	dyna	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	1358.000000
	mean	2609.227726	2444.582507	2435.154977	2438.666326	2447.682840
	std	316.103879	84.830766	84.354171	83.150243	86.216530
	min	2304.599680	2232.723650	2159.839980	2121.180810	2168.296260
	25%	2465.365183	2386.436958	2375.266330	2385.458375	2388.951850
	50%	2519.831020	2442.906655	2436.797750	2440.628870	2450.276535
	75%	2587.250530	2506.891053	2491.668385	2491.223030	2504.249350
	max	4072.983730	2733.906470	2776.924320	2693.636310	2689.082940
elec	**count**	2000.000000	600.000000	1500.000000	1500.000000	1358.000000
	mean	-19248.819606	-18501.277757	-18452.968051	-18491.712335	-18498.977895
	std	1124.630222	169.503578	157.422261	155.059520	164.806341
	min	-25088.512700	-18980.039040	-18903.246980	-18945.635930	-19009.495480
	25%	-19039.084790	-18621.555853	-18559.635540	-18601.043140	-18611.831190
	50%	-18909.098010	-18503.871630	-18455.375420	-18494.269095	-18497.104710
	75%	-18806.948100	-18381.976115	-18346.495345	-18384.523120	-18382.111595
	max	-18531.748660	-18081.534330	-17909.935700	-17930.211920	-18066.782610
volume	**count**	2000.000000	600.000000	1500.000000	1500.000000	1358.000000
	mean	68921.000000	55889.676667	55048.193333	54958.400000	55133.882916
	std	0.000000	2247.366391	318.803833	299.607611	298.950013

	dyna	0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT
	min	68921.000000	54231.000000	54212.000000	53984.000000	54195.000000
	25%	68921.000000	54971.000000	54819.000000	54763.000000	54935.250000
	50%	68921.000000	55217.000000	55052.000000	54983.500000	55118.000000
	75%	68921.000000	55515.500000	55267.750000	55186.000000	55338.000000
	max	68921.000000	68921.000000	56218.000000	55695.000000	56038.000000
temp	**count**	2000.000000	600.000000	1500.000000	1500.000000	1358.000000
	mean	329.710920	349.881240	349.889160	350.130712	349.940812
	std	44.754296	3.697410	3.732945	3.783769	3.662321
	min	60.855870	336.808930	338.345780	338.119000	339.080360
	25%	339.580128	347.531137	347.368088	347.530240	347.495905
	50%	341.976945	349.839910	349.866105	350.190335	349.940150
	75%	343.972900	352.354632	352.364753	352.755190	352.344640
	max	358.361060	360.060390	363.652640	361.290520	362.596710

Densities

density 1: 867.0796999463153 kilogram / meter ** 3

density 2: 1069.2493419923762 kilogram / meter ** 3

density 3: 1085.5942108424022 kilogram / meter ** 3

density 4: 1087.3679000844272 kilogram / meter ** 3

density 5: 1083.906970437593 kilogram / meter ** 3

temp. 1: 329.71092049500004

temp. 2: 349.88123971666664

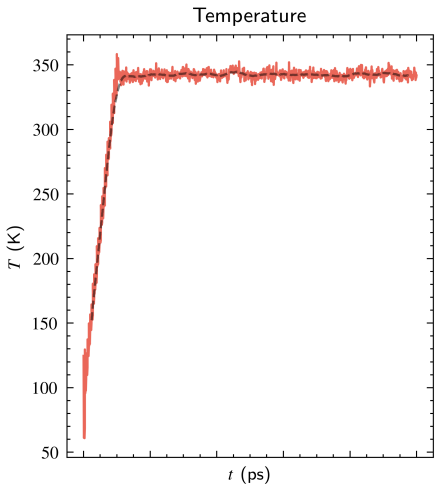
temp. 3: 349.88916012

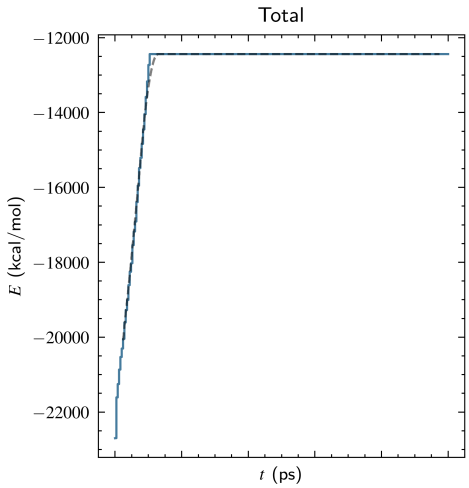
temp. 4: 350.1307124400001

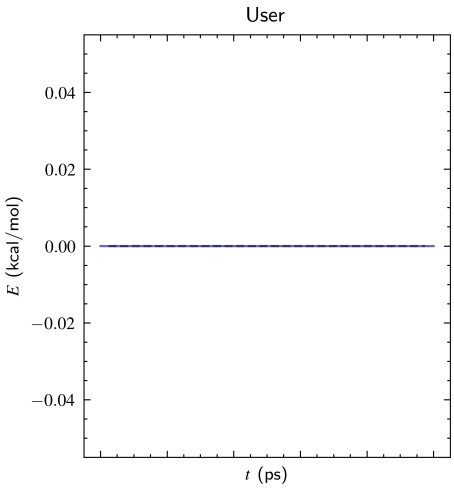
temp. 5: 349.9408122974963

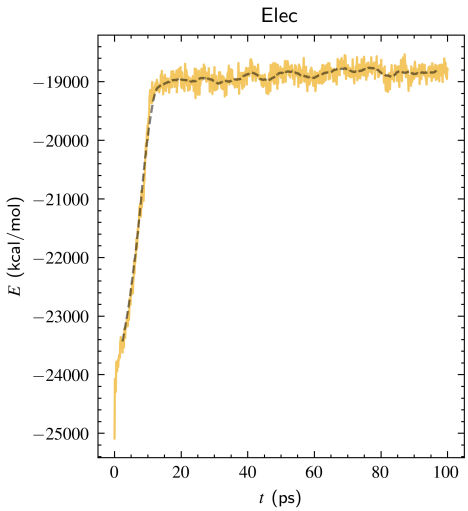
```
plotting
['3: DYNA RESTRT CPT', '2: DYNA RESTRT CPT', '4: DYNA RESTRT CPT', '0: DYNA STRT VERL', '1: DYNA RES
TRT CPT']
```

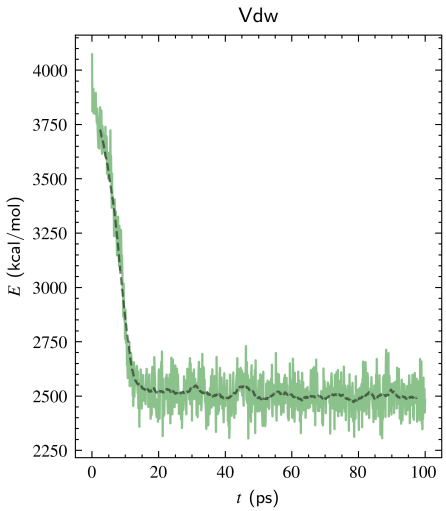
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
0: DYNA STRT VERL [100.0 ps]

