Supplementary materials

Crystal structure and spectroscopic analysis of 3-diethoxyphosphoryl-28-[1-(1-deoxy-β-D-glucopyranosyl)-1H-1,2,3-triazol-4-yl]carbonylbetulin

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Figure S1. Atom by atom superimposition of the compounds **2** (blue molecule) and **3** (violet molecule).

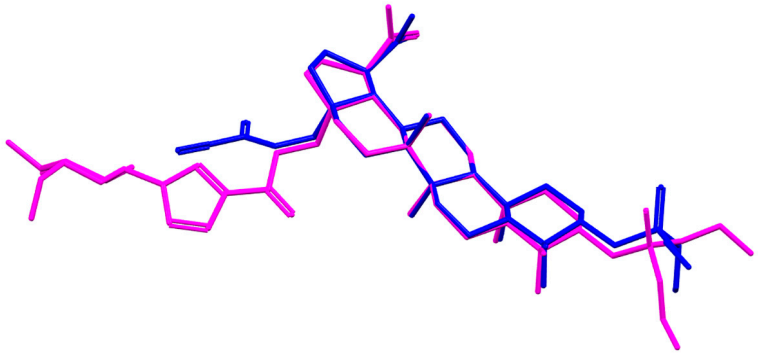
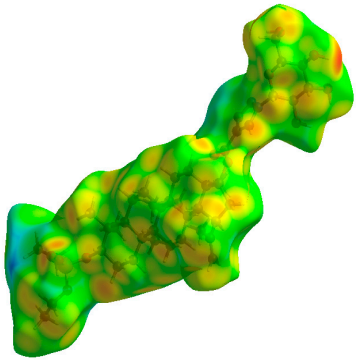
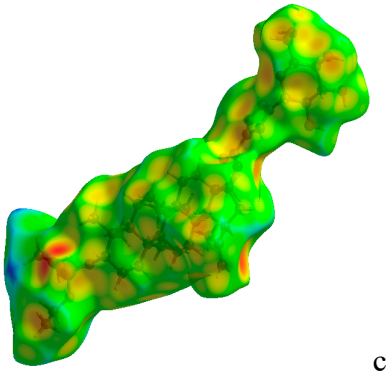
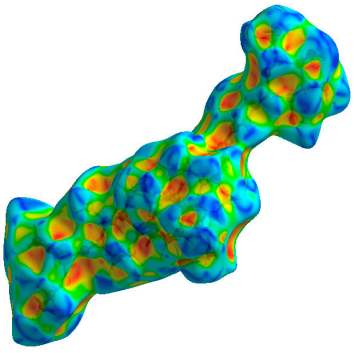
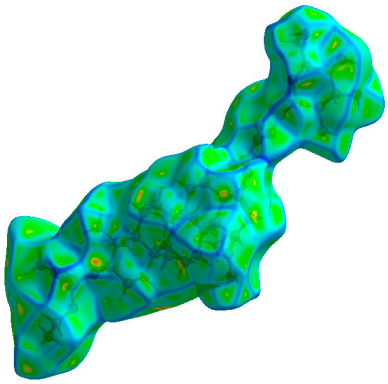


Figure S2. Hirshfeld surface mapped with a. d_{norm}, b. *di*, c. *de*, d. shape index, e. curvedness index and f. fragment patch for compound **3**.

a. 

b. 

c. 

d. 

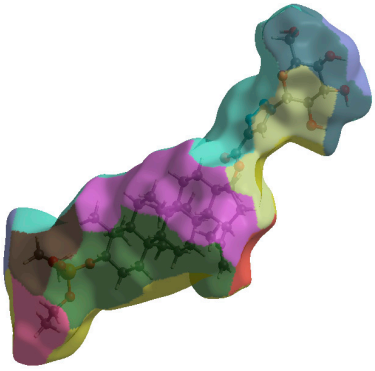
e. 

Table S1. Experimental data and refinement details of compound **3**.

Compound	**3**
Empirical formula	$C_{43}H_{70}N_3O_{11}P$
Formula weight	835.99
Temperature	100(1) K
Crystal system	monoclinic
Space group	P 21
Unit cell dimensions	
a [Å]	13.8397(12)
b [Å]	8.3259(3)
c [Å]	18.869(2)
α [°]	90
β [°]	95.161(10)
γ [°]	90
Volume	2165.4(3)
Z	2
Density (calculated) [Mg/m³]	1.282
Absorption coefficient [mm⁻¹]	1.076
F(000)	904
Crystal size [mm³]	0.330 *x* 0.030 *x* 0.020
Theta range for data collection [°]	3.206 to 73.880
Index ranges	$-17 \le h \le 17$ $-7 \le k \le 10$ $-23 \le l \le 23$
Reflections collected	17512
Independent reflections	6208 [R(int) = 0.0817]
Completeness to theta = 67.684°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.718 and 0.979
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6208/1/537
Goodness-of-fit on F2	1.036
Final R indices [I>2σ(I)]	R1 = 0.0919. wR2 = 0.0919
R indices (all data)	R1 = 0.1356. wR2 = 0.2470
Largest diff. peak and hole[eÅ⁻³]	0.797 and -0.553

Table S2. Experimental bond length in crystal structure of compound **3**.

Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]
P1-O1	1.5337	C5-C6	1.5370	C24-H24C	0.9800
P1-O4	1.4774	C5-C10	1.5697	C25-H25A	0.9800
P1-O5	1.5517	C6-H6A	0.9900	C25-H25B	0.9800
P1-O6	1.5782	C6-H6B	0.9900	C25-H25C	0.9800
O1-C3	1.4908	C6-C7	1.5322	C26-H26A	0.9800
O2-C28	1.4742	C7-H7A	0.9900	C26-H26B	0.9800
O2-C31	1.3532	C7-H7B	0.9900	C26-H26C	0.9800
O3-C31	1.1871	C7-C8	1.5401	C27-H27A	0.9800
O5-C34	1.4342	C8-C9	1.5641	C27-H27B	0.9800
O6-C36	1.4393	C8-C14	1.5920	C27-H27C	0.9800

O7-C38	1.4009	C8-C26	1.5599	C28-H28A	0.9900
O7-C42	1.4340	C9-H9A	1.0000	C28-H28B	0.9900
O8-H8	0.8400	C9-C10	1.5674	C29-H29A	0.9800
O8-C39	1.4257	C9-C11	1.5460	C29-H29B	0.9800
O9-H9	0.8400	C10-C25	1.5423	C29-H29C	0.9800
O9-C40	1.4029	C11-H11A	0.9900	C30-H30A	0.9500
O10-H10	0.8400	C11-H11B	0.9900	C30-H30B	0.9500
O10-C41	1.4382	C11-C12	1.5396	C31-C32	1.4815
O11-H11	0.8400	C12-H12A	0.9900	C32-C33	1.3595
O11-C43	1.4098	C12-H12B	0.9900	C33-H33	0.9500
N1-N2	1.3339	C12-C13	1.5269	C34-H34A	0.9900
N1-C32	1.3618	C13-H13	1.0000	C34-H34B	0.9900
N2-N3	1.3586	C13-C14	1.5887	C34-C35	1.5193
N3-C33	1.3499	C13-C18	1.5234	C35-H35A	0.9800
N3-C38	1.4476	C14-C15	1.5507	C35-H35B	0.9800
C1-H1A	0.9900	C14-C27	1.5474	C35-H35C	0.9800
C1-H1B	0.9900	C15-H15A	0.9900	C36-H36A	0.9900
C1-C2	1.5511	C15-H15B	0.9900	C36-H36B	0.9900
C1-C10	1.5360	C15-C16	1.5351	C36-C37	1.4522
C2-H2A	0.9900	C16-H16A	0.9900	C37-H37A	0.9800
C2-H2B	0.9900	C16-H16B	0.9900	C37-H37B	0.9800
C2-C3	1.4980	C16-C17	1.5397	C37-H37C	0.9800
C3-H3	1.0000	C17-C18	1.5680	C38-H38	1.0000
C3-C4	1.5505	C17-C22	1.5259	C38-C39	1.5226
C4-C5	1.5389	C17-C28	1.5174	C39-H39	1.0000
C4-C23	1.5365	C18-H18	1.0000	C39-C40	1.5219
C4-C24	1.5413	C18-C19	1.5553	C40-H40	1.0000
C21-H21B	0.9900	C19-H19	1.0000	C40-C41	1.5205
C21-C22	1.5454	C19-C20	1.5118	C41-H41	1.0000
C22-H22A	0.9900	C19-C21	1.5681	C41-C42	1.5003
C22-H22B	0.9900	C20-C29	1.4772	C42-H42	1.0000
C23-H23A	0.9800	C20-C30	1.3544	C42-C43	1.5222
C23-H23B	0.9800	C21-H21A	0.9900	C43-H43A	0.9900
C23-H23C	0.9800	C24-H24A	0.9800	C43-H43B	0.9900
C5-H5	1.0000	C24-H24B	0.9800		

Table S3. Experimental bond angle in crystal structure of compound **3**.

