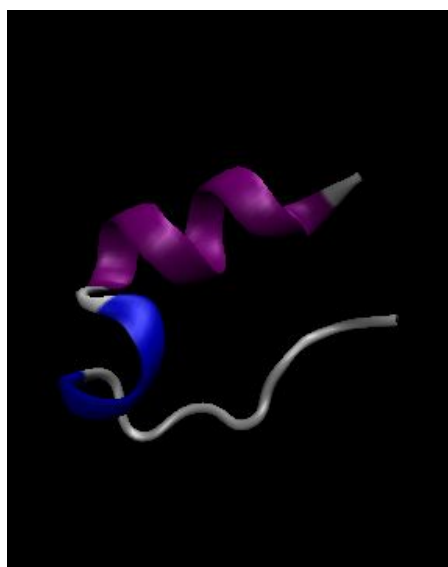


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Q2) 1L2Y - Finding all non bonded interactions



Molecule in New Cartoon Format

Non Bonded Interactions have been listed below

**1) Hydrophobic Interactions within 5 Angstroms**

Position	Residue	Chain	Position	Residue	Chain
2	LEU	A	19	PRO	A
2	LEU	A	3	TYR	A
3	TYR	A	18	PRO	A

## 2) Intra Protein Main Chain-Main Chain Hydrogen Bonds

POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
3	A	Y	N	1	A	N	O	3.24	3.34	75.49	83.32
4	A	I	N	1	A	N	O	2.92	2.25	122.94	123.98
4	A	I	N	2	A	L	O	3.41	3.37	83.89	74.89

## 3) Intra Protein Main Chain-Side Chain Hydrogen Bonds

POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
6	A	TRP	NE1	16	A	ARG	O	-	2.88	2.00	158.55	124.31
6	A	TRP	NE1	17	A	PRO	O	-	3.06	2.69	104.91	93.01
14	A	SER	OG	9	A	ASP	O	-	2.53	9.99	999.99	125.31

## 4) Intra Protein Side Chain-Side Chain Hydrogen Bonds

POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
8	A	LYS	NZ	5	A	GLN	OE1	-	2.8	9.9	999.99	999.99

										1	9		
16	A	AR	NE	9	A	ASP	OD2	-	3.4	2.9	111.75	999.99	
		G							3	0			

Dd-a = Distance Between Donor and Acceptor

Dh-a = Distance Between Hydrogen and Acceptor

A(d-H-N) = Angle Between Donor-H-N

A(a-O=C) = Angle Between Acceptor-O=C

MO = Multiple Occupancy

Note that angles that are undefined are written as 999.99

### 5) Intra protein Ionic Interactions within 6 Angstroms

Position	Residue	Chain	Position	Residue	Chain
8	LYS	A	9	ASP	A
9	ASP	A	16	ARG	A

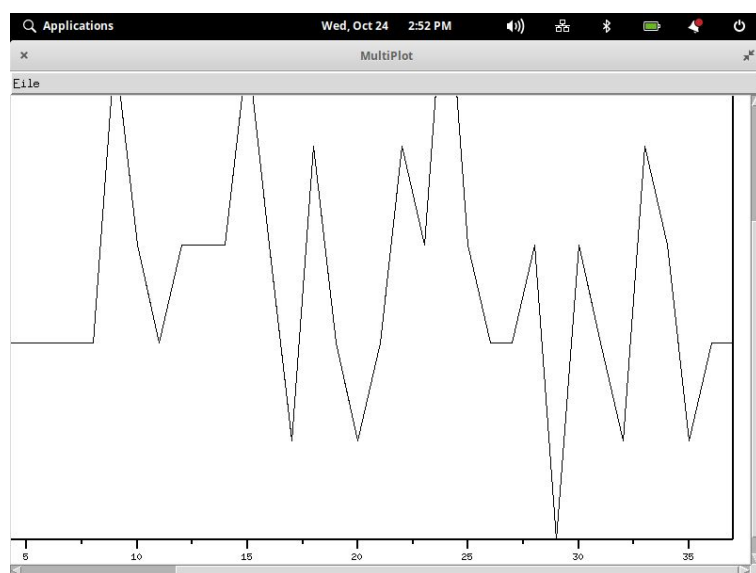
These were the non bonded interactions in the given protein.

Analysing the protein further- It contains 3 secondary structures:

- 1) Alpha-Helix- Purple
- 2) 3-10-Helix- Blue
- 3) Coils- White

Following is a graph of Hydrogen Bonds for the protein

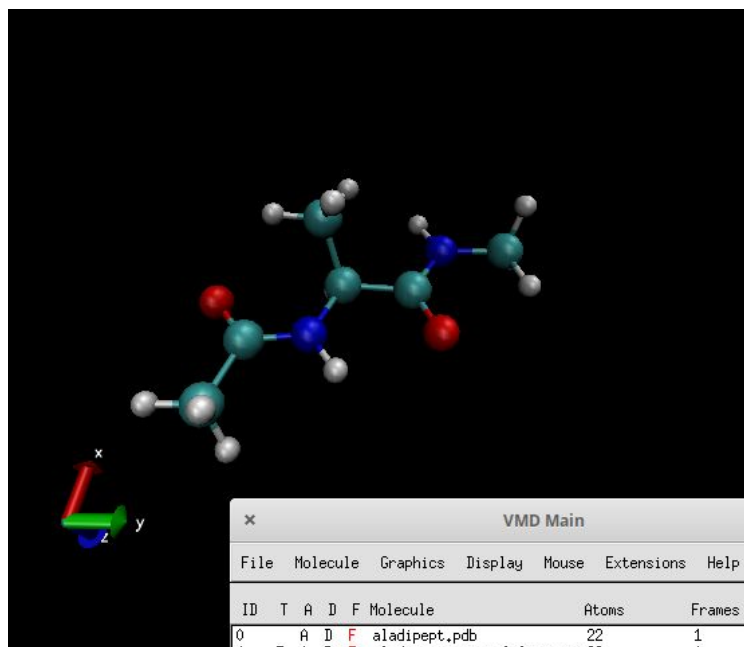
(Due to Resolution issues I had to take 2 pictures to complete represent the graph).



The graph was plotted using NAMD Plug in - HBonds

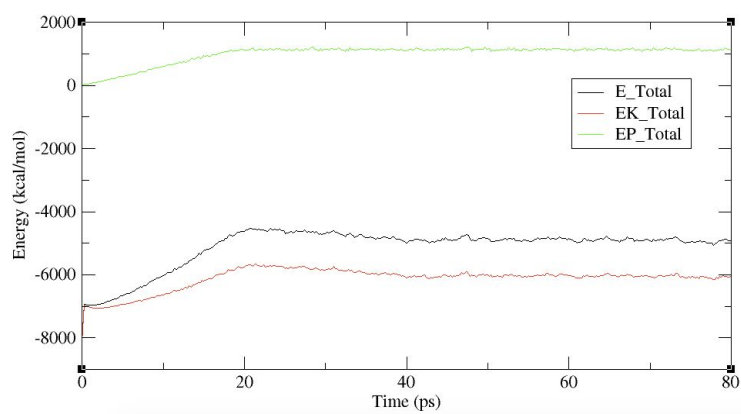
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## Q1) Alanine dipeptide

