

29

G19C1 HB

C	1.3976002	0.0549365	-0.9550754
O	0.7948440	0.0619255	-2.0396535
H	-0.3418659	0.1513155	0.1736674
N	0.6953091	0.1369980	0.2608918
C	1.2462394	0.1479677	1.5234437
N	0.3698628	0.3257246	2.5580764
H	-0.6147533	0.0680179	2.4219913
H	0.7708002	0.0883820	3.4596339
N	2.5463338	0.0609433	1.7694401
C	3.2605875	-0.0217654	0.6143655
N	4.6290127	-0.1192751	0.5197364
C	2.8168475	-0.0279512	-0.7185836
N	3.8697888	-0.1251140	-1.6117381
C	4.9390147	-0.1770151	-0.8243608
H	5.9699984	-0.2569826	-1.1697740
H	5.2720373	-0.1382821	1.3046048
N	-2.1971491	0.0058823	-0.0863734
C	-2.7740696	0.0624115	-1.2952881
N	-1.9728286	0.1505380	-2.3655058
H	-0.9403273	0.1389248	-2.2508051
H	-2.3786047	0.1882195	-3.2912921
C	-2.9585538	-0.1196772	1.0470806
O	-2.4970598	-0.1996356	2.1903114
N	-4.3566750	-0.1589005	0.8818017
H	-4.8962034	-0.2474432	1.7383546
C	-4.9657463	-0.0837983	-0.3354886
H	-6.0584422	-0.1212005	-0.3435690
C	-4.2110704	0.0291863	-1.4686679
H	-4.6767284	0.0856412	-2.4536924

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G19C2A HB

C	0.2489104	1.2646767	-1.5110775
N	0.5087529	0.3849741	-2.5391668
H	0.1133711	-0.5509639	-2.4456467
H	0.3457169	0.8137470	-3.4461661
N	0.0995386	0.7044574	-0.2635846
H	0.1020161	-0.3300393	-0.1823331
C	-0.0811067	1.4027815	0.9493736
O	-0.1903387	0.7940191	2.0212618
C	-0.1075213	2.8258309	0.7121224
N	-0.2639403	3.8757440	1.5988926
C	-0.2044327	4.9505975	0.8191374
H	-0.2900073	5.9814606	1.1634477
N	-0.0197725	4.6465579	-0.5142398
H	0.0617232	5.2949336	-1.2908608
C	0.0471550	3.2768745	-0.6085974
N	0.2262335	2.5635309	-1.7560662
C	-0.2382967	-3.1009506	-0.9226217
O	-0.4655869	-2.5031999	-2.1253855
H	-0.5920645	-3.2473810	-2.7397222
N	-0.2687521	-4.4327432	-0.9105807
C	-0.0442750	-4.9691716	0.3154719
H	-0.0590935	-6.0637471	0.3698787
C	0.1881149	-4.2093793	1.4505618
H	0.3599569	-4.6767492	2.4232372
C	0.1914804	-2.7941427	1.2995800
N	0.4370299	-1.9520580	2.3265525
H	0.4257854	-2.3345050	3.2641810
H	0.2125506	-0.9496580	2.2137450
N	-0.0188036	-2.2416775	0.0781530

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## G19C2B HB

N	-2.8692824	1.6707248	0.0163507
C	-3.5221709	0.4723011	-0.0444804
N	-4.8830577	0.3078159	-0.1566089
H	-5.5644135	1.0586213	-0.1992843
C	-5.1248023	-1.0497937	-0.1880665
H	-6.1360221	-1.4485482	-0.2722766
N	-4.0168469	-1.7802895	-0.1061679
C	-3.0106603	-0.8353470	-0.0154983
C	-1.5754472	-1.0078907	0.0902390
O	-0.9031441	-2.0377540	0.1218320
N	-0.9495199	0.2636312	0.1597922
H	0.0865424	0.2381454	0.2044818
C	-1.5654142	1.4872830	0.1263680
N	-0.7358866	2.5820579	0.2939209
H	0.2210853	2.4699301	-0.0383141
H	-1.1788062	3.4383927	-0.0282763
N	4.2364070	0.6505592	-0.1564897
C	4.5957469	-0.6452049	-0.0562140
N	5.9446524	-0.9072301	-0.0593282
H	6.5123050	-0.1561200	-0.4416530
H	6.2232070	-1.8379695	-0.3519011
C	3.6309525	-1.6677737	0.1024104
H	3.9158907	-2.7195540	0.1801970
C	2.2994847	-1.2740658	0.1566981
H	1.4745492	-1.9888623	0.2639564
N	1.9236925	0.0247530	0.0730491
C	2.9232531	0.8935094	-0.0813903
O	2.5358695	2.1888480	-0.1852730
H	3.3625279	2.6917108	-0.2797196

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## G17C1 HB

H	3.8119286	2.5389952	-0.2275625
N	3.8526162	1.5268945	-0.1718358
C	2.7775734	0.6837633	-0.0454803
C	3.3088686	-0.6169995	-0.0097870
N	4.6851034	-0.5752638	-0.1124076
C	4.9658596	0.7228301	-0.2067084
H	5.9677590	1.1420257	-0.3026266
N	2.5575561	-1.7563250	0.1104194
C	1.3706979	0.9406905	0.0274211
O	0.8040714	2.0525941	-0.0054572
N	0.6805662	-0.2595000	0.1458706
H	-0.3586422	-0.1840834	0.1610378
C	1.2632524	-1.5193029	0.1920500
N	0.3847025	-2.5537696	0.4109785
H	0.8027270	-3.4531503	0.1908255
H	-0.5795522	-2.4355724	0.0822990
C	-2.7761362	1.2857737	0.1072126
N	-1.9775853	2.3534657	0.2669117
H	-2.3857909	3.2791580	0.2672800
H	-0.9487472	2.2482182	0.1878530
N	-2.1959709	0.0832816	0.0085895
C	-2.9526393	-1.0497566	-0.1654968
O	-2.4862217	-2.1856116	-0.2826919
N	-4.3510972	-0.8834682	-0.2128248
H	-4.8883954	-1.7368565	-0.3393186
C	-4.9628930	0.3288231	-0.1004312
H	-6.0551140	0.3365075	-0.1502249
C	-4.2121544	1.4587188	0.0633705
H	-4.6809433	2.4397009	0.1533900

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## G17C2A HB

N	2.5719000	1.7438950	0.2479264
C	3.3229537	0.6106405	0.0597315
N	4.7002802	0.5662372	0.0042023
C	4.9762679	-0.7218777	-0.1904762
H	5.9782091	-1.1405842	-0.2870938
N	3.8569138	-1.5150272	-0.2644344
H	3.8119254	-2.5184403	-0.4087284
C	2.7837614	-0.6759853	-0.1068011
C	1.3730062	-0.9296402	-0.0960812
O	0.7982601	-2.0255635	-0.2311478
N	0.6862406	0.2675294	0.0965067
H	-0.3502686	0.1972703	0.0941746
C	1.2780454	1.5103803	0.2643267
N	0.3954410	2.5393546	0.5410447
H	0.8447754	3.4417043	0.4040507
H	-0.5168505	2.4710725	0.0889654
N	-2.2354325	-0.0835494	-0.0417632
C	-2.7919909	-1.2958952	0.2021662
N	-1.9514929	-2.3262264	0.4460533
H	-0.9528200	-2.2289508	0.2046402
H	-2.3437567	-3.2592911	0.4701644
C	-4.2071658	-1.4367454	0.2315286
H	-4.6784649	-2.4016434	0.4337765
C	-4.9632666	-0.2996511	-0.0064912
H	-6.0582671	-0.3461951	0.0029474
N	-4.4231974	0.9164297	-0.2693786
C	-3.0905684	0.9209232	-0.2643124
O	-2.4881549	2.1119985	-0.5268551
H	-3.2285242	2.7314112	-0.6495493

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G17C2B HB

C	-1.4834913	1.5827914	0.1336674
N	-2.5794000	0.7484989	0.3135173
H	-3.4339026	1.2143108	0.0168415
H	-2.4838840	-0.1874157	-0.0793399
N	-0.2608394	0.9377998	0.1566376
H	-0.2470850	-0.0996808	0.1952425
C	0.9914603	1.5579162	0.0793069
O	2.0556433	0.9270220	0.0925168
C	0.7950077	2.9813152	-0.0112293
C	-0.4771083	3.5766788	-0.0385259
N	-1.6613334	2.8806041	0.0310280
N	-0.3655295	4.9472470	-0.1490267
N	1.6925680	4.0133403	-0.1084267
C	0.9479054	5.1653127	-0.1868911
H	1.4194463	6.1447050	-0.2700795
H	2.7030301	3.9211319	-0.1171681
O	-2.1866128	-2.5372570	-0.2189263
H	-2.6919313	-3.3628520	-0.3097929
C	-0.8952391	-2.9264824	-0.0982076
N	-0.0243038	-1.9276528	0.0555411
C	1.2719334	-2.3068539	0.1556602
H	1.9886418	-1.4835068	0.2629080
C	1.6640148	-3.6392001	0.1166220
H	2.7141515	-3.9260771	0.2081286
C	0.6403474	-4.6027743	-0.0426668
N	-0.6530384	-4.2407699	-0.1585823
N	0.8986621	-5.9521761	-0.0300355
H	0.1486037	-6.5221769	-0.4111041
H	1.8311393	-6.2374813	-0.3105780

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G91C1 HB

N	1.2500906	-1.0858228	-0.1602082
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C	1.3330497	0.2633606	-0.0829156
N	0.3275543	1.1924834	-0.1173100
H	-0.6869504	0.9528038	-0.1786715
C	0.9318313	2.4212776	-0.0001702
H	0.3398421	3.3368944	0.0020607
N	2.2640758	2.3699558	0.1032996
C	2.5160654	1.0124566	0.0525560
C	3.7102389	0.2655558	0.1050418
O	4.9160343	0.8522412	0.2280818
H	4.7329374	1.8078626	0.2637930
N	3.6813826	-1.0603557	0.0256727
C	2.4656325	-1.6600076	-0.0995006
N	2.5027121	-3.0529794	-0.1148416
H	3.4190662	-3.3913823	-0.3999595
H	1.7542267	-3.4548031	-0.6742902
C	-3.9398157	-1.6272654	0.2352627
H	-4.1896271	-2.6807927	0.3687578
C	-4.9104159	-0.6643189	0.2390136
H	-5.9721838	-0.8875037	0.3759936
N	-4.5752416	0.6443532	0.0657529
H	-5.2811900	1.3754780	0.0789074
C	-3.2441898	1.0889371	-0.1092531
O	-3.0084365	2.2862021	-0.2265571
N	-2.2708775	0.1097634	-0.1311253
C	-2.5786926	-1.1762476	0.0392037
N	-1.5779992	-2.0792942	-0.0005640
H	-1.7740286	-3.0382176	0.2559528
H	-0.5942409	-1.7695231	-0.0595486

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G91C2A HB

N	-0.1736452	1.2674121	-1.0900341
C	-0.1012753	1.3416837	0.2582105
N	-0.1606515	0.3289630	1.1804014
H	-0.2371919	-0.6789332	0.9378528
C	-0.0375407	0.9220278	2.4154063
H	-0.0502707	0.3262984	3.3284779
N	0.0921492	2.2512613	2.3740074
C	0.0531822	2.5148208	1.0176963
C	0.1329704	3.7135980	0.2793241
O	0.2760626	4.9125878	0.8743862
H	0.3041294	4.7245172	1.8291954
N	0.0599784	3.6947003	-1.0465631
C	-0.0858162	2.4855528	-1.6562072
N	-0.0922202	2.5323937	-3.0464338
H	-0.3591362	3.4533004	-3.3864279
H	-0.6451969	1.7869968	-3.4623421
N	0.1554176	-4.6297808	0.6953303
C	0.3300102	-4.9003655	-0.6214482
H	0.5309825	-5.9483380	-0.8723622
C	0.2662966	-3.9384893	-1.6187107
H	0.4107861	-4.1983136	-2.6702071
C	0.0010596	-2.6017512	-1.2143969
N	-0.1305435	-1.5862523	-2.1044790
H	-0.1411511	-0.6122720	-1.7675894
H	0.2249418	-1.7433923	-3.0401945
N	-0.1755687	-2.3148203	0.0955479
C	-0.0833414	-3.3426016	0.9507606
O	-0.2538061	-2.9848122	2.2444819
H	-0.1509073	-3.8155675	2.7396279

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G91C2B HB

N	-1.6663190	0.3983851	-2.2493110
C	-0.8501998	0.1553166	-3.2867222

N	-1.1335769	0.1861246	-4.6362722
H	-2.0358634	0.3972783	-5.0510544
C	0.0327642	-0.1339041	-5.3031441
H	0.0714647	-0.1801457	-6.3918179
N	1.0622451	-0.3700627	-4.4941680
C	0.5115947	-0.1919282	-3.2364440
C	1.0624478	-0.2643786	-1.9417409
O	2.3634037	-0.5437932	-1.7202037
H	2.7599421	-0.6689374	-2.6003912
N	0.3067301	-0.0336953	-0.8767852
C	-1.0171726	0.2718491	-1.0754324
N	-1.7556795	0.4302708	0.0730803
H	-1.1994386	0.5684773	0.9244515
H	-2.5803156	1.0112808	-0.0463574
N	-0.5699742	-0.3890168	4.9483026
C	0.7274042	-0.0643104	5.1413915
H	1.0808495	-0.1203572	6.1783435
C	1.6038418	0.3094139	4.1259255
H	2.6504169	0.5467803	4.3320586
C	1.0682418	0.3738145	2.8182419
N	1.7844464	0.7760814	1.7230263
H	1.3888116	0.4673297	0.8261098
H	2.7926235	0.6853159	1.7978399
N	-0.2335714	0.0849407	2.6073908
C	-0.9550160	-0.3010655	3.6724626
O	-2.2364068	-0.6511167	3.4239060
H	-2.3178251	-0.6347537	2.4544060

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G92C1 HB

N	0.3317398	0.1273957	1.2002177
H	-0.6791986	0.1902279	0.9524620
C	0.9256583	0.0113167	2.4347001
H	0.3245346	0.0137370	3.3445622
N	2.2554237	-0.0989532	2.4004532
C	2.5287413	-0.0534285	1.0457822
C	3.7108512	-0.1119527	0.2784582
O	4.9115652	-0.2431134	0.8650482
H	5.5392497	-0.2593792	0.1205445
N	3.6664988	-0.0315123	-1.0522226
C	2.4536635	0.0995167	-1.6536550
N	2.4828891	0.1152217	-3.0484837
H	3.3930407	0.4132744	-3.3925996
H	1.7303350	0.6774363	-3.4399729
N	1.2503252	0.1628732	-1.0654238
C	1.3455576	0.0856536	0.2842359
N	-2.2740264	0.1353246	0.1068939
C	-3.2496344	0.1057383	1.0841816
O	-3.0183994	0.2250060	2.2818425
N	-4.5782904	-0.0811545	0.6361072
H	-5.2860888	-0.1012547	1.3652916
C	-4.9094699	-0.2540054	-0.6735669
H	-5.9696078	-0.3998072	-0.8990008
C	-3.9368257	-0.2398774	-1.6344847
H	-4.1833344	-0.3711552	-2.6890587
C	-2.5789890	-0.0318887	-1.1794810
N	-1.5762570	0.0266759	-2.0813942
H	-0.5951902	0.0713606	-1.7614510
H	-1.7635071	-0.2576615	-3.0344582

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G92C2A HB

N	0.9279192	0.6446357	-0.0993461
C	1.3874657	-0.6182242	-0.1217376
O	0.5454265	-1.6285191	-0.2238278

H	-0.3962516	-1.2592885	-0.2099826
C	2.7857371	-0.8294162	-0.0328366
N	3.5688128	-1.9729398	-0.0309189
C	4.8011851	-1.4933966	0.0932683
H	5.7055996	-2.1016203	0.1307379
N	4.8570210	-0.1156893	0.1744883
H	5.6849763	0.4635377	0.2685328
C	3.5610518	0.3406652	0.0939471
N	3.1378188	1.6192977	0.1403511
C	1.8059406	1.6857580	0.0294722
N	1.2334408	2.9452565	-0.0232264
H	1.8309940	3.6635178	0.3762963
H	0.2693242	2.9860012	0.2986126
N	-2.0255208	-0.7889759	-0.0979497
C	-2.9534835	-1.7619531	0.0500049
H	-2.5702618	-2.7888258	0.0764360
C	-4.3106057	-1.5009559	0.1589527
H	-5.0428841	-2.3045531	0.2641602
C	-4.6860181	-0.1347243	0.1170973
N	-6.0083017	0.2488691	0.1524537
H	-6.6433620	-0.3736429	0.6414709
H	-6.1338455	1.2339745	0.3721547
N	-3.7858392	0.8500090	-0.0167489
C	-2.4996251	0.4774041	-0.1244855
O	-1.6283752	1.4671778	-0.2708322
H	-0.7002737	1.0689843	-0.2755529

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G92C2B HB

N	-0.3007972	2.9947553	1.5701628
C	-0.0660924	1.6891934	1.7549462
N	-0.0700548	1.2162228	3.0539041
H	-0.5843662	1.8152990	3.6931224
H	-0.2865267	0.2262200	3.1444589
N	0.2401166	0.7572825	0.8012505
C	0.3172992	1.1248825	-0.4869257
O	0.5926964	0.2127703	-1.4087254
H	0.5565925	-0.6870429	-0.9488755
C	0.1082796	2.4832084	-0.8220491
N	0.1190613	3.1746322	-2.0233430
C	-0.1642557	4.4192299	-1.6558524
H	-0.2423926	5.2673757	-2.3369232
N	-0.3603707	4.5681005	-0.2967589
H	-0.5824769	5.4225015	0.2039462
C	-0.1890265	3.3254779	0.2695078
N	0.1806915	-2.2468059	-0.3961989
C	0.1836064	-2.6592704	0.8932691
O	0.4829049	-1.7516288	1.8199833
H	0.5130778	-0.8551757	1.3677564
N	-0.0819606	-3.8959014	1.3371727
C	-0.3827804	-4.7844279	0.3706841
H	-0.5995600	-5.8037584	0.7137144
C	-0.4369023	-4.4827246	-0.9892225
H	-0.6901121	-5.2371604	-1.7375621
C	-0.1423767	-3.1506576	-1.3432422
N	-0.0958945	-2.7188102	-2.6506547
H	-0.6530448	-3.2531736	-3.3095006
H	-0.1713409	-1.7105930	-2.7720392

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G19C1 ST

N	0.2809258	2.1324506	-0.6751233
C	1.6172781	1.9101274	-0.9170598
H	2.1234543	2.3684099	-1.7658543
N	2.1944917	1.1100686	-0.0216545

C	1.1539437	0.7682737	0.8162379
C	1.1101711	-0.2293495	1.8610403
O	1.9621599	-1.0328503	2.2319970
N	-0.1883440	-0.2392346	2.4515803
H	-0.3165432	-0.9785862	3.1421189
C	-1.3021841	0.4181983	1.9809500
N	-2.5063186	0.0934148	2.6108209
H	-2.4260443	0.0649281	3.6276993
H	-3.2157006	0.7752471	2.3415206
N	-1.2996547	1.2553779	0.9690229
C	-0.0510247	1.3748202	0.4187026
H	-0.3829378	2.5031261	-1.3540783
N	-1.8618947	-0.7150382	-1.5330740
C	-1.6232525	-1.6316655	-0.5549940
H	-2.4879858	-2.0008766	0.0036025
C	-0.3366128	-2.0319774	-0.3137111
H	-0.0999404	-2.7749383	0.4495317
C	0.6864050	-1.4353879	-1.1400155
N	1.9890556	-1.8238513	-0.9456145
H	2.6400053	-1.1400756	-1.3312879
H	2.2156668	-2.0451863	0.0244863
N	0.4447716	-0.5506867	-2.0999720
C	-0.8417730	-0.0834047	-2.2809611
O	-1.1443800	0.8575540	-3.0150511
H	-2.7922905	-0.3276780	-1.6666980

29

G17C2B ST

N	0.1761429	1.5322626	-0.3292571
C	0.5380056	0.8372410	-1.4596848
N	1.8100175	0.8096400	-1.9953669
C	1.7204479	-0.0513091	-3.0127221
H	2.5361072	-0.3169786	-3.6852265
N	0.4626830	-0.5812918	-3.1549863
H	0.1437363	-1.2470543	-3.8530921
C	-0.3076869	-0.0272545	-2.1674438
C	-1.6620957	-0.3127448	-1.7594495
O	-2.4760191	-1.0804902	-2.2641857
N	-1.9410420	0.4573217	-0.6127835
H	-2.8784264	0.3371078	-0.2298888
C	-1.0526655	1.2821437	0.0577048
N	-1.5815954	1.9178106	1.1783012
H	-2.0460881	1.2638292	1.8122700
H	-0.8175187	2.3722215	1.6792763
N	-0.8639892	-1.2812644	2.0841448
C	-0.2593159	-1.8036362	0.9901128
H	-0.8375617	-2.5557944	0.4387958
C	1.0011858	-1.4186438	0.5458116
H	1.4599176	-1.8588380	-0.3431824
C	1.6536756	-0.4043667	1.2879540
N	2.8720432	0.1064672	0.9006706
H	3.0640860	0.9842982	1.3816420
H	2.9452396	0.2253838	-0.1130221
N	1.1078395	0.0792133	2.4206970
C	-0.1075011	-0.3933234	2.7342283
O	-0.6810950	0.1435376	3.8425338
H	0.0052806	0.7326901	4.1992810