Bond Angle	[°]	Bond Angle	[°]	Bond Angle	[°]	Bond Angle	[°]
O1-P1-O4	115.25	C5-C6-C7	111.11	C14-C15-H15A	108.43	C4-C24-H24B	109.47
O1-P1-O5	107.05	H6A-C6-H6B	108.02	C14-C15-H15B	108.43	C4-C24-H24C	109.47
O1-P1-O6	101.66	H6A-C6-C7	109.41	C14-C15-C16	115.40	H24A-C24-H24B	109.47
O4-P1-O5	109.78	H6B-C6-C7	109.41	H15A-C15-H15B	107.47	H24A-C24-H24C	109.47
O4-P1-O6	113.64	C6-C7-H7A	108.82	H15A-C15-C16	108.42	H24B-C24-H24C	109.47
O5-P1-O6	108.96	C6-C7-H7B	108.82	H15B-C15-C16	108.43	C10-C25-H25A	109.47
P1-O1-C3	125.43	C6-C7-C8	113.72	C15-C16-H16A	109.34	C10-C25-H25B	109.47
C28-O2-C31	118.23	H7A-C7-H7B	107.68	C15-C16-H16B	109.34	C10-C25-H25C	109.47
P1-O5-C34	121.34	H7A-C7-C8	108.82	C15-C16-C17	111.42	H25A-C25-H25B	109.47
P1-O6-C36	120.49	H7B-C7-C8	108.82	H16A-C16-H16B	107.98	H25A-C25-H25C	109.47
C38-O7-C42	111.87	C7-C8-C9	109.54	H16A-C16-C17	109.34	H25B-C25-H25C	109.47
H8-O8-C39	109.47	C7-C8-C14	109.50	H16B-C16-C17	109.34	C8-C26-H26A	109.47
H9-O9-C40	109.47	C7-C8-C26	107.47	C16-C17-C18	105.66	C8-C26-H26B	109.47
H10-O10-C41	109.47	C9-C8-C14	108.22	C16-C17-C22	117.23	C8-C26-H26C	109.47
H11-O11-C43	109.47	C9-C8-C26	112.23	C16-C17-C28	110.57	H26A-C26-H26B	109.47
N2-N1-C32	107.92	C14-C8-C26	109.86	C18-C17-C22	101.59	H26A-C26-H26C	109.47
N1-N2-N3	106.61	C8-C9-H9A	105.69	C18C17-C28	110.99	H26B-C26-H26C	109.47
N2-N3-C33	111.16	C8-C9-C10	115.79	C22-C17-C28	110.28	C14-C27-H27A	109.47
N2-N3-C38	121.99	C8-C9-C11	110.15	C13-C18-C17	111.35	C14-C27-H27B	109.47
C33-N3-C38	126.56	H9A-C9-C10	105.69	C13-C18-H18	107.18	C14-C27-H27C	109.47
H1A-C1-H1B	107.89	H9A-C9-C11	105.69	C13-C18-C19	118.95	H27A-C27-H27B	109.47
H1A-C1-C2	109.18	C10-C9-C11	112.96	C17-C18-H18	107.18	H27A-C27-H27C	109.47
H1A-C1-C10	109.18	C1-C10-C5	108.09	C17-C18-C19	104.43	H27B-C27-H27C	109.47
H1B-C1-C2	109.18	C1-C10-C9	108.58	H18-C18-C19	107.18	O2-C28-C17	108.48
H1B-C1-C10	109.18	C1-C10-C25	107.39	C18-C19-H19	109.20	O2-C28-H28A	110.00
C2-C1-C10	112.13	C5-C10-C9	106.34	C18-C19-C20	113.14	O2-C28-H28B	110.00
C1-C2-H2A	109.71	C5-C10-C25	112.65	C18-C19-C21	104.74	C17-C28-H28A	110.00
C1-C2-H2B	109.71	C9-C10-C25	113.61	H19-C19-C20	109.20	C17-C28-H28B	110.00
C1-C2-C3	109.81	C9-C11-H11A	108.64	H19-C19-C21	109.20	H28A-C28-H28B	108.37
