

Chemical Evolution of Biomolecule Building Blocks. Can Thermodynamics Explain The Accumulation of Glycine in Prebiotic Ocean?

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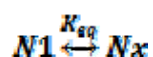
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Selection of the interval of relative Gibbs free energy studied

There is no way to discuss all the possible C₂H₅NO₂ species characterized in our calculations and we had to provide a reasonable (and necessarily arbitrary) truncation for the number of species discussed. We decided it should be based on thermochemical considerations as it is presented below.

A thermodynamic equilibrium between the isomer having the lowest Gibbs free energy, N1, and the one with the xth lowest Gibbs free energy, Nx can be written as:



Only those species are considered which underpopulate N1 by a factor of 1/(6.022·10²³) (=1/N_A). This simply means that only one molecule of Nx can be found in 1 mol C₂H₅NO₂, which should be a reasonable lower limit for considering all the important isomers.

The equilibrium constant, K_{eq}, can be expressed as:

$$\left(e^{-\frac{\Delta G^0}{RT}} \right) = K_{eq} = \frac{[Nx]}{[N1]} = \frac{1}{6.22 \cdot 10^{23}} = 1.66 \cdot 10^{-24}$$

Then, relative Gibbs free energy at 25°C, Δ_{rel}G⁰(g), can be calculated as:

$$\Delta_{rel}G^0 = -RT \ln K_{eq} = -8.314 \frac{J}{mol \cdot K} \cdot 298.15K \cdot \ln \left(\frac{1}{6.22 \cdot 10^{23}} \right)$$
$$\Delta_{rel}G^0 = 135.7 \frac{kJ}{mol}$$

Coordinates and energies

Notation:

DE(MP2)=E(MP2/G3MP2Large)-E(MP2/6-31G(d)) in Hartree

E(QCISD(T))= E(QCISD(T)/6-31G(d)) in Hartree

E(ZPE)=zero-point energy scaled by 0.96 in Hartree

E(HLC)=High level correction in Hartree

dfH=G3MP2B3 heat of formation in kJ/mol (calculated at 1 atm and 298.15 K)

S(scaled)=Entropy (in J/molK) calculated with scaled (by 0.96) B3LYP/6-31G(d) vibrational frequencies

S(Unscaled) =Entropy (in J/molK) calculated with UNscaled B3LYP/6-31G(d) vibrational frequencies

G=G3MP2B3 sum of electronic and thermal Free Energies in Hartree (calculated at 1 atm and 298.15 K)

Cv(Unscaled)=Heat capacity in J/molK calculated with UNscaled B3LYP/6-31G(d) vibrational frequencies

Coordinates and energies for the 18 lowest lying **gas** phase structures of C₂H₅NO₂

N1 val+05_120 DE(MP2)=-0.333434 E(QCISD(T))=-283.671467 E(ZPE)=0.074033 E(HLC)=-0.150615

C	-0.22845	2.36132	0.60173
C	0.00584	-1.22903	0.27046
N	0.36535	-0.10219	-0.59697
O	-0.96666	1.86176	1.36041
O	0.48644	2.94981	-0.11362
H	-1.04681	-1.13658	0.55547
H	0.59630	-1.17392	1.19072
H	0.15675	-2.22806	-0.17120
H	-0.15330	-0.15833	-1.47191
H	1.34974	-0.15557	-0.85268

N2 val+05_16 DE(MP2)=-0.336812 E(QCISD(T))=-283.666875 E(ZPE)=0.076835 E(HLC)=-0.150615

C	0.23264	0.63759	0.17164
C	-0.50662	-1.74014	-0.10402
N	0.49073	-0.68610	-0.01032
O	1.07220	1.49383	0.38740
O	-1.10052	0.91278	0.06223
H	-1.33313	-1.40818	-0.73466
H	-0.04786	-2.61848	-0.56622
H	-0.91114	-2.02874	0.87569
H	1.45169	-0.93547	0.17123
H	-1.16068	1.87660	0.17682

N3 val+03_47 DE(MP2)=-0.334791 E(QCISD(T))=-283.663561 E(ZPE)=0.076631 E(HLC)=-0.150615

C	0.50274	0.20616	0.02556
C	-1.81810	-0.12827	-0.12359
N	1.71036	-0.20454	-0.47448
O	0.34265	1.10678	0.82534
O	-0.50202	-0.51908	-0.53460
H	-2.01811	0.91039	-0.40065
H	-2.49825	-0.80017	-0.64896
H	-1.93533	-0.23489	0.95831
H	2.52562	0.10816	0.03035
H	1.76345	-1.09795	-0.94138

N4 val+03_37 DE(MP2)=-0.342478 E(QCISD(T))=-283.646569 E(ZPE)=0.075636 E(HLC)=-0.150615

C	0.10286	0.03673	-0.01242
C	-1.41972	-0.03714	0.15927
N	0.75391	-1.13894	-0.20263
O	0.66926	1.12377	0.02600
O	-1.93908	1.24903	0.34381

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H	-1.85740	-0.51680	-0.73179
H	-1.65140	-0.68503	1.02081
H	1.75760	-1.12773	-0.31694
H	0.27307	-2.02561	-0.22901
H	-1.15609	1.83660	0.30870

N5 val+05_118 DE(MP2)=-0.339888 E(QCISD(T))=-283.651387 E(ZPE)=0.077490 E(HLC)=-0.150615

C	0.50232	0.79255	0.25601
C	-0.60469	-0.24574	-0.00165
N	-0.02739	-1.58823	-0.16819
O	0.30499	1.98287	0.21376
O	1.68841	0.24300	0.55820
H	-1.25635	-0.23853	0.87889
H	-1.20745	0.10343	-0.84800
H	-0.62955	-2.30952	0.21820
H	1.53810	-0.73418	0.49585
H	0.11321	-1.80796	-1.15146

N7 val+05_128 DE(MP2)=-0.338536 E(QCISD(T))=-283.632342 E(ZPE)=0.072367 E(HLC)=-0.150615

C	1.55331	-2.12600	0.00636
C	-1.61829	1.20528	0.29045
N	0.43198	-1.72678	-0.22509
O	2.58625	-2.64604	0.23835
O	-0.63892	0.87016	-0.69673
H	-2.05556	2.19321	0.09812
H	-2.41993	0.45740	0.34802
H	-1.09547	1.23377	1.24842
H	-1.07865	0.82669	-1.55989
H	0.12319	-0.76248	-0.39332

N8 val+07_21 DE(MP2)=-0.338224 E(QCISD(T))=-283.642556 E(ZPE)=0.077184 E(HLC)=-0.150615

C	-0.17821	-1.05349	0.65131
C	-0.79094	1.05815	-0.38120
N	-1.13843	-0.29434	0.05685
O	0.93611	-0.63504	0.93611
O	0.24162	1.09105	-1.33077
H	-1.67578	1.49910	-0.84382
H	-0.52980	1.63182	0.51619
H	-1.92888	-0.76649	-0.36293
H	-0.50333	-2.08777	0.87178
H	1.03472	0.78151	-0.85782

N9 val+03_43 DE(MP2)=-0.334988 E(QCISD(T))=-283.640165 E(ZPE)=0.077089 E(HLC)=-0.150615

C	-0.97384	1.13573	-0.04638
C	-0.42779	-1.14662	-0.23683
N	0.87678	-1.11215	0.34839
O	-0.92978	1.08239	1.16166
O	-0.75293	0.12055	-0.88899
H	-1.21363	2.04373	-0.62127
H	-1.24299	-1.34740	0.46774
H	-0.45687	-1.86771	-1.05406
H	0.84916	-0.83138	1.32248
H	1.37218	-1.99014	0.24717

N10 val+05_125 DE(MP2)=-0.333046 E(QCISD(T))=-283.635533 E(ZPE)=0.073843 E(HLC)=-0.150615

C	-1.05381	1.55421	0.34962
C	0.77949	-1.58273	-0.33983
N	-0.12591	-1.70713	0.54575
O	-0.15249	1.44602	-0.45873
O	-1.54601	0.59618	1.12232
H	-1.58227	2.50313	0.53502
H	0.91579	-0.59822	-0.78878
H	1.42456	-2.40270	-0.67376
H	-1.05430	-0.26770	0.94360
H	-0.19293	-2.65778	0.91899

N11 val+07_114 DE(MP2)=-0.331613 E(QCISD(T))=-283.632471 E(ZPE)=0.072677 E(HLC)=-0.150615

C	0.49415	2.10323	0.88994
C	-0.26469	-1.48680	0.30787
N	-0.32511	-0.77709	-0.84152
O	0.00284	-1.02966	1.41179
O	0.29211	2.08597	-0.30926
H	0.75472	3.04914	1.40500
H	-0.48708	-2.56166	0.16012
H	0.42541	1.18592	1.49961
H	-0.55312	-1.23063	-1.71369
H	-0.13834	0.22748	-0.83176

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N12	val+05_98	DE(MP2)=-0.328101	E(QCISD(T))=-283.627829	E(ZPE)=0.065878	E(HLC)=-0.150615
C	1.25491	0.31327	-0.07308		
C	-0.59944	1.92796	-0.03851		
N	-0.09083	0.63638	-0.00967		
O	-1.77877	2.18777	0.01795		
O	1.68224	-0.81914	-0.04638		
H	1.90237	1.20514	-0.15121		
H	0.19432	2.69274	-0.11885		
H	-0.75741	-0.12807	0.06352		
H	-0.64367	-3.18508	0.21868		
H	-0.05303	-2.73628	0.15804		
N13	val+07_12	DE(MP2)=-0.337392	E(QCISD(T))=-283.623541	E(ZPE)=0.073309	E(HLC)=-0.150615
C	0.34486	1.72945	2.13304		
C	0.14459	-0.77347	-0.43203		
N	-0.34281	0.56230	-0.76601		
O	0.38955	2.86490	2.09498		
O	-0.30096	-1.14752	0.84647		
H	-0.20803	-1.57140	-1.10314		
H	1.24480	-0.73809	-0.50072		
H	-1.34784	0.53399	-0.93164		
H	0.09933	0.90920	-1.61584		
H	-0.05610	-0.41605	1.44058		
N14	val+03_12	DE(MP2)=-0.342479	E(QCISD(T))=-283.623134	E(ZPE)=0.075148	E(HLC)=-0.150615
C	0.43418	-0.32829	0.18268		
C	-1.90979	-0.62817	0.12905		
N	-0.55989	-1.08191	0.36729		
O	0.48805	0.97447	-0.24405		
O	1.68484	-0.77647	0.41441		
H	-2.04338	0.45986	-0.03407		
H	-2.53743	-0.89094	0.98822		
H	-2.33034	-1.13872	-0.74685		
H	-0.41308	1.28781	-0.42342		
H	2.30103	-0.05534	0.20665		
N15	val+05_13	DE(MP2)=-0.346204	E(QCISD(T))=-283.620087	E(ZPE)=0.075758	E(HLC)=-0.150615
C	0.02001	-0.29982	0.29977		
C	0.98266	0.85876	0.11426		
N	0.46291	-1.48390	0.22528		
O	2.28769	0.41686	-0.12484		
O	-1.28358	0.00611	0.53921		
H	0.61975	1.48056	-0.72334		
H	0.94248	1.49138	1.01879		
H	2.23182	-0.56058	-0.10798		
H	-0.26799	-2.18397	0.36522		
H	-1.40426	0.97050	0.55563		
N16	val+05_132	DE(MP2)=-0.333273	E(QCISD(T))=-283.610066	E(ZPE)=0.066053	E(HLC)=-0.150615
C	1.24215	1.92149	-0.19701		
C	1.05935	-1.54750	-0.70517		
N	-1.69182	0.57788	0.38046		
O	0.78225	2.92569	0.07921		
O	0.86260	-2.73138	-0.86302		
H	0.26790	-0.84464	-0.37811		
H	-1.93287	1.55188	0.55973		
H	-2.34735	0.24735	-0.32652		
H	-1.91738	0.06691	1.23299		
H	2.05727	-1.08958	-0.88107		
N17	val+03_28	DE(MP2)=-0.339943	E(QCISD(T))=-283.627047	E(ZPE)=0.076660	E(HLC)=-0.150615
C	0.52342	-0.28199	-0.34110		
C	-1.82134	-0.55774	-0.33149		
N	0.58861	0.80321	0.32048		
O	-0.53532	-1.02983	-0.71902		
O	1.63321	-0.89064	-0.80055		
H	-2.02779	0.42924	-0.76294		
H	-2.53363	-1.28367	-0.72481		
H	-1.91315	-0.50878	0.76037		
H	-0.32111	1.15583	0.60739		
H	2.36990	-0.32594	-0.50982		
N18	val+07_107	DE(MP2)=-0.340010	E(QCISD(T))=-283.608598	E(ZPE)=0.068409	E(HLC)=-0.150615
C	3.07641	-0.68082	-1.44404		
C	-0.08019	0.64201	0.68128		
N	-0.10988	-0.43171	0.00141		

O	4.10271	-0.80790	-1.91396
O	-2.77895	-1.00600	0.89293
H	0.78476	1.31400	0.75096
H	-0.97582	0.91961	1.24026
H	-1.89394	-1.12606	0.49033
H	0.78080	-0.60045	-0.47701
H	-3.32791	-0.73176	0.14373

Coordinates and energies for the 18 lowest lying water phase structures of C₂H₅NO₂

N1 val+05_120 DE(MP2)=-0.332803 E(QCISD(T))=-283.675892 E(ZPE)=0.073731 E(HLC)=-0.150615

C	-0.19672	2.35831	0.63269
C	-0.03121	-1.23991	0.23537
N	0.37195	-0.08067	-0.57116
O	-0.69467	1.85205	1.56326
O	0.27688	2.96899	-0.24638
H	-1.10754	-1.18599	0.42911
H	0.48029	-1.20017	1.20270
H	0.18299	-2.21880	-0.22217
H	-0.08660	-0.12612	-1.48035
H	1.36983	-0.13849	-0.77067

N2 val+05_16 DE(MP2)=-0.337361 E(QCISD(T))=-283.676410 E(ZPE)=0.076473 E(HLC)=-0.150615

C	0.23367	0.63390	0.17683
C	-0.52833	-1.73687	-0.04092
N	0.39398	-0.69309	0.38732
O	1.05706	1.49887	0.45499
O	-0.97792	0.91803	-0.37525
H	-1.54477	-1.50290	0.28438
H	-0.52985	-1.86695	-1.12997
H	-0.22108	-2.67548	0.42391
H	1.31221	-0.95860	0.71230
H	-1.00768	1.88678	-0.46379

N3 val+05_65 DE(MP2)=-0.334809 E(QCISD(T))=-283.672572 E(ZPE)=0.076384 E(HLC)=-0.150615

C	0.56419	-0.46168	-0.17224
C	-0.96652	1.30671	0.13752
N	0.90707	-1.70953	0.25968
O	-0.48178	0.01756	0.54524
O	1.08996	0.13139	-1.10239
H	-0.18300	2.06292	0.23179
H	-1.32011	1.27836	-0.89638
H	-1.79218	1.53267	0.81248
H	1.80764	-2.05509	-0.03977
H	0.58803	-2.01171	1.17006

N4 val+03_37 DE(MP2)=-0.342664 E(QCISD(T))=-283.659246 E(ZPE)=0.075704 E(HLC)=-0.150615

C	0.10039	0.03003	-0.01472
C	-1.42156	-0.04450	0.15881
N	0.75376	-1.13154	-0.20097
O	0.65470	1.13329	0.02104
O	-1.93241	1.25416	0.35219
H	-1.86334	-0.51294	-0.73331
H	-1.65693	-0.69096	1.01706
H	1.75815	-1.12675	-0.31839
H	0.27727	-2.02241	-0.22153
H	-1.13703	1.82653	0.30562

N5 val+05_78 DE(MP2)=-0.339841 E(QCISD(T))=-283.660883 E(ZPE)=0.076574 E(HLC)=-0.150615

C	0.51755	0.47160	-0.69470
C	-0.00513	-0.44336	0.39336
N	0.38765	-1.82508	0.13484
O	0.94739	0.10950	-1.77072
O	0.40940	1.76967	-0.34136
H	0.71798	2.30359	-1.09877
H	-1.09399	-0.26470	0.45070
H	0.40767	-0.11213	1.35271
H	-0.07937	-2.42694	0.81082
H	0.03215	-2.09974	-0.77978

N6 val+05_118 DE(MP2)=-0.340673 E(QCISD(T))=-283.660471 E(ZPE)=0.078079 E(HLC)=-0.150615

C	0.55882	0.86631	0.32186
C	-0.57479	-0.14691	-0.04598
N	0.07491	-1.50171	-0.10564

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O	0.22070	2.05751	0.40970
O	1.69509	0.32733	0.48681
H	-1.35759	-0.15366	0.71257
H	-1.01722	0.08841	-1.01393
H	-0.29715	-2.17009	0.57181
H	1.07565	-1.23364	0.14460
H	0.04318	-1.93585	-1.03021

N7 val+05_128 DE(MP2)=-0.337731 E(QCISD(T))=-283.641414 E(ZPE)=0.072179 E(HLC)=-0.150615

C	1.54964	-1.62327	-0.90501
C	-1.46307	1.22007	0.14512
N	0.36085	-1.75625	-0.72911
O	2.70713	-1.61523	-1.15135
O	-1.44576	-0.13093	0.62816
H	-0.48195	1.70009	0.24208
H	-1.73334	1.17075	-0.91149
H	-2.21282	1.81543	0.67817
H	-0.29502	-1.14394	-0.20854
H	-1.19774	-0.11152	1.56666

N8 val+07_4 DE(MP2)=-0.338837 E(QCISD(T))=-283.653204 E(ZPE)=0.076959 E(HLC)=-0.150615

C	0.22425	-0.65910	-0.63942
C	-1.17367	1.06321	0.35515
N	-1.07576	-0.16558	-0.19594
O	1.16765	-0.74036	0.40616
O	-0.21652	1.82896	0.48523
H	-2.19468	1.32791	0.67795
H	-1.87008	-0.79078	-0.15291
H	0.08485	-1.66437	-1.03760
H	1.31439	0.18191	0.68421
H	0.58279	0.00020	-1.43912

N9 val+03_43 DE(MP2)=-0.334856 E(QCISD(T))=-283.648868 E(ZPE)=0.076876 E(HLC)=-0.150615

C	-0.99775	1.15854	-0.06946
C	-0.41676	-1.14002	-0.20866
N	0.89180	-1.11908	0.36735
O	-1.00536	1.13080	1.14387
O	-0.72838	0.13437	-0.87935
H	-1.22259	2.05443	-0.66741
H	-1.22222	-1.31478	0.50899
H	-0.47544	-1.86251	-1.02134
H	0.86281	-0.99340	1.37355
H	1.41419	-1.96133	0.15237

N10 val+05_125 DE(MP2)=-0.334485 E(QCISD(T))=-283.641171 E(ZPE)=0.072732 E(HLC)=-0.150615

C	-1.59129	1.63193	0.20884
C	1.14359	-2.02958	0.26650
N	0.07197	-1.35751	0.13389
O	-2.47146	0.86811	-0.14229
O	-0.33477	1.30995	0.47555
H	-1.75104	2.71328	0.34774
H	2.05959	-1.51461	0.55891
H	1.20958	-3.10846	0.10408
H	-0.19875	0.30684	0.34319
H	-0.72533	-1.93666	-0.14220

