

Supporting Information for *A Transition State “Trapped”? Modeling Biphenyl
Torsional Rotation with a QM-cluster Model of Engineered Threonyl-tRNA
Synthetase*

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Potential Energy Scans

Cluster models of the torsional conformations were obtained by freezing C_α and select C_β atoms (Figure 2) to their x-ray crystallographic coordinates using Gaussian09 freeze codes, along with using generalized redundant internal coordinates to constrain the p-biphenylalanine C_β position, a select H- C_β - C_γ -H dihedral angle (Figure 3), and the two central C-C dihedral angles characteristic of the rotating biphenyl rings. To reproduce the constrained dihedral scans, the redundant internal coordinates below should be used with “opt(modred)” in Gaussian09:

115 114 121 120 F

113 114 121 122 F

268 31 111 112 F

111 F

Table S1. List of residues included in the QM cluster model. Total charge of model is neutral.

Species/residue label	Protonated R group?	Species/residue charge	Trim N-side	Trim R-group	Trim C-side
4S02					
Y ¹⁰	N/A	0	H	H	-
BIF ¹¹	N/A	0	-	-	-
E ¹²	N	-1	-	-	-
Y ¹³	N/A	0	-	-	H
R ³⁴	Y	+1	H	-	-
M ³⁵	N/A	0	-	-	-
E ³⁶	N/A	0	-	H	H
V ³⁸	N/A	0	H	-	H
V ⁴⁰	N/A	0	H	-	-
A ⁴¹	N/A	0	-	H	-
F ⁴² W	N/A	0	-	-	H
F ⁷⁷	N/A	0	H	-	-
V ⁷⁸	N/A	0	-	H	-
Y ⁷⁹ A	N/A	0	-	-	H
A ¹¹⁵	N/A	0	H	-	H
I ¹²¹	N/A	0	H	-	H
F ¹²³ Y	N/A	0	H	-	-
K ¹²⁴	N/A	0	-	H	-
I ¹²⁵	N/A	0	-	-	H
4S0J					
F ⁴² F	N/A	0	-	-	H
Y ⁷⁹ S	N/A	0	-	-	H
F ¹²³ V	N/A	0	H	-	-

4S0L						
F ⁴² F	N/A	0	-	-	H	
Y ⁷⁹ V	N/A	0	-	-	H	
W ⁸¹	N/A	0	H	-	H	
F ¹²³ V	N/A	0	H	-	-	
4S0I						
F ⁴² F	N/A	0	-	-	H	
Y ⁷⁹ S	N/A	0	-	-	H	
F ¹²³ A	N/A	0	H	-	-	
4S0I_W81						
F ⁴² F	N/A	0	-	-	H	
Y ⁷⁹ S	N/A	0	-	-	H	
W ⁸¹	N/A	0	H	-	H	
F ¹²³ A	N/A	0	H	-	-	
4S0K						
F ⁴² F	N/A	0	-	-	H	
Y ⁷⁹ V	N/A	0	-	-	H	
W ⁸¹	N/A	0	H	-	H	
F ¹²³ A	N/A	0	H	-	-	
4S03						
F ⁴² F	N/A	0	-	-	H	
Y ⁷⁹ I	N/A	0	-	-	H	
F ¹²³ A	N/A	0	H	-	-	
4S03_W81						
F ⁴² F	N/A	0	-	-	H	
Y ⁷⁹ I	N/A	0	-	-	H	
W ⁸¹	N/A	0	H	-	H	
F ¹²³ A	N/A	0	H	-	-	

Table S2. Comparison of calculated Φ among constrained and unconstrained cluster models. Experimental Φ are from their respective PDB crystal structures.

Model	Conditions	Experimental Φ (degrees)	Φ at $dE/d\Phi = 0$ (degrees)	Unconstrained model Φ (degrees)	Relaxation Energy (kcal/mol)
4S02	Gas	26	28.4	29.0	0.84
	Gas+GD3BJ	26	18.8	31.1	2.2
	CPCM	26	25.3	24.9	0.83
	CPCM+GD3BJ	26	24.8	31.9	0.90
4S0J	CPCM+GD3BJ	35	32.1	33.2	0.38
4S0L	CPCM+GD3BJ	21	25.2	32.0	2.3
4S0I	CPCM+GD3BJ	15	28.0	27.4	0.92

4S0I_W81	CPCM+GD3BJ	15	28.7	29.6	1.4
4S0K	CPCM+GD3BJ	20	23.0	26.7	0.39
4S03	Gas	0	2.3	-27.5	1.4
	Gas+GD3BJ	0	-0.4	9.4	0.53
	CPCM	0	2.8	-28.9	2.4
	CPCM+GD3BJ	0	-2.1	-6.7	0.33
4S03_W81	Gas	0	10.5	-26.7	1.9
	Gas+GD3BJ	0	-7.6	-13.1	0.33
	CPCM	0	10.5	-28.7	2.5
	CPCM+GD3BJ	0	-2.5	-10.9	0.48

Table S3. Thermal flexibility of biphenyl within the protein clusters at 310K, and root mean square deviation (RMSD) values between the trimmed x-ray crystal structure and its respective optimized unconstrained model.

Model	Conditions	Thermally Allowed Displacement from $\Phi_{\min}$ (degrees)		Thermal Range (degrees)	RMSD of Cluster Model (Angstroms)	Resolution of Crystallized Enzyme (Angstroms)
4S02	Gas	-12.6	+10.5	23.1	0.73	1.95
	Gas+GD3BJ	-15.0	+15.0	30.0	0.87	1.95
	CPCM	-12.4	+9.8	22.2	0.95	1.95
	CPCM+GD3BJ	-13.0	+10.5	23.5	0.78	1.95
4S0J	CPCM+GD3BJ	-8.6	+8.7	17.3	0.47	2.1
4S0L	CPCM+GD3BJ	-10.1	+9.8	19.9	0.87	2.5
4S0I	CPCM+GD3BJ	-12.1	+10.2	22.3	0.57	2.36
4S0I_W81	CPCM+GD3BJ	-10.4	+9.6	20.0	0.53	2.36
4S0K	CPCM+GD3BJ	-16.2	+9.9	26.1	0.53	2.1
4S03	Gas	-16.3	+19.7	36.0	0.62	2.05
	Gas+GD3BJ	-12.6	+15.2	27.8	0.52	2.05
	CPCM	-14.9	+19.8	34.7	0.58	2.05
	CPCM+GD3BJ	-12.1	+13.3	25.4	0.37	2.05
4S03_W81	Gas	-20.0	+14.4	34.4	0.78	2.05
	Gas+GD3BJ	-10.4	+15.7	26.1	0.66	2.05
	CPCM	-18.8	+15.8	34.6	0.85	2.05
	CPCM+GD3BJ	-11.5	+14.0	25.5	0.47	2.05

Table S4. Average RMSD calculations between the original PDB crystal structure and structures from the MD simulation

Enzyme	RMSD of Entire Enzyme (Å)	RMSD of Cluster Model Residues (Å)
4S02	0.52	0.30
4S0J	0.35	0.31
4s0L	0.36	0.30
4S0I	0.37	0.31
4S0K	0.36	0.30
4S03	0.33	0.28

BiPhe-Water Distances

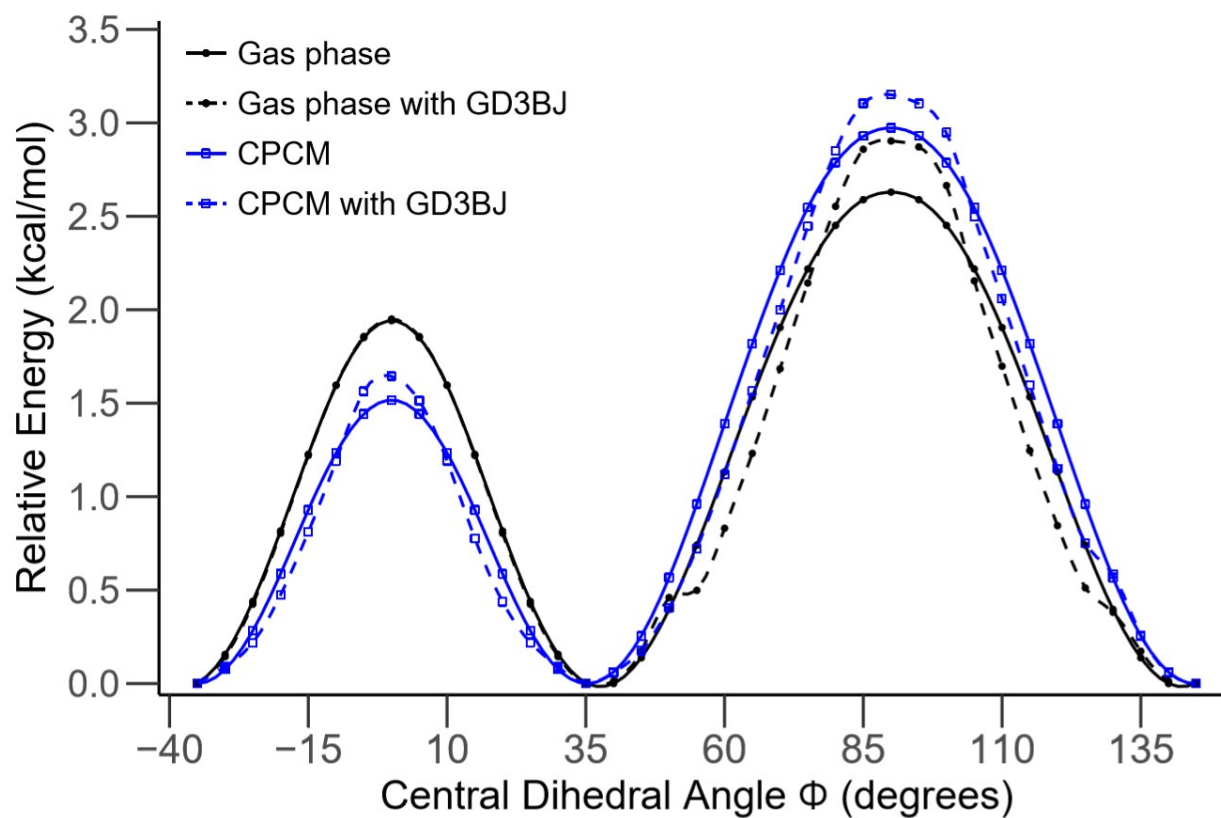
The MD simulations reinforce the expectation that the BiPhe residue has no significant interaction with the solvent, as anticipated by the hydrophobic residues surrounding the side chain and the absence of nearby waters in the crystal structure. The distance between the oxygen of the nearest water to the nearest atom of BiPhe (which is consistently the solvent-exposed atom H9 or H10, two hydrogens on the terminal ring of BiPhe) was measured and averaged for each of the MD simulations. The average of the shortest distance ranges from 2.85 Å (s , or standard deviation, of 0.33 Å) of 4S02 to 3.04 Å ($s = 0.39$ Å) of 4S0J, indicating no strong solvent-BiPhe residue interaction.

Table S6. Residue interactions with BIF¹¹ within the 4S0x enzymes. C_{MC} indicates a main chain contact with BIF¹¹. C_{SC} indicates a side chain contact with BIF¹¹. O_{MC} indicates a main chain overlap with BIF¹¹. O_{SC} indicates a side chain overlap with BIF¹¹. HB indicates the main chain hydrogen bonds with the BIF¹¹ main chain. (*) indicates the residues were included in the model for inter-model consistency and no distinct BIF¹¹-residue interaction was detected. (**) indicates the residue main chain was included for structural integrity and no distinct BIF¹¹-residue interaction was detected.

Residue Position	1Y2Q		4S02						4S0J						4S0L				
			CMC	CSC	OMC	OSC	HB		CMC	CSC	OMC	OSC	HB		CMC	CSC	OMC	OSC	HB
10	Y	Y	*	*	*	*	*	Y	1					Y	1				
12	E	E	1					E	1					E	1				
13	Y	Y		11				Y	9			2		Y		8			
34	R	R	2	2	1			R	2	1	1			R	2		1		
35	M	M	3		1		1	M	3		1		1	M	3		1		1
36	E	E	**	**	**	**	**	E	**	**	**	**	**	E	**	**	**	**	**
38	V	V		3				V		3				V		3			
40	V	V		7				V		8				V		7			
41	A	A	**	**	**	**	**	A	**	**	**	**	**	A	**	**	**	**	**
42	F	W		6			1	F		5		1		F		5			
77	F	F		11			4	F		11		2		F		4		1	
78	V	V	**	**	**	**	**	V	**	**	**	**	**	V	**	**	**	**	**
79	Y	A		4				S		7		1		V		13		4	
81	F	W						W						W		1			
115	A	A		5			3	A		5		2		A		5			
121	K	I		10				I		7				I		6			
123	F	Y		10				V		7		3		V		10		1	
124	K	K	1		1			K	2					K	1				
125	I	I	1	6			1	I	1	7				I		7			

Residue Position	1Y2Q	4S0I						4S0K						4S03					
			CMC	CSC	OMC	OSC	HB		CMC	CSC	OMC	OSC	HB		CMC	CSC	OMC	OSC	HB
10	Y	Y	*	*	*	*	*	Y	*	*	*	*	*	Y		1			
12	E	E	1					E	2					E	2				
13	Y	Y		6				Y		6				Y		7			
34	R	R	1		1			R	2	1	1			R	2	1	1		
35	M	M	3		1		1	M	3		1		1	M	3				1
36	E	E	**	**	**	**	**	E	**	**	**	**	**	E	**	**	**	**	**
38	V	V		1				V		1				V	*	*	*	*	*
40	V	V		7				V		6				V		5			
41	A	A	**	**	**	**	**	A	**	**	**	**	**	A	**	**	**	**	**
42	F	F		5				F		5				F		4			
77	F	F		8		1		F		7		1		F		4		2	
78	V	V	**	**	**	**	**	V	**	**	**	**	**	V	**	**	**	**	**
79	Y	S		4				V		14				I		15		2	
81	F	W						W		2				W					
115	A	A		6		1		A		6				A	*	*	*	*	*
121	K	I		7				I		9		1		I		8			
123	F	A		3				A		8		1		A		9		1	
124	K	K	2		1			K	2					K	3				
125	I	I	1	7		1		I		6				I	1	8		1	

Figure S1. Potential energy curves for the torsional rotation of free biphenyl.