H2A-C2-H2B	108.19	C9-C11-H11B	108.64	C20-C19-C21	111.23	C20-C29-H29A	109.47
H2A-C2-C3	109.70	C9-C11-C12	114.49	C19-C20-C29	117.66	C20-C29-H29B	109.47
H2B-C2-C3	109.70	H11A-C11-H11B	107.59	C19-C20-C30	121.84	C20-C29-H29C	109.47
O1-C3-C2	107.93	H11A-C11-C12	108.64	C29-C20-C30	120.50	H29A-C29-H29B	109.47
O1-C3-H3	108.70	H11B-C11-C12	108.64	C19-C21-H21A	110.50	H29A-C29-H29C	109.47
O1-C3-C4	108.74	C11-C12-H12A	109.28	C19-C21-H21B	110.50	H29B-C29-H29C	109.47
C2-C3-H3	108.70	C11-C12-H12B	109.28	C19-C21-C22	106.15	C20-C30-H30A	120.00
C2-C3-C4	113.97	C11-C12-C13	111.68	H21A-C21-H21B	108.68	C20-C30-H30B	120.00
H3-C3-C4	108.70	H12A-C12-H12B	107.95	H21A-C21-C22	110.50	H30A-C30-H30B	120.00
C3-C4-C5	105.89	H12A-C12-C13	109.28	H21B-C21-C22	110.50	O2-C31-O3	125.49
C3-C4-C23	107.30	H12B-C12-C13	109.28	C17-C22-C21	103.52	O2-C31-C32	109.06
C3-C4-C24	111.17	C12-C13-H13	107.65	C17-C22-H22A	111.06	O3-C31-C32	125.43
C5-C4-C23	109.92	C12-C13-C14	110.92	C17-C22-H22B	111.06	N1-C32-C31	121.87
C5-C4-C24	114.85	C12-C13-C18	114.05	C21-C22-H22A	111.06	N1-C32-C33	109.87
C23-C4-C24	107.48	H13-C13-C14	107.65	C21-C22-H22B	111.06	C31-C32-C33	128.06
C4-C5-H5	104.18	H13-C13-C18	107.65	H22A-C22-H22B	109.03	N3-C33-C32	104.43
C4-C5-C6	113.55	C14-C13-C18	108.68	C4-C23-H23A	109.47	N3-C33-H33	127.79
C4-C5-C10	118.25	C8-C14-C13	105.97	C4-C23-H23B	109.47	C32-C33-H33	127.79
H5-C5-C6	104.18	C8-C14-C15	110.85	C4-C23-H23C	109.47	O5-C34-H34A	109.84
H5-C5-C10	104.18	C8-C14-C27	111.77	H23A-C23-H23B	109.47	O5-C34-H34B	109.84
C6-C5-C10	110.76	C13-C14-C15	111.11	H23A-C23-H23C	109.47	O5-C34-C35	109.21
C5-C6-H6A	109.41	C13-C14-C27	110.21	H23B-C23-H23C	109.47	H34A-C34-H34B	108.27
C5-C6-H6B	109.41	C15-C14-C27	106.99	C4-C24-H24A	109.47	H34A-C34-C35	109.84
H34B-C34-C35	109.84	N3-C33-C32	104.43	O5-C34-C35	109.21	C34-C35-H35B	109.47
C34-C35-H35A	109.47	N3-C33-H33	127.79	H34A-C34-H34B	108.27	C34-C35-H35C	109.47
C34-C35-H35B	109.47	C32-C33-H33	127.79	H34A-C34-C35	109.84	H35A-C35-H35B	109.47
C34-C35-H35C	109.47	O5-C34-H34A	109.84	H34B-C34-C35	109.84	H35A-C35-H35C	109.47
H35A-C35-H35B	109.47	O5-C34-H34B	109.84	C34-C35-H35A	109.47	H35B-C35-H35C	109.47
O6-C36-H36B	109.38	H37B-C37-H37C	109.47	C38-C39-H39	109.94	O10-C41-H41	108.89
O6-C36-C37	111.27	O7-C38-N3	108.31	C38-C39-C40	108.07	O10-C41-C42	105.87

