

Supporting Information

for

Computational Evidence for the Substrate-Assisted Catalytic Mechanism of O-GlcNAcase. A DFT Investigation.

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Contents

Figure S1

Figure S2

Figure S3

Figure S4

Figure S5

Figure S6

Table S1

m0

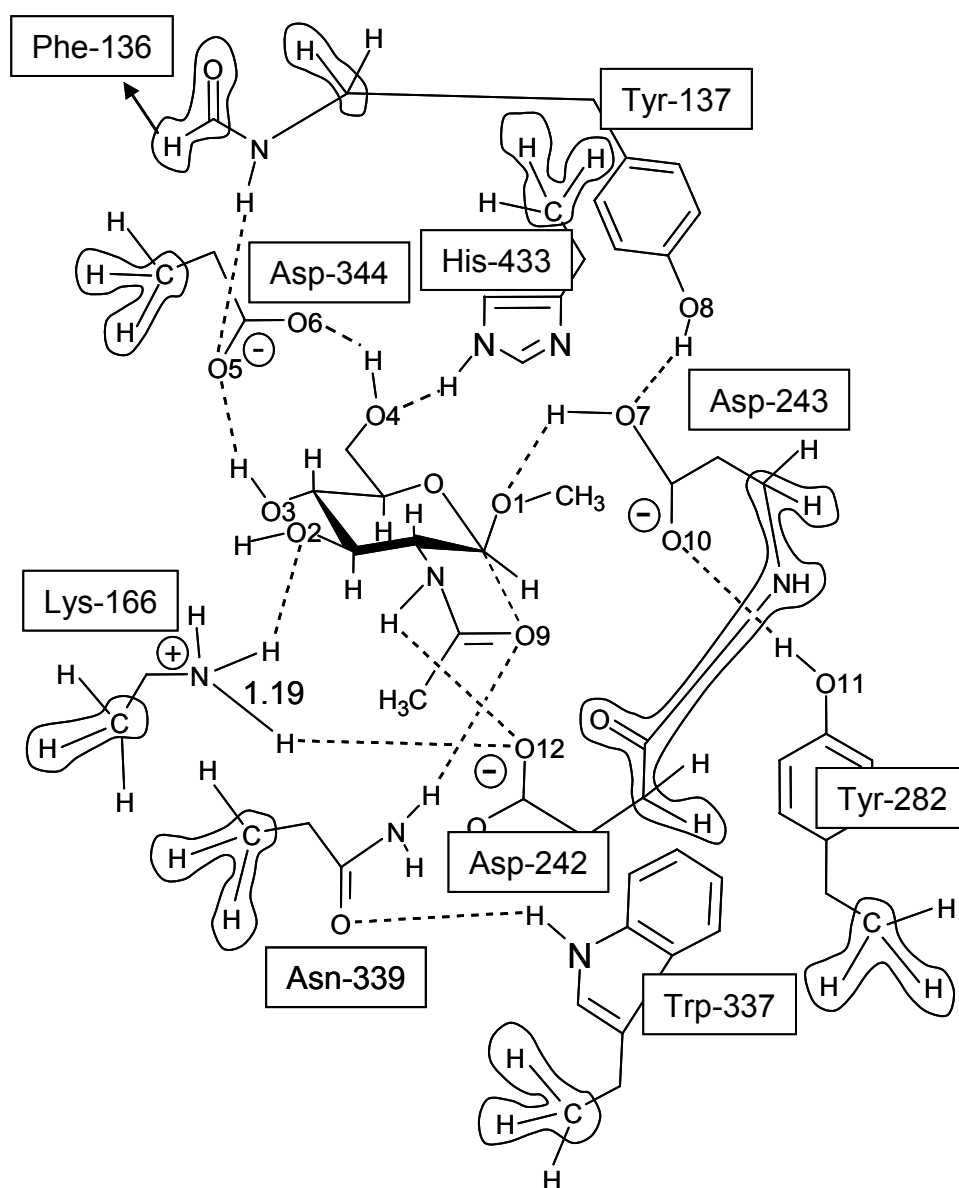


Figure S1. Two-dimensional schematic representation of the structure of the critical point **m0**. The frozen atoms are marked by contour lines.

m0

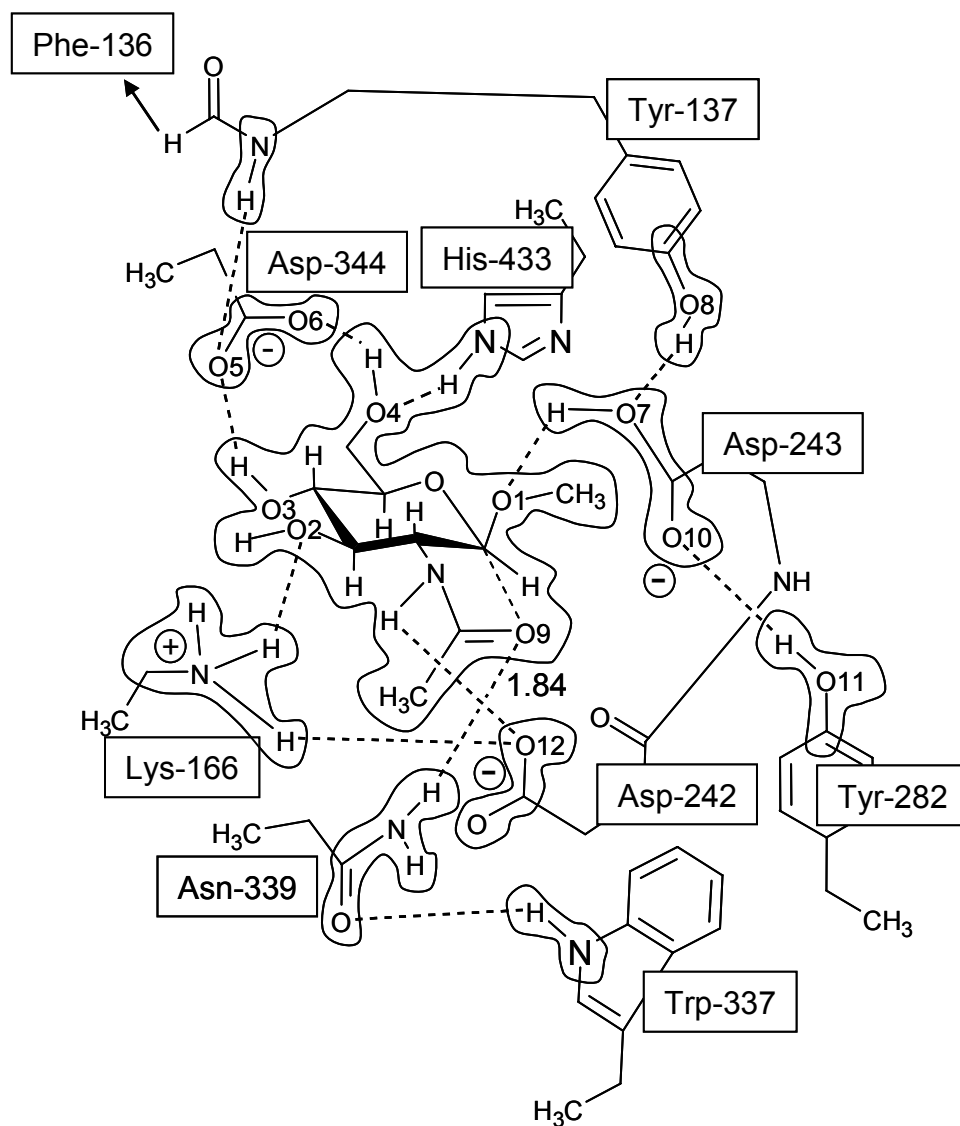
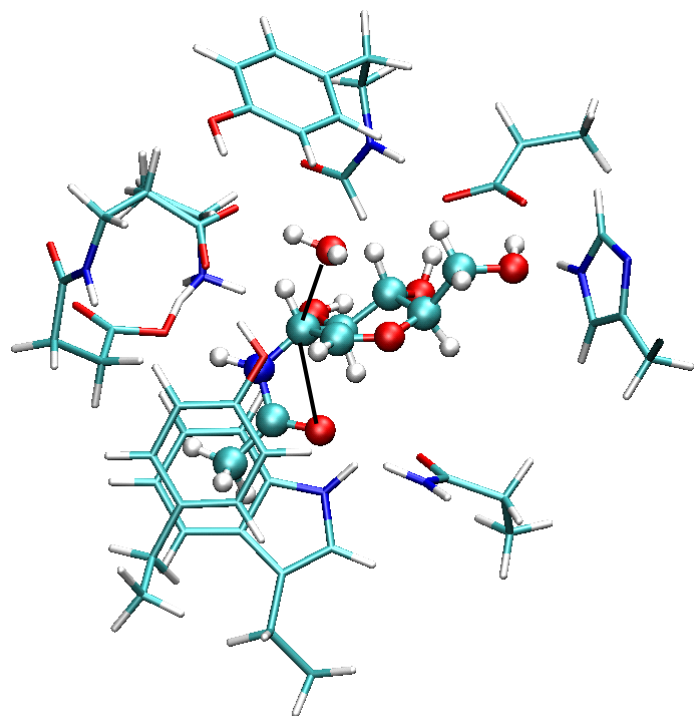


Figure S2. Two-dimensional schematic representation of the structure of the critical point **m0**. The atoms marked by contour lines are described by the DZVP basis set. The 3-21G* basis has been used for all remaining atoms.



ts2

Figure S3. A three-dimensional representation of **ts2**. For the atoms directly involved in the process a ball-and-stick representation is used. The two main components of the reaction coordinate (approach of the nucleophile and departure of the water) are highlighted by two straight lines.