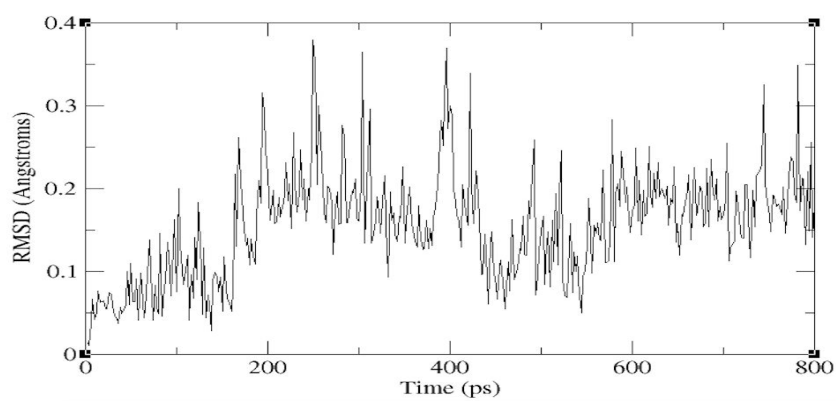


The alanine dipeptide has been shown in the CPK format

- 1)
- 2) Energy - Time graph for Alanine Dipeptide

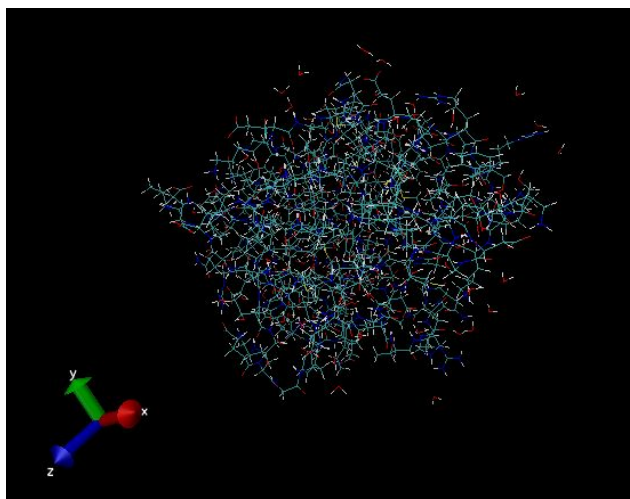


## RMSD Graph for Alanine Dipeptide

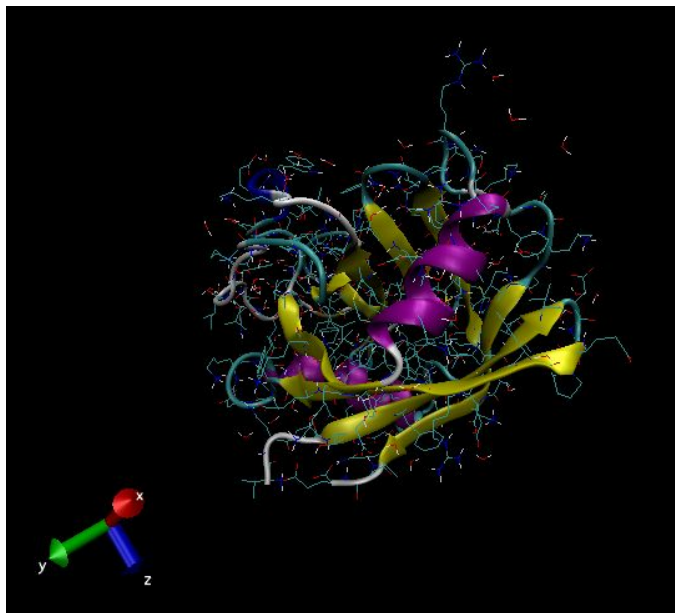


A protein containing Alanine Dipeptide

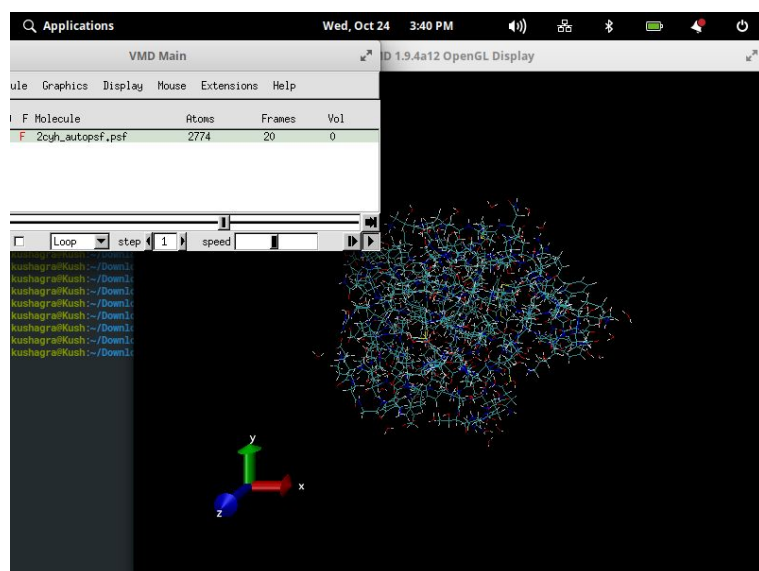
Simulations for 2cyh have been shown



CPK format



New Cartoon



Final dcd final loaded in psf contains 20 frames

LOG final of production follows:

Charm++: standalone mode (not using charmrun)

Charm++> Running in Multicore mode: 1 threads

Charm++> Using recursive bisection (scheme 3) for topology aware partitions

Converse/Charm++ Commit ID: v6.8.2-0-g26d4bd8-namd-charm-6.8.2-build-2018-Jan-11-30463

Warning> Randomization of virtual memory (ASLR) is turned on in the kernel, thread migration may not work! Run 'echo 0 > /proc/sys/kernel/randomize\_va\_space' as root to disable it, or try running with '+isomalloc\_sync'.

CharmLB> Load balancer assumes all CPUs are same.

Charm++> Running on 1 unique compute nodes (12-way SMP).

Charm++> cpu topology info is gathered in 0.000 seconds.

Info: NAMD Git-2018-10-19 for Linux-x86\_64-multicore

Info:

Info: Please visit <http://www.ks.uiuc.edu/Research/namd/>

Info: for updates, documentation, and support information.

Info:

Info: Please cite Phillips et al., J. Comp. Chem. 26:1781-1802 (2005)

Info: in all publications reporting results obtained with NAMD.

Info:

Info: Based on Charm++/Converse 60800 for multicore-linux64-iccstatic

Info: Built Fri Oct 19 01:57:46 CDT 2018 by jim on ganymede.ks.uiuc.edu

Info: 1 NAMD Git-2018-10-19 Linux-x86\_64-multicore 1 Kush kushagra

Info: Running on 1 processors, 1 nodes, 1 physical nodes.

Info: CPU topology information available.

Info: Charm++/Converse parallel runtime startup completed at 0.001194 s

CkLoopLib is used in SMP with a simple dynamic scheduling (converse-level notification) but not using node-level queue

Info: 49.2773 MB of memory in use based on /proc/self/stat

Info: Configuration file is production.conf

Info: Working in the current directory /home/kushagra/Downloads

TCL: Suspending until startup complete.

Info: EXTENDED SYSTEM FILE 2cyhsemi.xsc

Info: SIMULATION PARAMETERS:

Info: TIMESTEP 2

Info: NUMBER OF STEPS 50000

Info: STEPS PER CYCLE 20

Info: LOAD BALANCER Centralized

Info: LOAD BALANCING STRATEGY New Load Balancers -- DEFAULT

Info: LDB PERIOD 4000 steps

Info: FIRST LDB TIMESTEP 100

Info: LAST LDB TIMESTEP -1

Info: LDB BACKGROUND SCALING 1

Info: HOM BACKGROUND SCALING 1

Info: MIN ATOMS PER PATCH 40

Info: VELOCITY FILE 2cyhsemi.vel

Info: CENTER OF MASS MOVING INITIALLY? NO

Info: DIELECTRIC 1

Info: EXCLUDE SCALED ONE-FOUR

Info: 1-4 ELECTROSTATICS SCALED BY 1

Info: MODIFIED 1-4 VDW PARAMETERS WILL BE USED

Info: DCD FILENAME 2cyhfinal.dcd

Info: DCD FREQUENCY 2500

Info: DCD FIRST STEP 2500



Info: DCD FILE WILL CONTAIN UNIT CELL DATA  
Info: XST FILENAME 2cyhfinal.xst  
Info: XST FREQUENCY 5000  
Info: NO VELOCITY DCD OUTPUT  
Info: NO FORCE DCD OUTPUT  
Info: OUTPUT FILENAME 2cyhfinal  
Info: BINARY OUTPUT FILES WILL BE USED  
Info: RESTART FILENAME 2cyhfinal.restart  
Info: RESTART FREQUENCY 2500  
Info: BINARY RESTART FILES WILL BE USED  
Info: SWITCHING ACTIVE  
Info: VDW FORCE SWITCHING ACTIVE  
Info: SWITCHING ON 10  
Info: SWITCHING OFF 12  
Info: PAIRLIST DISTANCE 16  
Info: PAIRLIST SHRINK RATE 0.01  
Info: PAIRLIST GROW RATE 0.01  
Info: PAIRLIST TRIGGER 0.3  
Info: PAIRLISTS PER CYCLE 2  
Info: PAIRLISTS ENABLED  
Info: MARGIN 0  
Info: HYDROGEN GROUP CUTOFF 2.5  
Info: PATCH DIMENSION 18.5  
Info: ENERGY OUTPUT STEPS 500  
Info: CROSSTERM ENERGY INCLUDED IN DIHEDRAL  
Info: TIMING OUTPUT STEPS 1000  
Info: LANGEVIN DYNAMICS ACTIVE  
Info: LANGEVIN TEMPERATURE 303.15  
Info: LANGEVIN USING BBK INTEGRATOR  
Info: LANGEVIN DAMPING COEFFICIENT IS 1 INVERSE PS  
Info: LANGEVIN DYNAMICS NOT APPLIED TO HYDROGENS  
Info: USING VERLET I (r-RESPA) MTS SCHEME.  
Info: C1 SPLITTING OF LONG RANGE ELECTROSTATICS  
Info: PLACING ATOMS IN PATCHES BY HYDROGEN GROUPS  
Info: RIGID BONDS TO HYDROGEN : ALL  
Info: ERROR TOLERANCE : 1e-08  
Info: MAX ITERATIONS : 100  
Info: RIGID WATER USING SETTLE ALGORITHM  
Info: RANDOM NUMBER SEED 1540374229  
Info: USE HYDROGEN BONDS? NO  
Info: COORDINATE PDB 2cyh\_autopsf.pdb  
Info: STRUCTURE FILE 2cyh\_autopsf.psf  
Info: PARAMETER file: CHARMM format!  
Info: PARAMETERS toppar/par\_all36m\_prot.prm  
Info: PARAMETERS toppar/par\_all36\_na.prm  
Info: PARAMETERS toppar/par\_all36\_carb.prm  
Info: PARAMETERS toppar/par\_all36\_lipid.prm  
Info: PARAMETERS toppar/par\_all36\_cgenff.prm

