

29

G19C1 HB

C	1.4060135	0.0327715	-0.9520837
O	0.7962259	0.0404286	-2.0376940
H	-0.3521448	0.0647904	0.1581405
N	0.6832495	0.0605847	0.2573825
C	1.2216807	0.0506784	1.5213732
N	0.3542253	0.1075912	2.5562984
H	-0.6620558	0.0349785	2.4344495
H	0.7503633	0.0141142	3.4782147
N	2.5282251	0.0091798	1.7587833
C	3.2473867	-0.0143508	0.6192000
N	4.6179653	-0.0567181	0.5338882
C	2.8114895	-0.0038397	-0.7126937
N	3.8842108	-0.0384779	-1.5908368
C	4.9378219	-0.0686698	-0.8153612
H	5.9654784	-0.1000073	-1.1487281
H	5.2568650	-0.0729529	1.3166370
N	-2.1981648	0.0068426	-0.0756093
C	-2.7503761	0.0157779	-1.3004656
N	-1.9213539	0.0481635	-2.3477216
H	-0.8825240	0.0524140	-2.2153750
H	-2.2995819	0.0521465	-3.2824628
C	-2.9664695	-0.0326398	1.0413275
O	-2.5255868	-0.0499901	2.1982381
N	-4.3676240	-0.0553790	0.8605298
H	-4.9213499	-0.0862767	1.7071911
C	-4.9472080	-0.0445452	-0.3701186
H	-6.0306335	-0.0664423	-0.3996745
C	-4.1776009	-0.0087828	-1.4866701
H	-4.6270303	-0.0004677	-2.4714287

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G19C2A HB

C	0.0523503	1.2655358	-1.5311996
N	0.1254116	0.4186588	-2.5902563
H	0.0268991	-0.5851157	-2.4853747
H	-0.0217867	0.8302243	-3.4985386
N	0.0822761	0.7079931	-0.2769580
H	0.1066356	-0.3252822	-0.1853404
C	0.0581014	1.4248121	0.9444096
O	0.0870669	0.8099504	2.0211040
C	-0.0020141	2.8320434	0.7136557
N	-0.0437075	3.8949766	1.6022591
C	-0.0995735	4.9555199	0.8373775
H	-0.1431230	5.9792118	1.1812138
N	-0.0985138	4.6488690	-0.5144209
H	-0.1326677	5.2951433	-1.2907451
C	-0.0350699	3.2808722	-0.6113944
N	-0.0132849	2.5690072	-1.7571919
C	-0.0167250	-3.1385915	-0.9274657
O	0.0105605	-2.5833627	-2.1756526
H	-0.0509516	-3.3359410	-2.7899356
N	-0.1005437	-4.4635577	-0.8886123
C	-0.1222658	-4.9694870	0.3662543
H	-0.1917878	-6.0516620	0.4389476
C	-0.0638785	-4.1905044	1.4972886
H	-0.0840934	-4.6320063	2.4873988
C	0.0231644	-2.7838286	1.3207115
N	0.0923885	-1.9242719	2.3458084
H	0.0480970	-2.2789707	3.2881426
H	0.1066602	-0.8956347	2.1966954
N	0.0452195	-2.2591315	0.0653868

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G19C2B HB

N	-2.8593927	1.6552188	-0.0089909
C	-3.5189557	0.4731989	-0.0288964
N	-4.8826078	0.3194272	-0.0915333
H	-5.5600606	1.0685138	-0.1225691
C	-5.1328407	-1.0431104	-0.0955183
H	-6.1412466	-1.4295890	-0.1380789
N	-4.0396841	-1.7619946	-0.0424236
C	-3.0141228	-0.8314504	0.0009483
C	-1.5910598	-1.0107387	0.0586747
O	-0.9128295	-2.0372930	0.0788715
N	-0.9426466	0.2591731	0.0917279
H	0.0939264	0.2218289	0.1098553
C	-1.5504170	1.4805257	0.0603520
N	-0.7375457	2.5809801	0.1594909
H	0.2443708	2.4949616	-0.0726410
H	-1.1818342	3.4530142	-0.0898406
N	4.2523478	0.6373236	-0.0701750
C	4.5842126	-0.6692295	-0.0306943
N	5.9156437	-0.9519685	-0.0194988
H	6.5556838	-0.1989115	-0.2274842
H	6.2278342	-1.8944832	-0.1941398
C	3.5947352	-1.6739358	0.0299584
H	3.8492123	-2.7270886	0.0590743
C	2.2809842	-1.2564308	0.0531153
H	1.4443592	-1.9514697	0.0954095
N	1.9315847	0.0492412	0.0223208
C	2.9483142	0.9011711	-0.0383280
O	2.5917655	2.2116123	-0.0778953
H	3.4211626	2.7184154	-0.1182091

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G17C1 HB

H	3.8648127	2.5270018	-0.0671090
N	3.8803404	1.5171112	-0.0590070
C	2.7798475	0.6814698	-0.0065090
C	3.2952717	-0.6227292	-0.0167551
N	4.6734794	-0.5871214	-0.0744551
C	4.9726207	0.6997114	-0.0973828
H	5.9756269	1.1011618	-0.1417822
N	2.5426745	-1.7480920	0.0232363
C	1.3912182	0.9395775	0.0366568
O	0.8116239	2.0518957	0.0412064
N	0.6746960	-0.2574270	0.0752982
H	-0.3619275	-0.1683318	0.0823008
C	1.2417476	-1.5189171	0.0743980
N	0.3779399	-2.5594528	0.1605855
H	0.7843260	-3.4749158	0.0452961
H	-0.6336377	-2.4460307	0.0491306
C	-2.7611193	1.2960251	0.0302483
N	-1.9353804	2.3480012	0.0801229
H	-2.3186895	3.2805733	0.0889365
H	-0.8984952	2.2224758	0.0773422
N	-2.2043529	0.0752871	0.0090159
C	-2.9686273	-1.0455790	-0.0529097
O	-2.5237544	-2.1987385	-0.0824670
N	-4.3706593	-0.8671723	-0.0858456
H	-4.9214446	-1.7152036	-0.1319349
C	-4.9541596	0.3605773	-0.0585355
H	-6.0375379	0.3871200	-0.0872107
C	-4.1883621	1.4792652	0.0006417
H	-4.6414120	2.4622002	0.0222694

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G17C2A HB

N	2.5840322	1.7454709	0.0352026
C	3.3305994	0.6140054	-0.0294371
N	4.7047035	0.5696854	-0.1222526
C	4.9927319	-0.7198409	-0.1585358
H	5.9908479	-1.1292498	-0.2294796
N	3.8941462	-1.5276110	-0.0965154
H	3.8692201	-2.5374401	-0.1094198
C	2.8036377	-0.6834558	-0.0123936
C	1.4130780	-0.9346694	0.0581020
O	0.8277901	-2.0378259	0.0652952
N	0.7043855	0.2730677	0.1213336
H	-0.3286958	0.1904102	0.1394789
C	1.2882639	1.5251960	0.1185677
N	0.4419108	2.5869932	0.2629312
H	0.8651019	3.4837919	0.0723246
H	-0.5469216	2.4875057	0.0589124
N	-2.2685425	-0.0653391	0.0149425
C	-2.8026777	-1.3141585	0.0508059
N	-1.9479247	-2.3444811	0.1458142
H	-0.9213690	-2.2037542	0.1312703
H	-2.3103170	-3.2847442	0.1444474
C	-4.2106718	-1.4843792	-0.0062316
H	-4.6608499	-2.4703103	0.0243754
C	-4.9818221	-0.3494717	-0.1004668
H	-6.0656846	-0.4160164	-0.1455026
N	-4.4662765	0.8999870	-0.1433240
C	-3.1392021	0.9331184	-0.0827672
O	-2.5717390	2.1726466	-0.1275360
H	-3.3172084	2.7949799	-0.1949488

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G17C2B HB

C	-1.4676781	1.5687900	0.0668192
N	-2.5622418	0.7446922	0.1733241
H	-3.4324647	1.1843307	-0.0920518
H	-2.4676643	-0.2352667	-0.0630107
N	-0.2417560	0.9470730	0.1256537
H	-0.2081010	-0.0869584	0.1597376
C	1.0047708	1.6026317	0.0933311
O	2.0705020	0.9714883	0.1318269
C	0.7904308	3.0065026	0.0106545
C	-0.4863986	3.5757211	-0.0521541
N	-1.6491245	2.8674726	-0.0305363
N	-0.3936046	4.9478785	-0.1459178
N	1.6717652	4.0680011	-0.0479782
C	0.9054670	5.1939841	-0.1383500
H	1.3502522	6.1777227	-0.1957610
H	2.6798826	4.0065626	-0.0239864
O	-2.2055989	-2.5953890	-0.0496271
H	-2.7190888	-3.4195541	-0.1088837
C	-0.8993682	-2.9628102	-0.0234661
N	-0.0367540	-1.9554858	0.0593972
C	1.2642734	-2.3190827	0.0761518
H	1.9701820	-1.4933671	0.1355173
C	1.6707300	-3.6356516	0.0205418
H	2.7213752	-3.9008785	0.0398707
C	0.6561178	-4.6137457	-0.0604341
N	-0.6463454	-4.2681132	-0.0884820
N	0.9255305	-5.9476702	-0.0820137
H	0.1644442	-6.5747568	-0.3002794
H	1.8639294	-6.2669851	-0.2656706

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G91C1 HB

N	1.2653503	-1.0751003	-0.0749695
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C	1.3569851	0.2659831	-0.0226769
N	0.3505425	1.1897924	-0.0126051
H	-0.6651556	0.9580819	-0.0322059
C	0.9605333	2.4248165	0.0463878
H	0.3717806	3.3306935	0.0659151
N	2.2771370	2.3697635	0.0739063
C	2.5423661	1.0099329	0.0317521
C	3.7264590	0.2639616	0.0283146
O	4.9482927	0.8373565	0.0722213
H	4.8086506	1.8008870	0.1042352
N	3.6901751	-1.0610314	-0.0269336
C	2.4790757	-1.6599057	-0.0720461
N	2.5082041	-3.0395435	-0.0724210
H	3.4004821	-3.4355449	-0.3353753
H	1.6985170	-3.4966122	-0.4675981
C	-3.9223354	-1.6518611	0.1081192
H	-4.1423163	-2.7095025	0.1754666
C	-4.9214409	-0.7334858	0.0543990
H	-5.9712626	-1.0041646	0.0770257
N	-4.6298806	0.5892562	-0.0309743
H	-5.3587142	1.2906628	-0.0704079
C	-3.2983665	1.0874347	-0.0683198
O	-3.1159724	2.2981054	-0.1373238
N	-2.3009901	0.1526264	-0.0217494
C	-2.5738188	-1.1524053	0.0640681
N	-1.5378498	-2.0099185	0.1123740
H	-1.7206158	-2.9989163	0.1810442
H	-0.5538743	-1.6922126	0.0512043

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G91C2A HB

N	-0.1796511	1.2891496	-1.0736650
C	-0.0654290	1.3667964	0.2624106
N	-0.0526737	0.3487748	1.1753808
H	-0.1146445	-0.6600462	0.9346898
C	0.0898295	0.9421999	2.4128787
H	0.1294270	0.3459819	3.3132537
N	0.1660594	2.2563948	2.3689390
C	0.0701026	2.5395212	1.0154319
C	0.0808283	3.7312974	0.2801140
O	0.2024171	4.9441811	0.8604228
H	0.2742677	4.7961433	1.8203802
N	-0.0379232	3.7104767	-1.0402607
C	-0.1571705	2.5079276	-1.6479153
N	-0.2198030	2.5498504	-3.0238991
H	-0.4594671	3.4548443	-3.4050880
H	-0.6582576	1.7567493	-3.4703613
N	-0.0246478	-4.6937301	0.6191540
C	0.1805915	-4.9219575	-0.6961131
H	0.2773678	-5.9653154	-0.9856076
C	0.2660567	-3.9220150	-1.6388759
H	0.4307980	-4.1471394	-2.6866009
C	0.1262280	-2.5873801	-1.1815216
N	0.1910447	-1.5279829	-2.0122738
H	0.0493154	-0.5578132	-1.6933521
H	0.3494169	-1.6880628	-2.9945209
N	-0.0764536	-2.3397646	0.1343161
C	-0.1357063	-3.4043434	0.9326674
O	-0.3346313	-3.1075269	2.2399862
H	-0.3530825	-3.9656666	2.6994905

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G91C2B HB

N	-1.6828583	0.2737159	-2.2666065
C	-0.8944369	0.1310343	-3.3305763

N	-1.2329444	0.1709879	-4.6656375
H	-2.1596617	0.3170635	-5.0415256
C	-0.0654206	-0.0315042	-5.3870367
H	-0.0695066	-0.0446271	-6.4676813
N	0.9906983	-0.1964021	-4.6284106
C	0.4890563	-0.0984143	-3.3385314
C	1.0852423	-0.1740481	-2.0759811
O	2.4111221	-0.3747493	-1.8977983
H	2.8143523	-0.4546792	-2.7803441
N	0.3569521	-0.0379278	-0.9798926
C	-0.9872011	0.1749185	-1.1129643
N	-1.6730726	0.3013446	0.0454455
H	-1.2024739	0.1947202	0.9490798
H	-2.6578752	0.5064837	-0.0076278
N	-0.4728553	-0.0491324	5.1332193
C	0.8438770	0.2413865	5.1814103
H	1.2537258	0.3967880	6.1767888
C	1.6561540	0.3375900	4.0721415
H	2.7138564	0.5594861	4.1606645
C	1.0464144	0.1381454	2.8107352
N	1.7293720	0.2011416	1.6509418
H	1.2615596	0.0721625	0.7442446
H	2.7115072	0.4242115	1.6609455
N	-0.2798784	-0.1301844	2.7353744
C	-0.9341033	-0.2243022	3.9008477
O	-2.2508210	-0.5422987	3.8188388
H	-2.4286060	-0.7256947	2.8811170

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G92C1 HB

N	0.3446976	0.0103768	1.1784651
H	-0.6675203	0.0120251	0.9298801
C	0.9342904	-0.0168511	2.4256420
H	0.3281896	-0.0258163	3.3205285
N	2.2493715	-0.0320463	2.3989489
C	2.5466100	-0.0142276	1.0446303
C	3.7266400	-0.0156254	0.2933415
O	4.9394892	-0.0398590	0.8777310
H	5.5834695	-0.0365475	0.1456538
N	3.6878196	0.0149420	-1.0400930
C	2.4841552	0.0380484	-1.6528890
N	2.5181714	0.0116002	-3.0336063
H	3.4061661	0.2828307	-3.4335251
H	1.7067726	0.3969709	-3.4964742
N	1.2760523	0.0417319	-1.0668189
C	1.3668541	0.0132175	0.2763499
N	-2.3036725	-0.0032133	0.1469300
C	-3.3004879	0.0280870	1.0835261
O	-3.1177934	0.0616856	2.2951640
N	-4.6326377	0.0174778	0.5843887
H	-5.3608147	0.0395425	1.2872568
C	-4.9245063	-0.0171583	-0.7403867
H	-5.9744710	-0.0206366	-1.0116677
C	-3.9259042	-0.0440730	-1.6606611
H	-4.1468690	-0.0712922	-2.7198670
C	-2.5772701	-0.0354925	-1.1597442
N	-1.5409764	-0.0625383	-2.0182292
H	-0.5574686	-0.0378043	-1.6973211
H	-1.7224066	-0.0989980	-3.0090937

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G92C2A HB

N	0.9419311	0.6923755	-0.0338506
C	1.3645153	-0.5896068	-0.0355530
O	0.4872061	-1.5691125	-0.0578365

H	-0.4834588	-1.2047966	-0.0565973
C	2.7500884	-0.8360097	-0.0102571
N	3.5100058	-1.9985121	-0.0035657
C	4.7458153	-1.5702565	0.0357561
H	5.6262953	-2.1972342	0.0510694
N	4.8490457	-0.1868467	0.0572849
H	5.6959249	0.3636331	0.0851902
C	3.5659841	0.3052776	0.0269620
N	3.1864935	1.5877618	0.0379355
C	1.8524814	1.7038828	-0.0035627
N	1.3490189	2.9778155	-0.0641861
H	1.9953250	3.7150648	0.1751218
H	0.3772593	3.1289697	0.1651290
N	-2.0364663	-0.7866797	-0.0327622
C	-2.9706754	-1.7556032	-0.0134439
H	-2.5929488	-2.7744755	-0.0251999
C	-4.3214765	-1.4960626	0.0184962
H	-5.0521671	-2.2963844	0.0268878
C	-4.6899383	-0.1305023	0.0342275
N	-5.9956987	0.2626884	0.0268111
H	-6.7195885	-0.3989135	0.2605270
H	-6.1782060	1.2413081	0.1998980
N	-3.7796221	0.8534905	0.0227706
C	-2.4966601	0.4860381	-0.0147634
O	-1.6068945	1.4642735	-0.0320012
H	-0.6493434	1.0802557	-0.0522475

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G92C2B HB

N	-0.0377004	3.1402971	1.5208811
C	0.0257383	1.8222563	1.7587058
N	0.0953089	1.4361390	3.0702583
H	-0.1462883	2.1405095	3.7513256
H	-0.1075000	0.4762706	3.3090221
N	0.0687882	0.8258925	0.8319832
C	0.0591261	1.1347774	-0.4782319
O	0.0960773	0.1619018	-1.3706127
H	0.1015416	-0.7588119	-0.9062012
C	0.0084445	2.4877625	-0.8537460
N	-0.0169074	3.1391750	-2.0805177
C	-0.0758593	4.4077425	-1.7645473
H	-0.1092129	5.2279883	-2.4679781
N	-0.0929775	4.6352380	-0.3961461
H	-0.1338118	5.5282475	0.0752397
C	-0.0383648	3.4030324	0.2104648
N	0.0479987	-2.3129852	-0.3973531
C	0.0005596	-2.6604689	0.9097484
O	0.0401228	-1.6801438	1.8014973
H	0.0808100	-0.7670072	1.3416909
N	-0.0838410	-3.9019138	1.3953989
C	-0.1229370	-4.8697621	0.4665598
H	-0.1938389	-5.8858139	0.8490216
C	-0.0803676	-4.6472835	-0.8981040
H	-0.1106649	-5.4636132	-1.6106382
C	0.0099855	-3.3050211	-1.3090757
N	0.0992067	-2.9496274	-2.6227076
H	-0.1094406	-3.6370638	-3.3295170
H	0.0027448	-1.9784461	-2.8844036

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G19C1 ST

N	0.6758224	2.1954854	-0.2650695
C	1.9990813	1.8218945	-0.3852978
H	2.6550747	2.3082751	-1.0917756
N	2.3370521	0.8483069	0.4261437

C	1.1661083	0.5432334	1.0964195
C	0.8754017	-0.5280430	2.0002685
O	1.5633954	-1.4597419	2.4043271
N	-0.4997124	-0.4479478	2.4148064
H	-0.7839226	-1.2159432	3.0138369
C	-1.4423740	0.4207268	1.9322368
N	-2.7470990	0.2347827	2.3575625
H	-2.8721175	-0.0658439	3.3173853
H	-3.3363421	1.0233481	2.1160002
N	-1.1849706	1.3599515	1.0528595
C	0.1173208	1.3641568	0.6685268
H	0.1673310	2.7981964	-0.9005129
N	-1.7978449	-0.3941220	-1.8999557
C	-1.7594635	-1.4472816	-1.0470344
H	-2.7052427	-1.7863075	-0.6388070
C	-0.5671651	-2.0164062	-0.7303105
H	-0.5061572	-2.8525294	-0.0460967
C	0.5995081	-1.4374699	-1.3348979
N	1.8251358	-1.9633890	-1.0575857
H	2.6023355	-1.3569674	-1.2919962
H	1.9322486	-2.4588079	-0.1810314
N	0.5607807	-0.4070452	-2.1732507
C	-0.6278243	0.2048840	-2.4511382
O	-0.7595314	1.2393929	-3.1032192
H	-2.6644943	0.0898330	-2.0980267

29

G17C2B ST

N	0.1894604	1.5871339	-0.5617133
C	0.5204165	0.8417635	-1.6522322
N	1.7486332	0.8604981	-2.2795748
C	1.6434239	-0.0434118	-3.2423390
H	2.4226745	-0.2889818	-3.9499961
N	0.4269631	-0.6589757	-3.2737732
H	0.1108575	-1.3700722	-3.9191968
C	-0.3142769	-0.1023309	-2.2523783
C	-1.6139832	-0.4109084	-1.7592591
O	-2.4279160	-1.2458041	-2.1493701
N	-1.8841831	0.4258026	-0.6451436
H	-2.7899951	0.2738217	-0.2134915
C	-1.0072194	1.3328400	-0.0886826
N	-1.4701324	2.0364626	1.0023986
H	-2.0499044	1.5233110	1.6579153
H	-0.7205782	2.5394497	1.4629715
N	-0.8975150	-1.1293160	2.4212415
C	-0.4223999	-1.7852864	1.3413660
H	-1.0902277	-2.5258203	0.9079823
C	0.8118415	-1.5423381	0.7740240
H	1.1463335	-2.0798890	-0.1054561
C	1.5904126	-0.5237240	1.3645091
N	2.8020822	-0.1431002	0.8646419
H	3.1295661	0.7541009	1.2003641
H	2.9528265	-0.2894686	-0.1257768
N	1.1634208	0.1123291	2.4715605
C	-0.0416102	-0.2417409	2.9221788
O	-0.4798605	0.4266499	4.0210197
H	0.2558823	1.0099933	4.2776510