(a)

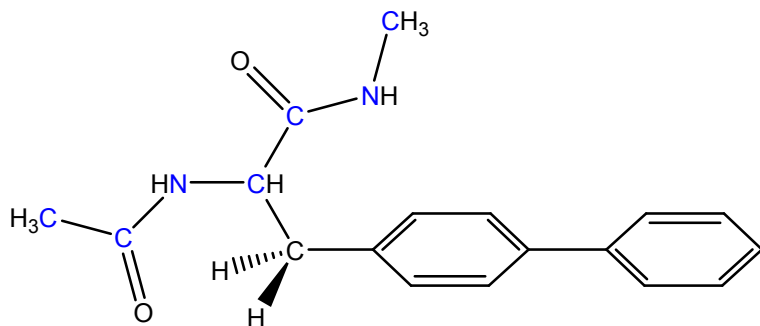
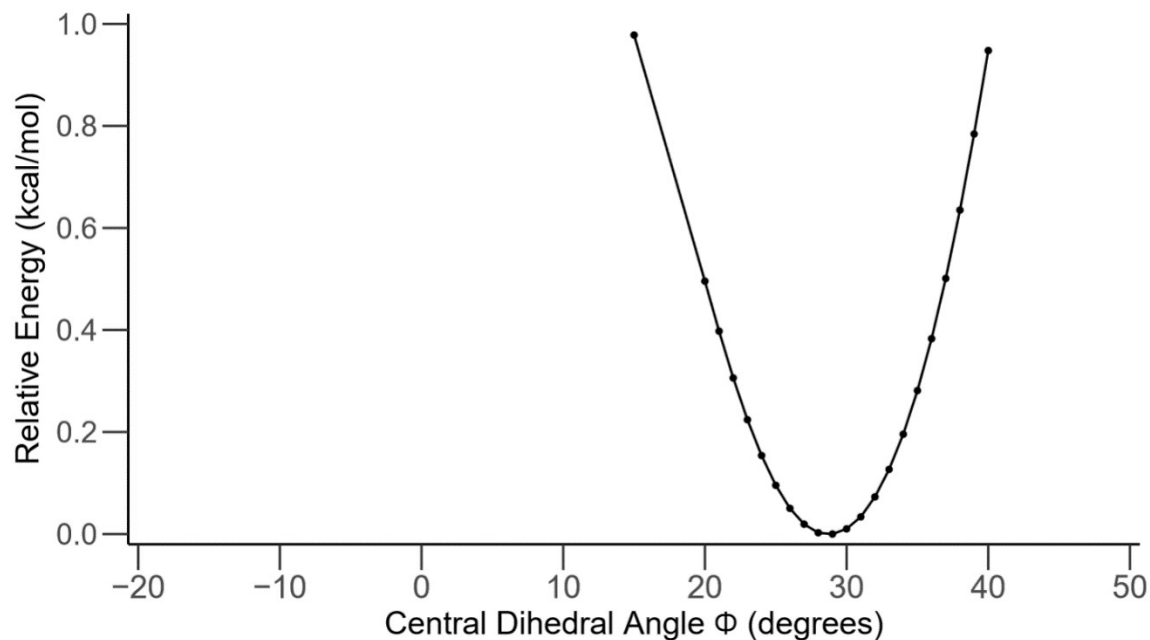


Figure S3. Potential energy curve near equilibrium for the torsional rotation of p-biphenylalanine within the (a) 4S0I_W81 and (b) 4S03_W81 protein cluster models. The 4S0I_W81 scan was only computed using the B3LYP/6-31G(d')+CPCM+GD3BJ level of theory. The 4S03_W81 scan was carried out in gas/aqueous phase, with and without GD3BJ.

a – 4S0I_W81



b – 4S03_W81

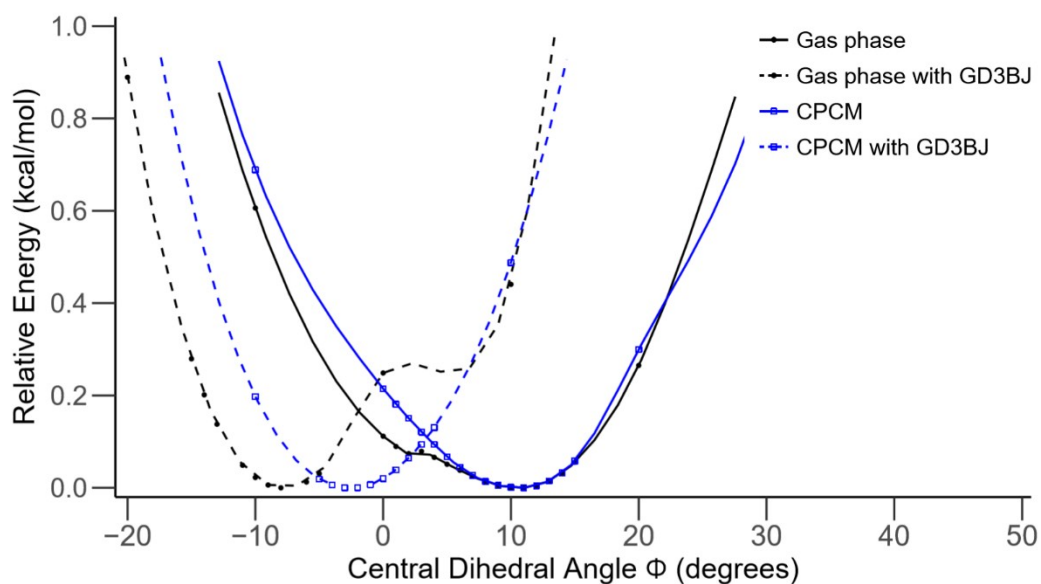
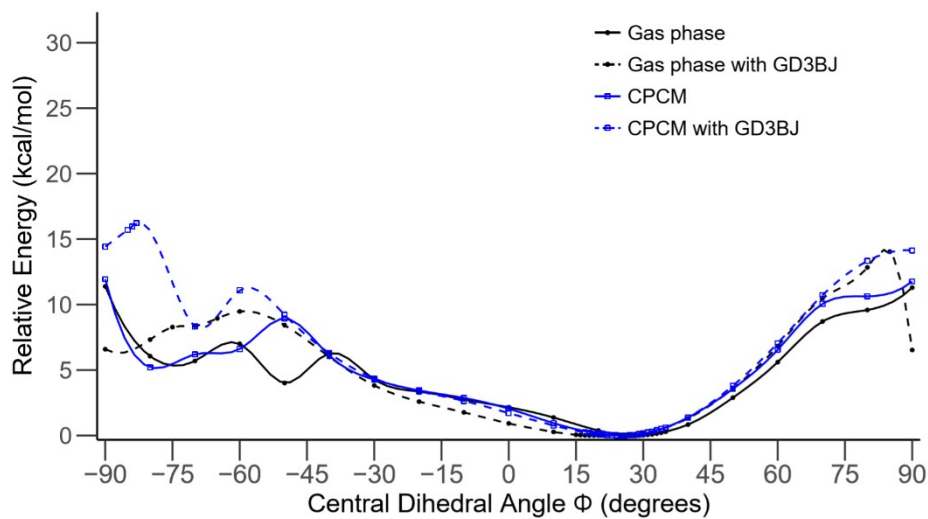
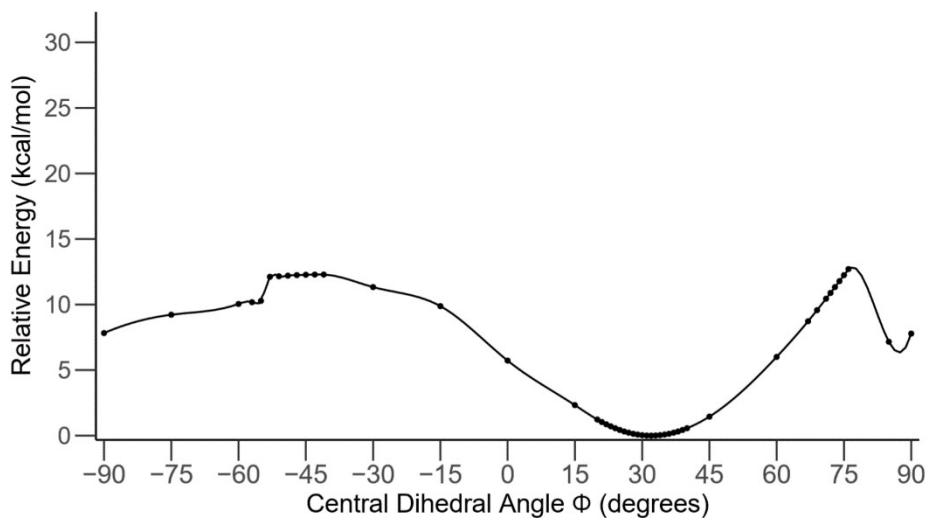


Figure S4. 180°-scan potential energy curves for the torsional rotation of p-biphenylalanine within the (a) 4S02, (b) 4S0J, (c) 4S0L, (d) 4S0I, (e) 4S0I_W81, (f) 4S0K, (g) 4S03, and (h) 4S03_W81 enzyme cluster models, calculated at the B3LYP/6-31G(d')+CPCM+GD3BJ level of theory unless otherwise labeled.