H36A-C36-H36B	108.00	O7-C38-H38	108.62	H39-C39-C40	109.95	C40-C41-H41	108.89
H36A-C36-C37	109.38	O7-C38-C39	110.29	O9-C40-C39	115.17	C40-C41-C42	113.80
H36B-C36-C37	109.38	N3-C38-H38	108.62	O9-C40-H40	107.74	H41-C41-C42	108.89
C36-C37-H37A	109.47	N3-C38-C39	112.29	O9-C40-C41	106.71	O7-C42-C41	110.95
C36-C37-H37B	109.47	H38-C38-C39	108.63	C39-C40-H40	107.74	O7-C42-H42	109.17
C36-C37-H37C	109.47	O8-C39-C38	107.07	C39-C40-C41	111.47	O7-C42-C43	107.06
H37A-C37-H37B	109.47	O8-C39-H39	109.95	H40-C40-C41	107.74	C41-C42-H42	109.17
H37A-C37-H37C	109.47	O8-C39-C40	111.79	O10-C41-C40	110.38	C41-C42-C43	111.27
H42-C42-C43	109.17	O11-C43-H43A	109.55	C42-C43-H43A	109.55	H43A-C43-H43B	108.10
O11-C43-C42	110.48	O11-C43-H43B	109.55	C42-C43-H43B	109.55		

Table S4. Experimental torsion angle in crystal structure of compound **3**.