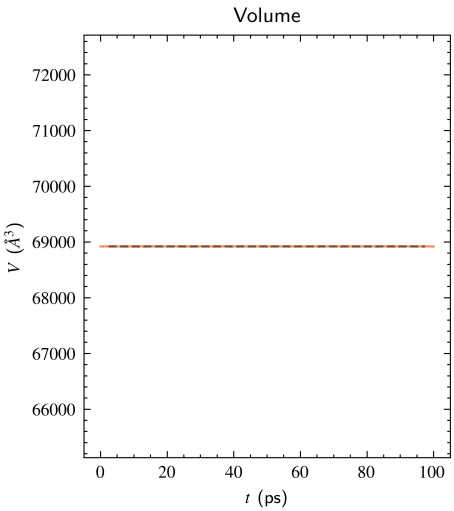




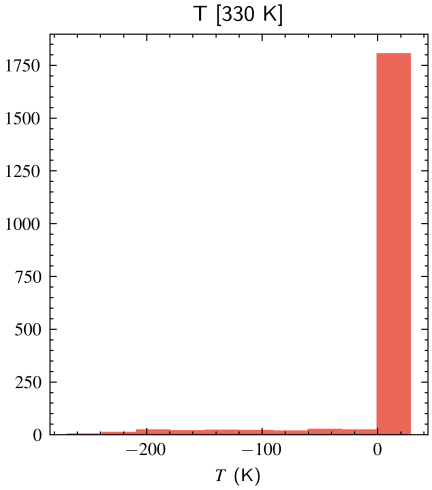


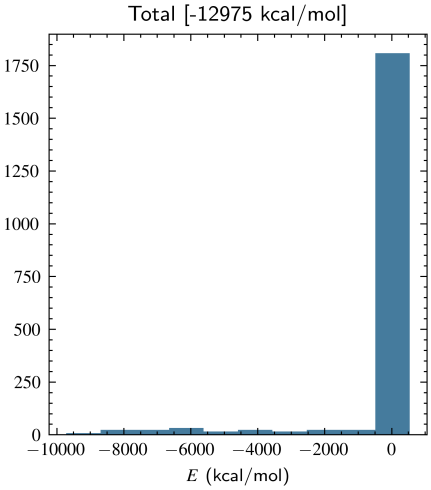


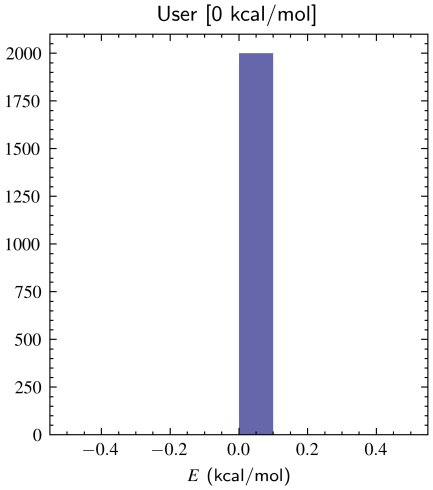


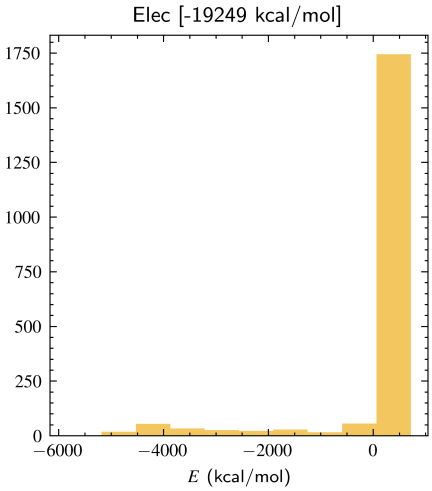


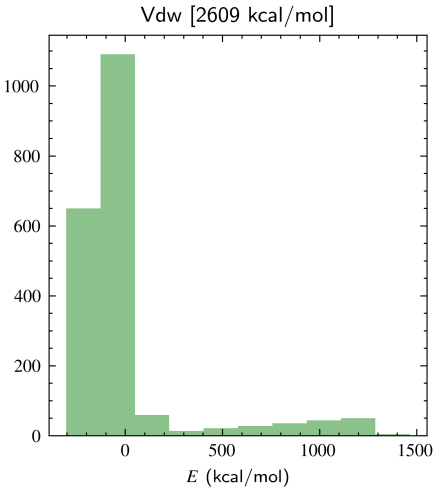
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
0: DYNA STRT VERL [100.0 ps]