29

G91C1 ST

N	-0.7385024	-0.9984888	-1.4531364
C	0.5185870	-0.6541298	-1.1646814
N	1.3027596	0.3187450	-1.7380187
H	0.9904135	1.0302393	-2.3869229
C	2.4985704	0.3289421	-1.0451873

H	3.2721964	1.0437539	-1.2843814
N	2.5626624	-0.5784667	-0.0963701
C	1.3248757	-1.2035329	-0.1583464
C	0.7226822	-2.2007256	0.6179613
O	1.3661306	-2.8193997	1.6342450
H	2.2747722	-2.4692045	1.6535936
N	-0.5312833	-2.5635849	0.3944600
C	-1.1908566	-1.9445558	-0.6135938
N	-2.5231621	-2.2956050	-0.7466238
H	-2.7584507	-3.1918631	-0.3398520
H	-2.9089784	-2.1290254	-1.6671793
N	0.6951722	1.9841375	1.2956494
C	-0.0291293	1.0466295	1.9561334
H	0.4430109	0.5682507	2.8070391
C	-1.2817832	0.7362900	1.5308805
H	-1.8717971	-0.0193719	2.0312462
C	-1.7429590	1.4231388	0.3609618
N	-2.9973662	1.1643093	-0.1108632
H	-3.1737747	1.5081138	-1.0463947
H	-3.3992763	0.2614307	0.1058251
N	-1.0242497	2.3178063	-0.3065413
C	0.2442626	2.6197124	0.1023161
O	1.0286633	3.3522271	-0.4975583
H	1.6547835	2.1799693	1.5530560

29

G91C2A ST

N	-1.3534444	-1.0692757	1.2168413
C	-1.3594718	-0.6787154	-0.0573254
N	-2.1265120	0.2893550	-0.6654473
H	-2.7676371	0.9190061	-0.2036518
C	-1.7220768	0.3545417	-1.9865276
H	-2.1553724	1.0710362	-2.6685630
N	-0.7824358	-0.5109327	-2.2878645
C	-0.5438657	-1.1645567	-1.0871205
C	0.3879853	-2.1345942	-0.7039566
O	1.2737597	-2.6695919	-1.5831724
H	1.0536014	-2.3034386	-2.4587674
N	0.4621254	-2.5455521	0.5496836
C	-0.4051218	-1.9976081	1.4408320
N	-0.2471246	-2.4146803	2.7387773
H	0.2500293	-3.2841793	2.8668340
H	-1.0196870	-2.2309169	3.3625979
N	0.0650919	2.2215701	1.6832751
C	0.9578713	1.2376977	1.9030272
H	1.0251215	0.8727082	2.9235860
C	1.7378680	0.6854102	0.9073825
H	2.4251592	-0.1268710	1.1123750
C	1.5483177	1.1936991	-0.3946129
N	2.2640468	0.7403648	-1.4699667
H	1.8495736	0.9496246	-2.3702570
H	2.6911844	-0.1729051	-1.3908642
N	0.6623930	2.1755413	-0.6461455
C	-0.0110397	2.6170520	0.4098765
O	-0.9223104	3.5900341	0.1418361
H	-1.2944207	3.8248687	1.0104610

29

G91C2B ST

N	-1.3156093	1.7187489	0.0586444
C	-0.6724336	1.1151039	-0.9425899
N	0.3362147	1.6022113	-1.7409584
H	0.8355076	2.4703981	-1.6021811
C	0.6880909	0.5839421	-2.6094107
H	1.4849446	0.7156907	-3.3266507

N	-0.0231252	-0.5072733	-2.4513073
C	-0.8777049	-0.1913073	-1.4052940
C	-1.8222317	-0.9359847	-0.6927537
O	-2.0897188	-2.2323967	-0.9802683
H	-1.5445996	-2.4688492	-1.7523410
N	-2.4725189	-0.4031924	0.3304088
C	-2.1965109	0.8888231	0.6452560
N	-2.8666866	1.3760158	1.7437798
H	-3.7205153	0.8912673	1.9828204
H	-2.8814447	2.3822930	1.8337867
N	2.4724902	1.0674575	0.7965782
C	1.5832969	1.1729671	1.8034092
H	1.5334619	2.1446073	2.2883299
C	0.7515437	0.1490890	2.2115502
H	0.0264785	0.2921931	3.0039503
C	0.8532375	-1.0628507	1.5020435
N	0.0705033	-2.1504768	1.7902575
H	0.0540765	-2.8624550	1.0699236
H	-0.8361836	-1.9552098	2.1958252
N	1.7561827	-1.2118975	0.5166562
C	2.4992968	-0.1389296	0.2335087
O	3.3851432	-0.2862446	-0.7827810
H	3.2578902	-1.1966442	-1.1030887

29

G92C1 ST

N	0.9361192	1.2226786	-1.3300852
C	0.6182806	-0.0751867	-1.3495900
N	-0.3074996	-0.7072949	-2.1413163
H	-1.0080611	-0.2527270	-2.7140467
C	-0.3246200	-2.0321827	-1.7468701
H	-1.0116110	-2.7350751	-2.1951070
N	0.5456705	-2.3178518	-0.8089332
C	1.1501883	-1.0974945	-0.5394376
C	2.1023999	-0.6598781	0.3852287
O	2.6714850	-1.5118953	1.2675461
H	3.3027311	-0.9720610	1.7784067
N	2.4616318	0.6192410	0.4463755
C	1.8645068	1.4921097	-0.4005224
N	2.2156201	2.8166555	-0.2377632
H	3.1029717	2.9715689	0.2211082
H	2.0304614	3.4064170	-1.0381235
N	-1.9787857	1.7241080	0.3555750
C	-1.0879869	1.7424489	1.3765814
H	-0.6743757	2.7050414	1.6544057
C	-0.7339561	0.5795235	1.9841621
H	-0.0137496	0.5680854	2.7915462
C	-1.3308393	-0.6172260	1.4684205
N	-1.0196556	-1.8210790	2.0327089
H	-1.2377883	-2.6231538	1.4535444
H	-0.1429640	-1.8884741	2.5319491
N	-2.1916277	-0.6375702	0.4581400
C	-2.5149598	0.5225525	-0.1873233
O	-3.1934656	0.5981676	-1.2105407
H	-2.1917682	2.5648066	-0.1665910

29

G92C2A ST

N	-1.6061074	-0.2555032	0.8624276
C	-1.2876852	-0.8910360	-0.2642305
N	-1.8932509	-0.7793703	-1.4927112
H	-2.6562714	-0.1567110	-1.7194973
C	-1.1830753	-1.5880981	-2.3643409
H	-1.4586144	-1.6642190	-3.4069191
N	-0.1902585	-2.2266500	-1.7959605

C	-0.2391176	-1.8070887	-0.4727597
C	0.5243672	-2.0669369	0.6709073
O	1.5654608	-2.9295652	0.6422899
H	1.9007861	-2.9577057	1.5576627
N	0.2698598	-1.4478962	1.8167865
C	-0.7622992	-0.5648988	1.8609849
N	-0.9710725	0.0531742	3.0669651
H	-0.1718142	0.0450227	3.6857365
H	-1.4496130	0.9427257	3.0029160
N	-0.5442318	2.6240166	-1.0078154
C	0.0788515	1.9439562	-1.9896967
H	-0.3346656	2.0645988	-2.9883431
C	1.1714094	1.1291018	-1.7771124
H	1.6324602	0.5732448	-2.5846877
C	1.6353364	1.0380711	-0.4475312
N	2.7239437	0.2832656	-0.1052230
H	2.8143723	0.0988512	0.8861098
H	2.9651698	-0.4888570	-0.7116754
N	1.0479526	1.7191614	0.5513129
C	-0.0045814	2.4513749	0.2037949
O	-0.6154510	3.0951129	1.2283723
H	-1.3619989	3.5663048	0.8180942

29

G92C2B ST

N	-1.0649477	1.7517858	-0.3007273
C	-0.6060150	0.9006596	-1.2220231
N	0.2773163	1.1330819	-2.2512321
H	0.8296652	1.9708718	-2.3753488
C	0.4742271	-0.0770157	-2.8909575
H	1.1596406	-0.1643065	-3.7213144
N	-0.2346861	-1.0580724	-2.3840748
C	-0.9133012	-0.4612923	-1.3328117
C	-1.7784394	-0.9627984	-0.3548312
O	-2.1483218	-2.2638030	-0.3092295
H	-1.7158535	-2.7076927	-1.0606593
N	-2.2535546	-0.1717889	0.5937098
C	-1.8694081	1.1294677	0.5787132
N	-2.3249259	1.8767697	1.6434122
H	-3.1683670	1.5300602	2.0794201
H	-2.2697531	2.8789465	1.5233935
N	2.5793832	-0.2610152	-0.3015394
C	2.2106996	-1.5150986	0.0233066
H	2.6118222	-2.3025345	-0.6095727
C	1.3596925	-1.8240898	1.0672754
H	1.0676406	-2.8468449	1.2765577
C	0.8753682	-0.7398558	1.8270843
N	0.0262006	-0.8966381	2.8903483
H	-0.4770213	-0.0535904	3.1428993
H	-0.5438373	-1.7318192	2.8896516
N	1.2523411	0.5186728	1.5467443
C	2.0572412	0.6698650	0.4929796
O	2.3569315	1.9520200	0.1635986
H	1.8446461	2.4981440	0.7864148

29

G19C2A TS

N	-0.5789221	4.0976801	0.9798766
C	-0.6667281	4.6241593	-0.2980519
H	-0.9948045	5.6400314	-0.4662032
N	-0.3174218	3.7700103	-1.2272640
C	0.0206504	2.6221831	-0.5308628
C	0.4701409	1.3468215	-0.9988534
O	0.6703196	0.9258134	-2.1390342
N	0.7017529	0.4805567	0.1137251

H	1.0352710	-0.4458883	-0.1527184
C	0.4922831	0.7625295	1.4378346
N	0.8043800	-0.2150212	2.3459900
H	0.7712908	-1.1909049	2.0650226
H	0.4716790	-0.0241519	3.2814743
N	0.0638416	1.9344676	1.8660888
C	-0.1371782	2.8051206	0.8489965
H	-0.7953925	4.5625008	1.8510744
N	0.5928523	-3.3077665	0.9901162
C	1.4878484	-2.9238034	0.0524400
H	2.5343804	-3.0077299	0.3346720
C	1.1273307	-2.4192733	-1.1792895
H	1.8644804	-2.1006955	-1.9061552
C	-0.2652118	-2.2933961	-1.4291100
N	-0.7330228	-1.7060330	-2.5600423
H	-1.7274464	-1.5125550	-2.5542824
H	-0.1535727	-0.9651898	-2.9479457
N	-1.1743495	-2.7566796	-0.5509846
C	-0.6873157	-3.2432897	0.5830765
O	-1.6115441	-3.7038250	1.4536041
H	-1.1076163	-4.0475475	2.2123696

29

G19C2B TS

N	-1.8736635	0.3851678	2.0958618
C	-2.2978883	1.6513661	1.7418966
H	-2.5177356	2.4026974	2.4863610
N	-2.3981250	1.8082608	0.4426129
C	-2.0217612	0.5826715	-0.0826314
C	-1.8708822	0.1729873	-1.4489086
O	-2.0707041	0.7626754	-2.4994014
N	-1.3815020	-1.1827667	-1.4856133
H	-1.2827667	-1.5495664	-2.4266310
C	-1.0215478	-1.9519513	-0.4161832
N	-0.5241179	-3.2063803	-0.6699156
H	0.0092299	-3.3279032	-1.5217719
H	-0.0787579	-3.6254555	0.1380043
N	-1.1593174	-1.5602858	0.8381699
C	-1.6768224	-0.3087156	0.9323594
H	-1.6836346	0.0447228	3.0287768
N	3.4623457	-0.6708811	0.1976618
C	3.8722936	0.4231309	-0.4721498
H	4.9020973	0.4014529	-0.8224555
C	3.0748981	1.5224956	-0.7288532
H	3.4503216	2.3793755	-1.2771349
C	1.7551944	1.4723209	-0.2299071
N	0.8799300	2.5086113	-0.3639347
H	-0.0981493	2.3391084	-0.1581485
H	1.0724719	3.2156257	-1.0572444
N	1.3200013	0.3940178	0.4474139
C	2.1960471	-0.6049158	0.6093688
O	1.7415605	-1.6952020	1.2686857
H	0.7735077	-1.5617913	1.4021178

29

G17C2A TS

N	-1.4960858	-1.1870019	0.1924686
C	-0.5540232	-2.0377077	0.6961833
N	-0.5316875	-2.5059787	1.9895092
C	0.5581724	-3.2553769	2.0496888
H	0.8933469	-3.7938920	2.9247282
N	1.2499769	-3.2971153	0.8749094
H	2.1044588	-3.8002038	0.6787082
C	0.5481627	-2.5108556	-0.0151298
C	0.8089219	-2.1504514	-1.3688671

O	1.7343609	-2.4742362	-2.1093631
N	-0.2300232	-1.2873578	-1.8125819
H	-0.1532559	-0.9949422	-2.7811962
C	-1.2929346	-0.8429648	-1.0599934
N	-2.2009125	-0.0357379	-1.7093024
H	-1.7758678	0.6909794	-2.2790340
H	-2.8407883	0.3788518	-1.0398327
N	1.1073072	3.7766857	-0.3109278
C	1.2279481	3.8335004	1.0323024
H	1.9065838	4.5921055	1.4146368
C	0.5519828	2.9971068	1.8961401
H	0.6809765	3.0721400	2.9699633
C	-0.3098782	2.0382674	1.3127651
N	-1.0629440	1.1739753	2.0390165
H	-1.4548812	0.3708686	1.5395808
H	-0.8422513	1.0392085	3.0144337
N	-0.4459791	1.9640369	-0.0278589
C	0.2701389	2.8270014	-0.7336156
O	0.1181159	2.7120815	-2.0825091
H	0.6964254	3.3960698	-2.4639485

29

G17C2B TS

N	-0.2820271	-0.5329509	0.3257632
C	0.6886108	-0.2869381	1.2441843
N	2.0463360	-0.3324753	0.9956937
C	2.6053544	-0.0241330	2.1559414
H	3.6696748	0.0318784	2.3365778
N	1.7004832	0.2241385	3.1444908
H	1.8893800	0.4704397	4.1063245
C	0.4532329	0.0621762	2.5757304
C	-0.8561611	0.1873811	3.1206348
O	-1.2143824	0.4764552	4.2613226
N	-1.8028837	-0.0918574	2.0967579
H	-2.7679822	-0.0766207	2.4093969
C	-1.5071057	-0.4325946	0.7881962
N	-2.5664732	-0.7279980	-0.0302970
H	-3.4446602	-0.2601504	0.1529210
H	-2.3196793	-0.7674896	-1.0245538
N	-1.2684216	-0.5635397	-2.7941201
C	-0.2839112	-1.4872536	-2.8427262
H	-0.6102422	-2.5149217	-2.9785901
C	1.0517538	-1.1892082	-2.6983071
H	1.8101890	-1.9628212	-2.7099701
C	1.3744280	0.1631804	-2.4678439
N	2.6601201	0.5797359	-2.2479655
H	2.7216188	1.5048830	-1.8400896
H	3.2606584	-0.0982067	-1.7961289
N	0.4251452	1.1139435	-2.4818661
C	-0.8260528	0.6832689	-2.6336852
O	-1.7932833	1.6337477	-2.5858713
H	-1.3210377	2.4722294	-2.4407376

29

G91C1 TS

N	0.3612519	0.4506188	-0.6897943
C	1.0976802	-0.6034915	-0.3118490
N	0.7314506	-1.9219185	-0.2077448
H	-0.2220241	-2.2917035	-0.3387879
C	1.8463380	-2.6025983	0.2319153
H	1.8148703	-3.6691210	0.4049305
N	2.9055285	-1.8399094	0.4061705
C	2.4466650	-0.5753341	0.0702478
C	3.0573479	0.6839590	0.0474892
O	4.3581692	0.8659585	0.3724222

H	4.7177284	-0.0113318	0.5956148
N	2.3687465	1.7625810	-0.2969795
C	1.0675528	1.5908264	-0.6350891
N	0.3746453	2.7574212	-0.9086810
H	0.9604114	3.5356216	-1.1814998
H	-0.4613952	2.6271071	-1.4623750
N	-3.1550826	-0.4288842	-1.1538925
C	-3.4540079	0.8699744	-0.9025940
H	-3.9865911	1.4103376	-1.6771905
C	-3.0831504	1.4337485	0.2765262
H	-3.3076075	2.4691229	0.4971596
C	-2.3952139	0.5806413	1.2001060
N	-2.0260420	1.0634281	2.4164405
H	-1.3953497	0.4862516	2.9563056
H	-1.9839145	2.0603898	2.5654043
N	-2.1143882	-0.6931854	0.9567305
C	-2.4078683	-1.2266468	-0.2568733
O	-2.0487180	-2.3494848	-0.6386883
H	-3.3540391	-0.8515520	-2.0523292

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G91C2A TS

N	0.0113177	4.1726862	0.4727393
C	0.8319974	3.1372201	0.2965473
N	2.1738073	3.0609266	0.6001470
H	2.7340482	3.7966449	1.0077758
C	2.5985517	1.7945417	0.2464552
H	3.6223582	1.4799959	0.3884374
N	1.6416390	1.0549158	-0.2604788
C	0.5219806	1.8767024	-0.2394961
C	-0.8190083	1.7183082	-0.6172446
O	-1.2546906	0.5591571	-1.1397012
H	-2.2080764	0.6729762	-1.3086756
N	-1.6851142	2.7121366	-0.4647999
C	-1.2392203	3.8826686	0.0643672
N	-2.1713431	4.8635414	0.1886979
H	-3.1210080	4.6873602	-0.0930913
H	-1.9089464	5.7503165	0.5857516
N	-0.9962873	-4.2742611	1.1886231
C	-0.7165028	-3.0218759	1.6053236
H	-1.1820695	-2.7197639	2.5410885
C	0.1000685	-2.1524298	0.9151788
H	0.3025005	-1.1497956	1.2716288
C	0.6574622	-2.6330942	-0.2945778
N	1.5001579	-1.8845503	-1.0461879
H	1.7302947	-2.2476662	-1.9600549
H	1.5885896	-0.8820341	-0.8726041
N	0.3905486	-3.8784597	-0.7397270
C	-0.4097327	-4.6047184	0.0312176
O	-0.6665680	-5.8562385	-0.4276238
H	-1.2572215	-6.2469242	0.2402312

29

G91C2B TS

N	0.6404487	-0.0204273	0.5143662
C	-0.4587146	-0.1084551	1.2734223
N	-1.7700697	-0.2088838	0.8781348
H	-2.0772999	-0.2374387	-0.1025869
C	-2.5252740	-0.2597375	2.0320805
H	-3.6026106	-0.3390398	1.9924004
N	-1.8120801	-0.2033243	3.1365903
C	-0.5076738	-0.1081869	2.6743879
C	0.7303962	-0.0010057	3.3206036
O	0.8466052	0.0271207	4.6682370
H	-0.0545248	-0.0402681	5.0316212

N	1.8510392	0.0850325	2.6206027
C	1.7502967	0.0651478	1.2680618
N	2.9513468	0.0991582	0.5914137
H	3.7319264	0.4564975	1.1246190
H	2.8927179	0.4001196	-0.3714454
N	-1.5855608	-0.3198753	-2.0123436
C	-1.0385746	-1.4463391	-2.5110196
H	-1.5494005	-2.3714393	-2.2576830
C	0.1007750	-1.4651308	-3.2862905
H	0.5112305	-2.3930548	-3.6669431
C	0.7047013	-0.2169025	-3.5450736
N	1.8201291	-0.0915952	-4.3195048
H	2.2795214	0.8079194	-4.3280742
H	2.3802793	-0.9045882	-4.5239314
N	0.1814907	0.9231002	-3.0632204
C	-0.9210250	0.7941960	-2.3255501
O	-1.4453544	1.9286859	-1.8162075
H	-0.8458450	2.6465341	-2.0841985