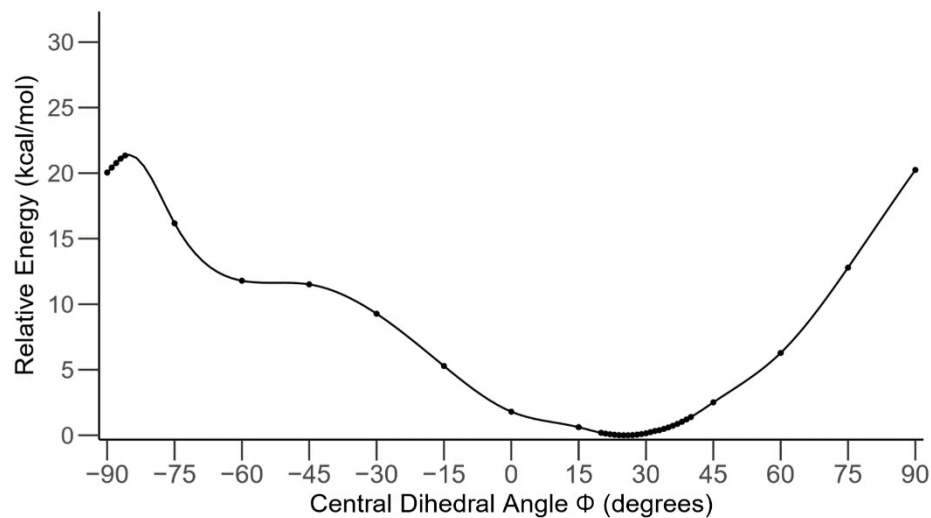
a – 4S02



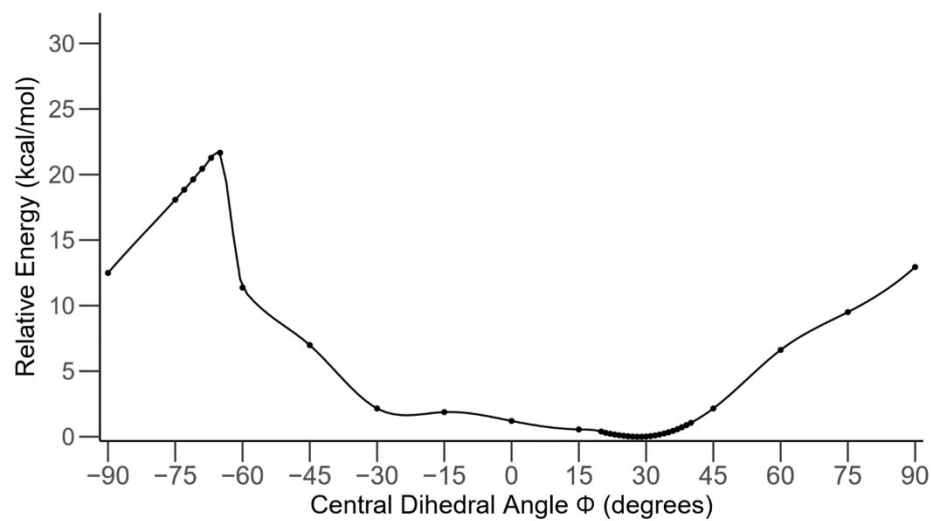
b – 4S0J



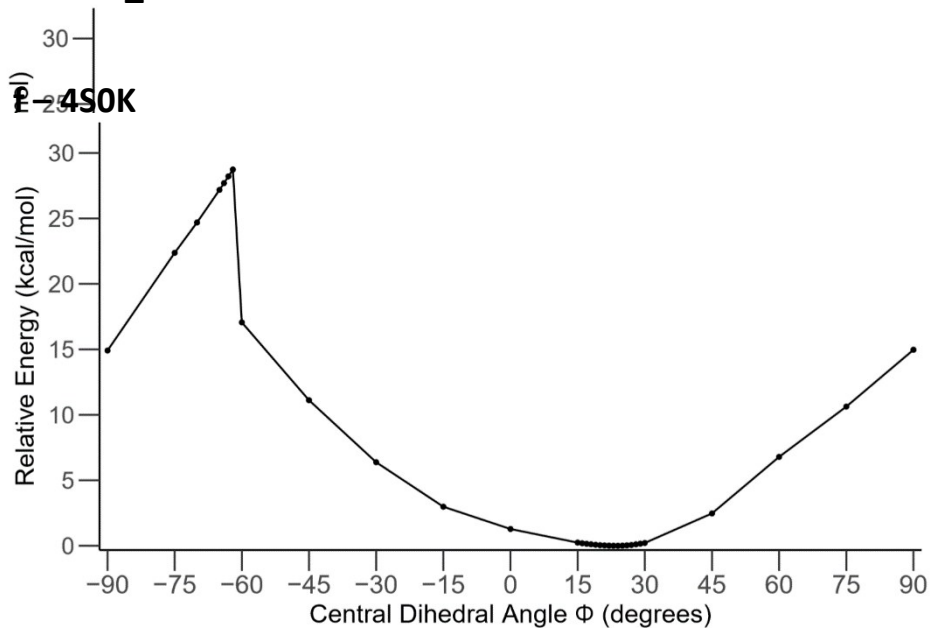
c – 4S0L



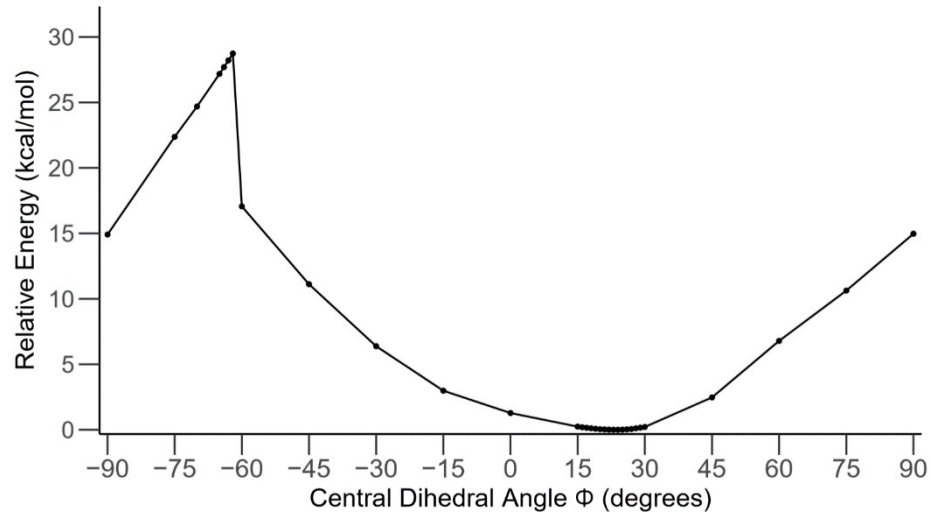
d – 4S0I



e – 4S0I_W81



f – 4S0K



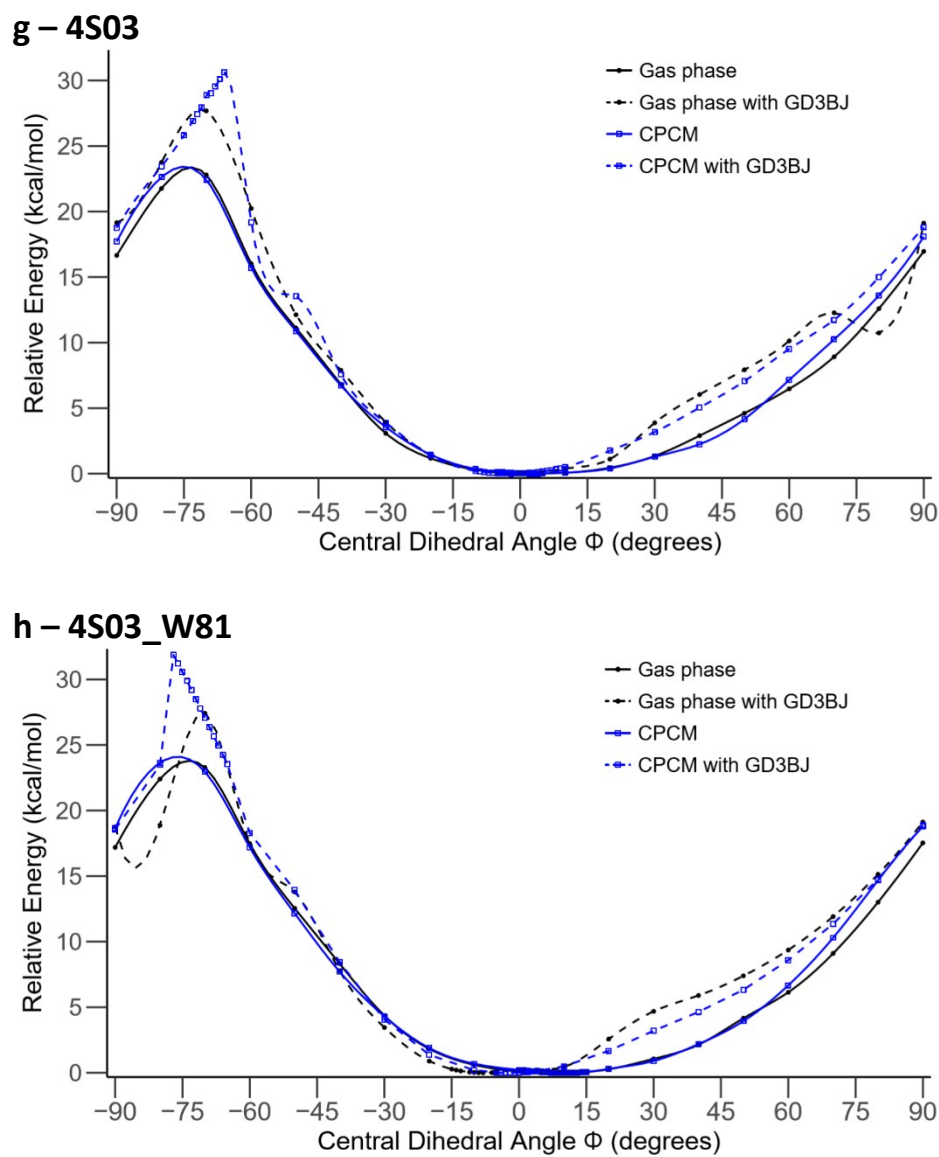


Figure S5.

Linear model between the computed thermal range for p-biphenylalanine within a given protein core model and the x-ray crystallographic resolution.

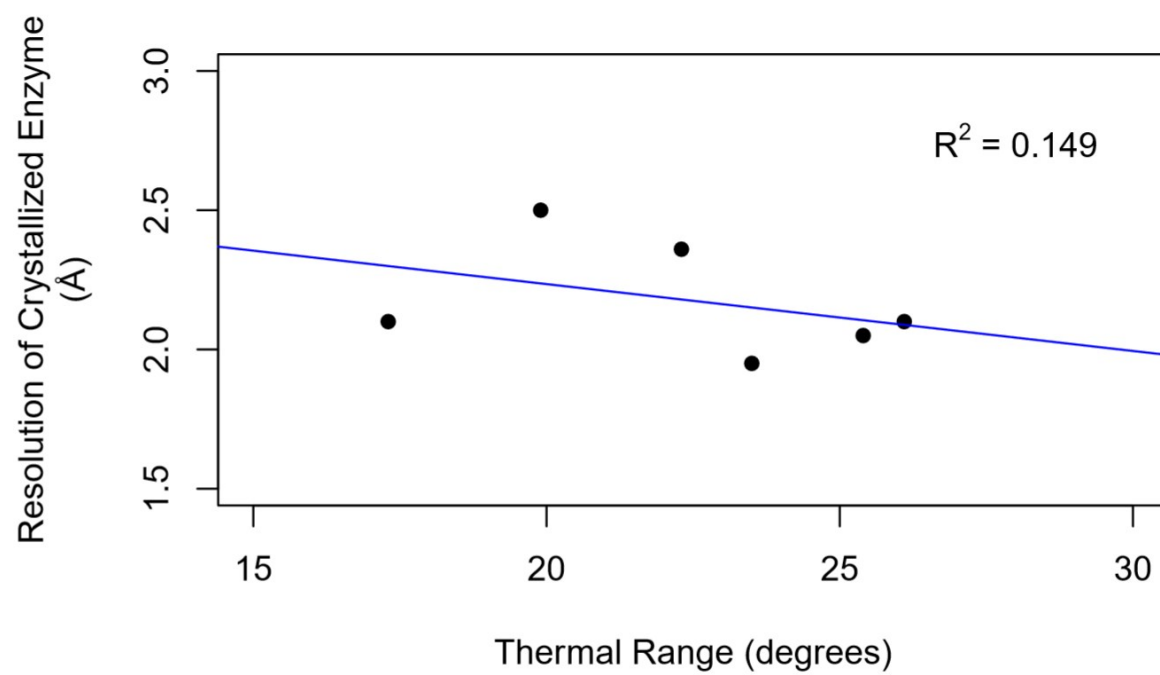


Figure S6. RMSD of non-hydrogen atoms of the whole protein and QM-cluster residues for MD simulations of (a) 4S02 (b) 4S0J (c) 4S0L (d) 4S0I (e) 4S0K and (f) 4S03 compared to their respective crystal structure with respect to a timescale of 10 ns.

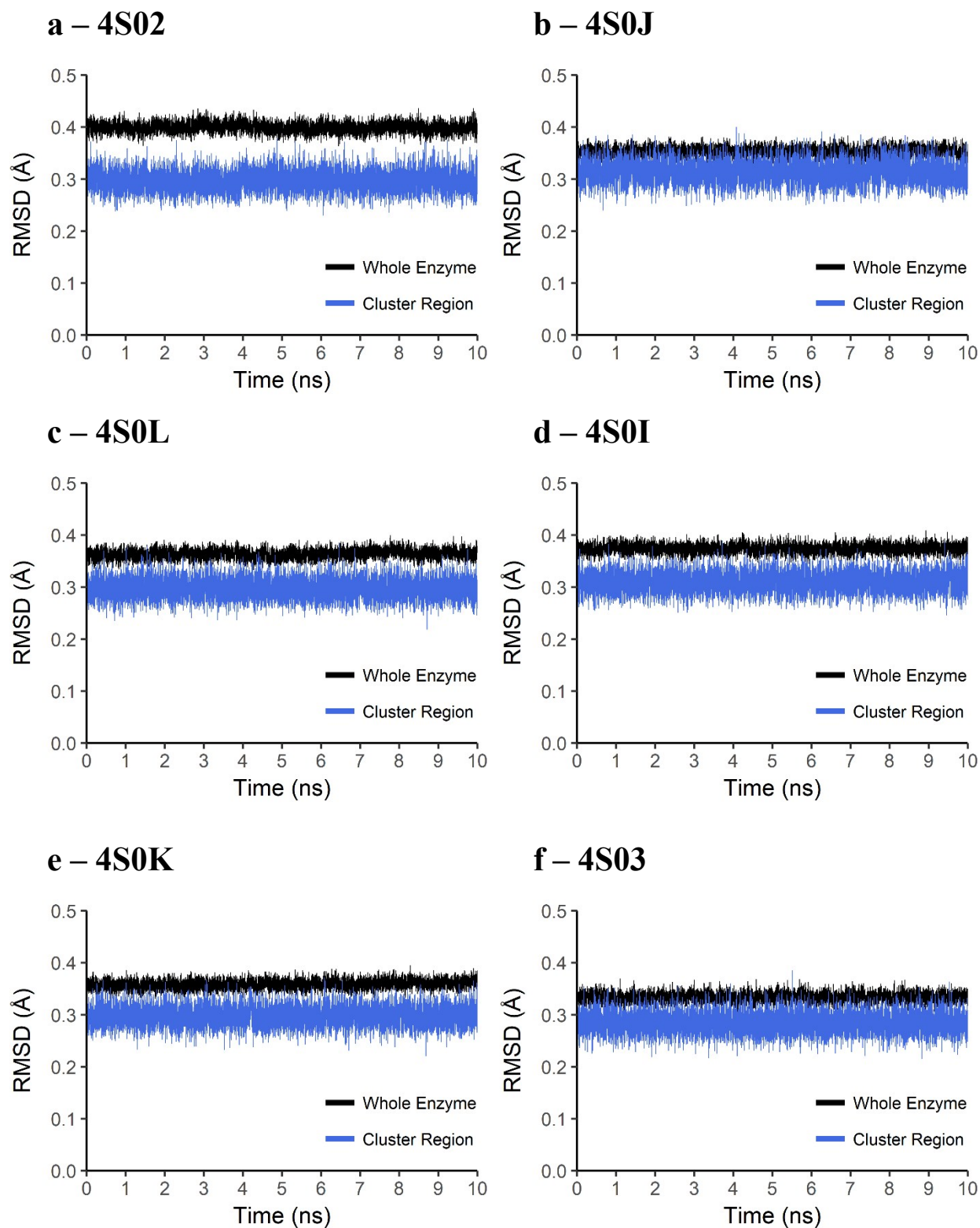


Figure S7. a) Average RMSD of non-hydrogen atoms of select residues within MD simulations compared to their respective crystal structure. **b)** Relative change in residue RMSD with respect to its value in the previous model. Note that the abnormal

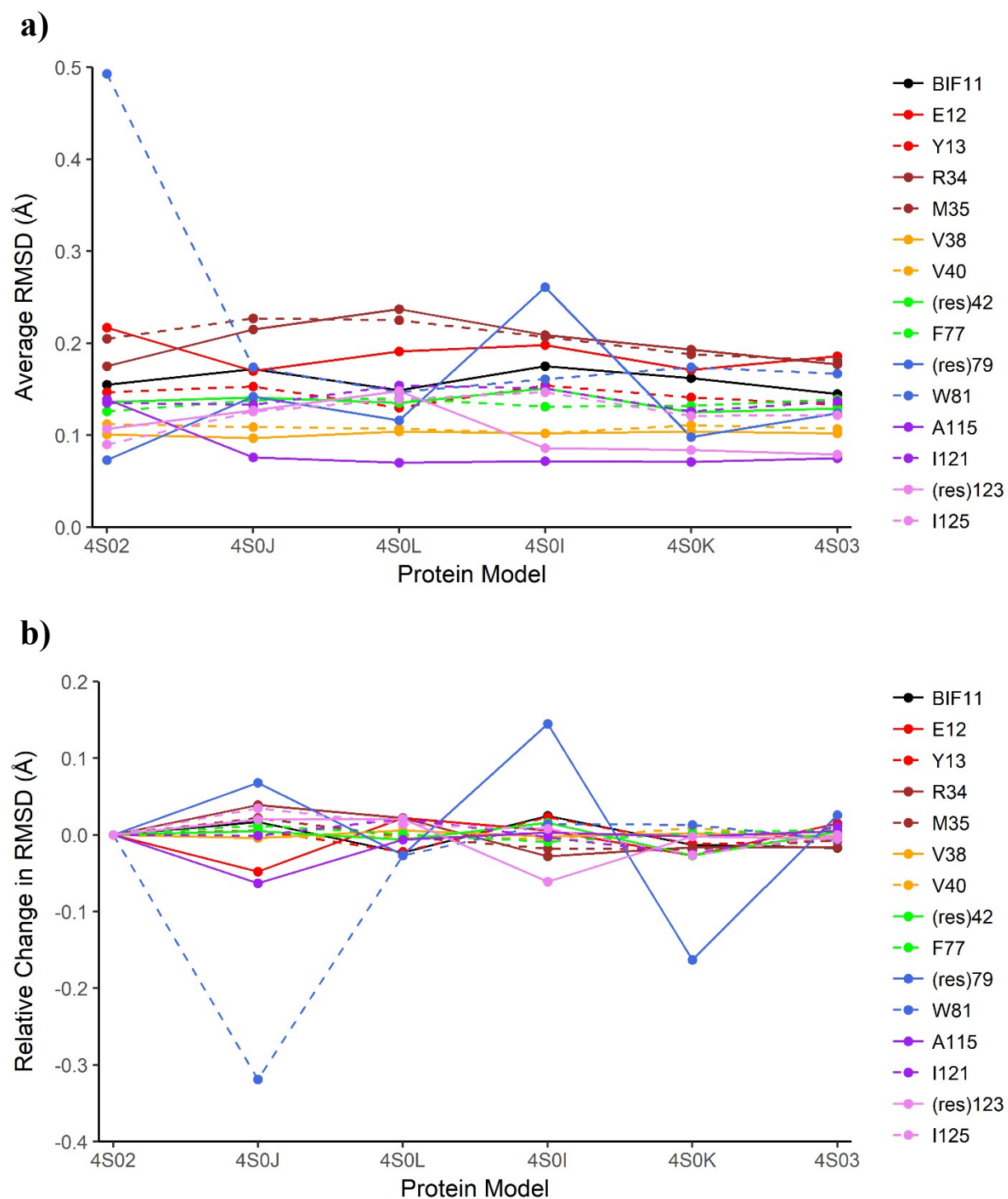
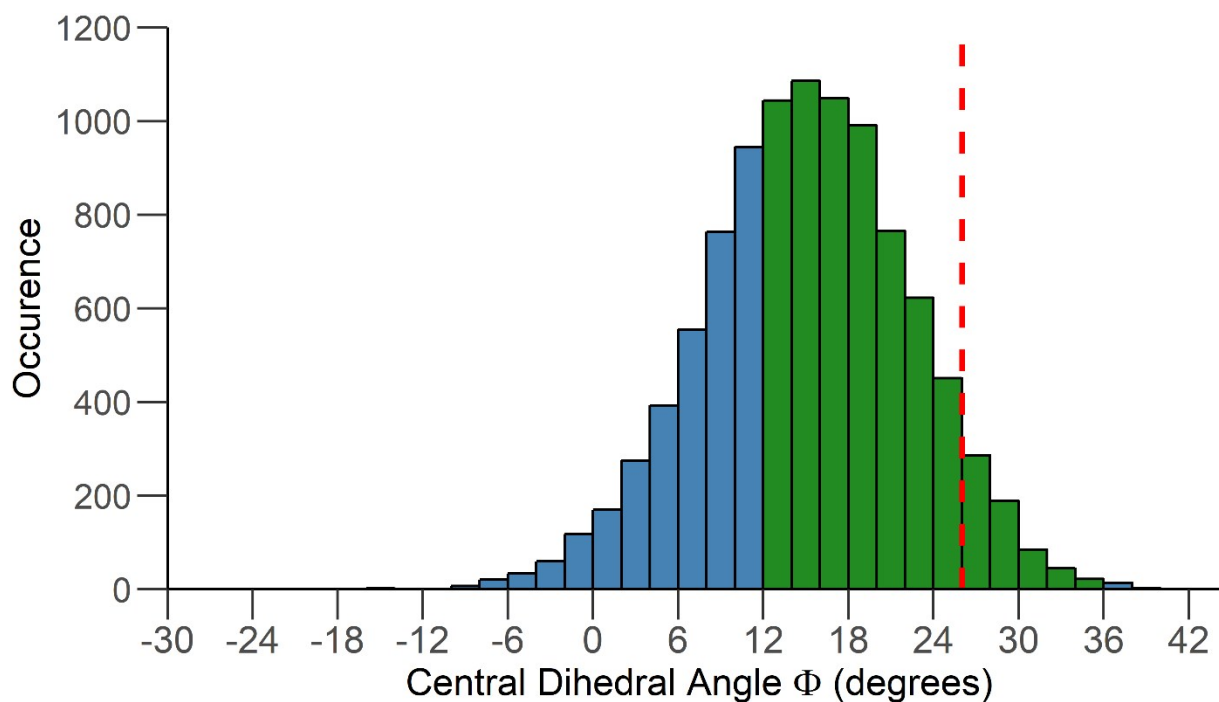
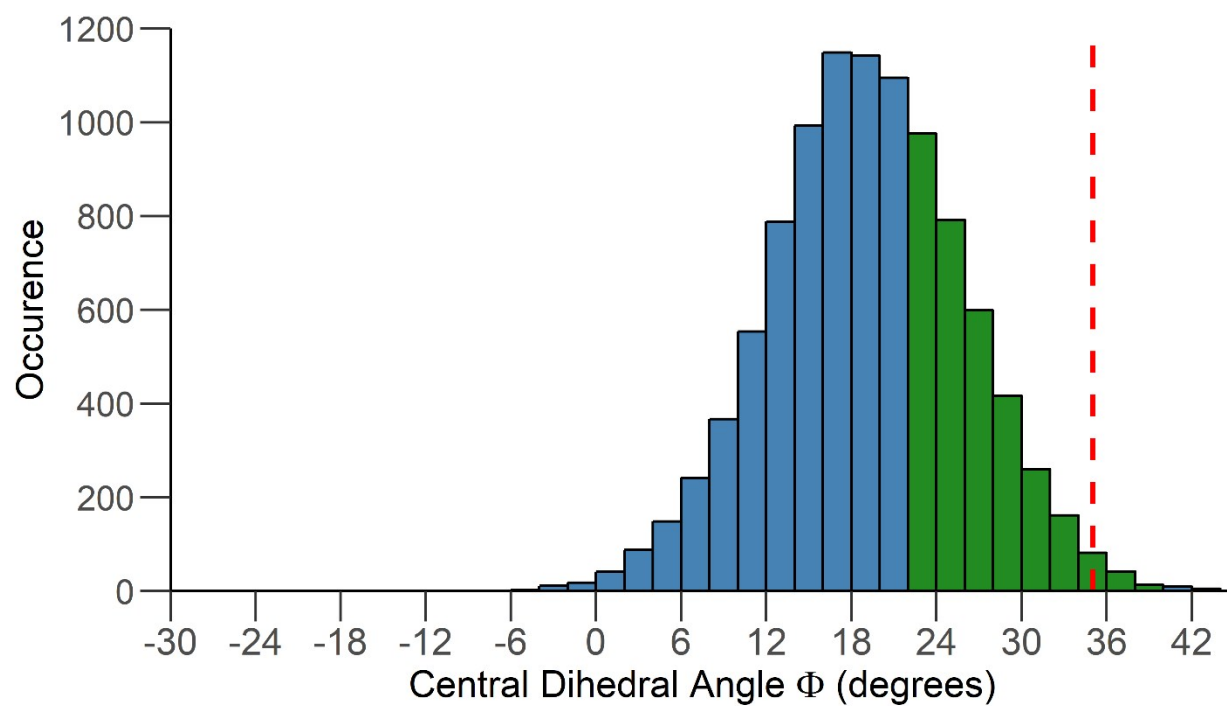