29

G91C1 ST

N	-0.6846102	-0.9024906	-1.4653696
C	0.5465594	-0.4391324	-1.1886943
N	1.2198141	0.6285743	-1.7384087
H	0.8087955	1.3483672	-2.3290478
C	2.4129826	0.7405999	-1.0590908

H	3.1120915	1.5471972	-1.2783158
N	2.5988436	-0.2053920	-0.1372101
C	1.4300349	-0.9402225	-0.2145621
O	0.9542915	-2.0367205	0.5330990
C	1.6913948	-2.6165130	1.5021083
H	2.5482286	-2.1545751	1.4867644
N	-0.2651258	-2.5177786	0.3205240
C	-1.0115338	-1.9150055	-0.6458567
N	-2.3331199	-2.3716391	-0.7368350
H	-2.4193610	-3.3234337	-0.3828214
H	-2.6879893	-2.2886226	-1.6891463
N	0.5191313	1.8110652	1.3654777
C	-0.1209315	0.7788244	1.9819377
H	0.3897578	0.3104799	2.8286127
C	-1.3462547	0.3772279	1.5233733
H	-1.8931047	-0.4399125	1.9952430
C	-1.8581463	1.0849589	0.3767029
N	-3.0987913	0.7291420	-0.1013644
H	-3.2516242	1.1040982	-1.0364662
H	-3.2819867	-0.2743070	-0.0476731
N	-1.2228226	2.0744107	-0.2354539
C	0.0214429	2.4721263	0.2177465
O	0.7249655	3.3163095	-0.3330154
H	1.4590611	2.0803612	1.6449418

29

G91C2A ST

N	-1.7533829	-0.0181033	0.4175257
C	-1.2017468	-0.6568297	-0.6283756
N	-1.3709944	-0.4170017	-1.9741242
H	-1.7915840	0.4274815	-2.3556476
C	-0.4834093	-1.2367020	-2.6356298
H	-0.3883653	-1.2117364	-3.7214010
N	0.2046525	-2.0491518	-1.8326678
C	-0.2478384	-1.6859589	-0.5758705
C	0.1624661	-2.0655529	0.7167707
O	1.1087191	-3.0145016	0.9154646
H	1.2978360	-3.3754899	0.0312756
N	-0.3292197	-1.4607105	1.7876777
C	-1.2482459	-0.4693495	1.5803034
N	-1.6529674	0.1908048	2.7287998
H	-1.5881605	-0.3867703	3.5626857
H	-2.5454814	0.6652118	2.6198132
N	-0.1051134	2.8016186	0.4597684
C	0.6424991	2.3142249	1.4747848
H	0.4827776	2.7718084	2.4571805
C	1.5520180	1.2735438	1.3165432
H	2.1224940	0.8782545	2.1601925
C	1.6962129	0.7509607	0.0109356
N	2.6085272	-0.2427263	-0.2850748
H	2.3641850	-0.7411595	-1.1407869
H	2.8115799	-0.8731015	0.4874846
N	0.9732219	1.2246583	-1.0223699
C	0.1055956	2.1931991	-0.7120281
O	-0.6905599	2.5850439	-1.7446624
H	-1.2457871	3.2784348	-1.3467487

29

G91C2B ST

N	-1.2738832	1.6884223	-0.5541213
C	-0.3873792	0.9540858	-1.2477419
N	0.7373581	1.3613912	-1.9316302
H	1.1402113	2.2936595	-1.9115337
C	1.3299303	0.2270520	-2.4436604
H	2.2610258	0.2803004	-3.0072948



N	0.6645493	-0.8951212	-2.1742818
C	-0.4028632	-0.4417062	-1.4211719
C	-1.4444850	-1.1199487	-0.7614611
O	-1.5583990	-2.4660834	-0.8034086
H	-0.8300194	-2.7653493	-1.3771334
N	-2.3329358	-0.4530772	-0.0348885
C	-2.1993377	0.9052110	0.0265615
N	-3.1038375	1.5352966	0.8732087
H	-3.9855790	1.0328413	0.9428572
H	-3.2211332	2.5207714	0.6491435
N	2.0358994	1.2813891	0.9765993
C	0.9480776	1.5102249	1.7451349
H	0.7598138	2.5578614	2.0083798
C	0.0770969	0.5129957	2.1766338
H	-0.8108934	0.7453750	2.7689911
C	0.3774276	-0.8039937	1.7688353
N	-0.4036151	-1.8835807	2.1447056
H	-0.2468051	-2.6803280	1.5291655
H	-1.3964407	-1.6541980	2.1798429
N	1.4718669	-1.0702528	1.0289117
C	2.2186359	-0.0107297	0.6803147
O	3.2951778	-0.2739725	-0.0989817
H	3.2352054	-1.2310945	-0.2612042

29

G92C1 ST

N	0.7073986	1.2200711	-1.3677054
C	0.3717412	-0.0834620	-1.3637464
N	-0.6539048	-0.6977366	-2.0443236
H	-1.4648325	-0.2131954	-2.4295945
C	-0.6526335	-2.0150240	-1.6381940
H	-1.4099371	-2.7134532	-1.9941795
N	0.3428867	-2.3349055	-0.8147124
C	0.9872246	-1.1241710	-0.6314105
C	2.0454520	-0.6999872	0.1967076
O	2.6708646	-1.5738871	1.0148164
H	3.3531777	-1.0363207	1.4570286
N	2.4244318	0.5745196	0.2285147
C	1.7354748	1.4636841	-0.5427412
N	2.1083343	2.7970094	-0.3814652
H	3.0822727	2.8894710	-0.1017049
H	1.8874313	3.3521057	-1.2056187
N	-1.8227999	1.7424750	0.4717022
C	-0.8186795	1.7978491	1.3882349
H	-0.3884433	2.7803143	1.5991616
C	-0.3818803	0.6393964	1.9727352
H	0.4188437	0.6457219	2.7134514
C	-1.0293995	-0.5749485	1.5463584
N	-0.6413947	-1.7659366	2.1177897
H	-0.8910581	-2.5593449	1.5276184
H	0.3389429	-1.7987766	2.3908820
N	-2.0027949	-0.6238376	0.6462692
C	-2.3887947	0.5365909	0.0043468
O	-3.1556057	0.5740840	-0.9590505
H	-2.0873466	2.5707109	-0.0555455

29

G92C2A ST

N	-1.6545197	0.0872979	0.7633858
C	-1.3320822	-0.7059610	-0.2702796
N	-1.8692712	-0.6994351	-1.5367173
H	-2.5733653	-0.0501083	-1.8738585
C	-1.1785458	-1.6420395	-2.2694044
H	-1.4101769	-1.8276616	-3.3190117
N	-0.2485465	-2.2915186	-1.5728816

C	-0.3405609	-1.7106880	-0.3190060
C	0.3423856	-1.8965915	0.9007320
O	1.3054923	-2.8360940	1.0150118
H	1.5740243	-2.7836057	1.9504993
N	0.0830875	-1.1277857	1.9517431
C	-0.8747128	-0.1595469	1.8284726
N	-1.0745252	0.6285754	2.9481706
H	-0.2421043	0.6527111	3.5328885
H	-1.3671845	1.5669226	2.6781628
N	-0.3109402	2.3420005	-1.3123272
C	0.3396140	1.5100437	-2.1598430
H	0.0133624	1.5360035	-3.2069014
C	1.3581546	0.6548767	-1.7575039
H	1.8543492	-0.0210345	-2.4574703
C	1.7160656	0.7054930	-0.3886599
N	2.7444539	-0.0651320	0.1201520
H	2.6833953	-0.1336752	1.1349690
H	2.8334077	-0.9814695	-0.3151325
N	1.1143758	1.5464992	0.4707538
C	0.1304477	2.2914096	-0.0494827
O	-0.4989066	3.0897655	0.8460303
H	-1.1883859	3.5283145	0.3182310

29

G92C2B ST

N	-0.6093422	1.7158970	-0.9513218
C	0.3279902	0.8291241	-1.3364179
N	1.6495411	1.0432041	-1.6625714
H	2.1661503	1.8948986	-1.4609478
C	2.1994408	-0.1919705	-1.9315760
H	3.2551536	-0.3001593	-2.1800221
N	1.3274222	-1.1964662	-1.8622931
C	0.1618209	-0.5596209	-1.4817714
C	-1.1212955	-1.0533409	-1.1747350
O	-1.4175992	-2.3682892	-1.2374350
H	-0.5962328	-2.8011993	-1.5317180
N	-2.0799147	-0.2299923	-0.7722735
C	-1.7676080	1.0950613	-0.6697582
N	-2.7841239	1.8746376	-0.1230745
H	-3.7073566	1.5244015	-0.3708509
H	-2.6682290	2.8626600	-0.3386716
N	2.1411616	-0.2333499	1.2089461
C	1.6224999	-1.4710329	1.3769329
H	2.3119660	-2.3048095	1.1985444
C	0.2955124	-1.7168550	1.7226584
H	-0.0926613	-2.7332976	1.8246254
C	-0.5234595	-0.5837511	1.9339029
N	-1.8479557	-0.6785433	2.3172391
H	-2.3531753	0.1748493	2.0735544
H	-2.3165019	-1.4979565	1.9357538
N	-0.0248473	0.6589619	1.8090983
C	1.2590843	0.7457107	1.4297208
O	1.7195189	2.0032802	1.2113859
H	0.9274136	2.5573399	1.3284851

29

G19C2A TS

N	-1.0884822	2.6274063	1.1081966
C	-1.1151903	3.2348807	-0.1252953
H	-1.8105731	4.0430036	-0.3528004
N	-0.2122193	2.7395701	-0.9725878
C	0.4180997	1.7570745	-0.2345034
C	1.4543170	0.8281119	-0.6307751
O	2.0540481	0.7111715	-1.6960846
N	1.7166883	-0.0585671	0.4494024

H	2.4459831	-0.7466189	0.2649782
C	1.0679576	-0.1104295	1.6611092
N	1.4879123	-1.1336519	2.5145439
H	1.3442909	-2.0419469	2.0610203
H	0.9038503	-1.0996079	3.3513536
N	0.1515879	0.7519989	2.0436297
C	-0.1180494	1.6575475	1.0585479
H	-1.7111196	2.7962484	1.8925113
N	-0.3140962	-2.7422450	0.3535098
C	0.4199202	-2.8339440	-0.7847847
H	1.1474761	-3.6540257	-0.8225602
C	0.2868149	-1.9545223	-1.8499085
H	0.9014501	-2.0394663	-2.7484586
C	-0.6529100	-0.9033157	-1.6913184
N	-0.8273161	0.0486874	-2.6671557
H	-1.2769090	0.8904167	-2.3065644
H	0.0384952	0.2838898	-3.1516429
N	-1.4306803	-0.8145235	-0.5951646
C	-1.2161436	-1.7464955	0.3426382
O	-2.0243733	-1.6495067	1.4219573
H	-1.7673730	-2.4044891	1.9771271

29

G19C2B TS

N	-2.7913346	-1.0706256	0.9946616
C	-3.4017839	0.1632526	0.9722204
H	-4.2685531	0.3866287	1.5945872
N	-2.8277291	1.0145678	0.1223044
C	-1.7984005	0.2762222	-0.4293486
C	-0.8031452	0.6669185	-1.4045309
O	-0.6405419	1.7349581	-1.9863300
N	0.0786007	-0.4276953	-1.6292386
H	0.8122900	-0.2447358	-2.3133140
C	0.0925711	-1.6364673	-0.9704338
N	1.1255856	-2.4969686	-1.3189811
H	2.0317178	-2.0240478	-1.2318053
H	1.1170158	-3.2833274	-0.6684613
N	-0.8237427	-2.0062269	-0.0965835
C	-1.7444410	-1.0194829	0.1050115
H	-3.0441273	-1.8727483	1.5637161
N	2.8507572	-0.3032030	0.1659208
C	2.8884165	0.9163552	-0.4251726
H	3.6957464	1.0696003	-1.1517996
C	1.9712281	1.9276291	-0.1683697
H	2.0122457	2.8878501	-0.6865671
C	0.9429037	1.6322536	0.7589584
N	-0.0412098	2.5467949	1.0545091
H	-0.8639922	2.1126705	1.4710672
H	-0.3051283	3.1179909	0.2522546
N	0.9147095	0.4513025	1.4081709
C	1.8663568	-0.4326094	1.0641489
O	1.8183420	-1.6351444	1.6813349
H	0.9978862	-1.6037457	2.2021949

29

G17C2A TS

N	-1.4707111	-0.7981081	-1.2509877
C	-0.5355082	-1.5805221	-0.6075844
N	-0.8276059	-2.6678306	0.1888446
C	0.3589933	-3.0548546	0.6624575
H	0.5236125	-3.9026923	1.3275724
N	1.3965893	-2.2759365	0.2137320
H	2.3838245	-2.3627290	0.4362113
C	0.8430929	-1.3187661	-0.5912775
C	1.4482864	-0.2107896	-1.2896829

O	2.6295266	0.1144931	-1.3579160
N	0.4171882	0.4960105	-1.9390735
H	0.7121048	1.3297258	-2.4453657
C	-0.9394013	0.2420184	-1.8476324
N	-1.7311323	1.1826365	-2.5089515
H	-1.5314003	2.1164316	-2.1385625
H	-2.7088509	0.9658418	-2.3129639
N	1.2839451	1.7357202	1.4893057
C	1.1024554	0.7132489	2.3569461
H	1.9603142	0.4650479	2.9935932
C	-0.0837706	-0.0061162	2.4480293
H	-0.2020512	-0.8362221	3.1487012
C	-1.1353691	0.3884553	1.5850074
N	-2.3599894	-0.2444027	1.5906627
H	-2.8145946	-0.1277244	0.6836801
H	-2.2831566	-1.2390722	1.8034703
N	-0.9956536	1.4315262	0.7424454
C	0.2086657	2.0134283	0.7437039
O	0.3426068	3.0134111	-0.1668102
H	1.2578166	3.3201377	-0.0411663

29

G17C2B TS

N	-0.3078115	-0.6723097	0.2047046
C	0.6816882	-0.3981462	1.1187059
N	2.0396350	-0.4900671	0.8767375
C	2.6025899	-0.1284562	2.0319178
H	3.6750869	-0.0844158	2.2218414
N	1.6866098	0.1932950	3.0008374
H	1.8680465	0.4916456	3.9544491
C	0.4497158	0.0296744	2.4335850
C	-0.8722435	0.2150753	2.9808900
O	-1.2018733	0.5654769	4.1104726
N	-1.8087785	-0.0893791	1.9706298
H	-2.7825419	-0.0670087	2.2709677
C	-1.5216605	-0.5046595	0.6754390
N	-2.6306747	-0.8097040	-0.1008236
H	-3.3721999	-0.1140213	-0.0200413
H	-2.3544428	-0.8994230	-1.0868931
N	-1.1969073	-0.5507846	-2.7792305
C	-0.1497756	-1.4007146	-2.8972177
H	-0.3992878	-2.4288556	-3.1848778
C	1.1658119	-1.0352824	-2.6483732
H	1.9881728	-1.7490560	-2.7299242
C	1.3875664	0.3031232	-2.2571947
N	2.6591406	0.7692629	-1.9640456
H	2.5936571	1.6590557	-1.4698268
H	3.1618238	0.0962596	-1.3841024
N	0.3774148	1.1873232	-2.1953218
C	-0.8436159	0.6911665	-2.4357822
O	-1.8768269	1.5565795	-2.2798988
H	-1.4438822	2.3894856	-2.0268654

29

G91C1 TS

N	0.2387860	0.3874231	-0.8447718
C	0.9709197	-0.6749290	-0.4471480
N	0.6036979	-1.9959158	-0.3412438
H	-0.3695390	-2.3485627	-0.3739094
C	1.7060600	-2.6640817	0.1399219
H	1.6736150	-3.7360049	0.3376405
N	2.7793551	-1.8929438	0.3311263
C	2.3139141	-0.6421217	-0.0279475
C	2.9183488	0.6320743	0.0017771
O	4.2031830	0.8061420	0.3697290

H	4.5354893	-0.0870241	0.5690015
N	2.2196628	1.7166794	-0.3161455
C	0.9273438	1.5298042	-0.7076010
N	0.2039378	2.7144506	-0.9124240
H	0.8200584	3.4711769	-1.2067729
H	-0.5550485	2.5656361	-1.5763995
N	-3.3921113	-0.5256088	-0.7195356
C	-3.5714115	0.8217836	-0.6259153
H	-4.3238751	1.2682265	-1.2817064
C	-2.8169707	1.5372356	0.2629904
H	-2.9283250	2.6168625	0.3687464
C	-1.8920253	0.7802739	1.0677704
N	-1.1239855	1.4533982	1.9843666
H	-0.3497867	0.8863652	2.3265931
H	-0.8316281	2.3797788	1.6772052
N	-1.7674095	-0.5380939	1.0122293
C	-2.4285056	-1.2248655	0.0256253
O	-2.1985828	-2.4072135	-0.2688355
H	-3.8706204	-1.0710864	-1.4318578

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G91C2A TS

N	-1.9641282	1.3989188	0.3656103
C	-0.8034684	2.0592293	0.2226558
N	-0.3721147	3.1675731	0.9216844
H	-0.9135718	3.6862250	1.6063326
C	0.9243691	3.4137801	0.5255863
H	1.5000869	4.2438776	0.9367891
N	1.3753986	2.5571894	-0.3904360
C	0.2932773	1.7144179	-0.5931992
C	0.0918886	0.5545739	-1.3763930
O	1.0557131	0.1176972	-2.2020442
H	0.7489446	-0.7604206	-2.4970257
N	-1.0397862	-0.1331483	-1.2843815
C	-1.9950416	0.3026892	-0.4112549
N	-3.1440512	-0.4680859	-0.3739733
H	-2.9412906	-1.4516807	-0.5403235
H	-3.6714577	-0.3197264	0.4833693
N	-0.7244772	-2.3484313	1.0871759
C	-0.4384276	-1.2324340	1.7984955
H	-1.1862573	-0.9263541	2.5397913
C	0.7232924	-0.4902194	1.6181420
H	0.9342879	0.4027111	2.2123586
C	1.6188775	-0.9457456	0.6194290
N	2.7963206	-0.2818337	0.3473365
H	3.1650678	-0.5580198	-0.5618090
H	2.7179284	0.7341759	0.4123182
N	1.3690086	-2.0617247	-0.0910583
C	0.2196712	-2.6853595	0.1965560
O	-0.0086819	-3.7982696	-0.5361373
H	-0.8569034	-4.1310262	-0.1980708

29

G91C2B TS

N	0.4655948	-0.0161502	0.2428998
C	-0.5365708	-0.1091642	1.1388549
N	-1.8888454	-0.2369775	0.9155418
H	-2.3068863	-0.3077835	-0.0216401
C	-2.4883723	-0.2794660	2.1541458
H	-3.5693482	-0.3778641	2.2584246
N	-1.6341309	-0.1876040	3.1759223
C	-0.4106861	-0.0824225	2.5390261
C	0.9054032	0.0574785	3.0287859
O	1.1750343	0.1105457	4.3485669
H	0.3113645	0.0322532	4.7904916

N	1.9306352	0.1505962	2.1904717
C	1.6547157	0.1055885	0.8553870
N	2.7737100	0.1447044	0.0236132
H	3.5565107	0.6151881	0.4727028
H	2.5473818	0.5365677	-0.8880041
N	-1.7144282	-0.4423624	-1.9257967
C	-0.9872178	-1.5382397	-2.2392083
H	-1.4522143	-2.5045359	-2.0106991
C	0.2786810	-1.4822180	-2.8076877
H	0.8440527	-2.3874924	-3.0399164
C	0.7996171	-0.1929582	-3.0513638
N	2.0372677	-0.0064778	-3.6328684
H	2.3878947	0.9444731	-3.5526428
H	2.7297386	-0.7255119	-3.4463709
N	0.0918424	0.9148989	-2.7759305
C	-1.1058312	0.7152598	-2.2112261
O	-1.8022668	1.8172766	-1.8648734
H	-1.2163341	2.5576486	-2.0958387