29

G92C1 TS

N	-0.4402712	0.3775660	0.6444886
C	0.6098464	1.1265886	0.2764412
N	1.9209726	0.7468314	0.1712976
H	2.2804391	-0.2100250	0.3015974
C	2.6142880	1.8632845	-0.2479145
H	3.6814219	1.8228887	-0.4165558
N	1.8679747	2.9323202	-0.4102154
C	0.5936992	2.4890490	-0.0865843
C	-0.6712310	3.0854783	-0.0441160
O	-0.8502101	4.3885123	-0.3436008
H	-1.8062815	4.5490497	-0.2410138
N	-1.7492083	2.3785138	0.2952894
C	-1.5834226	1.0719817	0.6090368
N	-2.7477167	0.3680475	0.8728643
H	-3.5229670	0.9400982	1.1810118
H	-2.6037505	-0.4804498	1.4046014
N	0.4434900	-3.1389443	1.1854066
C	-0.8538552	-3.4563787	0.9513565
H	-1.3831706	-3.9759292	1.7423414
C	-1.4296182	-3.1201692	-0.2326556
H	-2.4635066	-3.3630901	-0.4412901
C	-0.5888127	-2.4483620	-1.1799390
N	-1.0826726	-2.1178871	-2.4032143
H	-0.5140303	-1.4978311	-2.9641135
H	-2.0807532	-2.0884163	-2.5470010
N	0.6831888	-2.1484212	-0.9524651
C	1.2289316	-2.4076851	0.2635889
O	2.3519442	-2.0331479	0.6271691
H	0.8756079	-3.3137548	2.0843330

29

G92C2A TS

N	0.1467507	1.5832874	1.8673790
C	-0.6837055	0.5474522	1.9720943
N	-2.0300743	0.5484894	2.2520499
H	-2.6127236	1.3669287	2.3577987
C	-2.4472947	-0.7723808	2.2376327
H	-3.4796323	-1.0358968	2.4191028
N	-1.4781330	-1.6211664	1.9922701
C	-0.3661366	-0.8090097	1.8234967
C	0.9632006	-1.0767083	1.4904151
O	1.4256931	-2.3297793	1.2729816
H	0.6716487	-2.9351258	1.3877575
N	1.8339011	-0.0893401	1.3387058

C	1.3854711	1.1831870	1.5329832
N	2.3174324	2.1573104	1.3469837
H	3.2796625	1.9011950	1.2033717
H	2.0643538	3.1164960	1.5167657
N	-1.5371161	0.2610831	-3.2105317
C	-0.5943843	-0.3019441	-3.9921636
H	-0.8970534	-0.5300932	-5.0114055
C	0.6837972	-0.5851307	-3.5580090
H	1.4173252	-1.0371675	-4.2164465
C	0.9881158	-0.2511238	-2.2170404
N	2.2220296	-0.4449686	-1.6792693
H	2.3080341	-0.3649596	-0.6647863
H	2.8591346	-1.0691328	-2.1500907
N	0.0638641	0.3121995	-1.4140887
C	-1.1244936	0.5237586	-1.9652226
O	-2.0494565	1.0809800	-1.1414076
H	-2.8459311	1.1684931	-1.6945892

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G92C2B TS

N	-0.4914272	1.2968325	-1.5851613
C	-1.0469660	1.5322779	-0.3917777
N	-2.3708946	1.4641925	-0.0316505
H	-3.1369593	1.1792776	-0.6270230
C	-2.4315444	1.7306298	1.3275816
H	-3.3742389	1.7307637	1.8559340
N	-1.2584201	1.9725364	1.8613528
C	-0.3798296	1.8490714	0.7956101
C	1.0158722	1.8803294	0.7074143
O	1.8071777	2.0983902	1.7811257
H	1.2214523	2.2298632	2.5484421
N	1.6271813	1.6531311	-0.4447410
C	0.8547429	1.3856006	-1.5286100
N	1.5325160	1.2081009	-2.6999471
H	2.5190439	1.0095032	-2.6192610
H	1.0322097	0.7564945	-3.4517924
N	-1.2637937	-3.1317022	-0.1051916
C	-0.4618094	-3.6718429	0.8308557
H	-0.8402335	-4.5719423	1.3107841
C	0.7669067	-3.1538045	1.2003984
H	1.3728262	-3.6234291	1.9672032
C	1.1810113	-1.9880002	0.5241345
N	2.3812483	-1.3754525	0.7512568
H	2.4862031	-0.4367115	0.3797020
H	2.8730164	-1.5798694	1.6081346
N	0.4087292	-1.4370013	-0.4259755
C	-0.7630919	-2.0323446	-0.6715056
O	-1.5451109	-1.4443527	-1.6027350
H	-1.0957366	-0.6024730	-1.8567694

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G19C1W1 HB

O	-1.6806704	-0.0489708	0.8091566
C	-0.5305550	-0.0339146	1.2957624
C	-0.1414108	0.0023571	2.6654568
N	-0.8952322	0.0343611	3.8291864
C	-0.0114853	0.0677823	4.7946962
H	-0.2349183	0.0999982	5.8511888
N	1.2912671	0.0581859	4.3283508
H	2.1376670	0.0771167	4.8804317
C	1.2287503	0.0158443	2.9555086
N	2.2796241	-0.0060964	2.1153642
C	1.9013594	-0.0447842	0.8409291
N	2.8335335	-0.0951485	-0.1321415
H	3.7951779	-0.0285637	0.1617951

H	2.6019443	-0.0437515	-1.1318924
N	0.5838857	-0.0523065	0.4431621
H	0.3681615	-0.0608167	-0.5770549
C	0.9643105	0.0232949	-3.2534931
O	2.1597630	0.0296655	-2.9300892
N	0.6451513	0.0634515	-4.6277023
H	1.4325668	0.0927467	-5.2626965
C	-0.6369223	0.0614122	-5.0820492
H	-0.7737281	0.0925871	-6.1570488
C	-1.6715710	0.0204373	-4.2053997
H	-2.6967419	0.0174930	-4.5530242
C	-1.3437804	-0.0191194	-2.8049167
N	-2.3030373	-0.0589413	-1.8749269
H	-2.0630826	-0.0678728	-0.8603207
H	-3.2727192	-0.0524844	-2.1528910
N	-0.0696402	-0.0182284	-2.3766373
O	-3.7993301	0.0060839	2.9852210
H	-3.0165812	0.0274577	3.5674864
H	-3.3640295	-0.0176046	2.1153742

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G19C2AW1 HB

C	-1.8394624	-1.2404454	-0.0654969
N	-2.8834122	-0.3787031	-0.1458343
H	-2.7604562	0.6246811	-0.0569843
H	-3.7990914	-0.7730858	0.0026998
N	-0.5767114	-0.7006554	-0.1013723
H	-0.4686326	0.3323302	-0.1278878
C	0.6269969	-1.4368066	-0.0764371
O	1.7112278	-0.8295516	-0.1218338
C	0.3829402	-2.8371856	0.0001301
C	-0.9481049	-3.2696129	0.0402954
N	-2.0822814	-2.5413140	0.0117104
N	-0.8657723	-4.6375890	0.1158972
H	-1.6483602	-5.2757863	0.1587214
C	0.4830695	-4.9596690	0.1169444
H	0.8147630	-5.9869123	0.1693769
N	1.2603270	-3.9089458	0.0491356
C	1.0416013	2.8094559	-0.0416492
N	2.0587198	1.9476147	-0.1345796
H	3.0165683	2.2582902	-0.0813444
H	1.8864266	0.9327612	-0.1533253
C	1.2189614	4.2151916	0.0556172
H	2.2097612	4.6546916	0.0679675
C	0.0886594	4.9926259	0.1332991
H	0.1617767	6.0743351	0.2089779
N	-1.1672940	4.4862354	0.1241462
C	-1.2065583	3.1620753	0.0322252
O	-2.4561134	2.6058014	0.0243273
H	-3.0697469	3.3584431	0.0907590
N	-0.2154626	2.2834657	-0.0524317
O	4.4508317	-0.1332901	0.0399399
H	5.1535154	-0.7838309	0.1682043
H	3.6305380	-0.6621336	-0.0034878

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G19C2BW1 HB

C	-1.8659584	-1.1980391	0.0664558
N	-2.8796041	-0.2861738	0.1671314
H	-2.7017356	0.6929693	-0.0206414
H	-3.7970022	-0.6376459	-0.0649182
N	-0.5905022	-0.7089963	0.1026229
H	-0.4550629	0.3221034	0.1288327
C	0.6018105	-1.4756689	0.0700607
O	1.6939921	-0.8992102	0.1007352

C	0.2910490	-2.8730900	-0.0004239
N	1.1184353	-3.9836372	-0.0501180
C	0.3018916	-5.0060840	-0.1158843
H	0.5951301	-6.0444695	-0.1673226
N	-1.0272512	-4.6260024	-0.1131915
H	-1.8359134	-5.2308416	-0.1534027
C	-1.0538621	-3.2537829	-0.0382499
N	-2.1648756	-2.4850506	-0.0132477
C	0.7872552	4.7095164	-0.0476908
N	1.1673171	6.0141770	-0.0643617
H	0.4654606	6.7096370	-0.2717771
H	2.1341506	6.2567272	-0.2131590
N	-0.5402658	4.4731627	-0.0880353
C	-0.8991991	3.1945857	-0.0314102
O	-2.2328994	2.9331685	-0.0709181
H	-2.6787808	3.7955058	-0.1347186
N	-0.1251548	2.1183177	0.0542835
C	1.2028906	2.3719141	0.0844176
H	1.8358310	1.4896405	0.1448205
C	1.7163977	3.6496579	0.0376317
H	2.7854641	3.8253663	0.0660517
O	3.9500835	-2.9247113	-0.0018960
H	3.4723605	-2.0776602	0.0418327
H	3.2002860	-3.5481306	-0.0272614

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G17C1W1 HB

C	0.5461820	1.2998306	-0.0657242
O	1.7187045	0.8150275	-0.0948854
C	0.1607200	2.6507520	0.0069532
C	-1.1940248	3.0285011	0.0455279
N	-2.2334553	2.1619663	0.0045874
C	-1.8736821	0.8931492	-0.0747676
H	-3.7710410	0.2353169	-0.0354425
N	-2.8193449	-0.0722427	-0.1626097
H	-2.6014719	-1.0707989	-0.0894541
N	0.8841725	3.8259703	0.0741130
H	1.9103346	3.8682024	0.0632199
C	-0.0394501	4.8206209	0.1468314
H	0.2555508	5.8590331	0.2093629
N	-1.2965220	4.3970872	0.1332282
N	-0.5581304	0.4599535	-0.1029956
H	-0.3600007	-0.5614412	-0.1222200
N	0.0579861	-2.3820603	-0.0370957
C	-0.9901100	-3.2452670	0.0072508
O	-2.1791200	-2.9079767	-0.0107608
N	-0.6867918	-4.6236863	0.0805263
H	-1.4830231	-5.2480360	0.1116064
C	0.5882516	-5.0929927	0.1199537
H	0.7113206	-6.1684859	0.1798730
C	1.6344129	-4.2291250	0.0848699
H	2.6545292	-4.5891988	0.1171699
C	1.3227614	-2.8271156	0.0043434
N	2.2976379	-1.9095860	-0.0346773
H	3.2614376	-2.2013253	0.0151533
H	2.0727929	-0.8948742	-0.0652129
O	3.5481317	2.8637217	-0.0270335
H	3.0078158	2.0299734	-0.0477580
H	3.9922196	2.8901824	-0.8858277

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G17C2AW1 HB

N	-2.2330349	-0.0286266	2.2086225
C	-1.1854058	-0.0294949	3.0691643
N	-1.2745687	-0.0574196	4.4391841

C	-0.0122974	-0.0503418	4.8496047
H	0.2939805	-0.0668098	5.8864376
N	0.8994216	-0.0197359	3.8422509
H	1.9268961	-0.0001238	3.8719284
C	0.1630845	-0.0045449	2.6743047
C	0.5385916	0.0218617	1.3179303
O	1.7027658	0.0436201	0.8255328
N	-0.5772976	0.0219160	0.4836942
H	-0.3879723	0.0320167	-0.5364806
C	-1.8853196	-0.0037748	0.9380991
N	-2.8534108	-0.0012906	-0.0129336
H	-2.6595231	0.0224530	-1.0061565
H	-3.8055715	-0.0256683	0.3154693
N	-0.7089715	0.0211864	-4.7324725
C	0.5827232	-0.0449334	-5.1266163
H	0.7496234	-0.0663512	-6.2002567
C	1.6405185	-0.0841906	-4.2485882
H	2.6643667	-0.1366622	-4.6014945
C	1.3389880	-0.0521729	-2.8626343
N	2.2867937	-0.0859618	-1.9123049
H	2.0469538	-0.0434601	-0.9075771
H	3.2560970	-0.1355389	-2.1832665
N	0.0466739	0.0146406	-2.4480710
C	-0.8663222	0.0454872	-3.4137245
O	-2.1537868	0.1113787	-2.9686576
H	-2.7042514	0.1262754	-3.7714984
O	3.5497168	0.0719026	2.8780347
H	3.0199311	0.0571310	2.0392855
H	4.0080369	0.9234731	2.8658650

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G17C2BW1 HB

H	-3.7551888	-0.0016109	-0.6930681
N	-2.8444043	0.2272476	-0.3194983
H	-2.6810732	-0.0430671	0.6432142
C	-1.8281026	0.0944667	-1.2357669
N	-2.1217508	0.0213107	-2.5145075
C	-1.0285234	-0.0246734	-3.3231764
N	-1.0529748	-0.1033039	-4.6945815
C	0.2275693	-0.1291166	-5.0437466
H	0.5834315	-0.1889209	-6.0629465
N	1.0883011	-0.0730659	-3.9932946
H	2.1162868	-0.0740241	-3.9681241
C	0.2979248	-0.0042606	-2.8648078
C	0.6175112	0.0578521	-1.4874863
O	1.7413743	0.0704500	-0.9285854
N	-0.5500337	0.1065710	-0.7209873
H	-0.4199232	0.1252858	0.3096918
N	-0.0911624	0.0332874	2.1236015
C	-0.8979890	-0.0695529	3.1750948
O	-2.2187452	-0.1537223	2.8722726
H	-2.6912128	-0.2208980	3.7201151
N	-0.5793829	-0.1039349	4.4655406
C	0.7375958	-0.0257125	4.7461737
N	1.0734385	-0.0447907	6.0593810
H	2.0363711	-0.0533331	6.3526245
H	0.3477321	-0.1737996	6.7479099
C	1.6990038	0.0783026	3.7161523
H	2.7606238	0.1359467	3.9272961
C	1.2247963	0.1029457	2.4223306
H	1.8865698	0.1758744	1.5627605
O	3.6658854	-0.0587964	-2.8599508
H	4.1790890	0.7600608	-2.8270730
H	3.0801107	-0.0226713	-2.0540182

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G91C1W1 HB

H	-0.0223639	-0.9468912	-4.8002891
O	-0.0082381	0.0551349	-4.7031115
C	0.0035887	0.4117047	-3.4219913
N	0.0342774	1.7233372	-3.1772453
C	-0.0061870	-0.4865116	-2.3307874
C	0.0194425	0.0959637	-1.0581149
C	0.0523481	2.1522345	-1.9012883
N	0.0484344	1.4094942	-0.7763114
N	0.0298762	3.5233494	-1.7412611
H	0.4165157	3.8703910	-0.8746989
H	0.2985110	4.0388260	-2.5692169
N	-0.0243229	-1.8740940	-2.2129522
N	0.0145765	-0.9459799	-0.1696119
C	-0.0118651	-2.0950743	-0.9122185
H	-0.0196609	-3.0678903	-0.4433975
H	0.0180619	-0.8390480	0.8686363
O	0.1068029	-2.5116656	3.0943661
C	0.0532946	-1.3365034	3.4415154
N	0.0010011	-0.2750427	2.5818284
N	0.0401082	-1.0232727	4.8281045
H	0.0793726	-1.8167797	5.4552261
C	-0.0302375	0.2488475	5.2970856
H	-0.0381403	0.3743017	6.3742849
C	-0.0869383	1.2946456	4.4325841
H	-0.1434106	2.3127971	4.7950623
C	-0.0655058	0.9827352	3.0287685
N	-0.1192299	1.9704714	2.1178589
H	-0.0739687	1.7857612	1.0981154
H	-0.1699031	2.9271395	2.4313665
O	-0.0300863	-2.6304371	-4.8142034
H	-0.0342711	-2.6468353	-3.8135071
H	-0.8825379	-3.0036823	-5.0810864

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G91C2AW1 HB

C	-0.0849791	-2.1509100	1.9289461
N	-0.0851257	-3.5210546	1.7821344
H	-0.4624475	-3.8746770	0.9143687
H	-0.3495623	-4.0302675	2.6145032
N	-0.0757916	-1.4186527	0.7965462
C	-0.0253904	-0.1049252	1.0670073
N	-0.0065552	0.9292546	0.1671479
H	-0.0183883	0.8140404	-0.8679742
C	0.0451324	2.0853667	0.8998048
H	0.0677582	3.0554456	0.4254646
N	0.0602536	1.8757673	2.2016743
C	0.0173232	0.4902671	2.3331380
C	-0.0027592	-0.3970680	3.4343043
O	0.0194191	-0.0284720	4.7108897
H	0.0442833	0.9740680	4.8007538
N	-0.0551722	-1.7092693	3.2012075
C	-0.0900829	1.2032892	-3.5617678
O	-0.2109287	2.4648031	-3.0810382
H	-0.2433961	3.0383634	-3.8670322
N	-0.0286738	0.2642971	-2.6193759
C	0.0977243	-1.0138077	-3.0505021
N	0.1639886	-1.9818315	-2.1159705
H	0.2638487	-2.9391546	-2.4142417
H	0.0841782	-1.7893448	-1.1038937
C	0.1575974	-1.2888755	-4.4397018
H	0.2584435	-2.3019090	-4.8123787
C	0.0793975	-0.2147515	-5.2979937
H	0.1184928	-0.3630719	-6.3742413

N	-0.0472174	1.0651864	-4.8849984
O	0.0634454	2.6531203	4.7931180
H	0.0801957	2.6630671	3.7927185
H	0.9104257	3.0298636	5.0712837

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G91C2BW1 HB

C	1.5901352	3.1343879	-0.1308392
N	2.9517126	3.1301576	-0.2449219
H	3.4222704	3.9983736	-0.0387841
H	3.4371360	2.2688454	-0.0355593
N	1.0071319	4.3594787	-0.0967027
C	-0.3125349	4.4133746	-0.0326743
O	-0.8739099	5.6423422	0.0043118
H	-1.8379807	5.5147551	0.0544166
C	-1.0772257	3.2377776	0.0022953
N	-2.4414737	2.9994171	0.0827297
C	-2.5255220	1.6890161	0.0984909
H	-3.4458279	1.1249754	0.1575147
N	-1.2981995	1.0519239	0.0319966
H	-1.1403765	0.0467617	0.0415093
C	-0.3474250	2.0433182	-0.0300830
N	0.9813986	1.9310512	-0.0986133
C	-0.2678205	-5.3301849	-0.1094280
N	-0.8329868	-6.5569506	-0.2764160
H	-1.8353169	-6.6285600	-0.1749639
H	-0.2851245	-7.3873275	-0.1132856
N	-1.1118481	-4.2814590	-0.0696240
C	-0.5430713	-3.0838291	0.0565046
O	-1.4029275	-2.0269871	0.0890296
H	-2.2931881	-2.4110665	0.0037232
N	0.7433171	-2.7764249	0.1565009
C	1.5697621	-3.8423600	0.1129792
H	2.6293403	-3.6139692	0.1877178
C	1.1279600	-5.1422737	-0.0182374
H	1.8220593	-5.9738929	-0.0524597
O	2.5879616	-0.4514333	0.3611062
H	2.0325775	0.3279736	0.1414134
H	1.9322049	-1.1752265	0.3801051

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G92C1W1 HB

C	-1.4582148	-0.1200316	3.0581206
N	-2.8248382	-0.1545744	3.2606958
H	-3.3604031	-0.5937795	2.5243526
H	-3.0990441	-0.4161903	4.1981466
N	-0.7045018	-0.0334357	4.1753949
C	0.6203368	0.0591372	4.0477709
O	1.3483807	0.1469511	5.1766840
H	0.7037096	0.1295646	5.9079634
N	-1.0251044	-0.1324452	1.7873021
C	0.3156823	-0.0449594	1.7096045
C	1.2202872	0.0561357	2.7839149
N	2.5253295	0.1279280	2.3202454
C	2.3919938	0.0713808	1.0136108
H	3.2054360	0.1004302	0.3024721
N	1.0847555	-0.0349619	0.5835137
H	0.7166936	-0.0753613	-0.3877078
C	-1.6440567	0.0683228	-2.0080441
N	-2.3464684	0.0588017	-0.8603997
H	-1.8895165	-0.0131420	0.0657149
H	-3.3437399	0.2015025	-0.8939037
N	-0.3127625	-0.0521779	-1.9240090
C	0.4556209	-0.0584551	-3.0465067
O	1.6933094	-0.1672227	-3.0228586

N	-0.1973619	0.0673816	-4.2878304
H	0.4259439	0.0595043	-5.1090745
C	-1.5416654	0.1891168	-4.3850496
H	-1.9490852	0.2774391	-5.3861259
C	-2.3182326	0.1966783	-3.2682383
H	-3.3943016	0.2903193	-3.3381328
O	2.1940182	-0.1789364	-5.7005538
H	2.3043282	-0.2144435	-4.7137529
H	2.7268193	0.5760448	-5.9860656