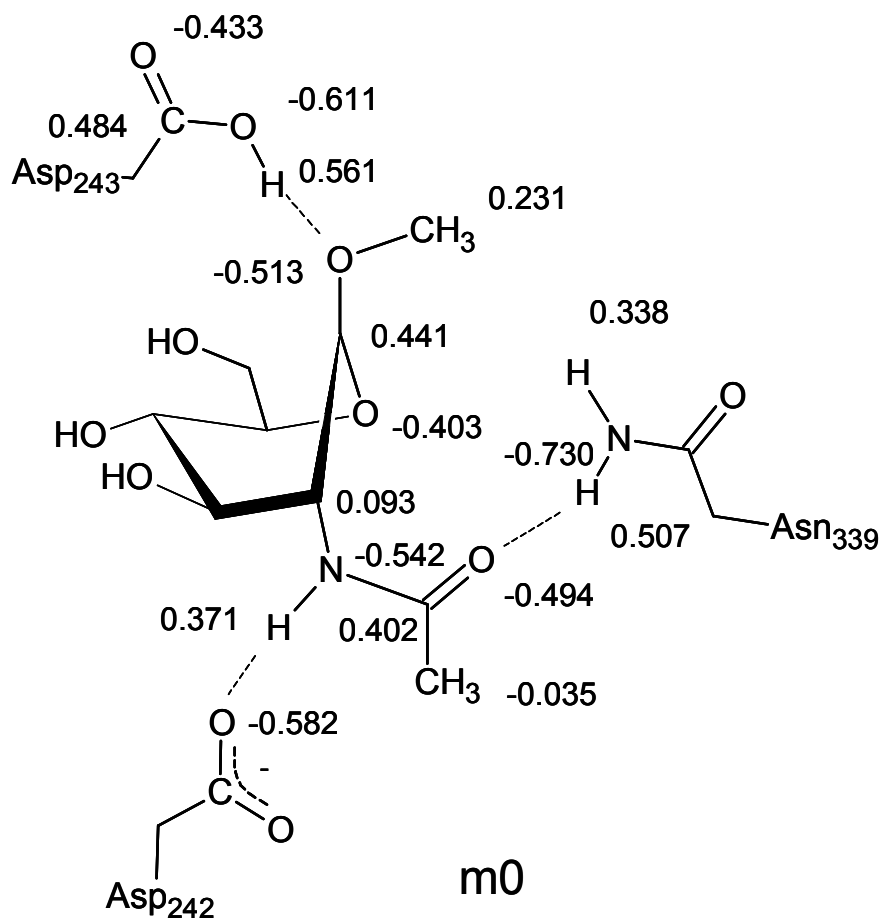


Figure S4. Net atomic charges (Mulliken) computed for **m0**.

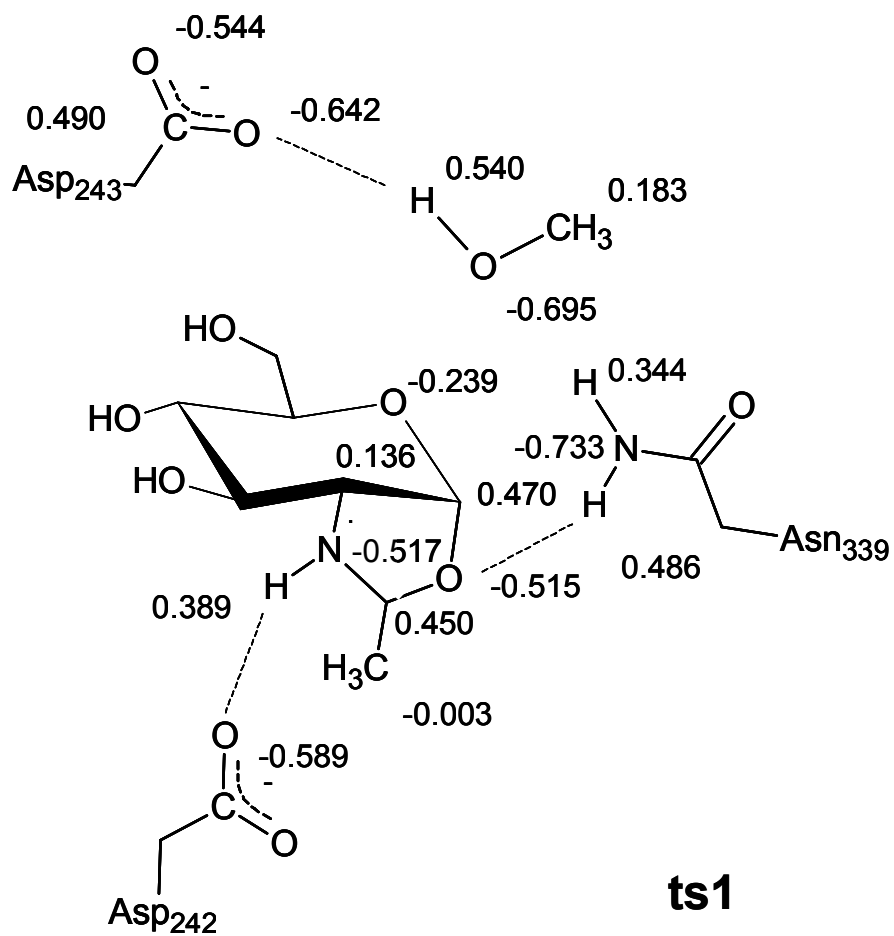


Figure S5. Net atomic charges (Mulliken) computed for **ts1**

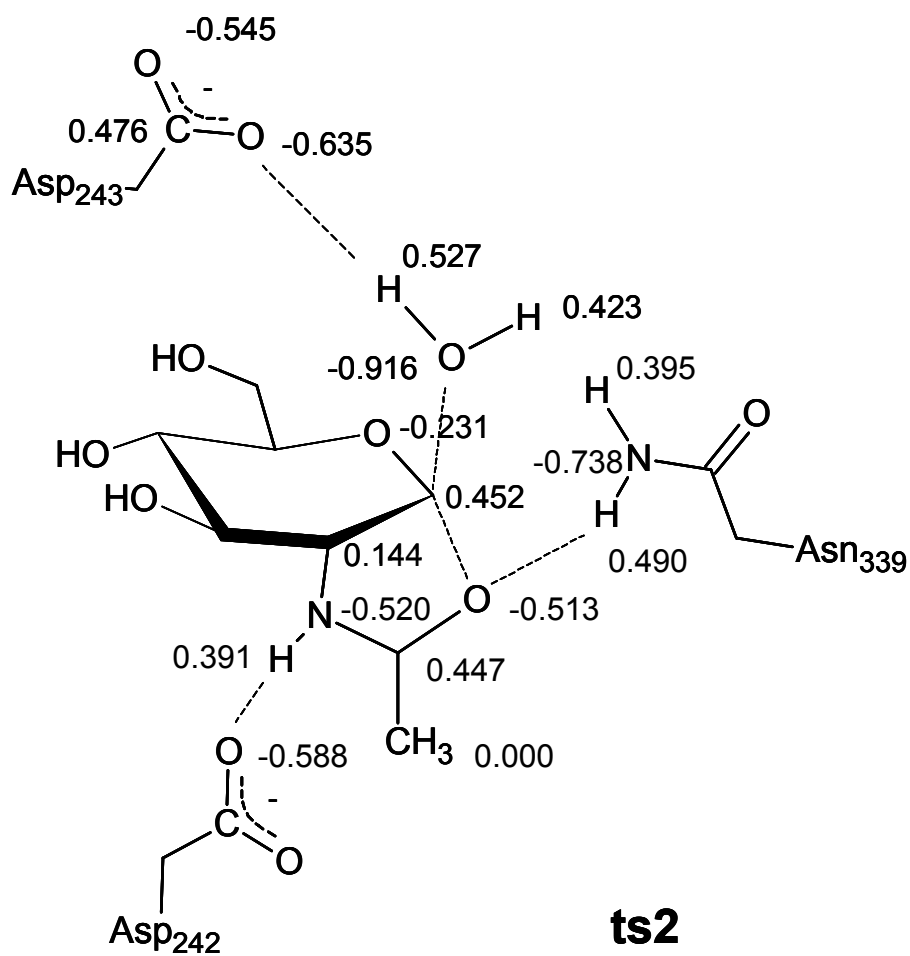


Figure S6. Net atomic charges (Mulliken) computed for **ts2**.

