

Supporting Information

Reaction Mechanism and Regioselectivity of Uridine Diphosphate Glucosyltransferase RrUGT3: A Combined Experimental and Computational Study

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CONTENTS

1. Supplementary Figures	1
Figure S1.	1
Figure S2.	1
Figure S3.	2
Figure S4.	2
Figure S5.	3
Figure S6.	3
Figure S7.	4
Figure S8.	4
Figure S9.	5
Figure S10.	5
Figure S11.	6
Figure S12.	6
2. Supplementary Tables.....	7
Table S1.....	7
Table S2.....	7
Table S3.....	8
Table S4.....	9
Table S5.....	9
Table S6.....	9
Table S7.....	10
Table S8.....	10
3. Cartesian Coordinates	11
4. Supplementary References.....	27

1. Supplementary Figures

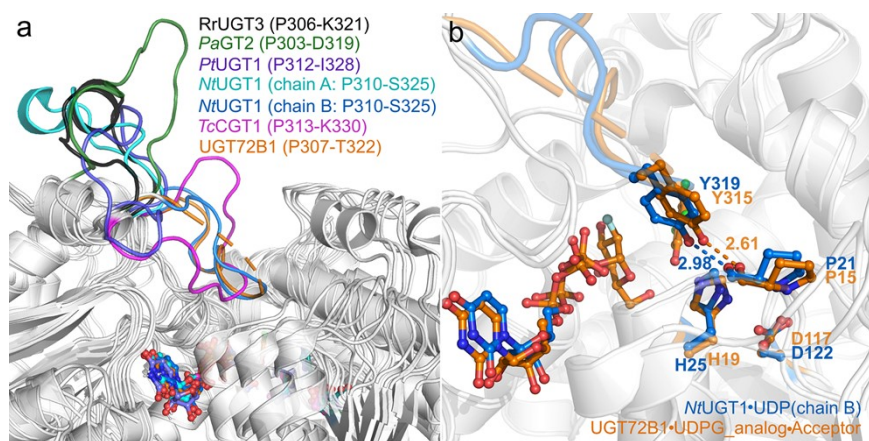


Figure S1. (a) Structural overlap of the homologous UGT enzymes. (b) The H-bond network analysis around the key tyrosine of the loop region of *UGT72B1* ternary complex and *NtUGT1* binary complex (chain B), with *UGT72B1* shown in orange and *NtUGT1* shown in blue. The distances are given in angstrom.

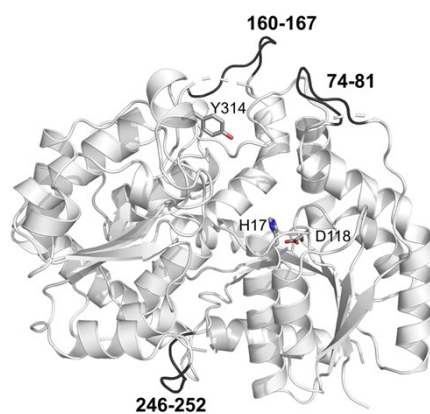


Figure S2. The added non-terminal residues that are missing in the crystal structure of *RrUGT3* using *MODELLER* (sequence: 74-81, 160-167 and 246-252).

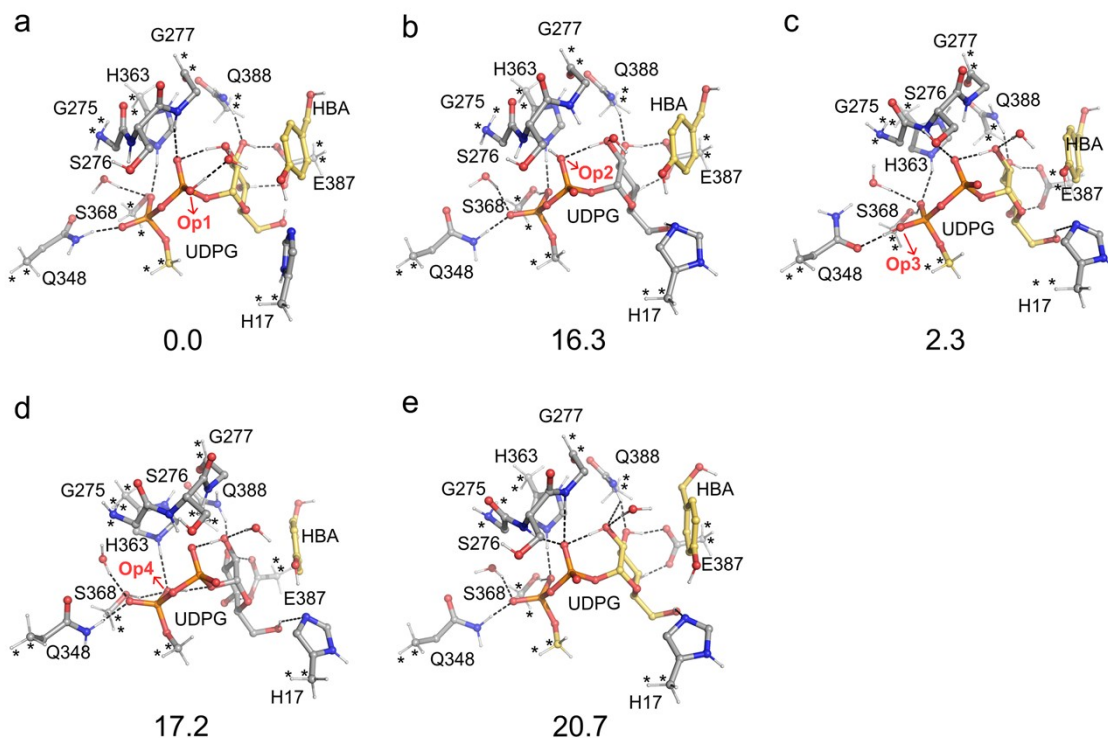


Figure S3. Optimized structures with the diphosphate group of UDPG is protonated at (a) Op1, (b) Op2, (c) Op3, (d) Op4, and (e) with the diphosphate group of UDPG was deprotonated. Fixed atoms during geometry optimizations are marked with stars. For clarity, most of the nonpolar hydrogens are hidden. The energy for the protonation of the diphosphate group of UDPG by a bulk proton was estimated using the following approximation: $\Delta E = E(\text{protonated form}) - E(\text{deprotonated form}) + 279.8 \text{ kcal/mol}$, in which 279.8 kcal/mol is the Gibbs free energy of a proton at pH = 7.¹ At the bottom of each figure, the energies relative to (a) are given in kcal/mol. The solvation effects were simulated using the SMD solvation model with $\epsilon=4$.

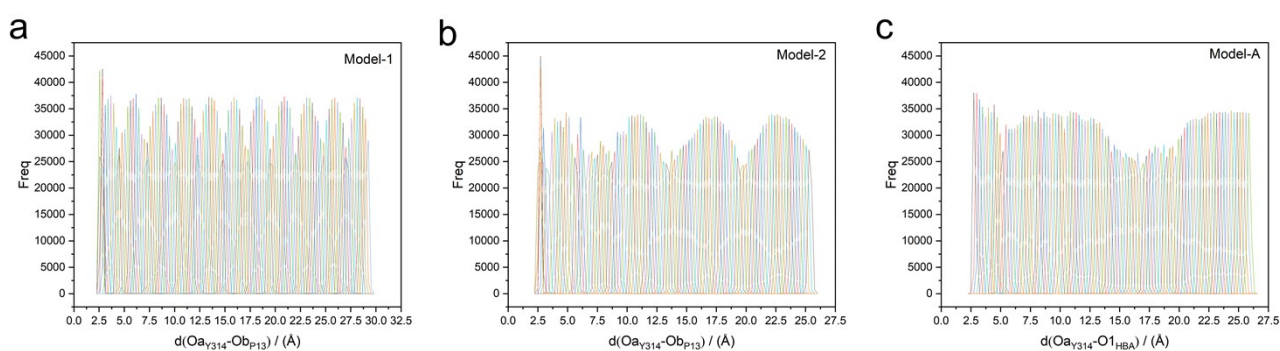


Figure S4. Histograms of constrained MD simulations from all windows of the US simulations for the “open-to-closed” transformation of (a) Model-1, (b) Model-2, and (c) Model-A.

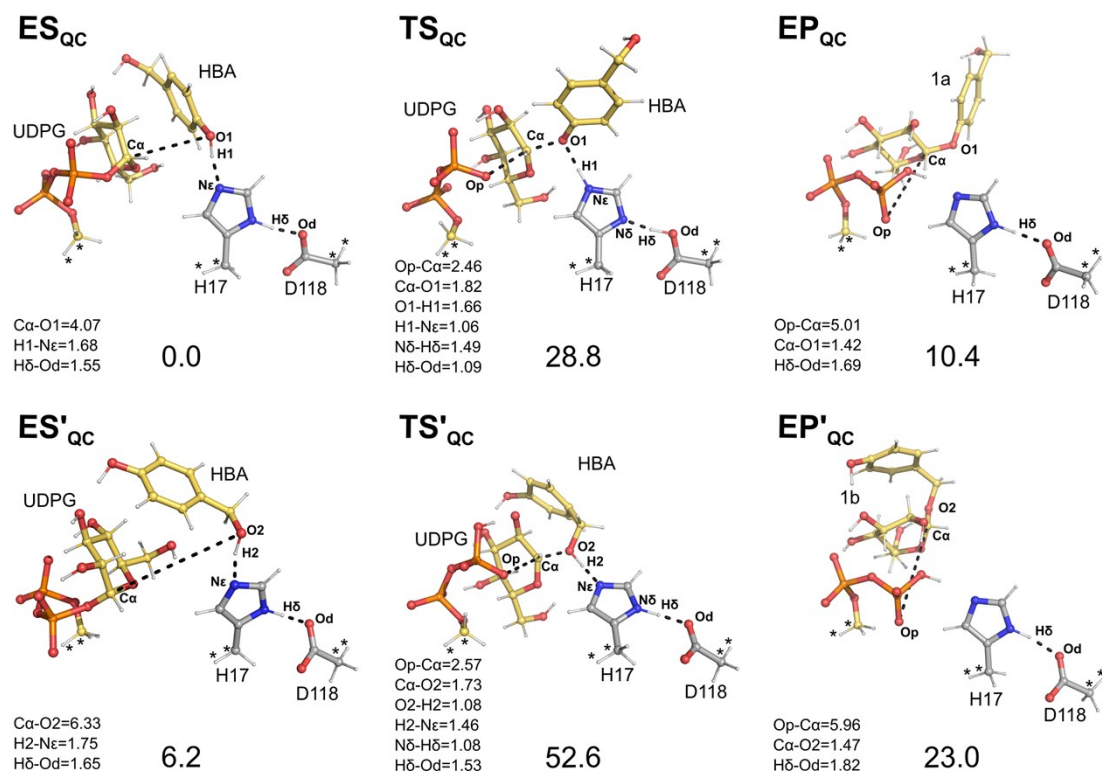


Figure S5. DFT optimized structures of Model-A_C (ES_{QC}, TS_{QC}, EP_{QC}) and Model-B_C (ES'_{QC}, TS'_{QC}, EP'_{QC}) with the diphosphate of UDPG in its deprotonated state. The energies relative to ES_{QC} are given in kcal/mol, and distances are given in angstrom. Fixed atoms during geometry optimizations are marked with stars.