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G92C2AW1 HB

C	-1.5485042	0.0881374	1.3847438
N	-2.4624720	0.1861046	0.3918263
H	-2.1485879	0.0954418	-0.5819908
H	-3.4296665	0.0489770	0.6382064
N	-0.2436470	0.0852504	1.0242267
C	0.5952122	0.0278928	2.0736933
N	1.9623224	0.0090812	2.0654597
H	2.5769286	0.0371429	1.2348994
C	2.3502130	-0.0576343	3.3932672
H	3.3964763	-0.0855907	3.6636360
N	1.3513881	-0.0831925	4.2424815
C	0.2287593	-0.0308919	3.4292685
C	-1.1537281	-0.0357239	3.6606714
O	-1.6531341	-0.1031776	4.9084103
H	-2.6225717	-0.0915249	4.8038099
N	-2.0203685	0.0229878	2.6535943
C	0.1010608	-0.0432104	-4.7284137
N	0.8161301	-0.0006799	-5.8918407
H	1.8125125	-0.1513018	-5.8138150
H	0.3736371	-0.2828313	-6.7531971
C	-1.3100484	-0.0958239	-4.7165866
H	-1.8974078	-0.1376595	-5.6265727
C	-1.9045306	-0.0854514	-3.4728559
H	-2.9874679	-0.1240102	-3.3787806
N	-1.2179113	-0.0285075	-2.3164112
C	0.1219023	0.0156082	-2.4517578
N	0.8150268	0.0080454	-3.5944400
O	0.8590415	0.0705921	-1.3455780
H	0.2989506	0.0790322	-0.4603208
O	3.4376315	0.0100517	-0.3692355
H	2.6490477	-0.0056472	-0.9574346
H	3.9317362	0.7960793	-0.6409536

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G92C2BW1 HB

C	1.8342072	1.5945254	-0.0016554
N	1.4252739	2.8846500	-0.0122339
H	0.4548932	3.1951353	0.0540927
H	2.1513235	3.5784407	0.0739908
N	0.8726548	0.6189856	-0.0691588
C	1.2440662	-0.6771243	-0.0760142
O	0.3224008	-1.6242187	-0.1433482
H	-0.6227928	-1.2296125	-0.1500635
C	2.6081556	-0.9989672	-0.0161531
N	3.3066796	-2.2008656	-0.0036466
C	4.5612748	-1.8361936	0.0612199
H	5.4083375	-2.5073245	0.0892213
N	4.7354687	-0.4592211	0.0932527
H	5.6090964	0.0461388	0.1430972
C	3.4797357	0.0997319	0.0444069
N	3.1648973	1.3945051	0.0578610
C	-3.1712890	-1.7618708	0.0564903
N	-2.7693026	-3.0631766	0.0549989

H	-3.4221298	-3.7797083	0.3306372
H	-1.7854268	-3.2793373	0.1357323
C	-4.5245298	-1.3879576	0.1545314
H	-5.3152679	-2.1217631	0.2598770
C	-4.7932107	-0.0322557	0.1052181
H	-5.8188726	0.3223779	0.1779242
N	-3.8566098	0.9216745	-0.0268613
C	-2.6042851	0.4661080	-0.1146435
N	-2.2133503	-0.8233892	-0.0789005
O	-1.6569375	1.3858078	-0.2518875
H	-0.6842952	1.0073492	-0.1984319
O	-1.2623059	4.0988441	0.1072270
H	-1.7257132	3.2556576	-0.0784546
H	-1.5882291	4.3644956	0.9782261

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G19C1W1 ST

N	-0.5104801	1.1194268	-2.8831881
C	-1.1580581	0.0526025	-3.4828702
H	-1.8611211	0.2021434	-4.2897965
N	-0.8163281	-1.1040979	-2.9699655
C	0.1069754	-0.7889747	-1.9893076
C	0.7888869	-1.6316771	-1.0486600
O	0.7339522	-2.8389027	-0.8501971
N	1.6409800	-0.8256194	-0.2213381
H	2.1543740	-1.3573670	0.4733527
C	1.7220309	0.5404563	-0.1986498
N	2.5477345	1.1042482	0.7403751
H	2.5222214	0.6632753	1.6558380
H	2.3995304	2.1042255	0.8209927
N	1.0687810	1.3095705	-1.0523023
C	0.3081438	0.5918578	-1.9177743
H	-0.6184902	2.1023213	-3.0971863
N	-1.4741654	0.9274015	1.1898591
C	-2.0368896	-0.2030327	0.7033978
H	-2.7905292	-0.0820138	-0.0663821
C	-1.6412902	-1.4187511	1.1677025
H	-2.0640728	-2.3336733	0.7760701
C	-0.5718450	-1.4140034	2.1143559
N	-0.0830961	-2.5988586	2.5742503
H	0.7604681	-2.5547020	3.1295920
H	-0.2257207	-3.4309888	2.0192780
N	0.0033205	-0.3062530	2.5814149
C	-0.4276486	0.9122418	2.1403506
O	0.0834105	1.9901434	2.4754036
H	-1.6311625	1.8387008	0.7456614
O	-0.6106104	3.4790861	0.1144446
H	-0.3522390	3.3871787	1.0561648
H	0.0702759	2.9394023	-0.3416662

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G19C2AW1 ST

N	2.4557539	-0.3282216	0.0249373
C	2.4860997	0.9747441	-0.4211066
H	3.2635216	1.6596802	-0.1169544
N	1.4924232	1.2570907	-1.2303519
C	0.7566007	0.0864815	-1.2999265
C	-0.4846615	-0.1886612	-1.9539053
O	-1.2159013	0.5254125	-2.6380761
N	-0.8722314	-1.5399290	-1.6993340
H	-1.7317447	-1.8109373	-2.1654974
C	-0.2124495	-2.4420006	-0.9032098
N	-0.7508203	-3.7043666	-0.8032566
H	-1.7600685	-3.7816160	-0.8271831
H	-0.3267534	-4.2447960	-0.0590340

N	0.9179301	-2.1762654	-0.2877344
C	1.3419931	-0.9126403	-0.5190195
H	3.0408313	-0.7351993	0.7425907
N	-1.2075775	-0.9161434	1.9789497
C	-2.0678901	-0.1890758	1.2343296
H	-2.9743855	-0.7021357	0.9202247
C	-1.8427991	1.1190337	0.8692336
H	-2.5415648	1.6678830	0.2503282
C	-0.6431179	1.7103155	1.3309314
N	-0.3301663	3.0017271	1.0445070
H	0.6195621	3.2551434	1.2879033
H	-0.6400819	3.3459021	0.1291959
N	0.2283661	1.0135414	2.0905888
C	-0.1104416	-0.2442070	2.3465152
O	0.8106391	-0.9485469	3.0558005
H	0.4328157	-1.8421101	3.1344140
O	-0.4984986	3.3142975	-1.8633479
H	0.3709988	2.8684397	-1.7733750
H	-1.0232301	2.5964702	-2.2650932

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G19C2BW1 ST

N	-0.8658260	3.4348726	-0.1241342
C	-0.3116269	3.4491819	-1.3891425
H	-0.6156935	4.1713553	-2.1332268
N	0.5940529	2.5126120	-1.5560026
C	0.6452094	1.8555792	-0.3349253
C	1.3990494	0.6996261	0.0667640
O	2.2378072	0.0452629	-0.5410830
N	1.0106768	0.3101357	1.3862337
H	1.4049490	-0.5716674	1.7080964
C	0.0528433	0.9053708	2.1685369
N	-0.1740502	0.3459431	3.3902629
H	-0.0035385	-0.6595278	3.4748145
H	-0.9977197	0.7018503	3.8558858
N	-0.6125957	1.9915042	1.8052862
C	-0.2742500	2.4005914	0.5636641
H	-1.5797126	4.0524970	0.2377696
N	-1.0498546	-2.3248657	0.2638380
C	-1.6825728	-1.1656814	-0.0291921
H	-2.3806434	-0.8068409	0.7220072
C	-1.4455428	-0.4395044	-1.1731423
H	-1.9468351	0.5019117	-1.3612190
C	-0.4475636	-0.9366757	-2.0451874
N	-0.0032342	-0.2293678	-3.1196039
H	0.8728598	-0.5746898	-3.4944328
H	-0.0262382	0.7831554	-3.0217009
N	0.1074986	-2.1440367	-1.8307781
C	-0.2223475	-2.7493372	-0.6962248
O	0.3781869	-3.9357660	-0.4442471
H	0.9910693	-4.0804063	-1.1866946
O	0.2188970	-2.3972624	2.7263711
H	0.6669179	-3.2427478	2.8591633
H	-0.3301083	-2.5124769	1.9008543

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G17C1W1 ST

N	-1.7331342	1.0757871	-1.0704088
C	-0.9489000	1.8960219	-0.3218420
N	-0.4376526	3.1078341	-0.7453285
C	0.2977936	3.5316152	0.2711596
H	0.8339741	4.4700240	0.2992964
N	0.3133550	2.6662242	1.3245872
H	0.7856560	2.7796020	2.2104979
C	-0.4863098	1.6006815	0.9621306

C	-0.7077941	0.3404947	1.5885720
O	-0.2395182	-0.0904218	2.6468562
N	-1.5615499	-0.4323700	0.7753569
H	-1.7319887	-1.3973560	1.0704734
C	-2.0141327	-0.0698987	-0.4794795
N	-2.8304276	-0.9732708	-1.0939301
H	-2.7158741	-1.9524426	-0.8266027
H	-2.9806973	-0.7850179	-2.0752348
N	2.2051286	-1.4963498	0.7545676
C	2.7600256	-0.2741725	0.5641577
H	3.4515509	0.0726723	1.3229178
C	2.4294461	0.4535150	-0.5340142
H	2.8550901	1.4330558	-0.7070951
C	1.4607921	-0.1242527	-1.4171611
N	1.0747070	0.5536651	-2.5297349
H	0.2181061	0.2181037	-2.9537080
H	1.1679683	1.5615532	-2.5212299
N	0.9112995	-1.3218565	-1.2192798
C	1.2573384	-2.0502432	-0.1291413
O	0.7862382	-3.1626334	0.1622829
H	2.3676133	-2.0208929	1.6055313
O	-1.8647241	-3.3187241	0.2482908
H	-2.0919017	-4.0853339	0.7895148
H	-0.8770626	-3.3658212	0.1076340

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G17C2AW1 ST

N	-1.4694212	-1.0437677	-0.5876556
C	-0.6993472	-2.1640151	-0.6394680
N	-0.5990544	-3.0048509	-1.7295913
C	0.2715614	-3.9305007	-1.3564248
H	0.5847204	-4.7678827	-1.9642629
N	0.7563727	-3.7405290	-0.0961109
H	1.4173579	-4.3179461	0.4056914
C	0.1419846	-2.6011960	0.3873504
C	0.3435947	-1.8611473	1.5895987
O	1.1064338	-2.0896320	2.5293293
N	-0.4849430	-0.7149611	1.5628389
H	-0.3522129	-0.0399425	2.3210631
C	-1.3286390	-0.3619270	0.5309071
N	-2.0699431	0.7680380	0.7273105
H	-1.8141577	1.3991880	1.4782561
H	-2.4804481	1.1665458	-0.1040221
N	-0.3097305	3.5822743	-0.8936831
C	-0.6252055	2.8846419	-2.0082183
H	-1.3624754	3.3428896	-2.6620913
C	-0.0709654	1.6625276	-2.3183374
H	-0.3624006	1.1159477	-3.2068886
C	0.8812168	1.1471924	-1.4105880
N	1.5345257	-0.0264565	-1.6278471
H	2.0276135	-0.4056190	-0.8296293
H	1.0964930	-0.7062492	-2.2355642
N	1.2096835	1.8192819	-0.2887787
C	0.5889235	2.9759962	-0.1213122
O	0.9062258	3.6251078	1.0450213
H	0.3819452	4.4462081	1.0236786
O	-0.3429926	1.8652986	2.9706395
H	-0.1015849	1.9778950	3.8997684
H	0.2896566	2.4094397	2.4598354

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G17C2BW1 ST

N	1.0256122	0.5482832	-1.7740063
C	1.9907448	0.3022845	-0.8464264
N	3.1159576	-0.4686435	-1.0593872

C	3.7529361	-0.4560541	0.1016654
H	4.6949613	-0.9487380	0.2974060
N	3.1083868	0.2643301	1.0629598
H	3.4006648	0.4230683	2.0174140
C	1.9649219	0.7632025	0.4713282
C	0.8498165	1.4553241	1.0261791
O	0.6568169	1.8213947	2.1864694
N	-0.1128690	1.6568011	0.0104499
H	-1.0072838	2.0607148	0.3006114
C	0.0081329	1.2382239	-1.2994892
N	-1.0128436	1.5906008	-2.1257804
H	-1.8342470	2.0564152	-1.7627661
H	-1.0115761	1.2019429	-3.0546448
N	-2.1418035	-0.8067311	1.4962780
C	-0.9574500	-1.2762269	1.9439055
H	-0.7470482	-1.0995417	2.9946495
C	-0.0349320	-1.9119040	1.1378737
H	0.9176040	-2.2502628	1.5286804
C	-0.3698496	-2.0643528	-0.2245520
N	0.4585180	-2.6617920	-1.1277026
H	0.2597969	-2.4348715	-2.0945372
H	1.4464882	-2.6640636	-0.9091758
N	-1.5581250	-1.6277019	-0.6890619
C	-2.3403589	-1.0313259	0.2058317
O	-3.5201631	-0.5338784	-0.2879653
H	-3.5147798	-0.7563997	-1.2359635
O	-3.0479397	2.2836465	-0.0338934
H	-3.4156551	2.7891517	0.7038996
H	-3.3792577	1.3693505	0.0826385

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G91C1W1 ST

N	-0.6721882	-0.5924505	2.4189253
C	-1.2801692	-0.0411403	1.3658935
N	-2.4832187	-0.4043361	0.8025863
H	-3.0730791	-1.1671083	1.1033883
C	-2.7101158	0.4484585	-0.2586734
H	-3.5917053	0.3657575	-0.8768184
N	-1.7505722	1.3258894	-0.4183564
C	-0.8309744	1.0322984	0.5847848
C	0.4397204	1.5504159	0.9277995
O	1.0844005	2.4890456	0.2463929
H	0.6085305	2.6974321	-0.6389516
N	1.0740928	1.0387627	1.9862951
C	0.4974884	0.0255087	2.6687343
N	1.2472987	-0.4808172	3.7098249
H	1.9486174	0.1500366	4.0735628
H	0.7288190	-1.0093506	4.3980712
N	1.7759605	-0.2118057	-1.4050405
C	1.9931503	-1.0023943	-0.3257154
H	2.8188569	-0.7347566	0.3218116
C	1.1643532	-2.0529437	-0.0824721
H	1.2942766	-2.6746792	0.7928395
C	0.0903219	-2.2370236	-1.0083411
N	-0.8100431	-3.2457162	-0.8050386
H	-1.4290467	-3.4505616	-1.5782569
H	-0.5614168	-4.0118981	-0.1970821
N	-0.1337263	-1.4531122	-2.0565423
C	0.6790508	-0.3835043	-2.2850093
O	0.5272211	0.4390566	-3.1952699
H	2.3345665	0.6199516	-1.5562609
O	-0.1257321	2.8781674	-2.0444289
H	0.1563906	2.1306663	-2.6241633
H	-0.9792801	2.5346596	-1.6876582

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G91C2AW1 ST

N	1.0614618	0.7641810	-1.9560997
C	1.3685579	0.5073391	-0.6868007
N	2.2660222	-0.4223391	-0.2031516
H	2.7662069	-1.1052252	-0.7550849
C	2.2257131	-0.3561304	1.1691294
H	2.8120151	-1.0166911	1.7895071
N	1.3965694	0.5634651	1.6061411
C	0.8376556	1.1163875	0.4575871
C	-0.1718658	2.0737666	0.2239253
O	-0.8451956	2.7158849	1.1862477
H	-0.5987032	2.3612002	2.0874405
N	-0.5168463	2.3600617	-1.0263903
C	0.1037895	1.7081651	-2.0373187
N	-0.3471737	2.0157927	-3.2959337
H	-0.8557009	2.8835089	-3.3848618
H	0.2510949	1.7489925	-4.0643425
N	-0.4116383	-2.5712160	-1.3887016
C	-1.3388083	-1.6249088	-1.6420329
H	-1.5959235	-1.4767559	-2.6872954
C	-1.9284246	-0.8599284	-0.6580645
H	-2.6504015	-0.0885753	-0.8986656
C	-1.5031511	-1.0958099	0.6682483
N	-2.0120387	-0.4045221	1.7273916
H	-1.4692576	-0.4162843	2.5826158
H	-2.4889266	0.4656153	1.5371061
N	-0.5783758	-2.0342964	0.9515488
C	-0.1066629	-2.7010509	-0.0944232
O	0.8442992	-3.6302261	0.1993210
H	1.0430159	-4.0535847	-0.6549129
O	-0.2320489	1.4594197	3.5230159
H	0.1326453	1.9215598	4.2906025
H	0.5443405	1.0394589	3.0432290

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G91C2AW1 ST

N	0.5062267	0.0823960	1.7006433
C	0.4674211	1.0888205	0.8193121
N	-0.5025824	2.0444790	0.6436917
H	-1.4435489	2.0500960	1.0629452
C	-0.1028283	2.8095739	-0.4323741
H	-0.7119168	3.6271660	-0.7909516
N	1.0577298	2.4539394	-0.9426928
C	1.4277786	1.3705555	-0.1634609
C	2.5078479	0.4840877	-0.2251055
O	3.4948421	0.6040936	-1.1444598
H	3.2965949	1.4007882	-1.6686423
N	2.5867647	-0.5420607	0.6086446
C	1.5910200	-0.6864180	1.5206128
N	1.6895437	-1.8170739	2.3118397
H	2.6318631	-2.1666432	2.4251445
H	1.1353310	-1.7866976	3.1571627
N	-2.3425757	-0.0295009	-1.1897509
C	-1.3165620	-0.0389888	-2.0663419
H	-1.3365675	0.7358555	-2.8279378
C	-0.2767622	-0.9443080	-2.0198363
H	0.5457769	-0.8961821	-2.7235237
C	-0.3164700	-1.9070705	-0.9894991
N	0.6485476	-2.8601786	-0.8293735
H	0.6738299	-3.2780196	0.0938555
H	1.5621280	-2.6441196	-1.2063996
N	-1.3403817	-1.9340300	-0.1158393
C	-2.2582800	-0.9868915	-0.2732001
O	-3.2510666	-0.9696996	0.6695930

H	-3.0280410	-1.6834607	1.2928827
O	-3.3107200	1.8471658	1.3916452
H	-3.4115557	0.8846524	1.2504993
H	-3.7723155	2.2249597	0.6280225

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G92C1W1 ST

N	-0.4214487	1.7400446	0.5279866
C	0.7460833	1.0833144	0.4871753
N	1.7191879	1.1521475	-0.4715119
H	1.6513227	1.6026868	-1.4062707
C	2.6884456	0.2475317	-0.0983475
H	3.5639738	0.0931748	-0.7133219
N	2.4444268	-0.3793232	1.0324653
C	1.2165373	0.1355270	1.4225259
C	0.3453019	-0.1117362	2.4866513
O	0.6408944	-1.0179576	3.4462216
H	-0.1077623	-0.9884406	4.0702947
N	-0.8221271	0.5211436	2.5787377
C	-1.1474462	1.4004980	1.6001225
N	-2.4122949	1.9570353	1.6976961
H	-2.7974577	1.9569607	2.6332312
H	-2.5190342	2.8285725	1.1962088
N	-2.0464490	-0.2782182	-1.6698737
C	-2.3244704	-0.9166991	-0.5060191
H	-3.2627067	-0.6721377	-0.0231674
C	-1.4216323	-1.7867404	0.0160942
H	-1.6123007	-2.2937437	0.9523300
C	-0.1997669	-1.9541175	-0.7106696
N	0.7428741	-2.8218246	-0.2526613
H	1.6629697	-2.7059012	-0.6594663
H	0.7428358	-3.0390766	0.7348799
N	0.0765228	-1.3108708	-1.8435828
C	-0.8191355	-0.4265220	-2.3500149
O	-0.6285936	0.2805649	-3.3529572
H	-2.6673344	0.4315423	-2.0382701
O	1.5184336	1.9024985	-3.1286602
H	1.1493758	2.7470725	-3.4222165
H	0.8106152	1.2362893	-3.3403444

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G92C2AW1 ST

N	1.9055732	1.5203525	-0.5388578
C	0.7844838	2.2081170	-0.3117306
N	0.3427154	3.3333352	-0.9707036
H	0.8385593	3.8292763	-1.6984700
C	-0.9007024	3.6429654	-0.4443312
H	-1.4650315	4.4935750	-0.8003905
N	-1.2867279	2.8166237	0.4973899
C	-0.2355682	1.9137521	0.6060217
C	-0.0277148	0.7571558	1.3784626
O	-0.9225840	0.3583447	2.2760529
H	-0.6481519	-0.5529370	2.6150525
N	1.0804982	0.0279816	1.1800792
C	1.9804689	0.4351751	0.2494876
N	3.1082771	-0.3374450	0.1327518
H	3.0287395	-1.2873278	0.4664763
H	3.6275344	-0.2150448	-0.7255002
N	0.5601511	-2.1711964	-1.7682551
C	0.1194308	-1.0227798	-2.3229026
H	0.7027805	-0.6431515	-3.1576093
C	-0.9913069	-0.3416503	-1.8736310
H	-1.3130591	0.5849691	-2.3342824
C	-1.6696496	-0.8906729	-0.7632339
N	-2.7809226	-0.3067780	-0.2303917