Table S1. Cartesian coordinates (Å), absolute total energy values (ET, hartee/particle) and Mulliken atomic charges for the various critical points located on the PES

m0, ET = -3892.764131

C	12.705893	-2.212052	3.766753	0.351157
O	11.602497	-1.666010	3.838112	-0.540096
N	12.991590	-3.455598	4.263721	-0.536609
H	13.914181	-3.868789	4.081811	0.440191
C	12.051410	-4.126827	5.187677	-0.282886
H	11.062679	-3.706714	4.989188	0.214522
C	12.079630	-5.669697	5.049117	-0.474482
H	13.105545	-6.008935	5.240152	0.219705
H	11.449167	-6.081026	5.848549	0.189024
C	11.618471	-6.212050	3.709518	-0.002890
C	10.264086	-6.479342	3.465831	-0.229796
H	9.531682	-6.267650	4.239702	0.173832
C	9.837092	-7.021783	2.253149	-0.263323
H	8.788104	-7.230267	2.067212	0.166090
C	10.776460	-7.312312	1.260904	0.409726
O	10.315002	-7.851478	0.082110	-0.606184
H	11.059733	-7.928097	-0.543327	0.495576
C	12.132558	-7.055601	1.484607	-0.301641
H	12.868663	-7.290677	0.718754	0.177824
C	12.544884	-6.502204	2.699462	-0.262469
H	13.596944	-6.287333	2.861051	0.283990
C	9.369252	-4.106927	-0.624293	-0.598127
H	8.904265	-5.051766	-0.321197	0.212766
H	9.142015	-3.941141	-1.687275	0.217356
C	10.879431	-4.223530	-0.418870	-0.320724
H	11.155389	-4.115028	0.637069	0.251183
H	11.229184	-5.205302	-0.755878	0.227627
N	11.632388	-3.223620	-1.239865	-0.827962
H	11.269836	-2.279258	-1.094777	0.372891
H	12.633366	-3.231739	-0.980823	0.481640
H	11.604982	-3.541352	-2.383680	0.439230
C	10.127385	-5.687502	-6.519331	-0.454880
H	10.601416	-6.159402	-7.390439	0.172490
C	11.214217	-4.832931	-5.798851	-0.476634
H	12.096727	-5.445914	-5.608107	0.235219
H	11.529102	-4.017231	-6.463991	0.227614
C	10.777631	-4.195634	-4.458422	0.656092
O	9.636175	-3.778522	-4.223430	-0.512024
O	11.806383	-4.100317	-3.594889	-0.582282
C	9.616630	-6.752682	-5.532985	0.674685
O	8.758226	-6.479231	-4.691189	-0.500857
C	15.624266	-5.138434	-11.056425	-0.542501
H	15.433193	-4.389702	-11.838641	0.177473
C	15.149844	-4.571845	-9.684046	-0.438913
H	15.801957	-3.743186	-9.381496	0.204889
H	14.138334	-4.163253	-9.795435	0.190778
C	15.129792	-5.637876	-8.598658	-0.011231
C	16.316078	-6.094284	-8.002344	-0.222926
H	17.265427	-5.667480	-8.310753	0.182907
C	16.299085	-7.056785	-6.994732	-0.248090
H	17.215132	-7.379828	-6.511966	0.182493
C	15.079557	-7.581580	-6.554798	0.436180
O	15.109957	-8.504765	-5.541732	-0.613928
H	14.218862	-8.605088	-5.150235	0.500480
C	13.888633	-7.160058	-7.152165	-0.296938
H	12.942239	-7.567535	-6.808005	0.161048
C	13.922295	-6.195850	-8.163908	-0.229226

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C	18.782406	1.874198	-6.417431	-0.548814
H	18.657367	2.777840	-5.813825	0.191607
C	17.464842	1.063731	-6.486661	-0.451308
H	16.698120	1.722153	-6.918062	0.189702
H	17.603187	0.243260	-7.207843	0.198984
C	16.942116	0.498689	-5.197715	0.009656
C	17.652767	0.032177	-4.117509	-0.168956
H	18.715867	0.033452	-3.939114	0.182842
N	16.794958	-0.520053	-3.176331	-0.337793
H	17.142046	-1.161868	-2.463666	0.447081
C	15.503408	-0.469687	-3.667599	0.086960
C	14.306647	-0.972859	-3.143910	-0.282758
H	14.302082	-1.522579	-2.209608	0.240426
C	13.146490	-0.790180	-3.890508	-0.198239
H	12.213764	-1.219943	-3.544115	0.179099
C	13.169423	-0.107856	-5.127027	-0.194170
H	12.243581	0.017829	-5.677753	0.165329
C	14.359793	0.382904	-5.652494	-0.226142
H	14.370799	0.889940	-6.611796	0.159193
C	15.551909	0.195289	-4.931795	-0.027863
C	21.207931	-1.153388	-1.795575	-0.615452
H	20.264547	-0.625040	-1.616426	0.238265
C	20.881912	-2.673509	-1.922329	-0.447758
H	21.591296	-3.177338	-2.590283	0.162639
H	20.971083	-3.142757	-0.933360	0.208590
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H	17.262231	-5.468420	7.424911	0.157240
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H	15.416287	-5.601838	5.893070	0.171518
H	16.220690	-4.063152	5.635902	0.175956
C	16.422968	-5.453509	4.027196	0.449924
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H	24.139646	-10.144425	-0.338389	0.197292
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N	10.150301	-7.975048	-5.648305	-0.702393
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H	10.609792	-9.904653	-5.095283	0.219035
C	10.361416	-8.727576	-3.305605	-0.481003
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C	14.812774	-3.475610	-5.536900	-0.747411
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N	14.447661	-4.769448	-3.509195	-0.541729
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C	14.804944	-5.419231	-2.252368	-0.141288
H	13.858294	-5.731959	-1.803620	0.233540
C	15.477640	-4.486894	-1.246051	0.071600
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H	16.093537	-4.643900	1.831721	0.534287
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ts1, ET = -3892.737821

C	12.704534	-2.224795	3.747439	0.350557
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N	12.990775	-3.462383	4.253522	-0.534196
H	13.908263	-3.884493	4.078644	0.436438
C	12.045902	-4.136002	5.171241	-0.283279
H	11.059163	-3.712284	4.970920	0.216891
C	12.072962	-5.676856	5.002188	-0.474103
H	13.097311	-6.021748	5.195407	0.211544
H	11.436567	-6.105291	5.787893	0.189258
C	11.622149	-6.192818	3.645340	-0.000677
C	10.266022	-6.431733	3.379703	-0.232835
H	9.526770	-6.215179	4.146272	0.167505
C	9.846099	-6.952570	2.156331	-0.259130
H	8.795170	-7.139089	1.956759	0.162251
C	10.785792	-7.257617	1.162039	0.407935
O	10.315518	-7.766869	-0.011661	-0.612892
H	11.039709	-7.872206	-0.686678	0.510625
C	12.146704	-7.030901	1.412833	-0.305263
H	12.885698	-7.284417	0.656609	0.194244
C	12.551313	-6.495861	2.640425	-0.265546
H	13.606110	-6.305176	2.816101	0.253531
C	9.365273	-4.120063	-0.641448	-0.599475
H	8.917522	-5.067778	-0.323059	0.224488
H	9.113924	-3.968022	-1.701071	0.216599
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H	11.177523	-4.151380	0.577004	0.249641
H	11.227960	-5.187524	-0.862225	0.248650
N	11.586918	-3.176439	-1.273121	-0.827289
H	11.188616	-2.250370	-1.105022	0.374112
H	12.583875	-3.159918	-1.007806	0.482616
H	11.578010	-3.455015	-2.407441	0.435024
C	10.121784	-5.711533	-6.533757	-0.454842
H	10.598873	-6.184274	-7.402663	0.169882
C	11.210797	-4.855458	-5.813028	-0.478666
H	12.073246	-5.484408	-5.587993	0.240604
H	11.559981	-4.064984	-6.492672	0.217700
C	10.777101	-4.170986	-4.497604	0.660438
O	9.629956	-3.785878	-4.246837	-0.504295
O	11.824798	-3.979903	-3.659565	-0.589152
C	9.608662	-6.774116	-5.545852	0.676326
O	8.750600	-6.497636	-4.704713	-0.504838
C	15.620884	-5.180522	-11.070316	-0.543510
H	15.430505	-4.432280	-11.852985	0.177390
C	15.139731	-4.608393	-9.701028	-0.436786
H	15.783767	-3.767317	-9.413577	0.198872
H	14.126394	-4.207088	-9.823835	0.191593
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C	16.290797	-6.041103	-7.920849	-0.239583
H	17.247018	-5.646703	-8.252420	0.176387
C	16.255063	-6.903161	-6.824762	-0.245008
H	17.165786	-7.177886	-6.302706	0.174536
C	15.027858	-7.378690	-6.341213	0.428816
O	15.039906	-8.146064	-5.212176	-0.632753
H	14.122463	-8.304242	-4.855122	0.520746
C	13.851568	-7.037262	-7.017884	-0.300908
H	12.902950	-7.419455	-6.654773	0.184403
C	13.903901	-6.171958	-8.116229	-0.233425