Torsion Angle	[°]	Torsion Angle	[°]	Torsion Angle	[°]
O4-P1-O1-C3	15.84	H6B-C6-C7-H7A	55.28	C28-C17-C18-C13	-52.83
O5-P1-O1-C3	138.25	H6B-C6-C7-H7B	-61.80	C28-C17-C18-H18	-169.74
O6-P1-O1-C3	-107.53	H6B-C6-C7-C8	176.74	C28-C17-C18-C19	76.76
O1-P1-O5-C34	50.35	C6-C7-C8-C9	-49.20	C16-C17-C22-C21	158.06
O4-P1-O5-C34	176.12	C6-C7-C8-C14	-167.73	C16-C17-C22-H22A	38.81
O6-P1-O5-C34	-58.85	C6-C7-C8-C26	72.98	C16-C17-C22-H22B	-82.69
O1-P1-O6-C36	171.21	H7A-C7-C8-C9	72.26	C18-C17-C22-C21	43.51
O4-P1-O6-C36	46.75	H7A-C7-C8-C14	-46.27	C18-C17-C22-H22A	-75.74
O5-P1-O6-C36	-76.00	H7A-C7-C8-C26	-165.56	C18-C17-C22-H22B	162.75
P1-O1-C3-C2	111.32	H7B-C7-C8-C9	-170.66	C28-C17-C22-C21	-74.24
P1-O1-C3-H3	-6.40	H7B-C7-C8-C14	70.81	C28-C17-C22-H22A	166.51
P1-O1-C3-C4	-124.58	H7B-C7-C8-C26	-48.48	C28-C17-C22-H22B	45.00
C31-O2-C28-C17	-124.73	C7-C8-C9-H9A	-65.46	C16-C17-C28-O2	68.73
C31-O2-C28-H28A	114.91	C7-C8-C9-C10	51.12	C16-C17-C28-H28A	-170.91
C31-O2-C28-H28B	-4.38	C7-C8-C9-C11	-179.18	C16-C17-C28-H28B	-51.62
C28-O2-C31-O3	5.95	C14-C8-C9-H9A	53.86	C18-C17-C28-O2	-174.33
C28-O2-C31-C32	-172.92	C14-C8-C9-C10	170.45	C18-C17-C28-H28A	-53.98
P1-O5-C34-H34A	53.45	C14-C8-C9-C11	-59.85	C18-C17-C28-H28B	65.31
P1-O5-C34-H34B	-65.53	C26-C8-C9-H9A	175.25	C22-C17-C28-O2	-62.55
P1-O5-C34-C35	173.96	C26-C8-C9-C10	-68.16	C22-C17-C28-H28A	57.81
P1-O6-C36-H36A	2.25	C26-C8-C9-C11	61.54	C22-C17-C28-H28B	177.10
P1-O6-C36-H36B	-115.84	C7-C8-C14-C13	-175.94	C13-C18-C19-H19	29.51
P1-O6-C36-C37	123.20	C7-C8-C14-C15	-55.28	C13-C18-C19-C20	-92.33
C42-O7-C38-N3	170.09	C7-C8-C14-C27	63.99	C13-C18-C19-C21	146.37
C42-O7-C38-H38	52.28	C9-C8-C14-C13	64.71	C17-C18-C19-H19	-95.37
C42-O7-C38-C39	-66.66	C9-C8-C14-C15	-174.63	C17-C18-C19-C20	142.79
C38-O7-C42-C41	58.83	C9-C8-C14-C27	-55.36	C17-C18-C19-C21	21.48
C38-O7-C42-H42	-61.52	C26-C8-C14-C13	-58.13	H18-C18-C19-H19	151.13
C38-O7-C42-C43	-179.58	C26-C8-C14-C15	62.52	H18-C18-C19-C20	29.29
H8-O8-C39-C38	-169.88	C26-C8-C14-C27	-178.21	H18-C18-C19-C21	-92.02
H8-O8-C39-H39	70.71	C7-C8-C26-H26A	-44.43	C18-C19-C20-C29	-61.80
H8-O8-C39-C40	-51.70	C7-C8-C26-H26B	-164.43	C18-C19-C20-C30	117.74
H9-O9-C40-C39	-42.51	C7-C8-C26-H26C	75.57	H19-C19-C20-C29	176.36
H9-O9-C40-H40	77.74	C9-C8-C26-H26A	76.06	H19-C19-C20-C30	-4.10
H9-O9-C40-C41	-166.80	C9-C8-C26-H26B	-43.94	C21-C19-C20-C29	55.77
H10-O10-C41-C40	49.86	C9-C8-C26-H26C	-163.94	C21-C19-C20-C30	-124.69
H10-O10-C41-H41	-69.62	C14-C8-C26-H26A	-163.50	C18-C19-C21-H21A	125.03
H10-O10-C41-C42	173.45	C14-C8-C26-H26B	76.50	C18-C19-C21-H21B	-114.65
H11-O11-C43-C42	102.53	C14-C8-C26-H26C	-43.50	C18-C19-C21-C22	5.19
H11-O11-C43-H43A	-18.25	C8-C9-C10-C1	-171.74	H19-C19-C21-H21A	-118.12
H11-O11-C43-H43B	-136.68	C8-C9-C10-C5	-55.64	H19-C19-C21-H21B	2.21
C32-N1-N2-N3	-1.08	C8-C9-C10-C25	68.85	H19-C19-C21-C22	122.05
N2-N1-C32-C31	-174.80	H9A-C9-C10-C1	-55.16	C20-C19-C21-H21A	2.47
N2-N1-C32-C33	0.45	H9A-C9-C10-C5	60.95	C20-C19-C21-H21B	122.80
N1-N2-N3-C33	1.37	H9A-C9-C10-C25	-174.56	C20-C19-C21-C22	-117.36
N1-N2-N3-C38	175.62	C11-C9-C10-C1	59.93	C19-C20-C29-H29A	70.16
N2-N3-C33-C32	-1.07	C11-C9-C10-C5	176.04	C19-C20-C29-H29B	-49.84