H	-3.0210090	-0.6214765	0.7013650
H	-2.8902012	0.6901070	-0.3703106
N	-1.2506925	-2.0354140	-0.1880162
C	-0.1747126	-2.5907723	-0.7364242
O	0.2357112	-3.7341867	-0.1283501
H	1.0125804	-4.0312666	-0.6338674
O	0.0450692	-2.0751983	2.7703372
H	-0.4645391	-2.6176231	2.1435606
H	0.7393267	-1.6643406	2.2040549

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G92C2BW1 ST

N	0.0226772	-0.6068196	1.8895646
C	-0.6655088	-1.3060197	0.9846881
N	-2.0093771	-1.5903100	0.9545303
H	-2.7121012	-1.1873550	1.5603482
C	-2.2460350	-2.2817556	-0.2206394
H	-3.2445301	-2.5893144	-0.4950465
N	-1.1628633	-2.5009143	-0.9270661
C	-0.1627228	-1.8905985	-0.1859076
C	1.1866643	-1.6502968	-0.4421754
O	1.8132043	-2.0782534	-1.5599416
H	1.1550004	-2.5604771	-2.0917945
N	1.9159717	-0.9380078	0.4082814
C	1.3068600	-0.4600758	1.5293842
N	2.0976313	0.3107675	2.3397509
H	3.0971516	0.2245353	2.2255681
H	1.7486117	0.4876010	3.2701361
N	-2.2224876	0.9445613	-1.0711135
C	-1.1898860	0.8128308	-1.9295862
H	-1.3956396	0.2290859	-2.8232982
C	0.0660081	1.3421606	-1.7142414
H	0.8773032	1.1901218	-2.4159906
C	0.2504303	2.0799850	-0.5231899
N	1.4350407	2.6673294	-0.2022104
H	1.5004132	2.9712659	0.7610982
H	2.2890865	2.2486926	-0.5772805
N	-0.7713733	2.2443034	0.3416985
C	-1.9196644	1.6524821	0.0135787
O	-2.9167819	1.7551124	0.9349105
H	-2.5348424	2.2853421	1.6565649
O	3.7330294	0.8854115	-0.7233942
H	4.1278628	0.5476983	-1.5386980
H	3.2127573	0.1232956	-0.3593195

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G19C1W1 TS

N	-4.3204804	1.1358065	-0.4416087
C	-4.3812288	0.5593133	-1.7012668
H	-5.1698337	0.8103581	-2.3965308
N	-3.4063895	-0.2853152	-1.9242300
C	-2.6624619	-0.2691931	-0.7541959
C	-1.4725264	-0.9729937	-0.3994517
O	-0.8148280	-1.7916911	-1.0601179
N	-1.0478367	-0.6207817	0.9017056
H	-0.1669797	-1.0351597	1.2262910
C	-1.6824212	0.2600193	1.7478405
N	-1.1181154	0.4446928	2.9606048
H	-0.2738500	-0.0671141	3.2219795
H	-1.5625257	1.0950370	3.5875128
N	-2.7919017	0.9145469	1.4271438
C	-3.2145565	0.6122924	0.1835959
H	-4.9600556	1.8097564	-0.0437960
N	4.3113635	0.9192645	-0.0161403
C	4.3993996	1.0886391	-1.3631378

H	5.2508339	1.6496663	-1.7313113
C	3.4468769	0.5652810	-2.1743253
H	3.5019843	0.6904979	-3.2482502
C	2.3707711	-0.1535849	-1.5401879
N	1.4012941	-0.7074963	-2.2791116
H	0.6023399	-1.1834127	-1.8234724
H	1.3930149	-0.5832065	-3.2793330
N	2.2914136	-0.3027169	-0.2109891
C	3.2486011	0.2121691	0.5868306
O	3.2681760	0.1125963	1.8298434
H	5.0089011	1.2957490	0.6132524
O	1.1615596	-1.1677263	2.8260347
H	1.9755629	-0.7138210	2.4520883
H	1.4386270	-2.0610916	3.0643792

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G19C2AW1 TS

N	0.9842917	-4.5860093	0.2658132
C	0.4875676	-4.6757987	1.5566398
H	0.6948892	-5.5338811	2.1802209
N	-0.2283447	-3.6356345	1.9023058
C	-0.2044849	-2.8154380	0.7858736
C	-0.8001603	-1.5375348	0.5584984
O	-1.5112298	-0.8533012	1.3047704
N	-0.4780129	-1.0603377	-0.7376853
H	-0.8448933	-0.1373421	-0.9787261
C	0.2631434	-1.7263226	-1.6847683
N	0.4634765	-1.0814784	-2.8668899
H	-0.1929569	-0.3451093	-3.1226752
H	0.8408354	-1.6576512	-3.6051985
N	0.8052946	-2.9162197	-1.4838347
C	0.5473880	-3.3892532	-0.2459864
H	1.5593795	-5.2614683	-0.2186859
N	0.9295555	4.5261014	-0.1275842
C	1.0769809	4.6129846	1.2144644
H	1.6297514	5.4763991	1.5756011
C	0.5709096	3.6829308	2.0929426
H	0.7079719	3.7871826	3.1635272
C	-0.1331569	2.5803087	1.5403735
N	-0.6885219	1.6187998	2.2979966
H	-1.0703666	0.7657699	1.8647306
H	-0.5091878	1.6069800	3.2898850
N	-0.2862650	2.4712573	0.1974812
C	0.2503028	3.4492824	-0.5130750
O	0.0691930	3.3223698	-1.8671910
H	0.5048949	4.0940864	-2.2682751
O	-1.4186242	1.1029805	-2.7424578
H	-0.9580514	1.9153882	-2.4437618
H	-2.3490408	1.2362198	-2.5174526

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G17C1W1 TS

N	1.5060586	3.0315817	-0.6879793
C	0.2810946	3.5589836	-0.4534820
N	-0.1183516	4.8352111	-0.7921964
C	-1.3691320	4.9134117	-0.3730134
H	-2.0018815	5.7848479	-0.4713918
N	-1.8217852	3.7679206	0.2170419
H	-2.7313289	3.5997087	0.6232523
C	-0.7656873	2.8767182	0.1785776
C	-0.6409362	1.5423657	0.6306903
O	-1.5071120	0.8427962	1.1980929
N	0.6455142	1.0595249	0.3591265
H	0.8696955	0.1097571	0.6730249
C	1.6452788	1.7886529	-0.2679044

N	2.8150410	1.1295804	-0.4814214
H	3.0251271	0.3106874	0.0959505
H	3.5771241	1.7204688	-0.7809585
N	0.1893838	-4.6596422	-0.6494327
C	-1.1380288	-4.8530897	-0.8723186
H	-1.4277655	-5.8008137	-1.3114982
C	-2.0270607	-3.8810712	-0.5477517
H	-3.0874598	-4.0196720	-0.7176767
C	-1.4917676	-2.6696811	0.0203727
N	-2.3107808	-1.6678656	0.3693157
H	-1.9321896	-0.7740927	0.7326307
H	-3.3007975	-1.7451064	0.1959665
N	-0.1815178	-2.4899389	0.2286725
C	0.6950349	-3.4697301	-0.0814527
O	1.9255813	-3.4032041	0.0968266
H	0.8751813	-5.3678015	-0.8789260
O	2.6231870	-1.0850054	1.2175831
H	2.3792605	-1.9681057	0.8130525
H	2.7517335	-1.2498450	2.1599379

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G17C2AW1 TS

N	-2.6799169	-0.7772230	1.5224820
C	-3.3985939	-0.4926103	0.4070768
N	-4.7305945	-0.7890210	0.2173548
C	-5.0086335	-0.3088364	-0.9824168
H	-5.9767545	-0.3609216	-1.4610174
N	-3.9423474	0.2852728	-1.5944997
H	-3.9177626	0.7210054	-2.5056869
C	-2.8868976	0.1781313	-0.7100231
C	-1.5307219	0.5661971	-0.8062089
O	-0.9590945	1.1339636	-1.7595056
N	-0.8388045	0.2089759	0.3616490
H	0.1796666	0.3482468	0.3426931
C	-1.4197856	-0.4034179	1.4625653
N	-0.5788457	-0.6444068	2.5161273
H	0.0844858	0.1097298	2.7247497
H	-1.0873692	-0.9783978	3.3262295
N	4.4948781	-0.6907217	0.2864635
C	4.7168443	-0.8715300	-1.0346585
H	5.6768083	-1.3065743	-1.2999594
C	3.8041997	-0.5295189	-2.0036320
H	4.0167314	-0.6792978	-3.0562761
C	2.5698030	0.0247814	-1.5732690
N	1.6189080	0.4107702	-2.4389475
H	0.6925808	0.7461754	-2.1223211
H	1.7542740	0.2362974	-3.4224493
N	2.3161946	0.1927883	-0.2478589
C	3.3051325	-0.1671837	0.5628891
O	3.0561115	0.0404477	1.8905738
H	3.8536292	-0.2680697	2.3561123
O	1.0854759	1.7591758	2.8608182
H	1.8857813	1.3510619	2.4732757
H	0.8348436	2.4583538	2.2408021

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G17C2BW1 TS

N	-1.8248879	-0.2292691	2.3139577
C	-0.7609526	0.0955073	3.0905535
N	-0.8311029	0.4960804	4.4064846
C	0.4259440	0.7092542	4.7558398
H	0.7489399	1.0379617	5.7337930
N	1.3201391	0.4751855	3.7517185
H	2.3253242	0.5706433	3.7857467
C	0.5725245	0.0758659	2.6608125

C	0.9409055	-0.2955374	1.3474592
O	2.0807745	-0.3580212	0.8509006
N	-0.2100932	-0.6197103	0.6043465
H	-0.0326740	-0.9242471	-0.3503285
C	-1.5120155	-0.5890121	1.0870473
N	-2.4928925	-1.0110432	0.2397377
H	-2.3689714	-0.9493386	-0.7756740
H	-3.4254198	-0.8280179	0.5848759
N	-1.6392491	-0.7065779	-2.6237671
C	-0.5219888	-1.4707018	-2.6808492
H	-0.6828287	-2.5410496	-2.5758660
C	0.7484031	-0.9625347	-2.8249079
H	1.6244353	-1.5977588	-2.8375038
C	0.8622440	0.4486255	-2.9370696
N	2.0632759	1.0535136	-3.0688161
H	2.0649612	2.0613776	-2.9840672
H	2.8778088	0.5512599	-2.7081819
N	-0.2397544	1.2271469	-2.9339495
C	-1.4054290	0.6004255	-2.7751903
O	-2.5066937	1.3816966	-2.7295423
H	-2.1873872	2.2963306	-2.8254157
O	3.7581941	-0.4546262	-1.3443050
H	4.3246583	-1.2295242	-1.2391609
H	3.1510142	-0.4624139	-0.5666936

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G91C1W1 TS

N	0.2902773	0.5490972	-1.0039224
C	-0.5488347	0.0499680	-1.9287213
N	-1.8856384	-0.2183106	-1.8216530
H	-2.4960128	0.0065459	-1.0047212
C	-2.2743321	-0.7140681	-3.0496529
H	-3.2999010	-1.0026029	-3.2327253
N	-1.2993879	-0.7961903	-3.9309746
C	-0.2014513	-0.3162208	-3.2364058
C	1.1387997	-0.1209848	-3.5905212
O	1.6202350	-0.4235247	-4.8139063
H	0.8764149	-0.7756467	-5.3353336
N	1.9997470	0.3881372	-2.7184655
C	1.5397880	0.6945673	-1.4862140
N	2.4914241	1.1709766	-0.6026544
H	3.3344135	1.5053006	-1.0510068
H	2.1370231	1.7664436	0.1346700
N	0.1393249	0.0886914	1.8841953
C	1.3051767	-0.5327712	2.1804893
H	1.9632655	-0.7385479	1.3435216
C	1.6104510	-0.8535285	3.4681409
H	2.5418704	-1.3450973	3.7183393
C	0.6425420	-0.4819404	4.4528969
N	0.8960928	-0.7032716	5.7728503
H	0.1329835	-0.5541094	6.4182942
H	1.6410536	-1.3224036	6.0517578
N	-0.5114617	0.1092485	4.1646632
C	-0.8182791	0.3999182	2.8713461
O	-1.8913261	0.9240555	2.5303453
H	-0.0375615	0.3484326	0.8969200
O	-3.3821871	0.4143977	0.3972263
H	-3.9943944	1.1623587	0.3704990
H	-2.8013906	0.5942418	1.1932901

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G91C2AW1 TS

N	-1.0970387	0.9345283	3.3530002
C	0.1565433	0.5418718	3.1199080
N	1.3037062	0.9434006	3.7703359

H	1.3529893	1.5888743	4.5460798
C	2.3638964	0.3162426	3.1439627
H	3.3842371	0.4778405	3.4605243
N	1.9899694	-0.4611727	2.1557592
C	0.6051902	-0.3426644	2.1290745
C	-0.4023210	-0.8650273	1.3001104
O	-0.0955421	-1.7374061	0.3360523
H	-0.8384849	-1.7899913	-0.3077037
N	-1.6671060	-0.4913667	1.4727997
C	-1.9536690	0.3703620	2.4813418
N	-3.2831823	0.6622293	2.6462452
H	-3.8864795	0.4617270	1.8623381
H	-3.5001108	1.4764503	3.2021798
N	-1.6440506	0.1348849	-3.6667152
C	-0.9539696	1.1004460	-4.3144997
H	-1.5049928	1.6423832	-5.0787524
C	0.3618730	1.4083655	-4.0473756
H	0.8761026	2.1961284	-4.5865925
C	1.0073025	0.6557876	-3.0324523
N	2.2813594	0.8601306	-2.6473356
H	2.6632629	0.2928345	-1.8724894
H	2.8339950	1.5785881	-3.0858749
N	0.3381323	-0.3282684	-2.3866922
C	-0.9211900	-0.5036122	-2.7476829
O	-1.5716073	-1.4936590	-2.0582771
H	-2.4893415	-1.4816072	-2.3806968
O	2.8032185	-1.0223588	-0.6148914
H	1.9090542	-1.3359779	-0.8451820
H	2.7352156	-0.8761294	0.3545994

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G92C1W1 TS

N	-1.3910386	-0.7469697	-1.7591552
C	-0.8688520	0.4542816	-1.4841553
N	-1.5044561	1.5333627	-0.9286503
H	-2.4142658	1.4579997	-0.4267396
C	-0.5499510	2.5047558	-0.7775134
H	-0.7818372	3.4493360	-0.3067056
N	0.6415898	2.1716332	-1.2345061
C	0.4584055	0.8713492	-1.6940711
C	1.2941815	-0.1037861	-2.2423146
O	2.6042423	0.1387849	-2.4816256
H	2.9522345	-0.6886226	-2.8623589
N	0.8287718	-1.3142358	-2.5370310
C	-0.4768801	-1.5796944	-2.2783527
N	-0.8812991	-2.8702222	-2.5397265
H	-0.3069032	-3.3822782	-3.1941181
H	-1.8795723	-2.9997988	-2.6281236
N	-0.0680599	-1.2114368	3.3775566
C	1.2793932	-1.3251853	3.4966664
H	1.6503853	-2.0584769	4.2037523
C	2.0923802	-0.5373317	2.7474721
H	3.1693931	-0.6092239	2.8311895
C	1.4517700	0.3882629	1.8521814
N	2.2043981	1.2220244	1.1044836
H	1.7576938	1.7534221	0.3485414
H	3.2008197	1.0757795	1.0477154
N	0.1246711	0.4844815	1.7332859
C	-0.6836163	-0.3024689	2.4826636
O	-1.9238603	-0.2964185	2.4582222
H	-0.6989382	-1.7884250	3.9194363
O	-3.6290176	0.7367690	0.6073968
H	-3.8289672	-0.0680061	0.1056602
H	-3.0124185	0.4175531	1.3201584

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G92C2AW1 TS

N	2.9941418	0.9155607	1.1747162
C	2.7379542	0.7677056	-0.1271856
N	3.2393330	1.5162988	-1.1710678
H	3.8711450	2.3006307	-1.0889775
C	2.7062934	1.0012557	-2.3337293
H	2.9380254	1.4212988	-3.3015887
N	1.9119007	-0.0200698	-2.1179947
C	1.9128685	-0.1861959	-0.7359494
C	1.2745833	-1.0959288	0.1387418
O	0.4817181	-2.0854232	-0.2284905
H	0.1876950	-1.9789255	-1.1992482
N	1.4799301	-0.9600919	1.4556988
C	2.3121584	0.0119622	1.8991304
N	2.4262161	0.1047431	3.2674882
H	2.2153049	-0.7408261	3.7786598
H	3.2147442	0.6417254	3.6009016
N	-4.0770266	0.7710344	-0.6732445
C	-4.4729056	0.7569026	0.6179745
H	-5.5017612	1.0562982	0.8018763
C	-3.6514184	0.3858435	1.6594541
H	-4.0084628	0.3800242	2.6833694
C	-2.3234703	0.0134663	1.3305809
N	-1.4264628	-0.3621124	2.2674680
H	-0.5006414	-0.7006277	2.0011820
H	-1.7171464	-0.4624841	3.2262714
N	-1.9002085	0.0361560	0.0481309
C	-2.8076759	0.3994382	-0.8436753
O	-2.3671857	0.3806934	-2.1392489
H	-3.1355735	0.6443798	-2.6754354
O	-0.2628013	-1.6231440	-2.7102576
H	0.5102180	-1.0202551	-2.8459815
H	-1.0146456	-1.0124428	-2.5824618

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G19C1W2 HB

N	-1.2479319	-0.1007836	5.0786438
C	-0.0114299	0.0346469	5.6915642
H	0.0834637	0.0486209	6.7682674
N	0.9742111	0.1388582	4.8368619
C	0.3613993	0.0693546	3.5950755
C	0.9077525	0.1158703	2.2786400
O	2.0962799	0.2301528	1.9276372
N	-0.1037086	0.0093380	1.3024320
H	0.2213529	0.0296843	0.3150954
C	-1.4479676	-0.1341878	1.5458282
N	-2.2555414	-0.2315551	0.4667421
H	-1.9101599	-0.1600507	-0.4954253
H	-3.2433867	-0.3187764	0.6441156
N	-1.9700138	-0.1860730	2.7661310
C	-1.0259254	-0.0804510	3.7229857
H	-2.1479691	-0.1990315	5.5278540
N	0.4472735	-0.1291047	-3.7697761
C	1.7782935	-0.1391569	-4.0378313
H	2.0501564	-0.1962117	-5.0857371
C	2.6939897	-0.0778807	-3.0365043
H	3.7554891	-0.0843443	-3.2483271
C	2.1873835	-0.0042302	-1.6965243
N	3.0099058	0.0568234	-0.6453311
H	2.6431773	0.1243265	0.3321153
H	4.0070433	0.0484903	-0.7958895
N	0.8629680	0.0085447	-1.4483279
C	-0.0276668	-0.0481441	-2.4616328
O	-1.2693065	-0.0324563	-2.2600378

H	-0.2278848	-0.1886405	-4.5574827
O	-1.2647320	-0.1277263	-5.9864675
H	-1.5327632	-0.9565339	-6.4074741
H	-2.0612394	0.1638009	-5.4623518
O	-3.1142050	0.5055821	-4.1510658
H	-3.3861399	1.4239519	-4.0157554
H	-2.4768889	0.3072165	-3.4102718

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G19C2AW2 HB

C	1.4188902	-2.0426562	0.0516829
N	0.6174939	-3.1312650	0.1196659
H	1.0732392	-4.0288631	0.0715654
H	-0.3887196	-3.0762240	-0.0080122
N	0.8043367	-0.8150891	-0.0097989
H	-0.2354355	-0.7692143	-0.0233648
C	1.4704344	0.4224617	-0.0516131
O	0.7960074	1.4698066	-0.1089148
C	2.8822834	0.2675029	-0.0191855
N	3.8987202	1.2097430	-0.0330684
C	4.9969488	0.4991466	0.0098889
H	6.0031838	0.8936407	0.0146437
N	4.7585607	-0.8667651	0.0514574
H	5.4453500	-1.6076529	0.0888965
C	3.3960135	-1.0338395	0.0356814
N	2.7355818	-2.2074466	0.0694678
C	-2.7993310	0.5679007	0.0624959
N	-2.0126183	1.6421866	0.1133073
H	-0.9948672	1.5302628	0.0434271
H	-2.3657173	2.5995856	0.1496453
N	-2.1875109	-0.6509518	-0.0251154
C	-2.9985472	-1.6990320	-0.0784747
O	-2.3565524	-2.9065571	-0.1672083
H	-3.0690552	-3.5690621	-0.1973282
N	-4.3241333	-1.7561855	-0.0598128
C	-4.9170650	-0.5403762	0.0333953
H	-6.0035970	-0.5458195	0.0556856
C	-4.2187205	0.6401852	0.0980314
H	-4.7239731	1.5958470	0.1739717
O	-1.9825827	4.5337949	0.1703677
H	-0.9958070	4.4873648	0.0939052
H	-2.2552819	5.0378220	-0.6083319
O	0.7527575	4.1986021	-0.2022360
H	1.3993786	4.5749097	0.4101375
H	0.9475949	3.2308299	-0.2089741