Info: PARAMETERS           toppar\_water\_ions.str  
Info: USING ARITHMETIC MEAN TO COMBINE L-J SIGMA PARAMETERS  
Info: BINARY COORDINATES   2cyhsemi.coor  
Info: SUMMARY OF PARAMETERS:  
Info: 953 BONDS  
Info: 2799 ANGLES  
Info: 6874 DIHEDRAL  
Info: 196 IMPROPER  
Info: 6 CROSSTERM  
Info: 355 VDW  
Info: 94 VDW\_PAIRS  
Info: 0 NBTHOLE\_PAIRS  
Info: TIME FOR READING PSF FILE: 0.27274  
Info: Reading pdb file 2cyh\_autopsf.pdb  
Info: TIME FOR READING PDB FILE: 0.00227118  
Info:  
Info: \*\*\*\*\*  
Info: STRUCTURE SUMMARY:  
Info: 2774 ATOMS  
Info: 2715 BONDS  
Info: 4668 ANGLES  
Info: 6695 DIHEDRALS  
Info: 439 IMPROPER  
Info: 162 CROSSTERMS  
Info: 0 EXCLUSIONS  
Info: 1503 RIGID BONDS  
Info: 6819 DEGREES OF FREEDOM  
Info: 1358 HYDROGEN GROUPS  
Info: 4 ATOMS IN LARGEST HYDROGEN GROUP  
Info: 1358 MIGRATION GROUPS  
Info: 4 ATOMS IN LARGEST MIGRATION GROUP  
Info: TOTAL MASS = 19635.9 amu  
Info: TOTAL CHARGE = 1 e  
Info: \*\*\*\*\*  
Info: Reading from binary file 2cyhsemi.coor  
Info:  
Info: Entering startup at 0.424172 s, 88.4844 MB of memory in use  
Info: Startup phase 0 took 2.69413e-05 s, 88.4844 MB of memory in use  
Info: ADDED 13964 IMPLICIT EXCLUSIONS  
Info: Startup phase 1 took 0.00183201 s, 89.5625 MB of memory in use  
Info: NONBONDED TABLE R-SQUARED SPACING: 0.0625  
Info: NONBONDED TABLE SIZE: 769 POINTS  
Info: ABSOLUTE IMPRECISION IN FAST TABLE ENERGY: 2.53117e-21 AT 11.9974  
Info: RELATIVE IMPRECISION IN FAST TABLE ENERGY: 1.68907e-16 AT 11.9974  
Info: INCONSISTENCY IN FAST TABLE ENERGY VS FORCE: 0.000290274 AT 0.251946  
Info: ABSOLUTE IMPRECISION IN VDWA TABLE ENERGY: 9.6778e-33 AT 11.9974  
Info: RELATIVE IMPRECISION IN VDWA TABLE ENERGY: 3.71539e-17 AT 11.9974  
Info: INCONSISTENCY IN VDWA TABLE ENERGY VS FORCE: 0.0040507 AT 0.251946

Info: ABSOLUTE IMPRECISION IN VDWB TABLE ENERGY: 9.34011e-27 AT 11.9974  
 Info: RELATIVE IMPRECISION IN VDWB TABLE ENERGY: 2.98256e-17 AT 11.9974  
 Info: INCONSISTENCY IN VDWB TABLE ENERGY VS FORCE: 0.00150189 AT 0.251946  
 Info: Startup phase 2 took 0.0023191 s, 93.7656 MB of memory in use  
 Info: Startup phase 3 took 1.78814e-05 s, 93.7656 MB of memory in use  
 Info: Startup phase 4 took 1.3113e-05 s, 93.7656 MB of memory in use  
 Info: Startup phase 5 took 1.19209e-05 s, 93.7656 MB of memory in use  
 Info: ORIGINAL ATOMS MINMAX IS -2.47032 -3.32062 -6.43733 37.0836 31.1611 34.2575  
 Info: ADJUSTED ATOMS MINMAX IS 0.253553 2.86954 0.134924 32.061 28.4026 28.5606  
 Info: PATCH GRID IS 2 BY 2 BY 2  
 Info: PATCH GRID IS 1-AWAY BY 1-AWAY BY 1-AWAY  
 Info: Reading from binary file 2cyhsemi.vel  
 Info: REMOVING COM VELOCITY 0.0807695 0.298655 0.10126  
 Info: LARGEST PATCH (2) HAS 400 ATOMS  
 Info: TORUS A SIZE 1 USING 0  
 Info: TORUS B SIZE 1 USING 0  
 Info: TORUS C SIZE 1 USING 0  
 Info: TORUS MINIMAL MESH SIZE IS 1 BY 1 BY 1  
 Info: Placed 100% of base nodes on same physical node as patch  
 Info: Startup phase 6 took 0.000880003 s, 94.1836 MB of memory in use  
 Info: Startup phase 7 took 1.69277e-05 s, 94.1836 MB of memory in use  
 Info: Startup phase 8 took 1.21593e-05 s, 94.1836 MB of memory in use  
 Info: Startup phase 9 took 1.19209e-05 s, 94.1836 MB of memory in use  
 Info: Startup phase 10 took 1.00136e-05 s, 94.1836 MB of memory in use  
 Info: Startup phase 11 took 1.19209e-05 s, 94.1836 MB of memory in use  
 LDB: Central LB being created...  
 Info: Startup phase 12 took 2.00272e-05 s, 94.1836 MB of memory in use  
 Info: CREATING 81 COMPUTE OBJECTS  
 Info: Startup phase 13 took 0.000224113 s, 94.1836 MB of memory in use  
 Info: Startup phase 14 took 1.69277e-05 s, 94.1836 MB of memory in use  
 Info: Startup phase 15 took 3.40939e-05 s, 95.293 MB of memory in use  
 Info: Finished startup at 0.429631 s, 95.293 MB of memory in use

TCL: Original numsteps 50000 will be ignored.

TCL: Running for 50000 steps

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW
BOUNDARY		MISC	KINETIC	TOTAL	TEMP	POTENTIAL	TOTAL3
TEMPAVG							

ENERGY:	0	527.7150	1409.3267	1606.0088	96.9235	-5574.1442	-389.2621
0.0000	0.0000	2119.9534	-203.4789	312.8931	-2323.4323	-180.1820	
312.8931							

OPENING EXTENDED SYSTEM TRAJECTORY FILE

LDB: ===== START OF LOAD BALANCING ===== 0.631356  
 LDB: ===== END OF LOAD BALANCING ===== 0.631413  
 LDB: ===== DONE WITH MIGRATION ===== 0.631505  
 LDB: ===== START OF LOAD BALANCING ===== 1.39879

LDB: ===== END OF LOAD BALANCING ===== 1.39883  
 LDB: ===== DONE WITH MIGRATION ===== 1.39895  
 Info: Initial time: 1 CPUs 0.00966485 s/step 0.0559308 days/ns 101.445 MB memory  
 LDB: ===== START OF LOAD BALANCING ===== 1.58899  
 LDB: ===== END OF LOAD BALANCING ===== 1.58902  
 LDB: ===== DONE WITH MIGRATION ===== 1.58913  
 LDB: ===== START OF LOAD BALANCING ===== 2.35179  
 LDB: ===== END OF LOAD BALANCING ===== 2.35183  
 LDB: ===== DONE WITH MIGRATION ===== 2.35193  
 Info: Initial time: 1 CPUs 0.00957305 s/step 0.0553996 days/ns 101.445 MB memory  
 LDB: ===== START OF LOAD BALANCING ===== 3.35809  
 LDB: ===== END OF LOAD BALANCING ===== 3.35813  
 LDB: ===== DONE WITH MIGRATION ===== 3.35827  
 Info: Initial time: 1 CPUs 0.0100194 s/step 0.0579829 days/ns 101.445 MB memory  
 LDB: ===== START OF LOAD BALANCING ===== 4.30884  
 LDB: ===== END OF LOAD BALANCING ===== 4.30889  
 LDB: ===== DONE WITH MIGRATION ===== 4.30905  
 Info: Benchmark time: 1 CPUs 0.00950525 s/step 0.0550072 days/ns 101.445 MB memory  
 Info: Benchmark time: 1 CPUs 0.00936836 s/step 0.054215 days/ns 101.445 MB memory  
 ENERGY: 500 523.8857 1514.7470 1579.7404 95.9324 -5540.7437 -390.9020  
 0.0000 0.0000 2043.3914 -173.9489 301.5930 -2217.3402 -152.5032  
 306.9397

Info: Benchmark time: 1 CPUs 0.00936223 s/step 0.0541796 days/ns 101.445 MB memory  
 Info: Benchmark time: 1 CPUs 0.00904113 s/step 0.0523213 days/ns 101.445 MB memory  
 Info: Benchmark time: 1 CPUs 0.00918434 s/step 0.0531501 days/ns 101.445 MB memory  
 Info: Benchmark time: 1 CPUs 0.00887648 s/step 0.0513685 days/ns 101.445 MB memory  
 TIMING: 1000 CPU: 9.36542, 0.00934727/step Wall: 9.37045, 0.00935089/step, 0.127276 hours  
 remaining, 101.445312 MB of memory in use.  
 ENERGY: 1000 551.9248 1432.3443 1570.2440 88.0978 -5545.6360 -372.9342  
 0.0000 0.0000 2067.3555 -208.6039 305.1300 -2275.9594 -186.7519  
 306.0568

ENERGY: 1500 536.2659 1397.8364 1586.1985 96.7186 -5545.4248 -413.7736  
 0.0000 0.0000 2065.9409 -276.2381 304.9212 -2342.1791 -250.2414  
 304.0004

TIMING: 2000 CPU: 18.8247, 0.00945923/step Wall: 18.8394, 0.00946894/step, 0.126252 hours  
 remaining, 101.445312 MB of memory in use.  
 ENERGY: 2000 529.0333 1458.5962 1590.7113 83.7352 -5564.2908 -410.4133  
 0.0000 0.0000 2018.1544 -294.4737 297.8682 -2312.6280 -273.3276  
 300.1189

ENERGY: 2500 546.9406 1451.4202 1566.6121 100.9116 -5581.2194  
 -414.0046 0.0000 0.0000 2019.7984 -309.5410 298.1108 -2329.3394  
 -286.9115 299.0639

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 2500

OPENING COORDINATE DCD FILE

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 2500

WRITING COORDINATES TO RESTART FILE AT STEP 2500

FINISHED WRITING RESTART COORDINATES

The last position output (seq=2500) takes 0.000 seconds, 102.113 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 2500

FINISHED WRITING RESTART VELOCITIES

The last velocity output (seq=2500) takes 0.000 seconds, 102.113 MB of memory in use

TIMING: 3000 CPU: 31.1676, 0.0123429/step Wall: 31.1821, 0.0123427/step, 0.161141 hours remaining, 102.113281 MB of memory in use.