N2-N3-C33-H33	178.92	C11-C9-C10-C25	-59.48	C19-C20-C29-H29C	-169.84
C38-N3-C33-C32	-175.00	C8-C9-C11-H11A	173.78	C30-C20-C29-H29A	-109.39
C38-N3-C33-H33	5.00	C8-C9-C11-H11B	-69.45	C30-C20-C29-H29B	130.61
N2-N3-C38-O7	48.77	C8-C9-C11-C12	52.16	C30-C20-C29-H29C	10.61
N2-N3-C38-H38	166.58	H9A-C9-C11-H11A	60.07	C19-C20-C30-H30A	-179.52
N2-N3-C38-C39	-73.26	H9A-C9-C11-H11B	176.83	C19-C20-C30-H30B	0.48
C33-N3-C38-O7	-137.91	H9A-C9-C11-C12	-61.55	C29-C20-C30-H30A	0.00
C33-N3-C38-H38	-20.09	C10-C9-C11-H11A	-55.01	C29-C20-C30-H30B	-180.00
C33-N3-C38-C39	100.06	C10-C9-C11-H11B	61.75	C19-C21-C22-C17	-30.67
H1A-C1-C2-H2A	-176.94	C10-C9-C11-C12	-176.63	C19-C21-C22-H22A	88.58
H1A-C1-C2-H2B	-58.23	C1-C10-C25-H25A	-90.76	C19-C21-C22-H22B	-149.91
H1A-C1-C2-C3	62.41	C1-C10-C25-H25B	149.24	H21A-C21-C22-C17	-150.50
H1B-C1-C2-H2A	-59.21	C1-C10-C25-H25C	29.24	H21A-C21-C22-H22A	-31.26
H1B-C1-C2-H2B	59.51	C5-C10-C25-H25A	150.34	H21A-C21-C22-H22B	90.25
H1B-C1-C2-C3	-179.85	C5-C10-C25-H25B	30.34	H21B-C21-C22-C17	89.17
C10-C1-C2-H2A	61.92	C5-C10-C25-H25C	-89.66	H21B-C21-C22-H22A	-151.58
C10-C1-C2-H2B	-179.36	C9-C10-C25-H25A	29.33	H21B-C21-C22-H22B	-30.07
C10-C1-C2-C3	-58.72	C9-C10-C25-H25B	-90.67	O2-C31-C32-N1	173.20
H1A-C1-C10-C5	-69.51	C9-C10-C25-H25C	149.33	O2-C31-C32-C33	-1.12
H1A-C1-C10-C9	45.46	C9-C11-C12-H12A	71.37	O3-C31-C32-N1	-5.66
H1A-C1-C10-C25	168.69	C9-C11-C12-H12B	-170.71	O3-C31-C32-C33	-179.98
H1B-C1-C10-C5	172.75	C9-C11-C12-C13	-49.67	N1-C32-C33-N3	0.38
H1B-C1-C10-C9	-72.27	H11A-C11-C12-H12A	-50.25	N1-C32-C33-H33	-179.62
H1B-C1-C10-C25	50.96	H11A-C11-C12-H12B	67.67	C31-C32-C33-N3	175.26
C2-C1-C10-C5	51.62	H11A-C11-C12-C13	-171.29	C31-C32-C33-H33	-4.74
C2-C1-C10-C9	166.59	H11B-C11-C12-H12A	-167.01	O5-C34-C35-H35A	-56.81
C2-C1-C10-C25	-70.17	H11B-C11-C12-H12B	-49.09	O5-C34-C35-H35B	-176.81
C1-C2-C3-O1	-177.82	H11B-C11-C12-C13	71.95	O5-C34-C35-H35C	63.19
C1-C2-C3-H3	-60.09	C11-C12-C13-H13	-62.32	H34A-C34-C35-H35A	63.70
C1-C2-C3-C4	61.29	C11-C12-C13-C14	55.21	H34A-C34-C35-H35B	-56.30
H2A-C2-C3-O1	61.54	C11-C12-C13-C18	178.31	H34A-C34-C35-H35C	-176.30
H2A-C2-C3-H3	179.27	H12A-C12-C13-H13	176.64	H34B-C34-C35-H35A	-177.32
H2A-C2-C3-C4	-59.35	H12A-C12-C13-C14	-65.83	H34B-C34-C35-H35B	62.68
H2B-C2-C3-O1	-57.18	H12A-C12-C13-C18	57.28	H34B-C34-C35-H35C	-57.32
H2B-C2-C3-H3	60.55	H12B-C12-C13-H13	58.72	O6-C36-C37-H37A	-69.88
H2B-C2-C3-C4	-178.06	H12B-C12-C13-C14	176.25	O6-C36-C37-H37B	170.12
O1-C3-C4-C5	-175.96	H12B-C12-C13-C18	-60.65	O6-C36-C37-H37C	50.11
O1-C3-C4-C23	66.66	C12-C13-C14-C8	-63.00	H36A-C36-C37-H37A	51.07
O1-C3-C4-C24	-50.59	C12-C13-C14-C15	176.51	H36A-C36-C37-H37B	-68.93
C2-C3-C4-C5	-55.53	C12-C13-C14-C27	58.08	H36A-C36-C37-H37C	171.07
C2-C3-C4-C23	-172.90	H13-C13-C14-C8	54.53	H36B-C36-C37-H37A	169.16
C2-C3-C4-C24	69.85	H13-C13-C14-C15	-65.96	H36B-C36-C37-H37B	49.16
H3-C3-C4-C5	65.86	H13-C13-C14-C27	175.62	H36B-C36-C37-H37C	-70.84
H3-C3-C4-C23	-51.51	C18-C13-C14-C8	170.86	O7-C38-C39-O8	-178.29
H3-C3-C4-C24	-168.77	C18-C13-C14-C15	50.37	O7-C38-C39-H39	-58.88
C3-C4-C5-H5	-63.65	C18-C13-C14-C27	-68.06	O7-C38-C39-C40	61.13
C3-C4-C5-C6	-176.34	C12-C13-C18-C17	172.68	N3-C38-C39-O8	-57.39
C3-C4-C5-C10	51.34	C12-C13-C18-H18	-70.40	N3-C38-C39-H39	62.02
C23-C4-C5-H5	51.95	C12-C13-C18-C19	51.22	N3-C38-C39-C40	-177.97
C23-C4-C5-C6	-60.74	H13-C13-C18-C17	53.32	H38-C38-C39-O8	62.77
C23-C4-C5-C10	166.94	H13-C13-C18-H18	170.24	H38-C38-C39-H39	-177.82
C24-C4-C5-H5	173.28	H13-C13-C18-C19	-68.15	H38-C38-C39-C40	-57.81
C24-C4-C5-C6	60.59	C14-C13-C18-C17	-63.01	O8-C39-C40-O9	70.51
C24-C4-C5-C10	-71.73	C14-C13-C18-H18	53.91	O8-C39-C40-H40	-49.74
C3-C4-C23-H23A	62.61	C14-C13-C18-C19	175.53	O8-C39-C40-C41	-167.74
C3-C4-C23-H23B	-57.39	C8-C14-C15-H15A	-42.03	C38-C39-C40-O9	-171.91
C3-C4-C23-H23C	-177.39	C8-C14-C15-H15B	74.36	C38-C39-C40-H40	67.85
C5-C4-C23-H23A	-52.09	C8-C14-C15-C16	-163.83	C38-C39-C40-C41	-50.15
C5-C4-C23-H23B	-172.09	C13-C14-C15-H15A	75.53	H39-C39-C40-O9	-51.90
C5-C4-C23-H23C	67.91	C13-C14-C15-H15B	-168.08	H39-C39-C40-H40	-172.14
C24-C4-C23-H23A	-177.74	C13-C14-C15-C16	-46.28	H39-C39-C40-C41	69.86