H	12.976936	-5.882241	-8.603084	0.177726
C	18.791715	1.833195	-6.441677	-0.550169
H	18.665393	2.738216	-5.840526	0.193157
C	17.478413	1.020687	-6.509813	-0.451334
H	16.715502	1.666507	-6.966363	0.193127
H	17.625764	0.182401	-7.208307	0.199896
C	16.939450	0.488232	-5.214869	0.009536
C	17.620234	0.108346	-4.084123	-0.155044
H	18.673592	0.160851	-3.861607	0.184769
N	16.739202	-0.421139	-3.145731	-0.351043
H	17.070557	-1.041983	-2.411892	0.424756
C	15.469230	-0.455812	-3.699903	0.093255
C	14.271031	-0.990631	-3.213768	-0.284863
H	14.234233	-1.485887	-2.250199	0.235382
C	13.145213	-0.905438	-4.028749	-0.202871
H	12.229757	-1.395366	-3.723826	0.193199
C	13.199355	-0.276421	-5.291313	-0.196711
H	12.298865	-0.223258	-5.893257	0.171230
C	14.391249	0.248712	-5.778411	-0.223976
H	14.429836	0.713777	-6.757883	0.162882
C	15.551026	0.144875	-4.992182	-0.030975
C	21.210071	-1.191801	-1.814380	-0.613759
H	20.268934	-0.657757	-1.636815	0.235039
C	20.875795	-2.708747	-1.946100	-0.448238
H	21.617577	-3.225120	-2.567419	0.166455
H	20.905541	-3.166692	-0.948168	0.213178
C	19.454327	-2.933792	-2.459044	0.424209
O	18.496940	-2.339315	-1.947230	-0.453793
N	19.291758	-3.818173	-3.476492	-0.732673
H	18.346244	-4.062267	-3.787665	0.486273
H	20.074271	-4.349725	-3.830731	0.344331
C	17.526448	-5.661788	6.355401	-0.573725
H	17.234137	-5.481610	7.405018	0.160979
C	16.360723	-5.166752	5.479238	-0.427336
H	15.432746	-5.685528	5.765705	0.177774
H	16.174281	-4.098825	5.656478	0.177741
C	16.531148	-5.357710	3.973766	0.453434
O	17.509699	-6.019570	3.544232	-0.520201
O	15.614273	-4.812940	3.255397	-0.616730
C	23.519229	-12.045904	-1.253177	-0.546740
H	22.876600	-12.372535	-2.076193	0.183106
C	23.289233	-10.541828	-0.915031	-0.448369
H	24.167392	-10.204845	-0.342245	0.198160
H	23.275884	-9.951554	-1.839902	0.180356
C	22.063582	-10.223030	-0.104599	0.227219
N	21.553778	-11.076987	0.880353	-0.566122
C	20.576288	-10.388600	1.477706	0.115017
H	19.958820	-10.737395	2.287991	0.193766
N	20.423337	-9.142809	0.922180	-0.391362
H	19.778100	-8.394736	1.204575	0.476122
C	21.363518	-9.033206	-0.086621	-0.204493
H	21.464823	-8.137717	-0.674964	0.169958
N	10.139958	-7.997721	-5.659094	-0.696134
H	10.832469	-8.128714	-6.382176	0.321799
C	9.928600	-9.139234	-4.743212	-0.221147
H	10.607641	-9.920352	-5.094834	0.211598
C	10.323020	-8.753747	-3.305467	-0.450170
H	9.733083	-7.878607	-3.010525	0.237841
H	10.073891	-9.564789	-2.607103	0.183650
C	11.812796	-8.438705	-3.157845	0.489898
O	12.594587	-8.629588	-4.126143	-0.543977
O	12.172984	-8.011898	-1.996914	-0.642244
H	13.735764	-8.037351	-1.739221	0.540288

O	16.556291	-4.666112	-4.123331	-0.514749
C	15.375090	-4.289330	-4.353979	0.449775
C	15.007162	-3.485049	-5.567499	-0.746635
H	13.974560	-3.141138	-5.521210	0.232423
H	15.162883	-4.100717	-6.457284	0.261037
H	15.666213	-2.615560	-5.623901	0.251273
N	14.405907	-4.629910	-3.490505	-0.516641
H	13.378256	-4.420837	-3.648520	0.389420
C	14.829965	-5.273916	-2.255604	-0.182770
H	13.961081	-5.781835	-1.830373	0.319005
C	15.430490	-4.317200	-1.223633	0.061423
O	14.437115	-3.427134	-0.701324	-0.715437
H	14.821486	-3.152091	0.159708	0.448370
H	16.232020	-3.728983	-1.684112	0.276050
C	16.012519	-5.123118	-0.059301	-0.116401
O	16.441451	-4.191123	0.903166	-0.678752
H	16.153017	-4.494487	1.833253	0.532757
H	15.225603	-5.773514	0.348496	0.239520
C	17.182907	-5.988118	-0.544034	0.009232
C	17.530283	-7.210054	0.334201	-0.274120
O	18.552118	-6.940417	1.273491	-0.695638
H	18.153173	-6.531175	2.099282	0.527898
H	16.621738	-7.586071	0.819779	0.217764
H	17.899707	-7.995093	-0.333527	0.218258
H	18.070292	-5.366961	-0.679246	0.281890
O	16.923078	-6.562455	-1.901787	-0.238842
C	15.866636	-6.328429	-2.585295	0.070380
H	15.764853	-6.924440	-3.489128	0.399952
O	14.723620	-8.065829	-1.530691	-0.694817
C	15.201635	-9.385581	-1.795546	-0.448566
H	14.930800	-10.065392	-0.976494	0.204267
H	16.293125	-9.346327	-1.865844	0.200542
H	14.798001	-9.773481	-2.737132	0.226895
H	19.005028	2.102578	-7.475048	0.180939
H	19.647447	1.273103	-6.067622	0.183380
H	21.646999	-0.801045	-2.732158	0.185133
H	21.814769	-1.026814	-0.923848	0.197170
H	24.565386	-12.098322	-1.551146	0.167528
H	23.298313	-12.647454	-0.372708	0.217643
H	18.420602	-5.056764	6.212697	0.194285
H	17.636693	-6.742427	6.278127	0.200461
H	15.002163	-6.048564	-11.293172	0.196043
H	16.699244	-5.330135	-11.043349	0.188283
H	9.324078	-5.072948	-6.910330	0.227041
H	8.921987	-9.554503	-4.757277	0.202236
H	13.583736	-1.698131	3.379250	0.141168
H	12.350341	-3.897732	6.189317	0.180120
H	8.923232	-3.331892	-0.033736	0.166152