29

G92C1 TS

N	-0.3777360	0.2532268	0.8008688
C	0.6807703	0.9963702	0.4091547
N	1.9942959	0.6117094	0.3041100
H	2.3347009	-0.3643152	0.3385119
C	2.6772314	1.7134252	-0.1584258
H	3.7498590	1.6698859	-0.3512874
N	1.9256681	2.7995894	-0.3372182
C	0.6635031	2.3530794	0.0099180
C	-0.6174052	2.9464833	0.0071588
O	-0.7798211	4.2378185	-0.3286030
H	-1.7406026	4.3818158	-0.2616492
N	-1.6999010	2.2342092	0.3220362
C	-1.5220844	0.9342854	0.6874112
N	-2.7062898	0.2059769	0.8854065
H	-3.4572442	0.8109336	1.2157109
H	-2.5447087	-0.5701674	1.5267324
N	0.5230500	-3.3922198	0.7563786
C	-0.8246475	-3.5724614	0.6670563
H	-1.2712261	-4.3102382	1.3393283
C	-1.5394819	-2.8395252	-0.2402205
H	-2.6186448	-2.9558117	-0.3462696
C	-0.7816167	-1.9322815	-1.0649777
N	-1.4538446	-1.1887598	-2.0034615
H	-0.8847044	-0.4233822	-2.3622499
H	-2.3799787	-0.8876391	-1.7045580
N	0.5353900	-1.8031665	-1.0089497
C	1.2218051	-2.4411217	-0.0060906
O	2.4018051	-2.2011153	0.2856757
H	1.0666747	-3.8498699	1.4837556

29

G92C2A TS

N	0.0436496	0.9600726	2.4718327
C	-0.8816118	0.1783495	1.8923805
N	-2.2539501	0.2739580	1.9467287
H	-2.7789512	1.0192540	2.3927382
C	-2.7603137	-0.7390350	1.1601628
H	-3.8341229	-0.8751046	1.0274086
N	-1.8227869	-1.5173341	0.6213430
C	-0.6512025	-0.9456167	1.0821507
C	0.7023416	-1.2581288	0.8569568
O	1.0807882	-2.2848861	0.0658895
H	0.2510661	-2.6782038	-0.2587665
N	1.6632915	-0.5196497	1.3958471

C	1.2832598	0.5492613	2.1601679
N	2.3351116	1.3289764	2.6165422
H	3.1914412	0.7989714	2.7538284
H	2.0793527	1.9060002	3.4135044
N	-1.3233471	0.4811987	-2.7747423
C	-0.4117317	-0.1695755	-3.5324241
H	-0.7779384	-0.5791273	-4.4814926
C	0.9162468	-0.3314023	-3.1551705
H	1.6294340	-0.8661297	-3.7876494
C	1.2981815	0.2304296	-1.9118173
N	2.5951394	0.1728849	-1.4506143
H	2.6371507	0.2318613	-0.4297178
H	3.1140546	-0.6304912	-1.7968626
N	0.4142782	0.8973476	-1.1435634
C	-0.8309960	0.9653388	-1.6267998
O	-1.7106110	1.6144723	-0.8255078
H	-2.5440157	1.5632824	-1.3246093

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G92C2B TS

N	-1.4412896	1.3633421	0.9098713
C	-0.5123434	1.5826750	-0.0377588
N	0.4758826	2.5399378	-0.0831477
H	0.7367308	3.1530247	0.6836016
C	1.2029732	2.3124404	-1.2324791
H	2.0642799	2.9288901	-1.4898447
N	0.7439072	1.3006813	-1.9669611
C	-0.3234877	0.8411539	-1.2177971
C	-1.1777497	-0.2677003	-1.3764522
O	-1.0421918	-1.1308647	-2.4088591
H	-0.3021251	-0.7793196	-2.9360800
N	-2.1224136	-0.5279337	-0.4833601
C	-2.2132759	0.3068680	0.5953435
N	-3.2766250	0.0433694	1.4405171
H	-3.5997061	-0.9184998	1.3984860
H	-3.1462769	0.4021067	2.3819067
N	2.4494928	0.0951542	0.6800166
C	2.6211819	-0.8074951	-0.3094506
H	3.4985578	-0.6549751	-0.9494654
C	1.7484076	-1.8648053	-0.5514867
H	1.9108888	-2.5678291	-1.3723013
C	0.6417001	-1.9827448	0.3174705
N	-0.2797700	-3.0076748	0.1917214
H	-1.1759248	-2.7353669	0.5947572
H	-0.4107643	-3.2977469	-0.7760543
N	0.4622706	-1.1208562	1.3361896
C	1.3659822	-0.1304668	1.4314305
O	1.1515132	0.7830409	2.4068971
H	0.2581912	0.5778415	2.7335291

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G19C1W1 HB

O	-1.6898301	-0.0457317	0.8030593
C	-0.5437513	-0.0464296	1.2916674
C	-0.1597485	0.0217427	2.6774780
N	-0.9287681	0.1115440	3.8255758
C	-0.0318854	0.1477257	4.8058894
H	-0.2662905	0.2199439	5.8678332
N	1.2667479	0.0878002	4.3482256
H	2.1165786	0.0960652	4.9034277
C	1.2127639	0.0049828	2.9763709
N	2.2811198	-0.0741641	2.1419894
C	1.8978039	-0.1428536	0.8728953
N	2.8284145	-0.3061169	-0.1094259
H	3.7736059	-0.0960126	0.1934679

H	2.5885282	-0.0549351	-1.0767236
N	0.5814813	-0.1201353	0.4615072
H	0.3793521	-0.1326433	-0.5620456
C	0.9814362	0.1370357	-3.2365343
O	2.1626794	0.2368945	-2.8865775
N	0.6804911	0.1861384	-4.6098466
H	1.4782795	0.2994352	-5.2291791
C	-0.5885923	0.0920962	-5.0987477
H	-0.7036718	0.1419210	-6.1848434
C	-1.6403034	-0.0549637	-4.2392134
H	-2.6645422	-0.1294319	-4.6073461
C	-1.3270882	-0.1003405	-2.8274820
N	-2.3105439	-0.2381513	-1.9275447
H	-2.0950993	-0.1912641	-0.9159707
H	-3.2741198	-0.2505996	-2.2358377
N	-0.0694234	-0.0188033	-2.3690141
O	-3.7976714	0.0866338	2.8945883
H	-3.0592802	0.1185709	3.5212441
H	-3.2859056	0.0342519	2.0739802

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G19C2AW1 HB

C	-1.7940496	-1.3453670	-0.2546132
N	-2.8609093	-0.5188411	-0.5120216
H	-2.7629193	0.4600653	-0.2407864
H	-3.7434662	-0.9436711	-0.2419814
N	-0.5516943	-0.7501800	-0.2692331
H	-0.4975098	0.2825719	-0.3659219
C	0.6819737	-1.4089847	-0.1209042
O	1.7442435	-0.7681852	-0.1696487
C	0.4909588	-2.8220474	0.0683402
C	-0.8253560	-3.3117673	0.0732751
N	-1.9994108	-2.6404892	-0.0786562
N	-0.6865478	-4.6644823	0.2704419
H	-1.4480006	-5.3337512	0.3228708
C	0.6661138	-4.9214708	0.3710277
H	1.0450016	-5.9310175	0.5313505
N	1.4179249	-3.8317999	0.2539762
C	0.9363319	2.8051464	-0.2630445
N	1.9626904	2.0386145	-0.6973533
H	2.9064748	2.2954398	-0.4182961
H	1.8161078	1.0230410	-0.6510832
C	1.0975863	4.1743806	0.0872406
H	2.0809032	4.6495411	0.0608742
C	-0.0379383	4.8746199	0.4601901
H	0.0237771	5.9318491	0.7423811
N	-1.2758807	4.3194643	0.5053945
C	-1.2965668	3.0343155	0.1573780
O	-2.5144880	2.4219171	0.1967967
H	-3.1218175	3.1219989	0.4934345
N	-0.2957608	2.2331621	-0.2239880
O	4.2986487	0.5236659	0.1958965
H	4.7129843	0.1169860	-0.5762356
H	3.5549527	-0.0833104	0.3468465

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G19C2BW1 HB

C	-1.8779929	-1.2337140	0.1148971
N	-2.8987979	-0.3179580	0.2656077
H	-2.7031612	0.6345286	-0.0392146
H	-3.7894178	-0.6829629	-0.0599633
N	-0.6061876	-0.7230204	0.1655009
H	-0.4878097	0.3100909	0.2100523
C	0.5991525	-1.4552228	0.1131199
O	1.6843555	-0.8671658	0.1611041



C	0.3123673	-2.8695897	0.0029123
N	1.1659525	-3.9553162	-0.0776552
C	0.3481436	-4.9998345	-0.1717808
H	0.6645488	-6.0395432	-0.2532785
N	-0.9813029	-4.6406801	-0.1573952
H	-1.7862951	-5.2567027	-0.2116818
C	-1.0323976	-3.2708622	-0.0447973
N	-2.1684969	-2.5188885	0.0016773
C	0.7449730	4.7163432	-0.0607684
N	1.0966617	6.0426677	-0.0808076
H	0.3905987	6.6583252	-0.4741333
H	2.0501404	6.2578338	-0.3525102
N	-0.5708198	4.4420501	-0.1725159
C	-0.9015378	3.1497408	-0.0818183
O	-2.2195275	2.8487429	-0.1959772
H	-2.6641992	3.7056805	-0.3116199
N	-0.1039105	2.0965492	0.0978209
C	1.2165303	2.3867465	0.1936128
H	1.8747135	1.5195278	0.3213978
C	1.6988281	3.6874253	0.1256486
H	2.7664046	3.9019497	0.2129377
O	3.9521784	-2.7879293	-0.0799903
H	3.4065151	-1.9932750	0.0143915
H	3.2456698	-3.4507858	-0.0963284

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G17C1W1 HB

C	0.5550561	1.2763806	-0.0641757
O	1.7242990	0.7991231	-0.0523018
C	0.1683298	2.6462885	0.0349410
C	-1.1868954	3.0360480	0.0257613
N	-2.2399560	2.1704505	-0.0989064
C	-1.8726264	0.9097666	-0.2068045
H	-3.7467228	0.2533802	-0.2066431
N	-2.8106691	-0.0687690	-0.4364922
H	-2.5950498	-1.0184143	-0.1135730
N	0.8983129	3.7987101	0.1807699
H	1.9299538	3.8192906	0.2080311
C	-0.0202844	4.8109130	0.2496444
H	0.2891755	5.8499452	0.3667388
N	-1.2884396	4.4021060	0.1613717
N	-0.5562656	0.4632095	-0.1822760
H	-0.3719229	-0.5627137	-0.2054250
N	0.0639183	-2.3750656	-0.0339586
C	-0.9943116	-3.2309766	0.1578497
O	-2.1694252	-2.8708014	0.2595731
N	-0.6979671	-4.6052998	0.2455954
H	-1.4990474	-5.2162976	0.3804676
C	0.5660799	-5.1047433	0.1529490
H	0.6749190	-6.1899096	0.2303388
C	1.6222180	-4.2555073	-0.0229844
H	2.6436260	-4.6315832	-0.0963436
C	1.3152558	-2.8445963	-0.1060118
N	2.3061169	-1.9536117	-0.2814663
H	3.2664424	-2.2692219	-0.2388053
H	2.0981376	-0.9415624	-0.2204522
O	3.5179494	2.9099162	0.0584802
H	3.0155164	2.0646459	0.0974168
H	3.7986035	2.9296264	-0.8667492

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G17C2AW1 HB

N	-2.2467121	-0.0380234	2.2172168
C	-1.1840323	-0.0490630	3.0799862
N	-1.2712950	-0.1002747	4.4518655

C	0.0024360	-0.0933377	4.8546436
H	0.3226303	-0.1258927	5.8964564
N	0.9103870	-0.0423489	3.8327877
H	1.9424165	-0.0097525	3.8466520
C	0.1670883	-0.0103786	2.6796650
C	0.5439080	0.0307941	1.3047232
O	1.7065284	0.0554396	0.8204417
N	-0.5780795	0.0381861	0.4898703
H	-0.3993369	0.0545133	-0.5318630
C	-1.8910563	0.0067483	0.9496865
N	-2.8469371	0.0271082	-0.0204175
H	-2.6292699	0.0663054	-1.0099929
H	-3.8058395	-0.0071536	0.2976090
N	-0.7244470	0.0201116	-4.7412853
C	0.5666768	-0.0778434	-5.1458860
H	0.7287453	-0.1159335	-6.2291407
C	1.6378847	-0.1282633	-4.2697419
H	2.6661749	-0.2069316	-4.6309721
C	1.3452964	-0.0720763	-2.8775732
N	2.3086071	-0.1111332	-1.9375125
H	2.0743835	-0.0538209	-0.9356094
H	3.2750752	-0.1861098	-2.2245263
N	0.0592701	0.0242203	-2.4526270
C	-0.8674221	0.0620591	-3.4176678
O	-2.1444065	0.1558354	-2.9560161
H	-2.6895023	0.1792681	-3.7619214
O	3.5174511	0.1516634	2.9299107
H	3.0239526	0.0425340	2.0869558
H	3.7785650	1.0818494	2.8885445

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G17C2BW1 HB

C	0.6081229	-0.1046206	-1.4498900
O	1.7232463	-0.1342483	-0.8826053
N	-0.5738989	-0.1949864	-0.7245865
C	-1.8494616	-0.1530423	-1.2607776
N	-2.8692729	-0.3528412	-0.3391875
H	-3.7599503	-0.0469905	-0.7246457
H	-2.6951657	0.0221307	0.5928445
N	-2.1335166	-0.0177005	-2.5356173
C	-1.0146948	0.0674074	-3.3293440
C	0.3086005	0.0207013	-2.8466507
N	1.1197293	0.1480811	-3.9441541
H	2.1513483	0.1387515	-3.8874806
C	0.2779241	0.2605036	-5.0177319
H	0.6624471	0.3733261	-6.0317111
N	-1.0182033	0.2182300	-4.6964142
H	-0.4671892	-0.2478673	0.3078452
O	-2.2231465	0.1638682	2.8638039
H	-2.6713987	0.2728903	3.7197210
C	-0.9060463	0.0720462	3.1643748
N	-0.5743412	0.1721284	4.4562518
C	0.7426679	0.0863542	4.7307490
N	1.0939363	0.1150770	6.0576028
H	0.3789152	0.4962107	6.6708267
H	2.0400801	0.4122805	6.2716537
C	1.6998541	-0.0830014	3.7020859
H	2.7690322	-0.1479633	3.9167154
C	1.2165274	-0.1650418	2.4023748
H	1.8766584	-0.2823978	1.5348888
N	-0.1044439	-0.0972269	2.1109032
O	3.6538340	-0.0262610	-2.8605984
H	3.1010433	0.0143274	-2.0462050
H	3.9546757	-0.9452055	-2.8472748

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G91C1W1 HB

H	-0.1435274	-0.9543992	-4.7602282
O	-0.1288759	0.0427839	-4.6860537
C	-0.0421123	0.4026434	-3.4112249
N	-0.0049504	1.7163237	-3.1694972
C	0.0213391	-0.4990789	-2.3103366
C	0.1205232	0.0958794	-1.0369873
C	0.0873895	2.1500354	-1.8887100
N	0.1543401	1.4195874	-0.7606111
N	0.0591082	3.5352462	-1.7358541
H	0.6060142	3.8490462	-0.9374571
H	0.3361318	4.0011211	-2.5972719
N	0.0179917	-1.8827415	-2.1949391
N	0.1779961	-0.9436261	-0.1448719
C	0.1102361	-2.0942257	-0.8777138
H	0.1350526	-3.0744799	-0.4017638
H	0.2115236	-0.8195430	0.8947672
O	0.2401703	-2.4859367	2.9954990
C	0.1057410	-1.3329650	3.3904000
N	0.1150792	-0.2316415	2.5582699
N	-0.0765812	-1.0732505	4.7681674
H	-0.0804335	-1.8917898	5.3707195
C	-0.2634653	0.1772119	5.2751007
H	-0.4031293	0.2545670	6.3569664
C	-0.2699568	1.2620944	4.4429938
H	-0.4151600	2.2709010	4.8321016
C	-0.0685117	1.0009659	3.0339034
N	-0.0418249	2.0274396	2.1616011
H	0.0289099	1.8535581	1.1444332
H	-0.2900070	2.9531638	2.4858939
O	-0.2335086	-2.6126815	-4.8065288
H	-0.0819188	-2.6632937	-3.8311689
H	-1.1689064	-2.8489043	-4.8813791

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G91C2AW1 HB

C	-0.1205220	-2.1484536	1.8993002
N	-0.1204948	-3.5314609	1.7503454
H	-0.6005321	-3.8373771	0.9077462
H	-0.4674974	-3.9934491	2.5876782
N	-0.0934297	-1.4181120	0.7688188
C	-0.0365384	-0.0973708	1.0479382
N	-0.0054278	0.9424320	0.1525156
H	0.0008892	0.8229726	-0.8833298
C	0.0457409	2.0931346	0.8888013
H	0.0774056	3.0747351	0.4161578
N	0.0486744	1.8815188	2.2081751
C	-0.0019324	0.4985516	2.3236496
C	-0.0393422	-0.4023255	3.4270306
O	-0.0283982	-0.0423039	4.7042972
H	0.0217352	0.9533765	4.7805185
N	-0.0999439	-1.7139957	3.1834771
C	-0.1163940	1.2097077	-3.5185088
O	-0.2613548	2.4449616	-2.9851579
H	-0.3465184	3.0310411	-3.7566094
N	0.0164404	0.2434441	-2.5999867
C	0.1719280	-1.0179973	-3.0655604
N	0.3391133	-2.0041662	-2.1565062
H	0.3567958	-2.9615446	-2.4834120
H	0.1892647	-1.8300898	-1.1515775
C	0.1844611	-1.2584151	-4.4673384
H	0.3078100	-2.2658645	-4.8722567
C	0.0328391	-0.1594280	-5.2990751
H	0.0324415	-0.2839074	-6.3881730

N	-0.1219436	1.1099981	-4.8482509
O	0.1826361	2.6061494	4.8355093
H	0.0883749	2.6661070	3.8545071
H	1.1215997	2.8009494	4.9650965

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G91C2BW1 HB

C	1.5292405	2.9974472	-0.1561379
N	2.8911520	3.1489929	-0.3216862
H	3.2396484	4.0551992	-0.0260819
H	3.4416396	2.3441811	-0.0275284
N	0.8072815	4.1547474	-0.1403552
C	-0.5133653	4.0535444	-0.0602740
O	-1.2218946	5.1994662	-0.0355005
H	-2.1532646	4.9228578	0.0246079
C	-1.1395223	2.7900362	0.0031471
N	-2.4660205	2.4100519	0.0995652
C	-2.3827747	1.0774838	0.1485190
H	-3.2342864	0.4008136	0.2234558
N	-1.0967988	0.5892550	0.0923553
H	-0.7889959	-0.4044985	0.1166609
C	-0.2749673	1.6822757	-0.0037683
N	1.0712466	1.7311969	-0.0803300
C	0.3314353	-4.8351159	-0.1109766
N	0.5068508	-6.1841878	-0.2972698
H	-0.3183945	-6.7437306	-0.1014633
H	1.3792253	-6.5802856	0.0362735
N	-0.9412404	-4.3921419	-0.0942636
C	-1.0947769	-3.0675662	0.0181786
O	-2.3618439	-2.5970002	0.0307095
H	-2.9220719	-3.3852381	-0.0686839
N	-0.1517911	-2.1264113	0.1273154
C	1.1220631	-2.5899667	0.1160164
H	1.9148043	-1.8369180	0.2055416
C	1.4226648	-3.9414916	-0.0032003
H	2.4576660	-4.2906272	-0.0208333
O	3.2496346	0.0485072	0.4556803
H	2.4164659	0.4990406	0.1816455
H	3.1620331	0.0765560	1.4187813

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G92C1W1 HB

C	-1.4575886	-0.1353693	3.0372583
N	-2.8348497	-0.1746009	3.2548328
H	-3.3181712	-0.7250827	2.5485712
H	-3.0490772	-0.4971223	4.1958990
N	-0.6991380	-0.0177752	4.1600930
C	0.6240236	0.0827835	4.0258029
O	1.3663980	0.2003671	5.1383256
H	0.7142313	0.1924894	5.8616117
N	-1.0371545	-0.1654010	1.7642147
C	0.3118596	-0.0675862	1.6775603
C	1.2247096	0.0589958	2.7498402
N	2.5292833	0.1298644	2.2971485
C	2.3843456	0.0475502	0.9729468
H	3.2049554	0.0690031	0.2551367
N	1.0825209	-0.0750138	0.5484284
H	0.7014218	-0.1149191	-0.4212974
C	-1.6791365	0.0873926	-2.0115728
N	-2.4178668	0.1131729	-0.8859072
H	-1.9750121	0.0138885	0.0414933
H	-3.4183991	0.2445977	-0.9510639
N	-0.3558828	-0.0557315	-1.8856781
C	0.4558126	-0.0777956	-2.9926456
O	1.6874433	-0.2009101	-2.9105092