N11 val+07_30 DE(MP2)=-0.335823 E(QCISD(T))=-283.633887 E(ZPE)=0.070800 E(HLC)=-0.150615

C	-1.93612	0.43786	-0.36718
C	1.60612	-0.02275	-0.11021
N	0.82165	-0.87491	0.59247
O	-1.68380	1.51727	-0.85674
O	2.03668	1.04479	0.30883
H	-1.97224	-0.49027	-0.96923
H	1.80669	-0.38466	-1.13477
H	0.65241	-0.69969	1.57542
H	-2.15544	0.31451	0.71070
H	0.60704	-1.79507	0.23302

N12 val+05_98 DE(MP2)=-0.329105 E(QCISD(T))=-283.638255 E(ZPE)=0.066029 E(HLC)=-0.150615

C	1.18310	0.28916	-0.01548
C	-0.50749	2.05809	-0.01790
N	-0.12764	0.72676	-0.01708
O	-1.66564	2.42305	-0.01983
O	1.50293	-0.88366	-0.01502
H	1.91275	1.11416	-0.01479
H	0.34975	2.74994	-0.01658
H	-0.86459	0.02518	-0.01815

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H	-0.55100	-3.50750	0.08914
H	-0.12146	-2.90048	0.06619
N13 val+07_110 DE(MP2)=-0.337363 E(QCISD(T))=-283.630256 E(ZPE)=0.072935 E(HLC)=-0.150615			
C	1.90623	-1.09920	1.21418
C	-0.81566	0.91130	-0.19867
N	-0.84191	-0.46911	-0.66580
O	2.06847	-2.19355	1.47430
O	0.50636	1.41437	-0.21148
H	-1.39314	1.61297	-0.81796
H	-1.24607	0.91994	0.81446
H	-1.74215	-0.89470	-0.44935
H	-0.74020	-0.49602	-1.67964
H	1.04155	0.76511	0.27986
N14 val+03_12 DE(MP2)=-0.342120 E(QCISD(T))=-283.636076 E(ZPE)=0.075099 E(HLC)=-0.150615			
C	0.43177	-0.34981	0.12132
C	-1.88180	-0.63519	-0.04278
N	-0.52438	-1.16856	-0.02610
O	0.39824	1.00093	0.27346
O	1.70519	-0.79361	0.14283
H	-2.05467	0.05882	-0.88008
H	-2.14701	-0.11300	0.89009
H	-2.58833	-1.46146	-0.15945
H	-0.52156	1.31533	0.25766
H	2.29676	-0.03115	0.26294
N15 val+03_10 DE(MP2)=-0.345859 E(QCISD(T))=-283.631194 E(ZPE)=0.075677 E(HLC)=-0.150615			
C	0.16008	0.12114	-0.31727
C	-1.33528	-0.01587	-0.10275
N	0.67214	1.28392	-0.33041
O	0.87616	-1.01366	-0.48614
O	-1.94299	1.24373	0.06675
H	-1.76660	-0.54392	-0.96788
H	-1.50693	-0.65299	0.77916
H	1.68272	1.25772	-0.48231
H	0.29976	-1.79677	-0.43992
H	-1.20527	1.88429	-0.01092
N16 val+07_25 DE(MP2)=-0.332316 E(QCISD(T))=-283.619113 E(ZPE)=0.066727 E(HLC)=-0.150615			
C	2.43079	0.06775	-2.04078
C	-0.85857	1.66642	0.64618
N	0.84873	-1.79297	0.11199
O	1.64938	0.89180	-1.95467
O	-1.00813	0.60472	1.21482
H	-1.44087	2.56308	0.92822
H	-0.13700	1.79417	-0.18015
H	0.32751	-2.17562	-0.67717
H	0.26555	-1.03623	0.47713
H	0.82092	-2.52372	0.82411
N17 val+03_28 DE(MP2)=-0.339522 E(QCISD(T))=-283.636967 E(ZPE)=0.076409 E(HLC)=-0.150615			
C	0.52542	-0.27685	-0.33822
C	-1.82801	-0.55513	-0.32931
N	0.58688	0.80967	0.32444
O	-0.52965	-1.02285	-0.71563
O	1.63461	-0.88942	-0.79967
H	-2.03253	0.42910	-0.76313
H	-2.53239	-1.28553	-0.72620
H	-1.91748	-0.51028	0.76098
H	-0.33074	1.15021	0.60411
H	2.38669	-0.33922	-0.51888
N18 val+07_107 DE(MP2)=-0.339459 E(QCISD(T))=-283.618535 E(ZPE)=0.067701 E(HLC)=-0.150615			
C	1.16640	-1.67315	-2.28420
C	-0.18441	1.17323	1.61414
N	0.13964	0.19041	0.87424
O	1.77741	-2.36826	-1.62063
O	-1.44310	-1.35865	-0.96665
H	-1.21849	1.52296	1.60748
H	0.50973	1.70623	2.27106
H	-0.93493	-0.81805	-0.31558
H	1.13344	-0.03939	0.97042
H	-1.36770	-0.84443	-1.78438
N19 val+07_39 DE(MP2)=-0.327443 E(QCISD(T))=-283.612408 E(ZPE)=0.056253 E(HLC)=-0.150615			
C	-1.31172	1.25486	1.25258

C	0.25222	2.70210	-1.53441
N	-0.36963	-1.42059	-0.41400
O	-1.49292	0.88772	2.31442
O	0.38857	1.66161	-1.97535
H	-0.10666	-0.61804	-0.98492
H	1.84864	-1.72571	2.22938
H	-1.32442	-1.64780	-0.69234
H	0.20203	-2.19420	-0.75313
H	1.31779	-1.61695	1.71818

Coordinates and thermochemical properties for the all $C_2H_5NO_2$ gas phase structures

Filename	dfH	S(scaled)	S(UNscaled)	G	Cv(UNscaled)
Units	kJ/mol	J/molK	J/molK	Hartree	J/molK
val+03_10:	-325.0	310.3	308.0	-284.069779	78.8
val+03_11:	-217.2	323.5	321.0	-284.030221	83.5
val+03_12:	-323.7	322.6	320.3	-284.070714	81.1
val+03_13:	95.8	313.2	310.7	-283.909839	83.8
val+03_14:	7.4	319.2	316.8	-283.944214	80.9
val+03_15:	-12.3	323.5	320.9	-283.952188	88.2
val+03_16:	-85.7	319.5	317.1	-283.979691	83.1
val+03_17:	-35.7	320.7	318.1	-283.960775	87.4
val+03_18:	-120.3	317.4	314.9	-283.992646	83.8
val+03_19:	-4.2	320.3	318.1	-283.948758	78.7
val+03_1:	-105.8	314.8	312.4	-283.986808	83.3
val+03_20:	-146.4	313.8	311.6	-284.002170	77.2
val+03_21:	-11.1	326.4	324.1	-283.952074	80.8
val+03_22:	-271.9	317.6	315.5	-284.050393	75.5
val+03_23:	59.5	330.6	328.1	-283.925646	83.7
val+03_24:	-28.0	325.3	322.9	-283.958398	82.8
val+03_25:	-128.3	329.6	327.2	-283.997082	81.4
val+03_26:	-168.9	321.0	318.9	-284.011551	76.7
val+03_27:	-79.6	320.2	317.8	-283.977436	83.3
val+03_28:	-324.9	306.9	304.8	-284.069362	75.7
val+03_29:	123.4	324.9	322.4	-283.900675	84.5
val+03_2:	-11.5	306.6	304.2	-283.949958	82.5
val+03_30:	102.6	318.4	316.1	-283.907857	79.9
val+03_31:	-35.7	318.6	316.5	-283.960561	76.9
val+03_32:	-148.2	319.6	317.4	-284.003532	78.5
val+03_33:	-346.6	316.8	314.6	-284.078773	77.0
val+03_34:	-296.7	320.8	318.3	-284.060210	83.3
val+03_35:	-228.5	314.7	312.4	-284.033551	81.2
val+03_36:	-419.8	316.7	314.5	-284.106613	77.7
val+03_37:	-383.7	324.6	322.2	-284.093783	81.8
val+03_38:	-366.1	316.2	314.0	-284.086131	78.6
val+03_39:	-204.3	320.2	317.9	-284.024962	78.1
val+03_3:	-140.0	312.3	309.8	-283.999544	84.4
val+03_40:	-135.6	309.5	307.3	-283.997566	78.4
val+03_41:	-97.0	322.9	320.7	-283.984382	77.9
val+03_42:	-130.7	313.0	310.8	-283.996111	77.2
val+03_43:	-344.7	311.0	308.9	-284.077380	75.5
val+03_44:	-165.4	316.6	314.4	-284.009741	77.5
val+03_45:	-190.1	314.6	312.5	-284.018917	75.6
val+03_46:	-223.5	316.6	314.3	-284.031838	80.1
val+03_47:	-406.2	315.3	313.1	-284.101288	79.3
val+03_48:	-94.9	320.0	317.8	-283.983274	77.8
val+03_49:	-61.6	315.7	313.5	-283.970099	76.1
val+03_4:	-279.9	310.1	307.6	-284.052611	85.1
val+03_50:	44.4	308.3	306.1	-283.928878	75.9
val+03_51:	-64.3	301.0	298.9	-283.969446	73.1
val+03_52:	-80.3	309.1	307.0	-283.976445	73.7
val+03_53:	-82.9	297.1	295.2	-283.976099	68.9
val+03_54:	-89.1	303.8	302.0	-283.979199	69.0
val+03_55:	-230.5	295.0	293.2	-284.032063	67.3
val+03_56:	-241.1	302.7	300.5	-284.036989	77.8
val+03_57:	-11.9	304.5	302.3	-283.949873	78.1
val+03_58:	-102.9	306.2	304.1	-283.984741	76.8
val+03_59:	166.7	313.5	311.3	-283.882887	77.7
val+03_5:	-278.4	317.2	314.6	-284.052854	87.3
val+03_60:	23.9	299.0	297.1	-283.935628	69.8
val+03_61:	-57.5	296.1	294.2	-283.966285	68.5
val+03_62:	-72.0	305.4	303.4	-283.972891	72.4
val+03_63:	-247.2	299.4	297.1	-284.038911	78.5
val+03_64:	-136.7	302.9	300.7	-283.997216	77.7

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val+03_65:	-209.4	302.5	300.3	-284.024884	77.3
val+03_66:	-78.2	314.0	311.6	-283.976231	81.3
val+03_67:	-236.1	295.8	293.6	-284.034293	76.2
val+03_68:	131.4	298.8	296.9	-283.894674	70.5
val+03_69:	41.3	303.1	301.2	-283.929457	69.9
val+03_6:	-292.5	310.7	308.5	-284.057450	78.8
val+03_70:	-21.1	307.2	305.2	-283.953708	74.4
val+03_71:	-68.6	310.4	308.4	-283.972152	72.0
val+03_72:	5.1	300.0	298.0	-283.942887	72.3
val+03_73:	-8.9	308.1	306.0	-283.949138	74.3
val+03_74:	-47.6	311.3	309.3	-283.964252	73.8
val+03_75:	-237.7	293.7	291.9	-284.034661	67.9
val+03_77:	-9.6	296.4	294.8	-283.948092	62.4
val+03_78:	-36.3	293.4	291.8	-283.957907	62.5
val+03_79:	-112.3	288.8	287.3	-283.986335	61.1
val+03_7:	-157.9	318.7	316.3	-284.007116	80.2
val+03_80:	213.2	308.0	305.9	-283.864531	75.1
val+03_81:	165.5	296.9	295.1	-283.881445	69.9
val+03_82:	42.9	307.9	305.9	-283.929393	74.2
val+03_83:	60.5	298.4	296.5	-283.921620	69.2
val+03_84:	-78.9	303.8	301.5	-283.975316	79.4
val+03_8:	-279.2	315.1	312.9	-284.052895	79.0
val+03_9:	-278.8	305.8	303.6	-284.051674	78.0
val+05_100:	-183.3	318.9	316.6	-284.016804	78.1
val+05_103:	-187.4	305.3	303.2	-284.016834	76.1
val+05_104:	-45.2	318.5	316.2	-283.964171	80.0
val+05_105:	-112.1	312.7	310.3	-283.988991	80.8
val+05_106:	-298.8	379.2	376.3	-284.067622	95.1
val+05_107:	-163.2	370.1	367.2	-284.014962	93.4
val+05_108:	-122.7	303.5	301.5	-283.991975	74.2
val+05_109:	-111.3	317.5	315.4	-283.989228	75.7
val+05_10:	-217.9	339.0	336.2	-284.032258	92.4
val+05_110:	-243.8	356.4	353.4	-284.044119	99.6
val+05_112:	34.4	302.2	300.3	-283.931997	68.5
val+05_113:	-67.2	406.2	403.3	-283.982510	94.8
val+05_114:	59.7	296.0	294.2	-283.921655	66.6
val+05_115:	25.8	292.4	290.7	-283.934157	64.8
val+05_116:	-46.3	384.6	381.8	-283.972102	93.7
val+05_117:	-379.4	312.1	309.7	-284.090725	80.8
val+05_118:	-386.7	306.9	304.9	-284.092923	74.2
val+05_11:	-199.8	346.6	343.7	-284.026211	92.9
val+05_121:	-273.3	391.3	388.2	-284.059280	98.4
val+05_122:	-310.6	373.8	371.1	-284.071527	91.9
val+05_123:	-197.7	370.9	367.5	-284.028206	107.2
val+05_124:	80.6	325.9	323.6	-283.917102	80.2
val+05_125:	-333.3	335.7	333.3	-284.075845	83.0
val+05_127:	-67.0	316.7	314.5	-283.972260	76.6
val+05_128:	-340.7	375.5	372.7	-284.083170	90.9
val+05_129:	5.4	315.0	312.8	-283.944485	77.8
val+05_12:	-380.9	332.7	330.3	-284.093632	83.1
val+05_131:	-278.5	447.1	443.4	-284.067625	115.6
val+05_132:	-275.4	473.1	469.3	-284.069382	117.5
val+05_133:	-72.6	307.7	305.6	-283.973378	75.8
val+05_134:	-228.5	314.5	312.2	-284.033531	81.2
val+05_135:	-100.0	317.1	315.1	-283.984847	72.6
val+05_136:	-53.2	314.5	312.6	-283.966764	72.4
val+05_137:	137.4	312.2	309.7	-283.893895	84.6
val+05_139:	96.0	362.2	358.9	-283.915332	103.3
val+05_13:	-325.0	310.3	308.1	-284.069787	78.8
val+05_141:	0.7	327.5	324.9	-283.947689	85.9
val+05_142:	-105.5	377.7	374.4	-283.993863	105.3
val+05_143:	112.2	355.7	352.5	-283.908449	103.8
val+05_144:	0.7	333.2	330.6	-283.948327	87.5
val+05_145:	-157.0	319.7	317.4	-284.006891	78.7
val+05_146:	113.8	321.0	318.4	-283.903876	87.8
val+05_147:	-67.2	312.2	309.7	-283.971800	83.2
val+05_148:	-131.4	314.6	312.3	-283.996562	80.7
val+05_149:	6.2	317.8	315.4	-283.944517	82.3
val+05_14:	-253.5	353.5	350.6	-284.047451	94.8
val+05_150:	-160.2	319.5	317.0	-284.008057	84.1
val+05_151:	205.9	343.5	340.8	-283.871365	89.8
val+05_152:	-13.9	327.2	324.5	-283.953216	89.3
val+05_153:	17.5	318.7	316.2	-283.940286	84.6
val+05_154:	-17.6	317.3	315.0	-283.953515	80.0
val+05_155:	103.5	318.6	316.2	-283.907542	82.5
val+05_156:	-163.7	306.8	304.5	-284.007978	78.6
val+05_157:	245.7	328.9	326.2	-283.854533	88.5

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val+05_158:	160.0	317.7	315.3	-283.885894	83.4
val+05_159:	145.7	320.2	317.9	-283.891631	80.4
val+05_15:	-228.5	314.3	311.9	-284.033479	81.1
val+05_160:	27.3	324.2	321.8	-283.937181	83.7
val+05_161:	-6.5	331.9	329.3	-283.950948	87.5
val+05_162:	257.8	329.1	326.6	-283.849973	85.9
val+05_17:	237.4	299.9	297.7	-283.854420	78.2
val+05_18:	234.2	310.5	308.1	-283.856830	81.7
val+05_19:	131.9	297.2	295.3	-283.894285	72.0
val+05_1:	233.8	390.9	387.6	-283.866130	105.6
val+05_20:	-252.2	387.4	384.2	-284.050838	103.6
val+05_21:	245.9	301.0	299.0	-283.851296	74.4
val+05_23:	-210.5	341.9	339.4	-284.029779	86.4
val+05_24:	164.7	309.8	307.7	-283.883240	76.5
val+05_25:	-241.8	400.7	397.9	-284.048390	92.2
val+05_26:	-301.8	367.1	364.4	-284.067424	88.2
val+05_27:	-114.1	353.6	350.9	-283.994396	90.5
val+05_28:	-11.3	312.0	309.5	-283.950502	84.5
val+05_29:	47.0	304.3	302.2	-283.927426	75.4
val+05_2:	-51.1	321.3	318.9	-283.966734	81.8
val+05_30:	157.2	307.7	305.5	-283.885829	77.0
val+05_31:	33.5	362.6	359.5	-283.939188	99.4
val+05_32:	214.7	326.1	323.5	-283.866045	87.6
val+05_33:	342.3	297.4	295.3	-283.814185	74.8
val+05_34:	-32.7	352.4	349.4	-283.963232	97.4
val+05_35:	-77.4	321.0	318.6	-283.976717	82.9
val+05_36:	156.7	312.0	309.9	-283.886538	75.0
val+05_37:	-171.1	345.9	343.1	-284.015217	91.9
val+05_38:	-107.5	321.8	319.3	-283.988259	84.8
val+05_39:	12.6	313.8	311.3	-283.941598	83.9
val+05_3:	157.2	333.7	330.9	-283.888786	92.7
val+05_40:	278.0	318.3	315.7	-283.841046	87.1
val+05_41:	-137.7	310.3	307.8	-283.998444	83.5
val+05_42:	110.6	303.6	301.3	-283.903128	80.9
val+05_43:	260.0	300.7	298.4	-283.845890	81.3
val+05_44:	-39.7	308.2	305.7	-283.960885	84.1
val+05_45:	-275.7	313.4	310.8	-284.051388	87.0
val+05_46:	-216.3	306.1	303.9	-284.027938	78.5
val+05_47:	-78.2	314.0	311.6	-283.976230	81.3
val+05_49:	-10.6	337.8	335.0	-283.953185	94.0
val+05_4:	-160.5	333.5	330.6	-284.009758	92.6
val+05_50:	-187.7	388.7	385.5	-284.026411	104.9
val+05_51:	-64.3	313.3	310.7	-283.970854	85.5
val+05_52:	190.1	366.3	363.4	-283.879953	93.4
val+05_53:	-4.2	315.0	312.7	-283.948145	78.4
val+05_54:	-259.7	363.0	360.0	-284.050923	96.3
val+05_55:	-32.5	312.0	309.5	-283.958595	84.4
val+05_56:	-131.7	318.9	316.6	-283.997134	80.3
val+05_57:	128.5	368.7	365.3	-283.903715	106.0
val+05_58:	-214.6	321.7	319.3	-284.029055	82.2
val+05_59:	-97.3	354.1	351.2	-283.988050	95.0
val+05_60:	217.7	326.2	323.8	-283.864910	81.4
val+05_61:	-75.6	308.2	306.1	-283.974552	76.0
val+05_62:	317.5	312.4	310.2	-283.825317	77.2
val+05_63:	-42.4	314.3	311.9	-283.962614	81.8
val+05_65:	-406.2	314.9	312.6	-284.101236	79.3
val+05_69:	-73.5	329.6	327.1	-283.976179	85.1
val+05_6:	-276.7	312.0	309.5	-284.051587	83.9
val+05_70:	305.2	313.8	311.5	-283.830166	79.7
val+05_71:	208.3	313.4	311.1	-283.867020	80.7
val+05_72:	-29.0	305.1	302.9	-283.956452	75.6
val+05_73:	-322.9	348.6	345.9	-284.073348	90.3
val+05_74:	-322.9	348.6	345.9	-284.073350	90.3
val+05_76:	-51.3	313.7	311.7	-283.965922	73.1
val+05_77:	-128.2	322.2	320.0	-283.996183	78.7
val+05_78:	-380.5	314.3	312.1	-284.091374	77.0
val+05_79:	-344.7	310.9	308.8	-284.077369	75.4
val+05_7:	-299.7	307.2	304.8	-284.059817	81.5
val+05_80:	-259.8	362.8	359.9	-284.050910	96.3
val+05_81:	-273.3	371.7	368.7	-284.057060	98.4
val+05_82:	-6.7	342.2	339.4	-283.952190	92.6
val+05_83:	-21.1	307.1	305.0	-283.953686	74.4
val+05_84:	256.8	333.2	330.9	-283.850814	80.5
val+05_85:	-22.0	354.2	351.7	-283.959392	85.2
val+05_86:	-10.3	308.1	306.1	-283.949685	74.3
val+05_88:	-78.9	304.0	301.7	-283.975342	79.4
val+05_8:	-84.0	381.1	378.0	-283.986056	100.3