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C	12.709892	-2.241313	3.763317	0.347930
O	11.606988	-1.694171	3.834061	-0.540038
N	12.998018	-3.479472	4.265271	-0.532073
H	13.921113	-3.887903	4.082688	0.438724
C	12.050855	-4.158640	5.178624	-0.284840
H	11.066319	-3.729572	4.978341	0.215637
C	12.070437	-5.698050	4.998040	-0.472826
H	13.090443	-6.051847	5.196657	0.211964
H	11.423211	-6.128666	5.773933	0.188266
C	11.629543	-6.194803	3.630712	-0.002230
C	10.271349	-6.368828	3.328784	-0.234643
H	9.522275	-6.122283	4.076707	0.165484
C	9.861363	-6.862449	2.090518	-0.259616
H	8.808475	-7.000270	1.862694	0.159482
C	10.812324	-7.200868	1.117441	0.403268
O	10.348389	-7.672104	-0.075471	-0.616475
H	11.080178	-7.778134	-0.744084	0.504881
C	12.175684	-7.045869	1.406557	-0.314075
H	12.926458	-7.337492	0.675757	0.217968
C	12.569609	-6.539907	2.649856	-0.261420
H	13.627374	-6.408264	2.857188	0.250865
C	9.378429	-4.122116	-0.637746	-0.600918
H	8.952981	-5.076390	-0.310556	0.232152
H	9.114809	-3.978790	-1.695286	0.214359
C	10.887151	-4.188009	-0.476305	-0.327999
H	11.195718	-4.119969	0.572931	0.254679
H	11.279241	-5.123189	-0.888494	0.257866
N	11.544655	-3.086560	-1.255116	-0.808706
H	11.097041	-2.185563	-1.075362	0.377453
H	12.541574	-3.034702	-0.989794	0.483877
H	11.536819	-3.343134	-2.348228	0.422010
C	10.144613	-5.689771	-6.535184	-0.455926
H	10.624882	-6.157944	-7.404551	0.172664
C	11.231806	-4.835589	-5.807238	-0.483836
H	12.084400	-5.472293	-5.563530	0.239611
H	11.600363	-4.053728	-6.487079	0.215237
C	10.785210	-4.135999	-4.506922	0.668580
O	9.630333	-3.784850	-4.252980	-0.496961
O	11.827672	-3.880554	-3.670624	-0.598196
C	9.630985	-6.756668	-5.552185	0.675328
O	8.771503	-6.484213	-4.711182	-0.504843
C	15.649651	-5.136348	-11.061830	-0.543686
H	15.458438	-4.381984	-11.837863	0.178393
C	15.169980	-4.576463	-9.685185	-0.436685
H	15.818945	-3.741640	-9.388986	0.196336
H	14.159248	-4.167681	-9.804924	0.190841
C	15.134606	-5.618898	-8.570705	-0.014619
C	16.310353	-6.107732	-7.973901	-0.248439
H	17.274953	-5.766893	-8.339493	0.176504
C	16.267601	-6.998036	-6.900068	-0.246117
H	17.180612	-7.350243	-6.430491	0.176856
C	15.034629	-7.423344	-6.378109	0.411918
O	15.047429	-8.232682	-5.287178	-0.610414
H	14.136081	-8.356320	-4.892609	0.518567
C	13.854778	-6.987319	-6.995763	-0.301612
H	12.901182	-7.330819	-6.608701	0.191084
C	13.914304	-6.094288	-8.071399	-0.238207

H	12.987008	-5.741945	-8.514567	0.179298
C	18.807986	1.861833	-6.401184	-0.550668
H	18.673436	2.762152	-5.795437	0.194601
C	17.501039	1.042434	-6.488603	-0.452217
H	16.736410	1.689306	-6.941087	0.194996
H	17.658181	0.214756	-7.197670	0.199132
C	16.959790	0.489937	-5.205022	0.006518
C	17.626594	0.155084	-4.053696	-0.144400
H	18.671584	0.249014	-3.807646	0.189205
N	16.742558	-0.388415	-3.123119	-0.355643
H	17.087837	-1.022021	-2.408415	0.415896
C	15.488580	-0.483094	-3.709842	0.098390
C	14.293819	-1.038410	-3.239625	-0.287933
H	14.243198	-1.505563	-2.261874	0.227056
C	13.184562	-1.000195	-4.082764	-0.209119
H	12.273172	-1.500563	-3.787059	0.201070
C	13.252991	-0.402428	-5.359300	-0.204596
H	12.364973	-0.385621	-5.981494	0.174652
C	14.440801	0.148621	-5.828494	-0.225037
H	14.490287	0.597287	-6.814966	0.166298
C	15.580741	0.096481	-5.010769	-0.027734
C	21.222349	-1.179316	-1.782408	-0.608153
H	20.266915	-0.671172	-1.612323	0.235916
C	20.942088	-2.707426	-1.908874	-0.459975
H	21.710848	-3.199849	-2.516808	0.174157
H	20.982361	-3.161576	-0.907976	0.218689
C	19.545382	-3.020636	-2.439832	0.429882
O	18.561792	-2.343019	-2.130488	-0.437141
N	19.438047	-4.106190	-3.260814	-0.722062
H	18.506290	-4.451862	-3.479096	0.452399
H	20.205435	-4.759233	-3.344607	0.351893
C	17.531037	-5.684470	6.364516	-0.574489
H	17.230548	-5.505918	7.411765	0.159708
C	16.371013	-5.190451	5.477162	-0.425134
H	15.441113	-5.706547	5.762519	0.176213
H	16.185962	-4.122080	5.653554	0.175561
C	16.533711	-5.377827	3.966493	0.446656
O	17.503822	-6.035226	3.515590	-0.514127
O	15.605684	-4.825294	3.265646	-0.617540
C	23.539906	-12.033573	-1.260623	-0.545841
H	22.897977	-12.357696	-2.085168	0.183504
C	23.311336	-10.529328	-0.921437	-0.447715
H	24.176057	-10.201151	-0.323491	0.197256
H	23.330811	-9.938132	-1.845979	0.178258
C	22.064698	-10.199356	-0.147864	0.226909
N	21.500398	-11.065839	0.796057	-0.566523
C	20.508348	-10.374591	1.365633	0.118544
H	19.848037	-10.731507	2.137821	0.195142
N	20.408210	-9.109705	0.842597	-0.387970
H	19.753105	-8.364017	1.108752	0.474418
C	21.390461	-8.994476	-0.124324	-0.204912
H	21.532569	-8.086719	-0.684692	0.166551
N	10.163439	-7.979382	-5.669490	-0.693880
H	10.857121	-8.106937	-6.392102	0.321664
C	9.951803	-9.124595	-4.758390	-0.220737
H	10.631265	-9.903002	-5.115339	0.213298
C	10.359725	-8.741191	-3.322606	-0.445789
H	9.753570	-7.885020	-3.007457	0.234437
H	10.144637	-9.566396	-2.629463	0.182474
C	11.847955	-8.384355	-3.194644	0.475876
O	12.619585	-8.592669	-4.171009	-0.551270
O	12.207089	-7.905616	-2.059239	-0.624805
H	13.791142	-8.206361	-1.497569	0.514797

O	16.401426	-5.041568	-3.946389	-0.403392
C	15.302717	-4.398519	-4.301393	0.486659
C	15.295958	-3.566519	-5.530637	-0.741633
H	15.373097	-4.216547	-6.407296	0.281287
H	16.166212	-2.904970	-5.511979	0.251948
H	14.391996	-2.960046	-5.576087	0.259205
N	14.294653	-4.558154	-3.489730	-0.486215
H	13.245914	-4.245941	-3.669248	0.427022
C	14.741243	-5.286328	-2.286024	-0.223041
H	13.955567	-5.950201	-1.925109	0.356337
C	15.270882	-4.338531	-1.213595	0.075377
O	14.247499	-3.542327	-0.610403	-0.723703
H	14.640518	-3.321795	0.265462	0.451199
H	16.014622	-3.665020	-1.662309	0.232521
C	15.962310	-5.149660	-0.115066	-0.123645
O	16.324174	-4.215371	0.878977	-0.690727
H	16.077987	-4.552134	1.812028	0.536361
H	15.252141	-5.890963	0.274327	0.257225
C	17.196014	-5.867274	-0.682948	0.032915
C	17.647623	-7.100355	0.128956	-0.306969
O	18.602988	-6.814802	1.142168	-0.695855
H	18.147775	-6.472366	1.962292	0.523226
H	16.766905	-7.610378	0.535601	0.225815
H	18.127059	-7.783254	-0.579165	0.218611
H	18.017369	-5.146556	-0.740413	0.259482
O	16.982963	-6.393269	-2.044991	-0.382375
C	15.938526	-6.071618	-2.834039	0.100501
H	15.661379	-6.935754	-3.439010	0.347531
O	14.678571	-8.303199	-1.064401	-0.691472
C	15.082202	-9.661310	-1.193752	-0.433021
H	14.399108	-10.343278	-0.664838	0.183708
H	16.076827	-9.760673	-0.748802	0.199976
H	15.140860	-9.972425	-2.246347	0.194961
H	19.022554	2.135431	-7.433201	0.183147
H	19.663687	1.300976	-6.028144	0.184818
H	21.660294	-0.784578	-2.698019	0.186603
H	21.825704	-1.017311	-0.890380	0.198817
H	24.586562	-12.083963	-1.557266	0.166604
H	23.318300	-12.638787	-0.382793	0.217004
H	18.424858	-5.078131	6.225476	0.192326
H	17.642283	-6.764702	6.283173	0.200236
H	15.031963	-6.003978	-11.288983	0.198498
H	16.728088	-5.285108	-11.033937	0.188681
H	9.346876	-5.050385	-6.910372	0.227859
H	8.945542	-9.540735	-4.775523	0.200743
H	13.589160	-1.712456	3.398390	0.140603
H	12.353669	-3.924126	6.198050	0.179461
H	8.934860	-3.336706	-0.027563	0.165486