ENERGY:	3000	516.1233	1438.1431	1597.4676	94.5048	-5648.0231	-354.5522
	0.0000	0.0000	2000.0168	-356.3196	295.1912	-2356.3364	-333.4457
	301.4019						

ENERGY:	3500	554.2769	1466.8232	1558.9378	86.3295	-5611.7861	-412.7397
	0.0000	0.0000	1966.2140	-391.9445	290.2020	-2358.1584	-371.9055
	295.2053						

TIMING: 4000 CPU: 45.9033, 0.0147357/step Wall: 45.9185, 0.0147364/step, 0.188299 hours remaining, 102.113281 MB of memory in use.

ENERGY:	4000	536.6707	1434.0221	1588.5915	86.7308	-5600.6145	-383.0617
	0.0000	0.0000	2001.6657	-335.9954	295.4345	-2337.6611	-312.5858
	296.7004						

LDB: ===== START OF LOAD BALANCING ===== 49.3782

LDB: ===== END OF LOAD BALANCING ===== 49.3782

LDB: ===== DONE WITH MIGRATION ===== 49.3784

LDB: ===== START OF LOAD BALANCING ===== 50.3451

LDB: ===== END OF LOAD BALANCING ===== 50.3452

LDB: ===== DONE WITH MIGRATION ===== 50.3453

ENERGY:	4500	506.8839	1433.5188	1586.0036	91.0080	-5567.7312	-378.6760
	0.0000	0.0000	2026.1825	-302.8105	299.0531	-2328.9930	-279.5896
	296.9637						

TIMING: 5000 CPU: 55.5592, 0.00965597/step Wall: 55.5774, 0.00965895/step, 0.120737 hours remaining, 102.113281 MB of memory in use.

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW
BOUNDARY		MISC	KINETIC	TOTAL	TEMP	POTENTIAL	TOTAL3
TEMPAVG							

ENERGY:	5000	474.5025	1429.1838	1559.1549	102.1483	-5562.5782	
	-392.2657	0.0000	0.0000	1982.8214	-407.0329	292.6532	-2389.8543
	-383.3910	294.9150					

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 5000

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 5000

WRITING COORDINATES TO RESTART FILE AT STEP 5000

FINISHED WRITING RESTART COORDINATES

The last position output (seq=5000) takes 0.000 seconds, 102.113 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 5000

FINISHED WRITING RESTART VELOCITIES

The last velocity output (seq=5000) takes 0.000 seconds, 102.113 MB of memory in use

ENERGY:	5500	537.1631	1398.0690	1564.4308	96.2775	-5577.4836	-422.4693
0.0000	0.0000	2027.9369	-376.0756	299.3120	-2404.0125	-353.8706	
							291.7868

TIMING: 6000 CPU: 64.9752, 0.00941596/step Wall: 64.992, 0.00941463/step, 0.115068 hours remaining, 102.113281 MB of memory in use.

ENERGY:	6000	507.7661	1449.2161	1550.7608	89.1381	-5588.3770	-346.9442
0.0000	0.0000	1950.8113	-387.6288	287.9287	-2338.4400	-367.0382	
							294.1112

ENERGY:	6500	543.3780	1415.9399	1550.2206	92.2176	-5605.9903	-408.4159
0.0000	0.0000	2030.5821	-382.0682	299.7024	-2412.6502	-357.9597	
							296.6896

TIMING: 7000 CPU: 74.6672, 0.00969196/step Wall: 74.6858, 0.00969376/step, 0.115787 hours remaining, 102.113281 MB of memory in use.

ENERGY:	7000	538.1372	1394.5279	1571.8326	82.7049	-5632.0304	-376.5202
0.0000	0.0000	2008.2834	-413.0647	296.4113	-2421.3481	-389.7480	
							295.2906

ENERGY:	7500	504.2295	1465.8990	1561.0474	96.2666	-5634.0099	-385.9378
0.0000	0.0000	2017.6166	-374.8886	297.7888	-2392.5052	-351.7093	
							294.2199

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 7500

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 7500

WRITING COORDINATES TO RESTART FILE AT STEP 7500

FINISHED WRITING RESTART COORDINATES

The last position output (seq=7500) takes 0.000 seconds, 102.113 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 7500

FINISHED WRITING RESTART VELOCITIES

The last velocity output (seq=7500) takes 0.000 seconds, 102.113 MB of memory in use

TIMING: 8000 CPU: 90.0271, 0.0153599/step Wall: 90.0427, 0.0153569/step, 0.179164 hours remaining, 102.113281 MB of memory in use.

ENERGY:	8000	523.9746	1403.0338	1566.6148	90.7985	-5590.4171	-443.3853
0.0000	0.0000	2063.1430	-386.2377	304.5082	-2449.3807	-360.4161	
							296.8777

LDB: ===== START OF LOAD BALANCING ===== 94.924

LDB: ===== END OF LOAD BALANCING ===== 94.9241

LDB: ===== DONE WITH MIGRATION ===== 94.9241

LDB: ===== START OF LOAD BALANCING ===== 96.0166

LDB: ===== END OF LOAD BALANCING ===== 96.0166

LDB: ===== DONE WITH MIGRATION ===== 96.0167

ENERGY: 8500 509.9643 1394.9666 1566.7047 96.5788 -5545.8992 -439.4488  
0.0000 0.0000 1982.4553 -434.6782 292.5992 -2417.1335 -411.3922  
295.4707

TIMING: 9000 CPU: 101.769, 0.0117417/step Wall: 101.793, 0.0117498/step, 0.133817 hours  
remaining, 102.113281 MB of memory in use.

ENERGY: 9000 527.4338 1415.6568 1554.1136 92.5963 -5607.8865 -411.6971  
0.0000 0.0000 1986.3382 -443.4449 293.1723 -2429.7830 -420.4413  
290.3577

ENERGY: 9500 521.4853 1435.4234 1541.1825 93.8082 -5599.3620 -374.5428  
0.0000 0.0000 2083.5407 -298.4646 307.5188 -2382.0053 -271.2547  
296.5898

TIMING: 10000 CPU: 111.442, 0.00967333/step Wall: 111.474, 0.00968097/step, 0.107566 hours  
remaining, 102.292969 MB of memory in use.

ETITLE: TS BOND ANGLE DIHED IMPRP ELECT VDW  
BOUNDARY MISC KINETIC TOTAL TEMP POTENTIAL TOTAL3  
TEMPAVG

ENERGY: 10000 514.0324 1459.9656 1574.0096 88.1220 -5564.4204  
-380.5331 0.0000 0.0000 2082.5442 -226.2798 307.3717 -2308.8240  
-201.6470 303.2483

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 10000  
WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 10000  
WRITING COORDINATES TO RESTART FILE AT STEP 10000  
FINISHED WRITING RESTART COORDINATES

The last position output (seq=10000) takes 0.000 seconds, 102.293 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 10000

FINISHED WRITING RESTART VELOCITIES

The last velocity output (seq=10000) takes 0.000 seconds, 102.293 MB of memory in use

ENERGY: 10500 534.2183 1460.3392 1579.7687 88.3898 -5604.8136  
-381.2172 0.0000 0.0000 2071.2681 -252.0467 305.7074 -2323.3148  
-225.4339 305.4872

TIMING: 11000 CPU: 120.866, 0.00942392/step Wall: 120.896, 0.00942263/step, 0.102078 hours  
remaining, 102.292969 MB of memory in use.

ENERGY: 11000 546.9572 1456.4829 1571.9916 100.3117 -5589.1404  
-407.1083 0.0000 0.0000 2079.3937 -241.1116 306.9067 -2320.5053  
-217.4042 304.7970

ENERGY: 11500 582.1593 1457.4117 1565.5660 97.9902 -5608.7998  
-400.2849 0.0000 0.0000 2035.7576 -270.1999 300.4663 -2305.9575  
-247.5741 303.1608

TIMING: 12000 CPU: 130.77, 0.00990396/step Wall: 130.798, 0.00990198/step, 0.104521 hours  
remaining, 102.292969 MB of memory in use.