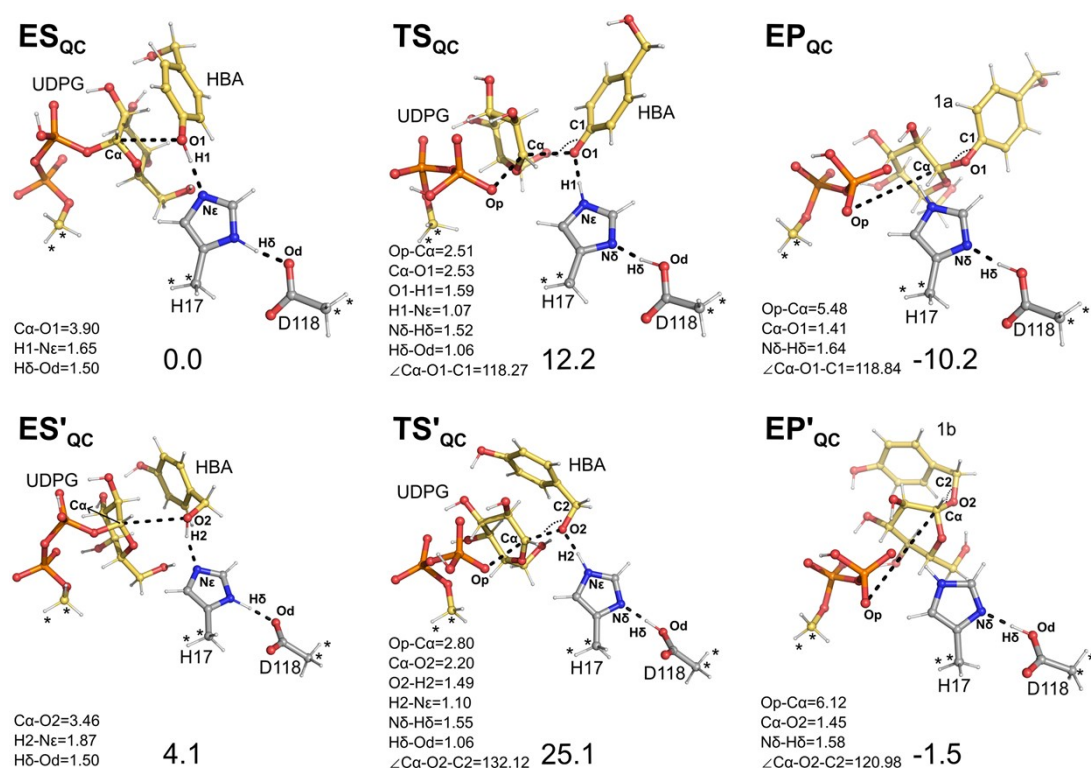


Figure S6. DFT optimized structures of Model-A_C (ES_{QC}, TS_{QC}, EP_{QC}) and Model-B_C (ES'_{QC}, TS'_{QC}, EP'_{QC}) with the diphosphate of UDPG in its singly protonated state. The calculated energies relative to ES_{QC} are given in kcal/mol. Key distances and angles are given in angstrom and degree, respectively. Fixed atoms during geometry optimizations are marked with stars.

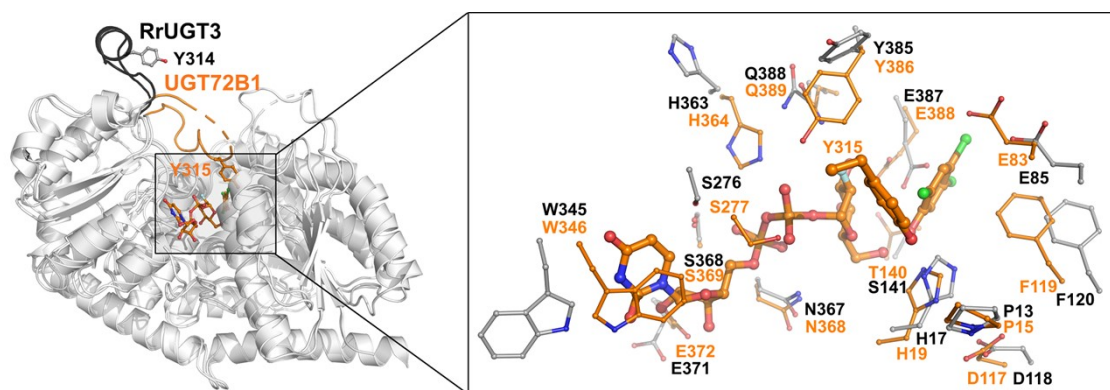


Figure S7. Comparison of the flexible loop region and binding pocket of apo-RrUGT3 with the homologous ternary complex of UGT72B1•UDP-2-deoxy-2-fluoro glucose•2,4,5-trichlorophenol. The RrUGT3 is shown in gray and the UGT72B1 is shown in orange.

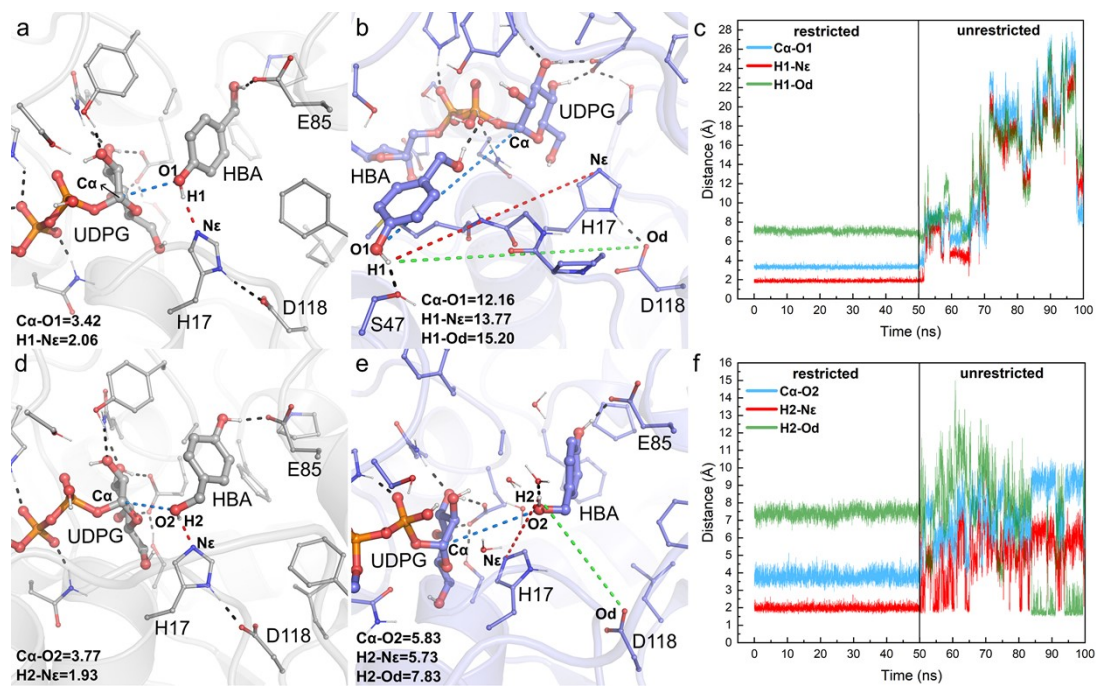


Figure S8. Geometry information of the starting and the final snapshots from the MD simulations of (a,b) Model-A₀ and (d,e) Model-B₀, and the fluctuation of key distances during the 50 ns of restricted and unrestricted MD simulations for (c) Model-A₀ and (f) Model-B₀. Key distances are given in angstrom.

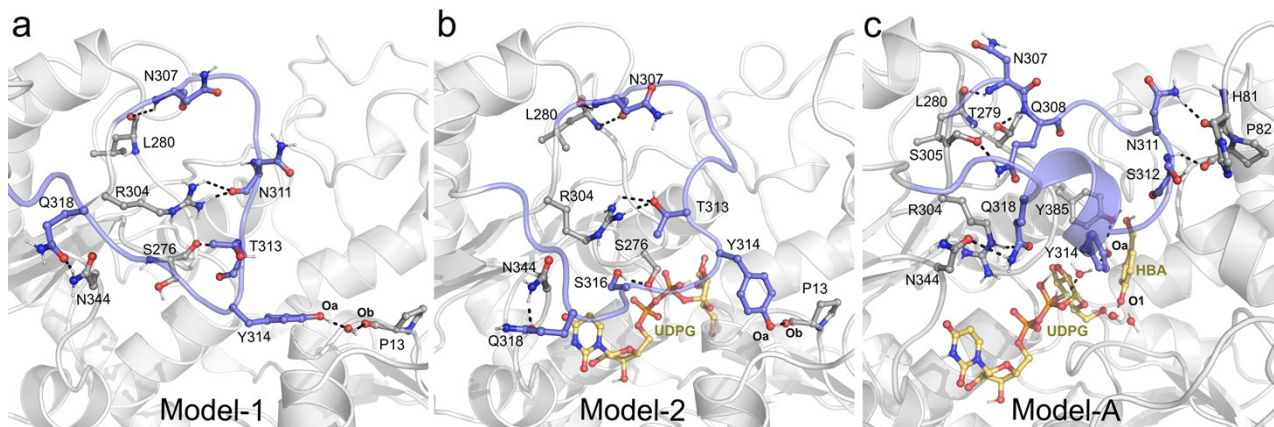


Figure S9. The hydrogen bond network analysis of the loop region of the most representative trajectory from (a) Model-1, (b) Model-2, and (c) Model-A in the “closed” state.

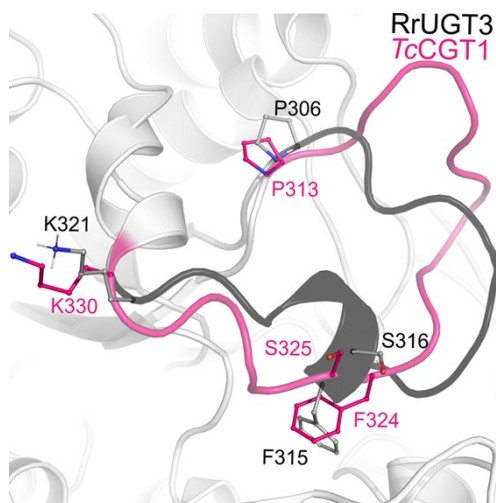


Figure S10. The overlap of Ω -1 loop region between the representative snapshot of the “closed” state of Model-A and the crystal structure of highly homologous enzyme *TcCGT1* (PDB ID: 6JTD). The Ω -1 loop region of Model-A is shown in black while the Ω -1 loop region of *TcCGT1* is shown in pink. The conserved residues in the Ω -1 loop region are shown as ball and sticks.

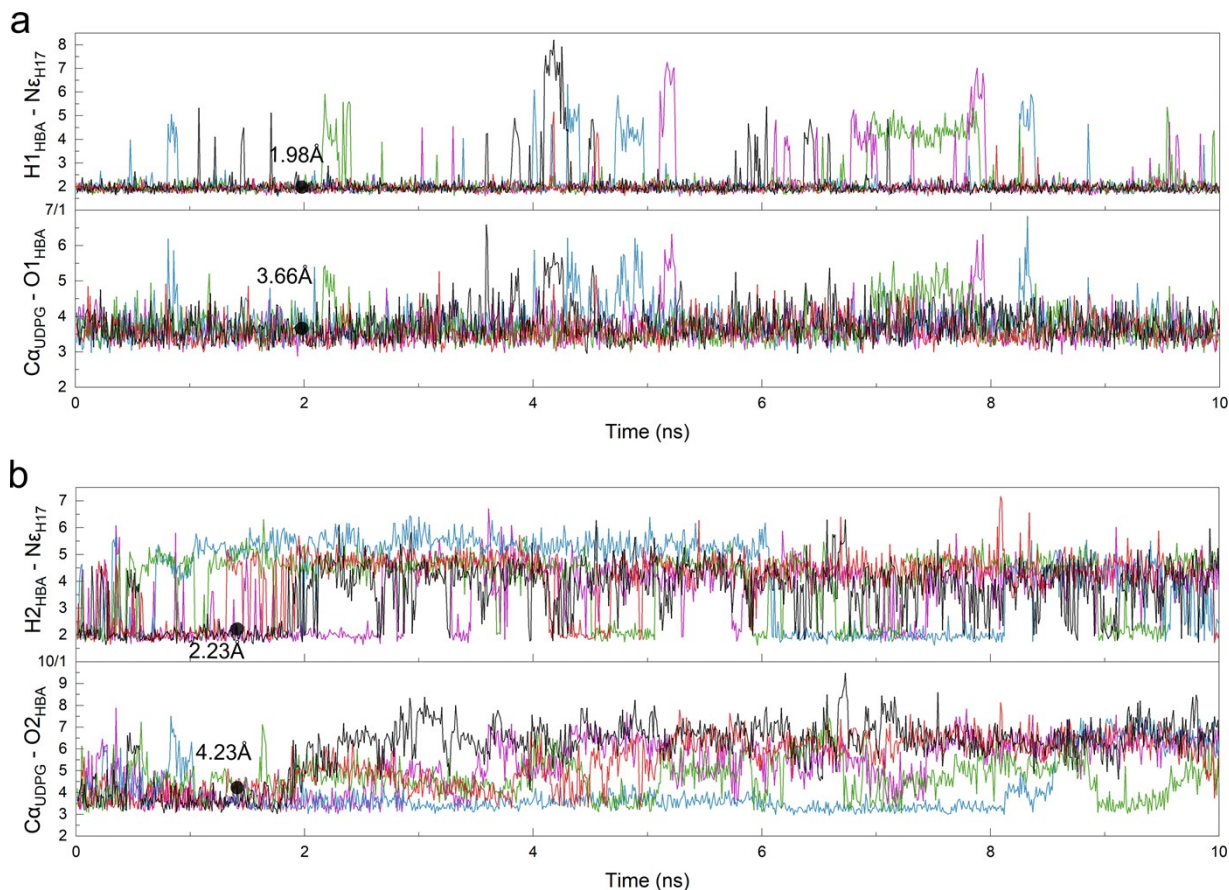


Figure S11. Fluctuation of key distances from five replicates unrestricted MD simulations of Model-A_C and Model-B_C. (a) The distances of Cα-O1 and H1-Nε for Model-A_C. (b) The distances of Cα-O2 and H2-Nε for Model-B_C. Distances are given in angstrom. The position of the obtained representative conformations in the MD trajectories were marked using black dots.