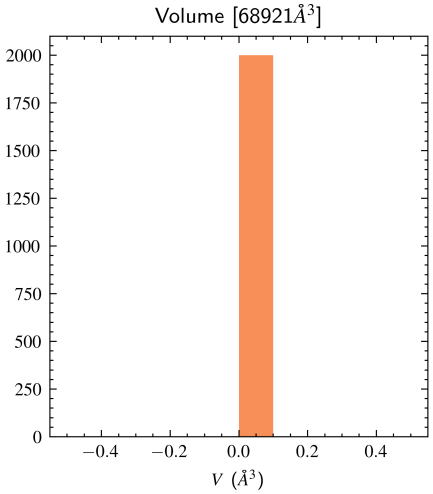




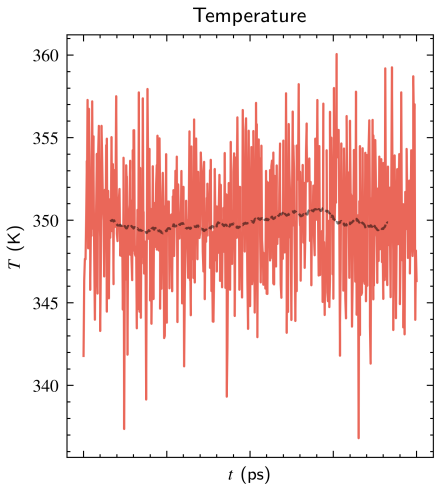


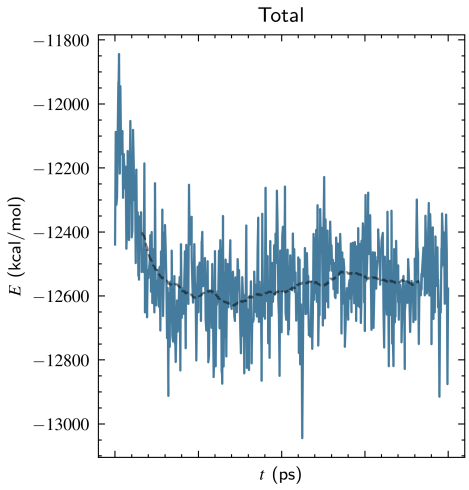


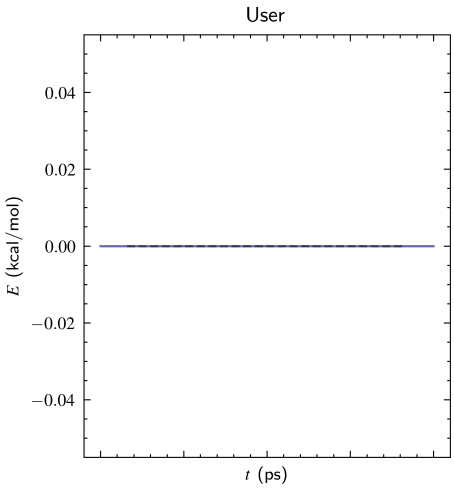


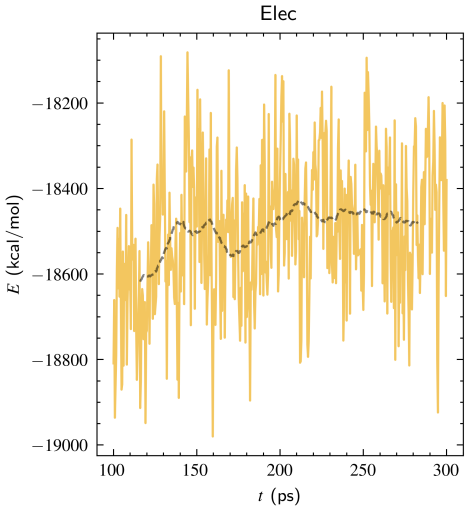


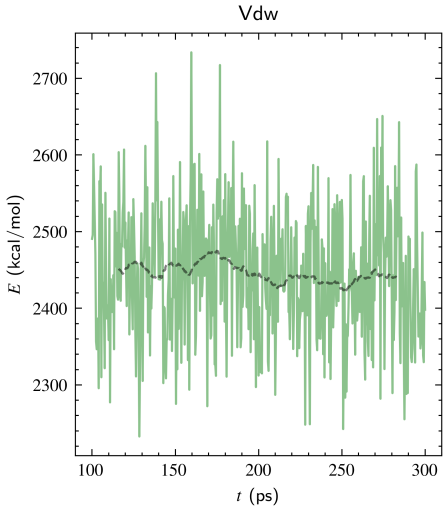
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
1: DYNA RESTRT CPT [200.0 ps]

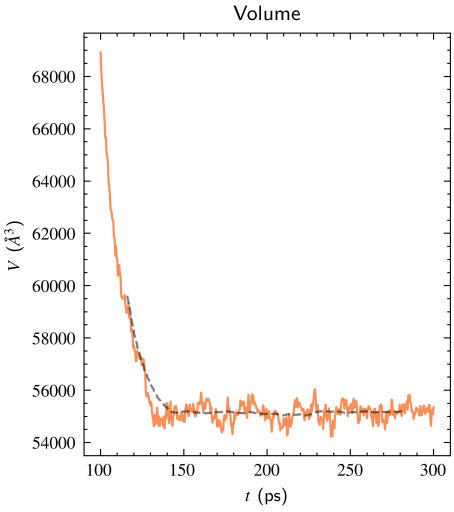




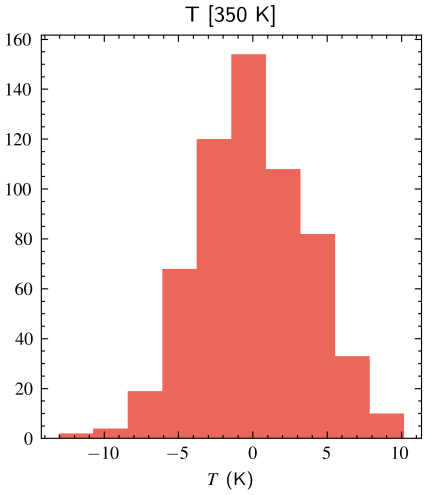


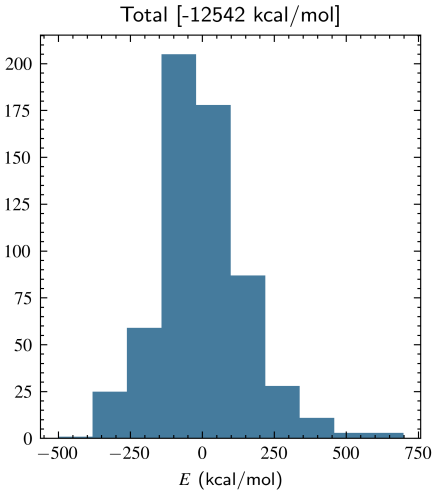


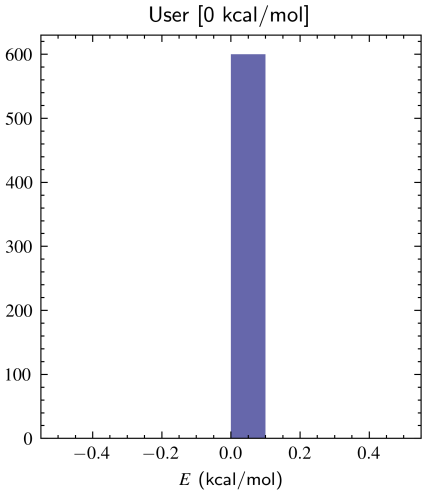


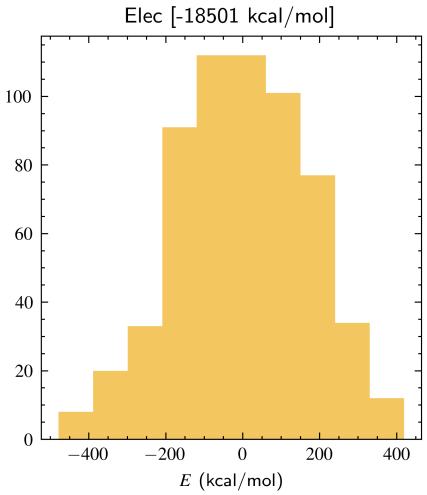


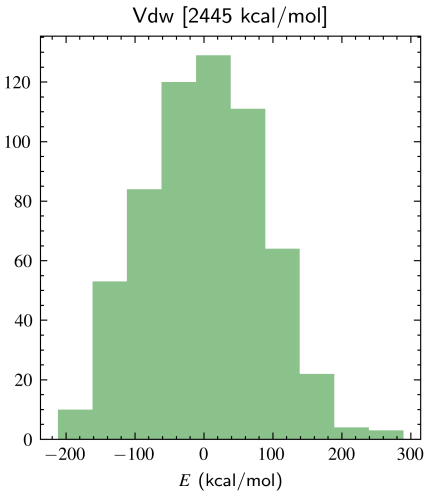
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
1: DYNA RESTRT CPT [200.0 ps]