ENERGY: 12000 526.5757 1434.2567 1575.8441 92.9895 -5603.9158  
-367.7024 0.0000 0.0000 2097.9164 -244.0357 309.6406 -2341.9521  
-220.0934 305.2913

LDB: ===== START OF LOAD BALANCING ===== 136.262

LDB: ===== END OF LOAD BALANCING ===== 136.262

LDB: ===== DONE WITH MIGRATION ===== 136.263

LDB: ===== START OF LOAD BALANCING ===== 138.009

LDB: ===== END OF LOAD BALANCING ===== 138.009

LDB: ===== DONE WITH MIGRATION ===== 138.009

ENERGY: 12500 534.4627 1445.7400 1557.1551 78.9669 -5546.0085  
-386.3441 0.0000 0.0000 2069.4265 -246.6014 305.4356 -2316.0279  
-221.2281 305.4626

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 12500

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 12500

WRITING COORDINATES TO RESTART FILE AT STEP 12500

FINISHED WRITING RESTART COORDINATES

The last position output (seq=12500) takes 0.000 seconds, 102.293 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 12500

FINISHED WRITING RESTART VELOCITIES

The last velocity output (seq=12500) takes 0.000 seconds, 102.293 MB of memory in use

TIMING: 13000 CPU: 148.2, 0.0174302/step Wall: 148.234, 0.0174356/step, 0.179199 hours remaining,  
102.292969 MB of memory in use.

ENERGY: 13000 562.0994 1419.3169 1573.4907 88.1033 -5533.5866  
-443.5282 0.0000 0.0000 2056.7865 -277.3179 303.5700 -2334.1044  
-254.6851 305.5006

ENERGY: 13500 566.6817 1423.6646 1561.4116 92.7336 -5538.1667  
-442.9440 0.0000 0.0000 2061.0267 -275.5925 304.1959 -2336.6192  
-249.7726 302.9361

TIMING: 14000 CPU: 161.828, 0.013628/step Wall: 161.859, 0.0136255/step, 0.136255 hours  
remaining, 102.292969 MB of memory in use.

ENERGY: 14000 556.5351 1434.0065 1574.1264 88.7530 -5549.7883  
-425.1484 0.0000 0.0000 2070.8927 -250.6229 305.6520 -2321.5156  
-225.8640 301.9263

ENERGY: 14500 505.9009 1408.8304 1601.1898 95.7142 -5558.9802  
-411.9477 0.0000 0.0000 2064.8840 -294.4086 304.7652 -2359.2926  
-269.0793 302.4530

TIMING: 15000 CPU: 171.444, 0.00961597/step Wall: 171.475, 0.00961595/step, 0.0934884 hours  
remaining, 102.292969 MB of memory in use.

ETITLE: TS BOND ANGLE DIHED IMPRP ELECT VDW  
BOUNDARY MISC KINETIC TOTAL TEMP POTENTIAL TOTAL3  
TEMPAVG



ENERGY: 15000 488.0104 1463.3978 1614.4479 100.4423 -5627.8239  
-408.1930 0.0000 0.0000 2049.7216 -319.9970 302.5273 -2369.7186  
-296.2076 301.2813

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 15000  
WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 15000  
WRITING COORDINATES TO RESTART FILE AT STEP 15000  
FINISHED WRITING RESTART COORDINATES

The last position output (seq=15000) takes 0.000 seconds, 102.293 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 15000  
FINISHED WRITING RESTART VELOCITIES

ENERGY: 15500 493.6709 1445.7454 1574.2464 91.1959 -5570.1230  
-363.3553 0.0000 0.0000 2079.9396 -248.6801 306.9873 -2328.6197  
-223.2896 304.8704

TIMING: 16000 CPU: 181.108, 0.00966398/step Wall: 181.141, 0.00966604/step, 0.0912904 hours  
remaining, 102.292969 MB of memory in use.

ENERGY: 16000 545.4255 1447.5572 1576.6898 94.1184 -5621.7585  
-386.4940 0.0000 0.0000 2044.6144 -299.8472 301.7735 -2344.4616  
-277.1509 303.4007

LDB: ===== START OF LOAD BALANCING ===== 184.476  
LDB: ===== END OF LOAD BALANCING ===== 184.476  
LDB: ===== DONE WITH MIGRATION ===== 184.476  
LDB: ===== START OF LOAD BALANCING ===== 185.939  
LDB: ===== END OF LOAD BALANCING ===== 185.939  
LDB: ===== DONE WITH MIGRATION ===== 185.939

ENERGY: 16500 503.7180 1496.5136 1571.3027 89.8118 -5553.2031  
-398.4880 0.0000 0.0000 2007.2447 -283.1003 296.2580 -2290.3450  
-261.5873 301.9208

TIMING: 17000 CPU: 195.644, 0.014536/step Wall: 195.674, 0.0145333/step, 0.133222 hours  
remaining, 102.292969 MB of memory in use.

ENERGY: 17000 508.0074 1426.3958 1579.6487 98.1613 -5608.2880  
-397.5421 0.0000 0.0000 2118.3629 -275.2540 312.6584 -2393.6169  
-250.3322 301.4860

ENERGY: 17500 549.1110 1450.2102 1568.4014 104.7512 -5645.1398  
-396.4177 0.0000 0.0000 2062.7991 -306.2845 304.4575 -2369.0836  
-281.3865 302.9082

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 17500  
WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 17500  
WRITING COORDINATES TO RESTART FILE AT STEP 17500  
FINISHED WRITING RESTART COORDINATES

The last position output (seq=17500) takes 0.000 seconds, 102.293 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 17500  
FINISHED WRITING RESTART VELOCITIES

TIMING: 18000 CPU: 207.892, 0.012248/step Wall: 207.926, 0.0122516/step, 0.108903 hours remaining, 102.292969 MB of memory in use.

ENERGY:	18000	521.8468	1490.6944	1585.1159	88.7504	-5625.2948
	-402.0541	0.0000	0.0000	2066.7582	-274.1832	305.0418
	-2340.9414					
	-248.4683	303.6994				

ENERGY:	18500	528.2718	1492.5860	1561.3700	87.6754	-5595.3264
	-442.1096	0.0000	0.0000	2069.0262	-298.5066	305.3766
	-2367.5328					
	-273.5973	301.8852				

TIMING: 19000 CPU: 217.556, 0.00966398/step Wall: 217.59, 0.00966392/step, 0.0832171 hours remaining, 102.292969 MB of memory in use.

ENERGY:	19000	564.0144	1442.2869	1569.5763	101.4832	-5640.0018
	-384.7967	0.0000	0.0000	2027.2087	-320.2289	299.2045
	-2347.4376					
	-297.2424	301.4311				

ENERGY:	19500	540.7841	1447.7379	1575.1416	91.6227	-5615.8629
	-406.4891	0.0000	0.0000	2037.8589	-329.2068	300.7764
	-2367.0656					
	-305.9044	302.8443				

TIMING: 20000 CPU: 227.264, 0.00970798/step Wall: 227.297, 0.00970742/step, 0.0808952 hours remaining, 102.484375 MB of memory in use.

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW
BOUNDARY		MISC	KINETIC	TOTAL	TEMP	POTENTIAL	TOTAL3
TEMPAVG							

ENERGY:	20000	512.9222	1465.1071	1574.5416	96.0066	-5621.9859
	-420.8422	0.0000	0.0000	2062.5696	-331.6810	304.4236
	-2394.2506					
	-307.2805	301.6558				

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 20000

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 20000

WRITING COORDINATES TO RESTART FILE AT STEP 20000

FINISHED WRITING RESTART COORDINATES

The last position output (seq=20000) takes 0.000 seconds, 102.484 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 20000

FINISHED WRITING RESTART VELOCITIES

LDB: ===== START OF LOAD BALANCING ===== 231.866

LDB: ===== END OF LOAD BALANCING ===== 231.866

LDB: ===== DONE WITH MIGRATION ===== 231.866

LDB: ===== START OF LOAD BALANCING ===== 233.433

LDB: ===== END OF LOAD BALANCING ===== 233.433

LDB: ===== DONE WITH MIGRATION ===== 233.433

ENERGY:	20500	552.4477	1444.7606	1545.8792	91.4251	-5558.1914
	-436.1708	0.0000	0.0000	2065.9626	-293.8869	304.9244
	-2359.8494					
	-270.0832	301.3812				

TIMING: 21000 CPU: 239.324, 0.0120599/step Wall: 239.355, 0.0120576/step, 0.097131 hours remaining, 102.484375 MB of memory in use.

ENERGY:	21000	545.0378	1411.3117	1558.1862	98.1206	-5560.3235
	-402.0121	0.0000	0.0000	2000.7982	-348.8811	295.3065
	-327.4868	299.8772				

ENERGY:	21500	516.1345	1431.8254	1556.2161	83.6984	-5612.2139
	-394.8434	0.0000	0.0000	2024.3220	-394.8609	298.7785
	-372.2455	300.3022				

TIMING: 22000 CPU: 253.34, 0.014016/step Wall: 253.371, 0.0140162/step, 0.109015 hours remaining, 102.484375 MB of memory in use.

ENERGY:	22000	517.2476	1414.6206	1557.6001	99.3892	-5563.8782
	-396.2152	0.0000	0.0000	2032.6689	-338.5671	300.0104
	-314.8345	297.0467				

ENERGY:	22500	547.4034	1414.3129	1557.0742	99.2650	-5598.0348
	-382.9825	0.0000	0.0000	2052.6407	-310.3212	302.9581
	-283.9830	300.3345				

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 22500

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 22500

WRITING COORDINATES TO RESTART FILE AT STEP 22500

FINISHED WRITING RESTART COORDINATES

The last position output (seq=22500) takes 0.000 seconds, 102.484 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 22500

FINISHED WRITING RESTART VELOCITIES

TIMING: 23000 CPU: 263.876, 0.010536/step Wall: 263.907, 0.010536/step, 0.0790203 hours remaining, 102.484375 MB of memory in use.