C24-C4-C23-H23B	62.26	C27-C14-C15-H15A	-164.13	O9-C40-C41-O10	-68.95
C24-C4-C23-H23C	-57.74	C27-C14-C15-H15B	-47.73	O9-C40-C41-H41	50.53
C3-C4-C24-H24A	66.61	C27-C14-C15-C16	74.07	O9-C40-C41-C42	172.19
C3-C4-C24-H24B	-53.39	C8-C14-C27-H27A	-165.19	C39-C40-C41-O10	164.52
C3-C4-C24-H24C	-173.39	C8-C14-C27-H27B	74.81	C39-C40-C41-H41	-76.00
C5-C4-C24-H24A	-173.19	C8-C14-C27-H27C	-45.19	C39-C40-C41-C42	45.66
C5-C4-C24-H24B	66.81	C13-C14-C27-H27A	77.25	H40-C40-C41-O10	46.51
C5-C4-C24-H24C	-53.19	C13-C14-C27-H27B	-42.75	H40-C40-C41-H41	166.00
C23-C4-C24-H24A	-50.54	C13-C14-C27-H27C	-162.75	H40-C40-C41-C42	-72.34
C23-C4-C24-H24B	-170.53	C15-C14-C27-H27A	-43.67	O10-C41-C42-O7	-169.44
C23-C4-C24-H24C	69.46	C15-C14-C27-H27B	-163.67	O10-C41-C42-H42	-49.09
C4-C5-C6-H6A	-75.77	C15-C14-C27-H27C	76.33	O10-C41-C42-C43	71.47
C4-C5-C6-H6B	42.40	C14-C15-C16-H16A	-68.93	C40-C41-C42-O7	-48.03
C4-C5-C6-C7	163.32	C14-C15-C16-H16B	173.03	C40-C41-C42-H42	72.32
H5-C5-C6-H6A	171.55	C14-C15-C16-C17	52.05	C40-C41-C42-C43	-167.13
H5-C5-C6-H6B	-70.29	H15A-C15-C16-H16A	169.26	H41-C41-C42-O7	73.63
H5-C5-C6-C7	50.63	H15A-C15-C16-H16B	51.23	H41-C41-C42-H42	-166.02
C10-C5-C6-H6A	60.08	H15A-C15-C16-C17	-69.75	H41-C41-C42-C43	-45.47
C10-C5-C6-H6B	178.24	H15B-C15-C16-H16A	52.87	O7-C42-C43-O11	-67.13
C10-C5-C6-C7	-60.84	H15B-C15-C16-H16B	-65.16	O7-C42-C43-H43A	53.65
C4-C5-C10-C1	-51.24	H15B-C15-C16-C17	173.85	O7-C42-C43-H43B	172.08
C4-C5-C10-C9	-167.67	C15-C16-C17-C18	-58.83	C41-C42-C43-O11	54.25
C4-C5-C10-C25	67.25	C15-C16-C17-C22	-171.10	C41-C42-C43-H43A	175.04
H5-C5-C10-C1	63.76	C15-C16-C17-C28	61.35	C41-C42-C43-H43B	-66.53
H5-C5-C10-C9	-52.68	H16A-C16-C17-C18	62.15	H42-C42-C43-O11	174.81
H5-C5-C10-C25	-177.76	H16A-C16-C17-C22	-50.12	H42-C42-C43-H43A	-64.41
C6-C5-C10-C1	175.22	H16A-C16-C17-C28	-177.67	H42-C42-C43-H43B	54.02
C6-C5-C10-C9	58.78	H16B-C16-C17-C18	-179.82	C22-C17-C18-C19	-40.48
C6-C5-C10-C25	-66.29	H16B-C16-C17-C22	67.92	H6A-C6-C7-H7A	173.44
C5-C6-C7-H7A	-65.64	H16B-C16-C17-C28	-59.64	H6A-C6-C7-H7B	56.36
C5-C6-C7-H7B	177.28	C16-C17-C18-C13	67.08	H6A-C6-C7-C8	-65.10
C5-C6-C7-C8	55.82	C16-C17-C18-H18	-49.84	C22-C17-C18-H18	73.02
C22-C17-C18-C13	-170.06	C16-C17-C18-C19	-163.34		