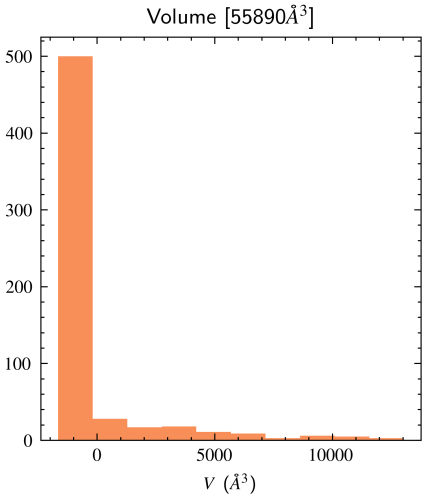




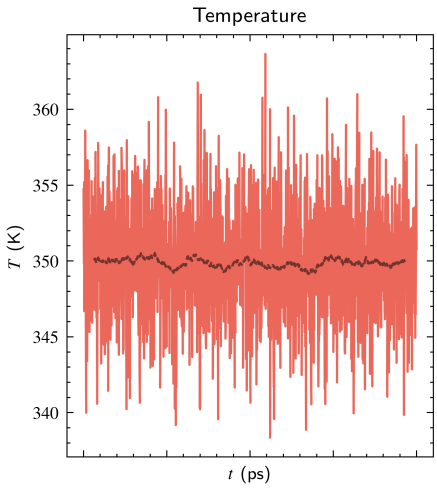


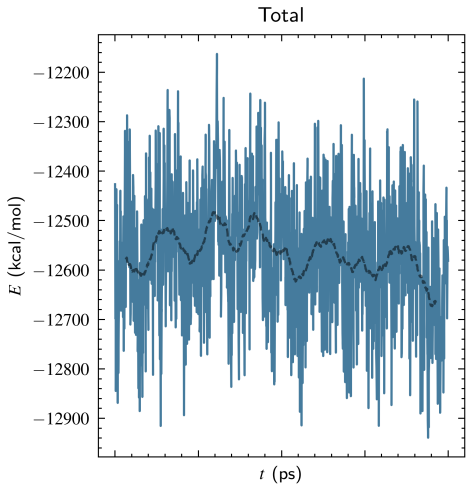


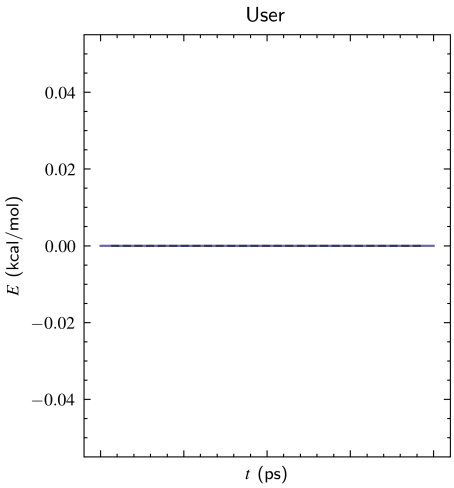


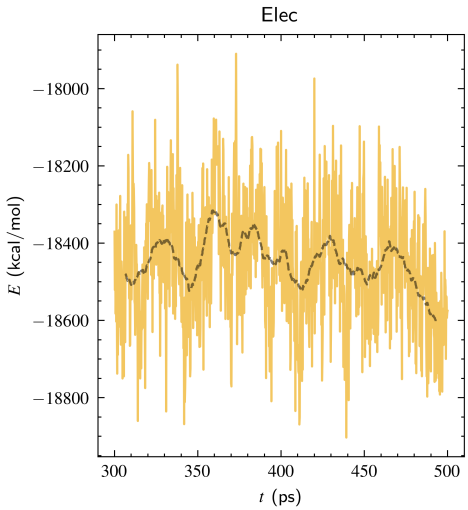


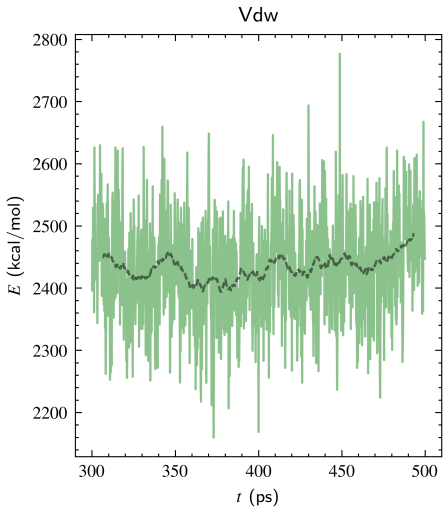
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
2: DYNA RESTRT CPT [200.0 ps]

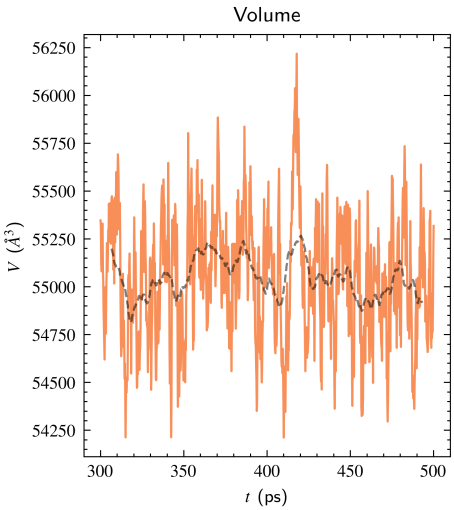




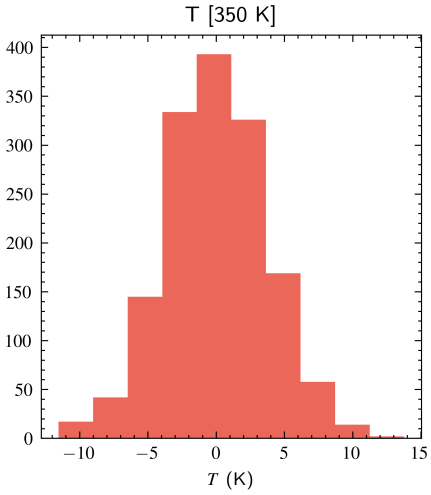


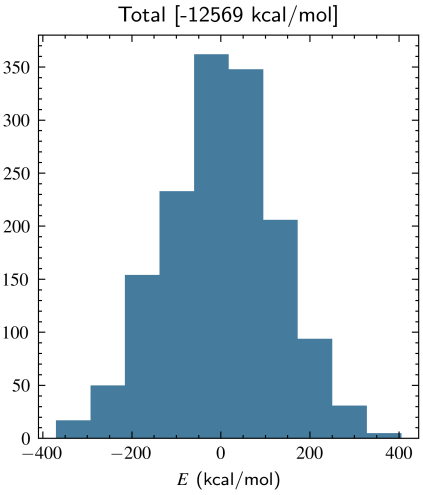


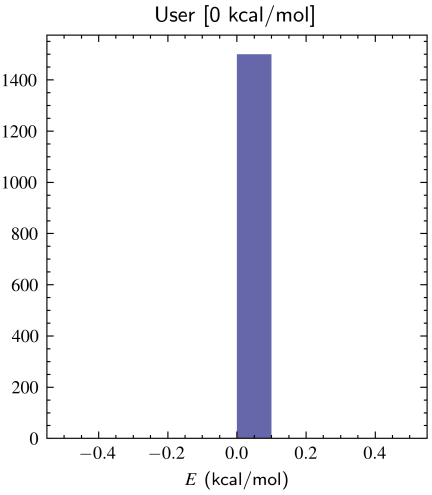


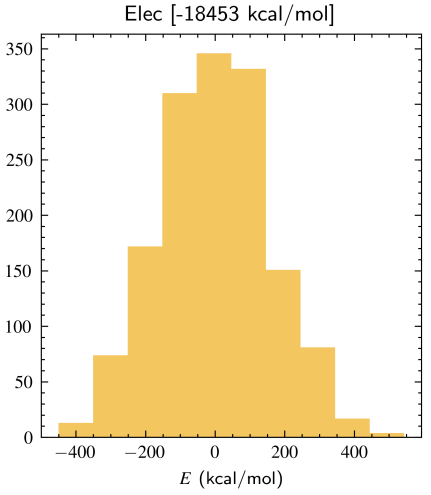


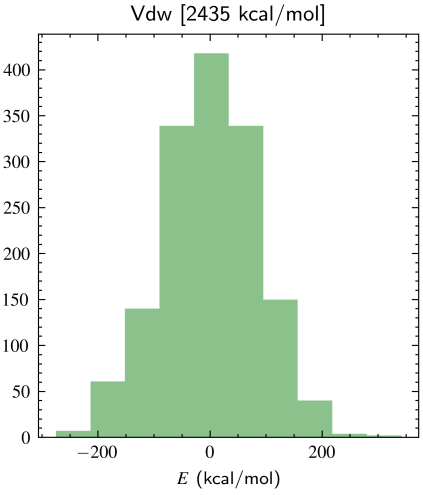
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
2: DYNA RESTRT CPT [200.0 ps]