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val+05_90:	19.3	301.8	299.6	-283.937688	75.7
val+05_91:	101.3	303.2	301.0	-283.906631	77.6
val+05_92:	-211.1	346.0	343.1	-284.030455	93.9
val+05_93:	-205.1	377.9	374.6	-284.031817	104.6
val+05_94:	52.6	312.9	310.5	-283.926273	81.6
val+05_95:	-280.3	356.2	353.2	-284.057997	95.6
val+05_96:	-115.6	317.4	315.0	-283.990833	83.1
val+05_97:	-48.1	325.9	323.3	-283.966101	86.6
val+05_98:	-317.3	365.8	362.6	-284.073179	102.4
val+05_99:	-124.3	311.9	309.5	-283.993534	82.4
val+05_9:	-214.6	320.5	318.1	-284.028899	82.1
val+07_100:	-205.1	386.8	383.5	-284.032823	104.6
val+07_101:	-31.7	307.6	305.3	-283.957758	78.7
val+07_102:	-11.1	307.0	304.9	-283.949856	76.4
val+07_103:	263.4	303.9	301.5	-283.844949	83.6
val+07_104:	19.3	301.7	299.5	-283.937675	75.7
val+07_105:	101.2	303.3	301.1	-283.906657	77.6
val+07_106:	53.1	311.4	309.1	-283.925904	81.0
val+07_107:	-287.0	426.6	423.1	-284.068544	110.7
val+07_109:	-11.5	313.7	311.5	-283.950787	77.4
val+07_10:	-51.1	321.3	319.0	-283.966736	81.8
val+07_110:	-57.0	365.2	362.1	-283.973938	99.1
val+07_111:	-103.2	364.4	361.3	-283.991446	99.5
val+07_112:	-425.9	368.7	366.0	-284.114840	88.4
val+07_113:	-51.2	321.6	319.2	-283.966794	81.9
val+07_114:	-322.9	348.7	346.0	-284.073370	90.3
val+07_115:	-66.7	341.0	337.9	-283.974900	99.6
val+07_117:	-59.5	341.1	338.3	-283.972169	94.1
val+07_119:	-197.7	371.3	367.9	-284.028248	107.2
val+07_11:	-312.1	365.7	362.9	-284.071154	91.7
val+07_120:	-99.0	329.8	327.5	-283.985937	78.3
val+07_121:	-72.6	307.7	305.6	-283.973357	75.7
val+07_122:	150.9	348.4	345.8	-283.892869	88.9
val+07_124:	-142.8	321.9	319.6	-284.001718	80.7
val+07_125:	-210.5	341.4	338.8	-284.029701	86.3
val+07_128:	-148.1	317.3	315.1	-284.003224	78.2
val+07_129:	-67.8	303.5	301.5	-283.971053	73.9
val+07_12:	-312.1	365.7	363.0	-284.071162	91.6
val+07_131:	-48.1	325.7	323.1	-283.966069	86.6
val+07_132:	-259.8	386.7	384.0	-284.053655	90.6
val+07_134:	-244.0	315.5	313.2	-284.039521	78.6
val+07_135:	-111.3	317.5	315.4	-283.989212	75.6
val+07_136:	257.9	316.9	314.5	-283.848541	83.7
val+07_137:	-22.3	314.6	312.4	-283.954984	77.7
val+07_138:	237.4	299.9	297.7	-283.854421	78.2
val+07_139:	159.0	301.3	299.3	-283.884431	73.9
val+07_13:	-139.7	367.4	364.5	-284.005692	93.2
val+07_140:	-425.8	368.1	365.5	-284.114766	88.4
val+07_141:	-175.4	353.2	350.7	-284.017684	84.4
val+07_142:	-86.4	318.3	316.1	-283.979820	79.9
val+07_143:	10.2	316.1	313.8	-283.942798	80.5
val+07_144:	309.0	309.9	307.7	-283.828273	76.9
val+07_145:	-12.8	352.5	349.2	-283.955688	104.2
val+07_146:	-124.5	386.9	383.4	-284.002119	110.1
val+07_148:	-236.2	314.3	311.9	-284.036439	80.9
val+07_14:	-166.7	366.8	364.0	-284.015924	92.5
val+07_150:	101.2	304.5	302.3	-283.906796	77.7
val+07_151:	52.6	312.9	310.6	-283.926284	81.6
val+07_152:	-310.6	373.9	371.1	-284.071543	91.9
val+07_153:	-48.2	325.8	323.3	-283.966121	86.6
val+07_154:	-67.2	404.6	401.7	-283.982334	94.8
val+07_155:	-72.6	308.0	305.9	-283.973402	75.8
val+07_158:	-46.3	384.4	381.5	-283.972055	93.7
val+07_15:	-311.1	367.1	364.6	-284.070933	85.6
val+07_16:	343.9	347.4	344.5	-283.819250	94.6
val+07_17:	-161.9	307.7	305.3	-284.007361	80.9
val+07_18:	-312.0	365.0	362.3	-284.071062	91.6
val+07_19:	-83.1	368.7	365.9	-283.984293	93.1
val+07_1:	201.6	308.1	305.8	-283.868974	81.0
val+07_21:	-359.6	308.8	306.7	-284.082821	74.4
val+07_22:	-118.1	353.6	350.7	-283.995917	95.3
val+07_23:	103.5	318.4	316.0	-283.907527	82.5
val+07_24:	-279.3	420.0	416.4	-284.064850	113.5
val+07_25:	-278.2	446.6	442.9	-284.067439	115.3
val+07_26:	-78.9	303.8	301.5	-283.975308	79.4
val+07_27:	-14.0	328.0	325.3	-283.953334	89.4
val+07_28:	-133.9	374.0	371.2	-284.004232	92.8

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val+07_29:	242.0	313.0	310.6	-283.854133	82.7
val+07_2:	-159.8	335.9	333.1	-284.009805	93.7
val+07_31:	181.9	303.8	301.6	-283.875982	77.2
val+07_32:	-22.1	355.4	352.9	-283.959537	85.3
val+07_36:	136.8	366.6	363.1	-283.900289	109.7
val+07_38:	363.5	352.7	349.4	-283.812389	104.2
val+07_39:	-221.6	366.2	363.2	-284.036747	98.7
val+07_3:	-43.7	314.8	312.2	-283.963146	86.9
val+07_40:	-163.2	369.2	366.4	-284.014879	93.4
val+07_41:	-103.2	364.4	361.4	-283.991459	99.5
val+07_42:	156.5	367.1	364.3	-283.892854	92.4
val+07_44:	-51.1	321.5	319.1	-283.966759	81.8
val+07_45:	-214.9	388.5	385.0	-284.036733	109.5
val+07_46:	-110.6	305.4	303.2	-283.987572	78.1
val+07_47:	-83.0	323.8	321.3	-283.979161	84.5
val+07_48:	-366.1	315.8	313.6	-284.086065	78.5
val+07_49:	-148.9	432.9	428.8	-284.016647	122.9
val+07_4:	-95.8	304.4	302.2	-283.981823	79.1
val+07_51:	-183.3	318.5	316.3	-284.016759	78.1
val+07_52:	401.4	322.6	320.1	-283.794529	85.4
val+07_53:	-32.7	352.9	349.9	-283.963294	97.5
val+07_54:	-70.2	315.0	312.6	-283.973267	83.6
val+07_55:	231.6	329.7	326.9	-283.859996	90.9
val+07_56:	79.7	311.4	309.1	-283.915760	80.6
val+07_57:	310.2	372.3	369.1	-283.834893	101.5
val+07_58:	-51.1	321.2	318.8	-283.966709	81.8
val+07_60:	-227.2	305.1	302.8	-284.031947	78.4
val+07_61:	110.3	313.9	311.5	-283.904398	83.4
val+07_62:	61.5	312.7	310.4	-283.922877	80.8
val+07_63:	-12.3	317.5	315.0	-283.951522	85.9
val+07_64:	-6.9	353.9	350.5	-283.953570	107.1
val+07_66:	21.6	325.7	322.9	-283.939511	91.5
val+07_69:	-78.3	335.1	332.6	-283.978661	84.6
val+07_6:	-196.1	313.5	311.3	-284.021063	79.7
val+07_71:	-245.3	352.2	349.2	-284.044205	98.8
val+07_72:	-85.2	334.0	331.3	-283.981149	90.8
val+07_74:	84.1	383.4	380.6	-283.922270	93.7
val+07_75:	-59.5	341.6	338.7	-283.972235	94.1
val+07_78:	-44.7	347.0	343.9	-283.967185	97.9
val+07_79:	-326.7	344.6	342.2	-284.074358	83.8
val+07_80:	-205.1	376.7	373.4	-284.031670	104.5
val+07_81:	-268.5	366.1	363.1	-284.054618	98.4
val+07_82:	-62.0	368.7	365.5	-283.976267	102.5
val+07_84:	-322.9	348.5	345.8	-284.073338	90.3
val+07_85:	151.8	375.4	371.9	-283.895578	109.1
val+07_86:	-51.3	313.7	311.7	-283.965937	73.1
val+07_87:	173.5	366.9	364.1	-283.886372	92.9
val+07_88:	242.0	313.0	310.6	-283.854134	82.7
val+07_89:	-322.9	348.7	346.0	-284.073360	90.3
val+07_8:	-120.2	318.4	315.8	-283.992708	88.4
val+07_90:	33.5	362.0	358.9	-283.939109	99.3
val+07_91:	83.6	377.6	374.7	-283.921810	94.4
val+07_92:	-386.7	306.6	304.6	-284.092882	74.2
val+07_93:	-386.7	306.9	304.8	-284.092918	74.2
val+07_94:	-259.7	362.9	359.9	-284.050904	96.2
val+07_95:	-221.6	369.0	365.9	-284.037067	98.8
val+07_97:	-11.5	313.6	311.4	-283.950784	77.4
val+07_98:	120.7	349.1	345.9	-283.904446	102.1
val+07_99:	-214.5	319.3	316.9	-284.028743	82.0
val+07_9:	233.7	354.9	352.1	-283.862065	93.7

val+03_10

C	0.16429	0.12606	-0.31760
C	-1.33185	-0.01017	-0.10219
N	0.68048	1.28242	-0.32808
O	0.87516	-1.02088	-0.48941
O	-1.94882	1.23403	0.06182
H	-1.75902	-0.54853	-0.96680
H	-1.49781	-0.64991	0.78273
H	1.69057	1.25783	-0.47990
H	0.28435	-1.79150	-0.44495
H	-1.22357	1.88826	-0.00732

val+03_11

C	0.22607	0.71955	0.12268
C	-1.25279	0.65508	-0.08195

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N	1.08074	-0.23302	0.14649
O	0.69641	1.98237	0.30517
O	0.47136	-1.49879	-0.05711
H	-1.52950	1.23136	-0.97184
H	-1.76497	1.10713	0.77447
H	-1.57660	-0.37844	-0.20038
H	1.66103	1.90558	0.42556
H	1.23674	-2.09062	-0.00500

val+03_12

C	0.43418	-0.32829	0.18268
C	-1.90979	-0.62817	0.12905
N	-0.55989	-1.08191	0.36729
O	0.48805	0.97447	-0.24405
O	1.68484	-0.77647	0.41441
H	-2.04338	0.45986	-0.03407
H	-2.53743	-0.89094	0.98822
H	-2.33034	-1.13872	-0.74685
H	-0.41308	1.28781	-0.42342
H	2.30103	-0.05534	0.20665

val+03_13

C	-0.04860	-0.97954	0.17409
C	1.26118	-1.12275	-0.04994
N	-0.86484	0.04659	-0.33371
O	-0.23006	1.18660	-0.73263
O	0.26575	1.93612	0.47031
H	-0.61598	-1.70791	0.74935
H	1.82112	-0.42189	-0.66083
H	1.78958	-1.98040	0.34847
H	-1.66785	0.28090	0.24705
H	1.11352	1.47607	0.62064

val+03_14

C	0.16977	-0.75453	-0.25464
C	1.47831	-0.99598	-0.24704
N	-1.72379	0.47065	0.24699
O	-0.42308	0.04047	0.69623
O	-1.59101	1.80212	-0.23679
H	-0.53007	-1.18144	-0.96978
H	2.13727	-0.54225	0.48566
H	1.90467	-1.67999	-0.97142
H	-2.16420	0.64177	1.15237
H	-1.57566	1.68078	-1.20088

val+03_15

C	-0.36661	0.54184	-0.21581
C	0.92459	0.23507	0.00694
N	-0.95265	1.78700	-0.03646
O	1.40712	-0.94886	-0.45939
O	1.75825	-1.79781	0.74456
H	-1.00482	-0.20899	-0.67390
H	1.63607	0.90558	0.49131
H	-1.94062	1.76641	0.18239
H	-0.44757	2.42119	0.57246
H	2.63675	-2.09563	0.44581

val+03_16

C	0.26404	0.09018	0.40703
C	1.46620	-0.10392	-0.14317
N	-1.66798	1.27213	-0.01394
O	-0.28261	1.35388	0.43161
O	2.18389	-1.26830	-0.12160
H	-0.32233	-0.69215	0.88837
H	2.00575	0.69574	-0.63895
H	-1.62125	1.57276	-0.99304
H	-2.08616	2.05820	0.48769
H	1.66715	-1.94793	0.34108

val+03_17

C	-0.19055	0.45414	-0.02474
C	1.13354	0.26924	-0.04279
N	-0.88777	1.64509	-0.24434
O	-1.15367	-0.53125	0.13459
O	-0.55080	-1.79293	0.47279
H	1.79377	1.12134	-0.15258
H	1.56675	-0.71431	0.05560

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H	-1.67405	1.76191	0.38852
H	-0.28083	2.45584	-0.21986
H	-0.56300	-2.22918	-0.40029

val+03_18			
C	0.15787	-0.06642	0.13024
C	1.47734	-0.17008	-0.05867
N	-1.56824	1.41029	-0.37249
O	-0.41493	1.11152	0.48352
O	-0.75266	-1.07892	0.10736
H	2.09084	0.72040	-0.07182
H	1.96007	-1.13569	-0.16316
H	-2.36381	1.12874	0.20608
H	-1.55498	2.43124	-0.33658
H	-0.34210	-1.85025	-0.31277

val+03_19			
C	0.97440	-0.54871	0.14629
C	-1.30824	-0.79717	-0.21700
N	0.03009	-0.49358	-0.69758
O	-2.27094	0.01260	-0.84954
O	-2.03937	1.37200	-0.39274
H	0.83605	-0.79219	1.21090
H	1.99612	-0.34717	-0.18090
H	-1.39934	-0.71671	0.87856
H	-1.57997	-1.81003	-0.54095
H	-1.41299	1.67526	-1.07735

val+03_1			
C	-0.12773	-0.41330	-0.01626
C	1.18406	-0.51899	-0.24597
N	-0.86429	0.80312	0.10140
O	1.90663	-1.68663	-0.24963
O	-0.08939	1.91336	-0.37824
H	-0.74740	-1.28494	0.19321
H	1.80998	0.33895	-0.45273
H	-1.67009	0.77690	-0.52603
H	1.30930	-2.42823	-0.06173
H	-0.00628	2.46387	0.41709

val+03_20			
C	1.68200	-0.12079	0.14433
C	-1.70701	-0.55320	-0.26140
N	0.57058	-0.20852	-0.47012
O	-0.45062	-0.63358	0.39749
O	-2.21214	0.74552	-0.33981
H	2.54323	0.17560	-0.44678
H	1.79532	-0.32990	1.20899
H	-2.34570	-1.22058	0.33209
H	-1.61344	-0.91038	-1.28880
H	-2.33162	1.07093	0.56710

val+03_21			
C	0.69757	-0.61222	-0.17429
C	-0.78238	-0.64497	0.14434
N	1.51508	-1.58623	-0.15275
O	-1.22107	0.49697	0.87116
O	-1.25310	1.59478	-0.09302
H	1.08222	0.36746	-0.47450
H	-1.37487	-0.74071	-0.77694
H	-1.02480	-1.48877	0.80226
H	1.04066	-2.45136	0.14128
H	-0.75549	2.26284	0.41165

val+03_22			
C	0.68198	-0.24504	-0.06028
C	-1.65821	-0.56951	-0.31402
N	1.87280	-0.34948	-0.47041
O	-0.32563	-0.85349	-0.73211
O	-2.27157	0.41119	-1.08919
H	0.34288	0.29873	0.83626
H	-1.65051	-0.31166	0.75741
H	-2.22595	-1.48612	-0.47322
H	2.49860	0.14598	0.16603
H	-1.83459	1.26180	-0.92248

val+03_23

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C	0.40106	1.14750	-0.09505
C	-1.04156	1.17913	0.31933
N	1.17006	0.12599	-0.15878
O	0.47521	-1.04257	0.18139
O	1.45768	-2.08043	0.33212
H	0.89497	2.07127	-0.39177
H	-1.33239	2.18709	0.62721
H	-1.69148	0.87911	-0.51342
H	-1.22355	0.47990	1.14105
H	1.67928	-2.26450	-0.60130

val+03_24

C	-0.07854	-0.14863	-0.10173
C	-2.38745	-0.16629	0.08481
N	-1.13024	-0.82405	-0.22078
O	1.12305	-0.75663	-0.37700
O	2.16280	0.25026	-0.25936
H	0.03376	0.89902	0.19957
H	-2.28123	0.88762	0.39161
H	-3.03984	-0.20652	-0.79518
H	-2.89652	-0.71110	0.88847
H	2.73292	-0.18967	0.39749

val+03_25

C	0.10686	-0.26912	0.23293
C	-2.23211	-0.28776	0.14247
N	1.21275	-0.71856	0.67839
O	-1.04024	-0.64299	0.83841
O	2.27933	-0.15959	-0.06999
H	0.03738	0.42472	-0.60954
H	-2.27523	0.79201	-0.05131
H	-3.05939	-0.56896	0.79566
H	-2.31797	-0.83186	-0.80656
H	3.04802	-0.57699	0.34706

val+03_26

C	1.61196	0.55220	-0.18863
C	-1.71981	-0.21186	0.12509
N	0.35050	0.77550	-0.18955
O	-0.31804	-0.44270	0.12302
O	2.22092	-0.61908	0.06082
H	2.28720	1.37170	-0.40791
H	-1.99422	0.53363	0.88041
H	-2.06435	0.12428	-0.85975
H	-2.17567	-1.17469	0.36991
H	1.50571	-1.26038	0.24029

val+03_27

C	0.21763	0.82787	0.12569
C	-1.24459	0.55538	-0.04932
N	0.73486	1.97728	-0.00784
O	1.05479	-0.22750	0.45114
O	0.32030	-1.47020	0.66614
H	-1.72925	1.49371	-0.32078
H	-1.68284	0.16394	0.87371
H	-1.41667	-0.19174	-0.83027
H	1.74511	1.95053	0.16662
H	0.76336	-2.02807	0.00090

val+03_28

C	0.52342	-0.28199	-0.34110
C	-1.82134	-0.55774	-0.33149
N	0.58861	0.80321	0.32048
O	-0.53532	-1.02983	-0.71902
O	1.63321	-0.89064	-0.80055
H	-2.02779	0.42924	-0.76294
H	-2.53363	-1.28367	-0.72481
H	-1.91315	-0.50878	0.76037
H	-0.32111	1.15583	0.60739
H	2.36990	-0.32594	-0.50982

val+03_29

C	0.25259	-0.94580	0.22269
C	1.40997	-1.12678	-0.41332
N	-1.50623	1.30303	-0.41256
O	0.02258	0.18692	0.94917
O	-1.41675	0.56619	0.76523