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G19C2BW2 HB

C	0.0531203	-1.8925490	-1.8288219
N	0.1463392	-1.1479113	-2.9705641
H	-0.0948273	-1.6341406	-3.8215340
H	-0.0264362	-0.1501508	-2.9443257
N	0.1079207	-1.2142048	-0.6438542
H	0.1417457	-0.1727038	-0.6714849
C	0.0839519	-1.7902022	0.6510182
O	0.1329811	-1.0559270	1.6433436
C	-0.0025243	-3.2181547	0.5585700
N	-0.0540589	-4.1886460	1.5470433
C	-0.1381395	-5.3231529	0.8971200
H	-0.1962156	-6.3040730	1.3461496
N	-0.1462056	-5.1510585	-0.4748373
H	-0.2003137	-5.8722773	-1.1807861
C	-0.0590603	-3.7995067	-0.7118106
N	-0.0394343	-3.2101252	-1.9274758
C	-0.0182726	4.3533772	-0.1655512

N	-0.0599048	5.6902162	0.0100137
H	-0.0849902	6.0932880	0.9442035
H	-0.1792867	6.2795402	-0.7998870
C	0.0847817	3.4531955	0.9230848
H	0.1241383	3.8086846	1.9454128
C	0.1306082	2.1109336	0.6267275
H	0.2033815	1.3457444	1.3960873
N	0.0833656	1.6395819	-0.6423151
C	-0.0165764	2.5769179	-1.5788348
O	-0.0718115	2.0996767	-2.8534719
H	-0.1452886	2.8799904	-3.4296249
N	-0.0718019	3.8956981	-1.4375831
O	0.0328207	-2.6887903	4.1787352
H	-0.0061221	-3.4330187	3.5497734
H	0.0811507	-1.9394361	3.5583890
O	-0.1179450	6.6510283	2.8107869
H	0.6765452	6.5501014	3.3546993
H	-0.8486330	6.3695352	3.3800909

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G17C1W2 HB

N	-1.9632151	2.7831552	-0.1625817
C	-1.0386760	3.7687514	-0.0623781
N	-1.3120167	5.1211515	-0.0633897
C	-0.1292160	5.6993960	0.0534559
H	0.0366941	6.7673881	0.0878644
N	0.9078492	4.8153548	0.1311447
H	1.8917707	5.0248221	0.2215652
C	0.3420094	3.5559772	0.0580779
C	0.9031963	2.2593305	0.0817830
O	2.1124500	1.9432438	0.1759403
N	-0.0988658	1.2923029	-0.0190894
H	0.2178640	0.3016883	-0.0107573
C	-1.4495908	1.5656334	-0.1356015
N	-2.2658120	0.4899801	-0.2308020
H	-1.9270735	-0.4732926	-0.1833220
H	-3.2524080	0.6793191	-0.3071403
N	0.4460671	-3.7807707	-0.1137142
C	1.7752362	-4.0535985	-0.1001982
H	2.0442995	-5.1032889	-0.1349827
C	2.6942789	-3.0542692	-0.0442411
H	3.7548292	-3.2706357	-0.0317239
C	2.1910303	-1.7121506	-0.0011923
N	3.0188928	-0.6624318	0.0551633
H	2.6578502	0.3155637	0.0998965
H	4.0149465	-0.8185694	0.0650714
N	0.8692866	-1.4577245	-0.0129980
C	-0.0262663	-2.4693925	-0.0629762
O	-1.2650568	-2.2629295	-0.0672615
H	-0.2330269	-4.5666199	-0.1660539
O	-1.2854459	-5.9768327	-0.0823137
H	-1.5451577	-6.4217637	-0.9011712
H	-2.0842002	-5.4415124	0.1830870
O	-3.1406841	-4.1246316	0.4633986
H	-3.4516937	-3.9570403	1.3638461
H	-2.4947392	-3.3916722	0.2656458

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G17C2AW2 HB

N	-1.7269620	-0.0256210	2.6964638
C	-2.7010983	-0.0206193	1.7528177
N	-4.0467343	0.0209616	2.0101433
C	-4.6051552	0.0083815	0.8061725
H	-5.6713169	0.0312928	0.6260519
N	-3.7223677	-0.0370438	-0.2251574

H	-3.9690020	-0.0762621	-1.2315152
C	-2.4706317	-0.0567404	0.3613939
C	-1.1616011	-0.0863536	-0.1551337
O	-0.7746773	-0.1093352	-1.3594579
N	-0.2091716	-0.0940991	0.8617776
H	0.7802279	-0.0929547	0.5545322
C	-0.5064348	-0.0761648	2.2096313
N	0.5542004	-0.1694000	3.0663372
H	1.4840652	0.0941115	2.7572008
H	0.3205465	0.0306037	4.0286315
N	4.9812107	0.2037450	0.4018720
C	5.2475720	-0.0332139	-0.9022768
H	6.2988199	-0.0364679	-1.1775620
C	4.2719322	-0.2564004	-1.8462875
H	4.5236425	-0.4380791	-2.8848190
C	2.9241776	-0.2335351	-1.4067714
N	1.8829066	-0.4349382	-2.2315778
H	0.9127499	-0.3451156	-1.8915953
H	2.0463531	-0.5807863	-3.2151596
N	2.6380200	-0.0068245	-0.0986429
C	3.6847912	0.1968054	0.6938797
O	3.3653641	0.4344920	1.9978661
H	4.2163587	0.5541896	2.4552068
O	-4.4477218	-0.0384845	-2.9357904
H	-3.5764243	0.2184746	-3.3445051
H	-4.6930885	-0.8701167	-3.3644244
O	-1.9293605	0.5849688	-3.6759607
H	-1.5208450	0.3454092	-2.7991996
H	-1.7399728	1.5261194	-3.7955039

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G17C2BW2 HB

N	2.6022266	-0.0234920	-2.0861298
C	1.5931838	0.0133986	-2.9957966
N	1.7651558	0.0256009	-4.3571816
C	0.5276003	0.0622718	-4.8374824
H	0.2800353	0.0805338	-5.8901515
N	-0.4435022	0.0734392	-3.8888306
H	-1.4626536	0.1182968	-4.0700183
C	0.2198094	0.0430141	-2.6763091
C	-0.2224325	0.0284148	-1.3335797
O	-1.3840246	0.0432168	-0.8540301
N	0.8654007	-0.0032445	-0.4555864
H	0.6329902	-0.0128797	0.5557118
C	2.1880508	-0.0261467	-0.8378168
N	3.1053039	-0.0428717	0.1703448
H	2.8499869	-0.1068392	1.1447426
H	4.0742867	-0.1022497	-0.0980558
N	0.1316480	-0.0124362	2.3387771
C	-1.2064287	0.0775185	2.5039968
H	-1.7805012	0.1124497	1.5814639
C	-1.8032131	0.1249961	3.7456560
H	-2.8797403	0.1949752	3.8497819
C	-0.9476576	0.0770375	4.8675816
N	-1.4142438	0.0803210	6.1447595
H	-0.7424559	0.1933466	6.8901779
H	-2.3720495	0.3330627	6.3311386
N	0.3897684	-0.0102910	4.7214849
C	0.8313579	-0.0519596	3.4683914
O	2.1760239	-0.1433548	3.2995375
H	2.5670909	-0.1589754	4.1902216
O	-3.7971945	-0.3724293	-1.8855409
H	-2.8823332	-0.2066871	-1.5140063
H	-3.9951246	-1.2925148	-1.6628166
O	-3.2004484	0.1313129	-4.4497978

H	-3.5988534	0.9819881	-4.6801014
H	-3.5495377	-0.0804420	-3.5389402

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G91C1W2 HB

N	-0.0148006	-2.6834402	3.8716714
C	-0.0386950	-1.3413686	3.5531012
H	-0.2569819	-2.8882166	4.8317536
H	-0.4105572	-3.3076604	3.1827292
N	0.0129196	-0.4999935	4.6098277
N	-0.0689158	-1.0247097	2.2438349
C	0.0464395	0.8034057	4.3657925
O	0.0950009	1.6209360	5.4392824
H	0.1101639	2.5345424	5.1016476
C	0.0233965	1.2834002	3.0510201
N	0.0404440	2.5573645	2.5045009
C	-0.0354470	0.3054586	2.0500551
N	-0.0538436	0.9964867	0.8709254
C	-0.0055865	2.3328507	1.2067515
H	-0.0751860	0.5585918	-0.0740184
H	-0.0082438	3.0955292	0.4411773
C	0.0186904	-1.9133196	-1.4979068
N	0.0229428	-2.5250342	-0.2997129
H	-0.0068209	-2.0019016	0.5934938
H	0.1170213	-3.5280264	-0.2634549
C	0.0861592	-2.6832747	-2.7045233
H	0.1467816	-3.7639422	-2.6961083
C	0.0717900	-1.9899132	-3.8740801
H	0.1224883	-2.4709482	-4.8449239
N	-0.0055905	-0.6372624	-3.8841693
H	-0.0122200	-0.1404704	-4.7972225
C	-0.0633095	0.1052230	-2.6966545
O	-0.1205176	1.3483260	-2.7377299
N	-0.0523824	-0.5755973	-1.5180513
H	-0.0915451	2.3478061	-4.0983409
O	-0.0428935	2.8523513	-4.9591996
H	0.7040520	3.4581429	-4.8575012
O	0.1083717	0.6013450	-6.3970244
H	0.1108040	1.5270066	-6.0231682
H	-0.6598761	0.5730287	-6.9842448

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G91C2AW2 HB

N	-1.2419740	0.0138575	-0.6862762
C	-1.4445080	-0.0071045	0.6436191
N	-0.5117664	0.0377892	1.6419117
H	0.5085855	0.0092404	1.4815297
C	-1.2169185	-0.0164127	2.8306290
H	-0.7057715	-0.0020572	3.7822750
N	-2.5209657	-0.0805351	2.6692910
C	-2.6793785	-0.0793153	1.2909416
C	-3.7996085	-0.1396605	0.4476332
O	-5.0605139	-0.1939161	0.9243550
H	-5.0008771	-0.1804717	1.8965432
N	-3.6596829	-0.1506983	-0.8684610
C	-2.4061767	-0.0872965	-1.3822824
N	-2.3120345	-0.1408502	-2.7311973
H	-3.1698588	-0.1320431	-3.2592065
H	-1.4129222	-0.0507173	-3.2027948
N	4.5758070	0.1573599	1.0815481
C	4.8525136	-0.3433009	-0.1424588
H	5.9051635	-0.3794261	-0.4114897
C	3.8881385	-0.7893373	-1.0187453
H	4.1486350	-1.1910859	-1.9910255
C	2.5398203	-0.7098726	-0.5927852

N	1.5131148	-1.1594578	-1.3472720
H	0.5615185	-0.8711040	-1.1010091
H	1.6662165	-1.2757591	-2.3409584
N	2.2405108	-0.1908649	0.6241729
C	3.2768594	0.1935181	1.3696734
O	2.9318902	0.6921585	2.5820781
H	3.7715617	0.9324716	3.0124306
O	0.5235314	1.9692557	-1.7715478
H	1.2864386	2.0335313	-1.1790467
H	-0.0986098	1.3504077	-1.3072760
O	0.4779156	0.2267523	-3.8671895
H	0.6485930	0.9437388	-3.2017242
H	0.5447563	0.6573707	-4.7303540

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G91C2BW2 HB

N	2.1427589	-2.1761318	-0.2455660
C	1.5012357	-3.3336993	-0.1100704
N	2.0480275	-4.6017894	-0.0929782
H	3.0296199	-4.8251061	-0.1844873
C	1.0119769	-5.4955588	0.0668737
H	1.1785238	-6.5619939	0.1097939
N	-0.1565732	-4.9035634	0.1550746
C	0.1230385	-3.5432787	0.0468652
C	-0.6695699	-2.3746114	0.0568999
O	-1.9950004	-2.3418102	0.1801325
H	-2.3790404	-3.2698109	0.2687145
N	-0.0687914	-1.1942201	-0.0739006
C	1.2830946	-1.1346096	-0.2202628
N	1.8015590	0.1060744	-0.3736035
H	1.2113956	0.9331303	-0.2572242
H	2.8022573	0.1917880	-0.4547775
N	-0.2565398	4.9630784	0.0108850
C	-1.5648310	4.7894547	-0.2778043
H	-2.1402025	5.7016483	-0.4107701
C	-2.1622667	3.5563680	-0.3960569
H	-3.2185411	3.4592554	-0.6195118
C	-1.3370278	2.4170157	-0.2203097
N	-1.8040369	1.1608737	-0.3103114
H	-1.1889629	0.3417038	-0.1880399
H	-2.7777481	1.0022596	-0.5155909
N	-0.0160271	2.5729744	0.0518920
C	0.4210160	3.8297719	0.1634513
O	1.7316613	3.9887633	0.4748377
H	2.0867375	3.0974911	0.6294785
O	1.1816347	7.5160870	0.3604480
H	0.6670877	6.6882121	0.2342305
H	2.0648327	7.1907033	0.5819941
O	-2.8652230	-4.8596299	0.3737044
H	-1.9229657	-5.1835558	0.3257182
H	-3.1877060	-5.1174983	1.2491157

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G92C1W2 HB

N	-0.9998737	2.2340025	-0.1455171
C	0.3279874	2.0571824	-0.0165593
N	1.0079748	0.8765361	0.0433824
H	0.5676190	-0.0653321	0.0079638
C	2.3406888	1.2094507	0.1787121
H	3.0965342	0.4400704	0.2499973
N	2.5719127	2.5033892	0.2076183
C	1.3085638	3.0624403	0.0857999
C	0.8065509	4.3676292	0.0407364
O	1.6150853	5.4407095	0.1230938
H	1.0278253	6.2171902	0.0696272

N	-0.5017429	4.5926603	-0.0935566
C	-1.3355437	3.5336680	-0.1759443
N	-2.6810205	3.8370575	-0.2551010
H	-2.8780506	4.7830028	-0.5531542
H	-3.2602026	3.1275352	-0.6827584
N	-0.6320436	-3.8843242	0.0800376
C	-1.9834838	-3.8726952	0.1706246
H	-2.4646974	-4.8428864	0.2296149
C	-2.6762592	-2.7023930	0.1832231
H	-3.7563025	-2.6927487	0.2541055
C	-1.9060063	-1.4976773	0.0889599
N	-2.5149894	-0.2975888	0.0866864
H	-1.9888801	0.5899792	0.0061504
H	-3.5168142	-0.2554428	0.1893245
N	-0.5700307	-1.5194854	-0.0030944
C	0.1102917	-2.6982137	-0.0073606
O	1.3522584	-2.7405425	-0.0820714
H	-0.1355700	-4.7976994	0.0785870
O	2.8253687	-4.9683169	-0.3052174
H	3.3151803	-4.8945305	-1.1357465
H	2.3316567	-4.1043354	-0.2124054
O	0.5915688	-6.4064591	-0.0210783
H	0.6831648	-6.9230827	0.7917310
H	1.5038881	-6.0367442	-0.1919300

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G92C2AW2 HB

N	-1.8347723	-0.1364802	3.5945046
C	-0.6422044	-0.0214702	4.1896227
N	-0.3807533	0.0187779	5.5381094
H	-1.0672095	-0.0244881	6.2784069
C	0.9951805	0.1344770	5.6736607
H	1.4585813	0.1886316	6.6488994
N	1.6291091	0.1687358	4.5294910
C	0.6187554	0.0730889	3.5812243
C	0.6176520	0.0445691	2.1742743
O	1.7320917	0.1104710	1.4804040
H	1.5490014	0.0438621	0.4616114
N	-0.5698222	-0.0531078	1.5373418
C	-1.7199287	-0.1369507	2.2609446
N	-2.8896263	-0.1825901	1.5424135
H	-2.8488672	-0.4928940	0.5819195
H	-3.7039765	-0.4653601	2.0687687
N	1.4063685	-0.0521606	-1.1321504
C	2.5167293	-0.1204472	-1.8985624
H	3.4579811	-0.1558753	-1.3569251
C	2.4832693	-0.1421889	-3.2690721
H	3.3937644	-0.1942921	-3.8543689
C	1.2032397	-0.0843216	-3.8827005
N	1.0589982	-0.0876387	-5.2198018
H	0.1415053	-0.0122136	-5.6863981
H	1.8847623	-0.0908689	-5.7975131
N	0.0838369	-0.0258827	-3.1261996
C	0.2355811	-0.0088644	-1.7965290
O	-0.8824139	0.0667032	-1.0923479
H	-0.6775204	0.0396906	-0.0757777
O	-1.4352211	0.2006605	-6.5806786
H	-1.7801144	-0.5730599	-7.0473804
H	-1.9913246	0.2653892	-5.7577969
O	-2.5396939	0.1564598	-4.1277622
H	-1.6429168	0.0625168	-3.7011140
H	-2.9400942	0.9198874	-3.6889397

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G92C2BW2 HB

N	3.3819259	-0.0955280	1.4920210
C	3.5737195	-0.0715444	0.1634143
N	4.7820659	-0.1146679	-0.4896090
H	5.6907542	-0.1680968	-0.0498897
C	4.5087374	-0.0720437	-1.8490340
H	5.3029938	-0.0949729	-2.5816835
N	3.2286378	-0.0041120	-2.1138876
C	2.6246091	-0.0004821	-0.8654692
C	1.2612908	0.0597605	-0.4905317
O	0.2528113	0.1363523	-1.2373199
H	-1.3927844	0.0545485	-0.7882999
N	1.0780507	0.0237714	0.8920650
C	2.0908681	-0.0505945	1.8231393
N	1.7464336	-0.0946840	3.1238380
H	0.7878674	0.0356554	3.4845944
H	2.5146795	-0.0795198	3.7771540
N	-3.8628770	-0.0736979	1.3770972
C	-4.8509926	-0.1459456	0.4774163
H	-5.8549176	-0.2008196	0.8961032
C	-4.7015132	-0.1561352	-0.9022513
H	-5.5535469	-0.2157181	-1.5678972
C	-3.3939583	-0.0815877	-1.4080942
N	-3.0844011	-0.0870159	-2.7154174
H	-2.1257355	0.0148614	-3.0937823
H	-3.8458428	-0.0946558	-3.3760713
N	-2.3913446	-0.0068279	-0.4925405
C	-2.6069798	-0.0025526	0.8893272
O	-1.5835342	0.0695336	1.6206502
H	0.0789587	0.0505496	1.1965080
O	-0.4983170	0.3189634	-3.7748144
H	0.0297652	0.2920225	-2.9362425
H	-0.0456766	-0.2920843	-4.3716505
O	-0.8755607	0.3138682	4.1623210
H	-1.3735881	0.2602716	3.3043433
H	-1.2689744	-0.3735302	4.7169440

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G19C1W2 ST

N	-2.2175672	1.1929609	2.1842136
C	-3.2074373	0.8106761	1.2984678
H	-4.1760813	1.2889530	1.2880288
N	-2.8279920	-0.1672244	0.5116940
C	-1.5268283	-0.4484532	0.9005525
C	-0.5858456	-1.3974580	0.3849903
O	-0.7167341	-2.2336277	-0.5146714
N	0.6557806	-1.2703917	1.0525936
H	1.4457184	-1.7895795	0.6516441
C	0.9398744	-0.4022239	2.0783276
N	2.1804726	-0.4912713	2.6242137
H	2.9154579	-0.9258818	2.0682606
H	2.4447042	0.2845347	3.2141485
N	0.0651320	0.4663190	2.5701353
C	-1.1245521	0.3925049	1.9398091
H	-2.2852502	1.8963826	2.9071465
N	1.2026410	2.1044458	-0.5737041
C	-0.0846653	2.3020866	-0.9696275
H	-0.6070084	3.1442135	-0.5309518
C	-0.6527887	1.4543081	-1.8616100
H	-1.6797253	1.5729798	-2.1785221
C	0.1635758	0.3727192	-2.3374761
N	-0.3544956	-0.5000432	-3.2280624
H	0.2107277	-1.3291282	-3.3699804
H	-1.3660317	-0.6729497	-3.1594885
N	1.4284977	0.1879063	-1.9440238
C	1.9749881	1.0163143	-1.0275068

O	3.1070152	0.8693829	-0.5250233
H	1.6331074	2.6871668	0.1330629
O	-2.8814231	-1.4304907	-2.1870138
H	-2.2288749	-1.9672462	-1.6844332
H	-3.2342161	-0.8782656	-1.4615848
O	3.4341876	-1.6344194	0.2884818
H	3.4328823	-0.7560016	-0.1909733
H	3.8393292	-2.2730374	-0.3114793