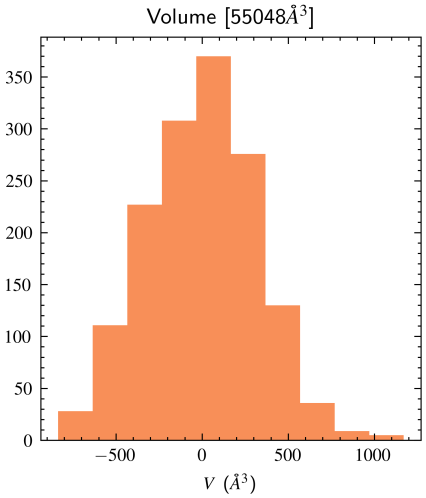




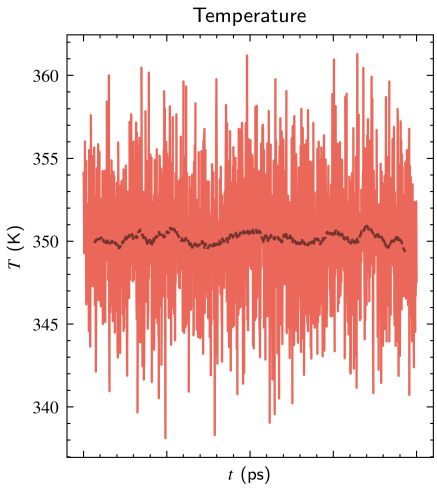


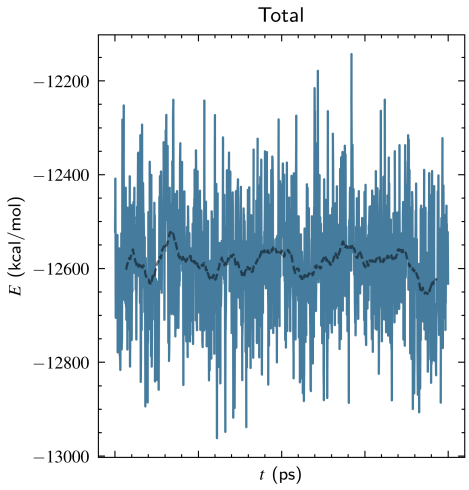


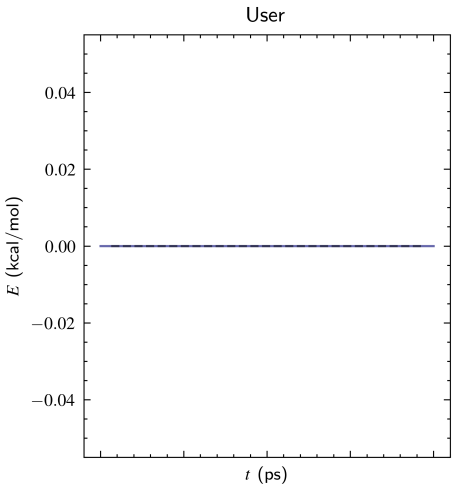


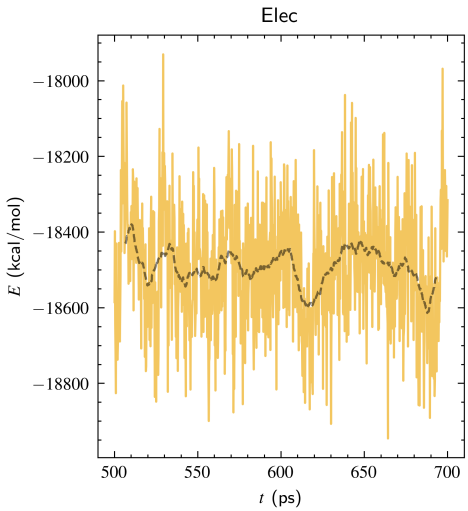


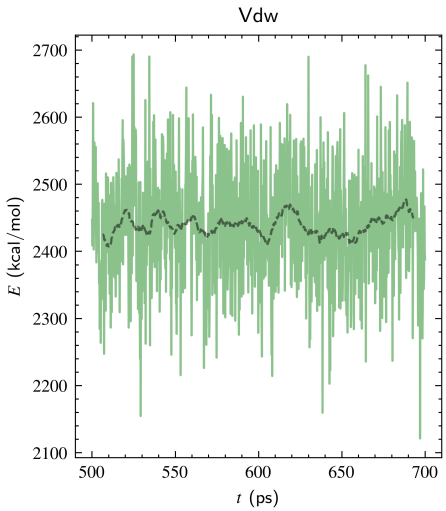
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
3: DYNA RESTRT CPT [200.0 ps]