ENERGY:	23000	532.6904	1447.2336	1571.7673	86.9396	-5612.8120
	-422.4700	0.0000	0.0000	2058.5566	-338.0945	303.8313
	-312.9257	298.5464				

ENERGY:	23500	527.4003	1481.6109	1562.6353	91.1706	-5629.1177
	-378.7318	0.0000	0.0000	2066.1252	-278.9072	304.9484
	-255.1582	302.5923				

TIMING: 24000 CPU: 277.036, 0.01316/step Wall: 277.069, 0.0131619/step, 0.0950584 hours remaining, 102.484375 MB of memory in use.

ENERGY:	24000	567.6490	1446.4768	1558.2191	94.8737	-5630.7738
	-398.0197	0.0000	0.0000	2094.5670	-267.0079	309.1462
	-243.3957	304.8548				

LDB: ===== START OF LOAD BALANCING ===== 282.762

LDB: ===== END OF LOAD BALANCING ===== 282.762

LDB: ===== DONE WITH MIGRATION ===== 282.762

LDB: ===== START OF LOAD BALANCING ===== 284.555

LDB: ===== END OF LOAD BALANCING ===== 284.555

LDB: ===== DONE WITH MIGRATION ===== 284.555

ENERGY:	24500	537.5665	1399.0325	1573.5651	91.4437	-5546.7624
	-410.1147	0.0000	0.0000	2121.9039	-233.3653	313.1810
	-206.5271	307.6991				-2355.2692

TIMING: 25000 CPU: 291.808, 0.0147716/step Wall: 291.846, 0.0147771/step, 0.102619 hours remaining, 102.656250 MB of memory in use.

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW
BOUNDARY		MISC	KINETIC	TOTAL	TEMP	POTENTIAL	TOTAL3
TEMPAVG							

ENERGY:	25000	548.3305	1491.0932	1552.9289	83.3444	-5566.6214
	-411.4759	0.0000	0.0000	2116.4815	-185.9189	312.3807
	-160.8941	308.7279				-2302.4004

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 25000

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 25000

WRITING COORDINATES TO RESTART FILE AT STEP 25000

FINISHED WRITING RESTART COORDINATES

The last position output (seq=25000) takes 0.000 seconds, 102.656 MB of memory in use

WRITING VELOCITIES TO RESTART FILE AT STEP 25000

FINISHED WRITING RESTART VELOCITIES

ENERGY:	25500	542.6128	1497.7556	1577.4433	97.8776	-5625.9787
	-387.3326	0.0000	0.0000	2077.1967	-220.4254	306.5825
	-198.0710	308.3075				-2297.6220

TIMING: 26000 CPU: 301.775, 0.00996797/step Wall: 301.818, 0.00997171/step, 0.0664781 hours remaining, 102.656250 MB of memory in use.

ENERGY:	26000	567.3300	1470.3663	1581.2074	86.9973	-5545.2565
	-430.1866	0.0000	0.0000	2063.5468	-205.9953	304.5678
	-184.6163	306.4052				-2269.5421

ENERGY:	26500	553.5625	1486.7291	1576.1251	74.6046	-5522.7671
	-444.5092	0.0000	0.0000	2076.5896	-199.6654	306.4929
	-177.2638	307.5581				-2276.2550

TIMING: 27000 CPU: 311.799, 0.010024/step Wall: 311.839, 0.0100212/step, 0.0640241 hours remaining, 102.656250 MB of memory in use.

ENERGY:	27000	531.7758	1460.0066	1561.8563	97.9838	-5594.9974
	-384.7142	0.0000	0.0000	2024.9816	-303.1076	298.8758
	-276.9923	302.8861				-2328.0891

ENERGY:	27500	550.7624	1467.3424	1551.3782	87.2462	-5599.5634
	-399.1158	0.0000	0.0000	2056.8230	-285.1270	303.5754
	-259.0033	302.8088				-2341.9500

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 27500

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 27500

WRITING COORDINATES TO RESTART FILE AT STEP 27500

FINISHED WRITING RESTART COORDINATES

WRITING VELOCITIES TO RESTART FILE AT STEP 27500

FINISHED WRITING RESTART VELOCITIES

TIMING: 28000 CPU: 324.299, 0.0125/step Wall: 324.341, 0.0125016/step, 0.0763985 hours remaining,  
102.656250 MB of memory in use.

ENERGY:	28000	551.3058	1470.1299	1571.2940	98.8510	-5515.9553
	-455.4253	0.0000	0.0000	2002.1961	-277.6037	295.5128
	-255.5192	304.4869				

LDB: ===== START OF LOAD BALANCING ===== 327.738

LDB: ===== END OF LOAD BALANCING ===== 327.738

LDB: ===== DONE WITH MIGRATION ===== 327.738

LDB: ===== START OF LOAD BALANCING ===== 328.873

LDB: ===== END OF LOAD BALANCING ===== 328.873

LDB: ===== DONE WITH MIGRATION ===== 328.873

ENERGY:	28500	544.2983	1445.3264	1559.0889	92.2264	-5567.3941
	-395.9730	0.0000	0.0000	2114.1608	-208.2663	312.0382
	-186.0606	304.7205				

TIMING: 29000 CPU: 337.502, 0.0132026/step Wall: 337.542, 0.0132017/step, 0.0770097 hours remaining,  
102.785156 MB of memory in use.

ENERGY:	29000	549.7516	1506.3462	1583.8539	100.7824	-5647.2330
	-372.7845	0.0000	0.0000	2080.2573	-199.0261	307.0342
	-173.5401	308.1707				

ENERGY:	29500	524.1909	1446.2069	1570.7042	89.3616	-5574.8590
	-390.0350	0.0000	0.0000	2114.5527	-219.8777	312.0960
	-194.0225	309.1966				

TIMING: 30000 CPU: 348.602, 0.0111/step Wall: 348.644, 0.0111011/step, 0.061673 hours remaining,  
102.785156 MB of memory in use.

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW
BOUNDARY		MISC	KINETIC	TOTAL	TEMP	POTENTIAL	TOTAL3
TEMPAVG							

ENERGY:	30000	525.2121	1465.1802	1590.0885	99.2205	-5553.9023
	-437.5714	0.0000	0.0000	2053.6906	-258.0819	303.1131
	-235.1103	306.0952				

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 30000

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 30000

WRITING COORDINATES TO RESTART FILE AT STEP 30000

FINISHED WRITING RESTART COORDINATES

WRITING VELOCITIES TO RESTART FILE AT STEP 30000

FINISHED WRITING RESTART VELOCITIES

ENERGY: 30500 500.4234 1472.5225 1570.2846 95.0388 -5594.6714  
-402.2356 0.0000 0.0000 2062.4472 -296.1904 304.4055 -2358.6377  
-273.8008 303.0333

TIMING: 31000 CPU: 359.054, 0.010452/step Wall: 359.096, 0.0104529/step, 0.055168 hours remaining, 102.785156 MB of memory in use.

ENERGY: 31000 519.4843 1407.5303 1564.7780 93.0215 -5607.1968  
-383.1314 0.0000 0.0000 2058.1545 -347.3597 303.7719 -2405.5142  
-322.4166 302.2282

ENERGY: 31500 530.8822 1420.7083 1569.7837 92.2419 -5560.4973  
-387.0846 0.0000 0.0000 2065.8478 -268.1180 304.9074 -2333.9658  
-242.7108 301.9455

TIMING: 32000 CPU: 369.934, 0.01088/step Wall: 369.977, 0.0108809/step, 0.0544043 hours remaining, 102.785156 MB of memory in use.

ENERGY: 32000 547.7778 1465.8221 1582.8561 91.1785 -5633.8285  
-393.4493 0.0000 0.0000 2085.2478 -254.3954 307.7708 -2339.6432  
-230.7440 304.3499

LDB: ===== START OF LOAD BALANCING ===== 375.912

LDB: ===== END OF LOAD BALANCING ===== 375.912

LDB: ===== DONE WITH MIGRATION ===== 375.912

LDB: ===== START OF LOAD BALANCING ===== 379.887

LDB: ===== END OF LOAD BALANCING ===== 379.887

LDB: ===== DONE WITH MIGRATION ===== 379.887

ENERGY: 32500 550.6296 1468.6038 1549.1410 97.2186 -5595.7686  
-415.8221 0.0000 0.0000 2028.7409 -317.2569 299.4307 -2345.9978  
-294.9175 302.5514

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 32500

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 32500

WRITING COORDINATES TO RESTART FILE AT STEP 32500

FINISHED WRITING RESTART COORDINATES

WRITING VELOCITIES TO RESTART FILE AT STEP 32500

FINISHED WRITING RESTART VELOCITIES

TIMING: 33000 CPU: 395.417, 0.0254831/step Wall: 395.484, 0.0255066/step, 0.120448 hours remaining, 102.785156 MB of memory in use.

ENERGY: 33000 534.6203 1465.4398 1551.8791 88.8565 -5558.2064  
-420.6233 0.0000 0.0000 1978.5052 -359.5287 292.0162 -2338.0340  
-336.5249 300.3363

ENERGY: 33500 526.9871 1434.7684 1592.0894 99.3750 -5569.8673  
-394.8583 0.0000 0.0000 2004.1227 -307.3830 295.7972 -2311.5057  
-284.5766 298.4423

TIMING: 34000 CPU: 409.659, 0.0142422/step Wall: 409.731, 0.0142475/step, 0.0633223 hours remaining, 102.785156 MB of memory in use.