Figure S8. Distribution of the BiPhe central dihedral angles in MD simulation snapshots of (a) 4S02 (b) 4S0J (c) 4S0L (d) 4S0I (e) 4S0K and (f) 4S03. The red dashed line represents the x-ray crystallographically determined value. Green is used to represent dihedral angle values within the thermal range calculated by our cluster models.

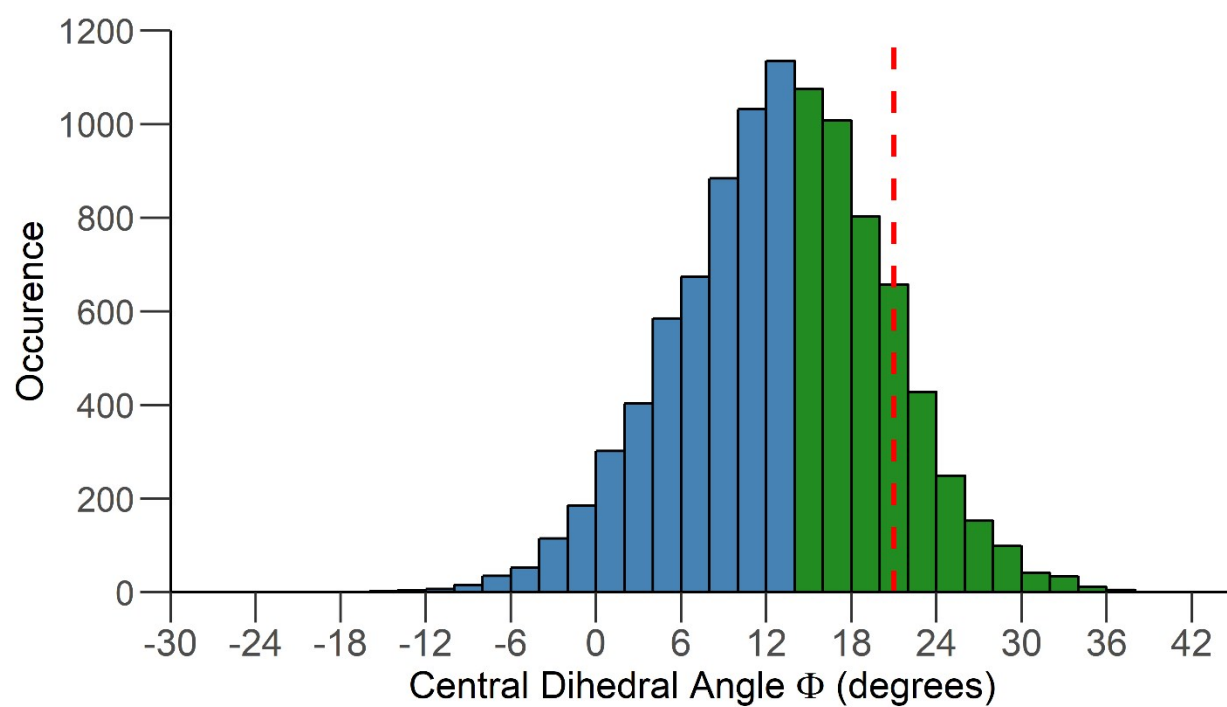
a – 4S02



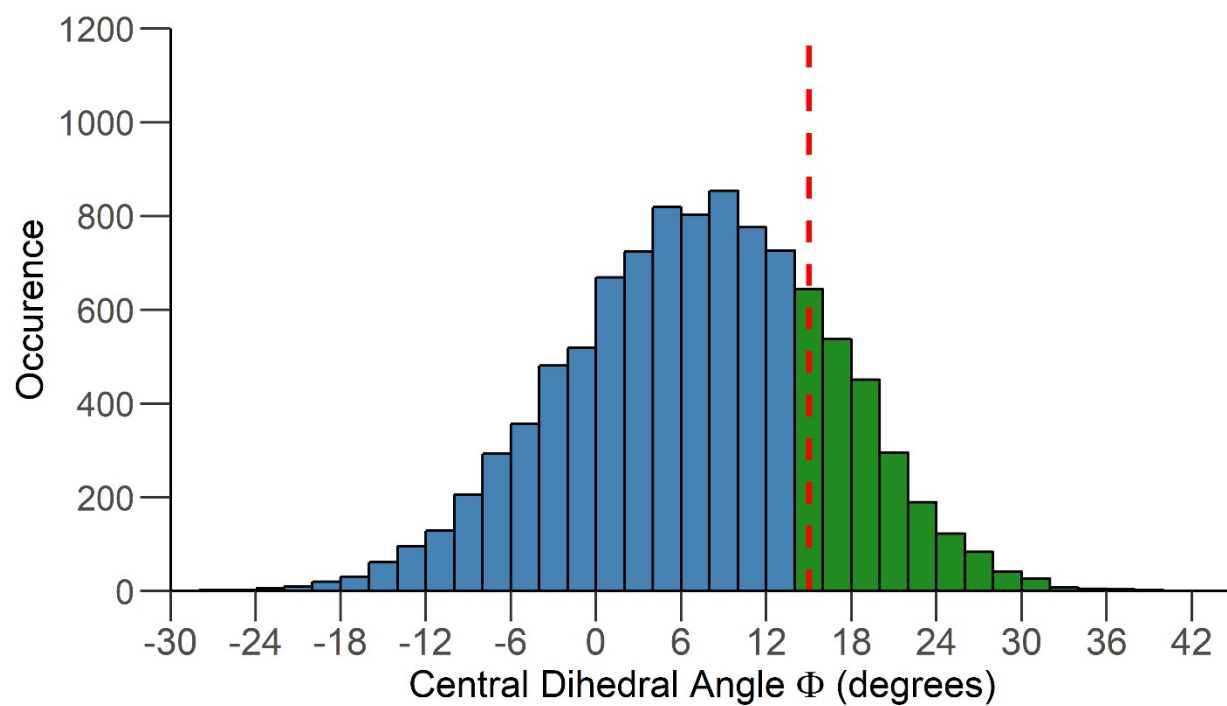
b – 4S0J



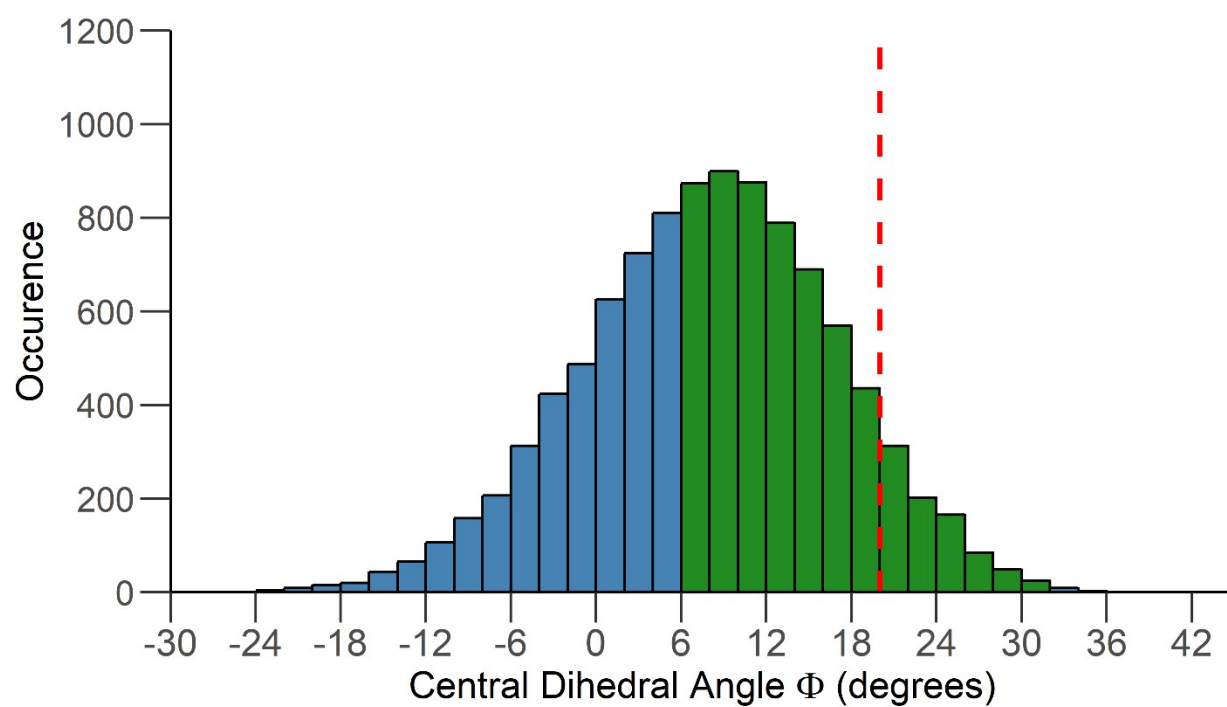
c – 4S0L



d – 4S0I



e – 4S0K



f – 4S03

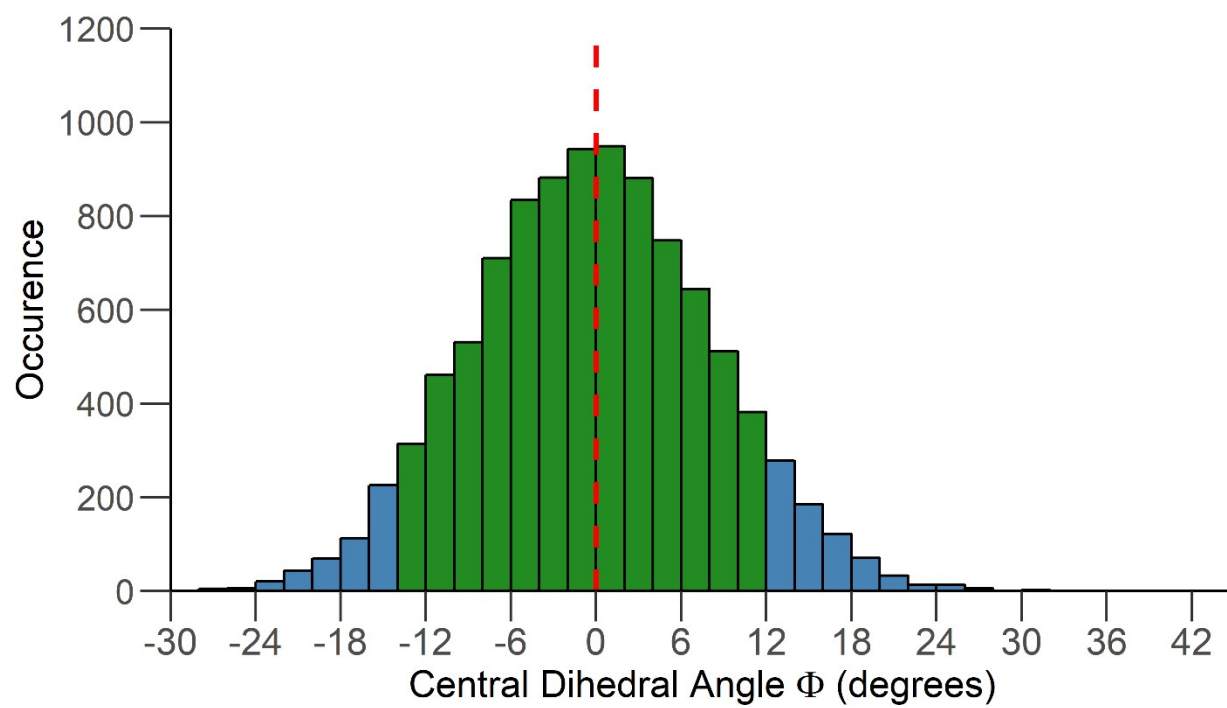
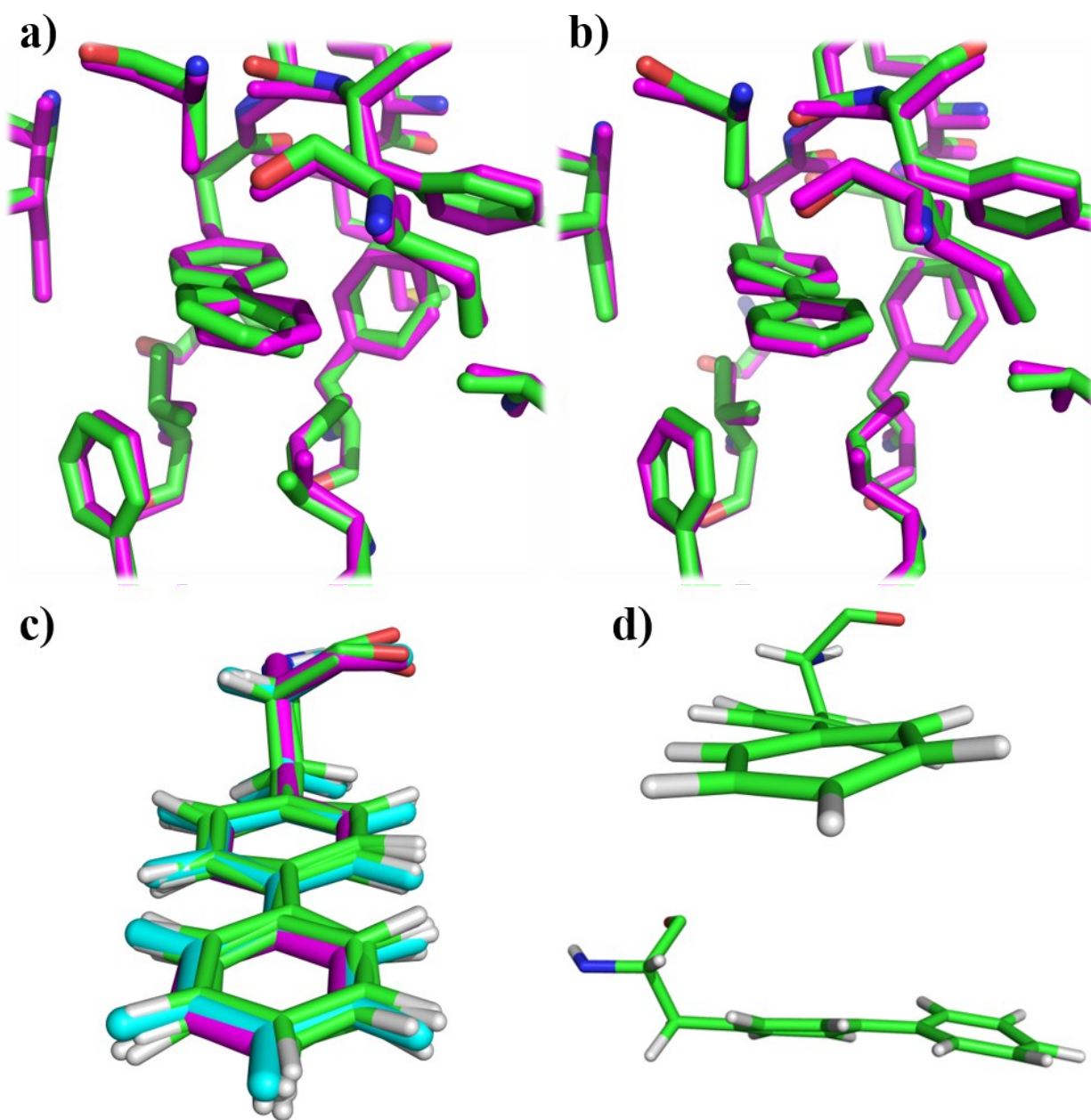