N	-0.1550327	0.0482552	-4.2497903
H	0.4957314	0.0259369	-5.0512380
C	-1.4986335	0.1840643	-4.3957011
H	-1.8721799	0.2681701	-5.4201809
C	-2.3188033	0.2117220	-3.2993510
H	-3.3993710	0.3208803	-3.4034046
O	2.2480759	-0.1356983	-5.6261651
H	2.3754264	-0.2758223	-4.6631766
H	2.6899898	0.7129710	-5.7663361

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G92C2AW1 HB

C	-1.5301142	0.3884287	1.4136489
N	-2.4687122	0.7501899	0.4785132
H	-2.1860064	0.5542212	-0.4890496
H	-3.4088260	0.4598400	0.7297504
N	-0.2428322	0.3701544	1.0146055
C	0.6128561	0.0545255	2.0149479
N	1.9778287	-0.0644344	1.9633191
H	2.5778596	0.0810423	1.1282117
C	2.3766498	-0.4059921	3.2384502
H	3.4295225	-0.5650612	3.4742244
N	1.3828984	-0.5180085	4.1175376
C	0.2664986	-0.2289127	3.3527901
C	-1.1180005	-0.1697954	3.6247789
O	-1.5848047	-0.4217302	4.8571353
H	-2.5492444	-0.3132247	4.7728794
N	-1.9940610	0.1307720	2.6690508
C	0.0758490	-0.3005711	-4.6415765
N	0.7658189	-0.3873409	-5.8320015
H	1.7743224	-0.4251663	-5.7055078
H	0.4086923	-1.0588063	-6.5044841
C	-1.3096115	-0.5794387	-4.5613861
H	-1.8856714	-0.9189579	-5.4253876
C	-1.9006448	-0.3883588	-3.3194798
H	-2.9698964	-0.5845181	-3.1748182
N	-1.2256259	0.0447035	-2.2307315
C	0.0861424	0.2713281	-2.4336541
N	0.7764261	0.1177795	-3.5757325
O	0.8161000	0.7015344	-1.3988284
H	0.2855888	0.6217051	-0.5313924
O	3.3887398	0.3815073	-0.4184226
H	2.6098877	0.3806057	-1.0102843
H	3.6948182	1.2957003	-0.4971117

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G92C2BW1 HB

C	1.4205219	1.6396779	0.0817377
N	0.7407298	2.8318564	0.1317724
H	-0.2709086	2.8046671	0.2942572
H	1.2257323	3.5343928	0.6823931
N	0.7103331	0.5680678	-0.4004991
C	1.2945768	-0.6361607	-0.4928103
O	0.5822008	-1.6768636	-0.9155803
H	-0.3793079	-1.3811289	-0.9141017
C	2.6574429	-0.7649364	-0.1439250
N	3.5386445	-1.8353823	-0.1357780
C	4.6674286	-1.2900377	0.3027517
H	5.6059317	-1.8279164	0.4415895
N	4.5640184	0.0593597	0.5804178
H	5.2927916	0.6751144	0.9265617
C	3.2673835	0.4272742	0.3001569
N	2.7111218	1.6419997	0.4514919
C	-2.6907281	-1.8602158	0.3054932
N	-2.1799561	-3.1316130	0.4058612

H	-2.4956495	-3.6788859	1.1999570
H	-1.1816584	-3.2054391	0.2182501
C	-3.9284747	-1.4837985	0.8729229
H	-4.5354471	-2.1836182	1.4519343
C	-4.3241738	-0.1649079	0.6741830
H	-5.2631209	0.2000909	1.1070880
N	-3.6056687	0.7433976	-0.0217685
C	-2.4661151	0.2732915	-0.5536742
N	-1.9822399	-0.9822253	-0.4301801
O	-1.7418468	1.1340508	-1.2647905
H	-0.7738687	0.8816051	-1.0939625
O	-2.2126861	3.4107422	0.3947733
H	-2.1322775	3.4391705	-0.5697257
H	-2.8363021	2.6665075	0.4712641

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G19C1W1 ST

N	-0.2542793	1.1465772	-2.7623390
C	-0.9519718	0.1412202	-3.3982587
H	-1.6083583	0.3474406	-4.2439011
N	-0.7225140	-1.0636932	-2.8803295
C	0.1758853	-0.8139621	-1.8628081
C	0.7378985	-1.7158421	-0.8789180
O	0.5555136	-2.9145148	-0.6934120
N	1.6171870	-0.9833934	-0.0304442
H	2.0613449	-1.5446800	0.6952944
C	1.7632401	0.3814369	0.0451429
N	2.5399320	0.8374323	1.0966947
H	2.2019944	0.4363573	1.9783074
H	2.4400122	1.8504112	1.1703752
N	1.2350769	1.2145850	-0.8323076
C	0.4798500	0.5529608	-1.7643720
H	-0.2859201	2.1423924	-2.9644776
N	-1.4734367	1.0431434	0.9164668
C	-2.0582388	-0.0732190	0.4098251
H	-2.7641049	0.0690823	-0.4138370
C	-1.7459710	-1.3034499	0.9257538
H	-2.1917084	-2.2185571	0.5355555
C	-0.7221926	-1.3191205	1.9325867
N	-0.3168992	-2.5350675	2.4257691
H	0.5230260	-2.4821125	2.9970825
H	-0.3200020	-3.2957213	1.7489003
N	-0.1394692	-0.2307959	2.4278432
C	-0.5041874	1.0085968	1.9352604
O	0.0165123	2.0665408	2.3120252
H	-1.5320923	1.9492327	0.4269779
O	-0.5258508	3.4758568	-0.0933094
H	-0.3473341	3.4876205	0.8656229
H	0.2218747	2.9171948	-0.3813915

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G19C2AW1 ST

N	-0.4172075	0.5306965	2.3941875
C	0.8684160	0.0654513	2.5134823
H	1.5551383	0.4557679	3.2639221
N	1.1540663	-0.8997178	1.6390818
C	-0.0028258	-1.0241502	0.8967135
C	-0.2906374	-1.8761491	-0.2350974
O	0.4155778	-2.6943291	-0.8219266
N	-1.6255406	-1.6480724	-0.6606965
H	-1.9293479	-2.2527972	-1.4232378
C	-2.5131762	-0.7258539	-0.1529915
N	-3.7673358	-0.7103453	-0.7537324
H	-3.7151865	-0.6862493	-1.7723194
H	-4.2906055	0.0967617	-0.4161978

N	-2.2623071	0.0558320	0.8731954
C	-0.9968795	-0.1422369	1.3495667
H	-0.8095377	1.3542946	2.8421957
N	-0.7703990	1.5264383	-1.4740034
C	0.0153749	0.6932212	-2.1987442
H	-0.4533982	0.2287748	-3.0755459
C	1.3358347	0.4144862	-1.8754711
H	1.9414478	-0.2776438	-2.4635490
C	1.8688466	1.0804357	-0.7418442
N	3.1789648	0.8987891	-0.3784495
H	3.3577281	1.2567957	0.5582064
H	3.4746959	-0.0807644	-0.4884458
N	1.1188964	1.9334122	-0.0134982
C	-0.1487812	2.0734799	-0.4190499
O	-0.9060933	2.8673363	0.3809802
H	-1.7952852	2.7972307	-0.0067391
O	3.1974376	-1.9898167	-0.1508574
H	2.7442283	-1.7427967	0.6766105
H	2.4500403	-2.4116490	-0.6083976

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G19C2BW1 ST

N	-3.3686442	-0.8161476	0.2083040
C	-3.5122112	-0.2679333	-1.0458930
H	-4.3308903	-0.5482737	-1.7089313
N	-2.5657465	0.6290884	-1.3289835
C	-1.7802925	0.6510997	-0.1891899
C	-0.5532818	1.3764693	0.0787292
O	0.0538030	2.1778840	-0.6235977
N	-0.0495988	0.9934395	1.3508412
H	0.8931345	1.3281318	1.5711422
C	-0.5948144	0.0699115	2.2142209
N	0.0643939	-0.0949258	3.4066034
H	1.0697246	0.0892781	3.3731797
H	-0.2052361	-0.9501162	3.8840183
N	-1.7220897	-0.5871446	1.9862395
C	-2.2528840	-0.2465688	0.7794614
H	-3.9672088	-1.5073917	0.6503672
N	2.1373852	-1.2274767	0.0804508
C	0.9256213	-1.7827625	-0.1715524
H	0.5820977	-2.5362698	0.5467284
C	0.1291123	-1.4145721	-1.2488584
H	-0.8505822	-1.8667610	-1.4206730
C	0.6300786	-0.3933617	-2.0964634
N	-0.1129160	0.1185652	-3.1299884
H	0.2651899	1.0163021	-3.4317004
H	-1.1064976	0.2039127	-2.8940106
N	1.8710866	0.1014422	-1.9179117
C	2.5245101	-0.3321217	-0.8368331
O	3.7360523	0.2287288	-0.5993011
H	3.8372793	0.8811162	-1.3138103
O	2.7077938	0.3416135	2.3480291
H	3.5146684	0.8007910	2.0802827
H	2.6519242	-0.3787358	1.6803870

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G17C1W1 ST

N	-1.8573605	0.3833674	-1.0652588
C	-1.3555812	1.3439495	-0.2223621
N	-1.2092229	2.6814886	-0.5400973
C	-0.6646420	3.2212608	0.5531327
H	-0.4265700	4.2777366	0.6797261
N	-0.4406949	2.3051724	1.5500634
H	-0.0564018	2.4715023	2.4748838
C	-0.8693001	1.0954912	1.0694258

C	-0.7513577	-0.2323874	1.6195113
O	-0.2304912	-0.5723874	2.6835282
N	-1.3169189	-1.1389545	0.7118937
H	-1.1803393	-2.1390051	0.9119863
C	-1.8043685	-0.8283374	-0.5488764
N	-2.3226020	-1.9010456	-1.2414626
H	-1.8487242	-2.7866278	-1.0474860
H	-2.4123924	-1.6885773	-2.2315273
N	2.4078503	-0.3381106	0.7237260
C	2.5355584	0.9931192	0.4694981
H	3.0883834	1.5862997	1.2031979
C	1.9733647	1.5157389	-0.6633309
H	2.0606512	2.5741564	-0.9102986
C	1.2411601	0.5958666	-1.4964801
N	0.6313053	1.0808256	-2.6243576
H	-0.1012787	0.4484932	-2.9463219
H	0.2646940	2.0261643	-2.5081014
N	1.1542827	-0.7106916	-1.2589031
C	1.7502002	-1.2313452	-0.1369045
O	1.7328070	-2.4300978	0.1793354
H	2.7510028	-0.7465023	1.5898926
O	-0.5869889	-3.8003214	0.0718709
H	-0.4284431	-4.6006972	0.5876548
H	0.3121356	-3.4033353	-0.0238100

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G17C2AW1 ST

N	-1.4204091	-0.8148409	-0.5586058
C	-0.6875216	-1.9725383	-0.6514796
N	-0.5639576	-2.7365036	-1.7962924
C	0.2670551	-3.7209961	-1.4454783
H	0.5899037	-4.5332793	-2.0969991
N	0.6928484	-3.6272281	-0.1445387
H	1.3145876	-4.2564503	0.3543405
C	0.0934075	-2.5099955	0.3816149
C	0.2654894	-1.8542935	1.6561463
O	0.9694316	-2.1930400	2.6052817
N	-0.5133509	-0.6837652	1.6581271
H	-0.3792699	-0.0524213	2.4573697
C	-1.2871227	-0.2198963	0.6085450
N	-2.0045400	0.9295365	0.8775483
H	-1.5975186	1.5332553	1.5912322
H	-2.2702039	1.4138219	0.0234251
N	-0.2406701	3.4764377	-0.7524547
C	-0.6884994	2.8982472	-1.8968473
H	-1.4491440	3.4574785	-2.4536364
C	-0.2286183	1.6723136	-2.3559717
H	-0.6116748	1.2208911	-3.2734008
C	0.7641359	1.0276682	-1.5749257
N	1.3569258	-0.1394922	-1.9876456
H	1.8471087	-0.6100530	-1.2285413
H	0.7428485	-0.7753840	-2.4968148
N	1.2160762	1.5721102	-0.4264794
C	0.6776145	2.7524169	-0.1107324
O	1.1370690	3.2870656	1.0646957
H	0.6762361	4.1440498	1.1145583
O	-0.1582068	1.7604244	3.0823422
H	0.0269104	2.0276536	3.9915108
H	0.5301894	2.2072772	2.5549883

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G17C2BW1 ST

N	0.6138938	-0.3204123	-1.5869497
C	1.7593538	-0.3490039	-0.8310142
N	2.6056906	-1.4367355	-0.7204265



C	3.5209119	-1.0548837	0.1756212
H	4.3697542	-1.6557782	0.5023349
N	3.3042084	0.2132221	0.6510830
H	3.8607869	0.7278062	1.3274045
C	2.1826809	0.6827582	0.0174392
C	1.3835676	1.8564598	0.2776337
O	1.5916603	2.7561765	1.0895278
N	0.2448560	1.8106757	-0.5443839
H	-0.4687022	2.5251879	-0.3580373
C	-0.1057798	0.7653542	-1.3864893
N	-1.2824484	0.9526666	-2.0824140
H	-1.9797607	1.5036845	-1.5736690
H	-1.6353678	0.0658780	-2.4348003
N	-2.0864209	0.1482015	1.2820372
C	-0.8540457	-0.1125362	1.7893269
H	-0.4714702	0.6150663	2.5148245
C	-0.0912692	-1.2088404	1.4129922
H	0.8965214	-1.3965162	1.8405580
C	-0.6349498	-2.0517297	0.4093792
N	0.0664632	-3.1180098	-0.0912716
H	-0.3407742	-3.4496505	-0.9644563
H	1.0669093	-2.9249758	-0.1991424
N	-1.8814818	-1.8467944	-0.0616937
C	-2.5176887	-0.7663982	0.4060707
O	-3.7531646	-0.5315189	-0.0961620
H	-3.9120002	-1.2809410	-0.6950537
O	-2.4375065	2.6195833	0.0129939
H	-3.2147294	3.1670206	0.1802537
H	-2.5175232	1.8755907	0.6528748

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G91C1W1 ST

N	-0.8034547	-2.3417529	-0.0662833
C	-1.3481406	-1.1161381	0.0337888
N	-2.3872030	-0.5943111	-0.7054364
H	-2.8063355	-1.0339535	-1.5187609
C	-2.5935055	0.6912393	-0.2673176
H	-3.3564414	1.3355939	-0.7035422
N	-1.7854210	1.0393210	0.7298235
C	-0.9852001	-0.0792550	0.9172264
C	0.1255054	-0.3555142	1.7645412
O	0.6766761	0.5133524	2.5997892
H	0.2397883	1.4285029	2.5030629
N	0.7022009	-1.5604518	1.6885910
C	0.2152939	-2.4676890	0.8014230
N	0.9469449	-3.6512267	0.7253906
H	1.4067534	-3.8680745	1.6070591
H	0.3874133	-4.4246702	0.3725543
N	1.9472582	0.9096037	-0.2571731
C	2.0707561	-0.3654527	-0.7167973
H	2.7846912	-1.0134489	-0.2033698
C	1.2932414	-0.7757946	-1.7673435
H	1.3382705	-1.8010994	-2.1356542
C	0.3780734	0.1994621	-2.2910005
N	-0.4833769	-0.1773192	-3.3096437
H	-0.8685416	0.6327239	-3.7936717
H	-0.1120375	-0.8798813	-3.9443115
N	0.2465411	1.4347504	-1.8322740
C	1.0113246	1.8372969	-0.7547516
O	0.9332475	2.9495767	-0.2278755
H	2.4455331	1.1997509	0.5822128
O	-0.3502587	2.8615055	2.2410517
H	0.1634574	3.1596687	1.4632396
H	-1.1482867	2.5213746	1.7848268

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G91C2AW1 ST

N	1.0792050	0.7366025	-1.9243647
C	1.3852736	0.3341712	-0.6826796
N	2.2008131	-0.7143939	-0.3105944
H	2.6174406	-1.3901051	-0.9436001
C	2.1931701	-0.7748746	1.0593382
H	2.7319874	-1.5464827	1.6076529
N	1.4617360	0.1882688	1.6156464
C	0.9357714	0.8821718	0.5351760
C	0.0135746	1.9566520	0.4129565
O	-0.5683034	2.5770742	1.4454171
H	-0.3501632	2.0916013	2.2852039
N	-0.3321452	2.3799018	-0.8012648
C	0.2057108	1.7590854	-1.8865960
N	-0.2792882	2.2012254	-3.1080967
H	-0.6087286	3.1624213	-3.0757368
H	0.3555651	2.0091938	-3.8786650
N	-0.5004854	-2.2620540	-1.5415571
C	-1.3430170	-1.2304447	-1.7865444
H	-1.5272758	-0.9923092	-2.8402654
C	-1.9354643	-0.4801205	-0.7784517
H	-2.6014273	0.3559216	-1.0048110
C	-1.6111033	-0.8359069	0.5542803
N	-2.1629407	-0.1795103	1.6293065
H	-1.6365717	-0.2785999	2.4961345
H	-2.4368722	0.7831278	1.4491553
N	-0.7831867	-1.8642215	0.8295155
C	-0.2911210	-2.4976826	-0.2404697
O	0.5666642	-3.5129630	0.0499960
H	0.7498462	-3.9030289	-0.8218785
O	-0.1443595	1.0358098	3.6007647
H	0.2604827	1.3692755	4.4127155
H	0.5913455	0.5710762	3.1270642

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G91C2BW1 ST

N	-0.0079428	-0.2029797	1.5493412
C	1.0741171	-0.5125853	0.8053091
N	2.2436039	0.1901239	0.6430682
H	2.3946962	1.1846613	0.9148342
C	2.9979596	-0.5241623	-0.2587278
H	3.9806891	-0.1724974	-0.5758712
N	2.4315468	-1.6611438	-0.6771748
C	1.2234601	-1.6513856	-0.0097569
C	0.1183452	-2.5232054	-0.0545911
O	0.1100754	-3.6310713	-0.8253066
H	0.9876599	-3.6562378	-1.2465831
N	-0.9793577	-2.2565604	0.6442887
C	-0.9748352	-1.1221440	1.4049968
N	-2.1852101	-0.8697106	2.0610767
H	-2.6389368	-1.7375549	2.3431857
H	-2.0508702	-0.2384094	2.8492789
N	0.3432616	2.1468272	-1.0558179
C	0.2773265	1.0620561	-1.8638849
H	1.1487016	0.8829279	-2.5041846
C	-0.8027114	0.1867375	-1.8770615
H	-0.8134942	-0.6947928	-2.5229383
C	-1.8775635	0.4825112	-1.0046447
N	-3.0033222	-0.3065528	-0.9264078
H	-3.4279664	-0.2228852	-0.0008997
H	-2.8133471	-1.2849261	-1.1400472
N	-1.8541810	1.5842141	-0.2283453
C	-0.7408969	2.3187024	-0.2896549
O	-0.6770159	3.3854023	0.5465128

H	-1.5133198	3.3471607	1.0417062
O	2.3135998	2.9384075	0.8455894
H	1.6165357	3.2773632	1.4274529
H	1.8203252	2.9017406	-0.0015642

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G92C1W1 ST

N	1.7447723	0.6990956	0.4049309
C	1.2492898	-0.5352582	0.1780733
N	1.3868716	-1.3144720	-0.9416395
H	1.7537896	-1.0429129	-1.8779191
C	0.6394752	-2.4441733	-0.7146995
H	0.5572402	-3.2214715	-1.4753115
N	0.0570312	-2.4987592	0.4850987
C	0.4374663	-1.2980854	1.0532187
C	0.1327682	-0.6591659	2.2701805
O	-0.7035036	-1.2399189	3.1608447
H	-0.7329821	-0.6086134	3.9028244
N	0.6125668	0.5485713	2.5529251
C	1.3774319	1.1643317	1.6058827
N	1.7455428	2.4778449	1.9116147
H	1.8208184	2.6209574	2.9169119
H	2.6000658	2.7444333	1.4255104
N	-0.6757278	2.0495918	-1.2824978
C	-1.1291257	2.1787983	-0.0060084
H	-0.8915786	3.1086132	0.5164234
C	-1.8265676	1.1451598	0.5580036
H	-2.2098337	1.2104476	1.5767788
C	-1.9821231	-0.0391281	-0.2449504
N	-2.6813635	-1.0986340	0.2778048
H	-2.4577656	-1.9715183	-0.1991165
H	-2.6019162	-1.1951009	1.2888081
N	-1.5161276	-0.1639427	-1.4846612
C	-0.8228982	0.8805366	-2.0468623
O	-0.3121823	0.8609496	-3.1767252
H	-0.1000280	2.7727502	-1.7056026
O	1.8037290	-0.7809094	-3.5884164
H	2.3943711	-0.0781188	-3.8917218
H	0.9295602	-0.3294554	-3.6085642