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H	-0.54017	-1.69056	0.27552
H	2.16100	-0.34475	-0.44699
H	1.64043	-2.08499	-0.86612
H	-2.22895	0.85150	-0.97192
H	-1.81197	2.23663	-0.13920

val+03_2

C	0.35736	-0.90714	-0.17819
C	1.69004	-0.97560	-0.18080
N	-0.39656	0.24230	-0.53161
O	-1.47998	0.31945	0.40664
O	0.35744	1.42041	-0.42889
H	-0.28288	-1.75510	0.03870
H	2.30975	-0.12418	-0.43696
H	2.18251	-1.91712	0.03451
H	-2.16500	0.77632	-0.11066
H	0.71453	1.42674	0.48737

val+03_30

C	1.81843	0.42388	0.10520
C	-2.14173	-0.47408	0.15582
N	0.71980	-0.07196	-0.31040
O	-1.46595	0.27506	-0.84622
O	-0.30466	0.86665	-0.22644
H	1.92218	1.44983	0.46143
H	2.68223	-0.23311	0.08970
H	-2.44756	0.16418	0.99327
H	-3.02604	-0.86701	-0.35550
H	-1.52190	-1.30414	0.51383

val+03_31

C	1.68457	0.54870	-0.12524
C	-1.54417	-0.00499	-0.02944
N	2.12858	-0.61621	0.05028
O	0.45753	1.09792	0.17218
O	-0.39466	0.10249	0.80282
H	2.27843	1.34795	-0.57239
H	-2.05839	0.95803	-0.11746
H	-2.18361	-0.72039	0.49683
H	-1.28807	-0.39066	-1.02293
H	1.41870	-1.20535	0.49436

val+03_32

C	0.84842	-1.30960	-0.04047
C	-0.53929	-0.69150	0.01979
N	-0.54340	0.46337	0.90984
O	1.22615	-2.02855	-0.93542
O	0.12609	1.52842	0.19355
H	1.49432	-1.06684	0.83304
H	-0.87807	-0.47267	-1.00305
H	-1.22125	-1.43873	0.45345
H	-1.50364	0.80006	0.99268
H	0.78758	1.82894	0.83689

val+03_33

C	0.74130	-1.00942	0.23892
C	-1.48664	0.03909	-0.07923
N	-0.09761	-0.15356	-0.42799
O	1.94306	-1.07089	0.06911
O	-1.70798	0.82349	1.07647
H	0.19231	-1.66327	0.94447
H	-1.99381	0.45480	-0.95956
H	-1.93120	-0.93269	0.14918
H	0.36063	0.50526	-1.04788
H	-1.37226	1.71799	0.90603

val+03_34

C	1.17474	-0.84490	0.19367
C	-0.26428	-0.49263	-0.18258
N	-0.41260	0.93836	-0.07204
O	1.98570	-1.29772	-0.57739
O	-1.06685	-1.26659	0.71178
H	1.42471	-0.63909	1.25874
H	-0.42247	-0.78133	-1.22804
H	-1.26587	1.27146	-0.51416
H	-0.43533	1.21514	0.90772
H	-1.98456	-1.24179	0.39721

val+03_35			
C	0.12083	1.01476	-0.07139
C	-1.38831	0.96517	0.01781
N	0.77194	-0.21822	-0.12772
O	0.78417	2.03634	-0.03817
O	0.04267	-1.30036	-0.67601
H	-1.75334	1.97256	0.22177
H	-1.81232	0.60081	-0.92372
H	-1.71844	0.28153	0.80675
H	1.69638	-0.16317	-0.54901
H	-0.00886	-1.93803	0.05598

val+03_36			
C	0.68427	-0.09985	0.01871
C	-1.46071	1.17968	0.21066
N	-0.01241	1.06066	0.15912
O	1.88657	-0.18011	-0.16181
O	-0.12724	-1.19303	0.12572
H	-1.71845	2.15169	0.63996
H	-1.92804	1.09742	-0.78007
H	-1.87103	0.39765	0.85192
H	0.54123	1.88477	-0.02219
H	0.47442	-1.95238	0.04158

val+03_37			
C	0.10286	0.03673	-0.01242
C	-1.41972	-0.03714	0.15927
N	0.75391	-1.13894	-0.20263
O	0.66926	1.12377	0.02600
O	-1.93908	1.24903	0.34381
H	-1.85740	-0.51680	-0.73179
H	-1.65140	-0.68503	1.02081
H	1.75760	-1.12773	-0.31694
H	0.27307	-2.02561	-0.22901
H	-1.15609	1.83660	0.30870

val+03_38			
C	1.04675	0.00648	0.07013
C	-0.46033	0.18766	-0.10119
N	-0.82275	1.57849	0.11206
O	1.83869	0.91235	-0.00087
O	1.47191	-1.26822	0.25628
H	-0.98727	-0.46135	0.61542
H	-0.69910	-0.20752	-1.10740
H	-1.61366	1.83902	-0.46976
H	-0.02881	2.15784	-0.15666
H	0.71058	-1.86767	0.33220

val+03_39			
C	0.74692	-0.89292	0.13827
C	-1.50340	0.24049	0.17999
N	-0.06857	0.17896	0.11510
O	1.95811	-0.79251	-0.05817
O	0.53329	1.39911	-0.21443
H	0.22423	-1.83607	0.36513
H	-1.81744	0.94929	0.95357
H	-1.92165	0.55430	-0.78368
H	-1.87529	-0.75622	0.43186
H	1.47300	1.11218	-0.31265

val+03_3			
C	-0.13052	-0.47019	-0.06489
C	1.18573	-0.61829	-0.24948
N	-0.82727	0.74696	0.09023
O	-1.04533	-1.47864	0.07497
O	-0.09271	1.84676	-0.43244
H	1.82097	0.24486	-0.38356
H	1.63535	-1.60511	-0.27558
H	-1.70712	0.71147	-0.42462
H	-0.57701	-2.32219	-0.01480
H	0.05440	2.39636	0.35447

val+03_40			
C	-0.08240	-0.73330	0.27238
C	1.33535	-0.73408	-0.29977
N	-0.30060	0.60819	0.92467

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O	-1.30072	1.15817	0.51305
O	-1.03781	-1.03271	-0.68349
H	-0.13630	-1.41910	1.13836
H	1.55269	-1.72382	-0.70982
H	1.41167	0.00133	-1.10665
H	2.06850	-0.49766	0.47714
H	-1.69227	-0.30201	-0.62728

val+03_41			
C	-0.04751	-0.70956	0.39690
C	-1.37131	-0.47637	-0.34356
N	1.03855	-0.90675	-0.60659
O	1.88664	-0.04377	-0.56859
O	-1.37084	0.71806	-1.10180
H	-0.10998	-1.64783	0.96391
H	0.21020	0.12316	1.06428
H	-2.19367	-0.50448	0.38825
H	-1.53479	-1.28626	-1.06084
H	-1.28188	1.46581	-0.49017

val+03_42			
C	1.13348	-1.01852	-0.22453
C	-0.32869	-1.13071	0.16616
N	-0.95793	1.03906	-0.31775
O	1.78724	-0.00349	-0.13977
O	-0.84903	0.04272	0.73161
H	1.57855	-1.96280	-0.61656
H	-0.89924	-1.44839	-0.72255
H	-0.42897	-1.91691	0.92844
H	-1.73960	1.60365	0.01835
H	-0.11802	1.60868	-0.18741

val+03_43			
C	-0.97384	1.13573	-0.04638
C	-0.42779	-1.14662	-0.23683
N	0.87678	-1.11215	0.34839
O	-0.92978	1.08239	1.16166
O	-0.75293	0.12055	-0.88899
H	-1.21363	2.04373	-0.62127
H	-1.24299	-1.34740	0.46774
H	-0.45687	-1.86771	-1.05406
H	0.84916	-0.83138	1.32248
H	1.37218	-1.99014	0.24717

val+03_44			
C	1.59853	-0.39565	0.09134
C	-1.75361	-0.31660	0.04879
N	0.45882	0.38255	0.07902
O	2.68659	0.01706	0.43593
O	-0.58448	-0.08066	-0.74029
H	1.37896	-1.43964	-0.19761
H	-2.10782	0.60786	0.52175
H	-2.50384	-0.68017	-0.65792
H	-1.56641	-1.07185	0.82056
H	0.59954	1.38648	-0.01466

val+03_45			
C	1.14459	-1.13416	0.13294
C	-1.16278	1.25667	-0.06719
N	-0.01086	0.79408	0.70887
O	1.87169	-1.83828	-0.50986
O	0.89834	0.15718	-0.22926
H	0.60380	-1.40908	1.05347
H	-0.88762	1.84964	-0.94974
H	-1.77820	1.86538	0.60396
H	-1.74870	0.39101	-0.38698
H	0.53314	1.60806	0.99799

val+03_46			
C	0.63193	0.98022	0.32078
C	-0.85427	0.80607	0.11499
N	0.71291	-1.38465	0.08878
O	1.18688	2.03478	0.49872
O	1.42827	-0.14334	0.30690
H	-1.31086	1.79572	0.15652
H	-1.06605	0.33196	-0.84732
H	-1.28504	0.15853	0.88370

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H	1.20882	-1.78140	-0.71227
H	1.00731	-1.94680	0.89022
val+03_47			
C	0.50274	0.20616	0.02556
C	-1.81810	-0.12827	-0.12359
N	1.71036	-0.20454	-0.47448
O	0.34265	1.10678	0.82534
O	-0.50202	-0.51908	-0.53460
H	-2.01811	0.91039	-0.40065
H	-2.49825	-0.80017	-0.64896
H	-1.93533	-0.23489	0.95831
H	2.52562	0.10816	0.03035
H	1.76345	-1.09795	-0.94138
val+03_48			
C	-0.58058	-1.11057	-0.21796
C	0.85354	-1.31980	0.24452
N	-1.44847	1.06734	-0.03458
O	-1.54621	2.12794	-0.54599
O	-0.72193	0.17013	-0.86462
H	-1.28562	-1.15111	0.61972
H	-0.87680	-1.85732	-0.96161
H	0.96695	-2.32010	0.67795
H	1.12748	-0.58086	1.00471
H	1.55053	-1.22654	-0.59435
val+03_49			
C	-0.42676	-1.15648	-0.04082
C	-0.99970	1.13640	0.02354
N	0.94170	-1.27641	0.58696
O	1.64264	-0.30855	0.40322
O	-0.68993	-0.01080	-0.76370
H	-1.12269	-1.32551	0.80020
H	-0.48797	-2.02209	-0.71303
H	-0.13661	1.47502	0.60531
H	-1.84216	0.93084	0.70090
H	-1.29092	1.92057	-0.67849
val+03_4			
C	-0.25160	0.02088	-0.12148
C	1.08291	-0.11888	-0.01331
N	-0.96346	1.21724	-0.17380
O	-1.06465	-1.06097	-0.26017
O	1.60383	-1.41193	-0.20324
H	1.78103	0.71005	0.04376
H	-1.86867	1.14047	0.27976
H	-0.44261	2.00729	0.18928
H	-0.45375	-1.81965	-0.33079
H	2.00085	-1.70330	0.63358
val+03_50			
C	0.55551	-0.15916	0.03902
C	-0.11144	1.16517	-0.02200
N	1.04859	0.83420	-0.88009
O	0.01980	-1.26578	-0.63598
O	-0.84649	-1.94030	0.32367
H	1.13247	-0.43301	0.92226
H	-1.04525	1.27260	-0.56831
H	0.01894	1.84743	0.81681
H	1.91419	1.24878	-0.53858
H	-1.71882	-1.64254	0.00589
val+03_51			
C	0.93804	-0.08625	-0.33577
C	0.38900	1.25604	-0.16203
N	0.12453	-1.26583	-0.37659
O	1.15432	0.62204	0.88551
O	-1.07884	-1.08069	0.38790
H	1.83503	-0.24179	-0.93869
H	-0.67139	1.36488	0.05339
H	0.86898	2.10834	-0.64454
H	0.61510	-2.01226	0.11962
H	-1.76747	-1.24118	-0.27720
val+03_52			
C	0.56473	0.54584	0.39839

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C	-0.40553	-0.46199	-0.16797
N	0.11894	1.81298	0.90880
O	0.82639	1.66176	-0.40740
O	-0.93061	-1.21037	0.91844
H	1.41874	0.12259	0.93012
H	-1.18708	0.08205	-0.72358
H	0.13055	-1.10184	-0.88698
H	-0.86544	1.92373	0.62816
H	-1.42299	-1.96234	0.55733

val+03_53

C	-0.01675	-0.33959	0.03582
C	-0.79266	0.98481	0.12428
N	0.99978	0.41307	-0.74900
O	0.37649	1.69809	-0.33371
O	-0.55596	-1.43315	-0.63037
H	0.33253	-0.71601	1.00310
H	-1.12313	1.32319	1.11181
H	-1.62641	1.04317	-0.58976
H	1.92018	0.41275	-0.29841
H	-0.68338	-1.15924	-1.55547

val+03_54

C	0.18718	-0.38145	0.04636
C	-0.59788	0.92000	-0.04933
N	0.61321	1.63681	0.46259
O	1.34572	0.34115	0.51204
O	-0.36717	-1.25723	0.97401
H	0.42622	-0.90353	-0.89320
H	-0.93291	1.21472	-1.04857
H	-1.42959	0.96935	0.65730
H	1.06380	2.11767	-0.32220
H	0.20752	-2.03639	1.04430

val+03_55

C	0.21941	-0.81821	0.06970
C	0.46271	1.14198	-0.30073
N	-0.22665	0.38424	0.75887
O	1.01455	-0.06575	-0.85737
O	-0.85517	-1.50096	-0.49803
H	0.85041	-1.50469	0.65267
H	-0.18826	1.68197	-1.00405
H	1.24970	1.80995	0.06883
H	-1.24154	0.46101	0.73394
H	-0.54748	-2.36953	-0.80373

val+03_56

C	0.39785	-0.61568	-0.34633
C	-0.29038	0.66590	-0.32657
N	-0.26843	-1.84665	-0.54784
O	0.20980	0.13858	0.90087
O	0.35378	1.76336	-0.87072
H	1.43125	-0.62099	-0.68676
H	-1.38317	0.70814	-0.38227
H	0.22742	-2.60942	-0.09179
H	-1.21243	-1.82112	-0.16985
H	0.06871	2.55267	-0.38174

val+03_57

C	0.65785	-0.06707	-0.27494
C	-0.32152	-1.12171	0.16766
N	0.26489	1.28763	-0.58910
O	1.05053	0.92098	0.64593
O	-1.08530	1.46891	-0.22390
H	1.45824	-0.42673	-0.92900
H	-1.09699	-0.69314	0.80217
H	0.21709	-1.89347	0.72880
H	-0.78594	-1.59827	-0.70326
H	-1.17325	2.43647	-0.25657

val+03_58

C	0.68572	-0.57361	-0.01391
C	-0.79905	1.36730	0.14102
N	0.48375	0.81841	-0.30201
O	1.23097	0.27347	0.92207
O	-0.33832	-1.37806	0.44979
H	1.38025	-1.08852	-0.68481