Figure S9. Overlay of select MD simulation snapshots of the 4S03 BiPhe core and the x-ray crystal structure (magenta) and average MD simulation structure (cyan). Models with the **a)** smallest and **b)** largest BiPhe dihedral angle are presented, along with five random intermediary angles (**c**). Viewing along the central BiPhe bond shows how snapshots outside the thermal range often have biphenyl ring distortion (**d**).



Cartesian coordinates of the unoptimized, starting cluster model structures

4S02

C	-3.335000	108.857002	5.976000
C	3.302000	108.438004	6.275000
C	3.335000	108.972000	4.826000
C	4.541000	108.489998	3.973000
C	6.687000	108.505997	7.927000
C	6.696000	107.877998	9.310000
C	2.342000	104.623001	5.174000
C	2.259000	105.103996	3.722000
C	-1.117000	103.671997	6.341000
C	-1.250000	103.157997	7.763000
C	-4.559000	104.955002	5.308000
C	-5.783000	104.744003	10.431000
C	-4.316000	104.685997	9.952000
C	-2.453000	106.879997	14.994000
C	-1.533000	106.432999	18.646000
C	1.361000	108.445000	19.948000
C	1.554000	109.931000	19.813000
C	-0.359000	102.705002	14.135000
C	0.036000	103.778000	13.128000
C	4.167000	105.695999	17.384001
C	7.659000	102.879997	14.115000
C	7.494000	104.327003	14.526000
C	11.128000	110.566002	12.421000
C	10.252000	109.388000	12.846000
C	5.858000	112.353996	9.221000
C	5.222000	111.651001	10.440000
C	2.805000	113.584999	7.347000
C	-0.673000	113.195999	8.689000
C	-0.639000	112.906998	10.236000
C	-0.099000	108.732002	7.959000
C	-0.334000	108.060997	9.304000
C	-2.290000	109.307999	6.999000
O	-2.447000	110.375999	7.614000
N	2.107000	108.922997	6.986000
C	4.496000	108.936996	7.047000
O	4.500000	110.032997	7.558000
C	4.192000	108.308998	2.474000
O	3.146000	108.893997	2.059000
O	4.905000	107.543999	1.735000
N	5.513000	108.119003	7.174000
C	6.873000	106.398003	9.340000
C	8.133000	105.805000	9.384000
C	5.764000	105.584999	9.282000
C	8.255000	104.434998	9.373000
C	5.876000	104.248001	9.220000
C	7.073000	103.689003	9.339000
O	7.075000	102.361000	9.297000
C	1.156000	103.731003	5.465000
O	1.135000	102.544998	5.100000
C	1.310000	106.267998	3.489000
C	1.316000	106.625999	1.987000
N	0.642000	107.896004	1.790000
C	-0.637000	108.050003	1.538000
N	-1.128000	109.292000	1.421000
N	-1.429000	106.997002	1.398000
N	0.173000	104.297997	6.140000
C	-2.233000	104.661003	6.027000
O	-2.063000	105.861000	6.140000
C	-0.239000	102.060997	8.103000
S	-0.587000	101.457001	9.787000
C	-1.884000	100.285004	9.610000
N	-3.374000	104.146004	5.604000
C	-3.742000	106.041000	9.534000
C	-3.436000	104.033997	11.015000
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H	6.483000	111.345001	18.214001
H	5.892000	113.569000	17.591999
H	2.941000	112.184998	21.521000
H	4.078000	115.496002	18.399000
H	1.857000	114.268997	21.514000
H	2.476000	115.903999	20.000000
H	8.196945	103.003777	14.671742
H	7.666000	103.101997	13.051000
H	8.064000	105.297997	13.743000
H	6.534000	105.125000	13.369000
H	6.981000	105.144997	14.888000
H	6.468977	102.845116	14.207602
H	10.797324	111.674271	11.706033
H	11.962000	110.454002	11.490000
H	9.842000	110.137001	13.287000
H	11.881000	108.273003	12.696000
H	11.707000	108.985001	14.072000
H	9.034000	108.417000	11.845000
H	9.061000	109.808998	11.091000
H	10.201000	108.742996	10.826000
H	10.927000	106.792000	14.224000
H	9.718000	107.789001	14.453000
H	9.894000	107.066002	13.055000
H	11.966905	111.218681	12.992634
H	6.181000	111.737000	8.439000
H	4.802000	111.709999	10.351000
H	6.316000	111.508003	10.771000
H	5.626000	112.921997	10.950000
H	7.070138	113.027962	9.060013
H	3.051959	113.559563	5.940181
H	4.231000	112.002998	7.357000
H	3.079000	114.473999	7.350000
H	-1.284326	113.901184	8.128566
H	0.865000	114.646004	7.962000
H	-0.583000	112.357002	8.202000
H	0.396000	112.762001	10.270000
H	-2.463000	112.931999	10.380000
H	-1.728000	111.584999	10.099000
H	-0.484000	114.445000	11.665000
H	0.271000	115.074997	10.424000
H	-1.311000	115.003998	10.436000
H	-2.419000	111.642998	12.336000

H	-0.837000	111.599998	12.287000
H	-1.583000	112.967003	12.573000
H	3.985000	107.433998	11.428000
H	2.403000	111.024002	12.249000
H	2.089000	106.834999	10.243000
H	0.509000	110.477997	10.981000
H	-0.888000	108.663002	10.048000
H	-0.234000	107.313004	9.622000
H	0.113000	109.736000	8.199000
H	7.569000	110.718002	15.015000
H	7.488000	108.592003	13.984000
H	5.660000	107.986000	12.621000
H	3.967000	111.572998	13.323000
H	5.843000	112.259003	14.609000
H	-1.264599	107.526466	7.026849

Cartesian coordinates and absolute energies for the computed cluster model ground states and near-coplanar transition states at the B3LYP/6-31G(d')+CPCM+GD3BJ. For the 4S02, 4S0J, 4S0I, and 4S03 models, the first 31 atoms are held frozen with “freeze codes”. For the 4S0L, 4S0I_W81, 4S0K, and 4S03_W81 models, the first 33 atoms are held frozen with “freeze codes”.

4S02

C	-5.600620	1.988496	-4.251357
C	-4.294521	-2.019919	0.900558
C	-5.692967	-2.640174	0.687636
C	-6.370856	-3.194494	1.971134
C	-2.135263	-4.062932	3.214664
C	-0.799837	-3.410038	3.527055
C	-5.715591	1.282754	2.839824
C	-7.137787	0.777687	2.577419
C	-5.147992	4.423226	0.828430
C	-3.790625	5.090417	0.956467
C	-6.639690	5.589614	-2.484373
C	-1.785565	7.267336	-3.671993
C	-2.032992	6.279389	-2.511110
C	3.337929	4.136036	-3.026087
C	7.062418	4.373988	-2.351641
C	8.894648	1.164463	-1.673108
C	8.863709	-0.082032	-2.515106
C	2.612760	5.732682	1.387304
C	1.732764	4.537342	1.043547
C	6.667234	0.998281	2.451920
C	3.847570	0.332320	7.186513
C	4.297849	-0.573612	6.061125
C	3.089112	-7.877541	4.736818
C	3.315019	-6.369859	4.844493
C	-0.800192	-6.187569	-0.082639
C	0.269509	-5.078302	-0.182176
C	-3.063763	-5.355963	-3.003734
C	-2.299098	-2.594837	-5.420382
C	-0.781519	-2.186508	-5.330316
C	-3.147268	0.232661	-1.945285
C	-1.889369	1.072373	-1.781045
C	-4.534295	0.995664	-3.850542
O	-4.022791	0.209829	-4.667191
N	-3.821312	-1.473574	-0.365494
C	-3.272719	-3.044307	1.329886
O	-2.614573	-3.701173	0.500568
C	-7.715526	-3.887342	1.662245
O	-8.537174	-3.251408	0.884609
O	-7.936665	-5.003431	2.170258
N	-3.142904	-3.195801	2.649270
C	-1.033574	-1.955425	3.894735
C	-1.343089	-1.556129	5.205071
C	-1.206533	-1.017722	2.860940
C	-1.845650	-0.277337	5.471854
C	-1.717653	0.255344	3.108766
C	-2.061765	0.617763	4.416216
O	-2.598938	1.853776	4.721001
C	-5.648536	2.773100	2.580967
O	-6.133083	3.617580	3.353825
C	-7.697925	1.321182	1.246301
C	-8.959717	0.604620	0.742762
N	-8.674057	-0.693274	0.124790
C	-8.280555	-0.851736	-1.138166
N	-8.192532	-2.108664	-1.627078
N	-8.057963	0.203353	-1.962966
N	-5.093224	3.086612	1.384655
C	-5.647956	4.343746	-0.615634

O	-5.667378	3.275399	-1.260086
C	-3.402204	5.384936	2.407863
S	-1.779757	6.236188	2.565313
C	-2.130525	7.815321	1.707338
N	-6.080616	5.506460	-1.136797
C	-2.488871	4.903213	-3.030584
C	-0.786413	6.147858	-1.617833
C	4.824061	3.983672	-3.285460
O	5.267757	3.495555	-4.341456
C	2.628298	2.757446	-3.002623
C	3.144435	1.870752	-1.855347
C	1.105087	2.933132	-2.922844
N	5.612981	4.422309	-2.275602
C	7.654724	3.261521	-1.524813
O	7.752801	3.330799	-0.282777
N	8.080164	2.216288	-2.247853
C	7.673009	-0.988730	-2.356328
C	7.674820	-2.160504	-1.622791
C	6.371995	-0.902863	-2.990617
N	6.458744	-2.809414	-1.766024
C	5.644325	-2.076126	-2.608105
C	5.753873	0.020298	-3.858842
C	4.358411	-2.351173	-3.089088
C	4.470954	-0.250428	-4.332913
C	3.782325	-1.425946	-3.954889
C	4.088549	5.378307	1.327110
O	4.642183	5.164712	0.231902
C	1.754670	3.472195	2.121359
C	2.859142	2.617569	2.284790
C	0.685508	3.367807	3.026449
C	2.895612	1.693039	3.334748
C	0.717238	2.443491	4.074701
C	1.824081	1.602493	4.231185
N	4.753143	5.296756	2.502801
C	6.126382	4.792967	2.589384
C	6.137210	3.339650	3.084754
O	5.735548	3.063418	4.227515
N	6.587147	2.437094	2.185325
C	5.907564	0.184096	1.394548
C	3.820800	-5.985131	6.252019
C	2.023170	-5.618740	4.469257
C	4.193263	-4.502540	6.402881
C	-1.512011	-6.408305	-1.407327
O	-1.210121	-7.329260	-2.183658
C	1.298755	-5.296896	-1.266754
C	1.061257	-4.883107	-2.591074
C	2.517793	-5.930713	-0.984701
C	2.000306	-5.105147	-3.599361
C	3.470284	-6.157919	-1.982719
C	3.209022	-5.748089	-3.297359
O	4.103730	-5.931592	-4.328252
N	-2.468327	-5.482826	-1.684338
C	-2.882441	-3.956811	-3.509393
O	-3.034438	-2.964366	-2.769151
N	-2.572263	-3.873956	-4.810760
C	-0.655540	-0.689768	-5.690291
C	0.091841	-3.090766	-6.210045
C	0.720875	-0.076322	-5.397610
N	-4.208893	1.043737	-2.539478
C	-3.665391	-0.167551	-0.574724
C	-0.747591	0.346152	-1.108323
C	-0.116645	0.890147	0.019115
C	0.908434	0.204992	0.672278
C	1.348491	-1.047691	0.210120
C	0.748615	-1.570081	-0.952887
C	-0.290015	-0.892403	-1.590540
C	3.387713	-2.511632	3.061576
C	4.248276	-3.381778	2.381845
C	4.164445	-3.477305	0.988755
C	3.236436	-2.707181	0.284310
C	2.367279	-1.827017	0.955114
C	2.455752	-1.742882	2.359729