ENERGY: 34000 525.1093 1438.0360 1561.3356 89.5298 -5571.5422  
-436.7235 0.0000 0.0000 2096.5889 -297.6660 309.4447 -2394.2550  
-270.9119 301.5701

ENERGY: 34500 534.7491 1463.4718 1523.4888 91.4498 -5588.6961  
-396.8758 0.0000 0.0000 1989.2834 -383.1290 293.6070 -2372.4124  
-360.8321 299.9873

TIMING: 35000 CPU: 419.583, 0.00992397/step Wall: 419.658, 0.00992617/step, 0.0413591 hours  
remaining, 102.785156 MB of memory in use.

ETITLE: TS BOND ANGLE DIHED IMPRP ELECT VDW  
BOUNDARY MISC KINETIC TOTAL TEMP POTENTIAL TOTAL3  
TEMPAVG

ENERGY: 35000 535.0867 1434.6280 1554.8809 97.5357 -5608.2573  
-395.2732 0.0000 0.0000 2054.8228 -326.5765 303.2802 -2381.3993  
-302.3369 298.8014

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 35000  
WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 35000  
WRITING COORDINATES TO RESTART FILE AT STEP 35000  
FINISHED WRITING RESTART COORDINATES  
WRITING VELOCITIES TO RESTART FILE AT STEP 35000  
FINISHED WRITING RESTART VELOCITIES

ENERGY: 35500 523.9438 1427.3549 1563.1368 96.8475 -5628.3384  
-363.2322 0.0000 0.0000 1977.1903 -403.0972 291.8221 -2380.2875  
-379.0585 297.9091

TIMING: 36000 CPU: 429.407, 0.00982397/step Wall: 429.481, 0.00982325/step, 0.0382015 hours  
remaining, 102.941406 MB of memory in use.

ENERGY: 36000 570.3414 1451.7974 1551.7639 85.8720 -5561.8858  
-445.0127 0.0000 0.0000 2020.7756 -326.3483 298.2550 -2347.1238  
-304.0630 298.3635

LDB: ===== START OF LOAD BALANCING ===== 432.827  
LDB: ===== END OF LOAD BALANCING ===== 432.827  
LDB: ===== DONE WITH MIGRATION ===== 432.827  
LDB: ===== START OF LOAD BALANCING ===== 433.783  
LDB: ===== END OF LOAD BALANCING ===== 433.783  
LDB: ===== DONE WITH MIGRATION ===== 433.783

ENERGY: 36500 520.6376 1455.8177 1577.1282 87.2791 -5611.3535  
-399.8361 0.0000 0.0000 2070.9476 -299.3794 305.6601 -2370.3270  
-278.1914 298.5071

TIMING: 37000 CPU: 439.231, 0.00982398/step Wall: 439.303, 0.00982247/step, 0.03547 hours  
remaining, 102.941406 MB of memory in use.

ENERGY: 37000 574.0467 1421.4571 1579.1386 84.9275 -5567.3480  
-432.4861 0.0000 0.0000 2052.4571 -287.8071 302.9310 -2340.2642  
-264.5470 300.6960

ENERGY: 37500 550.1975 1494.6263 1576.5321 98.3563 -5580.2077  
-429.5657 0.0000 0.0000 2043.3138 -246.7474 301.5815 -2290.0612  
-222.5628 302.9086

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 37500

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 37500

WRITING COORDINATES TO RESTART FILE AT STEP 37500

FINISHED WRITING RESTART COORDINATES

WRITING VELOCITIES TO RESTART FILE AT STEP 37500

FINISHED WRITING RESTART VELOCITIES

TIMING: 38000 CPU: 465.093, 0.0258617/step Wall: 465.202, 0.0258983/step, 0.0863276 hours  
remaining, 102.941406 MB of memory in use.

ENERGY: 38000 535.9252 1463.6623 1541.3389 101.2171 -5498.0896  
-472.8722 0.0000 0.0000 2094.2750 -234.5433 309.1031 -2328.8183  
-209.5575 304.5671

ENERGY: 38500 546.2482 1471.2479 1582.5452 99.2644 -5560.4408  
-419.4991 0.0000 0.0000 2033.1829 -247.4513 300.0863 -2280.6343  
-225.6188 305.5867

TIMING: 39000 CPU: 485.106, 0.0200128/step Wall: 485.219, 0.0200175/step, 0.0611647 hours  
remaining, 102.941406 MB of memory in use.

ENERGY: 39000 521.7965 1473.3316 1565.2726 87.7308 -5596.0212  
-408.3740 0.0000 0.0000 2098.8483 -257.4155 309.7781 -2356.2638  
-231.7165 305.7762

ENERGY: 39500 541.0736 1443.1870 1577.0501 91.6616 -5647.3873  
-384.0048 0.0000 0.0000 2101.4913 -276.9286 310.1682 -2378.4199  
-251.6141 304.8114

TIMING: 40000 CPU: 495.898, 0.010792/step Wall: 496.013, 0.0107943/step, 0.0299842 hours  
remaining, 102.941406 MB of memory in use.

ETITLE: TS BOND ANGLE DIHED IMPRP ELECT VDW  
BOUNDARY MISC KINETIC TOTAL TEMP POTENTIAL TOTAL3  
TEMPAVG

ENERGY: 40000 550.8082 1450.5841 1562.9847 93.0243 -5618.1019  
-404.0383 0.0000 0.0000 2078.2111 -286.5279 306.7322 -2364.7390  
-261.7016 305.2070

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 40000

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 40000

WRITING COORDINATES TO RESTART FILE AT STEP 40000

FINISHED WRITING RESTART COORDINATES



WRITING VELOCITIES TO RESTART FILE AT STEP 40000

FINISHED WRITING RESTART VELOCITIES

LDB: ===== START OF LOAD BALANCING ===== 499.374

LDB: ===== END OF LOAD BALANCING ===== 499.374

LDB: ===== DONE WITH MIGRATION ===== 499.374

LDB: ===== START OF LOAD BALANCING ===== 500.364

LDB: ===== END OF LOAD BALANCING ===== 500.364

LDB: ===== DONE WITH MIGRATION ===== 500.364

ENERGY: 40500 537.8898 1427.0075 1560.1357 84.8900 -5628.6804  
-379.1026 0.0000 0.0000 2062.1029 -335.7571 304.3547 -2397.8600  
-312.4171 300.5712

TIMING: 41000 CPU: 507.643, 0.0117453/step Wall: 507.767, 0.0117537/step, 0.0293843 hours remaining, 102.941406 MB of memory in use.

ENERGY: 41000 515.0984 1464.5944 1585.3953 104.2255 -5609.0320  
-405.7156 0.0000 0.0000 2042.2694 -303.1646 301.4274 -2345.4339  
-279.4245 300.7573

ENERGY: 41500 559.8762 1451.6256 1561.5956 94.1046 -5586.7215  
-415.2647 0.0000 0.0000 2054.5702 -280.2140 303.2429 -2334.7842  
-257.4277 302.4432

TIMING: 42000 CPU: 522.747, 0.0151039/step Wall: 522.871, 0.0151035/step, 0.0335633 hours remaining, 103.097656 MB of memory in use.

ENERGY: 42000 531.4476 1465.5735 1578.2904 88.1504 -5600.7112  
-395.0170 0.0000 0.0000 2087.8164 -244.4498 308.1499 -2332.2663  
-222.1564 304.8051

ENERGY: 42500 511.9259 1482.7713 1599.9337 85.6626 -5568.9136  
-431.1376 0.0000 0.0000 2089.1010 -230.6567 308.3395 -2319.7577  
-205.3795 305.7024

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 42500

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 42500

WRITING COORDINATES TO RESTART FILE AT STEP 42500

FINISHED WRITING RESTART COORDINATES

WRITING VELOCITIES TO RESTART FILE AT STEP 42500

FINISHED WRITING RESTART VELOCITIES

TIMING: 43000 CPU: 532.699, 0.00995196/step Wall: 532.823, 0.00995194/step, 0.019351 hours remaining, 103.300781 MB of memory in use.

ENERGY: 43000 556.3910 1411.2977 1575.6581 84.8612 -5590.3238  
-375.9869 0.0000 0.0000 2144.7997 -193.3030 316.5603 -2338.1027  
-168.3193 308.6923

ENERGY: 43500 536.7583 1471.7297 1586.0072 93.2241 -5627.7766  
-374.6140 0.0000 0.0000 2111.4003 -203.2710 311.6307 -2314.6713  
-178.4155 309.6238

TIMING: 44000 CPU: 542.687, 0.00998798/step Wall: 542.814, 0.00999144/step, 0.0166524 hours remaining, 103.300781 MB of memory in use.

ENERGY:	44000	555.4597	1461.7595	1577.4770	97.4407	-5621.3886
	-369.7415	0.0000	0.0000	2107.4348	-191.5584	311.0454
	-166.7266	309.3828				-2298.9932

LDB: ===== START OF LOAD BALANCING ===== 546.17

LDB: ===== END OF LOAD BALANCING ===== 546.17

LDB: ===== DONE WITH MIGRATION ===== 546.171

LDB: ===== START OF LOAD BALANCING ===== 547.153

LDB: ===== END OF LOAD BALANCING ===== 547.153

LDB: ===== DONE WITH MIGRATION ===== 547.153

ENERGY:	44500	570.3776	1433.4225	1584.8821	99.8304	-5587.5123
	-397.9257	0.0000	0.0000	2114.0262	-182.8992	312.0183
	-155.8573	310.2428				-2296.9254

TIMING: 45000 CPU: 554.61, 0.0119229/step Wall: 554.743, 0.0119291/step, 0.0165682 hours remaining, 103.300781 MB of memory in use.