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H	-0.61980	2.36172	0.55741
H	-1.32358	0.74222	0.86913
H	-1.41307	1.47645	-0.76145
H	-0.45257	-2.11559	-0.16843

val+03_59

C	-1.56084	0.61522	0.10792
C	-0.65576	-0.54623	-0.08849
N	-0.29337	0.54941	0.84863
O	0.59928	1.47262	0.17401
O	1.85794	1.39369	0.85416
H	-2.44873	0.54870	0.73087
H	-1.60780	1.34553	-0.69606
H	-0.09981	-0.58686	-1.02136
H	-0.85315	-1.50028	0.39308
H	2.28613	0.65140	0.38544

val+03_5

C	0.68202	0.02280	0.11114
C	-0.64345	-0.04708	-0.06649
N	-1.48487	1.07943	-0.28909
O	1.33642	1.20640	0.28293
O	1.55856	-1.03511	0.13343
H	-1.12638	-1.01902	-0.12317
H	-2.15593	1.19841	0.46917
H	-0.92307	1.92672	-0.32737
H	2.24881	1.08146	-0.02649
H	1.10249	-1.81953	-0.20816

val+03_60

C	-0.71755	-0.73871	0.20396
C	-1.61918	0.43133	-0.18250
N	0.35282	0.26217	0.50149
O	-0.47331	1.30928	-0.17559
O	1.43907	-0.03945	-0.34612
H	-0.42705	-1.37128	-0.63840
H	-0.97684	-1.34716	1.07396
H	-2.10399	0.38760	-1.16406
H	-2.35577	0.71354	0.57968
H	2.17471	0.44367	0.06747

val+03_61

C	1.08069	0.97442	-0.06914
C	0.96251	-1.02711	-0.08991
N	0.18037	0.03057	-0.77342
O	1.98414	-0.08682	0.27279
O	-1.15114	0.10376	-0.25008
H	0.59246	1.43049	0.80467
H	1.54792	1.73735	-0.70306
H	1.33741	-1.82643	-0.74008
H	0.42276	-1.44030	0.77482
H	-1.69273	0.14366	-1.05398

val+03_62

C	-0.47147	1.55383	-0.26345
C	0.39755	-0.60135	0.44304
N	0.61177	0.62678	-0.34723
O	0.61596	1.78973	0.59791
O	-0.09315	-1.60116	-0.41053
H	-1.40351	1.23747	0.21157
H	-0.58240	2.24108	-1.10283
H	-0.34549	-0.45871	1.23648
H	1.36333	-0.86135	0.89597
H	0.58850	-1.77372	-1.08025

val+03_63

C	-0.04136	-0.19933	0.28722
C	-0.34688	1.23274	0.32516
N	-1.05071	-1.18427	0.36673
O	0.13318	0.59599	-0.89937
O	1.13745	-0.71588	0.80026
H	-1.37802	1.58799	0.28526
H	0.35413	1.92208	0.79704
H	-0.73026	-2.04534	-0.07119
H	-1.89946	-0.87203	-0.09492
H	1.85392	-0.21444	0.37931

val+03_64			
C	0.24390	-0.05962	0.33663
C	-0.90885	-0.96864	-0.02986
N	0.04452	1.24677	0.87440
O	0.50201	0.99762	-0.54573
O	1.33187	-0.69675	0.89694
H	-1.73093	-0.39367	-0.46459
H	-0.58688	-1.70562	-0.77631
H	-1.26589	-1.51036	0.85186
H	-0.95027	1.48328	0.76080
H	1.56435	-1.45271	0.33457

val+03_65			
C	-0.62742	0.40348	-0.16508
C	-0.01745	-0.91380	0.11805
N	0.51959	-0.08707	-0.94979
O	-0.43869	1.39256	0.80200
O	-0.58159	-2.10982	-0.32487
H	-1.55639	0.46240	-0.73183
H	0.56072	-0.98790	1.04274
H	1.37813	0.36736	-0.63752
H	-0.50660	2.25562	0.36298
H	-1.22020	-2.39473	0.34822

val+03_66			
C	-0.57589	-0.31484	0.28357
C	-1.14178	1.05603	0.14058
N	-0.04335	0.56806	-0.73498
O	-1.20555	-1.48043	-0.13377
O	1.23037	1.10877	-0.32393
H	0.06129	-0.49812	1.14404
H	-2.07981	1.23586	-0.38042
H	-0.86651	1.78621	0.89752
H	-1.40711	-1.37044	-1.07769
H	1.61385	1.37660	-1.17451

val+03_67			
C	0.03192	-0.24575	-0.09532
C	-0.45073	1.11915	0.17941
N	0.41316	0.80005	-1.00811
O	0.96580	-0.75290	0.80998
O	-0.75833	-1.22696	-0.67792
H	-1.46910	1.39703	-0.07837
H	-0.00758	1.65449	1.01622
H	1.37492	1.07649	-0.80953
H	1.42665	-1.47517	0.34821
H	-1.25740	-1.64733	0.04222

val+03_68			
C	0.37254	0.00458	0.26802
C	-0.43732	-1.18159	-0.18877
N	-0.33729	1.20589	0.73769
O	0.99574	0.74738	-0.81160
O	0.64764	1.97332	-0.02441
H	1.13243	-0.26985	1.01064
H	-1.18243	-0.88037	-0.93228
H	0.22214	-1.92928	-0.64242
H	-0.94182	-1.64761	0.66495
H	-1.18443	1.29012	0.15788

val+03_69			
C	0.38102	-0.13441	-0.22817
C	-0.50358	-1.25477	0.25555
N	0.62375	1.79997	0.29179
O	1.13252	0.51810	0.80434
O	-0.31806	1.06986	-0.57111
H	1.03967	-0.45441	-1.05108
H	-1.12949	-1.61699	-0.56777
H	0.11242	-2.08832	0.61142
H	-1.14397	-0.90490	1.06996
H	0.01931	2.12896	1.06125

val+03_6			
C	1.36848	-0.08898	-0.20078
C	-0.10452	0.05171	0.15582
N	1.87459	-0.88189	-1.05226
O	-0.52403	1.39607	0.04666

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O	-0.82849	-0.81096	-0.68611
H	2.02441	0.60254	0.33811
H	-0.26028	-0.19244	1.21624
H	1.12534	-1.45537	-1.46213
H	-0.34228	1.67792	-0.86667
H	-1.76402	-0.73981	-0.43987
val+03_70			
C	0.96588	0.27021	-0.10959
C	-1.40548	-0.29167	0.16398
N	0.00004	-0.69619	0.15007
O	0.69174	1.41684	-0.89328
O	0.91204	1.45893	0.60655
H	1.96035	-0.15444	-0.26125
H	-1.50533	0.58800	0.80214
H	-1.99936	-1.10225	0.59468
H	-1.79835	-0.04465	-0.83143
H	0.17747	-1.55967	-0.34997
val+03_71			
C	0.70139	0.45676	0.09427
C	-1.04828	-1.09089	-0.17172
N	0.50881	1.88650	0.09796
O	0.00111	-0.34130	-0.78045
O	1.72463	1.16894	-0.47527
H	0.88467	-0.00171	1.07110
H	-1.85650	-0.44001	0.18770
H	-1.43825	-1.75557	-0.94413
H	-0.67371	-1.69366	0.66707
H	-0.02747	2.08334	-0.75862
val+03_72			
C	0.43606	0.03803	-0.14505
C	-0.45052	1.28901	-0.08342
N	-0.02746	-1.23037	-0.55968
O	1.18533	0.70040	-1.21341
O	0.51627	1.99606	-0.88071
H	1.06701	-0.09002	0.74394
H	-1.40973	1.16859	-0.60933
H	-0.60966	1.76514	0.89014
H	-0.17301	-1.89027	0.19442
H	-0.82770	-1.19677	-1.18301
val+03_73			
C	0.85581	0.64236	-0.39252
C	0.01659	-0.24435	0.50098
N	-0.88813	-1.13544	-0.22279
O	0.23422	1.77721	-0.92300
O	1.32381	1.85422	0.11497
H	1.53853	0.13398	-1.08353
H	-0.56635	0.40642	1.16023
H	0.67901	-0.85059	1.13166
H	-0.37004	-1.77077	-0.82734
H	-1.50785	-0.59265	-0.82187
val+03_74			
C	0.87916	0.27254	-0.08738
C	0.63655	1.72176	-0.08494
N	-0.66878	-1.38135	-0.48986
O	1.56753	1.07432	0.82232
O	-0.02991	-0.58830	0.53808
H	1.45658	-0.21580	-0.87341
H	-0.26876	2.09630	0.39010
H	1.09478	2.37083	-0.83120
H	-0.62536	-2.32371	-0.09831
H	-1.65150	-1.10559	-0.42609
val+03_75			
C	0.44974	-0.42892	0.11002
C	0.41946	1.53565	-0.15043
N	-0.52019	-1.42916	-0.03270
O	0.70698	0.45068	-1.02429
O	0.01053	0.67273	0.91068
H	1.38475	-0.87883	0.47287
H	-0.38561	2.19270	-0.50931
H	1.31234	2.12597	0.10580
H	-0.15670	-2.27430	-0.46152

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H	-1.33689	-1.09501	-0.53753
val+03_77			
C	-0.88400	-0.00087	-0.07180
C	0.34454	-0.86227	0.31507
N	0.93304	1.33905	0.25933
O	-0.48781	1.33372	0.27299
O	1.27656	0.09063	0.84323
H	-1.10777	-0.07773	-1.14508
H	-1.78388	-0.23146	0.50324
H	0.76585	-1.37790	-0.55945
H	0.14303	-1.59137	1.10327
H	1.17796	1.22800	-0.74059
val+03_78			
C	-0.32189	1.15827	-0.52345
C	0.37679	-0.97230	-0.26692
N	-0.84088	-0.18365	-0.29452
O	1.10772	1.12551	-0.24045
O	1.32984	-0.16227	0.41684
H	-0.40492	1.45757	-1.57381
H	-0.83203	1.88562	0.11837
H	0.71665	-1.18106	-1.28878
H	0.26230	-1.89475	0.30706
H	-1.24346	-0.20965	0.64085
val+03_79			
C	0.15336	-1.04901	-0.11229
C	0.91188	1.09175	-0.07814
N	-0.94712	-0.07634	0.03237
O	1.26606	-0.24086	-0.44638
O	-0.22395	0.98537	0.73954
H	0.36246	-1.61270	0.81190
H	-0.07194	-1.73650	-0.93396
H	0.70296	1.67134	-0.98896
H	1.70675	1.55298	0.51572
H	-1.60167	-0.39122	0.75140
val+03_7			
C	0.65386	0.52720	-0.13436
C	-0.81749	0.52236	-0.46798
N	1.36734	-0.45816	0.25505
O	-1.36757	1.83258	-0.44081
O	0.60099	-1.64107	0.32916
H	1.18969	1.47015	-0.23694
H	-1.34846	-0.17156	0.19828
H	-0.96312	0.15328	-1.49045
H	-1.37809	2.12680	0.48304
H	1.24556	-2.27998	0.67090
val+03_80			
C	-0.13223	-0.12742	0.37561
C	0.14749	-1.42074	-0.38535
N	-0.38743	0.95949	-0.59397
O	-0.04950	2.21071	0.01629
O	0.86653	1.57085	-0.92991
H	-1.05617	-0.20737	0.96093
H	0.69161	0.15789	1.03742
H	-0.67089	-1.65937	-1.07187
H	1.07366	-1.34028	-0.96325
H	0.25712	-2.24937	0.32119
val+03_81			
C	-0.64890	1.06734	0.12273
C	0.29469	-1.18290	0.17869
N	0.00712	0.03798	0.93754
O	0.60674	1.63701	-0.28886
O	1.21058	0.89050	0.85801
H	-1.24842	0.70410	-0.72076
H	-1.21959	1.76324	0.74884
H	-0.63372	-1.76334	0.13446
H	0.65979	-0.98163	-0.83792
H	1.03912	-1.76189	0.72987
val+03_82			
C	1.05488	-1.39239	0.24550
C	-1.05670	1.39021	-0.09710

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N	0.27882	-0.44034	-0.50081
O	1.66481	-0.14894	0.05126
O	-0.66146	0.10485	0.38536
H	1.44859	-2.23550	-0.32559
H	0.71309	-1.61656	1.25696
H	-0.23227	2.10644	-0.00695
H	-1.38495	1.32919	-1.14025
H	-1.88751	1.69604	0.54232

val+03_83

C	-0.12577	1.39108	0.04499
C	-0.02552	-1.67250	0.13658
N	0.49489	-0.44733	-0.45803
O	-0.66842	0.39744	-0.81699
O	0.79278	0.48897	0.65109
H	-0.85895	1.80913	0.74860
H	0.38370	2.19260	-0.51216
H	-0.79453	-1.47352	0.89043
H	0.82620	-2.19696	0.58087
H	-0.43167	-2.27541	-0.68158

val+03_84

C	0.03977	0.18052	0.20883
C	-1.25624	-0.55189	-0.03852
N	1.18702	-0.63059	0.25397
O	-0.04395	1.31342	1.05856
O	0.21635	1.40378	-0.43093
H	-2.06890	0.17288	-0.10368
H	-1.19518	-1.12139	-0.97064
H	-1.46807	-1.24924	0.78016
H	1.99521	-0.10126	0.56870
H	1.06208	-1.46043	0.82505

val+03_8

C	0.45693	-0.29980	-0.04082
C	-1.84206	-0.42105	-0.24106
N	-0.51553	-0.48706	-0.82301
O	1.72927	-0.35359	-0.50074
O	-2.68361	0.44411	-0.97002
H	0.36187	-0.09067	1.03759
H	-1.80876	-0.13049	0.83006
H	-2.30916	-1.40926	-0.30787
H	2.33728	-0.16813	0.23085
H	-2.19353	1.27075	-1.10439

val+03_9

C	-0.63494	-0.81942	0.07634
C	1.57464	-0.21252	-0.35992
N	0.64150	-1.04320	-0.57563
O	-0.84020	0.45089	0.65910
O	-1.60413	-1.07521	-0.90600
H	-0.70071	-1.52198	0.91813
H	1.47137	0.67059	0.28161
H	2.54426	-0.38257	-0.83127
H	-0.92916	1.07544	-0.08293
H	-2.46614	-1.00431	-0.46492

val+05_100

C	1.14518	-0.47921	0.63387
C	-0.37819	1.13756	-0.08920
N	-1.65540	0.56795	-0.34416
O	0.75180	0.24808	-0.39704
O	2.12961	-1.25395	0.15169
H	-0.29455	1.41262	0.96331
H	-0.21504	2.00447	-0.73137
H	-1.81135	-0.24149	0.25251
H	-1.74297	0.26899	-1.31246
H	2.43359	-1.78361	0.90484

val+05_103

C	0.22520	0.31889	-0.21820
C	-1.25347	0.26605	-0.10457
N	1.01759	-0.72279	-0.21135
O	2.31719	-0.56540	-0.31740
O	0.85189	1.48551	-0.33820
H	-1.59244	0.82631	0.77476
H	-1.72376	0.71956	-0.98496

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H	-1.60077	-0.76811	-0.01593
H	0.63912	-1.66746	-0.12361
H	1.80984	1.17994	-0.38985

val+05_104			
C	0.22338	0.87738	-0.17132
C	-1.26990	0.92419	-0.17617
N	0.89812	-0.23234	-0.27620
O	2.12877	-0.43434	-0.28837
O	0.08702	-1.39885	-0.39626
H	0.84976	1.75414	-0.07996
H	-1.59990	1.96305	-0.09627
H	-1.68872	0.49959	-1.09667
H	-1.69963	0.36192	0.66218
H	0.78771	-2.07715	-0.46105

val+05_105			
C	0.63636	-0.48769	-0.24882
C	-0.97320	1.21415	0.27250
N	0.01502	0.59493	-0.63147
O	0.19170	1.18369	-1.75442
O	1.53816	-1.04469	-1.08906
H	0.42962	-0.92579	0.71875
H	-0.64228	2.23710	0.46301
H	-1.92697	1.24092	-0.25844
H	-1.07146	0.66154	1.21062
H	1.91205	-1.82816	-0.66108

val+05_106			
C	2.12962	-1.16358	0.46216
C	-0.85900	0.02065	-0.24326
N	-1.06313	-1.36284	0.11422
O	2.37478	-1.55462	1.50309
O	-0.28761	0.65017	0.89480
H	-0.17219	0.04087	-1.10279
H	-1.78365	0.56042	-0.53208
H	-1.83752	-1.45456	0.76811
H	-1.27328	-1.92014	-0.70940
H	-0.30512	1.60753	0.74025

val+05_107			
C	2.08606	-1.37127	-1.15766
C	-0.65894	0.97958	0.46507
N	-0.29865	-0.43586	0.40875
O	1.33141	-1.85139	-1.86793
O	-1.27628	-1.09814	-0.41748
H	-0.00944	1.46152	1.20489
H	-1.71068	1.15011	0.73707
H	-0.47221	1.43395	-0.51220
H	-0.46007	-0.84597	1.32965
H	-0.72670	-1.48543	-1.12036

val+05_108			
C	0.88886	-1.27894	-0.32623
C	-1.16360	-0.12295	0.36310
N	0.10088	-0.25534	-0.46703
O	0.24143	0.69780	-1.30110
O	-1.35149	1.20999	0.65745
H	0.66222	-2.01218	0.43530
H	1.74486	-1.36056	-0.98223
H	-1.95822	-0.55111	-0.26666
H	-1.05292	-0.70143	1.28269
H	-1.03901	1.66972	-0.15408

val+05_109			
C	0.43821	-0.09627	-0.16470
C	-0.89369	0.07558	0.49357
N	0.85139	-1.26593	-0.58504
O	0.27455	-2.39089	-0.48047
O	-1.55066	1.25779	0.04289
H	1.09578	0.74726	-0.34215
H	-1.48644	-0.83343	0.32907
H	-0.77948	0.20381	1.57684
H	1.76833	-1.27138	-1.06103
H	-1.77229	1.12486	-0.89218

val+05_10

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C	-0.86532	1.09402	-0.02538
C	-2.22117	0.55499	0.18967
N	-1.11393	-0.08339	-0.63480
O	0.02883	1.86292	0.25036
O	1.62273	-0.62838	0.14241
H	-2.44493	0.15804	1.18094
H	-3.08700	0.85127	-0.39772
H	2.14456	-0.69627	-0.67133
H	-0.56605	-0.90214	-0.36190
H	1.46907	0.33074	0.24106

val+05_110

C	1.40398	-1.26195	-0.12813
C	0.48037	-0.35544	0.14385
N	-0.85625	-0.42794	-0.40059
O	2.21425	-2.06608	-0.39837
O	-1.28576	2.04920	1.05526
H	0.71367	0.46866	0.81133
H	-0.86585	-0.48524	-1.41599
H	-1.40064	1.25924	0.48484
H	-1.38860	-1.21293	-0.03087
H	-1.07109	2.75467	0.42718

val+05_112

C	0.43239	-0.04370	0.19194
C	-0.16954	1.22157	-0.19323
N	-0.36812	-1.29278	0.06242
O	-0.97463	-1.59251	1.22609
O	0.84284	0.57278	-1.00998
H	1.14464	-0.15056	1.00560
H	-1.17344	1.23283	-0.61768
H	0.14775	2.14140	0.29383
H	0.28352	-2.03588	-0.27528
H	-1.01710	-1.14725	-0.74382

val+05_113

C	0.00672	-0.61350	0.23157
C	0.18172	-2.08528	-0.02214
N	-0.48720	3.27239	0.22909
O	-0.89018	4.05362	-0.60812
O	-0.21281	0.20841	-0.63525
H	0.09137	-0.30054	1.29468
H	-0.56629	-2.65033	0.54947
H	1.16571	-2.40876	0.34209
H	0.08492	-2.30610	-1.08725
H	-0.44187	2.30681	-0.20916

val+05_114

C	0.01553	-0.69142	-0.08719
C	1.04339	0.42624	0.04665
N	-1.12943	0.30259	-0.04918
O	-2.07745	0.21613	-0.84201
O	0.12252	1.45391	-0.30259
H	-0.03540	-1.12728	-1.08470
H	-0.08052	-1.46485	0.68185
H	1.88960	0.36251	-0.64882
H	1.44138	0.52909	1.06956
H	-1.36211	0.63206	0.90294

val+05_115

C	-0.99421	0.38877	0.18136
C	0.99996	0.44166	-0.24159
N	0.02868	-0.75267	-0.05469
O	0.24769	-1.65340	0.86453
O	-0.09193	1.34852	-0.36037
H	-1.93986	0.32215	-0.36411
H	-1.12777	0.44869	1.26589
H	1.64524	0.41729	-1.12437
H	1.55861	0.51992	0.69617
H	-0.16181	-1.14743	-1.00182

val+05_116

C	-0.49569	1.93646	0.21295
C	-0.10213	-1.51032	0.11938
N	0.52642	-0.54351	-0.81188
O	1.23559	-1.05478	-1.64840
O	-1.14958	1.49081	1.12772