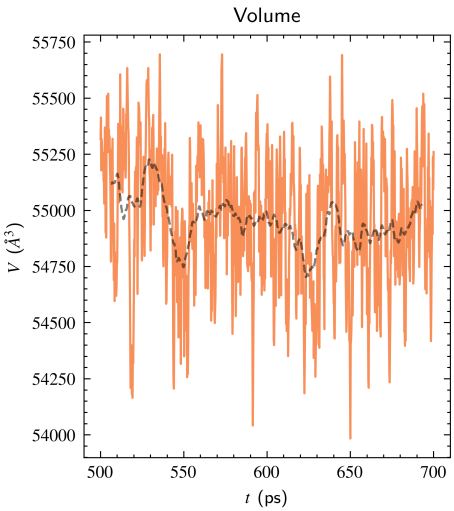




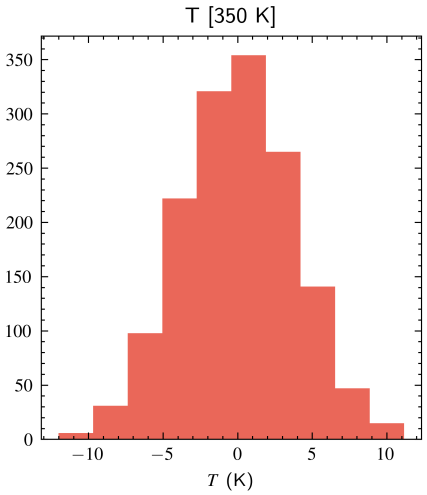


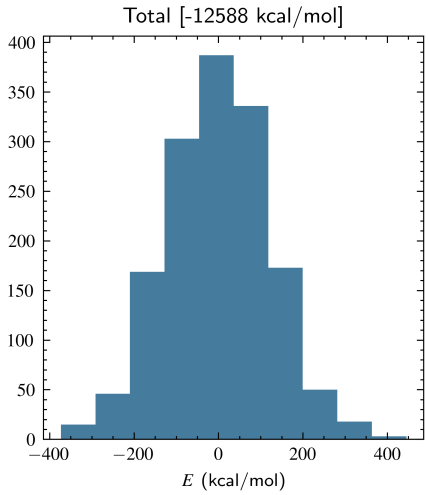


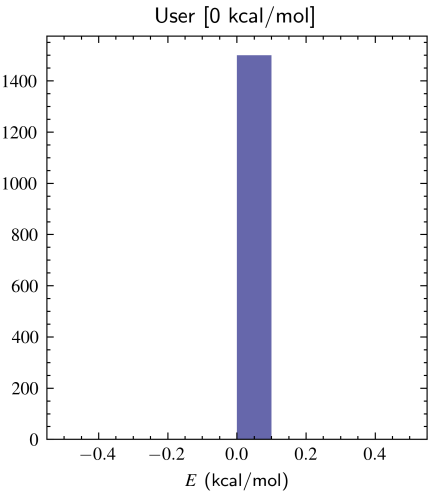


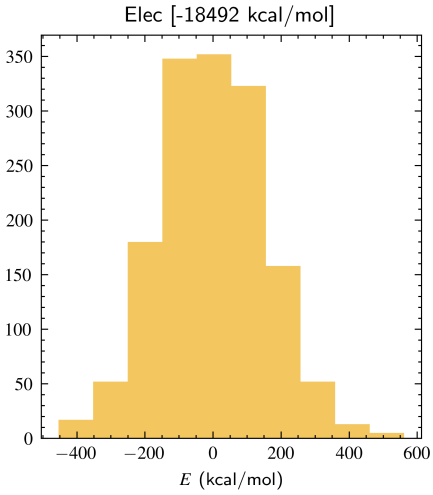


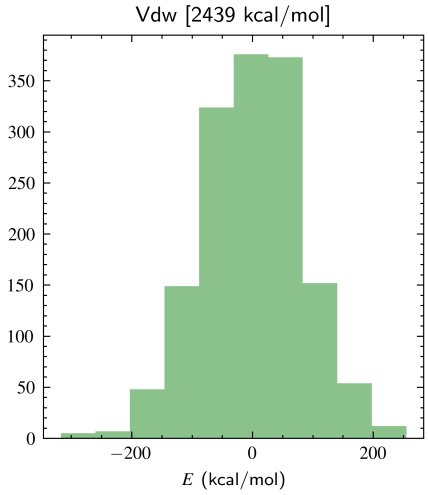
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
3: DYNA RESTRT CPT [200.0 ps]

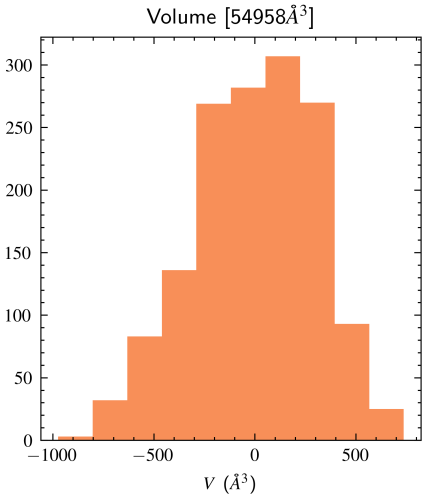




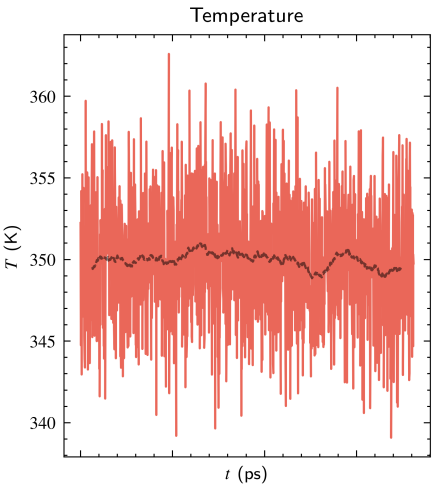


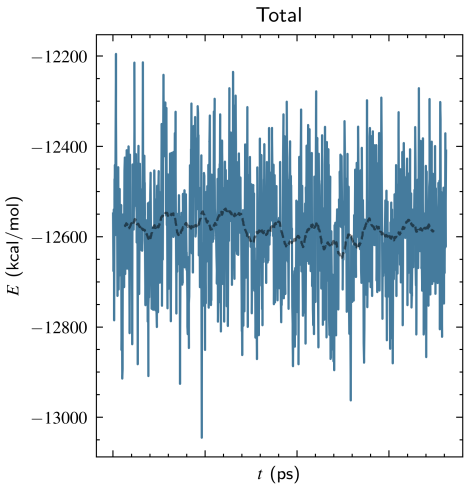


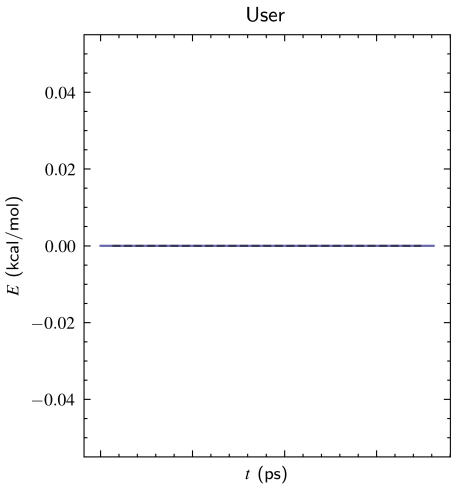


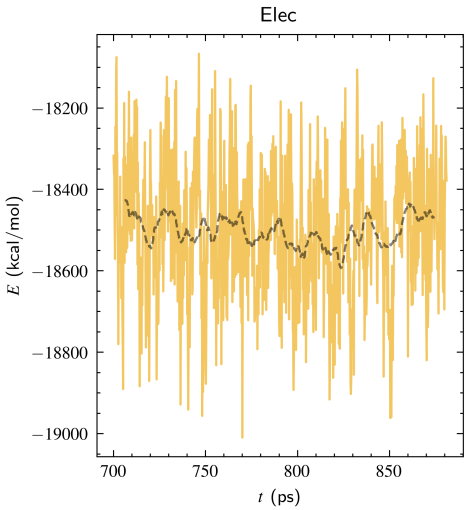


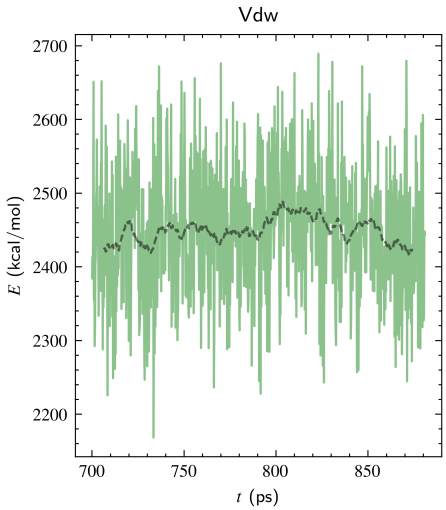
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
4: DYNA RESTRT CPT [181.0 ps]