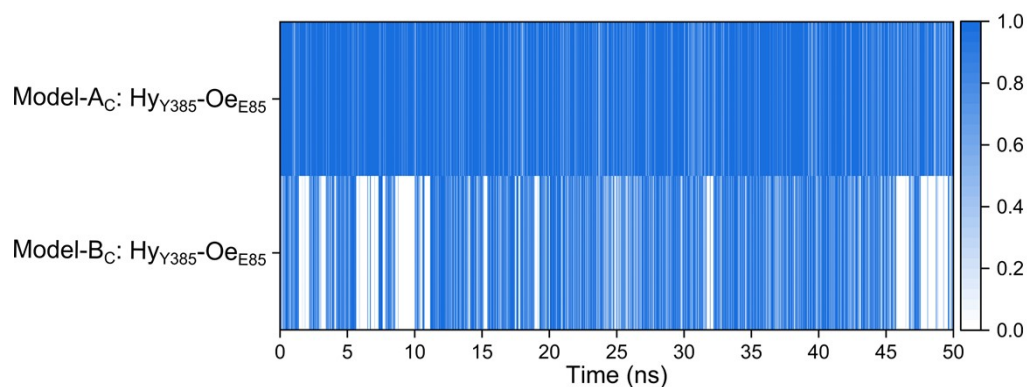


Figure S12. The heatmap of hydrogen bond interactions between Hy_{Y385} and Oe_{E85} from unrestricted MD simulations of Model-A_C and Model-B_C.

2. Supplementary Tables

Table S1. Strains and plasmids used in this study.

Strain	Host	Genotype/Description	Source
Rr3	<i>E. coli</i> BL21(DE3)	pETM11- <i>RrUGT3</i>	This study
Rr3-WT / GF-9	<i>E. coli</i> BL21(DE3)	pET28b- <i>RrUGT3</i>	Guo F., et al., 2022 ²
Rr3-H17A	<i>E. coli</i> BL21(DE3)	pET28b- <i>RrUGT3(H17A)</i>	This study
Rr3-D118A	<i>E. coli</i> BL21(DE3)	pET28b- <i>RrUGT3(D118A)</i>	This study
Rr3-F120A	<i>E. coli</i> BL21(DE3)	pET28b- <i>RrUGT3(F120A)</i>	This study
Rr3-Y314A	<i>E. coli</i> BL21(DE3)	pET28b- <i>RrUGT3(Y314A)</i>	This study
Rr3-E85A	<i>E. coli</i> BL21(DE3)	pET28b- <i>RrUGT3(E85A)</i>	This study

Table S2. Primers used in this study.

Plasmid	Primer	Sequence (5'-3')
pETM11- <i>RrUGT3</i>	RrUGT3-F	AAAACCATGGCTGGCACCCACACATC
	RrUGT3-R	AAAACCTCGAGTTAATGCTTCATAGAAGAACGC
pET28b (+)- <i>RrUGT3(H17A)</i>	H17A-F	TGGGCGCACTGATCCCGATGGCCGA
	H17A-R	GGATCAGTGCGCCCATGCCCGGGCT
pET28b (+)- <i>RrUGT3(D118A)</i>	D118A-F	GTTGTTGCACTGTTCCGGCACTGATGCATTC
	D118A-R	GAACAGTGCAACAACCAGAGAAACCAGGTT
pET28b (+)- <i>RrUGT3(F120A)</i>	F120A-F	GATCTGGCAGGCACTGATGCATTCGACCCG
	F120A-R	AGTGCCCTGCCAGATCAACAACCAGAGAAAC
pET28b (+)- <i>RrUGT3(Y314A)</i>	Y314A-F	AGCACCGCATTCTCTGTACAAAGCCA
	Y314A-R	AGAGAATGCGGTGCTGTTCGGGATTTGGT
pET28b (+)- <i>RrUGT3(E85A)</i>	E85A-F	CGTATCGCAACCCCTGATCTCCCTGACCGTT
	E85A-R	CAGGGTTGCGATACGCGGATGAGCTGGAGA

Table S3. Diffraction-data collection and refinement statistics.

	RrUGT3
PDB code	8YP7
Data collection statistics	
X-ray source	BL19U1, SSRF
Wavelength (Å)	0.97915
Space group	$P2_12_12_1$
Unit-cell dimensions (Å or °)	a = 69.19, b = 70.83, c = 92.66, $\alpha = \beta = \gamma = 90.00$
Resolution range (Å)	46.33–1.87 (1.91–1.87)
Number of unique reflections	38051 (2124)
Completeness (%)	99.2 (87.6)
Mean I/sigma(I)	20.6 (1.4)
Multiplicity	13.1 (13.2)
R_{merge}	0.090 (2.018)
R_{measure}	0.093 (2.099)
$CC_{1/2}$ (%)	100 (58.5)
Refinement statistics	
Resolution (Å)	1.87
$R_{\text{work}} / R_{\text{free}}$ (%)	17.95/21.21
Protein atoms	3419
Water	160
B factor (Å ²)	
Protein	32.32
Water	37.13
RMSD in bond lengths (Å)	0.010
RMSD in bond angles (°)	1.62
Ramachandran plot (%)	
favored	97.25%
allowed	2.52%

Table S4. Estimation of the pK_a of the enzyme-bound substrate (UDPG). “H” represents that one phosphate group of diphosphate of UDPG is protonated, “D” represents the diphosphate of UDPG is deprotonated. The pK_a value of acetic acid in aqueous solution was taken from previous study (measured to be 4.76)³ and been used as a reference. All the calculations were carried out at the B3LYP/def2-SVP level of theory.

The pK_a of the UDPG when Op1 atom was protonated.	
Deprotonation energy of the enzyme-bound substrate.	$\Delta E_1 = E(\mathbf{E:H})_{\epsilon=4} - E(\mathbf{E:D})_{\epsilon=4} = 300.5$ kcal/mol
Deprotonation energy of the acetic acid in aqueous solution.	$\Delta E_2 = E(\text{CH}_3\text{COOH})_{\epsilon=78} - E(\text{CH}_3\text{COO}^-)_{\epsilon=78} = 281.7$ kcal/mol
$\Delta pK_a = (\Delta E_1 - \Delta E_2) / 2.303RT = 18.8 / 1.37 = 13.72$, The pK_a of enzyme-bound substrate: $13.72 + 4.76 = \mathbf{18.48}$	
The pK_a of the UDPG when Op2 atom was protonated.	
Deprotonation energy of the enzyme-bound substrate.	$\Delta E_1 = E(\mathbf{E:H})_{\epsilon=4} - E(\mathbf{E:D})_{\epsilon=4} = 284.3$ kcal/mol
$\Delta pK_a = (\Delta E_1 - \Delta E_2) / 2.303RT = 2.6 / 1.37 = 1.90$, The pK_a of enzyme-bound substrate: $1.91 + 4.76 = \mathbf{6.66}$	
The pK_a of the UDPG when Op3 atom was protonated.	
Deprotonation energy of the enzyme-bound substrate.	$\Delta E_1 = E(\mathbf{E:H})_{\epsilon=4} - E(\mathbf{E:D})_{\epsilon=4} = 298.3$ kcal/mol
$\Delta pK_a = (\Delta E_1 - \Delta E_2) / 2.303RT = 16.6 / 1.37 = 12.12$, The pK_a of enzyme-bound substrate: $12.13 + 4.76 = \mathbf{16.88}$	
The pK_a of the UDPG when Op4 atom was protonated.	
Deprotonation energy of the enzyme-bound substrate.	$\Delta E_1 = E(\mathbf{E:H})_{\epsilon=4} - E(\mathbf{E:D})_{\epsilon=4} = 283.4$ kcal/mol
$\Delta pK_a = (\Delta E_1 - \Delta E_2) / 2.303RT = 1.7 / 1.37 = 1.24$, The pK_a of enzyme-bound substrate: $1.26 + 4.76 = \mathbf{6.00}$	

Table S5. The MM-PBSA calculated binding free energies of the substrates (UDPG and HBA) to the enzyme at the “open” and “closed” state of Model-A and Model-B.

	Type	Binding free energy (kcal/mol)
Open	Model-A _O	-24.5
	Model-B _O	-13.7
Closed	Model-A _C	-36.2
	Model-B _C	-39.1

Table S6. Calculated energies of Model-A_C (ES, TS, EP) and Model-B_C (ES', TS', EP') by using QM/MM methods.

		E_{BS1} (a.u.)	E_{BS2} (a.u.)	E_{ZPE} (a.u.)	E (a.u.)	ΔH (kcal/mol)
Model-A _C	ES	-4961.330013	-4966.502371	1.260096	-4965.242275	0
	TS	-4961.293482	-4966.474077	1.256475	-4965.217602	15.5
	EP	-4961.314626	-4966.495776	1.258661	-4965.237115	3.2
Model-B _C	ES'	-4654.614496	-4659.399765	1.152152	-4658.247612	0
	TS'	-4654.575962	-4659.366772	1.150675	-4658.216097	19.8
	EP'	-4654.608626	-4659.396798	1.153087	-4658.243711	2.4

Table S7. DFT calculated energies of stationaries for the phenolic and alcoholic glycosylation from Model-A_C and Model-B_C, with the diphosphate of UDPG in its deprotonated state. The solvation effects were calculated using the SMD solvation model with $\epsilon=78$.

Deprotonated at diphosphate of UDPG		E _{BS1} (a.u.)	E _{solvation} (a.u.)	E _{BS2} (a.u.)	E _{ZPE} (a.u.)	E (a.u.)	ΔE (kcal/mol)
Phenolic glycosylation	ES _{QC}	-2775.252844	-2775.701499	-2778.009746	0.503928	-2777.954473	0
	TS _{QC}	-2775.130937	-2775.639980	-2777.894465	0.494886	-2777.908622	28.8
	EP _{QC}	-2775.206209	-2775.678714	-2777.967823	0.502466	-2777.937862	10.4
Alcoholic glycosylation	ES' _{QC}	-2775.245427	-2775.691444	-2778.001698	0.503102	-2777.944613	6.2
	TS' _{QC}	-2775.117734	-2775.603938	-2777.880888	0.496520	-2777.870572	52.6
	EP' _{QC}	-2775.194245	-2775.661120	-2777.953429	0.502398	-2777.917906	23.0

Table S8. DFT calculated energies of stationaries from the phenolic and alcoholic glycosylation from Model-A_C and Model-B_C. The solvation effects were calculated using the SMD solvation model with $\epsilon=78$.