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H	-0.91844	2.09597	-0.79949
H	0.56569	2.23510	0.32904
H	0.19113	-1.21396	1.13294
H	0.19174	-2.53704	-0.11469
H	-1.18582	-1.36193	0.04943

val+05_117			
C	-0.44582	-0.07779	0.28948
C	0.66596	0.85330	-0.21166
N	-0.08143	-1.38927	0.35731
O	-1.54726	0.35581	0.59135
O	1.81625	0.18264	-0.71816
H	0.22404	1.54440	-0.94028
H	1.00509	1.45312	0.63936
H	-0.71089	-2.03923	0.80652
H	0.89407	-1.63058	0.25131
H	1.60668	-0.12429	-1.61384

val+05_118			
C	0.50232	0.79255	0.25601
C	-0.60469	-0.24574	-0.00165
N	-0.02739	-1.58823	-0.16819
O	0.30499	1.98287	0.21376
O	1.68841	0.24300	0.55820
H	-1.25635	-0.23853	0.87889
H	-1.20745	0.10343	-0.84800
H	-0.62955	-2.30952	0.21820
H	1.53810	-0.73418	0.49585
H	0.11321	-1.80796	-1.15146

val+05_11			
C	0.47162	1.02701	0.11813
C	-0.89009	1.42049	-0.08162
N	1.36243	0.13886	0.14227
O	0.26561	2.34392	0.28771
O	-0.73704	-1.68092	-0.75575
H	-1.62295	1.29821	0.71156
H	-1.27527	1.57598	-1.08566
H	0.16542	-1.35460	-0.57167
H	2.28241	0.52506	0.37009
H	-0.92065	-2.26431	-0.00476

val+05_121			
C	-0.27627	1.33236	-0.14361
C	-0.79376	0.45463	0.98570
N	0.72028	-1.18513	-0.62557
O	-0.93752	1.57916	-1.12765
O	-0.29984	0.46883	2.09090
H	0.72399	1.77335	0.04922
H	-1.69649	-0.13505	0.72352
H	0.61409	-2.06259	-0.11907
H	1.72078	-1.03500	-0.74437
H	0.32823	-1.32335	-1.55557

val+05_122			
C	0.27967	-1.71025	-0.20243
C	-0.77895	2.37960	-0.15202
N	0.97271	-0.57432	0.08218
O	0.75267	-2.72613	-0.67939
O	-0.47553	1.92510	0.92913
H	-0.79921	-1.60476	0.03359
H	-0.50789	1.87323	-1.09806
H	-1.34341	3.32678	-0.24532
H	0.54437	0.19657	0.58720
H	1.97967	-0.59893	-0.01299

val+05_123			
C	0.30617	1.23009	0.07486
C	-0.18496	0.37750	-1.05475
N	-1.19408	-0.46801	-0.92534
O	-0.12065	2.22138	0.62401
O	1.27251	0.40611	0.22462
H	0.37366	0.34812	-1.98288
H	0.64288	-2.03773	2.34609
H	-1.77420	-0.43616	-0.09501
H	0.84688	-1.46844	1.91189
H	-1.29211	-1.28526	-1.51540

val+05_124			
C	0.18427	0.44469	-0.88659
C	-0.23094	1.27534	0.09573
N	0.28801	-1.71903	0.49623
O	-0.07322	-2.82448	0.08817
O	1.02158	-0.57476	-0.71215
H	-0.21548	0.55260	-1.90175
H	-0.96517	2.04853	-0.10345
H	0.19245	1.23249	1.09681
H	1.14678	-1.66731	1.06783
H	-0.43068	-1.00587	0.74248

val+05_125			
C	-1.05381	1.55421	0.34962
C	0.77949	-1.58273	-0.33983
N	-0.12591	-1.70713	0.54575
O	-0.15249	1.44602	-0.45873
O	-1.54601	0.59618	1.12232
H	-1.58227	2.50313	0.53502
H	0.91579	-0.59822	-0.78878
H	1.42456	-2.40270	-0.67376
H	-1.05430	-0.26770	0.94360
H	-0.19293	-2.65778	0.91899

val+05_127			
C	0.58272	0.37437	-0.21094
C	-1.70587	-0.12161	-0.13790
N	1.74758	-0.21273	-0.19220
O	2.85587	0.26032	0.22557
O	-0.45164	-0.26226	-0.81228
H	0.48244	1.37753	0.19057
H	-1.97108	0.93739	-0.02355
H	-2.44775	-0.61472	-0.76781
H	-1.67785	-0.59865	0.84922
H	1.74448	-1.16764	-0.59169

val+05_128			
C	1.55331	-2.12600	0.00636
C	-1.61829	1.20528	0.29045
N	0.43198	-1.72678	-0.22509
O	2.58625	-2.64604	0.23835
O	-0.63892	0.87016	-0.69673
H	-2.05556	2.19321	0.09812
H	-2.41993	0.45740	0.34802
H	-1.09547	1.23377	1.24842
H	-1.07865	0.82669	-1.55989
H	0.12319	-0.76248	-0.39332

val+05_129			
C	1.95857	-0.43490	0.11487
C	-1.56808	-0.29327	0.18501
N	0.75340	-0.16793	-0.29947
O	0.37179	0.37301	-1.34321
O	-0.25015	-0.59238	0.64867
H	2.07812	-0.91868	1.07059
H	2.77227	-0.15090	-0.53383
H	-1.71663	0.78165	0.05171
H	-2.20331	-0.66619	0.99111
H	-1.79688	-0.81301	-0.74923

val+05_12			
C	0.40919	0.85547	0.10780
C	0.58091	-0.66160	0.19080
N	-0.50659	1.27470	-0.80091
O	1.07318	1.59334	0.82171
O	-0.31266	-1.31833	-0.70149
H	0.40585	-0.94933	1.23715
H	1.63268	-0.88021	-0.04320
H	-1.02851	0.60414	-1.34570
H	-0.67886	2.26416	-0.90041
H	-0.15628	-2.27215	-0.64764

val+05_131			
C	1.53132	-0.28499	0.37488
C	-0.63062	2.32058	0.52717
N	-1.26561	-0.79540	0.00008

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O	1.96821	-1.40721	0.26026
O	-1.73766	2.57796	0.46049
H	1.22579	0.14298	1.35015
H	1.42281	0.40705	-0.48356
H	-1.97477	-0.89147	0.72575
H	-1.76967	-0.68458	-0.87877
H	-0.78451	-1.69202	-0.05456

val+05_132			
C	1.24215	1.92149	-0.19701
C	1.05935	-1.54750	-0.70517
N	-1.69182	0.57788	0.38046
O	0.78225	2.92569	0.07921
O	0.86260	-2.73138	-0.86302
H	0.26790	-0.84464	-0.37811
H	-1.93287	1.55188	0.55973
H	-2.34735	0.24735	-0.32652
H	-1.91738	0.06691	1.23299
H	2.05727	-1.08958	-0.88107

val+05_133			
C	1.08774	-0.63307	0.45861
C	-0.65986	1.02787	-0.25693
N	-0.30946	-0.39078	0.00310
O	1.82865	0.25612	0.77717
O	-0.84797	-0.88584	1.17368
H	1.26354	-1.71186	0.52424
H	-0.20544	1.36260	-1.19449
H	-1.74802	1.07704	-0.30173
H	-0.28507	1.60757	0.58361
H	-0.56390	-0.96344	-0.82005

val+05_134			
C	-0.10887	-0.77528	0.12169
C	1.37543	-0.48591	0.08963
N	-0.95099	0.33614	0.06368
O	-0.59657	-1.88432	0.25173
O	-0.44490	1.48632	-0.58793
H	1.91048	-1.41420	0.29357
H	1.64862	0.27222	0.83103
H	1.66574	-0.09728	-0.89195
H	-1.88200	0.11383	-0.28115
H	-0.44353	2.16428	0.10880

val+05_135			
C	-0.38343	-0.29491	0.01418
C	1.08287	-0.67816	-0.03030
N	-0.61467	1.20044	-0.08961
O	-1.78655	1.56368	-0.08734
O	0.36198	1.93839	-0.16466
H	-0.96469	-0.71893	-0.80863
H	-0.87399	-0.58238	0.94803
H	1.16474	-1.76753	0.04933
H	1.63726	-0.22624	0.79564
H	1.54818	-0.36235	-0.96725

val+05_136			
C	1.02110	-0.56814	-0.07730
C	-0.48970	-0.37708	-0.08922
N	-0.74957	1.09299	0.06515
O	1.75264	0.19493	-0.66691
O	-0.51430	1.48484	1.33270
H	1.41196	-1.45700	0.45436
H	-0.98873	-0.85475	0.75407
H	-0.89022	-0.75901	-1.04154
H	-1.71962	1.28781	-0.26160
H	-0.11965	1.55461	-0.62410

val+05_137			
C	0.03830	-0.05524	0.01281
C	1.26058	-0.45151	-0.25101
N	-1.02612	-1.08027	-0.22950
O	-0.73491	1.05238	0.46209
O	-2.15069	-0.63868	-1.01971
H	2.06035	0.26124	-0.01821
H	-1.42921	-1.46141	0.63709
H	-0.51402	-1.80825	-0.74277

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H	-0.13273	1.81143	0.46458
H	-2.14075	0.32042	-0.80567
val+05_139			
C	0.44137	-1.22085	-0.13483
C	1.61541	-1.39000	0.09410
N	-0.89637	-1.02824	-0.31895
O	-2.85759	0.44606	1.15111
O	-2.59303	1.28523	-0.00984
H	2.65507	-1.54008	0.26851
H	-1.13895	-0.13302	-0.74749
H	-2.17373	-0.24878	1.00102
H	-1.35188	-1.78935	-0.81729
H	-2.25630	2.08563	0.43044
val+05_13			
C	0.02001	-0.29982	0.29977
C	0.98266	0.85876	0.11426
N	0.46291	-1.48390	0.22528
O	2.28769	0.41686	-0.12484
O	-1.28358	0.00611	0.53921
H	0.61975	1.48056	-0.72334
H	0.94248	1.49138	1.01879
H	2.23182	-0.56058	-0.10798
H	-0.26799	-2.18397	0.36522
H	-1.40426	0.97050	0.55563
val+05_141			
C	-1.40275	0.32530	-0.05475
C	-0.39856	-0.55050	0.00326
N	-2.73432	-0.15002	0.20486
O	0.93985	-0.34855	-0.20956
O	1.19585	1.03249	-0.57179
H	-1.21230	1.36707	-0.30830
H	-3.16926	0.40776	0.93910
H	-3.31856	-0.02439	-0.62159
H	-0.55379	-1.59965	0.23975
H	1.62593	1.33989	0.24792
val+05_142			
C	0.24070	0.30453	-1.12456
C	1.24281	0.78656	-0.65396
N	-2.62052	-0.45920	0.35656
O	-0.79526	-0.28799	-1.67617
O	2.25907	1.49968	-0.16294
H	-2.19364	0.07313	1.11300
H	-1.50725	-0.40342	-0.97332
H	-3.51843	-0.02422	0.15226
H	-2.81106	-1.39305	0.71532
H	2.97007	0.88939	0.09441
val+05_143			
C	0.66815	0.86272	0.33196
C	1.25641	0.19745	1.15666
N	-2.32360	-0.39898	0.20766
O	-0.02150	1.61868	-0.46779
O	-0.59827	0.78919	-1.56160
H	1.90730	-0.34238	1.80371
H	-3.07856	0.15304	0.61103
H	-1.35812	0.37645	-1.03897
H	-1.62860	-0.54360	0.94089
H	-2.70842	-1.31187	-0.02876
val+05_144			
C	-0.44155	0.76885	-0.13259
C	-1.39580	-0.37907	-0.21192
N	0.80118	0.49425	-0.08675
O	-2.73516	0.05249	-0.37525
O	1.45957	-0.83049	-0.17903
H	-1.30665	-0.98653	0.71083
H	-1.13175	-1.04548	-1.04768
H	1.55192	1.17430	-0.06544
H	-2.71981	1.00907	-0.20968
H	1.09456	-1.31739	0.58210
val+05_145			
C	1.49854	-0.31551	-0.35562

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C	-0.88998	0.40447	0.33085
N	0.57142	0.43759	0.28709
O	1.00227	-1.37785	-0.99789
O	-1.47198	1.51436	-0.31255
H	-1.24996	-0.54753	-0.08488
H	-1.22677	0.45465	1.36907
H	0.96776	1.24769	0.74808
H	0.03026	-1.51805	-0.92225
H	-1.16917	1.51788	-1.23510

val+05_146

C	-0.80115	0.25016	-0.09306
C	-1.66963	-0.96468	0.05501
N	0.43064	0.10352	0.13996
O	1.38546	1.14247	0.04214
O	1.16922	-1.02414	0.59981
H	-2.28940	-0.83150	0.95152
H	-2.36722	-1.01614	-0.78816
H	-1.13233	-1.91728	0.14594
H	0.82549	1.85862	-0.31930
H	1.98652	-0.98904	0.06643

val+05_147

C	0.50118	-0.92753	0.27021
C	-1.17171	0.86104	0.21595
N	0.17455	0.34100	0.17079
O	1.87166	-1.00561	0.18084
O	1.10671	1.41322	0.00146
H	-1.27396	1.55837	1.05393
H	-1.39913	1.38799	-0.71652
H	-1.84285	0.01242	0.34506
H	2.09709	-1.94225	0.25571
H	1.95976	0.93575	-0.01163

val+05_148

C	1.78892	-1.14594	0.22814
C	-0.34758	-0.01730	0.01877
N	0.96004	-0.42527	-0.49314
O	-0.35752	1.27908	0.54178
O	-1.21567	-0.13591	-1.07962
H	2.69321	-1.28112	-0.40356
H	-0.58333	-0.68011	0.85361
H	1.10973	-0.09331	-1.45599
H	-0.14093	1.89054	-0.18377
H	-2.08628	0.17674	-0.78581

val+05_149

C	0.88116	1.25492	-0.13956
C	-1.20222	-0.00105	-0.20601
N	0.26875	0.14561	-0.01812
O	-1.72847	1.17307	-0.71016
O	0.83155	-1.09700	0.48677
H	1.94407	1.14012	0.10602
H	-1.61029	-0.27601	0.77705
H	-1.36442	-0.83902	-0.89887
H	-0.98908	1.82618	-0.63106
H	0.94135	-1.64752	-0.31126

val+05_14

C	-0.05677	0.66219	-0.06714
C	-2.03902	0.72978	-0.11259
N	-1.04487	-0.18089	0.45264
O	-0.96576	1.63138	-0.48194
O	1.13408	0.64204	-0.15489
H	-2.57782	0.36191	-0.99179
H	-2.71422	1.18058	0.61869
H	2.52261	-2.30675	0.56145
H	-1.02781	-1.18528	0.31736
H	2.27968	-1.61865	0.41562

val+05_150

C	0.63981	0.37108	-0.30700
C	-0.65079	-0.42302	-0.24448
N	1.50257	-0.08455	0.56277
O	-1.75173	0.43005	-0.45914
O	-0.78807	-1.11064	0.99483
H	-0.62214	-1.16092	-1.06617

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H	2.41588	0.34837	0.65294
H	1.29360	-0.84384	1.22104
H	-1.38583	1.32823	-0.52591
H	-1.67872	-1.49306	1.01872

val+05_151

C	-0.96286	0.45021	0.31145
C	-1.94175	-0.49820	-0.28609
N	0.25557	0.42424	0.20944
O	1.29295	-0.67906	-0.64377
O	2.55785	-0.20572	-0.20088
H	-2.42440	0.00205	-1.13457
H	-2.73378	-0.72927	0.43283
H	-1.47973	-1.42718	-0.64207
H	1.02500	1.00589	0.54295
H	2.77615	-0.84307	0.50491

val+05_152

C	1.40671	0.82043	-0.58515
C	-1.01925	1.20469	-0.10831
N	0.36838	1.60878	-0.43769
O	1.59083	-0.37477	-0.53042
O	0.12755	-1.48244	-0.21685
H	-1.34616	1.75744	0.77789
H	-1.67831	1.43884	-0.95035
H	-1.00733	0.13020	0.08372
H	0.54953	2.59582	-0.56196
H	0.64004	-2.02629	0.40663

val+05_153

C	0.61073	1.36590	-0.98261
C	-1.23260	-0.00661	-0.06602
N	1.54305	0.55931	-0.51078
O	-0.67085	1.14383	-0.76010
O	1.46090	-0.76015	0.14838
H	-0.92467	-0.01374	0.98242
H	-2.31324	0.13082	-0.13341
H	-0.93155	-0.93794	-0.54543
H	2.49181	0.70960	-0.82505
H	1.60792	-0.54652	1.08710

val+05_154

C	1.76962	0.13257	0.05755
C	-1.49363	-0.71022	0.32244
N	0.56850	0.40820	0.55385
O	-0.65346	0.31238	-0.22177
O	1.71214	-0.40051	-1.16056
H	-0.99108	-1.68417	0.32673
H	-2.37106	-0.74406	-0.32922
H	-1.81023	-0.46052	1.34344
H	0.44993	0.99296	1.37117
H	0.78147	-0.41114	-1.48661

val+05_155

C	0.12197	-1.39461	-0.45545
C	-1.16416	-1.00910	0.21127
N	1.04766	-0.48779	-0.26705
O	-1.22726	0.23394	0.95660
O	-1.35068	1.31441	-0.01926
H	-1.97644	-1.02682	-0.52634
H	-1.39148	-1.76903	0.97241
H	0.90137	0.38182	0.25776
H	1.97555	-0.61618	-0.65540
H	-2.23994	1.63955	0.20906

val+05_156

C	0.99681	0.24268	-0.89382
C	-1.10475	-0.71687	-0.04258
N	1.33667	0.31440	0.40001
O	-0.28578	-0.17161	-1.08518
O	-1.42611	0.19810	0.97694
H	-1.99557	-1.08684	-0.56074
H	-0.58200	-1.54205	0.45117
H	2.27648	0.62617	0.59890
H	0.70191	0.24343	1.19592
H	-1.89046	0.94698	0.56827