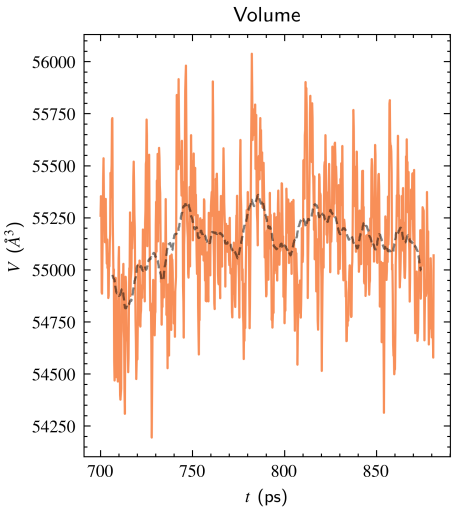




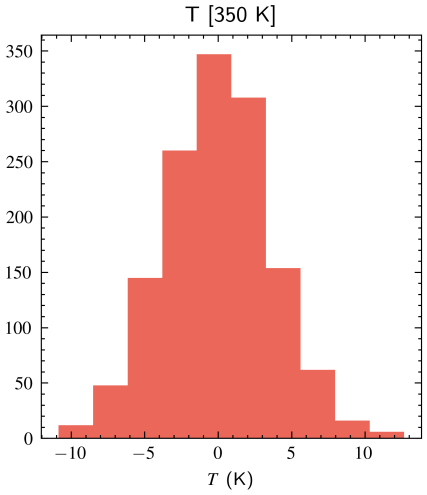


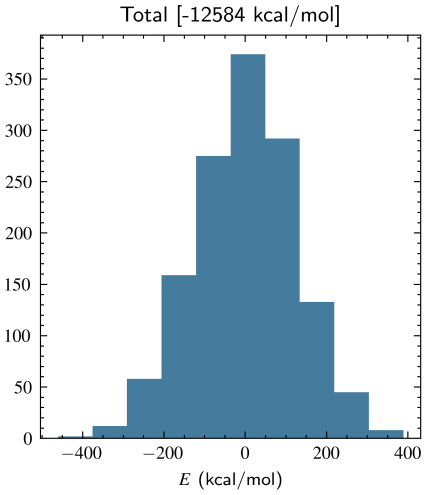


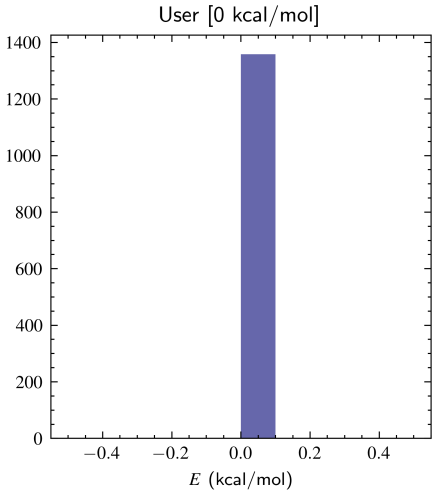


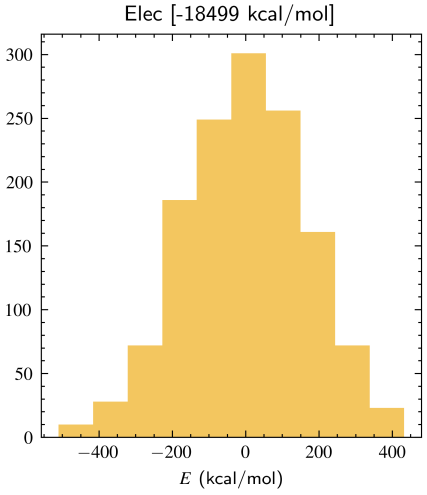


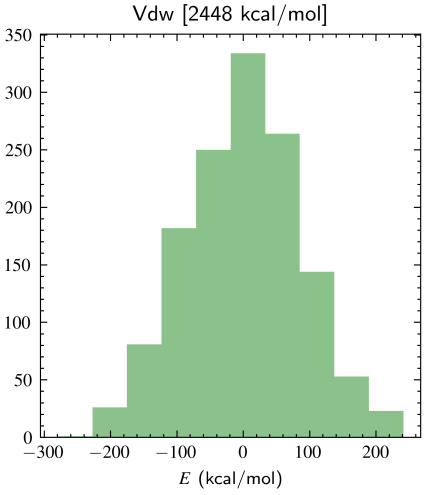
_home_boittier_pcbach_sims4_kmdcm_water_k350_dynamics.log
4: DYNA RESTRT CPT [181.0 ps]