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G92C2AW1 ST

N	-2.2646534	-0.2235960	0.8428563
C	-1.0316063	0.0167414	1.3207069
N	-0.3704371	-0.6479070	2.3280405
H	-0.6626909	-1.5358117	2.7266902
C	0.8743177	-0.0775996	2.4373123
H	1.6111278	-0.4440551	3.1519989
N	1.0640192	0.9497709	1.6106952
C	-0.1210871	1.0081507	0.8979298
C	-0.5889054	1.8063199	-0.1658087
O	0.1910238	2.7730761	-0.6988076
H	-0.3628048	3.1680932	-1.3972479
N	-1.7944205	1.6132721	-0.6816221
C	-2.5699092	0.6155180	-0.1581140
N	-3.8359622	0.5142992	-0.7046234
H	-3.8828467	0.8562478	-1.6604596
H	-4.2436648	-0.4088309	-0.5829569
N	-0.6495984	-1.5220518	-1.4841728
C	0.0827274	-0.6182697	-2.1767520
H	-0.4214048	-0.1413953	-3.0262716
C	1.3899261	-0.2842447	-1.8472006
H	1.9595960	0.4535673	-2.4156320
C	1.9660780	-0.9690794	-0.7472881
N	3.2731123	-0.7460356	-0.3873057

H	3.4770796	-1.1399015	0.5294313
H	3.5269381	0.2476236	-0.4535511
N	1.2649686	-1.8832519	-0.0459429
C	0.0037569	-2.0741293	-0.4522632
O	-0.7081435	-2.9333638	0.3206494
H	-1.6059199	-2.8816914	-0.0512397
O	3.1339672	2.1335456	-0.0533293
H	2.4534127	2.5622472	-0.5918904
H	2.5879851	1.8479495	0.7059154

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G19C1W1 TS

N	-4.8645335	0.6696250	-0.2145669
C	-4.8778052	0.3156327	-1.5487007
H	-5.7697676	0.4386209	-2.1634581
N	-3.7168547	-0.1732743	-1.9728904
C	-2.9170426	-0.1274255	-0.8444150
C	-1.5433272	-0.5297137	-0.6647438
O	-0.7780805	-1.0309662	-1.4970379
N	-1.1277156	-0.2839583	0.6598756
H	-0.1672506	-0.5609421	0.9092835
C	-1.9075139	0.2290913	1.6777831
N	-1.2724544	0.4109107	2.8786256
H	-0.4772834	-0.2112076	3.0480681
H	-1.9253645	0.5305485	3.6467298
N	-3.1738509	0.5890512	1.5385724
C	-3.6052743	0.3922331	0.2626271
H	-5.6264292	1.0621072	0.3289995
N	4.7132243	0.6640278	0.2688139
C	4.9522469	0.8715714	-1.0571377
H	5.9116902	1.3238996	-1.3222384
C	4.0067429	0.5145207	-1.9763263
H	4.1715383	0.6667426	-3.0441653
C	2.7854674	-0.0678515	-1.4596917
N	1.8259102	-0.4598975	-2.3146704
H	0.9088296	-0.7486449	-1.9406282
H	1.8969743	-0.2086263	-3.2921820
N	2.5653940	-0.2649665	-0.1551132
C	3.5227014	0.0906868	0.7517969
O	3.4126878	-0.0589185	1.9795802
H	5.3961077	0.9190560	0.9766868
O	1.0089585	-1.2076534	2.4593084
H	1.8815776	-0.7593717	2.3230436
H	1.1927665	-2.1084339	2.1632031

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G19C2AW1 TS

N	-0.2573944	-5.2038036	0.3828152
C	0.0110724	-5.0583723	1.7283589
H	-0.0095582	-5.9086621	2.4101822
N	0.2875602	-3.8050496	2.0749399
C	0.1953344	-3.1122793	0.8816068
C	0.3668292	-1.7047163	0.6060828
O	0.6194442	-0.7802801	1.3870957
N	0.1966946	-1.4576578	-0.7696894
H	0.3143411	-0.4826104	-1.0945851
C	-0.1551589	-2.3756426	-1.7301045
N	-0.2446187	-1.8722898	-3.0125054
H	-0.5026103	-0.8860420	-3.0532320
H	-0.7890998	-2.4769616	-3.6211147
N	-0.3490239	-3.6621341	-1.5034936
C	-0.1441927	-3.9585467	-0.1875299
H	-0.4930204	-6.0584730	-0.1114410
N	0.0492940	5.3844010	-0.1416385
C	-0.2227455	5.3994199	1.1865798

H	-0.3085471	6.3905283	1.6468405
C	-0.3795685	4.2526215	1.9489143
H	-0.5885182	4.3048146	3.0201494
C	-0.2497938	3.0036004	1.2809258
N	-0.4075521	1.8220457	1.9227182
H	-0.0313625	0.9617267	1.5046129
H	-0.3959599	1.8430706	2.9360963
N	-0.0020738	2.9698058	-0.0500021
C	0.1388664	4.1572623	-0.6559569
O	0.4143056	4.0640248	-1.9800856
H	0.4763374	4.9888621	-2.2744064
O	0.0383651	1.0001171	-2.0849993
H	0.7827504	1.4267761	-2.5335388
H	-0.1329191	1.6495929	-1.3627511

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G17C1W1 TS

N	1.5286631	3.1521472	-0.6210161
C	0.2644417	3.6406126	-0.4182599
N	-0.1535605	4.9242635	-0.7049631
C	-1.4323556	4.9401629	-0.3338262
H	-2.0970782	5.8008042	-0.4121276
N	-1.8681339	3.7409234	0.1752958
H	-2.7898909	3.5118987	0.5317926
C	-0.7906257	2.8929985	0.1285420
C	-0.6464547	1.5260479	0.5343945
O	-1.5231748	0.8042376	1.0439095
N	0.6547393	1.1001983	0.2803441
H	0.9192361	0.1467147	0.5734594
C	1.6643282	1.8935884	-0.2586839
N	2.8598483	1.2405331	-0.4616140
H	3.0489295	0.4843907	0.2004817
H	3.6204464	1.9003431	-0.5987071
N	0.2786987	-4.7044608	-0.6573733
C	-1.0423107	-4.9364069	-0.8991767
H	-1.2997453	-5.8904167	-1.3671335
C	-1.9668526	-3.9906451	-0.5556729
H	-3.0312747	-4.1507480	-0.7344916
C	-1.4590649	-2.7773115	0.0491878
N	-2.3209670	-1.8177241	0.4338556
H	-1.9481620	-0.9035568	0.7330035
H	-3.2899288	-1.8810478	0.1497267
N	-0.1602908	-2.5614885	0.2760317
C	0.7532037	-3.5197773	-0.0649197
O	1.9764259	-3.4133635	0.1136108
H	0.9901798	-5.3868053	-0.9043143
O	2.4141453	-0.9913002	1.2551252
H	2.3019969	-1.8699420	0.8139178
H	2.1587075	-1.1849099	2.1663081

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G17C2AW1 TS

N	-3.7109858	0.2700890	1.4966166
C	-4.0402423	0.0965800	0.1743075
N	-5.3147401	0.1757636	-0.3460731
C	-5.1481937	-0.0371402	-1.6498812
H	-5.9483626	-0.0529241	-2.3901077
N	-3.8372708	-0.2450759	-2.0051337
H	-3.4646693	-0.4321518	-2.9301482
C	-3.1093544	-0.1675734	-0.8456173
C	-1.6993385	-0.2781225	-0.5993468
O	-0.7932529	-0.4669364	-1.4293413
N	-1.4624820	-0.1391970	0.7643930
H	-0.4846376	-0.2139990	1.1009492
C	-2.4240564	0.1363766	1.7228441

N	-1.9259750	0.2053765	3.0153842
H	-0.9764968	0.5739452	3.0684111
H	-2.5814638	0.6805562	3.6312234
N	5.4113984	-0.1243098	0.1683353
C	5.4460145	0.1136537	-1.1653862
H	6.4424013	0.1436222	-1.6213653
C	4.3110856	0.3046742	-1.9386418
H	4.3786355	0.4857461	-3.0141004
C	3.0553993	0.2489614	-1.2749248
N	1.8835304	0.4508879	-1.9275659
H	1.0071525	0.1187085	-1.5072550
H	1.9123905	0.4028736	-2.9396706
N	3.0025026	0.0343128	0.0598779
C	4.1786960	-0.1463271	0.6776687
O	4.0651583	-0.3865219	2.0059115
H	4.9842032	-0.4866192	2.3081575
O	0.9888501	0.0544001	2.0540817
H	1.3800036	-0.6933260	2.5285334
H	1.6647796	0.2021329	1.3522786

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G17C2BW1 TS

N	-7.9809978	-3.4589990	8.3279977
C	-6.9769980	-3.2009991	9.1999974
N	-7.0149980	-3.3829991	10.5759970
C	-5.8389984	-2.9969992	11.0089969
H	-5.5759984	-3.0279992	12.0599966
N	-4.9859986	-2.5549993	10.0229972
H	-4.0389989	-2.2089994	10.0709972
C	-5.7499984	-2.7029992	8.8889975
C	-5.3719985	-2.3939993	7.5519979
O	-4.3189988	-1.9279995	7.1179980
N	-6.4069982	-2.6889992	6.6839981
H	-6.2479982	-2.5959993	5.6949984
C	-7.6239979	-3.1729991	7.0789980
N	-8.5289976	-3.3289991	6.1489983
H	-8.3889976	-3.0179992	5.1879985
H	-9.4189974	-3.6659990	6.4669982
N	-6.4249982	-2.6099993	3.6849990
C	-5.0689986	-2.6599993	3.6519990
H	-4.5649987	-3.6119990	3.5269990
C	-4.3769988	-1.5219996	3.8289989
H	-3.2999991	-1.5529996	3.8519989
C	-5.1219986	-0.3269999	3.9919989
N	-4.5079987	0.7869998	4.3009988
H	-5.0949986	1.5729996	4.4949987
H	-3.5659990	0.6969998	4.6649987
N	-6.4349982	-0.2699999	3.9429989
C	-7.0899980	-1.4199996	3.7729989
O	-8.4169976	-1.5139996	3.8119989
H	-8.7519975	-0.6199998	3.8449989
O	-2.5329993	-0.1520000	6.1189983
H	-1.7559995	-0.3679999	6.6489981
H	-3.1869991	-0.8009998	6.4659982

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G91C1W1 TS

N	0.2556354	0.7032173	-1.0134743
C	-0.5642518	0.1221535	-1.9205435
N	-1.9114597	-0.1201552	-1.8459316
H	-2.5492315	0.1543689	-1.0574117
C	-2.2535548	-0.7340506	-3.0288135
H	-3.2817899	-1.0374886	-3.2285796
N	-1.2350361	-0.9158834	-3.8742121
C	-0.1724758	-0.3762989	-3.1775616

C	1.1914594	-0.2359638	-3.5022823
O	1.6978712	-0.6669978	-4.6706205
H	0.9440608	-1.0502777	-5.1536901
N	2.0299090	0.3470319	-2.6503826
C	1.5211249	0.7765342	-1.4660084
N	2.4659825	1.3114270	-0.5826027
H	3.2998814	1.6113424	-1.0852533
H	2.0770893	2.0645846	-0.0166335
N	0.1705762	0.2199714	1.8876389
C	1.4234125	-0.2108961	2.1942982
H	2.1504664	-0.1853222	1.3771478
C	1.7139198	-0.6099430	3.4731975
H	2.7143936	-0.9438519	3.7523467
C	0.6305621	-0.5387989	4.4146797
N	0.8674756	-0.8564199	5.7316673
H	0.0174306	-1.0001992	6.2709463
H	1.6074544	-1.5262405	5.9136344
N	-0.5931215	-0.1275622	4.1124666
C	-0.8728595	0.2669639	2.8239570
O	-1.9969939	0.6535384	2.4740948
H	-0.0221048	0.5088673	0.9132147
O	-3.4779498	0.6320817	0.2281085
H	-3.7209782	1.5678108	0.2172661
H	-2.9584159	0.5672270	1.0658540

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G91C2AW1 TS

N	2.2529680	-0.4508920	1.0020433
C	1.2421909	-0.2740900	1.8691791
N	1.0213229	-0.9400696	3.0579081
H	1.6356279	-1.6335481	3.4731145
C	-0.1658821	-0.4675110	3.5722528
H	-0.5712334	-0.8372987	4.5145546
N	-0.7398435	0.4612837	2.8108334
C	0.1368873	0.5921039	1.7451017
C	0.1346293	1.3765401	0.5702370
O	-0.8798024	2.2143033	0.3124068
H	-0.8049748	2.4255749	-0.6421314
N	1.1299805	1.2692454	-0.3035243
C	2.1163895	0.3576811	-0.0635828
N	3.1058710	0.3124382	-1.0299760
H	2.7442507	0.5507636	-1.9521268
H	3.6223445	-0.5635211	-1.0143889
N	0.3783633	-0.1657638	-2.9862408
C	0.6542774	-1.4406462	-2.6154381
H	1.4853145	-1.9258060	-3.1419227
C	-0.0401613	-2.1170592	-1.6226378
H	0.2265782	-3.1373842	-1.3353635
C	-1.1198563	-1.4263540	-1.0070921
N	-1.9084084	-1.9870849	-0.0530204
H	-2.4720916	-1.3210986	0.5016684
H	-1.5506994	-2.8111072	0.4158180
N	-1.4376206	-0.1679728	-1.3884212
C	-0.6468001	0.3718759	-2.3161978
O	-0.9284545	1.6784757	-2.5828510
H	-0.2469520	1.9380370	-3.2273667
O	-3.1730728	0.2246306	1.2018429
H	-2.8140359	0.7347869	0.4570604
H	-2.5735418	0.4909242	1.9230886

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G92C1W1 TS

N	-0.9927552	-1.4972331	-0.4736063
C	-0.5918948	-0.5548448	-1.3537413
N	-1.3855167	0.2726977	-2.1016196

H	-2.4078232	0.3369777	-1.9161774
C	-0.5366065	1.1280315	-2.7551337
H	-0.9142246	1.9172403	-3.4062640
N	0.7619833	0.8965790	-2.5339581
C	0.7331923	-0.1680985	-1.6508860
C	1.7140962	-0.8511044	-0.9057534
O	3.0246618	-0.5441219	-1.0295373
H	3.4657915	-1.1672828	-0.4235476
N	1.3757768	-1.7896728	-0.0250832
C	0.0509087	-2.0573481	0.1526480
N	-0.2332619	-2.9723131	1.1681140
H	0.5194443	-3.6477531	1.2848333
H	-1.1320427	-3.4272937	1.0178511
N	-0.5581657	0.1711775	2.5967234
C	0.7789403	0.1560385	2.8435896
H	1.1203044	-0.4526686	3.6849074
C	1.6169077	0.8774594	2.0376163
H	2.6943882	0.8965121	2.2070082
C	1.0000427	1.5682548	0.9329941
N	1.8019320	2.2642103	0.0655427
H	1.3576347	2.4269239	-0.8395281
H	2.7423137	1.8900657	-0.0374046
N	-0.3098202	1.5930056	0.7093503
C	-1.1525079	0.9057541	1.5525535
O	-2.3830327	0.8739791	1.4480068
H	-1.1981138	-0.3942160	3.1483219
O	-3.7252644	-0.0275656	-0.7987792
H	-3.3521752	-0.8913910	-0.5572162
H	-3.3979061	0.5003328	-0.0395879

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G92C2AW1 TS

N	-2.0315823	1.1776044	0.7721215
C	-0.7376776	1.2393626	1.1329479
N	0.0232856	2.3712553	1.3381385
H	-0.2977932	3.3284988	1.2324107
C	1.2916293	1.9572995	1.6590078
H	2.0969965	2.6633315	1.8604753
N	1.4125022	0.6320672	1.6972572
C	0.1469117	0.1668585	1.3630294
C	-0.4210729	-1.1374594	1.2430011
O	0.2196673	-2.2742730	1.4466680
H	1.2144215	-2.1089801	1.5001828
N	-1.7078484	-1.2358590	0.8918801
C	-2.4125699	-0.1040616	0.6491763
N	-3.6810553	-0.3253547	0.0991261
H	-4.0857087	-1.1955998	0.4426136
H	-4.3001440	0.4699528	0.2496472
N	1.5157773	1.3178014	-1.6220862
C	0.2656455	1.7218112	-1.9537257
H	0.1254160	2.8028523	-2.0755640
C	-0.7965689	0.8448364	-2.1337831
H	-1.7970930	1.1990972	-2.3914759
C	-0.5241930	-0.5330171	-1.9457055
N	-1.4958197	-1.4914276	-2.1258814
H	-1.2499971	-2.3587182	-1.6488925
H	-2.4286619	-1.1748392	-1.8570542
N	0.7129176	-0.9642126	-1.6250232
C	1.6353671	-0.0074919	-1.4920046
O	2.8774736	-0.4677383	-1.1673546
H	3.4137877	0.3414032	-1.0958286
O	2.7766068	-1.7634463	1.4337459
H	2.6311365	-0.8334610	1.7087794
H	2.9235455	-1.6408971	0.4790502



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G19C1W2 HB

N	-1.2544139	0.0273455	5.0670915
C	-0.0377370	0.2752026	5.6702330
H	0.0500826	0.3971994	6.7500834
N	0.9707976	0.3446993	4.8075923
C	0.3625744	0.1279703	3.5835828
C	0.9247866	0.0869022	2.2566702
O	2.1077300	0.2377127	1.9142842
N	-0.0771239	-0.1609357	1.3010190
H	0.2420857	-0.1620535	0.3100786
C	-1.4162754	-0.3598203	1.5542933
N	-2.1865807	-0.6810276	0.4689839
H	-1.8647950	-0.3792091	-0.4581561
H	-3.1801283	-0.5745684	0.6480016
N	-1.9608957	-0.3187429	2.7617269
C	-1.0213484	-0.0734566	3.7156085
H	-2.1585016	-0.0740638	5.5167829
N	0.4227431	-0.0909152	-3.7755318
C	1.7490307	-0.1118309	-4.0760093
H	1.9988267	-0.1428706	-5.1403302
C	2.6918569	-0.0899112	-3.0841765
H	3.7584561	-0.1000359	-3.3140400
C	2.2012997	-0.0481435	-1.7292211
N	3.0543100	-0.0133763	-0.6962878
H	2.7027948	0.0629202	0.2777982
H	4.0502448	-0.0197576	-0.8736236
N	0.8854822	-0.0385673	-1.4507422
C	-0.0319293	-0.0431293	-2.4606574
O	-1.2648166	-0.0085528	-2.2360411
H	-0.2748596	-0.1184084	-4.5496439
O	-1.3701311	-0.0674300	-5.8850014
H	-1.7323732	-0.9324462	-6.1212306
H	-2.1141561	0.3389294	-5.3773064
O	-3.1478872	0.7992626	-4.0644710
H	-3.1743240	1.7477166	-3.8804713
H	-2.5570201	0.4620746	-3.3536937

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G19C2AW2 HB

C	1.4872809	-1.9945768	0.2363844
N	0.6920282	-3.0834478	0.4907155
H	1.1861861	-3.9606976	0.3565396
H	-0.2587896	-3.0644730	0.1195386
N	0.8312907	-0.7948412	0.0709983
H	-0.2126204	-0.7881821	0.0712578
C	1.4420700	0.4530887	-0.1085635
O	0.7427489	1.4744784	-0.2411156
C	2.8735549	0.3407735	-0.1059586
N	3.8464906	1.3142562	-0.2425058
C	4.9810441	0.6260626	-0.1636636
H	5.9810480	1.0550409	-0.2301826
N	4.7862006	-0.7290572	0.0150679
H	5.4973715	-1.4476841	0.1072196
C	3.4286992	-0.9388141	0.0581828
N	2.8043798	-2.1347963	0.2284620
C	-2.7661440	0.4853215	0.2216835
N	-2.0240443	1.5711303	0.4913138
H	-1.0203417	1.5094243	0.2864444
H	-2.4238652	2.5142945	0.4334321
N	-2.1114949	-0.6905357	0.0080940
C	-2.8838297	-1.7537042	-0.2359367
O	-2.1848655	-2.9051134	-0.4641553
H	-2.8770632	-3.5729483	-0.6123560
N	-4.2094846	-1.8533236	-0.2924004

C	-4.8494390	-0.6750721	-0.0659502
H	-5.9443804	-0.7115375	-0.1012215
C	-4.1915903	0.5145563	0.1928971
H	-4.7357927	1.4452365	0.3695285
O	-2.2852638	4.3891909	0.1375305
H	-1.3033572	4.4067337	0.0949114
H	-2.5226574	4.6507803	-0.7618510
O	0.4782653	4.2351162	-0.1546649
H	1.0246378	4.4749887	0.6051853
H	0.7477368	3.3090015	-0.3145905