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val+05_157
C 0.87435 1.93342 0.92486
C -0.90196 0.38329 0.20463
N 0.45072 0.84160 0.47716
O 1.47971 -0.27334 -0.01442
O 1.12095 -1.54938 0.53199
H 1.96920 1.95279 0.99946
H -1.02725 0.24782 -0.87390
H -1.58904 1.14379 0.57285
H -1.07342 -0.56488 0.71687
H 0.76664 -2.00012 -0.25740

val+05_158
C 0.54748 0.89859 -0.39258
C -1.26530 -1.09822 -0.01855
N 0.88771 -0.15941 0.19893
O 0.04783 -1.25416 0.52467
O 2.14592 -0.53537 0.74670
H 1.43190 1.53615 -0.49812
H -1.75665 -0.21431 0.39596
H -1.77632 -2.01332 0.28844
H -1.23431 -1.01258 -1.10875
H 2.11153 -1.51166 0.74189

val+05_159
C 0.61968 -1.60998 -1.10945
C -0.95805 -0.45243 0.31806
N 0.38475 -0.91285 -0.02048
O -0.99916 0.92501 0.60397
O -0.73944 1.63877 -0.64028
H 1.71277 -1.81218 -1.10605
H -1.60271 -0.74099 -0.51598
H -1.29444 -0.90556 1.25940
H 1.08475 -0.60151 0.66503
H -1.61055 2.05632 -0.77203

val+05_15
C 0.55653 0.34760 -0.15278
C -0.80527 0.95961 0.08975
N 0.57537 -1.02498 -0.40435
O 1.60021 0.97475 -0.19914
O -0.48085 -1.78903 0.14713
H -0.69453 2.04441 0.11335
H -1.21611 0.60757 1.04170
H -1.51494 0.67415 -0.69372
H 1.47254 -1.45690 -0.19546
H -0.92045 -2.17061 -0.63149

val+05_160
C 1.53078 0.00042 -0.40783
C -1.36303 -0.36030 0.09486
N 0.93704 0.22451 0.67180
O -0.57080 0.13314 1.10974
O -1.60746 0.66210 -0.85630
H 0.87843 -0.31666 -1.22985
H -2.28860 -0.68813 0.59210
H -0.88955 -1.23534 -0.39056
H 1.33833 0.55600 1.54092
H -2.06774 0.26585 -1.61358

val+05_161
C 1.48603 -0.97091 0.09178
C -1.90497 -0.33516 0.05827
N 1.82690 0.29927 0.18163
O 0.37636 -1.35968 -0.23863
O -0.75251 0.01494 -0.63743
H -2.68446 0.38750 -0.23937
H -2.27148 -1.34070 -0.20425
H -1.79872 -0.27836 1.15560
H 1.09313 0.97897 -0.02368
H 2.74842 0.58323 0.47250

val+05_162
C 2.65754 -0.38038 0.11197
C -1.46548 0.27161 -0.34099
N 1.67976 0.28747 -0.27792
O -0.47551 1.30062 -0.34113

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O	0.52483	0.93711	0.60378
H	2.67730	-0.55092	1.19538
H	-1.91523	0.16689	0.65164
H	-2.21838	0.60896	-1.06001
H	-1.04465	-0.68877	-0.66273
H	1.41733	0.60592	-1.21068

val+05_17

C	0.50458	1.17660	0.06490
C	-1.01085	-1.00754	-0.08341
N	0.21738	-0.22045	-0.25621
O	0.21637	0.61775	-1.37037
O	1.32023	-1.08565	-0.17649
H	-0.46959	1.59799	0.38087
H	-1.85125	-0.33362	-0.23977
H	-1.01295	-1.42102	0.92672
H	-1.01277	-1.80964	-0.82458
H	2.01837	-0.43213	0.05664

val+05_18

C	1.05216	0.87726	1.04820
C	0.41056	-0.11194	0.19556
N	-0.06856	1.30513	0.02098
O	-0.48739	-0.95162	0.84569
O	-1.34721	-1.56102	-0.18663
H	2.00461	1.19642	0.61281
H	0.75256	-0.54814	-0.74937
H	-0.96872	1.53900	0.42981
H	0.08552	1.72438	-0.89675
H	-1.24864	-2.49448	0.07190

val+05_19

C	-0.24767	0.43749	0.73499
C	0.43513	-0.70215	0.01017
N	0.37133	1.35132	-0.31917
O	1.04466	0.28653	-1.01507
O	-0.29252	-1.71215	-0.57680
H	-1.33137	0.42827	0.56705
H	1.29426	-1.20379	0.46849
H	-0.23309	1.89094	-0.95844
H	1.09691	1.98549	0.03067
H	-1.14272	-1.32804	-0.85519

val+05_1

C	0.59237	2.76936	0.42889
C	0.99388	3.89834	0.56705
N	-0.27281	-0.45434	-0.16859
O	-1.15867	-0.92590	0.76996
O	-1.43227	-2.36654	0.48458
H	0.23803	1.76390	0.30347
H	1.34746	4.89696	0.69025
H	-0.69729	-0.57093	-1.09219
H	0.57355	-1.02876	-0.13268
H	-1.14636	-2.74900	1.33485

val+05_20

C	0.15144	1.10067	-0.12025
C	1.32694	-0.94171	-0.00121
N	0.14049	2.30321	-0.49224
O	1.29506	0.36416	-0.38435
O	0.44733	-1.54735	0.55192
H	-0.62069	0.52841	0.39444
H	2.30340	-1.35755	-0.28398
H	-2.91498	-1.85021	0.90314
H	-0.75233	2.73041	-0.23796
H	-2.17336	-1.85953	0.85068

val+05_21

C	0.35725	0.00331	-0.49232
C	-0.26909	1.13656	0.20601
N	0.67927	0.20566	0.87150
O	-1.68741	-1.28347	0.06825
O	-0.41402	-1.22189	-0.73884
H	1.09335	0.10547	-1.28793
H	-1.29205	0.99411	0.53577
H	0.05350	2.14282	-0.05671
H	1.61770	0.58669	0.97910

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H	-0.78511	-1.15836	-1.63723
val+05_23			
C	1.01223	1.20623	-0.38160
C	-0.81140	0.94134	-0.12397
N	0.39210	0.09349	-0.19668
O	0.03084	2.14642	-0.35126
O	-1.48441	-1.90032	0.55984
H	2.05915	1.45619	-0.53565
H	-1.52485	0.80510	-0.93765
H	-1.29327	0.97529	0.85329
H	-0.57258	-1.58934	0.40877
H	-1.66583	-2.45669	-0.21199
val+05_24			
C	0.21512	1.81786	0.78793
C	-0.47114	-0.56427	-0.27210
N	0.45981	0.36565	0.41352
O	0.96591	1.34135	-0.47066
O	-1.18592	-1.32972	0.64976
H	-0.81867	1.96423	0.39662
H	-1.16137	0.08089	-0.81628
H	0.11345	-1.17119	-0.97669
H	1.20481	-0.08978	0.94405
H	-0.69842	-2.14531	0.84025
val+05_25			
C	-0.24629	-1.39539	0.37855
C	0.91352	2.39279	-0.19712
N	0.45683	-0.36819	0.16065
O	2.10915	2.52872	-0.31845
O	-1.58880	-1.27445	0.51204
H	0.12799	-2.42374	0.47628
H	0.24103	2.22817	-1.06201
H	0.40427	2.44169	0.78559
H	1.44340	-0.61413	0.08455
H	-1.97329	-2.14887	0.67371
val+05_26			
C	-0.02961	1.65706	-0.02179
C	-0.39307	-2.66153	0.62012
N	-0.50910	-1.41451	0.41423
O	1.07943	1.20185	0.14548
O	-0.29138	2.95610	-0.24599
H	-0.95450	1.06744	-0.01106
H	0.55565	-3.19049	0.78676
H	-1.29245	-3.28425	0.63849
H	0.40357	-0.94414	0.42088
H	0.56835	3.42118	-0.24311
val+05_27			
C	-1.14828	-1.76307	0.42921
C	0.29166	2.42697	-0.31887
N	-0.51369	-0.68630	0.17656
O	1.34261	1.84684	-0.50256
O	0.82518	-0.92175	-0.11458
H	-0.67420	-2.74532	0.41306
H	-2.20331	-1.66979	0.66738
H	0.22665	3.52837	-0.41114
H	-0.62993	1.88215	-0.05527
H	1.16600	-0.01740	-0.28098
val+05_28			
C	0.74401	0.84055	-0.40955
C	0.73501	-0.64536	-0.20680
N	-0.79280	1.26474	0.14055
O	1.30192	0.17354	0.77624
O	-0.45809	-1.31413	0.15067
H	1.42485	-1.28850	-0.75763
H	-0.65956	1.94035	0.89166
H	-1.32214	0.44892	0.48063
H	-1.28064	1.71839	-0.63103
H	-0.23276	-1.98179	0.81897
val+05_29			
C	0.59988	0.85626	-0.23574
C	-0.82644	1.16176	-0.45156

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N	-0.30754	0.72105	0.88069
O	1.25387	-0.24289	-0.83134
O	0.29996	-1.33739	-0.97440
H	1.36338	1.62968	-0.16658
H	-1.40158	0.44956	-1.03663
H	-1.17633	2.19085	-0.49099
H	-0.53298	-0.26653	1.00672
H	0.80308	-2.03566	-0.51896

val+05_2			
C	-0.34984	0.28537	0.28883
C	0.78974	1.11163	0.46432
N	-0.03229	-0.93913	-0.26733
O	1.93300	0.76754	0.11003
O	0.08677	-2.22642	0.67402
H	-1.36680	0.48663	0.58995
H	0.61175	2.11060	0.90550
H	-0.68103	-1.35468	-0.93315
H	0.93451	-0.84962	-0.62960
H	0.44129	-1.80152	1.47841

val+05_30			
C	0.62994	1.00162	-0.01342
C	-0.76355	1.43168	0.25463
N	-0.27562	0.12410	0.75543
O	-0.67826	-0.91425	-0.17757
O	-1.93410	-1.41183	0.30312
H	1.46630	1.38935	0.56135
H	0.86530	0.67359	-1.02223
H	-1.47305	1.38722	-0.56539
H	-0.98326	2.14934	1.04024
H	-1.63980	-1.97552	1.04495

val+05_31			
C	0.83677	-0.71586	0.27251
C	2.08595	-1.08555	0.42534
N	-0.35219	-0.40615	0.22504
O	-3.15887	-0.10571	0.52903
O	-2.86850	0.57938	-0.72310
H	2.81473	-0.40406	0.85009
H	2.40949	-2.07297	0.11505
H	-0.69832	0.04904	-0.62718
H	-2.24581	-0.37316	0.78123
H	-3.11387	1.48904	-0.47833

val+05_32			
C	-1.37134	0.97928	-0.30746
C	-0.08172	0.64462	-0.52160
N	-2.04806	-0.31707	0.27698
O	0.42264	-0.65164	-0.39824
O	1.39850	-0.69905	0.74777
H	0.64182	1.37057	-0.88853
H	-2.47460	-0.07675	1.17282
H	-2.80340	-0.61111	-0.34393
H	-1.37653	-1.09564	0.39722
H	2.21880	-0.83071	0.23877

val+05_33			
C	-0.92200	1.61364	0.05847
C	0.54834	1.18346	0.10975
N	0.15099	-0.14908	-0.51276
O	-1.03875	0.38939	-0.98891
O	-0.03888	-1.23200	0.40360
H	-1.42542	1.17593	0.94803
H	1.18720	1.66241	-0.64557
H	1.10304	1.06415	1.04642
H	0.71452	-0.58663	-1.26149
H	-0.69845	-0.83618	1.01637

val+05_34			
C	-0.55812	0.24791	0.27564
C	-1.29317	-1.95673	0.04350
N	0.65214	-0.02646	0.12847
O	-1.64312	-0.70779	0.24610
O	1.02586	2.84109	0.57849
H	-0.94968	1.24514	0.44788
H	-2.27762	-2.47812	0.06488

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H	0.75808	-1.04431	-0.01501
H	1.33309	1.91941	0.49104
H	1.22446	3.22897	-0.28669

val+05_35			
C	-1.16897	0.95166	-0.15119
C	0.13743	1.21920	-0.25702
N	-1.01368	-1.36369	0.25861
O	-1.81351	-0.24382	-0.23223
O	1.09494	0.26890	-0.57476
H	-1.87705	1.76729	-0.03669
H	0.47993	2.24836	-0.16896
H	-0.27261	-1.46700	-0.44082
H	-1.67154	-2.12675	0.08828
H	1.82248	0.33306	0.06417

val+05_36			
C	-0.27322	1.30050	-0.37013
C	0.56034	0.05867	-0.20035
N	-0.17725	-1.25188	-0.02925
O	-0.69744	-1.68210	-1.19536
O	-1.50635	1.01600	0.00600
H	1.22868	0.25633	0.65617
H	1.17573	-0.08873	-1.09189
H	0.49051	-1.92747	0.40290
H	-0.90299	-1.09192	0.69895
H	-2.04731	1.81970	-0.08934

val+05_37			
C	0.85232	0.55659	-0.42337
C	-1.98554	1.26707	0.93860
N	2.03575	0.48163	-1.03989
O	-1.92259	0.07378	1.16916
O	0.54205	-0.67602	0.01719
H	-2.85946	1.85969	1.27506
H	2.56299	-0.38915	-1.12821
H	2.43777	1.31428	-1.44073
H	-1.17595	1.77988	0.39173
H	-0.32715	-0.59626	0.46466

val+05_38			
C	-0.68745	0.85024	0.06356
C	0.49488	0.25684	0.24951
N	0.67083	-1.06696	-0.25555
O	-0.93195	2.12996	0.47112
O	1.18807	-1.90376	0.82644
H	1.30870	0.75294	0.77877
H	-1.49106	0.32364	-0.44845
H	1.45650	-1.08498	-0.90529
H	-1.84836	2.35818	0.26360
H	0.40874	-2.43521	1.05509

val+05_39			
C	-1.57282	0.25488	0.16832
C	-0.29476	-0.05604	-0.15201
N	-0.13199	-1.53737	-0.27529
O	-1.84645	1.57621	0.40870
O	0.92211	0.63098	-0.18892
H	0.17779	-1.88954	-1.19253
H	0.47799	-1.96035	0.43781
H	-1.12993	-1.78497	-0.09866
H	-1.02156	2.10751	0.39282
H	1.04893	0.99149	-1.08367

val+05_3			
C	-0.77805	-0.39727	0.20868
C	0.56065	-0.38022	0.08482
N	1.20287	-1.71384	0.25806
O	-1.67604	0.43970	0.13769
O	-1.07704	2.10152	-0.25523
H	1.23268	0.43647	-0.14169
H	0.41313	-2.34900	0.45166
H	1.86353	-1.77335	1.04577
H	1.69652	-2.06288	-0.57572
H	-1.68865	2.52337	0.37327

val+05_40

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C	-0.96499	1.56076	-0.36270
C	-0.02876	0.90990	0.33568
N	-0.13572	-0.53571	0.04812
O	0.92319	-1.08281	-0.78058
O	-0.15162	-1.36606	1.18479
H	-0.91129	2.65060	-0.22523
H	0.79461	1.09515	1.02769
H	-1.03091	-0.56403	-0.48835
H	1.14375	-0.31484	-1.34522
H	-0.01327	-2.26617	0.82898

val+05_41

C	-0.35478	0.81029	-0.21283
C	-1.50633	1.47893	-0.18893
N	-0.15924	-0.57863	0.02957
O	0.85202	1.40981	-0.46578
O	-1.38778	-1.27943	0.20697
H	-1.50227	2.55763	-0.27886
H	-2.44419	0.94952	-0.09733
H	0.27652	-1.01294	-0.78581
H	1.51835	0.97240	0.09308
H	-1.36599	-1.51598	1.14862

val+05_42

C	0.19972	-0.17978	-0.81361
C	-0.88084	0.46959	-0.07384
N	-0.18351	-0.77877	0.45335
O	-0.77212	1.59603	0.73576
O	-0.73718	-2.11503	0.43031
H	1.19521	0.26702	-0.81246
H	-1.92975	0.29199	-0.30895
H	0.27298	-0.68000	1.36154
H	0.10718	1.97990	0.58285
H	-0.60049	-2.31785	-0.52014

val+05_43

C	0.28257	0.61719	1.06861
C	-0.41119	1.17913	-0.16504
N	0.03048	-0.20896	-0.08539
O	0.95048	-0.59322	-1.09349
O	-0.89253	-1.29770	0.06316
H	1.34637	0.85480	1.12895
H	-1.49271	1.31439	-0.14910
H	0.09744	1.72256	-0.96636
H	1.43705	-1.32863	-0.67325
H	-1.00507	-1.25555	1.03800

val+05_44

C	-0.03085	-0.29560	-0.37055
C	0.52991	0.79839	-1.13855
N	-0.46941	1.08275	0.08820
O	0.57829	-0.97616	0.70628
O	-1.02575	-1.07732	-0.91814
H	1.52660	1.05540	-0.75577
H	-1.39024	1.41726	-0.17846
H	-0.18055	1.32918	1.03395
H	1.51372	-1.08445	0.47666
H	-1.29232	-1.71044	-0.22924

val+05_45

C	-0.16588	0.53809	0.24869
C	-0.17461	-0.80680	0.21722
N	-1.30694	1.32612	0.34182
O	0.96281	1.30353	0.14351
O	-1.36691	-1.49120	0.47080
H	0.72774	-1.39872	0.07605
H	-2.09507	0.77807	0.67006
H	-1.16169	2.15533	0.90904
H	1.73118	0.71187	0.14188
H	-1.70512	-1.83497	-0.37238

val+05_46

C	0.49005	-0.47197	0.37966
C	-0.80553	0.26377	0.40516
N	-0.18307	-0.09924	-0.85988
O	0.49298	-1.84365	0.65697
O	-0.91905	1.62533	0.67137

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H	1.43389	0.04571	0.56340
H	-1.67892	-0.28937	0.74791
H	-0.61817	-0.91240	-1.29550
H	0.59282	-1.95758	1.61583
H	-0.49541	2.07782	-0.07712

val+05_47

C	0.54333	0.10670	0.27714
C	-0.53391	0.91863	-0.35568
N	-0.62224	-0.56284	-0.26485
O	1.77528	-0.16635	-0.30352
O	-1.51485	-0.96827	0.79460
H	0.61767	0.14464	1.36025
H	-1.18401	1.48172	0.30931
H	-0.44215	1.29778	-1.37130
H	1.59618	-0.59019	-1.15908
H	-2.03410	-1.66311	0.35883

val+05_49

C	0.91165	-0.37673	0.39323
C	2.21250	-0.36695	0.43947
N	-0.35393	-0.37425	0.31473
O	-2.72170	-0.00395	-0.88538
O	-1.21489	-0.76865	1.21119
H	2.76283	0.49190	0.82315
H	2.80014	-1.22206	0.10610
H	-0.81465	-0.02542	-0.55373
H	-3.11713	0.85631	-0.67820
H	-2.59063	-0.42370	-0.00028

val+05_4

C	-0.19157	1.30131	1.25159
C	0.41556	1.54417	-0.02818
N	-0.80466	0.18838	1.50908
O	1.46813	1.02268	-0.42729
O	0.30387	-1.54228	-0.37528
H	-0.04241	2.38813	-0.58828
H	-0.81900	-0.60528	0.84379
H	0.08172	-1.64334	-1.31325
H	-1.15060	0.00476	2.44825
H	0.98687	-0.83524	-0.36833

val+05_50

C	0.15222	0.14674	0.35906
C	1.42534	0.28713	0.05244
N	-1.08210	0.05149	0.45878
O	2.29666	-0.71611	-0.31379
O	-3.59244	-0.27029	-1.12241
H	1.90853	1.25358	0.13667
H	-1.41365	-0.14949	1.41152
H	-2.68714	-0.15031	-0.77781
H	1.79205	-1.51737	-0.52591
H	-3.84978	0.62204	-1.39606

val+05_51

C	-0.98648	0.31814	-0.50603
C	0.28178	0.06467	-0.15319
N	-1.75178	-1.00584	-0.26749
O	1.27611	1.01472	-0.17534
O	0.81098	-1.15014	0.27324
H	-2.60721	-0.81141	0.25663
H	-1.20357	-1.72457	0.23955
H	-2.04684	-1.41044	-1.16014
H	0.81608	1.83861	-0.41307
H	1.58493	-0.94873	0.82505

val+05_52

C	0.33426	-0.73617	0.30793
C	-0.76609	-1.50287	0.28847
N	0.42470	0.56006	-0.17579
O	0.23243	2.37287	1.31295
O	0.91351	3.33507	0.92770
H	1.24890	-1.08532	0.78085
H	-0.76095	-2.48173	0.75250
H	-1.69422	-1.17066	-0.16948
H	-0.33024	0.89126	-0.76353
H	1.33562	0.89240	-0.46308