		E _{BS1} (a.u.)	E _{solvation} (a.u.)	E _{BS2} (a.u.)	E _{ZPE} (a.u.)	E (a.u.)	ΔE (kcal/mol)
Phenolic glycosylation	ES _{QC}	-2775.924509	-2776.156672	-2778.671749	0.514545	-2778.389367	0
	TS _{QC}	-2775.905777	-2776.134291	-2778.653164	0.511730	-2778.369948	12.2
	EP _{QC}	-2775.943864	-2776.177497	-2778.687509	0.515550	-2778.405592	-10.2
Alcoholic glycosylation	ES' _{QC}	-2775.925046	-2776.151087	-2778.671777	0.515012	-2778.382778	4.1
	TS' _{QC}	-2775.880553	-2776.115337	-2778.625713	0.511163	-2778.349334	25.1
	EP' _{QC}	-2775.935485	-2776.168099	-2778.674999	0.515790	-2778.391823	-1.5

3. Cartesian Coordinates

QM/MM Calculations

ES			
C	41.247197	41.506468	52.043255
H	41.824883	42.402202	52.312661
H	40.797584	41.159796	52.988410
C	42.140786	40.438987	51.490888
N	43.096523	39.820799	52.278221
H	43.265304	39.969397	53.307957
C	43.719019	38.887190	51.526081
H	44.509463	38.241813	51.906082
N	43.220744	38.853211	50.293759
C	42.233737	39.817427	50.259126
H	41.656275	39.994406	49.353300
C	43.268744	41.393025	56.968233
H	42.304903	41.889300	57.149816
H	44.034748	42.158248	57.172203
C	43.289950	41.075187	55.457977
O	43.048198	42.059151	54.716801
O	43.520140	39.910009	55.040476
C	42.127234	32.776443	49.542814
H	42.233173	32.151547	48.642784
H	42.277590	33.810496	49.182039
O	43.086885	32.393224	50.488896
H	43.255044	33.195527	51.030783
C	44.194488	44.210014	42.790966
H	44.140104	43.494540	43.624753
H	45.105559	44.821919	42.949661
O	43.020649	44.988402	42.793341
H	42.995458	45.530438	41.968905
C	48.581854	49.236725	45.690515
H	48.342643	50.032246	46.413220
H	47.941490	49.384296	44.802545
C	48.353672	47.859921	46.287023
C	48.071798	47.691323	47.650847
H	47.959071	48.569729	48.286534
C	47.927854	46.423992	48.223610
H	47.730808	46.317025	49.292257
C	48.051847	45.276749	47.426924
O	47.979057	44.020338	47.937650
H	47.700726	44.030014	48.910183
C	48.268154	45.427303	46.048046
H	48.360543	44.538477	45.421050
C	48.422001	46.698562	45.495586
H	48.621169	46.778437	44.422896
C	43.093562	36.467630	37.449154
H	44.060126	35.973631	37.640510
H	43.282952	37.205208	36.656888
C	42.638151	37.065770	38.742279
N	43.571418	37.292066	39.738337
H	44.581958	37.160688	39.632761
C	42.972694	37.726685	40.846153
H	43.458208	37.944329	41.791378
N	41.669348	37.809227	40.594519
H	40.947076	38.054484	41.320493
C	41.422831	37.412694	39.293510
H	40.411089	37.477656	38.897891
C	49.170436	36.787328	41.025293
H	49.721809	37.232487	40.179786
H	48.106451	36.989099	40.853666
C	49.607828	37.445584	42.314323
C	50.957228	37.561857	42.689484
H	51.738069	37.129072	42.056058
C	51.324913	38.252425	43.848082
H	52.378828	38.335512	44.122786
C	50.352853	38.875889	44.646629
O	50.670748	39.693223	45.690731
H	51.287818	39.260389	46.348562
C	49.001477	38.719126	44.310190
H	48.237107	39.148655	44.958590
C	48.644047	37.999069	43.173099
H	47.583633	37.842069	42.962289
C	45.335849	31.772842	46.865854
H	44.881899	31.394363	47.791741
H	46.114829	32.498975	47.147136
C	44.303247	32.542684	46.039148
O	43.077909	32.354082	46.296985
O	44.743442	33.362224	45.195297
C	44.697051	33.799015	41.129375
H	43.638951	33.922727	40.854140
H	44.727413	33.716961	42.222964
C	45.424000	35.053770	40.687666
O	45.797407	35.255622	39.518942
N	45.561387	35.985284	41.649216
H	45.923947	36.898939	41.374928
H	45.091172	35.892958	42.562345
P	39.387055	39.613451	42.908140
P	42.152957	40.336603	43.893188
C	41.720664	36.472733	48.274675
O	42.894112	36.368679	49.064283

C	41.990641	36.880838	46.828815	H	44.167841	39.117831	48.781147
O	42.733399	38.115172	46.877607	H	50.991118	37.391900	47.101188
C	42.713731	35.792486	46.015404	O	44.968602	41.545260	45.184284
O	41.833343	34.702093	45.863536	H	45.191175	42.040115	46.027092
C	43.167857	36.353634	44.655506	H	45.819356	41.588166	44.687724
O	43.855521	35.407435	43.872440	O	38.911745	39.207383	39.268276
C	44.037502	37.590604	44.911564	H	38.856590	39.944823	38.641857
O	44.631058	38.101171	43.731517	H	38.805533	39.633121	40.145034
C	43.223179	38.625225	45.700430	O	43.134861	34.896992	51.524491
O	38.637789	40.369823	41.848142	H	43.810740	35.314027	52.115896
O	43.063642	40.097310	42.713671	H	43.138119	35.410490	50.691141
O	39.916417	38.226114	42.596942	O	47.042269	43.876311	50.348598
O	42.503595	41.617971	44.732143	H	46.395085	44.586898	50.573772
O	40.633864	40.586348	43.452477	H	46.514231	43.051178	50.305317
O	42.078552	39.074418	44.880076	O	45.623296	42.982737	47.257443
C	38.404937	40.482881	45.286732	H	46.573350	43.227476	47.354521
O	38.531856	39.497394	44.297837	H	45.406748	42.619597	48.151038
H	44.149320	38.885711	43.394964	O	45.287579	41.874838	49.692899
H	42.313937	33.851630	46.029780	H	45.056728	40.995708	49.315571
H	43.069993	37.264600	49.443960	H	44.458225	42.320933	50.004108
H	41.019993	37.196291	48.723834	H	40.445119	41.795014	51.363933
H	41.217945	35.496966	48.250649	H	43.365738	40.597777	57.707313
H	41.016081	37.065034	46.343073	H	41.093038	32.732977	49.884304
H	43.617750	35.488343	46.573493	H	44.323695	43.639546	41.871217
H	42.265952	36.678947	44.103246	H	49.613075	49.379410	45.367575
H	44.108512	34.610988	44.418860	H	42.427024	35.709297	37.038393
H	44.864994	37.291814	45.578323	H	49.272925	35.709876	40.896223
H	43.838288	39.499449	45.956598	H	45.831055	30.940312	46.366123
H	38.180071	39.987653	46.241484	H	45.043770	32.881633	40.653704
H	39.309537	41.097046	45.396614	H	37.597026	41.192026	45.106569
H	43.535085	41.687174	44.857047				
C	45.972833	38.797729	48.167028	TS			
C	45.886325	37.410092	48.333630	C	41.290464	41.557258	52.077903
C	47.041417	36.635773	48.220740	H	41.829926	42.480618	52.329187
C	48.285746	37.209747	47.940400	H	40.852209	41.207237	53.025519
C	48.346566	38.599869	47.755189	C	42.257208	40.537990	51.567070
C	47.203522	39.392430	47.862737	N	43.148175	39.903016	52.419867
C	49.524339	36.340691	47.864974	H	43.221197	39.990757	53.488220
O	44.873940	39.599704	48.282388	C	43.928729	39.085760	51.701993
O	50.401644	36.657171	46.807077	H	44.709999	38.445777	52.105557
H	44.923700	36.937528	48.528508	N	43.575574	39.165280	50.423299
H	46.963298	35.551887	48.345804	C	42.537274	40.053374	50.308825
H	49.288783	39.077230	47.487789	H	42.083040	40.262521	49.345315
H	47.237520	40.473685	47.709139	C	43.236673	41.415431	57.005766
H	49.209778	35.290157	47.736738	H	42.279920	41.917079	57.210332
H	50.051498	36.376765	48.840985	H	44.010280	42.176667	57.193831

C	43.220484	41.096990	55.501703	C	51.062954	38.395474	43.946263
O	42.964901	42.066492	54.752310	H	52.089079	38.555626	44.284993
O	43.438152	39.923378	55.083495	C	49.996982	38.869747	44.726754
C	42.305486	32.631259	49.716225	O	50.171468	39.651379	45.827976
H	42.450261	31.954489	48.859495	H	50.931620	39.345923	46.405634
H	42.523569	33.635141	49.318642	C	48.684741	38.584631	44.327125
O	43.184372	32.271752	50.745469	H	47.851240	38.897047	44.958065
H	43.354230	33.097343	51.249474	C	48.457336	37.879934	43.150621
C	44.141801	44.011999	42.938023	H	47.431452	37.610764	42.887892
H	43.945921	43.227401	43.685220	C	45.435111	31.771092	46.888611
H	45.081919	44.524121	43.225614	H	44.985492	31.379557	47.811504
O	43.037765	44.886106	42.917007	H	46.216112	32.494258	47.174995
H	43.062934	45.429781	42.094643	C	44.388821	32.536199	46.071004
C	48.642981	49.236677	45.685601	O	43.168006	32.305840	46.330743
H	48.384719	50.010971	46.424022	O	44.798820	33.381070	45.239267
H	48.000243	49.391853	44.800741	C	44.699385	33.820003	41.166712
C	48.438889	47.841298	46.244174	H	43.626602	33.918527	40.943100
C	48.044591	47.628428	47.572969	H	44.785020	33.757384	42.260648
H	47.860039	48.487606	48.219826	C	45.388290	35.081694	40.672182
C	47.865038	46.340155	48.091162	O	45.822121	35.225631	39.521705
H	47.560016	46.196829	49.129476	N	45.445333	36.075305	41.587137
C	48.069735	45.217842	47.275444	H	45.795296	36.977481	41.265583
O	47.899820	43.947265	47.711490	H	44.996861	36.006388	42.510395
H	47.543943	43.893657	48.657393	P	39.341277	39.618263	42.721811
C	48.455561	45.413889	45.937608	P	41.980460	40.241742	43.943117
H	48.631434	44.548200	45.299299	C	41.626664	35.966591	48.453498
C	48.627614	46.701921	45.438840	O	42.885905	35.887462	49.085520
H	48.928380	46.814296	44.392789	C	41.728859	36.475976	47.025720
C	43.168086	36.438059	37.523508	O	42.144501	37.867803	47.155480
H	44.119060	35.937816	37.774315	C	42.633906	35.628587	46.122833
H	43.402973	37.166147	36.731357	O	41.872767	34.519477	45.729069
C	42.650935	37.085924	38.765641	C	43.190313	36.436183	44.931919
N	43.525426	37.663978	39.673082	O	43.972569	35.631048	44.083739
H	44.536382	37.782199	39.554788	C	44.015460	37.583132	45.554742
C	42.850612	38.135361	40.726806	O	44.648738	38.481738	44.674014
H	43.238539	38.702241	41.580022	C	43.180811	38.327974	46.573436
N	41.562946	37.876757	40.530669	O	38.509120	40.318448	41.680158
H	40.799398	38.063560	41.257981	O	43.142348	40.032798	42.964489
C	41.399964	37.238833	39.322336	O	39.810146	38.196694	42.432930
H	40.401909	37.008823	38.958732	O	42.147887	41.662915	44.694586
C	49.180722	36.811786	40.987369	O	40.625608	40.586585	43.063149
H	49.795204	37.256286	40.186614	O	41.709145	39.121501	44.918357
H	48.130779	37.011065	40.733659	C	38.506883	40.513068	45.149314
C	49.506042	37.470468	42.309260	O	38.564832	39.525148	44.164036
C	50.817479	37.718800	42.744082	H	44.017177	38.882369	44.027184
H	51.664716	37.395164	42.131360	H	42.367884	33.680515	45.945096