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G19C2AW2 ST

N	-2.9031646	-1.5439670	1.2354233
C	-3.6737719	-0.4505657	0.8901784
H	-4.6047740	-0.2303497	1.3918510
N	-3.1451920	0.2500814	-0.0844354
C	-1.9703297	-0.4152167	-0.3999227
C	-0.9463002	-0.0967335	-1.3489321
O	-0.8707549	0.8286504	-2.1625387
N	0.1172005	-1.0293886	-1.2528391
H	0.9432149	-0.8252560	-1.8206522
C	0.1770789	-2.1080202	-0.4051773
N	1.2654678	-2.9146487	-0.5195649
H	2.0777478	-2.5659029	-1.0208370
H	1.4173961	-3.5497280	0.2503543
N	-0.7737780	-2.4102667	0.4651387
C	-1.7963742	-1.5327778	0.4190554
H	-3.1058218	-2.2330273	1.9469944
N	2.0107137	-0.1434484	1.8277122
C	0.7713801	0.2830787	2.1683301
H	0.2740160	-0.2857438	2.9492411
C	0.1494760	1.3547161	1.5701781
H	-0.8501303	1.6618536	1.8524636
C	0.8641490	2.0316146	0.5491723
N	0.3595118	3.1077495	-0.0922320
H	0.8844114	3.3952886	-0.9089106
H	-0.6630158	3.1897992	-0.1817166
N	2.1049896	1.6212775	0.1933096
C	2.5671159	0.5773138	0.8570895
O	3.8087898	0.1462161	0.4416844
H	4.0218609	-0.5951491	1.0372428
O	3.0198115	-1.0588838	-2.0023104
H	3.4050193	-0.7791349	-2.8433203
H	3.4189525	-0.4844208	-1.3143478
O	-2.3657123	2.9472880	-1.0016599
H	-2.9401817	2.2966225	-0.5509941
H	-1.9295088	2.3638465	-1.6607022

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G19C2BW2 ST

N	3.8731147	0.2946024	-0.9917388
C	3.6946289	1.6176154	-0.6382761
H	4.3510640	2.3959816	-0.9994306
N	2.6659778	1.7921186	0.1554521
C	2.1400493	0.5209615	0.3362087
C	1.0057985	0.0811620	1.0904646
O	0.2199322	0.7199247	1.7957913
N	0.8212476	-1.3164918	0.9231021
H	-0.0294463	-1.7029428	1.3336659
C	1.5948971	-2.1566430	0.1553343
N	1.2312185	-3.4656903	0.1307770
H	0.2431316	-3.6799824	0.3030687
H	1.7070311	-4.0146820	-0.5716749
N	2.6652841	-1.7521774	-0.5133663
C	2.8741091	-0.4266317	-0.3812675
H	4.5921782	-0.0841679	-1.5927172

N	-2.2896166	-1.0202277	-0.9059784
C	-1.2763287	-0.2478507	-1.3709345
H	-0.4766443	-0.7799465	-1.8786885
C	-1.2170137	1.1112810	-1.1957722
H	-0.3718424	1.6950567	-1.5375342
C	-2.2773212	1.7108175	-0.4699795
N	-2.2703397	3.0277692	-0.1627161
H	-2.9836464	3.3164224	0.4946551
H	-1.3442415	3.4519621	-0.0266073
N	-3.3384520	0.9737136	-0.0749678
C	-3.2624569	-0.3323358	-0.3042823
O	-4.2922105	-1.0880459	0.1523867
H	-4.8943862	-0.4635610	0.5935468
O	0.3415627	3.4478932	0.8982966
H	1.2339096	3.2750461	0.5383114
H	0.1938498	2.6206447	1.4072267
O	-1.5434873	-3.2044804	0.5605741
H	-2.3097334	-3.5346908	1.0472249
H	-1.9047163	-2.5219340	-0.0792789

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G17C1W2 ST

N	0.6945941	-0.4294393	-2.4327933
C	-0.6189515	-0.3709307	-2.0929674
N	-1.5973894	-1.2284938	-2.5438139
C	-2.6961619	-0.8339046	-1.9130260
H	-3.6694690	-1.2894542	-2.0321487
N	-2.5060080	0.2313356	-1.0895342
H	-3.1409744	0.6422380	-0.4004556
C	-1.1642612	0.5433357	-1.1824282
C	-0.3577105	1.4474095	-0.4502992
O	-0.6881212	2.2396201	0.4611272
N	0.9764445	1.3395988	-0.8508988
H	1.6730857	1.8126714	-0.2636096
C	1.4479375	0.4434958	-1.7944991
N	2.7791518	0.5338199	-2.0822143
H	3.3861036	0.9199410	-1.3624296
H	3.1407847	-0.2644792	-2.5856499
N	0.7598399	-2.0946847	0.5556726
C	-0.5816251	-2.2270733	0.7181634
H	-1.0798611	-2.9495827	0.0833903
C	-1.2322806	-1.4454326	1.6193511
H	-2.3022456	-1.5198370	1.7581624
C	-0.4392932	-0.4837951	2.3245653
N	-1.0333399	0.3559991	3.2137227
H	-0.4499459	1.1329982	3.5008357
H	-2.0056597	0.5931564	3.0394671
N	0.8788864	-0.3651602	2.1672688
C	1.5220174	-1.1456299	1.2651218
O	2.7332854	-1.0559419	0.9933392
H	1.2456139	-2.5919128	-0.1812613
O	-3.1340634	1.6311204	1.3466806
H	-2.2360431	1.9859712	1.0670283
H	-3.6953216	2.4096207	1.4647424
O	3.4806044	1.4759972	0.6066489
H	3.2821783	0.5622591	0.9571009
H	3.7556127	2.0039342	1.3668309

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G17C2AW2 ST

N	-0.9509010	-2.2351337	-0.0200575
C	0.3148330	-1.9268065	0.3803290
N	1.4551445	-2.5813794	-0.0230146
C	2.4427958	-1.8953568	0.5431893
H	3.4927011	-2.1262949	0.4299914

N	2.0234425	-0.8477528	1.2994252
H	2.5571831	-0.0556585	1.6832417
C	0.6488994	-0.8408499	1.1997693
C	-0.3285475	0.0519279	1.7114583
O	-0.1986439	1.0738413	2.4109462
N	-1.6021882	-0.3540327	1.2867228
H	-2.3668807	0.2765547	1.5215404
C	-1.8645991	-1.4081392	0.4365109
N	-3.1877400	-1.5865846	0.1158958
H	-3.7348255	-0.7329102	0.0206117
H	-3.3236726	-2.2647378	-0.6223740
N	1.1452434	2.1739956	-0.7417170
C	2.0949057	1.3820060	-1.2877808
H	3.1237072	1.6678833	-1.0854849
C	1.8092176	0.2623853	-2.0340643
H	2.5945945	-0.3662910	-2.4352081
C	0.4442730	-0.0547239	-2.2082385
N	0.0414310	-1.1640514	-2.8892545
H	-0.9129204	-1.4440372	-2.6967561
H	0.6938284	-1.9385084	-2.8978587
N	-0.5247466	0.7435118	-1.7160458
C	-0.1016190	1.7907824	-1.0231158
O	-1.1012599	2.5621697	-0.5050129
H	-0.6681727	3.2089290	0.0793574
O	-3.7176223	1.3706270	0.1652589
H	-2.9295152	1.8006536	-0.2229877
H	-4.3331634	2.0877275	0.3669556
O	2.4457354	1.8387798	2.1289344
H	2.2807793	2.3029147	1.2894955
H	1.5217799	1.6824332	2.4462925

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G17C2BW2 ST

N	-1.3816383	1.8409342	0.1353998
C	-2.1767585	0.7928143	-0.2058525
N	-3.3934526	0.5011153	0.3755803
C	-3.7906234	-0.6122633	-0.2215550
H	-4.7246989	-1.1202722	-0.0267670
N	-2.9027479	-1.0767933	-1.1453455
H	-2.9922998	-1.8966342	-1.7301338
C	-1.8505960	-0.1816256	-1.1552547
C	-0.5635084	-0.2569860	-1.7528633
O	-0.0995603	-1.1548058	-2.4763954
N	0.1969981	0.8530821	-1.3613236
H	1.1873923	0.8889219	-1.6368929
C	-0.2183528	1.8323938	-0.4819163
N	0.6710433	2.8468323	-0.2998115
H	1.6222264	2.7176826	-0.6289390
H	0.5030660	3.4574116	0.4852068
N	1.8933377	-1.4828458	0.6800357
C	0.6911665	-2.0996926	0.7333436
H	0.5912296	-2.9862197	0.1140915
C	-0.3689506	-1.6402290	1.4832005
H	-1.3248275	-2.1502787	1.4826830
C	-0.1692530	-0.4445270	2.2078475
N	-1.1518045	0.1358053	2.9486635
H	-0.9865316	1.1058058	3.1861651
H	-2.1083070	-0.0635227	2.6816421
N	1.0325008	0.1670294	2.1995943
C	1.9706273	-0.3976912	1.4455122
O	3.1770995	0.2392255	1.4276123
H	3.0842114	0.9827320	2.0495983
O	2.7325556	-1.3484992	-2.1683588
H	2.6867892	-1.5931827	-1.2192062
H	1.7889277	-1.3818651	-2.4474774

O	3.0942018	1.2504873	-1.4114944
H	3.1139891	0.3704150	-1.8779887
H	3.3707316	1.0008239	-0.5111469

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G91C1W2 ST

N	0.6201243	-0.3139621	-2.1866593
C	1.1868514	-0.0655923	-1.0011551
N	1.9862850	-0.8997251	-0.2548560
H	2.1051873	-1.9268456	-0.3869373
C	2.2721719	-0.2332997	0.9037066
H	2.8611355	-0.6897293	1.6853995
N	1.7551397	0.9789481	0.9564974
C	1.0550640	1.1059219	-0.2399667
C	0.1947098	2.0897893	-0.7648155
O	-0.1339484	3.2258168	-0.1355629
H	0.1897814	3.2055851	0.8049815
N	-0.3803805	1.8864640	-1.9465008
C	-0.1398010	0.7182978	-2.5873199
N	-0.8370359	0.5457598	-3.7669253
H	-1.1526449	1.4023944	-4.2015575
H	-0.4537879	-0.1499427	-4.3927678
N	-1.9571385	-1.2848452	-0.3643105
C	-2.3612397	-0.0413621	-0.0009669
H	-2.9611548	0.5082174	-0.7159842
C	-1.9815295	0.4663433	1.2010681
H	-2.2733843	1.4623056	1.5050563
C	-1.1187723	-0.3530245	1.9953035
N	-0.6838578	0.1034252	3.2010427
H	0.0508290	-0.4503225	3.6228851
H	-0.6069391	1.1074152	3.3287045
N	-0.7142370	-1.5695144	1.6296152
C	-1.1090837	-2.0789124	0.4351115
O	-0.7572680	-3.1815392	-0.0169973
H	-2.1475045	-1.6441421	-1.2920715
O	0.6390521	2.8360200	2.4921996
H	1.2515205	2.1292803	2.1069271
H	1.2078429	3.4880321	2.9251601
O	1.8810519	-3.6433450	-0.1594737
H	1.9599070	-4.2118314	-0.9382042
H	0.8992672	-3.5910717	0.0114118

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G91C2AW2 ST

N	-0.8017616	-0.9758489	2.4729087
C	-1.3432884	-0.5279325	1.3419767
N	-2.2923186	-1.1570326	0.5664454
H	-2.6718449	-2.0792702	0.7285420
C	-2.5444256	-0.3378616	-0.5087900
H	-3.2356101	-0.6173151	-1.2904029
N	-1.8475776	0.7748829	-0.4803799
C	-1.0783329	0.6810152	0.6775801
C	-0.1214239	1.5110115	1.3028041
O	0.2807540	2.7044239	0.8658964
H	0.0801526	2.8747663	-0.0976815
N	0.4484447	1.1006719	2.4352168
C	0.0967554	-0.0958545	2.9530444
N	0.7838578	-0.4739205	4.0820008
H	1.2279595	0.2762197	4.5925647
H	0.3578579	-1.2061017	4.6325064
N	0.5482239	-2.6815874	-0.9166679
C	1.3780487	-2.3234472	0.0866862
H	1.5047056	-3.0516679	0.8829524
C	2.0221933	-1.1077474	0.1382980
H	2.6579727	-0.8414914	0.9740492

C	1.7622992	-0.1992245	-0.9129193
N	2.3308185	1.0351343	-0.9520812
H	1.8809318	1.7449261	-1.5256293
H	2.7067034	1.3885031	-0.0825737
N	0.9415947	-0.5356253	-1.9327167
C	0.4025776	-1.7504962	-1.8611482
O	-0.4247420	-2.0615325	-2.8902108
H	-0.7133395	-2.9743074	-2.7137798
O	0.4063988	3.2691752	-1.7363022
H	0.3445600	4.1811533	-2.0500374
H	-0.1414748	2.6939804	-2.3669570
O	-0.9359779	1.4742291	-3.0489314
H	-1.4391345	1.2947732	-2.2142548
H	-0.2590439	0.7617023	-3.0200802

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G91C2BW2 ST

N	0.4597811	2.2355567	-0.5488060
C	1.0954139	1.0874014	-0.3071111
N	1.8741567	0.7689855	0.7832699
H	1.8900628	1.2941778	1.6760268
C	2.2690581	-0.5323278	0.6145366
H	2.8707940	-1.0416826	1.3527548
N	1.8359274	-1.0719026	-0.5066809
C	1.0831406	-0.0662727	-1.1057805
C	0.2678426	-0.0065715	-2.2540684
O	0.0652693	-1.0291542	-3.0983015
H	0.4576102	-1.8669534	-2.7271418
N	-0.3853723	1.1166090	-2.5317816
C	-0.2556505	2.1654933	-1.6847023
N	-1.0059669	3.2725504	-2.0051297
H	-1.3103079	3.3305933	-2.9663879
H	-0.7228639	4.1367942	-1.5649718
N	-1.0680659	0.4982306	2.3683225
C	-1.8528292	0.8653440	1.3278491
H	-2.1833076	1.8990706	1.3284241
C	-2.1910200	0.0193953	0.2957148
H	-2.7860497	0.3650892	-0.5405307
C	-1.6422313	-1.2824349	0.3315725
N	-1.8307817	-2.1855851	-0.6672968
H	-1.1608080	-2.9459413	-0.7235867
H	-2.1435970	-1.8301829	-1.5602693
N	-0.8995515	-1.6859011	1.3822469
C	-0.6726337	-0.7743601	2.3219554
O	0.0980715	-1.1744158	3.3666427
H	0.3046957	-2.1088993	3.1882814
O	1.2195987	1.9122834	3.2695983
H	1.4994819	1.4349269	4.0638820
H	0.3072301	1.5593102	3.0958832
O	0.9321661	-3.2554579	-1.7637660
H	1.5820044	-3.8601535	-2.1483521
H	1.4474818	-2.6261735	-1.1710309

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G92C1W2 ST

N	-0.9035077	-1.2954765	0.8107671
C	-1.2256327	-0.0015788	0.6676617
N	-1.9593112	0.5737554	-0.3314780
H	-2.1961934	0.1076959	-1.2216098
C	-1.9530148	1.9319510	-0.0751296
H	-2.4328784	2.6245479	-0.7512653
N	-1.3104226	2.2696996	1.0197322
C	-0.8386241	1.0587708	1.5079335
C	-0.0404515	0.6786987	2.5922531
O	0.4117151	1.5805120	3.4859080

H	0.9315199	1.0706220	4.1345123
N	0.3157434	-0.5939387	2.7687002
C	-0.1112166	-1.5098970	1.8720360
N	0.3803915	-2.7897086	2.0327670
H	0.6985225	-3.0099918	2.9669348
H	-0.1482746	-3.5199644	1.5717162
N	1.4053567	2.0015301	-1.2554644
C	2.2539875	1.4661845	-0.3427933
H	2.7712976	2.1601177	0.3100926
C	2.4110198	0.1194833	-0.2663140
H	3.0772755	-0.3217997	0.4628758
C	1.6058240	-0.6823612	-1.1410904
N	1.6830721	-2.0306631	-1.0847151
H	0.8714355	-2.5603684	-1.4315597
H	2.1192579	-2.4287012	-0.2634148
N	0.7569574	-0.1443109	-2.0242645
C	0.6230522	1.2147124	-2.1338256
O	-0.1505986	1.7739236	-2.9095861
H	1.2284924	2.9979174	-1.2874062
O	-0.9205363	-3.2806107	-1.2448364
H	-1.4436362	-2.9343742	-1.9890956
H	-1.0727386	-2.6075070	-0.5353753
O	-1.8066748	-0.9213664	-2.7716259
H	-0.8308923	-0.7430350	-2.6376555
H	-2.0176428	-0.4168390	-3.5710192

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G92C2AW2 ST

N	0.7977305	2.0417016	-1.5604952
C	0.1242051	2.0693239	-0.4097161
N	0.3220936	2.9123994	0.6601619
H	1.0371761	3.6224248	0.7323177
C	-0.5854552	2.5532487	1.6338955
H	-0.6265534	3.0604065	2.5867083
N	-1.3589630	1.5586573	1.2703958
C	-0.9298820	1.2348323	-0.0136287
C	-1.3059118	0.2421364	-0.9419836
O	-2.2419029	-0.6742433	-0.7459464
H	-2.4744935	-0.7479817	0.2509367
N	-0.6622805	0.1897337	-2.1146646
C	0.3374794	1.0718707	-2.3689878
N	0.9249361	0.9631210	-3.6014266
H	0.8102398	0.0863000	-4.0913087
H	1.8101935	1.4358792	-3.7120294
N	1.9812730	-0.0268914	1.8086396
C	2.3591390	-0.3586382	0.5541827
H	3.1928077	0.2058994	0.1455827
C	1.7416072	-1.3357702	-0.1927404
H	2.0600818	-1.5756754	-1.1997991
C	0.6392035	-1.9940749	0.4016151
N	-0.0416105	-2.9719773	-0.2425998
H	-0.9221653	-3.2424779	0.1762590
H	-0.0135439	-2.9721858	-1.2668720
N	0.2304801	-1.6682508	1.6497380
C	0.9412435	-0.7242585	2.2658419
O	0.5191578	-0.4327565	3.5198010
H	1.1217711	0.2637879	3.8339749
O	-2.5601087	-0.9189613	1.8307938
H	-1.7036010	-1.3778969	2.0022481
H	-2.3295877	0.0233948	2.0069745
O	-0.1656816	-2.3301492	-3.1243576
H	-0.5085720	-1.4386186	-2.8304389
H	-0.9067208	-2.7389017	-3.5931075

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G92C2BW2 ST

N	1.5510577	-0.5324411	-0.0575626
C	0.7283917	-1.5795493	-0.1836868
N	0.4507767	-2.5690939	0.7243016
H	0.6534687	-2.5316189	1.7413802
C	-0.5080897	-3.3723870	0.1396810
H	-0.9166364	-4.2215615	0.6693099
N	-0.8504406	-3.0071237	-1.0775798
C	-0.0807411	-1.8744885	-1.2936658
C	-0.0507962	-0.9398933	-2.3269379
O	-0.8286886	-1.0321957	-3.4302264
H	-1.3495116	-1.8508591	-3.3444090
N	0.7296630	0.1313949	-2.2438187
C	1.4993352	0.2739010	-1.1264138
N	2.2578393	1.4142435	-1.0869414
H	2.4381478	1.8791560	-1.9643317
H	2.9811983	1.4462107	-0.3840768
N	-0.8961760	0.1489194	2.2951096
C	-1.5951938	0.1273315	1.1365889
H	-2.1902744	-0.7647020	0.9617923
C	-1.5556963	1.1395342	0.2066128
H	-2.1108785	1.0812341	-0.7210992
C	-0.7276546	2.2501055	0.5008786
N	-0.6024323	3.3010472	-0.3434653
H	0.1471732	3.9412361	-0.1163205
H	-0.7587736	3.1400611	-1.3436213
N	-0.0421172	2.3023535	1.6634539
C	-0.1680227	1.2527861	2.4683768
O	0.5476534	1.2861573	3.6200454
H	1.0318698	2.1299317	3.5997648
O	0.2787418	-2.1132263	3.4418529
H	0.9723833	-1.7616617	4.0176351
H	-0.2491059	-1.3071803	3.1801239
O	-0.4035382	2.5342114	-3.1297732
H	-1.0454030	2.3697934	-3.8338197
H	0.0295545	1.6538536	-2.9683557

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G19C1W2 TS

N	1.1924460	3.9351870	-1.3392142
C	2.3700603	3.5555470	-0.7225706
H	3.3173754	4.0028812	-0.9863896
N	2.1911158	2.6230779	0.1805930
C	0.8265267	2.3761782	0.1633680
C	0.0330458	1.4478323	0.9013212
O	0.3696509	0.6131305	1.7632728
N	-1.3156618	1.5285755	0.5241104
H	-1.9710198	0.8562061	0.9663022
C	-1.8347837	2.3446880	-0.4476596
N	-3.1760087	2.2404664	-0.6512882
H	-3.6387354	1.4006900	-0.3112483
H	-3.5300208	2.6722819	-1.4920995
N	-1.1154365	3.2145744	-1.1409821
C	0.1854223	3.1804350	-0.7873289
H	1.0807808	4.6262609	-2.0685738
N	0.1444078	-1.9695460	0.5547764
C	1.4377145	-2.2337804	0.2388047
H	2.1780640	-1.5114945	0.5810567
C	1.7449610	-3.3545118	-0.4724514
H	2.7698141	-3.5803290	-0.7386696
C	0.6509548	-4.1972648	-0.8316094
N	0.8699818	-5.3310917	-1.5565854
H	0.0905532	-5.9668943	-1.6546511
H	1.8013899	-5.7099339	-1.6302813
N	-0.6164004	-3.9313212	-0.5274315