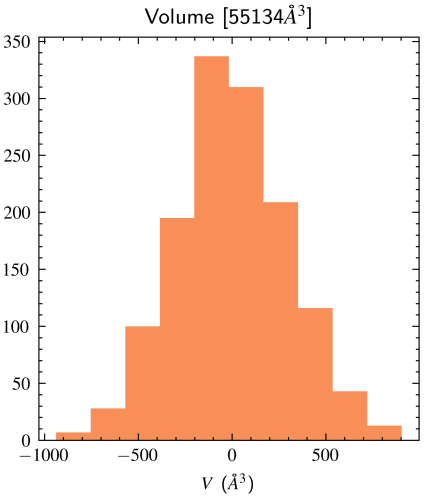












Trajectory info.

```
<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:165: 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 6.78464646 9.22287879 9.96494949] [2.87510157 1.07229085 1.05374866 1.00685434 1.00126781]
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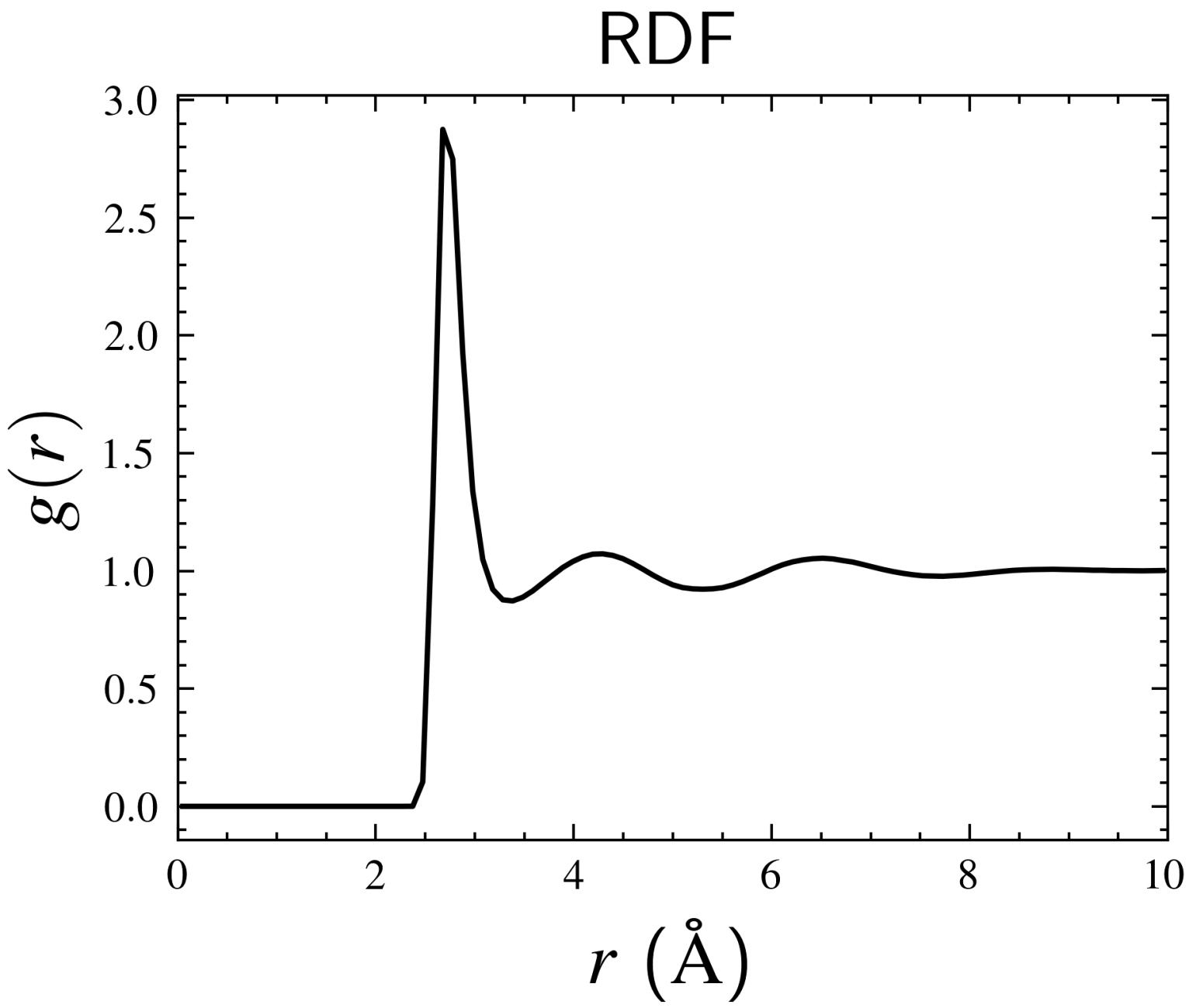


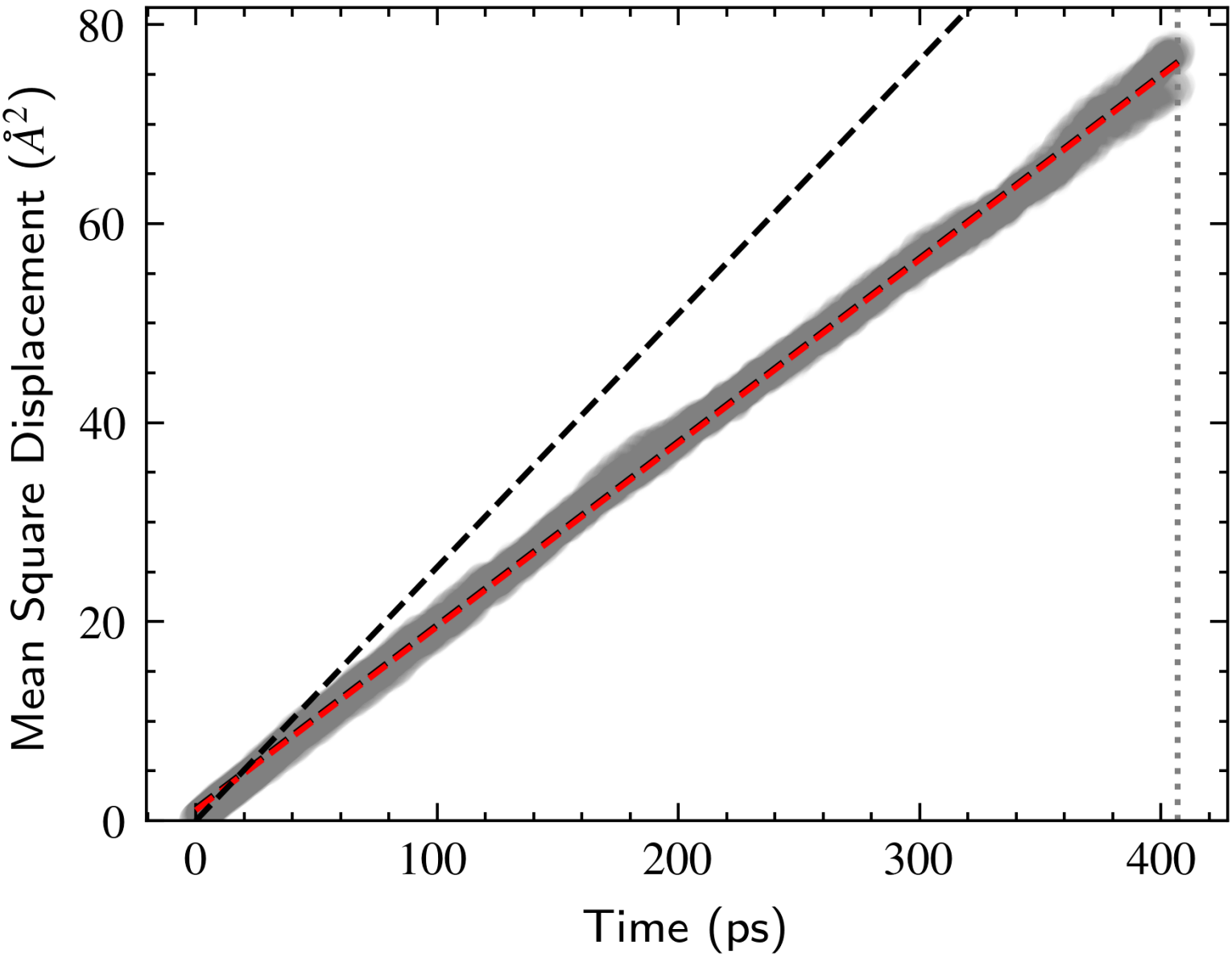
MSD and D

true ρ: 974

true D: 6.26e-05

```
0.0002
```

```
407.0166167328458
<Axes: xlabel='Time (ps)', ylabel='Mean Square Displacement ($\\AA^2$)'>
```

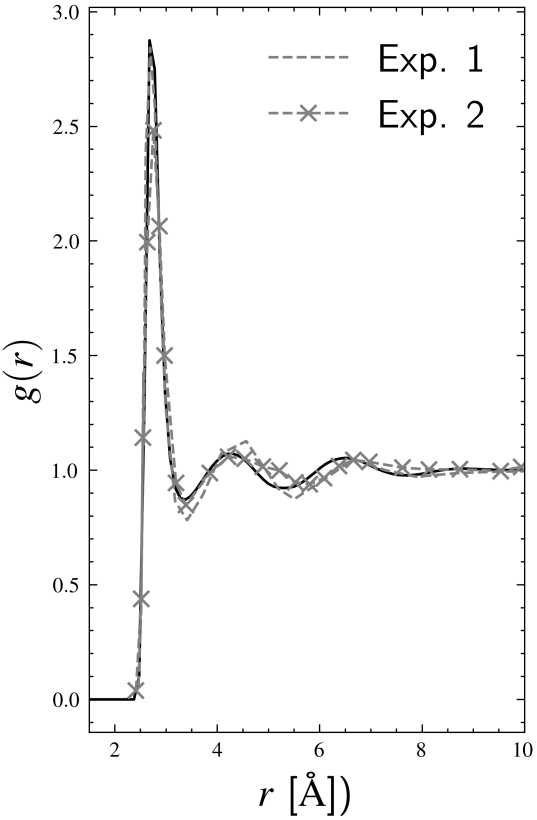


Structure and Transport

407.0166167328458

ρ = 1082 [kg/m^3] (error = 11.0%)

RDF



D = 1.9 [10^{-5} cm s^{-1}] (error = -70.0%)

MSD