H	43.440992	36.684927	48.846610	H	44.367226	42.161735	49.347505
H	40.934471	36.628272	49.001408	H	40.481942	41.804571	51.390011
H	41.175727	34.966036	48.425236	H	43.344597	40.614350	57.736990
H	40.735184	36.526142	46.564665	H	41.249561	32.634727	49.986553
H	43.502502	35.295136	46.717030	H	44.294453	43.510850	41.982191
H	42.358920	36.875044	44.354820	H	49.673064	49.401083	45.369425
H	44.225432	34.786543	44.544264	H	42.505267	35.690719	37.087364
H	44.837461	37.097991	46.107440	H	49.293237	35.734457	40.865836
H	43.370765	39.383764	46.747770	H	45.929384	30.939331	46.386680
H	38.363790	40.024658	46.123889	H	45.042278	32.900169	40.693008
H	39.407653	41.143182	45.187346	H	37.675730	41.207180	45.024976
H	42.989477	41.623409	45.224208				
C	45.685365	37.525613	48.244636	EP			
C	46.015075	36.160030	48.373699	C	41.339385	41.483793	51.939406
C	47.335696	35.744311	48.227636	H	41.913674	42.377360	52.220160
C	48.361514	36.653053	47.954168	H	40.920347	41.102063	52.883454
C	48.034506	38.012748	47.827741	C	42.243870	40.449255	51.345954
C	46.718451	38.448466	47.971103	N	43.173381	39.767767	52.125688
C	49.781264	36.156895	47.828232	H	43.296129	39.853125	53.193091
O	44.412869	37.922023	48.352116	C	43.846649	38.905245	51.357910
O	50.489459	36.663318	46.715318	H	44.612779	38.212384	51.700048
H	45.222497	35.441814	48.592159	N	43.377921	39.002332	50.110253
H	47.576546	34.681098	48.300645	C	42.386145	39.951856	50.070572
H	48.812276	38.738406	47.583091	H	41.877619	40.187752	49.140851
H	46.456285	39.504640	47.875961	C	43.212833	41.293608	56.804500
H	49.754093	35.054931	47.744949	H	42.234063	41.770228	56.963638
H	50.323688	36.376340	48.769128	H	43.952890	42.087045	56.994875
H	44.025849	38.671915	49.569328	C	43.254159	40.968900	55.293202
H	50.996691	37.455338	47.007936	O	43.052473	41.955422	54.549301
O	44.495898	41.185598	46.015758	O	43.450747	39.798081	54.857699
H	45.247195	41.835180	45.855205	C	42.256459	32.630287	49.726881
H	44.791244	40.352144	45.595614	H	42.395886	31.965070	48.860958
O	38.948856	39.096193	39.154783	H	42.482986	33.636811	49.342347
H	38.902011	39.827984	38.521348	O	43.134534	32.240704	50.748158
H	38.748751	39.525189	40.014638	H	43.273874	33.029851	51.313160
O	43.274359	34.827375	51.659110	C	44.094433	43.926533	43.025463
H	43.949079	35.300100	52.204106	H	43.852271	43.135107	43.750911
H	43.226643	35.297215	50.800577	H	45.047663	44.398485	43.339624
O	46.806952	43.561209	50.000572	O	43.025924	44.844380	43.000848
H	46.214410	44.284752	50.303808	H	43.063206	45.376422	42.171886
H	46.222538	42.837367	49.680274	C	48.631455	49.198650	45.711978
O	46.465849	42.873675	45.695323	H	48.366673	49.987696	46.432311
H	47.241788	42.477063	45.204091	H	47.985037	49.326390	44.825393
H	46.897321	43.131010	46.547872	C	48.437240	47.816533	46.308746
O	45.066275	41.608866	48.922431	C	48.022591	47.642676	47.637403
H	44.806346	41.510579	47.985957	H	47.819946	48.519895	48.253434

C	47.844459	46.370766	48.195055	O	45.766514	35.213968	39.567341
H	47.522384	46.259843	49.232117	N	45.363175	36.045652	41.637581
C	48.070075	45.224312	47.420195	H	45.691311	36.960652	41.333343
O	47.904293	43.966284	47.895471	H	44.865174	35.969963	42.534900
H	47.513552	43.933641	48.829247	P	39.263265	39.617245	42.675956
C	48.471554	45.379599	46.081615	P	41.831876	40.242819	44.013471
H	48.656898	44.493387	45.473954	C	41.849547	36.136812	48.549185
C	48.645622	46.652493	45.543900	O	43.036242	35.775664	49.261762
H	48.960114	46.731920	44.498947	C	42.204801	36.688542	47.178895
C	43.148930	36.456058	37.588357	O	43.251029	37.639108	47.461798
H	44.097175	35.957026	37.851891	C	42.738803	35.632161	46.197771
H	43.396444	37.190964	36.806506	O	41.772470	34.636510	45.982945
C	42.608610	37.090309	38.828188	C	43.192711	36.319538	44.892996
N	43.466697	37.649139	39.762998	O	43.658673	35.389146	43.938725
H	44.479105	37.772061	39.657940	C	44.309053	37.327044	45.224303
C	42.772571	38.098668	40.814257	O	44.766498	38.065373	44.119563
H	43.147295	38.628044	41.696006	C	43.862887	38.278917	46.351748
N	41.488838	37.847957	40.587411	O	38.451823	40.308114	41.610512
H	40.708546	38.025931	41.304869	O	43.065157	39.958502	43.143760
C	41.347690	37.235808	39.363375	O	39.691658	38.173735	42.427290
H	40.355918	37.019584	38.975053	O	41.960183	41.728192	44.652512
C	49.023992	36.795142	41.202471	O	40.570750	40.556944	42.980603
H	49.592449	37.283491	40.393404	O	41.408442	39.223627	45.038730
H	47.958974	36.959429	40.995098	C	38.464950	40.567205	45.099654
C	49.377320	37.422213	42.534425	O	38.478641	39.580490	44.113236
C	50.700150	37.663236	42.941864	H	44.098438	38.739766	43.831654
H	51.530976	37.365875	42.294027	H	42.219316	33.757046	46.090875
C	50.980148	38.307770	44.155658	H	43.755338	36.318725	48.904760
H	52.015343	38.487551	44.457368	H	41.283243	36.899013	49.111306
C	49.933981	38.751890	44.982496	H	41.214867	35.249617	48.434401
O	50.128942	39.512190	46.089184	H	41.338188	37.204476	46.736564
H	50.960844	39.272805	46.598063	H	43.633707	35.175419	46.660030
C	48.610867	38.474820	44.605114	H	42.335995	36.868728	44.463531
H	47.791752	38.786477	45.253842	H	43.998392	34.583051	44.410156
C	48.348799	37.805146	43.414892	H	45.167005	36.721247	45.548993
H	47.310175	37.564145	43.174824	H	43.135943	38.984796	45.935829
C	45.317716	31.725065	46.892117	H	38.367855	40.083518	46.081954
H	44.861242	31.348509	47.817413	H	39.361090	41.203783	45.100470
H	46.107131	32.439116	47.176397	H	42.705558	41.758140	45.307995
C	44.289680	32.503185	46.062452	C	45.977084	38.474324	47.514856
O	43.064448	32.312382	46.326989	C	46.045584	37.109417	47.828587
O	44.730652	33.323588	45.220218	C	47.221225	36.589930	48.362387
C	44.667495	33.782720	41.206476	C	48.323118	37.403379	48.617488
H	43.587440	33.864933	41.015781	C	48.205513	38.781870	48.381494
H	44.785705	33.714623	42.296104	C	47.045819	39.321841	47.832004
C	45.327601	35.060271	40.715292	C	49.640183	36.765651	48.963064

O	44.904015	39.059933	46.892580	C	44.247487	38.209173	49.400755
O	50.492146	36.703000	47.836769	H	44.971254	37.532993	49.854666
H	45.230181	36.434036	47.601054	N	43.849942	38.181193	48.128631
H	47.289336	35.515535	48.551653	C	42.899676	39.185739	48.020885
H	49.052166	39.443325	48.576032	H	42.405835	39.391340	47.073030
H	46.964474	40.384750	47.597533	C	43.940370	41.129521	54.555552
H	49.464216	35.727677	49.285843	H	42.996141	41.597641	54.883767
H	50.100209	37.287283	49.821033	H	44.719686	41.898399	54.659504
H	43.667354	38.480552	49.275977	C	43.792331	40.790856	53.068284
H	50.995405	37.544368	47.744957	O	43.769905	41.776268	52.287713
O	44.081494	41.667993	46.430582	O	43.666394	39.589626	52.705351
H	44.905980	42.158839	46.157864	C	42.511822	32.395616	48.605391
H	44.407842	40.748195	46.491788	H	42.908178	33.417709	48.481357
O	38.920576	39.079292	39.104899	H	42.749394	32.056980	49.629213
H	38.888658	39.815454	38.475654	O	43.082212	31.517095	47.639884
H	38.708799	39.505771	39.964082	H	43.726571	32.074026	47.136497
O	43.199946	34.755653	51.857901	C	45.221489	43.060379	40.752957
H	43.911756	35.203378	52.374533	H	45.160561	42.284695	41.532271
H	43.199598	35.197314	50.985199	H	46.158760	43.616417	40.921313
O	46.727410	43.616169	50.144452	O	44.080799	43.877182	40.893890
H	46.157293	44.362791	50.437199	H	44.214938	44.729113	40.425395
H	46.114910	42.906833	49.839001	C	47.694702	47.158874	42.148984
O	46.414053	42.832317	45.957978	H	47.086027	47.698146	42.889147
H	47.149363	42.378737	45.459660	H	47.189910	47.247687	41.173094
H	46.886566	43.137133	46.770469	C	47.833207	45.698609	42.529956
O	44.866747	41.722485	49.193845	C	47.336467	45.202720	43.745734
H	44.574289	41.782542	48.258809	H	46.850976	45.885185	44.448306
H	44.243701	42.339394	49.661085	C	47.440500	43.849013	44.079478
H	40.516888	41.780560	51.288641	H	47.036625	43.476496	45.022291
H	43.323546	40.530167	57.574543	C	48.054249	42.952204	43.197959
H	41.200291	32.637035	49.996194	O	48.095327	41.628223	43.524474
H	44.244106	43.438909	42.062194	H	48.789668	41.164641	42.978660
H	49.658146	49.369901	45.388489	C	48.566697	43.431757	41.981949
H	42.497689	35.709577	37.133695	H	49.032139	42.738877	41.282363
H	49.172306	35.726396	41.048031	C	48.443796	44.782868	41.655852
H	45.803121	30.883752	46.397506	H	48.809938	45.124930	40.683843
H	45.018907	32.873216	40.719262	C	43.403654	35.430327	35.695014
H	37.623456	41.252896	45.000749	H	44.369230	34.939978	35.911415
				H	43.589774	36.181751	34.912331
ES'				C	42.933606	36.089936	36.951294
C	41.917060	40.952128	49.768125	N	43.817365	36.812622	37.738422
H	42.552246	41.827120	49.967139	H	44.817399	36.964171	37.580230
H	41.507016	40.667258	50.750128	C	43.183924	37.298037	38.811685
C	42.747253	39.819277	49.241230	H	43.612291	37.926621	39.594529
N	43.613928	39.171705	50.097032	N	41.913239	36.923460	38.749844
H	43.683167	39.367589	51.150183	H	41.236686	37.188375	39.569033

C	41.721767	36.178704	37.604072	O	40.692084	37.632206	40.860032
H	40.739269	35.805407	37.322817	O	43.255987	41.046371	42.875781
C	49.096972	35.059320	39.337302	O	41.410302	40.052547	41.553973
H	49.526942	35.345751	38.363987	O	42.688861	38.530683	43.093897
H	48.027389	35.309839	39.308230	C	39.050115	40.147239	43.196897
C	49.811348	35.844682	40.410005	O	39.251048	39.041150	42.360562
C	51.211452	35.952805	40.407499	H	44.626798	37.890648	41.496567
H	51.799434	35.407448	39.664812	H	41.659648	33.596867	43.768268
C	51.874619	36.789517	41.302712	H	43.564312	36.484347	47.358044
H	52.962507	36.882734	41.267306	H	41.454908	36.890361	46.979177
C	51.137079	37.555188	42.214913	H	41.225237	35.216978	46.392623
O	51.723685	38.487057	43.017486	H	41.266181	36.974262	44.557434
H	52.712390	38.327948	43.085837	H	43.304357	34.734399	44.661648
C	49.743681	37.421287	42.270635	H	42.424657	36.179002	42.133873
H	49.182342	37.996499	43.006560	H	43.912033	33.847575	42.745042
C	49.095058	36.569391	41.377201	H	45.050458	36.208038	43.700878
H	48.004392	36.480212	41.421838	H	44.553964	38.605594	44.048121
C	43.568882	30.369946	44.541372	H	38.829373	39.782328	44.210144
H	43.001119	29.632579	43.955616	H	39.920875	40.815209	43.232047
H	43.093937	30.398059	45.536167	H	44.200467	41.012915	43.302567
C	43.298773	31.752448	43.931779	C	49.564566	36.610633	45.677798
O	44.222630	32.619012	43.835645	C	48.256422	36.270735	46.072042
O	42.102864	31.951474	43.626484	C	47.360553	37.254454	46.490855
C	44.602605	32.558669	39.505130	C	47.736165	38.609071	46.528308
H	43.531256	32.695634	39.305382	C	49.029013	38.941405	46.100210
H	44.713356	32.591259	40.597086	C	49.937347	37.964868	45.685646
C	45.344053	33.755185	38.911022	C	46.809121	39.672891	47.071108
O	45.864750	33.766444	37.788998	O	50.392335	35.620606	45.281724
N	45.346576	34.833329	39.723010	O	45.520620	39.721913	46.456288
H	45.781014	35.696602	39.402624	H	47.968210	35.217454	46.061447
H	44.863043	34.842784	40.631605	H	46.352431	36.960402	46.799601
P	40.163812	39.049807	41.000321	H	49.331064	39.992940	46.073791
P	42.879876	39.747930	42.078373	H	50.920282	38.250604	45.308232
C	41.927510	36.064434	46.419315	H	47.265981	40.664623	46.927729
O	43.123130	35.653719	47.050855	H	46.669181	39.534095	48.159815
C	42.174006	36.504830	44.977075	H	51.349064	35.912585	45.307725
O	43.228807	37.478917	45.041026	H	44.969180	38.985317	46.811353
C	42.541908	35.302722	44.102756	O	45.514800	40.697850	43.928507
O	41.376819	34.531464	43.935566	H	45.498095	40.392591	44.869204
C	43.187405	35.691614	42.765308	H	46.437567	40.978155	43.732366
O	43.670627	34.550707	42.079916	O	50.077210	40.610998	42.105579
C	44.314427	36.691634	43.034479	H	50.179067	40.674749	41.130034
O	45.016007	37.074629	41.871623	H	50.774467	40.015140	42.439761
C	43.761842	37.874118	43.840116	H	41.095846	41.263144	49.122414
O	39.529714	39.743730	39.843601	H	44.160219	40.326659	55.259218
O	43.823670	39.383554	40.951327	H	41.429661	32.504429	48.533602