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C	12.709892	-2.241313	3.763317	0.347920
O	11.606988	-1.694171	3.834061	-0.539691
N	12.998003	-3.479692	4.264929	-0.532998
H	13.920943	-3.888652	4.081999	0.438861
C	12.050855	-4.158640	5.178624	-0.284620
H	11.066109	-3.730002	4.978368	0.215573
C	12.070695	-5.698338	4.999992	-0.472750
H	13.091489	-6.050991	5.196623	0.212089
H	11.425820	-6.128194	5.778270	0.187953
C	11.626705	-6.198052	3.634779	-0.002406
C	10.268333	-6.380726	3.338621	-0.234644
H	9.520797	-6.137695	4.089248	0.164929
C	9.856364	-6.879328	2.102891	-0.259449
H	8.803406	-7.024006	1.879613	0.159008
C	10.805594	-7.213740	1.126703	0.402340
O	10.340587	-7.690532	-0.063913	-0.617023
H	11.071252	-7.786741	-0.735291	0.505385
C	12.169095	-7.049790	1.410060	-0.315022
H	12.918932	-7.339166	0.677704	0.223365
C	12.564856	-6.539344	2.650829	-0.262056
H	13.622721	-6.401821	2.853850	0.251559
C	9.378429	-4.122116	-0.637746	-0.600821
H	8.955172	-5.076890	-0.309241	0.232437
H	9.113030	-3.979824	-1.694983	0.214274
C	10.887624	-4.185303	-0.478603	-0.328359
H	11.197339	-4.117885	0.570331	0.254785
H	11.281025	-5.119235	-0.892334	0.258032
N	11.542619	-3.081577	-1.256610	-0.808664
H	11.093437	-2.181708	-1.075107	0.377423
H	12.539536	-3.028319	-0.990865	0.483851
H	11.534479	-3.336287	-2.350324	0.421849
C	10.144613	-5.689771	-6.535184	-0.455818
H	10.625359	-6.157726	-7.404406	0.172370
C	11.230968	-4.834208	-5.807160	-0.483509
H	12.083759	-5.470002	-5.561867	0.239530
H	11.599626	-4.053081	-6.487807	0.215076
C	10.783333	-4.132763	-4.507995	0.668954
O	9.627206	-3.786131	-4.253364	-0.497412
O	11.825934	-3.870358	-3.674073	-0.598158
C	9.630985	-6.756668	-5.552185	0.675919
O	8.771503	-6.484213	-4.711182	-0.504818
C	15.649650	-5.136348	-11.061831	-0.543728
H	15.458859	-4.382765	-11.838764	0.178485
C	15.169372	-4.574327	-9.686125	-0.436593
H	15.817660	-3.738447	-9.391424	0.196450
H	14.158443	-4.166351	-9.806962	0.190942
C	15.134205	-5.614132	-8.569051	-0.014687
C	16.309917	-6.100563	-7.970243	-0.248196
H	17.274501	-5.760179	-8.336318	0.176568
C	16.267143	-6.988234	-6.894185	-0.245712
H	17.180073	-7.338952	-6.423360	0.176569
C	15.034147	-7.413433	-6.372090	0.412267
O	15.046890	-8.220933	-5.279751	-0.611120
H	14.135266	-8.345086	-4.885840	0.516378
C	13.854394	-6.979695	-6.991528	-0.301549
H	12.900858	-7.323231	-6.604371	0.191245
C	13.913933	-6.089000	-8.069106	-0.238084

H	12.986672	-5.738407	-8.513722	0.179441
C	18.807985	1.861833	-6.401184	-0.550513
H	18.673737	2.762309	-5.795531	0.194603
C	17.500565	1.043438	-6.488681	-0.452274
H	16.736576	1.690883	-6.941431	0.194956
H	17.657052	0.215395	-7.197470	0.199016
C	16.958926	0.492202	-5.204875	0.006354
C	17.626005	0.155315	-4.054312	-0.144116
H	18.671480	0.246421	-3.809289	0.189214
N	16.741560	-0.386203	-3.123102	-0.355883
H	17.086515	-1.020624	-2.408949	0.416080
C	15.486743	-0.477492	-3.708688	0.098232
C	14.291059	-1.030182	-3.237833	-0.287668
H	14.240070	-1.497493	-2.260236	0.227410
C	13.181399	-0.989571	-4.080347	-0.208837
H	12.269213	-1.488249	-3.784256	0.200933
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C	15.579128	0.102293	-5.009511	-0.027741
C	21.222349	-1.179317	-1.782409	-0.608126
H	20.267157	-0.670668	-1.612310	0.235888
C	20.940962	-2.707074	-1.908755	-0.459785
H	21.710205	-3.200268	-2.515474	0.173960
H	20.979394	-3.160981	-0.907673	0.218684
C	19.544752	-3.019050	-2.441683	0.430024
O	18.560708	-2.342207	-2.132121	-0.437124
N	19.438350	-4.102627	-3.265319	-0.722335
H	18.506639	-4.447638	-3.484721	0.452717
H	20.205508	-4.755968	-3.348801	0.351687
C	17.531037	-5.684471	6.364516	-0.574458
H	17.230051	-5.505545	7.411559	0.159577
C	16.370935	-5.191482	5.476117	-0.424996
H	15.440988	-5.706648	5.763007	0.176192
H	16.186383	-4.122786	5.651056	0.175383
C	16.531562	-5.381103	3.965076	0.447086
O	17.499043	-6.041705	3.513135	-0.514114
O	15.603966	-4.826801	3.264899	-0.617808
C	23.539905	-12.033574	-1.260625	-0.545718
H	22.898458	-12.358293	-2.085325	0.183252
C	23.308377	-10.529944	-0.920845	-0.447789
H	24.170024	-10.201337	-0.318748	0.197319
H	23.330703	-9.937498	-1.844508	0.178140
C	22.057657	-10.203741	-0.152132	0.226656
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C	20.493578	-10.386539	1.352468	0.118481
H	19.830054	-10.747048	2.120237	0.195065
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H	19.738259	-8.375277	1.100776	0.475011
C	21.382241	-8.999508	-0.127022	-0.204894
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N	10.163439	-7.979382	-5.669490	-0.694134
H	10.857121	-8.106937	-6.392102	0.321460
C	9.951803	-9.124595	-4.758391	-0.220328
H	10.631798	-9.902686	-5.114996	0.212554
C	10.357075	-8.741965	-3.321400	-0.444246
H	9.749263	-7.886557	-3.007487	0.234956
H	10.140929	-9.567606	-2.629141	0.183029
C	11.844017	-8.380916	-3.189496	0.460547
O	12.618254	-8.583940	-4.165021	-0.548518
O	12.197226	-7.901433	-2.052726	-0.617940
H	13.789696	-8.145910	-1.490642	0.502261

O	16.401208	-5.027177	-3.952048	-0.404207
C	15.303670	-4.381984	-4.306567	0.487573
C	15.296886	-3.551627	-5.536977	-0.741789
H	15.369954	-4.202888	-6.413120	0.280950
H	16.168993	-2.892486	-5.521074	0.251762
H	14.394478	-2.942692	-5.581140	0.259396
N	14.295900	-4.539385	-3.494229	-0.485376
H	13.246497	-4.230172	-3.673792	0.426769
C	14.740596	-5.270839	-2.291858	-0.213589
H	13.952724	-5.932525	-1.933494	0.351581
C	15.270715	-4.328358	-1.215295	0.073474
O	14.246637	-3.533741	-0.610803	-0.723787
H	14.638014	-3.317030	0.266751	0.451133
H	16.016025	-3.653940	-1.660057	0.232793
C	15.958587	-5.145347	-0.118491	-0.126260
O	16.323866	-4.214531	0.877994	-0.690853
H	16.077039	-4.552588	1.810288	0.536246
H	15.245743	-5.884723	0.268740	0.262505
C	17.189893	-5.867046	-0.687296	0.039046
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O	18.589304	-6.827282	1.135884	-0.695961
H	18.137278	-6.482585	1.956912	0.522043
H	16.749476	-7.614193	0.522381	0.231239
H	18.111770	-7.788310	-0.589250	0.214900
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O	16.978968	-6.384883	-2.052723	-0.382474
C	15.935733	-6.058283	-2.840823	0.095242
H	15.655750	-6.920191	-3.447378	0.345517
O	14.674244	-8.212950	-1.041592	-0.938309
H	15.012165	-9.091849	-1.266461	0.407679
H	19.022553	2.135431	-7.433201	0.183036
H	19.663686	1.300975	-6.028145	0.184763
H	21.660294	-0.784579	-2.698020	0.186502
H	21.825704	-1.017312	-0.890381	0.198770
H	24.586561	-12.083963	-1.557268	0.166522
H	23.318299	-12.638788	-0.382795	0.217009
H	18.424858	-5.078132	6.225476	0.192038
H	17.642283	-6.764703	6.283173	0.200234
H	15.031962	-6.003978	-11.288984	0.198429
H	16.728087	-5.285108	-11.033938	0.188671
H	9.346876	-5.050385	-6.910372	0.227827
H	8.945542	-9.540736	-4.775524	0.200822
H	13.589160	-1.712456	3.398390	0.140465
H	12.353669	-3.924126	6.198050	0.179251
H	8.934860	-3.336706	-0.027563	0.165504