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G19C2BW2 HB

C	0.0733084	-1.9002416	-1.8500867
N	0.2050163	-1.1535360	-3.0014622
H	-0.1596828	-1.6385302	-3.8162451
H	-0.0635548	-0.1720116	-2.9434007
N	0.1816063	-1.2053597	-0.6727578
H	0.2505682	-0.1652476	-0.7169429
C	0.1556539	-1.7469023	0.6294837
O	0.2551775	-1.0056801	1.6128867
C	0.0027308	-3.1847385	0.5640513
N	-0.0710654	-4.1271154	1.5745728
C	-0.2170140	-5.2799946	0.9277796
H	-0.3104293	-6.2575571	1.4004358
N	-0.2415664	-5.1257417	-0.4405734
H	-0.3387856	-5.8540031	-1.1409549
C	-0.1009397	-3.7824768	-0.7022733
N	-0.0786695	-3.2117219	-1.9397345
C	0.0002561	4.3672912	-0.1834269
N	-0.0434737	5.7142586	-0.0135001
H	-0.1803281	6.0708645	0.9320656
H	-0.4003861	6.2524685	-0.7950336
C	0.2239253	3.4886716	0.9100337
H	0.3178011	3.8774525	1.9245781
C	0.2995041	2.1343838	0.6283619
H	0.4521550	1.3779387	1.4068023
N	0.1764342	1.6439751	-0.6321671
C	-0.0399838	2.5651410	-1.5709947
O	-0.1833528	2.0676875	-2.8276554
H	-0.3297415	2.8486881	-3.3879134
N	-0.1402730	3.8914688	-1.4410777
O	0.0041011	-2.5419738	4.1457923
H	-0.0393024	-3.3086117	3.5548192
H	0.1129363	-1.8488409	3.4779185
O	-0.2922702	6.2817572	2.8792511
H	0.4997822	6.2428338	3.4322779
H	-0.9463716	5.8037261	3.4068731

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G17C1W2 HB

N	-1.9456115	2.7750688	-0.3540747
C	-1.0343577	3.7595943	-0.0739256
N	-1.3219986	5.1048940	0.0399967
C	-0.1465638	5.6676861	0.3128773
H	0.0162432	6.7341832	0.4703704
N	0.8878115	4.7663260	0.3828227
H	1.8657543	4.9528370	0.5780775
C	0.3367522	3.5342192	0.1375025
C	0.9160348	2.2250762	0.0934929
O	2.1134575	1.9229053	0.2733801
N	-0.0689569	1.2862139	-0.1889694
H	0.2400174	0.2905960	-0.1985194
C	-1.4098090	1.5724049	-0.4083683
N	-2.1750734	0.4895436	-0.7755487

H	-1.8821315	-0.4289249	-0.4256050
H	-3.1680666	0.6845570	-0.6822905
N	0.4170088	-3.7741859	-0.0731043
C	1.7414730	-4.0790073	-0.1062052
H	1.9875060	-5.1445215	-0.1262904
C	2.6881376	-3.0901101	-0.1084756
H	3.7537302	-3.3238208	-0.1292724
C	2.2015442	-1.7340889	-0.0760226
N	3.0604822	-0.7023719	-0.0688420
H	2.7146774	0.2687424	0.0409383
H	4.0547856	-0.8866788	-0.0445615
N	0.8887654	-1.4500688	-0.0566880
C	-0.0349445	-2.4573163	-0.0382108
O	-1.2641357	-2.2263486	0.0068452
H	-0.2830235	-4.5473478	-0.0773539
O	-1.3758330	-5.8783894	0.0088804
H	-1.7315816	-6.1444256	-0.8501580
H	-2.1255583	-5.3616453	0.3933519
O	-3.1719228	-4.0435099	0.7972220
H	-3.2405214	-3.8329232	1.7379454
H	-2.5762137	-3.3357680	0.4636564

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G17C2AW2 HB

N	-1.7312851	-0.1116130	2.6959764
C	-2.7047401	-0.0671812	1.7316430
N	-4.0551314	-0.0207014	1.9759498
C	-4.5953928	0.0049418	0.7548472
H	-5.6661323	0.0423906	0.5515118
N	-3.6857455	-0.0187915	-0.2666454
H	-3.9081904	-0.0245583	-1.2849813
C	-2.4558964	-0.0647028	0.3396461
C	-1.1247200	-0.0951760	-0.1743325
O	-0.7413155	-0.0897952	-1.3746387
N	-0.2013045	-0.1451922	0.8569315
H	0.7971250	-0.1493673	0.5689717
C	-0.5131936	-0.1582556	2.2072802
N	0.5729380	-0.3076331	3.0532954
H	1.4299748	0.1555278	2.7489877
H	0.3118440	-0.0703533	4.0078124
N	4.9106363	0.4344056	0.3891224
C	5.2159548	-0.0008515	-0.8579944
H	6.2775141	0.0277908	-1.1289418
C	4.2682825	-0.4566177	-1.7618308
H	4.5510488	-0.7963319	-2.7611022
C	2.9127405	-0.4609084	-1.3345649
N	1.9003622	-0.9179307	-2.1118017
H	0.9396287	-0.6490007	-1.8525251
H	2.0927624	-1.0380213	-3.0994876
N	2.5908902	-0.0402026	-0.0872355
C	3.6096526	0.3787935	0.6725430
O	3.2380663	0.8087839	1.9076568
H	4.0742247	1.0667106	2.3339063
O	-4.3321865	0.0271981	-2.9471088
H	-3.5119731	0.4116498	-3.3399869
H	-4.3764800	-0.8436614	-3.3643278
O	-1.8783103	0.8998893	-3.6475289
H	-1.4680173	0.5219070	-2.8372558
H	-1.7487291	1.8496017	-3.5231692

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G17C2BW2 HB

N	2.6052097	-0.0599261	-2.1258347
C	1.5693739	0.0167481	-3.0226351
N	1.7164480	0.0542575	-4.3886447

C	0.4618196	0.1340255	-4.8401979
H	0.1835485	0.1832640	-5.8935194
N	-0.4905827	0.1471942	-3.8592154
H	-1.5175928	0.2329072	-4.0044682
C	0.2002727	0.0736947	-2.6744360
C	-0.2243115	0.0429784	-1.3073335
O	-1.3807193	0.0750711	-0.8254495
N	0.8797135	-0.0265341	-0.4660316
H	0.6661507	-0.0480545	0.5497894
C	2.2012629	-0.0743469	-0.8744039
N	3.1168370	-0.1430237	0.1397040
H	2.8508722	-0.1519450	1.1163942
H	4.0903385	-0.1748936	-0.1288070
N	0.1388627	-0.0269558	2.3206763
C	-1.2010474	0.0849481	2.4847523
H	-1.7803798	0.1116235	1.5542941
C	-1.7951679	0.1611773	3.7381032
H	-2.8788768	0.2424909	3.8496006
C	-0.9318019	0.1259404	4.8591564
N	-1.4064532	0.1343239	6.1469591
H	-0.7088343	0.3651458	6.8487675
H	-2.3160200	0.5586720	6.2948070
N	0.4046423	0.0226360	4.7125428
C	0.8448836	-0.0513289	3.4520828
O	2.1848468	-0.1598248	3.2789127
H	2.5582576	-0.1649185	4.1766470
O	-3.7423941	-0.7359266	-1.8898553
H	-2.9079681	-0.3949546	-1.4908197
H	-3.6042495	-1.6921034	-1.8623790
O	-3.2179675	0.3335803	-4.3063152
H	-3.5565789	1.2335845	-4.2073656
H	-3.5513097	-0.1091001	-3.4883834

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G91C1W2 HB

N	-0.2663677	-2.6596992	3.8788648
C	-0.1813382	-1.3143187	3.5277612
H	-0.5998822	-2.7698904	4.8338380
H	-0.8127693	-3.2025153	3.2145316
N	-0.0679383	-0.4588612	4.5808656
N	-0.1721167	-1.0302491	2.2122131
C	0.0753145	0.8343738	4.3130802
O	0.1853371	1.6748076	5.3594567
H	0.2736173	2.5615006	4.9671100
C	0.1004560	1.2911237	2.9798080
N	0.2261621	2.5525140	2.4301518
C	-0.0301052	0.2980631	1.9918017
N	0.0163512	0.9741426	0.8016210
C	0.1715131	2.3022355	1.1175465
H	-0.0180156	0.5132240	-0.1358523
H	0.2384568	3.0584086	0.3350715
C	0.0464622	-1.9927588	-1.5025094
N	0.0156336	-2.6354815	-0.3194512
H	-0.0486993	-2.1145534	0.5696528
H	0.0658063	-3.6453863	-0.3029796
C	0.1222012	-2.7386149	-2.7334194
H	0.1496854	-3.8291835	-2.7527787
C	0.1609551	-2.0042007	-3.8892268
H	0.2206342	-2.4591526	-4.8822196
N	0.1235037	-0.6463486	-3.8570782
H	0.1795448	-0.1073187	-4.7477530
C	0.0386725	0.0630686	-2.6568540
O	0.0014098	1.3060618	-2.6533169
N	0.0034967	-0.6556658	-1.4885523
H	-0.5174548	2.3775985	-3.9692341

O	-0.6933671	2.8770687	-4.7987738
H	-0.1282985	3.6543175	-4.6992262
O	0.2355568	0.7884184	-6.2292919
H	-0.1581842	1.6252240	-5.8801766
H	1.1360400	1.0604657	-6.4525754

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G91C2AW2 HB

N	-1.1747333	-0.0553983	-0.6966013
C	-1.4489735	-0.0682501	0.6286943
N	-0.5748153	-0.0576454	1.6844180
H	0.4511298	-0.0937088	1.5739190
C	-1.3472268	-0.0733614	2.8265146
H	-0.8920928	-0.0729779	3.8170780
N	-2.6613932	-0.0858663	2.5921467
C	-2.7243902	-0.0855144	1.2100650
C	-3.8063213	-0.0842643	0.3007902
O	-5.0840086	-0.0725660	0.7199300
H	-5.0381158	-0.0675365	1.6924832
N	-3.5960501	-0.0948950	-1.0087483
C	-2.3032504	-0.0936820	-1.4482323
N	-2.1383313	-0.1809296	-2.7999208
H	-2.9603537	0.0355739	-3.3510925
H	-1.2151598	0.0219099	-3.1903979
N	4.4667577	0.1940464	1.1627036
C	4.8012543	-0.2736236	-0.0660333
H	5.8709459	-0.2667447	-0.3054518
C	3.8759860	-0.7430153	-0.9863573
H	4.1829292	-1.1236798	-1.9633074
C	2.5075253	-0.7216314	-0.6027920
N	1.5242560	-1.2284343	-1.3917952
H	0.5687843	-0.9235142	-1.1632825
H	1.7035691	-1.2112168	-2.3940918
N	2.1524481	-0.2369998	0.6135312
C	3.1558450	0.1735472	1.4053739
O	2.7370026	0.6298760	2.6088101
H	3.5542343	0.8907701	3.0672274
O	0.7691873	1.9441300	-1.4736730
H	1.4721720	1.8058802	-0.8227037
H	0.0674618	1.3494319	-1.1325918
O	0.7022134	0.3638702	-3.7094006
H	0.8655671	1.0154189	-2.9891445
H	0.7868945	0.8960885	-4.5114249

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G91C2BW2 HB

N	2.161770	-2.055890	-0.258760
C	1.529210	-3.236300	-0.200050
N	2.082980	-4.491060	-0.358150
H	3.063710	-4.685110	-0.535990
C	1.069900	-5.408320	-0.224680
H	1.243980	-6.481120	-0.306180
N	-0.112540	-4.844300	0.008530
C	0.160400	-3.480890	0.027610
C	-0.641240	-2.316740	0.193190
O	-1.958980	-2.304860	0.371770
H	-2.314320	-3.241710	0.397140
N	-0.049010	-1.122750	0.149930
C	1.299610	-1.039830	-0.060490
N	1.818700	0.229530	-0.028120
H	1.135990	0.985530	-0.142580
H	2.702280	0.324730	-0.519500
N	-0.363410	4.933020	-0.105620
C	-1.655130	4.758370	-0.476430
H	-2.210150	5.674460	-0.709490

C	-2.277510	3.521490	-0.557570
H	-3.327060	3.429040	-0.847310
C	-1.486810	2.380600	-0.252570
N	-1.962610	1.120400	-0.287230
H	-1.346680	0.331410	-0.048630
H	-2.929040	0.949250	-0.529230
N	-0.184650	2.535660	0.093320
C	0.274970	3.792280	0.161940
O	1.564420	3.932380	0.558560
H	1.846480	3.039010	0.817700
O	1.773240	7.001140	0.327800
H	0.935750	6.552710	0.128680
H	2.299600	6.236870	0.592160
O	-2.815600	-4.803940	0.475520
H	-1.918300	-5.148900	0.258310
H	-2.924160	-5.058770	1.402730

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G92C1W2 HB

N	-1.0069700	2.2129089	-0.2048508
C	0.3243142	2.0012068	-0.0667642
N	0.9874503	0.8057166	-0.0674928
H	0.5204480	-0.1237395	-0.1410624
C	2.3176175	1.1058369	0.1064600
H	3.0668806	0.3145880	0.1468242
N	2.5812994	2.4097773	0.2148391
C	1.3272572	2.9825431	0.1073947
C	0.8455609	4.3080177	0.1334311
O	1.6828485	5.3459358	0.2923218
H	1.0999106	6.1259790	0.2763390
N	-0.4554654	4.5651793	-0.0072739
C	-1.3098247	3.5184966	-0.1659524
N	-2.6593102	3.8623828	-0.2427085
H	-2.7767773	4.8231370	-0.5567496
H	-3.1886330	3.2099238	-0.8168700
N	-0.6378072	-3.8422995	0.1696932
C	-1.9918321	-3.8707736	0.2801713
H	-2.4395222	-4.8575960	0.4297407
C	-2.7302321	-2.7191722	0.2046089
H	-3.8179839	-2.7353461	0.2878421
C	-1.9921658	-1.4984528	0.0019500
N	-2.6433665	-0.3209788	-0.1111983
H	-2.1096166	0.5618649	-0.1442111
H	-3.6233455	-0.2847546	0.1394899
N	-0.6607817	-1.4874389	-0.1129818
C	0.0638850	-2.6508291	-0.0287205
O	1.3036328	-2.6461563	-0.1169543
H	-0.1006154	-4.7328947	0.2458064
O	2.8906648	-4.8436611	-0.5307146
H	3.0617808	-4.7575081	-1.4779163
H	2.4243971	-4.0021049	-0.3237033
O	0.7507957	-6.2372982	0.2953188
H	1.0290282	-6.4934383	1.1854348
H	1.5924348	-5.8904356	-0.0911249

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G92C2AW2 HB

N	-1.8408387	-0.2621694	3.4961997
C	-0.6665222	-0.1149611	4.1414138
N	-0.4462603	-0.1592884	5.4990109
H	-1.1560085	-0.2989820	6.2108293
C	0.9090514	0.0266697	5.6900695
H	1.3459479	0.0365801	6.6892134
N	1.5918764	0.1859533	4.5620389
C	0.6111853	0.0998710	3.5866705

C	0.6502575	0.1712285	2.1721519
O	1.7844690	0.3483535	1.5238539
H	1.5972237	0.2829581	0.5308547
N	-0.5056762	0.0546215	1.4950733
C	-1.6749336	-0.1572848	2.1732519
N	-2.8106393	-0.2059556	1.3807120
H	-2.6476359	-0.5489289	0.4366825
H	-3.5908005	-0.6592779	1.8486512
N	1.4230946	0.0801565	-1.1405655
C	2.5333963	-0.0999336	-1.8995119
H	3.4850825	-0.1139692	-1.3557738
C	2.4975776	-0.2512128	-3.2734305
H	3.4122664	-0.3886906	-3.8547587
C	1.2150045	-0.2180142	-3.8917729
N	1.0537499	-0.3799501	-5.2245883
H	0.1410674	-0.1562568	-5.6549572
H	1.8785370	-0.3097738	-5.8078375
N	0.1009732	-0.0598499	-3.1440740
C	0.2590307	0.0873504	-1.8188004
O	-0.8715166	0.2713875	-1.1422475
H	-0.6522101	0.2659477	-0.1515532
O	-1.4769709	0.2418185	-6.3882571
H	-1.8886118	-0.5559319	-6.7473487
H	-2.0062772	0.3818729	-5.5691159
O	-2.6410212	0.2022938	-3.9321127
H	-1.7492107	-0.0150517	-3.5817049
H	-2.8508510	1.0033498	-3.4329268

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G92C2BW2 HB

N	2.2602758	-0.6407826	2.1048527
C	2.9143459	-0.4329310	0.9520913
N	4.1566212	-0.9105911	0.5891437
H	4.7749535	-1.4619884	1.1761242
C	4.3692206	-0.5363473	-0.7199707
H	5.2810338	-0.8079335	-1.2526138
N	3.3653488	0.1652425	-1.2403805
C	2.4570391	0.2470961	-0.1946579
C	1.1728981	0.8201839	-0.0772562
O	0.6205680	1.5193507	-1.0690502
H	-0.3714185	1.2782763	-1.0379501
N	0.4867568	0.6459924	1.0587324
C	1.0306612	-0.0911266	2.0822236
N	0.2523830	-0.2294842	3.1987915
H	-0.7685938	-0.2261685	3.0861154
H	0.5994173	-0.9370236	3.8394310
N	-3.6515329	-0.1233919	0.4243523
C	-4.0623553	-0.9628924	-0.5573527
H	-4.9950896	-1.5048677	-0.3611750
C	-3.3680964	-1.1753913	-1.7390097
H	-3.7279881	-1.8806635	-2.4921619
C	-2.1533554	-0.4607964	-1.9120684
N	-1.3765213	-0.6005418	-3.0135282
H	-0.3994279	-0.2764834	-3.0329377
H	-1.5973437	-1.3650981	-3.6402226
N	-1.7704503	0.4308875	-0.9686392
C	-2.5219202	0.5398654	0.1489797
O	-2.0904207	1.3959623	1.0825650
H	-1.0861756	1.3063905	1.0850959
O	1.3690007	0.2754290	-3.4973061
H	1.2179333	1.1494083	-3.1054279
H	2.1436781	0.0123504	-2.9671696
O	-2.7291540	-0.2627496	3.3005989
H	-2.7542131	0.7041740	3.2499970
H	-3.2041439	-0.4640512	2.4733792

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G19C1W2 ST

N	-1.2743017	0.8875049	2.6663432
C	-2.4916059	0.5185607	2.1384572
H	-3.4291980	0.9532596	2.4851504
N	-2.3790006	-0.4112767	1.1923748
C	-1.0178317	-0.6512066	1.1169478
C	-0.2697150	-1.5297027	0.2440580
O	-0.6763699	-2.2848071	-0.6436026
N	1.1087596	-1.4155167	0.5168228
H	1.7413371	-1.8135772	-0.1934889
C	1.6987035	-0.5910274	1.4475482
N	3.0606644	-0.7065164	1.5700061
H	3.5353366	-1.0101695	0.7188424
H	3.4712449	0.1233891	1.9895831
N	1.0321799	0.2227134	2.2555972
C	-0.3065568	0.1434543	2.0278350
H	-1.1086763	1.5305105	3.4350478
N	0.6146108	2.2675939	-0.3448568
C	-0.7438722	2.3902603	-0.4009041
H	-1.1985097	3.1517550	0.2384570
C	-1.4573530	1.5760659	-1.2361558
H	-2.5432302	1.6390585	-1.3095225
C	-0.7001148	0.6202937	-2.0098850
N	-1.3701380	-0.1940042	-2.8670645
H	-0.7809496	-0.9582039	-3.1949438
H	-2.2833142	-0.5188829	-2.5111170
N	0.6299966	0.5194010	-1.9532776
C	1.3284201	1.3168830	-1.0882805
O	2.5557680	1.2293096	-0.9064351
H	1.1656959	2.8017649	0.3217454
O	-3.3754382	-1.4927791	-1.3207479
H	-2.6055748	-2.0710018	-1.1660208
H	-3.3913581	-1.0487697	-0.4519198
O	3.2946778	-1.3659690	-1.2687061
H	3.0613736	-0.4103940	-1.3588490
H	3.2326672	-1.7001858	-2.1723194

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G19C2AW2 ST

N	-2.7817011	-1.7758434	1.0493946
C	-3.6128388	-0.7151314	0.7715963
H	-4.5827910	-0.5964734	1.2541954
N	-3.1003807	0.1138788	-0.1368272
C	-1.8775133	-0.4508498	-0.4544025
C	-0.8329328	0.0147370	-1.3401177
O	-0.7974610	1.0099109	-2.0694413
N	0.2727174	-0.8588358	-1.2787531
H	1.1119039	-0.5594568	-1.7939237
C	0.3811187	-1.9957898	-0.5107147
N	1.5350848	-2.7178907	-0.6727547
H	2.3235845	-2.2138587	-1.0759341
H	1.7417495	-3.3161552	0.1210582
N	-0.5665721	-2.4442415	0.2974592
C	-1.6529400	-1.6273881	0.2758697
H	-2.9566409	-2.5420102	1.6927091
N	1.8532414	-0.3017721	1.7993969
C	0.5727178	0.0372651	2.1044115
H	0.0520518	-0.6311004	2.7996886
C	-0.0656218	1.1495233	1.5752756
H	-1.0971747	1.4000650	1.8340722
C	0.6806329	1.9586567	0.6727928
N	0.1650963	3.1005146	0.1457386
H	0.7120141	3.4540438	-0.6359997