C	-0.9185047	-2.8002946	0.1602071
O	-2.0891368	-2.4873016	0.4535133
H	-0.0532029	-1.1240018	1.1037228
O	3.2241797	0.1723459	1.6080793
H	3.2904103	0.9871078	1.0747037
H	2.3357154	0.2934881	1.9969028
O	-3.3432238	-0.2684293	1.0204772
H	-3.8246307	-0.4393199	1.8409730
H	-2.8638210	-1.1310871	0.8056444

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G19C2AW2 TS

N	-0.4928603	1.7723142	-3.0420977
C	0.6018979	1.0975607	-3.5361661
H	1.2535375	1.5305942	-4.2807065
N	0.7510687	-0.0861259	-2.9872600
C	-0.2966356	-0.1957317	-2.0855747
C	-0.6466770	-1.2533009	-1.1855771
O	-0.1299271	-2.3593840	-1.0231094
N	-1.7563973	-0.8643610	-0.3897655
H	-1.9665374	-1.4782412	0.4000749
C	-2.4444505	0.3191525	-0.4749583
N	-3.5074940	0.4701287	0.3621642
H	-3.5496086	-0.1192221	1.1910358
H	-3.8649004	1.4116248	0.4363754
N	-2.1529245	1.2758019	-1.3441797
C	-1.0776467	0.9619982	-2.0951813
H	-0.8058009	2.6976168	-3.3024168
N	1.1421972	1.5400938	3.1139087
C	2.2780615	1.6866540	2.3904880
H	2.8503238	2.5897534	2.5869479
C	2.7073509	0.7705262	1.4576278
H	3.6197249	0.9199310	0.8923575
C	1.9020336	-0.3815367	1.2604120
N	2.2308505	-1.3677380	0.4024134
H	1.4744598	-2.0110547	0.1744775
H	2.8622039	-1.1674898	-0.3773603
N	0.7556634	-0.5424767	1.9692608
C	0.4802315	0.4224121	2.8275698
O	-0.6907885	0.2356692	3.5260301
H	-0.7747402	1.0121782	4.1063572
O	-2.6837327	-1.4333996	2.4052394
H	-1.9369994	-0.9681729	2.8410762
H	-2.6829329	-2.3286966	2.7688018
O	3.3672065	-0.9141745	-2.2843915
H	2.4553539	-0.7247274	-2.6264075
H	3.5913645	-1.7755502	-2.6634415

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G19C2BW2 TS

N	-3.3707051	-1.2729130	1.2408443
C	-3.9068679	-0.0629181	0.8473348
H	-4.8181288	0.3222995	1.2806626
N	-3.1875176	0.5320743	-0.0740541
C	-2.1245019	-0.3287319	-0.2982969
C	-1.0187087	-0.2223195	-1.1995895
O	-0.7442974	0.6492432	-2.0292383
N	-0.1558499	-1.3383545	-1.0463865
H	0.7021496	-1.2950849	-1.5963997
C	-0.3193726	-2.3790590	-0.1679370
N	0.6343571	-3.3597218	-0.1825652
H	1.5959381	-3.0841349	-0.3631309
H	0.5356356	-4.0112305	0.5854100
N	-1.3643452	-2.4987115	0.6330883
C	-2.2157936	-1.4575807	0.5178092

H	-3.7430839	-1.9074199	1.9342993
N	2.8555707	-0.5304456	-1.0612799
C	2.4500758	0.7127000	-1.4278135
H	2.4062131	0.8955147	-2.4975296
C	2.0673265	1.6866939	-0.5381910
H	1.7076862	2.6525696	-0.8688989
C	2.0909533	1.3478823	0.8362882
N	1.6792855	2.2098456	1.7897509
H	1.5967037	1.8407028	2.7268583
H	1.0621306	2.9861775	1.5158088
N	2.5434435	0.1339816	1.2321712
C	2.8941307	-0.6996499	0.2579240
O	3.3149224	-1.9367365	0.6618662
H	3.2775507	-1.9103354	1.6343460
O	-1.9049615	3.0056447	-1.0044966
H	-2.6060730	2.4482678	-0.6070647
H	-1.4357328	2.3396012	-1.5561512
O	-0.2395949	4.0708305	0.8511688
H	-0.8618805	3.6713411	0.1789781
H	-0.1132910	4.9842288	0.5635476

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G17C1W2 TS

N	1.2023078	-1.5195007	1.1604204
C	1.5352252	-0.3174792	1.7126153
N	1.3713384	0.0092710	3.0388982
C	1.7457184	1.2773917	3.1140462
H	1.7581964	1.8673681	4.0196091
N	2.1356330	1.7976819	1.9158274
H	2.4576463	2.7365584	1.7261074
C	2.0143010	0.7783584	0.9929021
C	2.1692431	0.7523297	-0.4201205
O	2.4638401	1.6764798	-1.1925772
N	1.9116194	-0.5453708	-0.8917734
H	1.9409667	-0.6961747	-1.9091573
C	1.3921655	-1.5726294	-0.1459887
N	1.0984540	-2.7067593	-0.8430207
H	0.9273667	-2.5896202	-1.8411094
H	0.5139330	-3.3681231	-0.3518831
N	-3.6212032	1.0541945	-0.5141136
C	-4.2763231	0.4967728	0.5357467
H	-5.2970564	0.8200252	0.7069058
C	-3.6441145	-0.4176858	1.3140687
H	-4.1478600	-0.8755893	2.1558146
C	-2.2876794	-0.7450092	0.9622374
N	-1.6203931	-1.6695235	1.6840664
H	-0.5976864	-1.7539923	1.5594063
H	-2.0050857	-1.9634188	2.5696739
N	-1.6494721	-0.1925510	-0.0758158
C	-2.2846037	0.7213601	-0.8514379
O	-1.8016092	1.3020690	-1.8330186
H	-4.0646492	1.7373712	-1.1152091
O	0.4947288	1.1661982	-3.3052480
H	1.2029317	1.5252498	-2.7305854
H	-0.3227319	1.2117274	-2.7476810
O	1.1685255	-1.3677486	-3.5113323
H	0.8324273	-0.4137989	-3.5522336
H	1.7076550	-1.4926266	-4.3032026

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G17C2AW2 TS

N	-0.3314671	-1.9936203	-0.8552800
C	-0.9054641	-1.0971777	-1.7091131
N	-2.2154043	-1.1225134	-2.1158468
C	-2.3350101	-0.0496041	-2.8932318

H	-3.2448448	0.2422651	-3.3982347
N	-1.1913416	0.6713851	-3.0128732
H	-0.9944453	1.5439568	-3.5250065
C	-0.2495861	0.0123255	-2.2505362
C	1.0896337	0.3375590	-1.9124107
O	1.7817528	1.3176789	-2.2472520
N	1.6191632	-0.6444287	-1.0591543
H	2.5437852	-0.4518167	-0.6690099
C	0.9267033	-1.7274520	-0.5636738
N	1.6321276	-2.5762926	0.2403682
H	2.4087015	-2.1710406	0.7598533
H	1.0464518	-3.2164980	0.7596568
N	-0.2886245	1.7143722	3.5901195
C	-1.6217776	1.5064398	3.6605683
H	-2.1780021	2.1995655	4.2861042
C	-2.2641410	0.4906444	2.9885219
H	-3.3370376	0.3555305	3.0649817
C	-1.4652854	-0.3641933	2.1891522
N	-1.9805883	-1.4153182	1.5098056
H	-1.4198344	-1.8171384	0.7475037
H	-2.9814765	-1.4483329	1.3801276
N	-0.1270273	-0.1732713	2.1041548
C	0.3430578	0.8436119	2.8072616
O	1.6998833	1.0310456	2.7128037
H	1.8843615	1.8156124	3.2585598
O	3.5106130	-0.5264762	1.1704737
H	2.9161758	0.0361174	1.7123443
H	4.4117334	-0.2623880	1.3964687
O	0.2326102	2.9175510	-3.8395145
H	0.9161890	2.4659460	-3.2748715
H	0.6522114	3.0232537	-4.7033696

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G17C2BW2 TS

N	-0.6186627	-1.7261690	1.8533051
C	-0.2562932	-0.6503425	2.5976669
N	0.5355899	-0.6960500	3.7274444
C	0.6889433	0.5724830	4.0771963
H	1.2450775	0.9132075	4.9393575
N	0.0594116	1.4462949	3.2414093
H	0.0527251	2.4555509	3.2934233
C	-0.5689204	0.6779043	2.2823662
C	-1.2077273	1.0283183	1.0703898
O	-1.3631632	2.1634902	0.5722197
N	-1.6301287	-0.1236452	0.3989352
H	-2.0827530	-0.0024647	-0.5183590
C	-1.3104185	-1.4142862	0.7757821
N	-1.7907085	-2.3945756	-0.0399395
H	-2.0718178	-2.1354220	-0.9846017
H	-1.4036403	-3.3134222	0.1165953
N	1.1067034	0.3423002	-2.9319206
C	2.0754728	-0.5920655	-2.8673215
H	2.3364269	-1.0658390	-3.8101430
C	2.6993810	-0.9637012	-1.6965609
H	3.4696856	-1.7261983	-1.6826315
C	2.2627652	-0.3141434	-0.5195768
N	2.7912264	-0.5963645	0.7055734
H	2.2597694	-0.2864599	1.5091980
H	3.2778159	-1.4733198	0.8229256
N	1.3227600	0.6446448	-0.5622530
C	0.7948544	0.9198979	-1.7584648
O	-0.1690935	1.8418896	-1.8243308
H	-0.4915543	2.0453419	-0.8969269
O	-2.6306319	-0.6611555	-2.2371482
H	-3.5621347	-0.6229259	-2.4904358

H	-2.1190914	-0.3397800	-3.0388973
O	-1.2243622	0.1880770	-4.3712293
H	-1.4790908	1.1054770	-4.5484201
H	-0.3046812	0.2749219	-3.9786681

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G91C1W2 TS

N	-0.9973179	0.5448330	-1.9967624
C	-0.2767423	-0.5489950	-1.7272943
N	-0.7108200	-1.7972062	-1.3669777
H	-1.6946041	-2.0782012	-1.1719072
C	0.4097184	-2.5441052	-1.1272431
H	0.3395450	-3.5709138	-0.8026157
N	1.5464686	-1.8935860	-1.3230167
C	1.1200473	-0.6293505	-1.7184617
C	1.8011974	0.5588055	-2.0169563
O	3.1543511	0.6409169	-2.0303029
H	3.4946492	-0.2516041	-1.8426968
N	1.1338445	1.6689355	-2.2889564
C	-0.2210343	1.6119902	-2.2607974
N	-0.8641214	2.7801537	-2.5776460
H	-0.3060799	3.6196596	-2.5089475
H	-1.8324756	2.8493194	-2.2987098
N	-0.4897000	1.0400422	3.7149497
C	0.6824845	0.7175030	4.3138051
H	0.8376259	1.0810031	5.3231642
C	1.5951203	-0.0330273	3.6448139
H	2.5370603	-0.3049742	4.1041957
C	1.2452960	-0.4377910	2.3098582
N	2.1148864	-1.1922305	1.6060672
H	1.9185693	-1.4594438	0.6403072
H	3.0165812	-1.4246093	1.9924395
N	0.0911271	-0.1130608	1.7221782
C	-0.8212397	0.6325611	2.3964290
O	-1.9211694	0.9985559	1.9664886
H	-1.1903502	1.5999291	4.1837237
O	-3.3233086	-2.2547176	-0.6149755
H	-3.4355183	-1.2676517	-0.4322077
H	-4.0303469	-2.4806591	-1.2344508
O	-3.2981390	0.3726921	-0.3300232
H	-2.8219228	0.5900223	0.5086586
H	-2.6109087	0.5383436	-1.0171901

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G91C2AW2 TS

N	1.1583851	-2.4328783	0.3864614
C	1.9930888	-1.4024239	0.2485496
N	3.1552674	-1.1635943	0.9491653
H	3.5605071	-1.7674589	1.6508860
C	3.6438528	0.0540832	0.5170055
H	4.5477532	0.4788440	0.9298134
N	2.8982328	0.6143480	-0.4058994
C	1.8611703	-0.2909749	-0.6023854
C	0.7209105	-0.3216905	-1.4166074
O	0.4447678	0.6671729	-2.2883994
H	-0.4688097	0.5026661	-2.5985927
N	-0.1351945	-1.3323394	-1.3359468
C	0.1006864	-2.3188890	-0.4376712
N	-0.8360951	-3.3176381	-0.4017038
H	-1.7511156	-3.0666717	-0.7514943
H	-0.8130770	-3.9102519	0.4159024
N	-3.1602743	-0.6150788	0.0764739
C	-2.9233107	-0.9278576	1.3702950
H	-3.5101292	-1.7495107	1.7738509
C	-1.9952627	-0.2808000	2.1518469

H	-1.8181732	-0.5788979	3.1790659
C	-1.2668367	0.7798269	1.5528219
N	-0.3096482	1.4623262	2.2078425
H	0.3536129	2.0867744	1.7109345
H	-0.0583644	1.1612816	3.1369012
N	-1.5307893	1.1425395	0.2741065
C	-2.4331477	0.4084377	-0.3682232
O	-2.6134180	0.7579350	-1.6708809
H	-3.2842559	0.1384570	-2.0085991
O	-0.2873521	3.4016601	-1.0663129
H	-0.8011523	2.6780387	-0.6293384
H	0.1565021	2.9324341	-1.7902633
O	1.6361856	3.0446269	0.8774960
H	2.2045273	2.4166494	0.3887827
H	1.0268087	3.3841617	0.1747990

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G91C2BW2 TS

N	0.9822374	0.3386478	1.6203409
C	1.2409688	0.9498223	0.4550055
N	2.2675643	0.6838479	-0.4162173
H	2.9315141	-0.1050752	-0.3382741
C	2.0828136	1.5020653	-1.5020183
H	2.7546392	1.4828839	-2.3472875
N	1.0307369	2.2855970	-1.3879326
C	0.4756489	1.9480825	-0.1558411
C	-0.7172477	2.3052960	0.5133810
O	-1.6165378	3.1722371	0.0541214
H	-1.3289633	3.5655412	-0.8279880
N	-1.0093191	1.7184367	1.6736420
C	-0.1647070	0.7920241	2.1707788
N	-0.5122774	0.2671915	3.3859680
H	-1.4791501	0.3895012	3.6513843
H	-0.0799040	-0.6091177	3.6423950
N	0.1198964	-3.5622266	-0.6952156
C	-0.9754711	-3.7175091	-1.4634162
H	-0.9654154	-4.5787740	-2.1277703
C	-2.0627071	-2.8629708	-1.4493973
H	-2.9201483	-3.0269708	-2.0926372
C	-1.9896738	-1.7739782	-0.5561326
N	-2.9932642	-0.8615068	-0.4025684
H	-2.7686857	-0.0221977	0.1176439
H	-3.6986958	-0.7805308	-1.1189833
N	-0.9150700	-1.6026399	0.2303622
C	0.0673810	-2.4965056	0.1038066
O	1.1635435	-2.2917805	0.8747542
H	1.0744968	-1.3836033	1.3089993
O	3.6146892	-1.7679981	-0.4299391
H	4.3649566	-2.0626936	0.1046211
H	2.8355118	-2.2367487	-0.0558159
O	-0.7496432	4.1004231	-2.3049721
H	-0.4085176	5.0059467	-2.2821024
H	0.0526291	3.5079825	-2.2193115

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G92C1W2 TS

N	0.5135887	2.1804710	0.6526734
C	0.0001302	1.7435056	-0.5051379
N	0.6464918	1.5712372	-1.6988529
H	1.6669187	1.6935383	-1.8780933
C	-0.2740395	1.0308910	-2.5584203
H	-0.0038075	0.7610616	-3.5694243
N	-1.4727096	0.8660979	-2.0329108
C	-1.3202952	1.3207308	-0.7294339
C	-2.1484150	1.3662582	0.3952466

O	-3.4350443	0.9578391	0.3392840
H	-3.7869024	1.0853147	1.2396463
N	-1.6899786	1.8012516	1.5653931
C	-0.3922038	2.1824400	1.6447342
N	0.0212936	2.6507545	2.8670734
H	-0.5505342	2.3843037	3.6556369
H	1.0200792	2.6668526	3.0205876
N	1.0652491	-3.4366095	1.0879920
C	0.0139370	-4.2456718	0.8035543
H	0.0124904	-5.2301862	1.2577140
C	-0.9724528	-3.8029350	-0.0167251
H	-1.8184209	-4.4334991	-0.2591838
C	-0.8279545	-2.4731255	-0.5487790
N	-1.7675655	-1.9987633	-1.3896018
H	-1.7347641	-1.0258965	-1.7166742
H	-2.6070337	-2.5310450	-1.5551376
N	0.2094454	-1.6796367	-0.2618773
C	1.1912148	-2.1228204	0.5639946
O	2.1940325	-1.4854969	0.9095061
H	1.8182753	-3.7356093	1.6947335
O	3.3932704	1.6449564	-1.9214098
H	3.9120097	2.4556915	-2.0151016
H	3.4544143	1.4022154	-0.9450903
O	3.1524466	1.0976495	0.6667327
H	2.3195640	1.6128061	0.7827273
H	2.8423054	0.1625352	0.7367308

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G92C2AW2 TS

N	-0.7319949	2.2304650	0.1353580
C	0.4372220	1.7710397	-0.3353583
N	1.6719375	1.8662545	0.2479537
H	1.8857572	2.2750314	1.1796072
C	2.5345183	1.1753587	-0.5655274
H	3.5805385	1.0740556	-0.3134573
N	1.9672757	0.6623535	-1.6380200
C	0.6357304	1.0354477	-1.5136148
C	-0.5309995	0.7538174	-2.2306532
O	-0.5023255	0.0063225	-3.3522021
H	-1.4288196	-0.0550669	-3.6502154
N	-1.7134872	1.1974239	-1.8138566
C	-1.7649855	1.9100420	-0.6646023
N	-3.0028123	2.3764531	-0.3027349
H	-3.7924887	1.9088951	-0.7240624
H	-3.1093507	2.6679390	0.6588179
N	-1.0867547	-3.2191835	1.6053908
C	-0.6664897	-4.1728248	0.7477995
H	-1.0905053	-5.1633217	0.8934708
C	0.2401112	-3.9349326	-0.2608552
H	0.5561425	-4.7253527	-0.9326333
C	0.7398897	-2.6137873	-0.3805420
N	1.6515562	-2.2771140	-1.3209649
H	1.8688636	-1.2904558	-1.4927680
H	1.8453714	-2.9316286	-2.0627542
N	0.3362907	-1.6409461	0.4693977
C	-0.5387757	-2.0213408	1.3879501
O	-0.9550527	-1.0386902	2.2436333
H	-1.5780413	-1.4879670	2.8425657
O	1.9830476	2.6652136	2.8895663
H	2.0250969	3.5814297	3.1962817
H	1.0440622	2.3698736	3.0647412
O	-0.5766332	1.8229668	2.9053735
H	-0.5745706	0.8506734	2.8202029
H	-0.7493475	2.1117600	1.9712837

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G92C2BW2 TS

N	3.5757745	0.0633053	0.5792689
C	2.6559372	-0.9012595	0.5494491
N	2.6328823	-2.0576001	1.3048536
H	3.3250498	-2.3334995	1.9877636
C	1.4759707	-2.7274833	0.9902273
H	1.2068937	-3.6602136	1.4640028
N	0.7593133	-2.1030331	0.0788647
C	1.4917819	-0.9562843	-0.2249752
C	1.2741295	0.1443119	-1.0885071
O	0.2764623	0.2714279	-1.9425863
H	-0.3623263	-0.5243963	-1.9289521
N	2.1387952	1.1649420	-1.0394580
C	3.2235990	1.0765274	-0.2337429
N	4.0339503	2.1843869	-0.2227475
H	3.9610271	2.7915438	-1.0262641
H	4.9551666	2.0566245	0.1712785
N	-3.4539189	0.2166929	0.7923915
C	-3.7169643	1.5141964	0.5270005
H	-4.7679841	1.7680499	0.4167217
C	-2.7421720	2.4743207	0.3670839
H	-2.9952957	3.5012358	0.1293342
C	-1.4013660	2.0373400	0.4680974
N	-0.3431739	2.8693923	0.2605160
H	0.5430377	2.4285774	0.0250219
H	-0.5282408	3.7344919	-0.2269340
N	-1.1167537	0.7659162	0.8042738
C	-2.1513076	-0.0603829	0.9369605
O	-1.8817275	-1.3496270	1.2214376
H	-0.9269364	-1.5032134	1.0391376
O	-3.9767198	-1.7827335	-1.1566855
H	-4.1745071	-2.6275870	-0.7274529
H	-4.0034214	-1.1273928	-0.4143145
O	-1.2732798	-1.8347925	-1.9549097
H	-0.8168391	-2.3041523	-1.2281596
H	-2.2290095	-1.7957733	-1.6968081