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW
BOUNDARY		MISC	KINETIC	TOTAL	TEMP	POTENTIAL	TOTAL3
TEMPAVG							

ENERGY:	45000	536.9994	1459.1237	1595.3141	98.2115	-5602.5933
	-381.4521	0.0000	0.0000	2033.1651	-261.2316	300.0837
	-238.0998	305.6627				-2294.3967

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 45000

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 45000

WRITING COORDINATES TO RESTART FILE AT STEP 45000

FINISHED WRITING RESTART COORDINATES

WRITING VELOCITIES TO RESTART FILE AT STEP 45000

FINISHED WRITING RESTART VELOCITIES

ENERGY:	45500	521.6228	1455.5904	1574.7467	111.3981	-5602.4937
	-376.2806	0.0000	0.0000	2065.1523	-250.2640	304.8048
	-223.5789	304.5059				-2315.4164

TIMING: 46000 CPU: 565.418, 0.0108082/step Wall: 565.562, 0.0108188/step, 0.0120209 hours remaining, 103.300781 MB of memory in use.

ENERGY:	46000	513.8371	1525.9308	1584.0248	90.0718	-5663.6019
	-384.0214	0.0000	0.0000	2129.7089	-204.0499	314.3330
	-179.2982	306.6575				-2333.7587

ENERGY:	46500	522.7833	1446.2126	1569.9277	97.1367	-5555.8506
	-412.5926	0.0000	0.0000	2101.2194	-231.1635	310.1281
	-205.9308	306.8229				-2332.3830

TIMING: 47000 CPU: 579.166, 0.013748/step Wall: 579.308, 0.013746/step, 0.011455 hours remaining, 103.457031 MB of memory in use.

ENERGY: 47000 527.9774 1445.9827 1563.3734 97.7786 -5531.7743  
-461.1893 0.0000 0.0000 2090.2676 -267.5840 308.5117 -2357.8516  
-243.4666 304.3990

ENERGY: 47500 535.6700 1412.2804 1546.2775 102.7396 -5543.7306  
-392.9060 0.0000 0.0000 2050.8706 -288.7985 302.6969 -2339.6691  
-264.6534 303.2868

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 47500

WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 47500

WRITING COORDINATES TO RESTART FILE AT STEP 47500

FINISHED WRITING RESTART COORDINATES

WRITING VELOCITIES TO RESTART FILE AT STEP 47500

FINISHED WRITING RESTART VELOCITIES

TIMING: 48000 CPU: 589.11, 0.00994398/step Wall: 589.252, 0.00994372/step, 0.00552429 hours  
remaining, 103.457031 MB of memory in use.

ENERGY: 48000 526.9699 1493.4987 1569.1180 83.8480 -5606.4782  
-401.0432 0.0000 0.0000 2053.0940 -280.9928 303.0251 -2334.0868  
-258.3303 304.0394

LDB: ===== START OF LOAD BALANCING ===== 594.764

LDB: ===== END OF LOAD BALANCING ===== 594.764

LDB: ===== DONE WITH MIGRATION ===== 594.764

LDB: ===== START OF LOAD BALANCING ===== 596.531

LDB: ===== END OF LOAD BALANCING ===== 596.531

LDB: ===== DONE WITH MIGRATION ===== 596.531

ENERGY: 48500 513.7201 1446.2377 1560.7539 108.0969 -5594.4494  
-400.3233 0.0000 0.0000 2034.5633 -331.4008 300.2900 -2365.9641  
-309.6698 303.5667

TIMING: 49000 CPU: 605.698, 0.016588/step Wall: 605.841, 0.0165898/step, 0.00460828 hours  
remaining, 103.457031 MB of memory in use.

ENERGY: 49000 540.6392 1459.4610 1547.8740 102.4680 -5610.8270  
-410.9085 0.0000 0.0000 2024.2493 -347.0439 298.7677 -2371.2932  
-324.0890 300.0600

ENERGY: 49500 535.0577 1458.9162 1581.6973 89.3077 -5638.4087  
-391.2205 0.0000 0.0000 2007.7806 -356.8696 296.3371 -2364.6502  
-335.4947 295.9533

TIMING: 50000 CPU: 615.798, 0.0100999/step Wall: 615.94, 0.0100987/step, 0 hours remaining,  
103.457031 MB of memory in use.

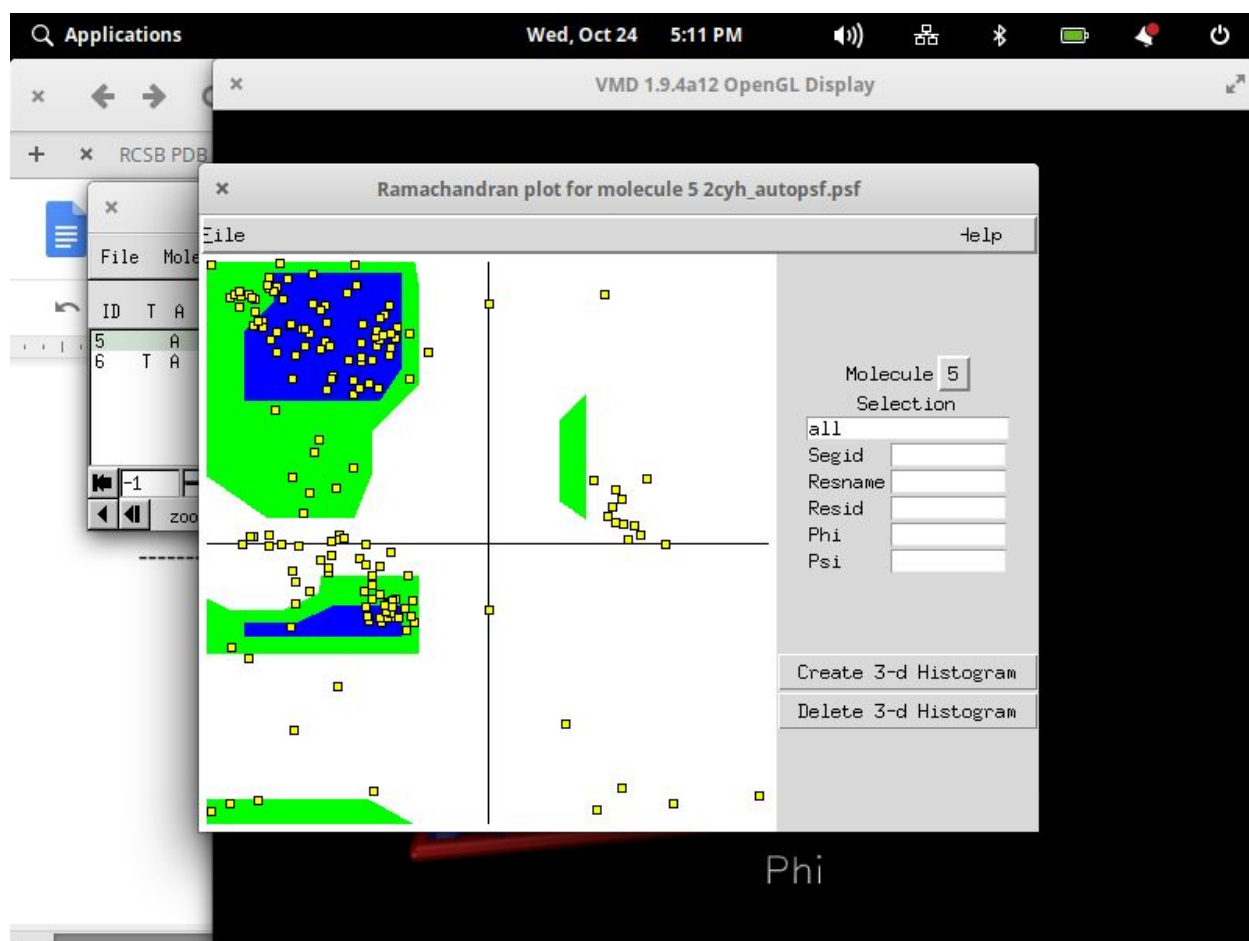
ETITLE: TS BOND ANGLE DIHED IMPRP ELECT VDW  
BOUNDARY MISC KINETIC TOTAL TEMP POTENTIAL TOTAL3  
TEMPAVG

ENERGY: 50000    528.6220    1392.4975    1584.7464    101.1052    -5586.7147  
-392.2814    0.0000    0.0000    1989.9427    -382.0823    293.7043    -2372.0250  
-358.5143    298.5692

WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 50000  
WRITING COORDINATES TO DCD FILE 2cyhfinal.dcd AT STEP 50000  
WRITING COORDINATES TO RESTART FILE AT STEP 50000  
FINISHED WRITING RESTART COORDINATES  
WRITING VELOCITIES TO RESTART FILE AT STEP 50000  
FINISHED WRITING RESTART VELOCITIES  
WRITING EXTENDED SYSTEM TO OUTPUT FILE AT STEP 50000  
CLOSING EXTENDED SYSTEM TRAJECTORY FILE  
WRITING COORDINATES TO OUTPUT FILE AT STEP 50000  
CLOSING COORDINATE DCD FILE 2cyhfinal.dcd  
WRITING VELOCITIES TO OUTPUT FILE AT STEP 50000  
=====

WallClock: 616.444275 CPUTime: 616.230408 Memory: 103.457031 MB  
[Partition 0][Node 0] End of program

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Ramachandran Plot for 2cyh