O	-3.934405	0.717922	0.268041
H	-5.200326	2.646740	-5.031150
H	-6.448615	1.453009	-4.694889
H	-5.944619	2.598377	-3.415974
H	-3.523576	-2.136094	-1.085532
H	-4.351125	-1.196259	1.644022
H	-6.318138	-1.853469	0.261785
H	-5.606857	-3.440188	-0.063243
H	-5.725823	-3.921277	2.471442
H	-6.547813	-2.367128	2.674480
H	-2.559621	-4.464094	4.146261
H	-3.616210	-2.534044	3.262640
H	-2.001108	-4.909532	2.533633
H	-0.312930	-3.959103	4.338962
H	-0.137289	-3.459749	2.653906
H	-1.219352	-2.260830	6.023405
H	-0.971209	-1.301052	1.841706
H	-2.093459	0.028021	6.483581
H	-1.864189	0.952883	2.290751
H	-2.702965	2.374252	3.901005
H	-5.012029	0.761003	2.189498
H	-7.131300	-0.319199	2.560478
H	-7.803952	1.083654	3.394528
H	-7.930000	2.387187	1.365522
H	-6.921011	1.261218	0.473147
H	-9.653158	0.416622	1.570435
H	-9.488439	1.229081	0.010640
H	-8.682744	-1.579959	0.678087
H	-8.274848	-2.851181	-0.917940
H	-7.584024	-2.272348	-2.424130
H	-7.783222	1.098200	-1.568832
H	-7.680799	0.001455	-2.884953
H	-5.429648	1.093383	3.880566
H	-4.728174	2.340860	0.794144
H	-5.899096	4.997246	1.424931
H	-3.026312	4.446448	0.495167
H	-3.796592	6.028963	0.383481
H	-4.172678	5.986453	2.903242
H	-3.297746	4.455717	2.978185
H	-1.255646	8.455458	1.848996
H	-2.285780	7.666267	0.636249
H	-3.004580	8.307646	2.144206
H	-6.108136	6.331268	-0.538361
H	-6.927691	6.624154	-2.679671
H	-5.900261	5.275742	-3.228262
H	-7.519527	4.943600	-2.582434
H	-2.685644	7.387715	-4.286603
H	-0.979096	6.902021	-4.321489
H	-1.493541	8.254240	-3.293922
H	-2.849816	6.687619	-1.892975
H	-2.730526	4.224418	-2.204332
H	-3.381571	4.993539	-3.662065
H	-1.697953	4.432802	-3.628782
H	-0.973375	5.473970	-0.773413
H	0.058045	5.744383	-2.189839
H	-0.484419	7.120660	-1.210889
H	3.160763	4.662339	-2.080878
H	2.869224	2.258124	-3.951546
H	2.655569	0.891509	-1.872639
H	4.223318	1.703235	-1.932904
H	2.934608	2.328653	-0.881523
H	0.606304	1.961555	-2.972228
H	0.812167	3.406945	-1.977855
H	0.730625	3.555873	-3.744839
H	2.913392	4.743206	-3.836504
H	7.470913	5.323936	-1.967160
H	5.189884	4.734647	-1.404692
H	7.340036	4.273184	-3.409579
H	9.932681	1.526051	-1.578111
H	8.021738	2.278304	-3.264606
H	8.531412	0.962508	-0.658445
H	8.976176	0.199729	-3.575139

H	9.762579	-0.665790	-2.272819
H	8.466169	-2.587280	-1.023821
H	6.215485	-3.703955	-1.347995
H	6.248986	0.941768	-4.144712
H	3.834593	-3.257474	-2.813544
H	3.988357	0.460457	-4.995442
H	2.788419	-1.615242	-4.340942
H	2.343906	6.122183	2.377040
H	0.704431	4.889163	0.905929
H	2.061223	4.122124	0.083493
H	3.691320	2.671395	1.590288
H	-0.170283	4.023951	2.906442
H	3.755543	1.045504	3.450470
H	-0.118998	2.382926	4.760377
H	1.844914	0.880016	5.039636
H	2.445845	6.531831	0.653485
H	6.685688	5.404654	3.315146
H	4.212065	5.324904	3.367326
H	6.587102	4.891049	1.598771
H	7.723084	0.692786	2.475200
H	6.927846	2.767934	1.282430
H	6.250575	0.832053	3.449630
H	5.978703	-0.887940	1.607201
H	4.846425	0.451218	1.379777
H	6.317228	0.357818	0.392458
H	4.623993	0.440458	7.953449
H	2.948874	-0.056652	7.681272
H	4.545709	-1.579003	6.420733
H	3.515480	-0.679230	5.302830
H	5.184661	-0.173193	5.554443
H	3.611087	1.336424	6.814845
H	2.761693	-8.158759	3.728660
H	2.312537	-8.203007	5.442201
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H	1.222562	-5.860733	5.181842
H	4.622053	-4.300077	7.391110
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H	3.319425	-3.853006	6.282954
H	4.003539	-8.439213	4.964832
H	-1.518710	-5.907740	0.692562
H	-0.245079	-4.124230	-0.337423
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H	0.128242	-4.382826	-2.835489
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H	1.819653	-4.782943	-4.617748
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H	4.899774	-6.386488	-3.993546
H	-0.326999	-7.135584	0.195358
H	-4.148739	-5.580024	-2.968583
H	-2.631088	-4.729960	-1.016736
H	-2.590268	-6.097363	-3.662761
H	-2.597914	-2.633402	-6.476263
H	-2.373909	-4.733666	-5.320503
H	-2.908097	-1.838666	-4.923322
H	-0.478057	-2.319905	-4.280842
H	-0.899054	-0.563236	-6.756322
H	-1.422401	-0.134899	-5.134203
H	1.156339	-2.865434	-6.084751
H	-0.052098	-4.148527	-5.958313
H	-0.158867	-2.956261	-7.270479
H	0.728944	0.994887	-5.629395
H	0.979449	-0.185644	-4.338069
H	1.513767	-0.547167	-5.989467
H	1.363985	0.647305	1.545847
H	1.072132	-2.527289	-1.341568
H	-0.433597	1.856983	0.398321
H	-0.772496	-1.348600	-2.447745
H	-1.589958	1.414607	-2.781848

H	-2.144657	1.967950	-1.202166
H	-2.974485	-0.637067	-2.597438
H	4.964219	-3.983317	2.933277
H	3.432641	-2.447369	4.141353
H	1.772777	-1.099893	2.901995
H	3.189697	-2.781006	-0.792889
H	4.815257	-4.157405	0.448431
H	-4.618873	1.770571	-1.954413
el energy= -6211.26291501			
zpe= -6208.961018			
th energy= -6208.852704			
th enthalpy= -6208.851760			
free energy= -6209.101991			

4S0J

C	-5.486889	-3.126252	3.630288
C	-4.181093	2.024683	-0.423490
C	-5.607141	2.431452	-0.181261
C	-6.218852	3.216271	-1.369450
C	-2.269356	4.783573	-2.094321
C	-0.826980	4.276447	-2.347788
C	-5.237045	-0.911064	-3.256388
C	-6.708735	-0.570413	-3.057897
C	-4.571210	-4.420896	-1.904899
C	-3.184237	-5.098949	-2.098957
C	-5.991593	-6.284897	1.092954
C	-1.098326	-7.766867	2.206663
C	-1.379534	-6.618886	1.168292
C	3.768479	-4.248627	2.584687
C	7.459414	-3.870522	2.097921
C	8.838707	-0.411543	2.583741
C	8.512947	0.441281	3.732403
C	3.369750	-4.848257	-2.094327
C	2.357572	-3.832557	-1.598641
C	7.275759	0.312560	-1.979938
C	4.452543	1.760993	-6.325909
C	4.574767	2.405462	-4.958987
C	2.505506	9.371448	-2.337869
C	2.876430	7.935922	-2.690881
C	-1.016017	6.243065	1.826460
C	0.353721	5.706147	2.292756
C	-3.730068	4.698583	3.896450
C	-2.780768	1.610533	5.842922
C	-1.215563	1.405298	5.795138
C	-3.101491	-0.757524	1.954852
C	-1.810056	-1.507796	1.590833
C	-4.437249	-2.051579	3.570840
O	-3.949055	-1.513690	4.580400
N	-3.684714	1.250726	0.709489
C	-3.252386	3.206534	-0.568787
O	-2.595709	3.665245	0.386954
C	-7.752737	3.400979	-1.297141
O	-8.439799	2.551388	-0.611138
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H	2.870757	10.029426	-0.667150
H	1.463423	9.850120	-1.727579
H	4.054649	8.215472	-1.922333
H	1.457124	8.068629	-3.532912
H	3.000645	8.677440	-4.122325
H	2.650418	6.304854	-1.117277
H	2.609093	7.624429	0.056964
H	1.234969	7.371442	-1.034026
H	2.719395	6.376219	-4.953097
H	4.008813	6.348567	-3.738429
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H	2.996880	10.447629	-2.385982
H	-1.854391	6.085626	1.211552
H	-0.253818	4.405479	2.052062
H	0.607623	5.666468	1.172303
H	0.628953	5.661193	2.939703
H	-0.966505	7.380441	2.028713
H	-4.442264	4.576995	4.541460
H	-2.795557	4.420956	2.432105
H	-2.901849	4.953686	5.335518
H	-3.091051	0.784019	7.035406
H	-3.078758	3.121311	6.578178
H	-3.156839	0.444206	5.299253
H	-0.786006	1.372392	5.108265
H	-1.051253	-1.100149	6.893462
H	-1.410880	-1.076845	5.173731
H	0.614228	1.536360	7.169647
H	-0.753184	2.649402	7.265859
H	-0.790072	1.119837	8.169705

H	0.892224	-1.950950	5.523509
H	0.985740	-0.398109	4.680932
H	1.361182	-0.493773	6.410012
H	1.394671	0.627176	-1.406864
H	1.093307	2.371154	2.522010
H	-0.270788	-1.059482	-0.786603
H	-0.568930	0.672351	3.132668
H	-1.224916	-1.947010	2.494829
H	-1.707296	-2.079706	0.799567
H	-2.834084	-0.072282	2.847302
H	5.414952	5.000390	-0.751868
H	3.925979	4.113950	-2.531269
H	2.041218	2.626296	-1.969007
H	3.177499	2.798865	2.181306
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zpe= -5846.448776			
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4S0I_W81

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C	-6.170651	-4.373903	1.195300
C	-1.909361	-4.844370	2.498873
C	-0.682997	-4.007743	2.951307
C	-6.428168	-0.065379	2.644037
C	-7.736645	-0.801802	2.304269
C	-6.459564	3.341180	0.931408
C	-5.285347	4.282136	1.114780
C	-7.897696	4.547947	-2.348518
C	-3.392515	7.173241	-3.061680
C	-3.518380	6.116410	-1.924259
C	2.098950	5.027151	-2.465459
C	5.636704	5.763652	-1.418756
C	7.883968	2.754487	-1.474575
C	7.941066	1.779631	-2.620783
C	0.967518	5.821139	2.050887
C	0.293354	4.559225	1.510103
C	5.818407	1.601507	2.882548
C	10.742417	-1.504455	0.854221
C	10.323817	-0.669470	-0.325848
C	2.799300	-0.072446	7.204895
C	3.173542	-0.827951	5.949473
C	3.644284	-8.203973	3.857853
C	3.656635	-6.683355	3.945493
C	-0.216456	-6.460020	-0.849401
C	0.766820	-5.341965	-0.858375
C	-2.325397	-5.553453	-3.767956
C	-2.231447	-2.433396	-5.861109
C	-0.783237	-1.853445	-5.704681
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O	-4.275395	0.024836	-4.976153
N	-3.874870	-2.083021	-0.842410
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O	-2.310733	-4.108714	-0.135571
C	-7.714823	-4.411525	1.147410
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O	-8.317323	-4.484041	2.244104
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C	-0.589496	-3.011523	5.285347
C	-1.676468	-1.748346	3.542939

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C	-6.651285	1.433826	2.486129
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C	-9.082381	-1.535168	-2.078476
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N	-9.172487	-0.861201	-3.260262
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C	-6.857737	3.303452	-0.535786
O	-6.513296	2.387775	-1.306061
C	-4.897456	4.456830	2.586809
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C	-3.713541	4.705309	-2.508840
C	-2.295191	6.165140	-0.992547
C	3.594487	5.156653	-2.600863
O	4.193437	4.929159	-3.669736
C	1.642819	3.567166	-2.732633
C	2.176645	2.600343	-1.661072
C	0.113226	3.477207	-2.831777
N	4.212257	5.534687	-1.462981
C	6.396975	4.588526	-0.863490
O	6.376232	4.284759	0.344860
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C	6.475356	-0.281402	-2.587978
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C	5.296038	-0.973135	-2.887125
C	4.375842	1.040307	-3.859524
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C	1.658267	2.571568	2.329281
C	-0.426366	3.101356	3.436776
C	1.864558	1.523699	3.232329
C	-0.219497	2.057637	4.341904
C	0.924540	1.258602	4.233116
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O	4.560800	1.209515	0.781442
C	9.960992	-1.479925	-1.542362
C	10.506853	-1.354340	-2.804684
C	8.965654	-2.530764	-1.631268
N	9.910084	-2.260293	-3.671576
C	8.959782	-2.992529	-2.987333
C	8.049558	-3.097517	-0.721913
C	8.083882	-3.991863	-3.433508
C	7.179925	-4.093825	-1.163841
C	7.197322	-4.537303	-2.507041
C	3.065859	-6.240388	5.305901
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C	3.055892	-4.726071	5.553269
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C	0.536679	0.362953	-5.558137

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O	-4.503592	-0.034539	-0.056139
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H	-7.013829	0.727151	-4.459278
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C	6.362399	0.142323	2.672256
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4S03

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H	-5.014190	-1.100293	3.702139
H	-6.080060	-1.549913	0.868563
H	-3.943655	-2.632988	0.901899
H	-3.843413	-1.127981	0.001912
H	-5.296492	0.838961	0.556557
H	-6.568591	0.678317	1.779320
H	-4.881191	0.902365	2.267985
H	-1.813689	-1.411023	1.407517
H	-2.730684	-0.025389	1.990926

H	-2.795663	-1.557402	2.871473
H	-11.027425	0.422134	1.774731
H	-11.273855	1.867047	0.768423
H	-9.893282	1.782340	1.874930
H	-8.952466	-0.140501	0.530476
H	-10.313522	-0.044244	-0.568831
H	-7.613604	2.711207	0.595976
H	-6.785231	3.883656	-1.481297
H	-10.470311	0.196963	-2.926512
H	-7.174948	3.739762	-4.295790
H	-10.134974	0.763506	-5.317865
H	-8.511624	2.507031	-5.997474
H	-3.187506	1.134209	7.591724
H	-1.576111	0.725735	6.978810
H	-2.647398	2.421318	5.436684
H	-2.468854	0.880915	4.583819
H	-4.053725	1.357191	5.213410
H	-2.934489	-0.386779	6.714096
H	-3.438609	8.620649	1.973760
H	-2.750158	8.988956	3.565517
H	-4.389452	6.480635	2.879162
H	-2.950713	7.271182	5.461547
H	-4.693222	7.317489	5.212951
H	-2.203246	5.276458	3.163638
H	-2.124773	6.445424	1.846905
H	-1.390675	6.836670	3.416033
H	-4.125378	5.250829	6.443108
H	-4.679727	4.795650	4.824250
H	-2.951084	4.772492	5.213870
H	-4.510408	8.944909	3.351162
H	1.057360	6.202846	-0.788669
H	-0.437826	4.380417	-1.564156
H	-1.313869	5.457594	-0.479328
H	-1.571590	5.573543	-2.225478
H	-0.080570	7.418611	-1.399865
H	3.737066	5.538926	-4.336427
H	2.390116	5.129275	-2.192652
H	2.137872	5.817916	-5.082505
H	2.544941	1.844354	-7.133038
H	2.126064	4.087778	-6.446376
H	2.852028	1.388959	-5.452208
H	0.404190	1.678813	-4.961829
H	1.097979	-0.355323	-7.143788
H	1.473310	-0.517123	-5.435332
H	-1.230980	1.834492	-6.838322
H	-0.148253	3.228688	-6.863150
H	0.096591	1.895351	-8.012797
H	-0.554552	-1.842210	-5.915284
H	-1.049677	-0.461461	-4.926942
H	-1.359130	-0.458176	-6.668003
H	-0.094780	1.199523	1.647711
H	-1.758823	1.589857	-2.317113
H	1.703753	-0.166144	0.745784
H	0.064388	0.223041	-3.196922
H	1.827781	-1.450394	-2.746959
H	2.474649	-1.659727	-1.116395
H	3.121645	0.634466	-3.040530
H	-5.176956	4.478749	1.722838
H	-3.640851	3.255213	3.259764
H	-1.771207	1.961158	2.380573
H	-2.909960	3.062394	-1.633605
H	-4.759933	4.384650	-0.736386
H	4.992193	-1.461848	-2.057637
e1	energy=	-6333.78971595	
	zpe=	-6331.335672	
	th energy=	-6331.222556	
	th enthalpy=	-6331.221612	
	free energy=	-6331.480620	