H	45.287978	42.544499	39.795088	H	48.681180	41.162683	42.954615
H	48.662233	47.655037	42.073008	C	48.452515	43.427891	41.949721
H	42.751432	34.676797	35.253578	H	48.799261	42.714913	41.202827
H	49.156471	33.971243	39.362109	C	48.351989	44.781320	41.629820
H	44.578515	29.989458	44.696087	H	48.628983	45.106103	40.623253
H	44.887692	31.579790	39.119658	C	43.431292	35.468014	35.620431
H	38.212763	40.785111	42.914006	H	44.404637	34.992810	35.832954
TS'				H	43.602845	36.215085	34.830581
C	41.844228	41.030570	49.799576	C	42.944358	36.118505	36.875472
H	42.480104	41.902214	50.007588	N	43.804207	36.828795	37.698092
H	41.424591	40.744789	50.776936	H	44.805678	36.990816	37.563815
C	42.673498	39.892972	49.282992	C	43.136257	37.290745	38.767973
N	43.509036	39.217551	50.150180	H	43.536865	37.913743	39.581565
H	43.578671	39.418309	51.218537	N	41.870148	36.912334	38.664112
C	44.130025	38.245618	49.463604	H	41.108615	37.159807	39.495359
H	44.839464	37.556151	49.919930	C	41.716925	36.194436	37.499769
N	43.749886	38.238756	48.183693	H	40.742779	35.825644	37.185026
C	42.834595	39.272277	48.055003	C	49.166732	35.016761	39.264698
H	42.340035	39.465762	47.104951	H	49.620164	35.287573	38.296940
C	43.913473	41.152669	54.582747	H	48.099966	35.276151	39.205253
H	42.982560	41.631552	54.932438	C	49.860270	35.819932	40.336748
H	44.703486	41.912055	54.674054	C	51.260662	35.911429	40.383197
C	43.729446	40.831024	53.099322	H	51.869257	35.332545	39.684298
O	43.687018	41.821726	52.328123	C	51.901472	36.772969	41.272179
O	43.596051	39.632045	52.722251	H	52.991226	36.849183	41.275390
C	42.462223	32.361458	48.662285	C	51.141382	37.584093	42.124379
H	42.866155	33.384404	48.589144	O	51.709332	38.528278	42.927584
H	42.683560	31.975837	49.672091	H	52.696337	38.374101	43.020493
O	43.038233	31.520202	47.668568	C	49.744476	37.472220	42.126418
H	43.656791	32.104411	47.165521	H	49.156152	38.083525	42.807139
C	45.150828	43.091194	40.758499	C	49.119896	36.590776	41.246851
H	45.109711	42.327893	41.547880	H	48.028255	36.509512	41.262942
H	46.098730	43.639586	40.885577	C	43.534537	30.535013	44.494217
O	44.028919	43.927725	40.936211	H	42.976204	29.816468	43.877050
H	44.143384	44.760086	40.428977	H	43.019690	30.560094	45.469756
C	47.713240	47.177062	42.160423	C	43.316263	31.931592	43.890967
H	47.110619	47.722213	42.901378	O	44.246204	32.794776	43.863272
H	47.203830	47.256693	41.186560	O	42.139620	32.141421	43.523223
C	47.860478	45.721235	42.551554	C	44.639002	32.617351	39.591742
C	47.499713	45.255288	43.825523	H	43.560896	32.779697	39.457646
H	47.122113	45.961683	44.570764	H	44.812810	32.638828	40.677145
C	47.602731	43.901388	44.160643	C	45.375547	33.805197	38.972503
H	47.331453	43.550595	45.158006	O	45.913841	33.788167	37.861498
C	48.049010	42.970164	43.214585	N	45.368037	34.911542	39.753767
O	48.020267	41.644213	43.523865	H	45.780379	35.765305	39.378060
				H	44.864031	34.971047	40.648206

P	39.948736	38.962747	40.637819	H	48.753688	39.353070	45.402678
P	42.543944	39.704418	41.863946	H	50.788676	37.971866	45.082471
C	41.547736	36.000269	46.491973	H	46.139594	39.265747	45.204713
O	42.731745	35.600335	47.165058	H	46.228525	39.065780	46.960345
C	41.852465	36.542209	45.099442	H	51.693909	35.739422	45.269626
O	42.731450	37.674867	45.289435	H	44.514706	37.840214	46.867977
C	42.413240	35.449884	44.195063	O	45.088954	41.303040	43.827582
O	41.314633	34.657351	43.832250	H	45.011004	42.072865	44.444357
C	43.206551	35.992404	43.002621	H	46.041883	41.263254	43.611357
O	43.727921	34.922905	42.232175	O	49.995070	40.637660	42.076645
C	44.344306	36.879146	43.558411	H	50.084947	40.690125	41.097951
O	45.125854	37.517837	42.597696	H	50.703650	40.050824	42.401966
C	43.824335	37.872686	44.608569	H	41.030113	41.339634	49.144014
O	39.165225	39.542244	39.504073	H	44.137287	40.343747	55.278174
O	43.704885	39.200546	40.994408	H	41.382263	32.484179	48.580472
O	40.395505	37.498346	40.572176	H	45.184334	42.563655	39.805270
O	42.812465	41.252483	42.256082	H	48.681896	47.669600	42.075703
O	41.251843	39.949859	40.869329	H	42.783930	34.703455	35.190969
O	42.141796	38.867358	43.045568	H	49.214233	33.928597	39.306042
C	39.163763	40.167490	42.925095	H	44.528359	30.132015	44.689093
O	39.190021	39.046749	42.094073	H	44.883604	31.638401	39.179562
H	44.566813	38.097839	42.019072	H	38.285845	40.796924	42.779702
H	41.654130	33.743358	43.642359				
H	43.140839	36.404180	47.541433	EP'			
H	40.997760	36.759566	47.074455	C	41.821908	41.012525	49.744178
H	40.899121	35.120110	46.373346	H	42.384145	41.906007	50.052388
H	40.953372	36.956406	44.618060	H	41.393351	40.615895	50.678615
H	43.128397	34.860333	44.796317	C	42.776282	40.010854	49.175424
H	42.543017	36.592000	42.362472	N	43.700832	39.418448	50.018641
H	43.962061	34.167904	42.834812	H	43.732701	39.572554	51.125936
H	45.016597	36.197418	44.104308	C	44.490448	38.619546	49.303281
H	44.076757	38.924512	44.457134	H	45.306010	38.019765	49.700256
H	39.138045	39.836058	43.973446	N	44.104472	38.664137	48.022563
H	40.024327	40.835813	42.781654	C	43.030797	39.520144	47.913314
H	43.642656	41.314814	42.791362	H	42.551904	39.689263	46.953041
C	49.779203	36.100490	45.484578	C	43.933194	41.172763	54.502834
C	48.558957	35.507272	45.835597	H	42.989461	41.643320	54.828514
C	47.417182	36.282350	46.013039	H	44.714871	41.935297	54.634703
C	47.465763	37.672660	45.848178	C	43.805603	40.897056	53.004850
C	48.698269	38.269088	45.549382	O	43.762499	41.910672	52.265664
C	49.851526	37.499749	45.383086	O	43.720870	39.708148	52.573267
C	46.222110	38.510799	46.004695	C	42.450967	32.230340	48.694768
O	50.807325	35.273986	45.218407	H	42.890075	33.238657	48.649731
O	45.050763	37.690760	45.993708	H	42.644336	31.811101	49.695684
H	48.533155	34.422016	45.940066	O	43.010262	31.388142	47.692055
H	46.469918	35.804025	46.266946	H	43.610566	31.969123	47.162884

C	45.080513	43.167932	40.795029	H	47.956066	36.512560	41.318579
H	45.062254	42.427628	41.605497	C	43.516742	30.433318	44.473789
H	46.034290	43.714792	40.877561	H	42.964895	29.692338	43.877939
O	43.967685	44.016280	40.984349	H	43.004257	30.475938	45.450079
H	44.074080	44.836145	40.454712	C	43.286925	31.811400	43.830365
C	47.702470	47.189790	42.169687	O	44.221100	32.670635	43.782522
H	47.103520	47.739974	42.910014	O	42.111704	32.011940	43.457980
H	47.192025	47.268863	41.196340	C	44.626242	32.584188	39.607923
C	47.843907	45.734686	42.564906	H	43.544797	32.740922	39.494699
C	47.509884	45.279113	43.849898	H	44.818745	32.600949	40.689894
H	47.157373	45.994201	44.599243	C	45.348160	33.777964	38.983819
C	47.609536	43.926112	44.189859	O	45.869562	33.767989	37.863581
H	47.361114	43.581071	45.195561	N	45.349686	34.876744	39.772994
C	48.024658	42.985095	43.238694	H	45.748275	35.735684	39.395539
O	47.994239	41.662551	43.556741	H	44.852660	34.925390	40.674496
H	48.640288	41.173160	42.975205	P	39.907581	38.903178	40.631806
C	48.400485	43.433129	41.961849	P	42.519494	39.542394	41.949492
H	48.721251	42.713248	41.210111	C	41.403579	35.797327	46.405016
C	48.304929	44.785591	41.637169	O	42.462879	35.200320	47.149928
H	48.561204	45.102655	40.622657	C	41.970916	36.404311	45.121964
C	43.382704	35.444057	35.666804	O	43.091255	37.157658	45.589904
H	44.354812	34.973229	35.894820	C	42.414300	35.296078	44.173056
H	43.569322	36.206719	34.895587	O	41.275122	34.594078	43.744023
C	42.861889	36.065993	36.923224	C	43.267276	35.839763	43.029073
N	43.701383	36.755195	37.782624	O	43.692889	34.786962	42.176794
H	44.703106	36.933455	37.665017	C	44.480073	36.585596	43.619693
C	43.011552	37.184813	38.851762	O	45.268066	37.189132	42.622548
H	43.402762	37.770161	39.699185	C	44.079091	37.619126	44.699997
N	41.748850	36.805411	38.711788	O	39.174567	39.566329	39.508123
H	40.963908	37.044303	39.521761	O	43.683551	38.847913	41.229050
C	41.621372	36.121400	37.523826	O	40.204606	37.401362	40.566680
H	40.654671	35.759297	37.180861	O	42.889328	41.119618	42.107471
C	49.078091	35.019893	39.301974	O	41.310634	39.745943	40.837845
H	49.499546	35.310321	38.325319	O	41.968394	38.953881	43.217316
H	48.005035	35.255046	39.272931	C	39.191706	40.224432	42.863751
C	49.780681	35.827631	40.364610	O	39.172821	39.062936	42.092743
C	51.181473	35.924267	40.394614	H	44.684884	37.803882	42.101209
H	51.783556	35.346735	39.688484	H	41.580148	33.675857	43.543232
C	51.831256	36.788164	41.275570	H	43.155344	35.884039	47.141665
H	52.920952	36.867199	41.267069	H	40.898364	36.578014	47.003267
C	51.078428	37.596826	42.136513	H	40.674372	35.017196	46.151110
O	51.651567	38.543015	42.934545	H	41.253227	37.066464	44.610070
H	52.635085	38.379472	43.035221	H	43.064392	34.625403	44.759194
C	49.682110	37.480126	42.152189	H	42.658388	36.532377	42.428222
H	49.101958	38.087079	42.842483	H	43.924539	34.006150	42.746943
C	49.047124	36.597146	41.281935	H	45.109068	35.826279	44.114005