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N	12.996532	-3.481098	4.263407	-0.532277
H	13.921062	-3.886157	4.085800	0.434855
C	12.050855	-4.158640	5.178624	-0.284454
H	11.065530	-3.731951	4.978085	0.217097
C	12.075524	-5.698747	5.003291	-0.473273
H	13.097858	-6.046519	5.201412	0.211245
H	11.433075	-6.129532	5.782889	0.189557
C	11.633740	-6.206760	3.640543	-0.001161
C	10.276687	-6.410323	3.351036	-0.233711
H	9.529637	-6.172877	4.103747	0.167800
C	9.865356	-6.923684	2.121535	-0.261440
H	8.813781	-7.085525	1.904361	0.161922
C	10.814529	-7.252723	1.143847	0.412029
O	10.355502	-7.752275	-0.038043	-0.612139
H	11.093611	-7.871166	-0.696431	0.511543
C	12.176003	-7.060801	1.418616	-0.303881
H	12.920893	-7.337434	0.676320	0.192764
C	12.572407	-6.537185	2.653529	-0.261975
H	13.628650	-6.379232	2.850220	0.250824
C	9.378429	-4.122116	-0.637746	-0.599947
H	8.935554	-5.073280	-0.324052	0.224887
H	9.135848	-3.968426	-1.698872	0.216508
C	10.888221	-4.207064	-0.449274	-0.325177
H	11.176650	-4.093372	0.602535	0.248960
H	11.261381	-5.175106	-0.799801	0.247039
N	11.590182	-3.171688	-1.275498	-0.825542
H	11.179326	-2.246126	-1.137670	0.374699
H	12.586893	-3.133260	-1.014284	0.480553
H	11.578028	-3.481339	-2.399648	0.436715
C	10.144613	-5.689771	-6.535184	-0.454298
H	10.620602	-6.160039	-7.406117	0.169879
C	11.234409	-4.836111	-5.815000	-0.479530
H	12.098357	-5.464706	-5.593471	0.241004
H	11.581553	-4.042731	-6.492296	0.217790
C	10.800765	-4.159789	-4.496948	0.659354
O	9.647978	-3.802771	-4.231247	-0.503443
O	11.852468	-3.942428	-3.669377	-0.588140
C	9.630985	-6.756668	-5.552185	0.676486
O	8.771503	-6.484213	-4.711182	-0.505166
C	15.649649	-5.136348	-11.061832	-0.543421
H	15.459319	-4.384816	-11.841286	0.177631
C	15.167952	-4.570444	-9.689745	-0.437440
H	15.812233	-3.730594	-9.399296	0.198772
H	14.154669	-4.168309	-9.810217	0.191936
C	15.143940	-5.602543	-8.566134	-0.010874
C	16.318098	-5.994869	-7.902048	-0.240870
H	17.273068	-5.590347	-8.224965	0.177057
C	16.281986	-6.858077	-6.806524	-0.243882
H	17.191711	-7.123818	-6.277987	0.174135
C	15.055960	-7.346306	-6.333206	0.426400
O	15.065609	-8.112683	-5.202044	-0.636265
H	14.145493	-8.270365	-4.848055	0.518591
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C	18.807984	1.861833	-6.401186	-0.550064
H	18.683154	2.765872	-5.797900	0.193203
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C	16.952215	0.519642	-5.175951	0.008620
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H	18.681324	0.183663	-3.818203	0.185332
N	16.743568	-0.397801	-3.110630	-0.353176
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C	15.476251	-0.432045	-3.671504	0.095374
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H	14.234001	-1.484039	-2.240102	0.233918
C	13.158254	-0.898089	-4.021478	-0.203077
H	12.253074	-1.416305	-3.733513	0.194056
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C	14.407468	0.278699	-5.753067	-0.224421
H	14.450041	0.750227	-6.729290	0.163036
C	15.562793	0.174636	-4.960529	-0.034271
C	21.222348	-1.179317	-1.782411	-0.612976
H	20.277107	-0.652856	-1.605942	0.236637
C	20.901312	-2.697550	-1.921203	-0.449336
H	21.642436	-3.203285	-2.552166	0.166627
H	20.944239	-3.164484	-0.927598	0.212074
C	19.479518	-2.935269	-2.426714	0.422565
O	18.523676	-2.311923	-1.948666	-0.450617
N	19.315713	-3.872994	-3.394596	-0.737568
H	18.371081	-4.112078	-3.710373	0.490139
H	20.100984	-4.401987	-3.746164	0.344530
C	17.531037	-5.684472	6.364516	-0.574620
H	17.235706	-5.506601	7.413559	0.161115
C	16.366084	-5.191712	5.484665	-0.427144
H	15.435577	-5.698505	5.785090	0.177371
H	16.189635	-4.119938	5.646243	0.177594
C	16.521495	-5.408983	3.979869	0.453263
O	17.468886	-6.116304	3.552527	-0.519849
O	15.623109	-4.835915	3.260053	-0.616109
C	23.539905	-12.033574	-1.260627	-0.546218
H	22.902318	-12.367276	-2.085177	0.183085
C	23.280909	-10.536498	-0.920805	-0.450636
H	24.138690	-10.183332	-0.327584	0.197715
H	23.273141	-9.942080	-1.843291	0.180184
C	22.026824	-10.260982	-0.136551	0.227552
N	21.472018	-11.188370	0.754154	-0.565673
C	20.457628	-10.551675	1.346021	0.119666
H	19.798195	-10.963360	2.091300	0.193941
N	20.333391	-9.264291	0.887348	-0.389572
H	19.658946	-8.549811	1.185645	0.474438
C	21.323560	-9.075287	-0.060402	-0.207513
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N	10.163439	-7.979382	-5.669490	-0.695339
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H	10.631851	-9.903929	-5.112072	0.212104
C	10.346841	-8.739980	-3.320448	-0.449664
H	9.769303	-7.853359	-3.034213	0.238184
H	10.081135	-9.539996	-2.616131	0.185311
C	11.840714	-8.446707	-3.170888	0.475796
O	12.616355	-8.616710	-4.149245	-0.544897
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C	15.408845	-4.246364	-4.364687	0.446730
C	15.055833	-3.423578	-5.570027	-0.742888
H	15.313294	-3.992312	-6.467367	0.256865
H	15.648667	-2.505647	-5.553096	0.256991
H	13.999192	-3.157975	-5.580693	0.229033
N	14.428079	-4.611374	-3.523523	-0.519854
H	13.408751	-4.355339	-3.676492	0.390871
C	14.839575	-5.269784	-2.289766	-0.183302
H	13.968975	-5.790177	-1.881960	0.327097
C	15.431393	-4.329801	-1.236983	0.064235
O	14.437698	-3.443581	-0.712101	-0.714195
H	14.822775	-3.168159	0.148495	0.448898
H	16.240353	-3.740255	-1.682783	0.275049
C	15.998009	-5.151329	-0.075025	-0.114737
O	16.427054	-4.228242	0.895980	-0.679694
H	16.152634	-4.536030	1.829852	0.533052
H	15.200420	-5.795770	0.321674	0.237199
C	17.165148	-6.024584	-0.555025	0.011229
C	17.465269	-7.279848	0.293922	-0.280963
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H	18.062151	-6.650993	2.088297	0.527114
H	16.538656	-7.650927	0.747083	0.222395
H	17.832437	-8.053947	-0.387616	0.217922
H	18.067331	-5.416792	-0.643346	0.282390
O	16.938954	-6.546196	-1.940771	-0.230861
C	15.887703	-6.309810	-2.628685	0.054502
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H	21.825703	-1.017312	-0.890383	0.196479
H	24.586561	-12.083963	-1.557270	0.166095
H	23.318299	-12.638788	-0.382797	0.218771
H	18.424858	-5.078133	6.225476	0.192770
H	17.642283	-6.764704	6.283173	0.202328
H	15.031961	-6.003979	-11.288985	0.196132
H	16.728086	-5.285108	-11.033939	0.188490
H	9.346876	-5.050385	-6.910372	0.226980
H	8.945542	-9.540737	-4.775524	0.202026
H	13.589160	-1.712456	3.398390	0.141588
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C	12.705893	-2.212052	3.766753	0.350181
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H	13.915238	-3.867015	4.082853	0.439965
C	12.051410	-4.126827	5.187677	-0.283187
H	11.063599	-3.704237	4.989371	0.214663
C	12.075762	-5.668862	5.043937	-0.474473
H	13.100354	-6.012319	5.234352	0.219697
H	11.442616	-6.082171	5.840180	0.189038
C	11.614889	-6.200882	3.700085	-0.003085
C	10.260005	-6.458732	3.450447	-0.229487
H	9.526378	-6.250277	4.224037	0.173841
C	9.833390	-6.987566	2.231379	-0.262966
H	8.783805	-7.189249	2.041342	0.166184
C	10.773919	-7.273202	1.239120	0.410898
O	10.314039	-7.801631	0.054678	-0.606251
H	11.060438	-7.874384	-0.568786	0.495250
C	12.130688	-7.025033	1.468435	-0.302206
H	12.867343	-7.257181	0.702235	0.176832
C	12.542578	-6.486053	2.689638	-0.262528
H	13.595095	-6.277490	2.855679	0.284803
C	9.369252	-4.106928	-0.624293	-0.596830
H	8.937907	-5.058570	-0.295129	0.216041
H	9.110261	-3.959697	-1.682633	0.216329
C	10.886488	-4.177568	-0.455900	-0.324342
H	11.179831	-4.086472	0.597030	0.251605
H	11.261704	-5.137982	-0.826477	0.227314
N	11.585045	-3.130319	-1.266318	-0.827399
H	11.184586	-2.205882	-1.095676	0.370772
H	12.588677	-3.101762	-1.017788	0.481844
H	11.549269	-3.441028	-2.417141	0.438224
C	10.127385	-5.687504	-6.519330	-0.454417
H	10.606238	-6.157817	-7.388442	0.171450
C	11.204344	-4.825307	-5.795363	-0.476715
H	12.079248	-5.438301	-5.571173	0.231796
H	11.538806	-4.025651	-6.470264	0.229201
C	10.738016	-4.158786	-4.480011	0.659406
O	9.587781	-3.755175	-4.270509	-0.510767
O	11.754243	-4.025562	-3.606542	-0.585202
C	9.616630	-6.752683	-5.532984	0.675015
O	8.758226	-6.479232	-4.691188	-0.500938
C	15.624266	-5.138437	-11.056425	-0.542548
H	15.433751	-4.393616	-11.842605	0.177758
C	15.147090	-4.556948	-9.689972	-0.439284
H	15.782962	-3.706964	-9.413019	0.203787
H	14.126774	-4.171694	-9.805777	0.191115
C	15.153968	-5.588249	-8.569467	-0.009433
C	16.342509	-5.951417	-7.916018	-0.222590
H	17.276965	-5.485290	-8.212863	0.183055
C	16.345220	-6.868911	-6.866433	-0.247470
H	17.262290	-7.118142	-6.343392	0.182649
C	15.142996	-7.441689	-6.438501	0.432116
O	15.191163	-8.310393	-5.377642	-0.610809
H	14.288256	-8.478954	-5.038947	0.498710
C	13.951595	-7.116888	-7.093623	-0.297606
H	13.017593	-7.563137	-6.763159	0.162632
C	13.965889	-6.196046	-8.146343	-0.230338