H	-0.8542799	3.1178504	-0.0134728
N	1.9545690	1.6356713	0.3490839
C	2.4303263	0.5407850	0.9415403
O	3.7164578	0.2283598	0.5734725
H	3.9201445	-0.5626852	1.1032920
O	3.0460010	-0.5734294	-2.0312452
H	3.4183964	-0.1783812	-2.8298985
H	3.4404510	-0.0606884	-1.3000255
O	-2.5288513	2.8794181	-0.8100030
H	-3.0332553	2.1246745	-0.4540483
H	-2.0647617	2.4148640	-1.5309930

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G19C2BW2 ST

N	3.7202134	0.5376698	-0.9223256
C	3.3984792	1.8369802	-0.6066617
H	3.9936716	2.6821763	-0.9516282
N	2.3053562	1.9253702	0.1485615
C	1.9094390	0.6101388	0.3245847
C	0.7801720	0.0590848	1.0419259
O	-0.0986093	0.6309655	1.6921680
N	0.7632125	-1.3450976	0.8958270
H	-0.0786188	-1.8237588	1.2378839
C	1.6675801	-2.1158426	0.1960674
N	1.4608214	-3.4699321	0.2457086
H	0.4861634	-3.7563359	0.3690616
H	1.9743766	-3.9651372	-0.4775027
N	2.7191063	-1.6288957	-0.4456961
C	2.7735613	-0.2737614	-0.3400277
H	4.5054464	0.2168864	-1.4808081
N	-1.9101648	-1.0410654	-1.0755004
C	-1.0171333	-0.1061112	-1.4960515
H	-0.1634749	-0.4839831	-2.0720294
C	-1.1400971	1.2441302	-1.2115426
H	-0.3897958	1.9710865	-1.5277107
C	-2.2650960	1.6394184	-0.4390411
N	-2.4592950	2.9453647	-0.0928363
H	-3.1791355	3.0482323	0.6200668
H	-1.5773884	3.4238345	0.1485116
N	-3.1894949	0.7341836	-0.0550282
C	-2.9355215	-0.5357384	-0.3829218
O	-3.8217298	-1.4614745	0.0679794
H	-4.4759732	-0.9381854	0.5619357
O	0.0429906	3.4691230	1.0790513
H	0.9189721	3.2897467	0.6905924
H	-0.1004085	2.6105040	1.5193002
O	-1.3686213	-3.2496666	0.5292834
H	-2.2430996	-3.3782649	0.9210588
H	-1.5745774	-2.6455794	-0.2238413

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G17C1W2 ST

N	0.1835490	-2.1855712	-1.0583427
C	0.1321908	-1.9981560	0.3002368
N	0.9249390	-2.6465189	1.2214874
C	0.5481159	-2.1261977	2.3942813
H	0.9590787	-2.4140495	3.3626538
N	-0.4441863	-1.1894641	2.2885010
H	-0.8337963	-0.5591255	3.0016555
C	-0.7157506	-1.0807952	0.9488009
C	-1.5554118	-0.1752913	0.2194332
O	-2.2677763	0.7519347	0.6591903
N	-1.4603471	-0.4387056	-1.1408599
H	-1.8249234	0.2921772	-1.7716813
C	-0.6296940	-1.3892394	-1.7207911

N	-0.7635223	-1.5134690	-3.0878400
H	-1.0229578	-0.6467368	-3.5595617
H	0.0617219	-1.9503074	-3.4915756
N	2.2431329	0.1745793	-0.5883926
C	2.3851989	0.1904675	0.7656048
H	3.0719691	-0.5419446	1.1958497
C	1.6685619	1.0935354	1.5055625
H	1.7679241	1.1490197	2.5901379
C	0.7643368	1.9441463	0.7773862
N	0.0127143	2.8610348	1.4661303
H	-0.7489214	3.2163269	0.8893008
H	-0.3160420	2.5371681	2.3774675
N	0.6336481	1.9205932	-0.5467088
C	1.3598316	1.0144956	-1.2783926
O	1.2534121	0.8845389	-2.5087388
H	2.6667288	-0.5659608	-1.1437413
O	-1.6454958	1.1136667	3.2557114
H	-2.0130878	1.0450026	2.3340978
H	-2.4268041	1.2628802	3.8053191
O	-1.3111675	1.3764170	-3.2838513
H	-0.3550108	1.4192568	-3.0403161
H	-1.5916304	2.2998135	-3.2689067

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G17C2AW2 ST

N	-0.9171493	-2.0464689	0.7475131
C	0.3548216	-1.5812429	0.9877676
N	1.5059515	-2.3273973	0.8691952
C	2.4834188	-1.4523368	1.1353802
H	3.5473734	-1.6912795	1.1357225
N	2.0334590	-0.1931540	1.4267938
H	2.5434074	0.7073610	1.4951811
C	0.6695810	-0.2497565	1.3229537
C	-0.3389358	0.7660059	1.4594099
O	-0.2173090	1.9815968	1.6936131
N	-1.5931681	0.1911868	1.2623937
H	-2.3806190	0.8449867	1.2170049
C	-1.8379124	-1.1173822	0.8804056
N	-3.1783929	-1.4161329	0.7078667
H	-3.7002760	-0.6589949	0.2602475
H	-3.2886354	-2.3107448	0.2363988
N	1.1479041	1.6340206	-1.3867447
C	2.0783752	0.6769593	-1.6342465
H	3.1261186	0.9934444	-1.5687820
C	1.7511169	-0.6364818	-1.9316885
H	2.5183321	-1.3938012	-2.1049834
C	0.3737109	-0.9647828	-1.9482131
N	-0.0490149	-2.2529199	-2.1782922
H	-0.9811642	-2.4035192	-1.7932240
H	0.5983057	-2.9453623	-1.8009836
N	-0.5741877	-0.0198925	-1.7775863
C	-0.1141037	1.2040471	-1.5032271
O	-1.0941362	2.1294913	-1.2923229
H	-0.6370514	2.8963061	-0.9038708
O	-3.6837131	1.3439429	-0.2437740
H	-2.9085041	1.5717073	-0.7899915
H	-4.2581864	2.1152631	-0.3287980
O	2.4752845	2.5149566	1.2441310
H	2.2292425	2.5669837	0.3042185
H	1.5781296	2.5408073	1.6377650

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G17C2BW2 ST

N	-1.2852010	1.7899480	0.4175850
C	-2.0876883	0.8398434	-0.1618594

N	-3.3338611	0.4661176	0.3025469
C	-3.7109665	-0.5186463	-0.5178027
H	-4.6668706	-1.0410765	-0.4733629
N	-2.7725421	-0.8064595	-1.4767657
H	-2.8265881	-1.5071237	-2.2103786
C	-1.7252380	0.0519543	-1.2662726
C	-0.3804098	0.0211344	-1.7738696
O	0.0906933	-0.7720918	-2.6011893
N	0.3698249	1.0117533	-1.1410346
H	1.3906489	1.0286096	-1.3014102
C	-0.0849302	1.8375099	-0.1230930
N	0.8238368	2.7892865	0.2696576
H	1.7950205	2.6025325	0.0242096
H	0.6495042	3.1609092	1.1976539
N	1.7190326	-1.5777846	0.4856459
C	0.4843484	-2.1158726	0.3247546
H	0.3966870	-2.8853339	-0.4503541
C	-0.6260805	-1.7180123	1.0587486
H	-1.6084498	-2.1712312	0.9038754
C	-0.4332166	-0.6862598	2.0110812
N	-1.4587225	-0.2121983	2.7875155
H	-1.2410840	0.7027393	3.1791834
H	-2.3641422	-0.2011548	2.3134822
N	0.7938065	-0.1589097	2.2093220
C	1.7728933	-0.6417709	1.4363018
O	3.0039197	-0.0886220	1.6307883
H	2.8722235	0.5272440	2.3731037
O	2.9136242	-1.0777652	-2.2010278
H	2.7350143	-1.4730423	-1.3269289
H	2.0106230	-1.0415099	-2.5715005
O	3.2230186	1.3041372	-0.9429854
H	3.3097751	0.5526435	-1.5771873
H	3.4254462	0.8494661	-0.1073353

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G91C1W2 ST

N	0.6201241	-0.3139620	-2.1866587
C	1.1868511	-0.0655923	-1.0011548
N	1.9862844	-0.8997248	-0.2548559
H	2.1051867	-1.9268451	-0.3869372
C	2.2721713	-0.2332996	0.9037063
H	2.8611347	-0.6897291	1.6853990
N	1.7551392	0.9789478	0.9564971
C	1.0550637	1.1059216	-0.2399666
C	0.1947097	2.0897887	-0.7648153
O	-0.1339484	3.2258159	-0.1355629
H	0.1897813	3.2055842	0.8049813
N	-0.3803804	1.8864635	-1.9465003
C	-0.1398010	0.7182976	-2.5873192
N	-0.8370357	0.5457596	-3.7669242
H	-1.1526446	1.4023940	-4.2015563
H	-0.4537878	-0.1499427	-4.3927666
N	-1.9571380	-1.2848448	-0.3643104
C	-2.3612390	-0.0413621	-0.0009669
H	-2.9611540	0.5082173	-0.7159840
C	-1.9815289	0.4663432	1.2010678
H	-2.2733837	1.4623052	1.5050559
C	-1.1187720	-0.3530244	1.9953029
N	-0.6838576	0.1034252	3.2010418
H	0.0508290	-0.4503224	3.6228841
H	-0.6069389	1.1074149	3.3287036
N	-0.7142368	-1.5695140	1.6296147
C	-1.1090834	-2.0789118	0.4351114
O	-0.7572678	-3.1815383	-0.0169973
H	-2.1475039	-1.6441416	-1.2920711

O	0.6390519	2.8360192	2.4921989
H	1.2515201	2.1292797	2.1069265
H	1.2078426	3.4880311	2.9251593
O	1.8810514	-3.6433440	-0.1594737
H	1.9599065	-4.2118302	-0.9382039
H	0.8992669	-3.5910707	0.0114118

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G91C2AW2 ST

N	-0.5889437	-0.9951154	2.5451226
C	-1.1083656	-1.0048108	1.3077011
N	-1.6242530	-2.0847927	0.6241678
H	-1.6183851	-3.0462143	0.9497533
C	-2.0243656	-1.6317428	-0.6068214
H	-2.4550807	-2.2945792	-1.3577294
N	-1.8342423	-0.3223523	-0.7724859
C	-1.2537118	0.0829998	0.4214329
C	-0.8231859	1.3384305	0.9314040
O	-0.9153096	2.4992488	0.2858160
H	-0.9776907	2.3662421	-0.6989142
N	-0.2962635	1.3934063	2.1559386
C	-0.1900139	0.2456064	2.8767628
N	0.4821734	0.3784663	4.0841302
H	0.4090052	1.3176375	4.4676277
H	0.2431230	-0.3525451	4.7495955
N	1.4500746	-2.0618112	-0.3841538
C	1.9667957	-1.3613118	0.6574875
H	2.2061715	-1.9383685	1.5576242
C	2.1709099	0.0115547	0.6242727
H	2.5669995	0.5477857	1.4899206
C	1.7980810	0.6874565	-0.5656932
N	1.9531202	2.0428548	-0.7196503
H	1.3318833	2.4202300	-1.4402611
H	1.8945424	2.5647891	0.1523040
N	1.3021086	0.0116470	-1.6229904
C	1.1694244	-1.3054694	-1.4493871
O	0.6496167	-1.9485562	-2.5330801
H	0.6332362	-2.8839799	-2.2690459
O	-0.5439087	2.5668926	-2.3210437
H	-1.0283723	3.2478505	-2.8076365
H	-0.7073623	1.7393490	-2.8560082
O	-1.2364990	0.3005313	-3.4941188
H	-1.6156835	0.0895578	-2.6143877
H	-0.4537501	-0.2745641	-3.4890611

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G91C2BW2 ST

N	0.7086847	2.1196361	0.1528314
C	1.2030148	0.8701370	0.1287900
N	1.8503437	0.2053614	1.1467834
H	1.8315443	0.4996748	2.1474204
C	2.1246742	-1.0497181	0.6784506
H	2.6238538	-1.7976991	1.2948998
N	1.7429979	-1.2487853	-0.5873613
C	1.1445305	-0.0485085	-0.9407262
C	0.4495740	0.4019836	-2.0952784
O	0.2381384	-0.3395059	-3.1915342
H	0.4953696	-1.2776465	-2.9987403
N	-0.0631741	1.6304418	-2.1088870
C	0.0897677	2.4105458	-1.0028974
N	-0.5642503	3.6353531	-1.0625764
H	-0.6695391	3.9724495	-2.0163975
H	-0.1566902	4.3236738	-0.4339134
N	-1.2079797	0.2824353	2.1911055
C	-1.8600170	0.9255455	1.1896480

H	-2.1189107	1.9731192	1.3761072
C	-2.1665866	0.3306963	-0.0274079
H	-2.6703700	0.8886112	-0.8198795
C	-1.7395543	-1.0066972	-0.2135520
N	-1.9600760	-1.6915141	-1.3814062
H	-1.3150329	-2.4680712	-1.5329333
H	-2.0543248	-1.1025772	-2.2057780
N	-1.1226483	-1.6791638	0.7815838
C	-0.9017997	-0.9862471	1.9032797
O	-0.2476744	-1.6563051	2.8926094
H	-0.1223567	-2.5474527	2.5229497
O	1.1553652	0.8195771	3.7496853
H	1.0511951	-0.0607524	4.1417219
H	0.2508733	0.9399599	3.3886949
O	0.6618457	-2.8894363	-2.4243319
H	1.2517058	-3.4854516	-2.9054970
H	1.2088934	-2.5560027	-1.6658837

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G92C1W2 ST

N	1.2472962	-0.3551937	-1.0800658
C	-0.0894952	-0.4601673	-1.2388515
N	-0.9453209	0.4579517	-1.7890659
H	-0.6968362	1.4552837	-1.9430002
C	-2.2081050	-0.0725085	-1.6499386
H	-3.0892923	0.4827881	-1.9716222
N	-2.2422213	-1.2881999	-1.0999472
C	-0.9081728	-1.5386474	-0.8342084
C	-0.2141694	-2.5943203	-0.2065876
O	-0.8694336	-3.6815184	0.2360922
H	-0.1710108	-4.2452520	0.6150326
N	1.1029904	-2.5279623	-0.0122602
C	1.7577774	-1.4134060	-0.4354960
N	3.1058781	-1.3406441	-0.0753039
H	3.5181040	-2.2663720	0.0280154
H	3.6419579	-0.7543493	-0.7146464
N	-1.8634673	0.4555295	1.6079037
C	-1.0250426	-0.4316720	2.2108924
H	-1.4829259	-1.3259231	2.6431358
C	0.3206489	-0.1836908	2.2431544
H	1.0136435	-0.8764030	2.7224312
C	0.7794866	1.0019977	1.5632178
N	2.1088459	1.2871980	1.5388855
H	2.3891005	1.8856624	0.7479956
H	2.7111440	0.4718985	1.6426438
N	-0.0559633	1.8539737	0.9637685
C	-1.4176821	1.6190195	0.9528035
O	-2.2302107	2.3448850	0.3792911
H	-2.8527777	0.2453190	1.4995931
O	2.6892683	2.2251203	-1.1283285
H	2.0552594	2.8749121	-1.4731091
H	2.2217991	1.3870524	-1.3144062
O	-0.0252009	3.0812151	-1.5204700
H	0.1002009	2.7855170	-0.5818321
H	-0.7960829	3.6597327	-1.4147235

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G92C2AW2 ST

N	0.5507038	2.2148207	-1.3076243
C	0.0211260	2.0591536	-0.0831216
N	0.2948584	2.7981804	1.0466257
H	0.9664133	3.5570411	1.1083126
C	-0.4413144	2.2612652	2.0740513
H	-0.4010040	2.6649987	3.0858866
N	-1.2004636	1.2357773	1.6946132

C	-0.9147657	1.0950810	0.3436732
C	-1.3657814	0.1952412	-0.6606999
O	-2.2284337	-0.7918760	-0.4780150
H	-2.3659145	-0.9481996	0.5193207
N	-0.8801212	0.3398751	-1.8993811
C	0.0517499	1.3029551	-2.1578413
N	0.4936543	1.3435874	-3.4681089
H	0.4722159	0.4302096	-3.9216799
H	1.3811055	1.8300627	-3.5634645
N	1.9717557	-0.0344156	1.5844856
C	2.3064331	-0.1185452	0.2719621
H	3.0524719	0.6027249	-0.0817181
C	1.7519201	-1.0432346	-0.6010863
H	2.0325530	-1.0870514	-1.6560470
C	0.7662978	-1.9157195	-0.0698077
N	0.1776903	-2.8756753	-0.8415073
H	-0.6940851	-3.2281070	-0.4541031
H	0.1396621	-2.6693709	-1.8449937
N	0.4082404	-1.8462909	1.2314013
C	1.0461828	-0.9209072	1.9627207
O	0.6598722	-0.8919579	3.2600168
H	1.1825662	-0.1676113	3.6435736
O	-2.3465757	-1.2983996	2.0470827
H	-1.4927977	-1.7740780	2.0609494
H	-2.0665937	-0.4062436	2.3393027
O	-0.1408750	-1.7133306	-3.5506308
H	-0.6583154	-1.0660441	-3.0082103
H	-0.7992117	-2.0768298	-4.1585270

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G92C2BW2 ST

N	1.5513672	-0.3270643	0.2798466
C	0.7385750	-1.3945020	0.4142004
N	0.4070564	-2.0883967	1.5507837
H	0.5595592	-1.7495413	2.5269448
C	-0.5032590	-3.0453731	1.1642159
H	-0.9446575	-3.7292179	1.8903659
N	-0.7681053	-3.0630587	-0.1461898
C	0.0122190	-2.0253660	-0.6155513
C	0.1316856	-1.4429006	-1.8874295
O	-0.5643484	-1.8831979	-2.9602538
H	-1.0778609	-2.6464457	-2.6395508
N	0.9155217	-0.3858843	-2.0740571
C	1.5809848	0.1121556	-0.9862205
N	2.3272657	1.2590514	-1.2421486
H	2.7184560	1.2646354	-2.1819167
H	3.0322782	1.4144836	-0.5246788
N	-1.1054196	0.6657208	2.0189063
C	-1.7791635	0.3399268	0.8869171
H	-2.4589289	-0.5175343	0.9616541
C	-1.6216665	1.0157243	-0.3143203
H	-2.1578316	0.7220473	-1.2192627
C	-0.7207834	2.1140635	-0.3243891
N	-0.5426440	2.8813833	-1.4343107
H	0.3260978	3.4096745	-1.4134459
H	-0.7455381	2.4225762	-2.3301714
N	-0.0440052	2.4575732	0.7937449
C	-0.2687663	1.6986284	1.8688484
O	0.4515107	2.0038016	2.9792879
H	1.0065311	2.7518629	2.7004211
O	0.2556824	-0.8579510	3.9828347
H	0.8950945	-0.1453963	4.1327392
H	-0.4498585	-0.3551547	3.5171785
O	-0.6811864	1.2282384	-3.8054770
H	-1.3180252	0.5493477	-4.0663173

H 0.0288049 0.6833184 -3.4076520

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G19C1W2 TS

N	1.2747370	3.8051043	-1.3794147
C	2.4324763	3.4023641	-0.7520660
H	3.4064986	3.8118814	-1.0190026
N	2.2190643	2.4830828	0.1854433
C	0.8490730	2.2901204	0.1553690
C	0.0100678	1.4037340	0.9200845
O	0.3193678	0.5895438	1.8092563
N	-1.3247889	1.5262823	0.5228226
H	-2.0089624	0.8799846	0.9622033
C	-1.8136943	2.3482271	-0.4667393
N	-3.1729958	2.2991970	-0.6432829
H	-3.6170344	1.4301526	-0.3424585
H	-3.4738859	2.6667180	-1.5406157
N	-1.0709222	3.1795836	-1.1812633
C	0.2369443	3.0998037	-0.8170171
H	1.1856529	4.4878439	-2.1258935
N	0.0912648	-1.9457724	0.6156090
C	1.4016114	-2.1543365	0.3082016
H	2.1165815	-1.4202218	0.7030256
C	1.7400316	-3.2394612	-0.4589242
H	2.7768614	-3.4346016	-0.7369691
C	0.6583285	-4.0890140	-0.8685405
N	0.9246617	-5.1743798	-1.6714972
H	0.1570666	-5.8399500	-1.7155615
H	1.8455378	-5.5906742	-1.5807748
N	-0.6175996	-3.8725922	-0.5706395
C	-0.9506215	-2.7662918	0.1713625
O	-2.1272248	-2.4870353	0.4622210
H	-0.1345802	-1.1319714	1.2002820
O	3.1836649	0.1475931	1.7442237
H	3.2010018	0.9355640	1.1729324
H	2.3062412	0.2762361	2.1407315
O	-3.3943542	-0.2080915	0.9715905
H	-3.8566266	-0.4037129	1.7977364
H	-2.9545558	-1.0730027	0.7514806