4S02 TS at $\Phi_{\text{gas}} = 9.3^\circ$

C	-5.125773	-2.414222	4.629480
C	-4.305883	2.043026	-0.246384
C	-5.678178	2.631211	0.150984
C	-6.472110	3.292549	-1.009725
C	-2.371683	4.298594	-2.562329
C	-1.072051	3.685885	-3.055035
C	-5.906061	-1.085986	-2.329911
C	-7.296079	-0.616150	-1.890228
C	-5.154490	-4.387502	-0.665870
C	-3.815678	-5.030285	-0.979308
C	-6.329582	-5.852942	2.655388
C	-1.386727	-7.592723	3.229881
C	-1.741229	-6.507997	2.189413
C	3.656188	-4.378574	2.387149
C	7.300679	-4.528240	1.348456
C	9.063905	-1.257800	0.788492
C	9.113325	-0.090829	1.736867
C	2.518320	-5.584424	-2.063091
C	1.675496	-4.430841	-1.533706
C	6.459017	-0.744555	-3.078777
C	3.207745	0.316006	-7.450801
C	3.762422	1.122368	-6.296631
C	2.690016	8.271561	-4.222843
C	2.903357	6.780967	-4.484359
C	-0.730955	6.133608	0.770819
C	0.342403	5.027848	0.671028
C	-2.710784	5.030348	3.805757
C	-1.725047	2.072412	5.885832
C	-0.222953	1.684904	5.618311
C	-2.898222	-0.443067	2.268742
C	-1.662142	-1.255916	1.913544
C	-4.037411	-1.436699	4.233554
O	-3.358850	-0.819125	5.064611
N	-3.685274	1.413621	0.910966
C	-3.390092	3.142368	-0.710917
O	-2.803704	3.871780	0.101717
C	-7.972234	3.101190	-0.779226
O	-8.478355	3.621981	0.260595
O	-8.583817	2.340678	-1.600712
N	-3.292381	3.312270	-2.041495
C	-1.281357	2.834823	-4.297064
C	-1.235647	3.416699	-5.579604
C	-1.615052	1.472887	-4.208271
C	-1.517088	2.677512	-6.727492
C	-1.908766	0.720634	-5.352316
C	-1.862163	1.323110	-6.615435
O	-2.138167	0.644925	-7.782241
C	-5.822836	-2.593280	-2.198555
O	-6.378873	-3.377495	-2.979038
C	-7.686683	-0.970245	-0.436503
C	-9.201912	-0.893368	-0.146160
N	-9.709393	0.485637	-0.094642
C	-10.575742	0.958685	0.798425
N	-10.662396	2.277177	1.005867
N	-11.415544	0.125690	1.497811
N	-5.161847	-3.000652	-1.077922
C	-5.504956	-4.467757	0.818971
O	-5.367588	-3.507883	1.589198
C	-3.575454	-5.155024	-2.497153
S	-2.210924	-6.299109	-2.961679
C	-3.004277	-7.920911	-2.653316
N	-5.968395	-5.663669	1.254938
C	-2.134464	-5.194186	2.891027
C	-0.582363	-6.296178	1.199377
C	5.170440	-4.304702	2.523500
O	5.729603	-4.081973	3.605275
C	2.987044	-3.169857	3.080797
C	3.358089	-1.856525	2.369026
C	1.464140	-3.358425	3.168238

N	5.851427	-4.488777	1.358842
C	7.909618	-3.385866	0.578197
O	7.973483	-3.363048	-0.663719
N	8.401006	-2.407756	1.363377
C	7.790697	0.510369	2.133868
C	6.999436	1.344082	1.370233
C	7.119143	0.360176	3.406764
N	5.881362	1.723121	2.095417
C	5.919906	1.134517	3.346357
C	7.417491	-0.339103	4.593107
C	5.033336	1.221969	4.428450
C	6.535125	-0.259621	5.666654
C	5.355063	0.514851	5.584885
C	4.009478	-5.282790	-2.103084
O	4.672559	-5.282759	-1.055148
C	1.418439	-3.364133	-2.583042
C	2.389585	-2.400805	-2.897517
C	0.222736	-3.375477	-3.322700
C	2.184730	-1.490357	-3.940173
C	0.005855	-2.455125	-4.352456
C	0.989593	-1.510116	-4.668697
N	4.569063	-5.042903	-3.320461
C	5.934717	-4.521390	-3.445885
C	5.862115	-3.029601	-3.805032
O	5.189896	-2.661126	-4.778107
N	6.533226	-2.203375	-2.968013
C	5.794156	-0.115126	-1.849300
C	3.445641	6.566514	-5.920042
C	1.607681	5.994265	-4.225123
C	3.853075	5.123110	-6.253059
C	-1.299838	6.233258	2.185570
O	-0.888436	7.041051	3.022982
C	1.518680	5.283036	1.598311
C	1.648100	4.605370	2.823571
C	2.497041	6.236711	1.273598
C	2.713794	4.860445	3.690790
C	3.567524	6.506626	2.131097
C	3.676639	5.817728	3.346966
O	4.703801	6.033022	4.241779
N	-2.266876	5.302589	2.453600
C	-2.496117	3.584105	4.149608
O	-2.712709	2.662710	3.345160
N	-2.075542	3.388175	5.412443
C	-0.015709	0.234379	6.116808
C	0.733843	2.684209	6.292851
C	1.408485	-0.318985	5.948631
N	-3.906904	-1.296250	2.888790
C	-3.540534	0.087713	0.995428
C	-0.589527	-0.456601	1.193737
C	-0.507464	-0.419450	-0.208516
C	0.456946	0.355794	-0.858413
C	1.392514	1.128765	-0.137821
C	1.313754	1.069565	1.269333
C	0.345058	0.301693	1.914640
C	3.584764	2.700563	-2.849885
C	4.356860	3.607202	-2.115313
C	4.155951	3.702910	-0.734531
C	3.201468	2.899980	-0.102805
C	2.418618	1.970537	-0.823076
C	2.635950	1.893101	-2.215454
O	-3.905439	-0.706158	0.101316
H	-4.712700	-3.137946	5.340500
H	-5.917772	-1.869858	5.157462
H	-5.553007	-2.940810	3.777420
H	-3.341114	2.014318	1.664581
H	-4.434189	1.277683	-1.012927
H	-6.260455	1.801999	0.570125
H	-5.536270	3.349650	0.965277
H	-6.228992	4.359581	-1.068155
H	-6.219331	2.835841	-1.971889
H	-2.859651	4.843798	-3.380129
H	-3.697473	2.631828	-2.668618

H	-2.181628	5.008197	-1.757613
H	-0.371496	4.496382	-3.279174
H	-0.624326	3.093151	-2.248578
H	-0.974038	4.466536	-5.678174
H	-1.637174	0.987351	-3.236784
H	-1.477635	3.127681	-7.712737
H	-2.165528	-0.330899	-5.256348
H	-2.369232	-0.271718	-7.578707
H	-5.120809	-0.612747	-1.738906
H	-7.399845	0.462413	-2.049200
H	-8.025889	-1.093033	-2.562507
H	-7.384555	-1.999797	-0.211056
H	-7.148383	-0.335543	0.278732
H	-9.744436	-1.465914	-0.912250
H	-9.391962	-1.370757	0.823978
H	-9.316136	1.207258	-0.767969
H	-9.875820	2.914994	0.668678
H	-11.483061	2.650898	1.458166
H	-11.367213	-0.865840	1.324138
H	-11.675311	0.397890	2.434357
H	-5.766603	-0.822567	-3.384350
H	-4.726592	-2.308429	-0.468498
H	-5.938872	-4.886272	-1.251252
H	-3.006953	-4.449461	-0.520379
H	-3.775942	-6.030233	-0.524292
H	-4.489649	-5.470333	-3.011615
H	-3.302143	-4.183509	-2.919362
H	-2.286591	-8.688134	-2.955970
H	-3.240777	-8.067377	-1.595423
H	-3.911964	-8.031679	-3.254566
H	-6.149867	-6.399322	0.588519
H	-6.616857	-6.894897	2.810327
H	-5.481049	-5.616008	3.302290
H	-7.164905	-5.203999	2.939953
H	-2.222139	-7.773779	3.917563
H	-0.520993	-7.282770	3.829713
H	-1.134258	-8.543704	2.744943
H	-2.615688	-6.862587	1.618919
H	-2.447413	-4.427339	2.173835
H	-2.963011	-5.352514	3.592946
H	-1.288318	-4.792183	3.462092
H	-0.841491	-5.549043	0.440908
H	0.315904	-5.947990	1.724042
H	-0.330135	-7.228060	0.678960
H	3.362842	-4.437352	1.332964
H	3.396605	-3.130714	4.099080
H	2.927794	-0.994451	2.887683
H	4.443418	-1.714500	2.342154
H	2.979574	-1.846181	1.338306
H	0.997839	-2.529945	3.713706
H	1.011896	-3.395194	2.168530
H	1.210646	-4.289672	3.690766
H	3.322076	-5.306253	2.873529
H	7.639762	-5.457904	0.874937
H	5.358669	-4.731599	0.502946
H	7.626826	-4.529412	2.390846
H	10.084958	-1.538148	0.488972
H	8.190325	-2.424369	2.352804
H	8.538372	-0.984808	-0.133162
H	9.656952	-0.386840	2.646560
H	9.742652	0.681041	1.271699
H	7.151716	1.709289	0.366385
H	5.116027	2.261206	1.718776
H	8.324420	-0.931760	4.677449
H	4.135560	1.829358	4.371230
H	6.751425	-0.801356	6.581483
H	4.690091	0.561046	6.441070
H	2.151315	-5.890182	-3.050003
H	0.715633	-4.835225	-1.194544
H	2.163762	-3.995340	-0.653020
H	3.318127	-2.370572	-2.336286
H	-0.529655	-4.123860	-3.095634

H	2.970305	-0.790928	-4.198038
H	-0.921149	-2.490285	-4.917605
H	0.829958	-0.802776	-5.475423
H	2.410710	-6.446151	-1.393983
H	6.451674	-5.054374	-4.251031
H	3.953073	-4.833731	-4.097218
H	6.453596	-4.699569	-2.503527
H	7.473384	-0.342871	-3.208704
H	7.036975	-2.599348	-2.174361
H	5.897613	-0.525779	-3.989918
H	5.799218	0.977244	-1.924343
H	4.752642	-0.437847	-1.756492
H	6.315440	-0.399160	-0.928855
H	3.983952	0.091894	-8.192434
H	2.402822	0.851874	-7.969117
H	4.203441	2.067428	-6.636554
H	2.973531	1.369291	-5.575783
H	4.540876	0.563521	-5.763336
H	2.803810	-0.643724	-7.108921
H	2.341984	8.454629	-3.198612
H	1.935860	8.683939	-4.907050
H	3.667229	6.411010	-3.780746
H	2.683249	6.908561	-6.637301
H	4.315087	7.224964	-6.061592
H	1.756974	4.914975	-4.327838
H	1.241314	6.185134	-3.208942
H	0.823105	6.303420	-4.930217
H	4.283741	5.059840	-7.259327
H	4.607160	4.754453	-5.545510
H	2.998156	4.439149	-6.218049
H	3.616272	8.841110	-4.368169
H	-1.534768	5.925411	0.061309
H	-0.114999	4.058095	0.893877
H	0.695794	4.977703	-0.367383
H	0.898458	3.871231	3.104347
H	2.423559	6.778315	0.334554
H	2.804179	4.346851	4.641019
H	4.308336	7.254997	1.859116
H	5.278175	6.736262	3.909823
H	-0.287998	7.105238	0.531270
H	-3.781793	5.261332	3.921471
H	-2.536092	4.644879	1.726842
H	-2.158465	5.706825	4.464241
H	-1.909755	2.030648	6.967155
H	-1.807733	4.195840	5.955242
H	-2.381282	1.340124	5.410037
H	-0.068021	1.720456	4.530981
H	-0.289368	0.193279	7.182907
H	-0.734470	-0.415041	5.599917
H	1.780646	2.448260	6.073646
H	0.555968	3.710303	5.949364
H	0.612670	2.663227	7.384878
H	1.449407	-1.376690	6.232848
H	1.755481	-0.244532	4.910785
H	2.131051	0.214552	6.576016
H	0.475159	0.342734	-1.941287
H	2.026510	1.608983	1.880437
H	-1.209206	-0.999989	-0.799233
H	0.325744	0.273989	2.998477
H	-1.258714	-1.676658	2.841272
H	-1.979531	-2.095297	1.284605
H	-2.658871	0.366734	2.958970
H	5.092135	4.232853	-2.611322
H	3.725826	2.616010	-3.921143
H	2.074530	1.188443	-2.816312
H	3.026795	3.051314	0.954592
H	4.714139	4.425440	-0.147492
H	-4.413843	-1.929751	2.276334
el energy= -6210.42801140			
zpe= -6208.114958			
th energy= -6208.005530			
th enthalpy= -6208.004586			

free energy= -6208.262108

4S0I TS at $\Phi_{\text{CPM+GD3BJ}} = -3.2^\circ$

C	-5.389216	-3.351708	3.267644
C	-4.130005	2.121589	-0.208850
C	-5.539751	2.570441	0.061942
C	-6.208736	3.356806	-1.070860
C	-2.083375	5.044390	-1.531958
C	-0.639896	4.623563	-1.916768
C	-5.189243	-0.477215	-3.304596
C	-6.672972	-0.145618	-3.061099
C	-4.558335	-4.093388	-2.274737
C	-3.169315	-4.682991	-2.425230
C	-6.018653	-6.277071	0.441524
C	-1.113230	-7.915336	1.409355
C	-1.367767	-6.691844	0.479911
C	3.683713	-4.514334	2.146694
C	7.390768	-4.191502	1.592570
C	8.776775	-0.841289	2.573970
C	8.448041	-0.152575	3.872042
C	3.334624	-4.537452	-2.563747
C	2.303085	-3.607810	-1.922145
C	7.017649	0.740407	-1.783096
C	4.206748	2.595482	-6.171520
C	4.225234	3.122949	-4.754430
C	2.555195	9.778096	-1.301262
C	2.963633	8.355708	-1.661969
C	-1.265712	6.228569	2.291357
C	-0.038891	5.385420	2.260922
C	-3.405740	4.257680	4.598593
C	-2.771001	0.858929	6.071817
C	-1.214994	0.667283	6.057676
C	-2.924691	-0.816226	1.920867
C	-1.576317	-1.439198	1.569260
C	-4.335866	-2.276748	3.345771
O	-3.941737	-1.797149	4.424059
N	-3.663819	1.253045	0.870659
C	-3.166122	3.304078	-0.223711
O	-2.599170	3.685427	0.818618
C	-7.708383	3.042361	-1.270820
O	-8.376140	2.636790	-0.248581
O	-8.176958	3.211818	-2.420702
N	-3.001010	3.925673	-1.399313
C	-0.515621	3.773988	-3.158821
C	0.083962	4.280087	-4.322403
C	-0.969713	2.439586	-3.178041
C	0.230466	3.491434	-5.469369
C	-0.857365	1.652473	-4.322156
C	-0.246850	2.174852	-5.470608
O	-0.123520	1.336251	-6.558497
C	-5.037943	-1.984621	-3.467300
O	-5.421703	-2.572384	-4.493262
C	-7.147142	-0.707925	-1.706902
C	-8.612300	-0.396917	-1.373594
N	-9.028548	-1.078195	-0.125701
C	-8.646482	-0.693267	1.106523
N	-8.218832	0.539632	1.362860
N	-8.683130	-1.610618	2.114214
N	-4.530686	-2.638438	-2.388907
C	-5.132061	-4.464656	-0.915818
O	-5.153601	-3.677164	0.048556
C	-2.594148	-4.466969	-3.828716
S	-0.885018	-5.108001	-4.036484
C	-1.155064	-6.905285	-3.817034
N	-5.575767	-5.730427	-0.826977
C	-1.982894	-5.522659	1.270906
C	-0.074810	-6.258078	-0.231092
C	5.138984	-4.361992	2.508070