H	13.030412	-5.930234	-8.630323	0.176484
C	18.782406	1.874196	-6.417432	-0.547005
H	18.656628	2.777964	-5.814324	0.192111
C	17.466381	1.058905	-6.478074	-0.453378
H	16.700956	1.704782	-6.929110	0.189828
H	17.611224	0.221539	-7.177859	0.198947
C	16.937211	0.531571	-5.174598	0.009791
C	17.645484	-0.004190	-4.124466	-0.166709
H	18.710313	-0.103394	-3.990320	0.185525
N	16.780302	-0.475595	-3.149155	-0.332902
H	17.102041	-1.123012	-2.430343	0.445734
C	15.479701	-0.297213	-3.580535	0.086925
C	14.262864	-0.665510	-2.994424	-0.272979
H	14.245360	-1.205137	-2.054827	0.234134
C	13.093886	-0.354337	-3.682221	-0.191041
H	12.134200	-0.645053	-3.269076	0.169406
C	13.128762	0.316327	-4.925138	-0.192794
H	12.195824	0.543337	-5.429221	0.165192
C	14.337685	0.673877	-5.511846	-0.226398
H	14.355593	1.176898	-6.473180	0.159919
C	15.537259	0.362365	-4.848294	-0.029931
C	21.207932	-1.153388	-1.795576	-0.616855
H	20.269784	-0.615777	-1.614954	0.239011
C	20.863988	-2.668569	-1.921778	-0.446935
H	21.568488	-3.183385	-2.586464	0.162195
H	20.940229	-3.137658	-0.931965	0.208118
C	19.416998	-2.864595	-2.369628	0.426894
O	18.502817	-2.245616	-1.804101	-0.464336
N	19.192192	-3.721511	-3.390516	-0.728268
H	18.231117	-3.915410	-3.694578	0.508391
H	19.947421	-4.266070	-3.781319	0.337880
C	17.535262	-5.643658	6.368002	-0.574422
H	17.256867	-5.466247	7.422523	0.158137
C	16.352433	-5.150605	5.513516	-0.422797
H	15.418541	-5.601557	5.885351	0.171545
H	16.225235	-4.065479	5.623334	0.176312
C	16.418921	-5.459286	4.017331	0.449586
O	17.313771	-6.226591	3.584987	-0.514267
O	15.499286	-4.896554	3.315266	-0.624476
C	23.538691	-12.003786	-1.252269	-0.546894
H	22.903016	-12.345125	-2.075617	0.181102
C	23.254213	-10.512183	-0.910980	-0.450245
H	24.091850	-10.151659	-0.293928	0.197257
H	23.257029	-9.909944	-1.828105	0.178751
C	21.976000	-10.269621	-0.155262	0.228561
N	21.479485	-11.178887	0.788128	-0.567892
C	20.415031	-10.580934	1.330936	0.107712
H	19.779344	-10.991279	2.097335	0.189637
N	20.203800	-9.336659	0.794294	-0.384527
H	19.476780	-8.656875	1.057103	0.497354
C	21.189372	-9.134853	-0.155336	-0.217628
H	21.252259	-8.223616	-0.724581	0.172529
N	10.150301	-7.975049	-5.648304	-0.701911
H	10.842887	-8.103520	-6.371782	0.326779
C	9.941438	-9.118418	-4.734204	-0.229902
H	10.607482	-9.905078	-5.099108	0.219949
C	10.370628	-8.731624	-3.308336	-0.477904
H	9.830783	-7.821504	-3.019317	0.260374
H	10.111231	-9.513159	-2.580701	0.210699
C	11.864499	-8.500026	-3.259660	0.465749
O	12.635285	-8.762542	-4.177252	-0.434024
O	12.286203	-8.002413	-2.087341	-0.598602
H	13.285831	-7.853978	-2.117860	0.568308

O	16.526589	-4.205301	-4.294922	-0.491160
C	15.300714	-4.017685	-4.400106	0.400995
C	14.715830	-3.217824	-5.545586	-0.745432
H	14.822000	-3.797145	-6.467936	0.231387
H	15.284853	-2.291794	-5.648524	0.254476
H	13.665103	-2.973168	-5.379697	0.213017
N	14.403559	-4.527961	-3.523903	-0.542829
H	13.388278	-4.334646	-3.660303	0.377404
C	14.774872	-5.201794	-2.286184	-0.132249
H	13.833598	-5.542858	-1.845343	0.237867
C	15.441279	-4.295217	-1.252116	0.066698
O	14.496409	-3.324900	-0.757554	-0.721889
H	14.883069	-3.076851	0.110337	0.444709
H	16.295665	-3.771299	-1.690817	0.287104
C	15.918731	-5.140259	-0.066300	-0.112996
O	16.346604	-4.235897	0.931913	-0.684454
H	16.048292	-4.559382	1.838563	0.533872
H	15.061628	-5.724479	0.303874	0.196323
C	17.042348	-6.093359	-0.520096	0.013453
C	17.180166	-7.397308	0.303632	-0.258997
O	18.189470	-7.338186	1.302163	-0.711334
H	17.838325	-6.874931	2.117017	0.527270
H	16.214716	-7.683034	0.743654	0.192218
H	17.475575	-8.187836	-0.394832	0.197208
H	17.986646	-5.548737	-0.446137	0.259798
O	16.925007	-6.423159	-1.938104	-0.397603
C	15.663140	-6.454669	-2.516473	0.131698
H	15.829952	-6.620110	-3.579164	0.291112
O	14.906011	-7.605100	-1.994142	-0.732827
H	15.417194	-8.398444	-2.234939	0.440387
H	18.994928	2.145633	-7.450427	0.176690
H	19.639348	1.315191	-6.044493	0.182898
H	21.643857	-0.760307	-2.712847	0.181150
H	21.812539	-0.988626	-0.904943	0.193211
H	24.584866	-12.053658	-1.550578	0.164397
H	23.319192	-12.607174	-0.372694	0.218198
H	18.428182	-5.036639	6.226045	0.191004
H	17.647626	-6.723954	6.288983	0.204114
H	15.007184	-6.007294	-11.280522	0.193724
H	16.702914	-5.285907	-11.029984	0.190338
H	9.328322	-5.049905	-6.894674	0.234093
H	8.935647	-9.535676	-4.748663	0.218939
H	13.583956	-1.683070	3.399181	0.146119
H	12.355633	-3.889576	6.206052	0.181949
H	8.925811	-3.320599	-0.015220	0.170643