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G19C2AW2 TS

N	-1.8091781	-1.8215462	-1.0397056
C	-1.7520715	-1.2918891	-2.3072535
H	-2.6075244	-1.3133102	-2.9823968
N	-0.5555396	-0.7822146	-2.6006816
C	0.1820900	-0.9858603	-1.4493420
C	1.5480708	-0.6267993	-1.1400933
O	2.4088069	-0.0839872	-1.8371907
N	1.8326443	-0.9691252	0.1993520
H	2.7253126	-0.6122333	0.5451667
C	0.9705226	-1.5257120	1.1177255
N	1.4798212	-1.6930495	2.3887097
H	2.0759649	-0.9023652	2.6523841
H	0.7092815	-1.7976552	3.0475571
N	-0.2557552	-1.9253737	0.8293247
C	-0.5819273	-1.6207038	-0.4563984
H	-2.6188151	-2.2207946	-0.5736498
N	-2.4474745	0.5785079	1.3857474
C	-2.5642246	1.0894483	0.1325571
H	-3.5573904	1.0105815	-0.3264486
C	-1.5154325	1.6746615	-0.5581881
H	-1.6315171	2.0695928	-1.5692694
C	-0.2647636	1.7476688	0.1139261
N	0.8174023	2.3295898	-0.4683612

H	1.7036216	2.1148226	-0.0140600
H	0.8298347	2.2894346	-1.4993591
N	-0.1386859	1.2810765	1.3791966
C	-1.2311008	0.7158286	1.9145142
O	-1.0433946	0.2243384	3.1635222
H	-1.9108917	-0.1520288	3.3927373
O	2.5650697	1.0340052	2.0828040
H	1.5910475	1.1930258	2.0128270
H	2.8684679	1.7258886	2.6851911
O	0.8019044	1.7201267	-3.3032812
H	0.1473039	1.0013270	-3.3803750
H	1.5907467	1.1786815	-3.1149479

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G19C2BW2 TS

N	-2.8624043	-1.8967814	1.2357671
C	-3.6549006	-0.8439025	0.8423261
H	-4.6381754	-0.6647580	1.2763428
N	-3.0853981	-0.0973186	-0.1014128
C	-1.8612721	-0.7047263	-0.3165770
C	-0.8046733	-0.3744945	-1.2478445
O	-0.7409873	0.5242630	-2.0888693
N	0.2635638	-1.2883275	-1.0957401
H	1.0834001	-1.0902623	-1.6754396
C	0.3318705	-2.3458506	-0.2161592
N	1.4709469	-3.1220736	-0.2938280
H	2.3409692	-2.5886801	-0.3662344
H	1.5021260	-3.7717203	0.4899619
N	-0.6400934	-2.6793591	0.6137577
C	-1.6993298	-1.8297112	0.5051218
H	-3.0786795	-2.6006141	1.9352932
N	2.8716026	0.2926213	-1.0507569
C	2.1203854	1.3993425	-1.2999318
H	2.0667848	1.7143369	-2.3477359
C	1.4210159	2.0914367	-0.3248027
H	0.7877985	2.9494246	-0.5527698
C	1.4998418	1.5904197	1.0016545
N	0.8466426	2.1980620	2.0239009
H	0.7887062	1.6594557	2.8818551
H	0.0496510	2.7952798	1.7649086
N	2.2628855	0.5074931	1.2837796
C	2.8894714	-0.0455778	0.2398073
O	3.6342929	-1.1564360	0.5272951
H	3.5529139	-1.2399322	1.4936945
O	-2.5588977	2.5205526	-1.1980920
H	-3.0817633	1.7833532	-0.8291544
H	-1.9104958	2.0042579	-1.7138913
O	-1.2809767	3.6836673	0.8881879
H	-1.7574200	3.2383348	0.1425496
H	-1.2407162	4.6010348	0.5904233

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G17C1W2 TS

N	0.4545570	-0.9315427	2.0777910
C	-0.2444296	0.2464345	1.9477992
N	-1.4963227	0.4835239	2.4759767
C	-1.8176155	1.6965251	2.0207181
H	-2.7413449	2.2287617	2.2485182
N	-0.8434468	2.2496959	1.2269137
H	-0.8463535	3.1603789	0.7780484
C	0.1758869	1.3357967	1.1715982
C	1.3934451	1.3220143	0.4081153
O	1.8241084	2.1954614	-0.3562023
N	2.0705803	0.1282478	0.6623312
H	2.9346521	-0.0577028	0.1297242



C	1.5851585	-0.9338351	1.3987916
N	2.4289154	-2.0222631	1.4401015
H	3.0113956	-2.1276497	0.6069765
H	1.9502000	-2.8683127	1.7353843
N	-2.2724589	0.2492794	-2.3786688
C	-3.4236652	-0.0936212	-1.7362841
H	-4.3592895	0.2849493	-2.1572134
C	-3.3560852	-0.8811218	-0.6210583
H	-4.2561321	-1.1829341	-0.0834382
C	-2.0375657	-1.2963834	-0.2009485
N	-1.9308318	-2.1322788	0.8732249
H	-1.0075742	-2.0897762	1.3221879
H	-2.6834675	-2.0404558	1.5512095
N	-0.9160678	-0.9499197	-0.8323343
C	-0.9911587	-0.1629965	-1.9565730
O	-0.0243925	0.2174829	-2.6249786
H	-2.2856349	0.8246411	-3.2166500
O	2.7315559	0.5532652	-2.5192156
H	2.6209002	1.3238921	-1.9310252
H	1.7942484	0.2871659	-2.6226935
O	4.0360618	-1.0990644	-0.9112428
H	3.5900258	-0.5865742	-1.6409304
H	4.9621646	-0.8345646	-0.9885742

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G17C2AW2 TS

N	0.7200092	-2.1262509	0.7593068
C	0.8564069	-1.6312678	-0.5158929
N	0.5960342	-2.3345353	-1.6702504
C	0.8148364	-1.4431204	-2.6455639
H	0.7147377	-1.6522334	-3.7110783
N	1.1984515	-0.2122661	-2.1903976
H	1.3570406	0.6802707	-2.6929416
C	1.2201746	-0.3068333	-0.8251779
C	1.4508456	0.6808768	0.1927447
O	1.6785496	1.8990536	0.0744695
N	1.3645126	0.0765709	1.4454917
H	1.4025147	0.7071143	2.2530879
C	0.9741976	-1.2318390	1.6890255
N	0.9372248	-1.5757109	3.0278455
H	0.5946417	-0.8219242	3.6276720
H	0.4364287	-2.4515640	3.1578098
N	-1.5074090	1.8599524	-0.7417545
C	-1.8006023	1.0399807	-1.7783454
H	-1.7986374	1.5028703	-2.7719591
C	-2.0694317	-0.3131282	-1.6160919
H	-2.2936530	-0.9603993	-2.4667587
C	-2.0047447	-0.8283047	-0.2990107
N	-2.2317061	-2.1630097	-0.0391972
H	-1.7833230	-2.4370403	0.8354464
H	-1.8906950	-2.7599574	-0.7939432
N	-1.7552328	-0.0246960	0.7577404
C	-1.5226678	1.2532295	0.4475467
O	-1.2354340	2.0551807	1.5186299
H	-0.9516159	2.8923169	1.1086647
O	0.2118583	1.1609856	3.7961438
H	-0.4541742	1.4417830	3.1392572
H	0.2313642	1.8864928	4.4326339
O	1.5337633	2.4561196	-2.6558289
H	1.4852152	2.4616488	-1.6731365
H	2.4290155	2.7862930	-2.8139132

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G17C2BW2 TS

N	-0.2172747	-1.8239975	1.4250702
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C	-0.3497235	-0.7694108	2.2907692
N	0.2027119	-0.7048796	3.5548408
C	-0.1083342	0.5188047	3.9862566
H	0.1420472	0.9216306	4.9681302
N	-0.8178680	1.2532087	3.0651399
H	-1.1727876	2.2000208	3.1608104
C	-0.9988112	0.4372026	1.9789193
C	-1.5306869	0.7074766	0.6756337
O	-1.9487486	1.7912306	0.2337508
N	-1.4855720	-0.4554308	-0.0911553
H	-1.8229314	-0.4001851	-1.0679762
C	-0.86150263	-1.6184642	0.2673622
N	-0.8631326	-2.6180189	-0.6741914
H	-1.0120503	-2.3099054	-1.6366298
H	-0.1546774	-3.3295760	-0.5247831
N	1.3120987	0.1911860	-2.3946290
C	2.2498682	-0.6701193	-1.9327903
H	2.6728283	-1.3592847	-2.6728999
C	2.6648713	-0.7077048	-0.6087526
H	3.4145959	-1.4221402	-0.2613507
C	2.0820776	0.2438320	0.2630280
N	2.4776467	0.3668523	1.5743064
H	1.8177276	0.9116871	2.1261048
H	2.7106402	-0.5106957	2.0348667
N	1.1640944	1.1247728	-0.1777181
C	0.8097014	1.0206171	-1.4672940
O	-0.1809827	1.8229664	-1.9061602
H	-0.7009670	2.1053039	-1.1164556
O	-1.9477624	-1.0000406	-2.8083719
H	-2.7972889	-1.2021408	-3.2221460
H	-1.4788038	-0.4431939	-3.4869805
O	-0.5511865	0.5429184	-4.4946834
H	-0.7628606	1.4095533	-4.1152155
H	0.2700455	0.3508498	-3.9890554

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G91C1W2 TS

N	-0.9272188	1.2593912	0.3705576
C	0.4093121	1.1451760	0.4964865
N	1.3926375	1.4647440	-0.4079538
H	1.2315447	1.7330743	-1.4024023
C	2.5836860	1.1021434	0.1792962
H	3.5357355	1.2539960	-0.3317848
N	2.4617979	0.6007814	1.4128710
C	1.0953605	0.6271115	1.6099013
C	0.2820331	0.1592491	2.6626455
O	0.8055942	-0.3973468	3.7750032
H	1.7707369	-0.3302255	3.6657359
N	-1.0408468	0.2079047	2.5689414
C	-1.5772702	0.7460715	1.4328284
N	-2.9588570	0.7778604	1.3831881
H	-3.3771778	0.1614026	2.0751950
H	-3.3121776	0.6121235	0.4405433
N	-0.9321377	-1.9780113	0.1285959
C	0.3575028	-2.3170307	0.4074866
H	0.5401363	-2.8075793	1.3678480
C	1.3449807	-2.0326584	-0.4981030
H	2.3859275	-2.2897514	-0.2976094
C	0.9322281	-1.3295371	-1.6857761
N	1.8598377	-0.9948337	-2.6357830
H	1.5659442	-0.2028893	-3.2132955
H	2.8236069	-0.9560381	-2.3194307
N	-0.3259266	-0.9899541	-1.9412192
C	-1.3165589	-1.2912656	-1.0388677
O	-2.5020290	-0.9743214	-1.1919333

H	-1.6668469	-2.1342973	0.8147059
O	0.7267004	1.7456085	-3.0689012
H	-0.2532120	1.6076254	-2.9053187
H	0.7402723	2.5646010	-3.5837649
O	-1.8411342	1.6168093	-2.3629989
H	-2.1530078	0.6933715	-2.3994682
H	-1.6645258	1.6828991	-1.4009377

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G91C2AW2 TS

N	0.8639998	-4.8459986	7.3139980
C	0.2229999	-3.6559990	7.3899979
N	0.4449999	-2.6879992	8.3219977
H	1.1419997	-2.7769992	9.0409975
C	-0.4379999	-1.6739995	8.0409977
H	-0.5069999	-0.7579998	8.6159976
N	-1.2079997	-1.9229995	7.0159980
C	-0.7699998	-3.1829991	6.5799982
C	-1.1379997	-4.0839989	5.5329984
O	-2.1189994	-3.8429989	4.6329987
H	-2.4889993	-4.7069987	4.3599988
N	-0.5309999	-5.2879985	5.4109985
C	0.4089999	-5.5689984	6.2969982
N	0.9559997	-6.7369981	6.1639983
H	0.6259998	-7.3069980	5.4109985
H	1.6769995	-6.9769980	6.8139981
N	-3.3889991	-8.1179977	5.5109985
C	-3.3739991	-8.7279976	6.7249981
H	-3.2899991	-9.8069973	6.7789981
C	-3.4589990	-7.9819978	7.8469978
H	-3.4409990	-8.4719976	8.8049975
C	-3.5689990	-6.5709982	7.6919978
N	-3.6349990	-5.7969984	8.7489975
H	-3.6739990	-4.7949987	8.5799976
H	-3.6119990	-6.1819983	9.6689973
N	-3.5999990	-5.9679983	6.5229982
C	-3.4909990	-6.7659981	5.4639985
O	-3.4729990	-6.1359983	4.2869988
H	-3.4369990	-6.8539981	3.6519990
O	-4.7399987	-3.3759991	5.8239984
H	-4.5509987	-4.3349988	5.8259984
H	-4.1559988	-3.0729991	5.1099986
O	-3.5749990	-2.9909992	8.2309977
H	-2.8119992	-2.4869993	7.8739978
H	-4.1619988	-2.9789992	7.4369979

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G91C2BW2 TS

N	1.4876714	1.1107957	-1.1757672
C	0.2040996	1.2976568	-0.8123561
N	-0.8741679	1.5382137	-1.6330691
H	-0.8760421	1.3727628	-2.6576072
C	-1.9734130	1.6128258	-0.8241790
H	-2.9749352	1.7622596	-1.2272674
N	-1.6919674	1.4869059	0.4753994
C	-0.3207947	1.2792532	0.4969680
C	0.6145197	1.0005942	1.5297900
O	0.3032733	0.8600263	2.8222165
H	-0.6896809	0.9007294	2.9335704
N	1.8977016	0.8257640	1.2118909
C	2.2588957	0.8841344	-0.0985835
N	3.6008311	0.6141175	-0.3428931
H	4.1865095	0.8354356	0.4586482
H	3.9307845	1.0412266	-1.2050726
N	-1.4555371	-1.5744690	-1.0804266

C	-1.9221182	-1.6943821	0.1849255
H	-3.0107025	-1.6368731	0.3022174
C	-1.1015594	-1.8490434	1.2984036
H	-1.5159718	-1.8946569	2.3083331
C	0.2907332	-1.9130298	1.0585136
N	1.2058636	-2.0948352	2.0755795
H	2.1230482	-1.7437777	1.7974610
H	0.9131628	-1.6523645	2.9459123
N	0.7807287	-1.8355011	-0.1946498
C	-0.1258814	-1.6455938	-1.1609424
O	0.3792024	-1.4844024	-2.4192065
H	1.3301283	-1.3257045	-2.2752651
O	-0.9516078	0.4337735	-4.1430408
H	-0.2113006	0.5628895	-4.7519684
H	-0.6943470	-0.3824979	-3.6737495
O	-2.3440370	0.8625674	3.0331970
H	-2.6877233	1.6466508	3.4843309
H	-2.4126946	1.1062863	2.0756943

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G92C1W2 TS

N	0.3978724	0.9309236	1.2285968
C	0.5104202	-0.4085869	1.1237557
N	-0.4154890	-1.3591170	1.4695747
H	-1.4010271	-1.1666749	1.7449517
C	0.1409557	-2.5705786	1.1251765
H	-0.3934137	-3.5064794	1.2975277
N	1.3717860	-2.4938010	0.6144403
C	1.6103602	-1.1322821	0.6099508
C	2.6740379	-0.3239990	0.1545039
O	3.7848698	-0.8765130	-0.3656944
H	4.3554650	-0.1142601	-0.5722661
N	2.5913210	1.0047780	0.1980744
C	1.4610063	1.5697595	0.7154291
N	1.4263881	2.9534616	0.7307763
H	2.1156203	3.3560452	0.1009470
H	0.4860025	3.3072338	0.5517230
N	0.1235936	0.8512257	-2.0029617
C	0.3567643	-0.4558528	-2.3110391
H	1.3044807	-0.6867038	-2.8054531
C	-0.5750193	-1.4050331	-1.9859476
H	-0.4073494	-2.4588834	-2.2117538
C	-1.7414256	-0.9347349	-1.2841498
N	-2.7158059	-1.8220103	-0.9139538
H	-3.2732094	-1.4901792	-0.1224621
H	-2.4287305	-2.7938751	-0.8539200
N	-1.9540210	0.3407107	-0.9787447
C	-1.0241926	1.2923179	-1.3173025
O	-1.1360420	2.4916115	-1.0347921
H	0.8230891	1.5627831	-2.1993273
O	-3.0646671	-0.6122504	1.7930163
H	-3.5502497	-0.5986526	2.6296213
H	-2.8854784	0.3602514	1.6303055
O	-2.3055405	1.9396247	1.5898615
H	-1.3512495	1.7253991	1.6533038
H	-2.3397105	2.2159684	0.6550595

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G92C2AW2 TS

N	-1.1741626	1.2602303	0.4565078
C	-0.5412991	1.3883959	-0.7289475
N	0.2293414	2.4337593	-1.1680029
H	0.4707695	3.2901770	-0.6179318
C	0.7168906	2.0555446	-2.3948672
H	1.3758944	2.7099783	-2.9670640

N	0.3111247	0.8502629	-2.8081084
C	-0.4908044	0.4286211	-1.7628997
C	-1.1782950	-0.7690920	-1.4805426
O	-1.1722194	-1.7908858	-2.3615351
H	-1.7009078	-2.4806390	-1.9192914
N	-1.8188731	-0.9399922	-0.3282634
C	-1.7748968	0.0674498	0.5876543
N	-2.4754114	-0.1672377	1.7622910
H	-2.4746240	-1.1550000	2.0094413
H	-2.1493004	0.4212745	2.5261113
N	0.2562189	-2.2191684	2.0809902
C	0.2240252	-3.1966747	1.1441508
H	-0.2867586	-4.1230577	1.4320817
C	0.7950092	-3.0599525	-0.1137003
H	0.7656425	-3.8673674	-0.8493250
C	1.3991279	-1.8121026	-0.4091780
N	1.9800837	-1.5718903	-1.6314237
H	2.0859034	-0.5774163	-1.8294373
H	1.5216468	-2.0484684	-2.4055374
N	1.4705969	-0.8302905	0.5128379
C	0.9054496	-1.1158709	1.6896124
O	1.0168611	-0.1325475	2.6260731
H	0.5963624	-0.5145485	3.4161330
O	0.8771386	4.4721400	0.5387416
H	0.2194760	5.1661714	0.6823757
H	0.7670879	3.9049677	1.3425769
O	0.2067066	2.6904994	2.4556563
H	0.8281629	1.9495572	2.5454901
H	-0.4469026	2.2804516	1.8470302

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G92C2BW2 TS

N	-0.5311364	0.0075659	-3.5899916
C	-0.4955156	0.9634247	-2.6476120
N	-1.1972564	2.1534716	-2.6429947
H	-1.8341596	2.4659045	-3.3697014
C	-0.9154336	2.7912399	-1.4645612
H	-1.3583174	3.7518650	-1.2008659
N	-0.0578825	2.1109519	-0.6992565
C	0.2223606	0.9661073	-1.4371107
C	1.0409774	-0.1779400	-1.2054943
O	1.8551916	-0.3548789	-0.1845133
H	1.8434000	0.4401637	0.4441824
N	0.9821553	-1.1809660	-2.0925174
C	0.2153555	-1.0436238	-3.2095521
N	0.1702609	-2.1651146	-4.0212725
H	1.0118713	-2.7316227	-3.9604240
H	-0.1154982	-1.9531097	-4.9735127
N	-0.7067947	-0.3005452	3.4418561
C	-0.4701274	-1.6153980	3.6559671
H	-0.3561820	-1.9166143	4.7039077
C	-0.3500254	-2.5480068	2.6344518
H	-0.1398101	-3.5996930	2.8440387
C	-0.4636009	-2.0594624	1.3096005
N	-0.3358859	-2.8824439	0.2200362
H	-0.0362433	-2.4112242	-0.6373460
H	0.1871240	-3.7354822	0.3965594
N	-0.7598789	-0.7643534	1.0738629
C	-0.8518419	0.0278316	2.1487024
O	-1.1153515	1.3343753	1.9345463
H	-0.9640556	1.4998424	0.9801973
O	0.9328342	1.9861240	3.9468232
H	0.2336649	2.6196817	3.7303897
H	0.3916726	1.1769893	4.0589328
O	1.9046626	1.7272407	1.3501165

H	1.2304245	2.2498235	0.8822161
H	1.6206579	1.7638469	2.2940036