H	43.741162	38.547247	44.223211	N	0	42.11379500	39.56033600	52.73191500
H	39.255799	39.952459	43.927138	C	0	42.40694500	38.36676800	52.18245600
H	40.028609	40.894357	42.619242	N	0	42.05597800	38.30565400	50.89901800
H	43.652639	41.233605	42.727980	H	-1	40.45102100	42.09765800	51.17319200
C	49.801599	36.139222	45.805995	H	0	41.95635700	42.41715800	52.06356800
C	48.516020	35.617353	46.005417	H	0	40.57132700	41.82804300	52.95205700
C	47.394394	36.420593	45.843404	H	0	42.38079500	39.84606200	53.76743600
C	47.518626	37.770372	45.486082	H	0	41.13016800	39.77336000	49.61943300
C	48.806737	38.305524	45.355462	H	0	42.88414800	37.56165300	52.73983500
C	49.942234	37.505076	45.509980	C	-1	43.37900000	41.42400100	57.03499500
C	46.292323	38.587158	45.157200	C	0	42.63516000	41.16427800	55.69740200
O	50.824204	35.272323	45.906605	O	0	41.86335000	42.03710600	55.27522500
O	45.130536	37.902791	45.623051	O	0	42.93197200	40.05830900	55.14066800
H	48.426974	34.559138	46.252155	H	-1	43.37096300	40.53611600	57.67579800
H	46.400035	35.996450	45.978486	H	0	42.93829200	42.28153700	57.56533000
H	48.929005	39.359344	45.083501	H	0	44.43750000	41.64863700	56.81480600
H	50.931829	37.926616	45.324675	P	0	37.17078400	38.45589900	44.16735600
H	46.213748	38.722347	44.068965	P	0	39.96322600	37.46839000	43.95707300
H	46.327909	39.590295	45.617180	C	0	38.58736900	37.71400500	49.49997800
H	51.712454	35.699188	45.730015	O	0	39.33567100	37.05299500	50.49285800
H	44.549688	38.219259	47.185139	C	0	38.77318200	37.13789900	48.10392400
O	45.028731	41.431907	43.827170	O	0	40.17795300	37.26040200	47.78813600
H	44.948213	42.215964	44.423276	C	0	38.34686600	35.67369200	48.01915600
H	45.988095	41.343290	43.669651	O	0	36.96082600	35.57011600	48.26916900
O	49.934655	40.642970	42.090827	C	0	38.68835400	35.07907900	46.65092400
H	50.003826	40.679286	41.109513	O	0	38.25181800	33.72794900	46.60235700
H	50.641938	40.051286	42.411611	C	0	40.19526000	35.24997200	46.46804600
H	41.003347	41.316027	49.091560	O	0	40.75444900	34.57829400	45.35956100
H	44.140212	40.359363	55.198240	C	0	40.56032400	36.74110400	46.56481100
H	41.377258	32.392342	48.600047	O	0	36.45178400	39.38205900	43.24650600
H	45.078389	42.624378	39.850248	O	0	40.00484800	36.09030700	43.36307400
H	48.673329	47.677402	42.081746	O	0	36.86342800	37.02850900	44.47273800
H	42.752003	34.681663	35.209599	O	0	41.33444700	38.26063900	43.55200600
H	49.154049	33.932999	39.332924	O	0	38.83701300	38.46790900	43.53539800
H	44.515925	30.046395	44.673764	O	0	39.92413200	37.54222600	45.55453000
H	44.871942	31.609198	39.187100	C	-1	37.99899400	40.51898600	45.59997500
H	38.294829	40.833983	42.753635	O	0	37.50198200	39.20264700	45.60323500

DFT Calculations (singly protonated at diphosphate of UDPG)

The numbers 0 and -1 represent the unfrozen and frozen atoms during the geometry optimization, respectively.

ES_{QC}

C	-1	41.09000000	41.73702800	51.98602800	H	0	40.38716200	34.96868200	44.52298700
C	0	41.53311700	40.33132300	51.74728000	H	0	36.70479500	34.73797500	47.84204400
C	0	41.50892200	39.54058200	50.61321600	H	0	40.26273600	37.33480400	50.41188900
					H	0	38.81772300	38.79656000	49.47330900
					H	0	37.52140400	37.60184500	49.75261600
					H	0	38.18248600	37.72363800	47.37920900
					H	0	38.91895000	35.11557500	48.78850500
					H	0	38.12317500	35.62416400	45.87490700

H	0	38.98080200	33.13862200	46.87278800	C	0	37.72454600	36.16155100	48.30372100
H	0	40.68077000	34.81167700	47.34529600	O	0	38.13597600	35.16834200	49.19459300
H	0	41.65103100	36.86789000	46.48538800	C	0	38.80353700	36.62085300	47.33058800
H	0	38.34808000	40.74405700	46.62096100	O	0	39.80115400	37.31120400	48.16899700
H	0	38.85373400	40.62995700	44.90991100	C	0	39.38706600	35.47526600	46.49483200
H	0	41.86679400	37.64289200	43.03214600	O	0	38.57888500	35.22953100	45.37133800
C	0	43.12042700	35.70821100	48.82773800	C	0	40.85061000	35.65437400	46.08446800
C	0	42.16464700	34.97727600	49.56702300	O	0	41.30192000	34.43035400	45.53146800
C	0	41.77487800	33.70824600	49.14305600	C	0	41.71091500	36.00923700	47.29701500
C	0	42.31332900	33.11405600	47.99004400	O	0	43.02793400	36.34365200	47.03345900
C	0	43.29727700	33.82810100	47.29053500	C	0	41.03868200	37.05252300	48.15377600
C	0	43.70299200	35.09304800	47.70030500	O	0	39.93967400	39.71995400	43.32208500
C	0	41.70787200	31.87190300	47.39011800	O	0	42.67566800	38.29160200	45.32986300
O	0	43.49710000	36.94775100	49.12892200	O	0	38.90542000	37.30654600	43.74566500
O	0	40.58333700	32.13488600	46.56243300	O	0	41.57123400	40.64343900	45.18607900
H	0	41.68950700	35.43658400	50.43446700	O	0	40.12983100	38.59472300	45.60732300
H	0	40.98844800	33.18539700	49.69612000	O	0	41.65513000	39.38667100	47.46055400
H	0	43.71908800	33.39965400	46.37615200	C	-1	37.99911900	40.51951400	45.60134200
H	0	44.44572500	35.66238400	47.13685100	O	0	37.86610000	39.33491900	44.84248600
H	0	41.35454800	31.19161900	48.18374100	H	-1	37.22855000	41.24368900	45.31670800
H	0	42.48454500	31.32486000	46.81599500	H	0	43.01164100	37.09066100	46.35669700
H	0	42.88949800	37.39008500	49.81229500	H	0	38.66109700	36.01230300	44.74886300
H	0	40.77711700	32.89510300	45.96222200	H	0	38.97663200	35.44560200	49.65155000
TS_{QC}					H	0	37.33291500	37.06139700	48.82448700
C	-1	41.08956900	41.73744600	51.98664200	H	0	36.90870200	35.75773900	47.67979300
C	0	41.09568100	40.23830100	51.97235400	H	0	38.42188400	37.41225300	46.67570600
C	0	40.81891800	39.37303800	50.92749100	H	0	39.35409000	34.56775500	47.12091900
N	0	41.39578100	39.48887900	53.09269000	H	0	40.93269100	36.46325800	45.34704800
C	0	41.29673500	38.21438300	52.72997400	H	0	40.61224100	34.20519600	44.88816200
N	0	40.94910600	38.09875300	51.43387000	H	0	41.70934200	35.11577600	47.95859700
H	-1	40.45147900	42.09747600	51.17275100	H	0	41.65551400	37.62049000	48.84476300
H	0	42.10155600	42.15227800	51.83524100	H	0	37.89779400	40.29866700	46.67920500
H	0	40.72851900	42.11411800	52.95472000	H	0	38.97994200	40.99850200	45.45364300
H	0	42.02508900	39.90658000	54.41414700	H	0	41.08260900	40.46846700	44.32635900
H	0	40.60523500	39.56087100	49.87509200	C	0	41.26666100	34.70578100	50.53457200
H	0	41.46997800	37.35543600	53.37646200	C	0	40.84646500	33.39362500	50.16834800
C	-1	43.37865500	41.42372800	57.03450900	C	0	41.63296300	32.28215000	50.44509500
C	0	42.45966200	41.23462100	55.83229700	C	0	42.87859700	32.40069900	51.09040800
O	0	41.73658400	42.12590400	55.42347300	C	0	43.30599300	33.69029700	51.44220100
O	0	42.58188000	40.03959400	55.31001500	C	0	42.52883900	34.81547300	51.18113400
H	-1	43.37123300	40.53612700	57.67581800	C	0	43.72296700	31.18299000	51.35633400
H	0	43.08340400	42.31750000	57.60010900	O	0	40.53311200	35.75222300	50.26216700
H	0	44.41214500	41.55381800	56.67236300	O	0	43.91289400	30.36865400	50.20370500
P	0	39.26054700	38.69660000	44.20916900	H	0	39.88245100	33.29255900	49.66435000
P	0	41.64960400	39.21963200	45.95525300	H	0	41.28762900	31.28852800	50.14170900
					H	0	44.28153900	33.81508400	51.92565100

H	0	42.89240500	35.81199700	51.44375000	O	0	37.34212300	39.28278100	45.82547700
H	0	43.25204700	30.52074600	52.10783400	H	-1	37.22845200	41.24373700	45.31709300
H	0	44.69543900	31.50402400	51.78586000	H	0	41.06981300	35.64779400	48.44393300
H	0	40.78496700	37.16654300	50.94118000	H	0	36.50758600	36.32276400	47.57729400
H	0	43.94940000	30.97812000	49.45287100	H	0	36.84760200	34.21142400	52.01176600
EP_{QC}					H	0	36.11933500	36.53362200	52.24605300
C	-1	41.08976500	41.73705800	51.98610000	H	0	35.16459800	36.07817900	50.79550900
C	0	41.49776300	40.33263300	51.71992400	H	0	37.46907800	37.06659500	50.32708500
C	0	41.40005800	39.67105600	50.51837600	H	0	36.83920900	34.25275600	49.32944700
N	0	42.02165700	39.47585000	52.67500700	H	0	38.76771900	36.33019100	48.22163200
C	0	42.21558800	38.31405600	52.04638000	H	0	38.02288100	35.20345500	46.57403200
N	0	41.85758700	38.39929900	50.74560800	H	0	39.34530700	33.65922900	49.55220700
H	-1	40.45121800	42.09778600	51.17309300	H	0	39.84280500	36.57082300	50.38125000
H	0	41.95744500	42.41855200	52.06393800	H	0	38.54493300	40.85322800	46.50039700
H	0	40.55198100	41.82466900	52.94290300	H	0	38.73034400	40.42909000	44.77895000
H	0	42.53349200	39.92688000	54.16665200	H	0	40.63291200	37.76521200	45.17645800
H	0	41.09296900	39.97668800	49.51446500	C	0	40.68226500	33.83397100	51.92992700
H	0	42.58031400	37.39637600	52.50369000	C	0	40.08027200	33.43102000	53.12940800
C	-1	43.37884600	41.42362700	57.03455900	C	0	40.21352900	32.11359800	53.56809200
C	0	42.58610300	41.16954600	55.74122100	C	0	40.93787800	31.17636400	52.81446100
O	0	41.67570200	41.90030700	55.40132300	C	0	41.52217600	31.59298900	51.60936400
O	0	43.01735500	40.11622700	55.07998500	C	0	41.40555700	32.90990400	51.16409700
H	-1	43.37110300	40.53630400	57.67606100	C	0	41.07578200	29.75223200	53.29974300
H	0	42.94508200	42.28096400	57.56449400	O	0	40.60415300	35.14087300	51.54559900
H	0	44.43146300	41.63155500	56.78290100	O	0	39.88612500	29.23375800	53.87221400
P	0	38.23220800	37.90329700	45.79281700	H	0	39.51284200	34.17200500	53.69480200
P	0	40.84318000	38.27729200	47.26390600	H	0	39.74053800	31.79470800	54.50066500
C	0	36.05276200	35.82491300	51.39384000	H	0	42.06960800	30.86734900	50.99915900
O	0	35.93199500	34.49216500	51.85247300	H	0	41.81488600	33.25427800	50.21180400
C	0	37.28370300	35.99111300	50.51374600	H	0	41.83982900	29.68352000	54.09573300
O	0	38.36039200	35.43215800	51.27099600	H	0	41.43575600	29.11756500	52.46370800
C	0	37.14437500	35.30377700	49.14805900	H	0	41.82101500	37.71796300	49.95197700
O	0	36.13826900	35.96810000	48.42204900	H	0	39.15862300	29.52355100	53.30400200
C	0	38.49417900	35.28318200	48.41988400	ES'_{QC}				
O	0	38.40958700	34.56717500	47.21312400	C	-1	42.05796400	41.09909000	49.97013600
C	0	39.60295000	34.70653700	49.30951700	C	0	42.37094500	39.68328300	49.61265600
O	0	40.86394300	34.70848900	48.70771400	C	0	42.16131200	38.94760600	48.45936200
C	0	39.60982700	35.52032200	50.61530000	N	0	42.99417300	38.83020700	50.49256200
O	0	39.12761900	37.90202600	44.56686600	C	0	43.13098300	37.64110800	49.87028700
O	0	41.27636200	37.30096600	48.37249300	N	0	42.64072200	37.66514700	48.63167200
O	0	37.25819100	36.77027300	46.05360200	H	-1	41.21407800	41.45359900	49.36910100
O	0	41.37336500	37.70076900	45.85467900	H	0	42.92158200	41.76450200	49.81106000
O	0	39.18072600	38.08158600	47.12067100	H	0	41.82007900	41.19920500	51.03630600
O	0	41.11066000	39.74412100	47.46320900	H	0	43.27942000	39.10402300	51.51705700
C	-1	37.99922000	40.51947000	45.60086500	H	0	41.70440500	39.25454700	47.51995500