O	5.533541	-4.281948	3.686244
C	2.872781	-3.265444	2.588815
C	3.307156	-2.009139	1.814823
C	1.364015	-3.506442	2.434913
N	5.960346	-4.307316	1.438378
C	7.888448	-2.782800	1.394370
O	7.982249	-2.249234	0.271118
N	8.230663	-2.177874	2.539045
C	6.958493	0.105584	4.024302
C	6.364128	1.192053	3.359577
C	6.135178	-0.759611	4.762838
C	4.985285	1.409691	3.429804
C	4.753358	-0.543057	4.838888
C	4.174833	0.542719	4.172617
C	4.768796	-4.117989	-2.308773
O	5.346398	-4.433175	-1.249248
C	2.266652	-2.250634	-2.588551
C	3.158063	-1.231550	-2.218840
C	1.389385	-2.027319	-3.664776
C	3.176273	-0.021995	-2.920223
C	1.399121	-0.814349	-4.357787
C	2.293727	0.195133	-3.982308
N	5.381052	-3.410573	-3.284226
C	6.711298	-2.827415	-3.111402
C	6.625736	-1.298201	-3.122282
O	6.186823	-0.696793	-4.116918
N	7.064363	-0.702979	-1.993124
C	6.434621	1.086276	-0.407619
O	5.082619	0.622106	-0.232712
C	2.809533	8.102608	-3.178986
C	2.132378	7.354653	-0.832157
C	3.289898	6.719119	-3.643393
C	-2.062457	5.958579	3.537429
O	-1.942565	6.617756	4.583683
N	-2.859742	4.869462	3.421595
C	-3.137890	2.773908	4.624431
O	-2.959556	2.103445	3.589933
N	-3.151297	2.241223	5.859568
C	-0.872391	-0.836342	5.999745
C	-0.560224	1.382330	7.249595
C	0.623757	-1.134227	5.802284
N	-3.907503	-1.871528	2.133134
C	-3.444527	-0.051030	0.701530
C	-0.547434	-0.385603	1.228683
C	-0.174267	-0.117136	-0.096085
C	0.731059	0.903195	-0.397620
C	1.302545	1.700019	0.616071
C	0.911437	1.430023	1.945136
C	0.006089	0.413765	2.240138
C	3.829371	3.851683	-1.271128
C	4.394592	4.610756	-0.240507
C	3.895271	4.466614	1.057848
C	2.873768	3.552283	1.325646
C	2.316977	2.746992	0.309008
C	2.799560	2.942818	-1.004503
O	-3.656385	-0.663877	-0.369016
H	-5.265374	-4.047784	4.101930
H	-6.381720	-2.891945	3.361510
H	-5.359903	-3.890569	2.320302
H	-3.390428	1.701335	1.747862
H	-4.071810	1.559002	-1.166331
H	-6.121408	1.659782	0.246050
H	-5.563378	3.138953	1.004016
H	-6.104015	4.439460	-0.913629
H	-5.719560	3.145108	-2.030462
H	-2.485726	5.713511	-2.304540
H	-3.418801	3.523210	-2.236912
H	-2.064466	5.587667	-0.584250
H	-0.050224	5.540236	-2.034480
H	-0.213802	4.082922	-1.059078
H	0.452795	5.301950	-4.330036
H	-1.396379	2.005090	-2.281125

H	0.714328	3.895346	-6.355652
H	-1.206570	0.626206	-4.327451
H	0.369214	1.789591	-7.269261
H	-4.578263	-0.113563	-2.474942
H	-6.821813	0.940921	-3.082465
H	-7.274888	-0.568764	-3.876521
H	-7.016235	-1.798149	-1.693256
H	-6.503192	-0.312888	-0.910102
H	-8.790728	0.675592	-1.267439
H	-9.277189	-0.767627	-2.161455
H	-9.251662	-2.070531	-0.221343
H	-8.243874	1.334815	0.671615
H	-7.921554	0.753517	2.310608
H	-9.142661	-2.499230	1.935640
H	-8.761854	-1.263845	3.066788
H	-4.849373	-0.000444	-4.230835
H	-4.280312	-2.106455	-1.556307
H	-5.225502	-4.477949	-3.081924
H	-2.499031	-4.222042	-1.684614
H	-3.204295	-5.758058	-2.200110
H	-3.241766	-4.919317	-4.588704
H	-2.527337	-3.396912	-4.050152
H	-0.204624	-7.399961	-4.034455
H	-1.448123	-7.145584	-2.792189
H	-1.913599	-7.271039	-4.515647
H	-5.531910	-6.331964	-1.648132
H	-6.362624	-7.301765	0.286368
H	-5.204916	-6.280511	1.175840
H	-6.841083	-5.682671	0.853910
H	-2.041263	-8.239370	1.895065
H	-0.391999	-7.651206	2.193552
H	-0.705994	-8.760952	0.842836
H	-2.094619	-7.001118	-0.288585
H	-2.209820	-4.671525	0.618980
H	-2.914986	-5.822631	1.765261
H	-1.288487	-5.172946	2.045527
H	-0.263712	-5.426937	-0.919667
H	0.675521	-5.930916	0.499721
H	0.356891	-7.082790	-0.811202
H	3.558444	-4.675755	1.069545
H	3.091838	-3.106546	3.655436
H	2.743738	-1.131090	2.145391
H	4.370122	-1.788386	1.952636
H	3.123474	-2.131611	0.741005
H	0.802253	-2.651246	2.823248
H	1.090968	-3.631082	1.379275
H	1.042387	-4.404231	2.977113
H	3.291213	-5.397155	2.668429
H	7.879147	-4.826939	0.834380
H	5.583602	-4.346092	0.492990
H	7.661676	-4.565269	2.589564
H	9.869958	-0.879491	2.431923
H	8.088927	-2.681252	3.414620
H	8.363634	-0.283593	1.724931
H	8.812464	-0.756234	4.716130
H	8.995242	0.798740	3.907724
H	6.986515	1.865854	2.776054
H	6.573243	-1.614297	5.270890
H	4.545494	2.240831	2.891716
H	4.130799	-1.228824	5.405711
H	3.102338	0.704420	4.219831
H	3.140877	-4.599326	-3.642493
H	1.320356	-4.084084	-2.004870
H	2.526381	-3.509262	-0.853139
H	3.849193	-1.370926	-1.394455
H	0.705663	-2.817098	-3.959656
H	3.893201	0.738295	-2.640810
H	0.723397	-0.651092	-5.189857
H	2.292205	1.139389	-4.511378
H	3.223614	-5.544930	-2.144476
H	7.361726	-3.139489	-3.946155
H	4.824957	-3.079298	-4.072939

H	7.125780	-3.208638	-2.170080
H	8.029654	1.172013	-1.854504
H	7.363029	-1.286451	-1.212496
H	6.409051	1.176434	-2.584151
H	7.020534	0.594529	0.375684
H	6.503134	2.172175	-0.250366
H	4.479259	1.285309	-0.598493
H	5.222008	2.452825	-6.560265
H	3.686978	3.283769	-6.849726
H	4.751483	4.083156	-4.689266
H	3.208624	3.282449	-4.374416
H	4.730103	2.420275	-4.080796
H	3.697456	1.626614	-6.229988
H	2.693300	9.973022	-0.230953
H	1.495167	9.945359	-1.535291
H	4.026490	8.214063	-1.405839
H	1.750331	8.235284	-3.449957
H	3.366550	8.880305	-3.721404
H	2.408516	6.317219	-1.032104
H	2.267837	7.530624	0.241814
H	1.063904	7.476446	-1.058276
H	3.238236	6.628902	-4.734730
H	4.330857	6.545003	-3.342181
H	2.684093	5.913147	-3.217086
H	3.140291	10.521345	-1.857540
H	-1.881160	6.026576	1.409920
H	-0.286172	4.319024	2.212056
H	0.580609	5.610443	1.385234
H	0.583344	5.546988	3.150346
H	-1.004392	7.293215	2.281094
H	-4.504580	4.404899	4.660376
H	-2.830472	4.318111	2.563505
H	-2.971046	4.752040	5.480776
H	-3.173715	0.532033	7.038882
H	-3.173426	2.877549	6.655164
H	-3.222398	0.241870	5.292901
H	-0.854681	1.137667	5.130057
H	-1.221798	-1.316571	6.926529
H	-1.449621	-1.292876	5.185152
H	0.532356	1.337481	7.194791
H	-0.842522	2.441348	7.279252
H	-0.870686	0.919153	8.195877
H	0.797059	-2.210985	5.693113
H	1.008870	-0.646058	4.898336
H	1.223783	-0.785062	6.649916
H	0.993649	1.056195	-1.435374
H	1.317138	2.006197	2.767950
H	-0.593483	-0.711556	-0.902475
H	-0.281204	0.239005	3.269941
H	-1.251684	-2.040370	2.426562
H	-1.719568	-2.119301	0.721932
H	-2.863606	-0.183082	2.823544
H	5.190889	5.317081	-0.451522
H	4.184471	3.971328	-2.286509
H	2.377223	2.384716	-1.829261
H	2.513740	3.471355	2.343751
H	4.300787	5.064680	1.868155
H	-4.246043	-2.352074	1.301228
el energy= -5848.63721550			
zpe= -5846.448337			
th energy= -5846.345908			
th enthalpy= -5846.344964			
free energy= -5846.584310			

4S0K TS at $\Phi_{\text{PCM+GD3BJ}} = 2.4^\circ$

C	6.241836	-2.042009	-4.140763
C	4.315932	2.685688	0.094023
C	5.606940	3.410561	-0.310959

C	6.170475	4.300774	0.810568
C	2.027266	5.026586	1.988531
C	0.791265	4.249358	2.481701
C	6.360059	0.152959	2.674835
C	7.667805	0.863362	2.310212
C	6.422232	-3.417758	1.308429
C	5.218231	-4.336053	1.545791
C	8.053631	-4.895716	-1.756459
C	3.517625	-7.598059	-2.279788
C	3.603914	-6.415444	-1.249401
C	-2.113651	-5.410707	-1.995383
C	-5.682406	-6.075021	-1.054569
C	-7.869459	-3.003786	-1.346397
C	-7.952478	-2.200308	-2.615441
C	-0.870436	-5.656110	2.470093
C	-0.065904	-4.517880	1.805570
C	-5.819354	-1.518580	2.671200
C	-10.767958	1.279383	0.837284
C	-10.175259	0.371029	-0.217747
C	-2.906215	0.741006	6.584857
C	-3.237795	1.357423	5.223034
C	-3.458851	8.557098	2.886844
C	-3.517466	7.047445	3.184226
C	0.359895	6.297190	-1.577555
C	-0.670776	5.209358	-1.334997
C	2.640676	5.121968	-4.323106
C	2.281577	1.821558	-6.118026
C	0.810560	1.232527	-5.955397
C	3.550102	-0.300464	-2.173123
C	2.398944	-1.207924	-1.747995
C	4.973782	-1.261973	-3.930424
O	4.298699	-0.799303	-4.867803
N	3.875871	1.808358	-0.990563
C	3.191608	3.668854	0.349142
O	2.423650	4.031541	-0.562586
C	7.581452	4.876434	0.546114
O	8.341770	4.272184	-0.302512
O	7.912566	5.882118	1.211334
N	3.110796	4.141832	1.602046
C	0.935257	3.533288	3.804455
C	0.212906	3.972065	4.927103
C	1.763487	2.404477	3.956951
C	0.307646	3.319666	6.159768
C	1.890999	1.761998	5.189447
C	1.154236	2.211602	6.294248
O	1.294934	1.518337	7.475453
C	6.591547	-1.358240	2.670797
O	7.253724	-1.915918	3.563208
C	8.112734	0.506570	0.879080
C	9.332900	1.301348	0.399016
N	9.738336	0.886672	-0.962187
C	9.097640	1.266943	-2.084687
N	8.336101	2.355718	-2.128665
N	9.224915	0.491800	-3.198821
N	6.089103	-2.024135	1.596708
C	6.891939	-3.519597	-0.130494
O	6.611454	-2.669893	-0.996739
C	4.766359	-4.305998	3.011171
S	3.468528	-5.579327	3.292931
C	2.944646	-5.111829	4.983304
N	7.614474	-4.618137	-0.403546
C	3.797890	-5.077975	-1.987806
C	2.358291	-6.379438	-0.353823
C	-3.593456	-5.587756	-2.194968
O	-4.141808	-5.498650	-3.309233
C	-1.655101	-3.986603	-2.409870
C	-2.241803	-2.924939	-1.464789
C	-0.122663	-3.893129	-2.458435
N	-4.257850	-5.868196	-1.052103
C	-6.453200	-4.863508	-0.579083
O	-6.521748	-4.544945	0.625459
N	-7.052746	-4.185253	-1.564235

C	-6.641953	-1.491999	-2.924425
C	-6.412088	-0.206954	-2.403923
C	-5.612287	-2.115978	-3.649668
C	-5.186012	0.438288	-2.596767
C	-4.382771	-1.473261	-3.842688
C	-4.164568	-0.195169	-3.315192
C	-2.363910	-5.403892	2.399339
O	-2.927313	-5.246914	1.298028
C	-0.100766	-3.199614	2.552651
C	-1.304912	-2.518065	2.794545
C	1.093586	-2.628445	3.026233
C	-1.322122	-1.329010	3.528474
C	1.083354	-1.426619	3.743679
C	-0.129586	-0.779313	4.011286
N	-3.048566	-5.346085	3.563096
C	-4.465525	-4.982416	3.590267
C	-4.660720	-3.460871	3.686793
O	-4.131181	-2.815776	4.607815
N	-5.446542	-2.931750	2.725330
C	-5.555130	-0.876974	1.294210
C	-6.101816	0.559159	1.289041
C	-4.068882	-0.917422	0.917658
C	-9.768119	1.098313	-1.471883
C	-10.176936	0.806558	-2.758292
C	-8.873156	2.235089	-1.576249
N	-9.583350	1.684883	-3.655452
C	-8.783212	2.574502	-2.965279
C	-8.133388	2.994375	-0.647408
C	-7.993923	3.637262	-3.426311
C	-7.362202	4.061504	-1.102722
C	-7.290689	4.379665	-2.479187
C	-3.843880	6.800680	4.673726
C	-2.191654	6.388732	2.769571
C	-3.998693	5.320906	5.056394
C	0.934611	6.212379	-2.970900
O	0.383577	6.729281	-3.957190
N	2.088453	5.497759	-3.042136
C	2.614975	3.619856	-4.508758
O	2.848939	2.828648	-3.575681
N	2.365837	3.223772	-5.770481
C	0.855143	-0.306523	-6.037844
C	-0.144138	1.864839	-6.976816
C	-0.484135	-0.989330	-5.711003
N	4.680865	-1.084667	-2.625631
C	4.044473	0.484672	-0.957481
C	1.227533	-0.411795	-1.227239
C	0.995862	-0.256262	0.146136
C	-0.045135	0.548123	0.612180
C	-0.897431	1.235394	-0.276087
C	-0.647649	1.081289	-1.656900
C	0.389738	0.274593	-2.118194
C	-3.313494	3.049586	2.051514
C	-4.177843	3.674231	1.146204
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