H	0	43.58238600	36.77182900	50.34727500	C	0	43.10835700	33.97268200	47.24888500
C	-1	43.78801300	40.90300600	54.80198000	C	0	44.35210100	34.39239100	46.75441900
C	0	43.67846700	40.68035200	53.27677600	C	0	44.89515900	33.70642700	45.65925000
O	0	43.66757100	41.67801600	52.54190400	C	0	44.19578800	32.67766700	45.02758000
O	0	43.57570600	39.45628400	52.94202700	C	0	44.99914900	35.66347100	47.26325000
H	-1	44.15962700	39.98292500	55.26501300	O	0	42.16470200	31.43317100	44.76809600
H	0	42.78592900	41.12169500	55.21063600	O	0	44.46562300	36.81457400	46.65564300
H	0	44.43987700	41.76075000	55.03049000	H	0	41.41561800	32.64744900	46.98304300
P	0	38.08395900	37.81462200	42.29529000	H	0	42.64461900	34.50355400	48.08278800
P	0	41.02902700	37.44474100	41.70233200	H	0	45.85792500	34.03158800	45.25282500
C	0	39.61578000	36.71924000	47.04909000	H	0	44.57662700	32.20100100	44.12235400
O	0	40.41277700	35.98819800	47.94470600	H	0	46.08127800	35.63195300	47.03772000
C	0	40.00538400	36.52942300	45.58818300	H	0	44.90132200	35.71728100	48.36561200
O	0	41.38651300	36.91857600	45.47740300	H	0	41.47063400	31.99505600	44.34064700
C	0	39.77994600	35.07971400	45.13879900	H	0	43.68099500	37.08168700	47.18820000
O	0	38.40520400	34.80400500	44.94132000					
C	0	40.54421800	34.68621500	43.87425300					
O	0	40.44059600	33.25826700	43.72403900	TS'qc				
C	0	41.98584300	35.16397100	43.92594500	C	-1	42.05795800	41.09910000	49.97013500
O	0	42.75968200	34.84456700	42.80339700	C	0	42.66648600	39.82673900	49.48453100
C	0	41.97429600	36.66864900	44.26059300	C	0	42.60494200	39.19653600	48.25610600
O	0	37.08196400	38.45831300	41.40311200	N	0	43.47944900	39.08490400	50.31755000
O	0	41.31050000	36.15985300	40.98558800	C	0	43.89005000	38.04205500	49.59927700
O	0	38.06633300	36.38154000	42.75508100	N	0	43.38848100	38.06997800	48.35076100
O	0	42.00976600	38.62061800	41.14140400	H	-1	41.21407500	41.45359700	49.36910400
O	0	39.60447300	38.09080100	41.50388200	H	0	42.80947300	41.90349700	50.03099500
O	0	41.24677800	37.47677800	43.27823800	H	0	41.68767700	40.96358300	50.99948200
C	-1	38.72298300	40.07292300	43.52695700	H	0	43.62584500	39.42953600	51.82501100
O	0	38.36525400	38.71620100	43.64444200	H	0	42.07491300	39.44271500	47.33900400
H	-1	37.99102800	40.64841300	42.95068300	H	0	44.54278700	37.24836200	49.96053300
H	0	42.26152400	35.13861900	42.01036900	C	-1	43.78802700	40.90300600	54.80196300
H	0	38.12492100	35.38533300	44.18953100	C	0	43.88176700	40.78059200	53.28081600
H	0	41.26245700	36.46848800	48.05078800	O	0	44.14724200	41.72987100	52.56878600
H	0	39.63097900	37.80113800	47.28393000	O	0	43.61852400	39.55775100	52.87503200
H	0	38.57415700	36.36972900	47.14478500	H	-1	44.15961200	39.98291700	55.26501000
H	0	39.39641100	37.19676700	44.96107200	H	0	42.72918300	41.01762100	55.08757800
H	0	40.13477200	34.42781700	45.95233500	H	0	44.34735700	41.78227600	55.14754000
H	0	40.03904100	35.14161900	43.01000200	P	0	39.30235000	38.81451900	41.26954700
H	0	39.49867600	33.09183600	43.89830600	P	0	42.05690200	40.03484000	41.93563900
H	0	42.48475400	34.71939200	44.79347300	C	0	40.29617800	36.10638600	46.29310200
H	0	43.00553800	37.04363100	44.31352000	O	0	41.29255100	35.20062800	46.67360900
H	0	38.78362300	40.48853500	44.54514900	C	0	40.62481600	36.89621000	45.03514800
H	0	39.71063400	40.18561900	43.04689400	O	0	41.76477500	37.76318600	45.40009300
H	0	42.60608600	38.20570600	40.50294600	C	0	40.86836300	36.01774900	43.79267300
C	0	42.92240300	32.31587400	45.48296200	O	0	39.62930200	35.71466400	43.21075700
C	0	42.40704200	32.93826900	46.63008100	C	0	41.82546500	36.73487500	42.83937100
					O	0	41.96505100	36.05112400	41.61445500

C	0	43.16372600	36.92831000	43.55048700	EP' _{QC}				
O	0	44.18664800	37.51588600	42.82767900	C	-1	42.05771400	41.09901300	49.97016300
C	0	42.90136600	37.68438800	44.83039700	C	0	42.39157400	39.69973200	49.59277700
O	0	38.18652500	39.45077200	40.50780700	C	0	42.31977600	39.11666600	48.34704300
O	0	43.11939600	39.23513600	41.19825300	N	0	42.78972200	38.75241300	50.51684600
O	0	39.72432000	37.36519100	41.02275000	C	0	42.93147300	37.61400900	49.83364700
O	0	42.29812700	41.62707800	41.56618100	N	0	42.66416600	37.80157300	48.52441800
O	0	40.61044300	39.82250400	41.16660100	H	-1	41.21416500	41.45381300	49.36911200
O	0	41.90613900	39.90079900	43.42996100	H	0	42.90587200	41.79364600	49.85162100
C	-1	38.72299200	40.07295500	43.52701000	H	0	41.76009400	41.14949900	51.02772000
O	0	39.00267700	38.83728800	42.90379700	H	0	43.03483900	39.23027500	52.00467400
H	-1	37.99103100	40.64838200	42.95065000	H	0	42.08505000	39.49176400	47.34821000
H	0	43.80178700	38.18138200	42.17442600	H	0	43.18043800	36.64340900	50.25575600
H	0	39.49172000	36.33482900	42.45109500	C	-1	43.78809300	40.90288600	54.80171600
H	0	42.18372500	35.64714100	46.62969600	C	0	43.71373500	40.64049800	53.28990900
H	0	40.05770900	36.82885500	47.10357400	O	0	44.17646500	41.41560600	52.47587000
H	0	39.37392400	35.54355500	46.06755400	O	0	43.11073700	39.50068000	53.02660000
H	0	39.82969600	37.60654600	44.77546000	H	-1	44.15958400	39.98293900	55.26507600
H	0	41.33168900	35.07320600	44.11817200	H	0	42.77860800	41.09292200	55.19968700
H	0	41.40143600	37.72048800	42.64858200	H	0	44.44592500	41.75570600	55.01038600
H	0	41.23425900	36.44672000	41.07453000	P	0	38.82109300	37.50794100	44.12790600
H	0	43.48934700	35.93877200	43.87380700	P	0	41.69209100	37.77811800	45.08480700
H	0	43.62268200	38.44466300	45.13196900	C	0	39.30671700	36.06640800	49.99488700
H	0	38.29586400	39.85610800	44.52187600	O	0	38.99640000	34.85455700	50.65471100
H	0	39.64937200	40.65311100	43.66484400	C	0	39.85412000	35.86347500	48.58861400
H	0	42.71650900	41.63472500	40.69470200	O	0	41.14310400	35.20529500	48.70206600
C	0	44.05434100	33.86688700	42.57073100	C	0	38.86111000	35.12382500	47.67044400
C	0	43.33921700	33.36985400	43.67344800	O	0	37.75504200	35.95846500	47.42505100
C	0	43.69168700	33.75030200	44.96663000	C	0	39.60537300	34.70168500	46.40563100
C	0	44.76644100	34.62977400	45.18303700	O	0	38.73675200	34.13115200	45.42506200
C	0	45.58950100	34.94903600	44.09536900	C	0	40.80358700	33.79223100	46.72980700
C	0	45.24693000	34.56446700	42.79611400	O	0	41.91348800	34.06501200	45.91423100
C	0	44.77179400	35.48110600	46.43888300	C	0	41.26259500	33.92048100	48.21762800
O	0	43.53245300	33.76795300	41.31261400	O	0	39.45703100	37.23368700	42.77717500
O	0	43.69577400	36.38122900	46.41274100	O	0	42.18601900	36.73104600	46.09733600
H	0	42.43071900	32.79441300	43.48188300	O	0	37.81906200	36.53773600	44.73221800
H	0	43.02577600	33.50072300	45.79610200	O	0	41.91564800	37.20171200	43.59551000
H	0	46.41943300	35.64652000	44.23977200	O	0	40.00770700	37.75548300	45.22241200
H	0	45.79701000	34.94578400	41.93457100	O	0	42.13394900	39.20356700	45.25039000
H	0	45.74919700	36.00703900	46.51680900	C	-1	38.72313500	40.07314400	43.52734500
H	0	44.69295900	34.83021500	47.34028000	O	0	38.05413000	38.96008300	44.09235800
H	0	42.90060300	34.53144100	41.25526200	H	-1	37.99100700	40.64816400	42.95046100
H	0	43.55941900	37.33697100	47.55258200	H	0	42.05939400	35.04934300	45.90957500
					H	0	37.78912700	36.29716700	46.50087900
					H	0	39.65746400	34.19997400	50.36292100
					H	0	40.04408000	36.66350100	50.56922400

H	0	38.38077100	36.65712100	49.90712300
H	0	40.05262100	36.84254500	48.12659100
H	0	38.49486700	34.23161900	48.19893200
H	0	40.03597000	35.61970500	45.99055000
H	0	38.30465700	34.91970300	45.00694200
H	0	40.51402900	32.75767000	46.53413400
H	0	42.33853800	33.66988800	48.21442900
H	0	39.17226900	40.70332900	44.31415000
H	0	39.52687100	39.74926800	42.84520500
H	0	41.03884900	37.15880700	43.10338000
C	0	38.35184400	31.19042600	45.75538300
C	0	37.77885400	31.66081000	46.94732700
C	0	38.50779800	31.61360600	48.12602800
C	0	39.81417100	31.09922200	48.13308000
C	0	40.27607400	30.42854600	46.99642200
C	0	39.53916700	30.45233800	45.80727300
C	0	40.75316400	31.66557700	49.17296400
O	0	37.83331600	31.58541600	44.55984800
O	0	40.62476100	33.07751000	49.21806100
H	0	36.83515100	32.20605500	46.89300800
H	0	38.13651900	32.13369100	49.01254100
H	0	41.29358100	30.02498000	46.98417900
H	0	39.95992700	30.07092100	44.87439800
H	0	41.79850300	31.36781000	48.95879000
H	0	40.50896700	31.32597200	50.19465700
H	0	37.98151500	32.56111000	44.59264700
H	0	42.58874300	37.13767900	47.71531700

4. Supplementary References

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