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val+05_53
C -0.62983 -0.13681 0.01132
C 0.00420 1.04450 -0.01324
N 0.08965 -1.38749 0.08007
O 1.31841 1.34611 0.00016
O 2.21789 0.21740 -0.19724
H -1.71817 -0.13465 -0.01078
H -0.55715 1.97581 -0.02392
H -0.14016 -1.99688 -0.70437
H 1.62568 -0.56956 -0.00911
H -0.13972 -1.89803 0.93211

val+05_54
C -0.87756 1.21641 -0.23594
C 0.65117 1.16913 -0.35094
N -0.13717 -1.29313 0.35053
O -1.61498 1.19313 -1.19285
O 1.23451 1.10438 -1.40710
H -1.24977 1.30928 0.80799
H 1.18016 1.23539 0.62513
H -0.90213 -1.70973 0.87918
H 0.72198 -1.74727 0.65678
H -0.27611 -1.55089 -0.62559

val+05_55
C -0.00792 0.03102 0.23977
C -1.25645 0.44422 0.00459
N 0.53515 -1.25263 0.02167
O 0.91567 0.89689 0.76576
O 2.08947 0.97071 -0.12992
H -2.05070 -0.25906 -0.22227
H -1.49612 1.49852 0.05834
H -0.09257 -1.87448 -0.47619
H 2.21352 0.01732 -0.32663
H 0.86123 -1.68991 0.88198

val+05_56
C 0.20453 0.33701 0.08696
C -0.03057 1.64962 0.04871
N -0.37378 -1.89207 -0.34648
O -0.62918 -0.51530 -0.65167
O 1.19956 -0.26141 0.75897
H -0.86098 2.03756 -0.52545
H 0.62297 2.32872 0.57882
H -1.25763 -2.23497 0.03384
H -0.25662 -2.32389 -1.26331
H 1.04040 -1.22776 0.65092

val+05_57
C 0.32345 0.17211 0.66132
C -0.02386 1.21744 -0.09591
N 0.56487 -1.17958 0.60908
O 0.40745 0.99100 1.83567
O 0.02281 2.12060 0.97204
H -0.28113 1.51158 -1.10066
H 0.28252 -2.39266 -1.89927
H -0.08511 -1.74073 1.15409
H 0.21959 -2.76033 -2.54341
H 1.52231 -1.44114 0.83105

val+05_58
C 0.46298 0.84973 0.20123
C 0.72737 -0.45828 -0.19531
N -0.39280 -1.40890 -0.04637
O -0.91710 0.99843 0.57013
O 1.19139 1.83582 0.25798
H 1.69854 -0.87475 -0.40066
H -0.28002 -2.12381 0.69016
H -0.99636 1.94081 0.79075
H -1.19366 -0.81124 0.22285
H -0.64615 -1.91152 -0.90797

val+05_59
C -0.07550 0.65561 0.54831
C 0.07982 2.10165 0.77715
N -0.25236 -2.30410 -0.14855

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O	1.15437	2.64225	0.99794
O	-0.01631	0.27944	-0.68866
H	-0.89300	2.63352	0.93487
H	-1.09402	-2.82587	-0.38411
H	-0.10948	-0.74282	-0.68603
H	0.54638	-2.91823	-0.29420
H	-0.29280	-2.07355	0.84469

val+05_60			
C	-0.05289	-0.70555	0.00911
C	-1.48086	-0.29417	-0.04859
N	0.88546	0.18528	0.16080
O	0.68233	1.50304	0.27615
O	1.94277	2.11704	0.41889
H	0.28835	-1.73026	-0.06750
H	-1.64865	0.40942	-0.87570
H	-2.12951	-1.16185	-0.18090
H	-1.77025	0.23372	0.87060
H	1.90073	0.02953	0.21403

val+05_61			
C	-0.13580	1.23813	-0.48770
C	-0.33172	-1.23630	0.03316
N	0.53183	-0.03809	-0.12871
O	0.25420	1.93041	-1.38697
O	1.05035	0.41362	1.06032
H	-0.92591	1.44933	0.24264
H	-1.14839	-0.95826	0.70046
H	0.28197	-1.99867	0.51572
H	-0.70776	-1.57760	-0.93687
H	1.25954	-0.21647	-0.84084

val+05_62			
C	0.72395	1.40439	-0.69630
C	-0.97090	-1.20776	-0.02167
N	0.97330	0.07903	-0.07256
O	1.58136	1.10382	0.60453
O	0.08927	-0.65624	0.76871
H	-0.25088	1.66959	-0.23611
H	-1.55069	-0.41909	-0.51335
H	-0.59245	-1.91773	-0.76946
H	-1.59821	-1.73963	0.69552
H	1.63884	-0.57429	-0.49662

val+05_63			
C	0.14458	0.08311	-0.11032
C	0.40496	-1.37621	0.05595
N	-1.03350	0.63269	-0.34166
O	1.14812	0.88926	-0.02257
O	0.76923	2.25443	-0.19881
H	-0.16149	-1.77805	0.90394
H	1.47055	-1.53348	0.23407
H	0.10803	-1.92921	-0.84260
H	-1.89243	0.11488	-0.43110
H	-0.89605	1.66497	-0.40799

val+05_65			
C	0.56452	-0.45449	-0.17222
C	-0.96555	1.30154	0.13803
N	0.90933	-1.70650	0.26440
O	-0.48444	0.01719	0.55343
O	1.09095	0.13864	-1.09280
H	-0.17872	2.05645	0.21942
H	-1.31778	1.26753	-0.89656
H	-1.78986	1.53541	0.81323
H	1.80327	-2.05208	-0.04988
H	0.58160	-2.01211	1.16893

val+05_69			
C	-0.58821	-1.75654	0.10444
C	1.06520	1.95319	-0.38608
N	-0.13020	-0.54807	-0.00823
O	1.79536	1.11189	-0.89232
O	-0.65894	0.53145	0.41340
H	-0.00279	-2.56245	-0.31667
H	-1.53096	-1.91331	0.61110
H	0.29722	2.49265	-0.96837

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H	1.20431	2.30506	0.65160
H	0.77941	-0.40088	-0.49778
val+05_6			
C	0.07630	-0.37432	-0.11628
C	0.96619	0.62635	-0.06947
N	0.53277	-1.71279	-0.00697
O	2.31045	0.42726	0.08009
O	-1.29340	-0.23569	-0.26544
H	0.70025	1.67621	-0.14542
H	0.10041	-2.17647	0.79273
H	2.41162	-0.54400	0.13587
H	0.26923	-2.25172	-0.83253
H	-1.50803	0.70926	-0.33107
val+05_70			
C	1.03116	0.80189	-0.02639
C	-0.83984	-1.12996	0.31646
N	0.31680	-0.49257	-0.45193
O	0.21959	1.76737	0.50699
O	1.20910	0.95286	1.32299
H	1.84322	1.12234	-0.69140
H	-0.43442	-1.26820	1.32895
H	-1.58374	-0.32320	0.38268
H	-0.00914	-0.33283	-1.40930
H	1.04899	-1.20301	-0.53845
val+05_71			
C	1.09148	-0.48262	0.49251
C	-1.33277	-0.49974	-0.02922
N	-0.03784	0.10468	0.24633
O	-0.09232	1.48101	0.15981
O	1.13990	2.03611	0.35518
H	1.93051	0.19213	0.61646
H	1.11323	-1.56088	0.55633
H	-2.09735	0.22550	0.25292
H	-1.41903	-0.73342	-1.09398
H	-1.44152	-1.40829	0.56586
val+05_72			
C	-0.86716	-0.37706	0.33430
C	0.42099	-1.12162	0.07241
N	-0.88201	0.89154	0.43513
O	1.57980	-0.33365	0.21955
O	1.56918	0.65793	-0.84328
H	-1.76551	-1.00941	0.40274
H	0.53535	-1.93037	0.80765
H	0.37464	-1.58234	-0.92776
H	-1.82686	1.24671	0.60328
H	0.92027	1.28638	-0.45384
val+05_73			
C	1.42303	1.29575	0.41982
C	-1.77958	-0.58332	0.30020
N	-0.90019	-1.04943	-0.61511
O	1.64179	0.49266	-0.46695
O	-1.57247	0.33815	1.07942
H	2.19658	2.03036	0.71967
H	-2.74361	-1.12833	0.28471
H	0.45583	1.31951	0.95071
H	0.02619	-0.62571	-0.69511
H	-1.14868	-1.81664	-1.22175
val+05_74			
C	-1.45640	-0.58855	-0.08956
C	1.81298	1.17400	-0.18360
N	-0.42509	-1.46308	-0.08892
O	-1.35343	0.63120	-0.11720
O	2.16147	0.00895	-0.16537
H	-2.44355	-1.08993	-0.06177
H	0.74643	1.45726	-0.17100
H	2.56462	1.98769	-0.21359
H	0.53654	-1.11842	-0.11311
H	-0.59506	-2.45752	-0.06517
val+05_76			
C	-0.62070	0.95798	-0.25626

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C	-0.51090	-0.41576	0.38509
N	0.88390	-0.95164	0.17067
O	-1.68952	1.47405	-0.49325
O	1.81446	-0.12799	0.68999
H	0.35033	1.44337	-0.46713
H	-1.27764	-1.09497	-0.00864
H	-0.60773	-0.32345	1.47029
H	1.00149	-1.10880	-0.85415
H	0.91201	-1.90850	0.57730

val+05_77

C	-1.20197	0.22748	0.01832
C	0.22090	0.75578	0.13600
N	1.19031	-1.34064	0.05468
O	-2.10959	0.59549	0.72731
O	1.15528	-0.03519	-0.57304
H	-1.35124	-0.50870	-0.80229
H	0.48226	0.86367	1.19745
H	0.26884	1.74876	-0.33122
H	2.11776	-1.37560	0.48775
H	1.24506	-1.97055	-0.74757

val+05_78

C	0.11898	0.66660	-0.66270
C	-0.42832	-0.57587	0.01510
N	0.54937	-1.66117	0.05287
O	-0.52055	1.42688	-1.35234
O	1.42273	0.87780	-0.35186
H	1.68070	1.69921	-0.81091
H	-1.30294	-0.88769	-0.56159
H	-0.79950	-0.24159	1.00400
H	1.36944	-1.36467	0.57748
H	0.15140	-2.45709	0.54705

val+05_79

C	-1.23421	0.71635	0.77535
C	0.88321	0.29870	-0.16547
N	0.62022	-0.98443	-0.74019
O	-0.32544	1.11939	-0.11966
O	-1.13120	-0.23319	1.51827
H	-2.10409	1.39070	0.74365
H	1.55436	0.86988	-0.80734
H	1.27584	0.27361	0.85760
H	0.39429	-1.67721	-0.03476
H	1.37983	-1.31110	-1.32575

val+05_7

C	0.60637	0.22567	-0.06610
C	-0.33304	-0.73152	-0.16321
N	0.15130	-2.08017	-0.00049
O	1.90751	-0.06095	0.16684
O	0.36157	1.54740	-0.18716
H	-1.37460	-0.48982	-0.35033
H	-0.29563	-2.55148	0.78507
H	1.90552	-1.04600	0.22639
H	-0.03008	-2.65064	-0.82549
H	1.20938	2.00721	-0.07501

val+05_80

C	1.10862	-0.11341	-0.45455
C	0.24655	1.13607	-0.23530
N	-1.21488	-0.95578	0.58251
O	2.00725	-0.43648	0.28577
O	0.40005	1.89200	0.69476
H	0.85658	-0.68044	-1.37753
H	-0.51333	1.30619	-1.02939
H	-2.17797	-0.62403	0.60600
H	-0.84217	-0.85046	1.52513
H	-1.24611	-1.95515	0.38640

val+05_81

C	-0.86314	-0.85692	0.31855
C	-1.08707	0.63867	0.15546
N	1.60688	0.22497	-0.22115
O	-1.13047	-1.64855	-0.55753
O	-1.14375	1.39176	1.10205
H	-0.50548	-1.15336	1.32639

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H	-1.25914	0.95818	-0.89351
H	2.14154	-0.63591	-0.32493
H	1.99107	0.72577	0.57841
H	1.80036	0.79169	-1.04522

val+05_82

C	1.08211	0.53611	0.67503
C	0.49662	-1.28273	0.83365
N	-1.13523	0.58193	-1.20805
O	0.26334	0.01713	1.53446
O	1.51013	-0.51379	0.04822
H	1.16974	1.57332	0.37814
H	1.04944	-1.92995	1.52861
H	-2.09281	0.87496	-1.01864
H	-1.07493	0.44381	-2.21601
H	-1.03282	-0.34530	-0.78731

val+05_83

C	-0.29016	0.88408	-0.18233
C	0.25181	-1.49609	0.05241
N	0.66447	-0.12523	-0.24678
O	-1.08757	0.95985	0.95230
O	-1.66480	0.63601	-0.41218
H	0.07082	1.83486	-0.57984
H	-0.30073	-1.49267	0.99354
H	1.14626	-2.11229	0.17715
H	-0.38710	-1.93860	-0.72360
H	1.25780	-0.04031	-1.06399

val+05_84

C	-0.54184	0.63146	-0.17222
C	0.81232	0.96114	0.35733
N	0.63803	0.00511	-0.73643
O	0.42639	-2.13138	-0.04034
O	-0.69761	-2.20561	0.48217
H	-1.17357	-0.05935	0.39272
H	-1.07871	1.36624	-0.76821
H	1.24550	1.93395	0.13262
H	1.13812	0.51359	1.29251
H	0.90538	0.34455	-1.65824

val+05_85

C	-0.58292	1.49743	-0.40742
C	1.11213	-1.69051	0.66297
N	-1.27800	0.36644	-0.95560
O	0.16258	0.68179	-1.27007
O	0.00099	-1.50454	1.11257
H	-0.87536	2.47244	-0.79887
H	-0.28275	1.48474	0.64280
H	1.45487	-1.19725	-0.26265
H	1.83214	-2.36359	1.17005
H	-1.17556	-0.38884	-0.26347

val+05_86

C	0.20678	-0.85628	-0.65948
C	0.52931	0.55444	-0.23485
N	-0.72240	1.27297	0.00802
O	1.21100	-1.81487	-0.54027
O	-0.00145	-1.79872	0.35315
H	1.05429	1.04522	-1.06412
H	1.22455	0.49626	0.61711
H	-0.54369	2.27024	0.09525
H	-0.45224	-0.95552	-1.52602
H	-1.12605	0.97176	0.89310

val+05_88

C	0.29161	-0.17544	0.44555
C	-0.58983	0.89463	-0.15034
N	0.42138	-1.34322	-0.32612
O	1.40199	0.28753	1.19737
O	0.19817	-0.39160	1.81721
H	-0.16973	1.25974	-1.09461
H	-1.58816	0.49331	-0.34831
H	-0.66156	1.72835	0.54949
H	1.13732	-1.95479	0.05580
H	0.60420	-1.15160	-1.30605

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val+05_8			
C	0.40465	1.58792	0.06109
C	-0.77840	1.78637	-0.47455
N	0.53796	-1.28879	-0.24836
O	1.46573	1.44846	0.54640
O	-0.11052	-2.48428	-0.68722
H	-1.32940	0.93240	-0.84522
H	-1.18094	2.78974	-0.53640
H	0.75106	-1.39546	0.74603
H	1.43290	-1.22072	-0.73838
H	0.48676	-3.23253	-0.50070

val+05_90			
C	-0.09695	-0.24064	-0.41072
C	-0.81119	1.03614	-0.10824
N	0.62206	0.81981	0.36892
O	1.61517	1.50698	-0.13685
O	-0.42447	-1.38176	0.30166
H	0.37395	-0.37645	-1.38188
H	-1.58349	1.02346	0.65692
H	-0.85727	1.81221	-0.86260
H	0.65252	0.56426	1.37144
H	-1.38064	-1.53473	0.22606

val+05_91			
C	-0.60150	1.20375	-0.47589
C	0.59523	0.97651	0.42464
N	-0.11120	-0.16938	-0.20011
O	0.39839	-0.95153	-1.07420
O	-0.99526	-0.83087	0.80646
H	-1.55159	1.46177	-0.02203
H	-0.43495	1.50792	-1.50303
H	0.46583	1.07859	1.49613
H	1.59081	1.12325	0.02141
H	-0.90445	-1.74260	0.46841

val+05_92			
C	0.55696	1.34289	-0.26851
C	-0.86716	1.35075	0.08575
N	-0.20059	0.36928	-0.88762
O	1.65969	1.81412	-0.23527
O	-0.93827	-1.59596	1.20991
H	-1.47822	2.15674	-0.32072
H	-1.25505	0.84590	0.96683
H	-0.60281	-1.28985	0.34703
H	-0.38423	0.42415	-1.88884
H	-0.13701	-1.84392	1.69473

val+05_93			
C	0.42446	0.55898	0.26950
C	-0.76248	0.93847	-0.18651
N	-0.06821	-2.14369	-0.10272
O	1.49938	0.32997	0.68858
O	-1.01842	2.30772	-0.32214
H	-1.46825	0.20160	-0.54632
H	-0.78109	-2.83205	-0.34118
H	0.70207	-2.28758	-0.75402
H	0.29004	-2.40205	0.81546
H	-1.56951	2.58003	0.43004

val+05_94			
C	0.63464	0.22120	-0.25310
C	1.42440	-0.79466	0.06207
N	-0.60034	0.49655	0.48087
O	-0.71440	1.71192	0.87927
O	-1.72786	0.07933	-0.50070
H	0.80638	0.97569	-1.00944
H	2.35888	-0.95569	-0.46408
H	1.17504	-1.49854	0.85253
H	-0.75770	-0.22306	1.21015
H	-2.15075	0.95837	-0.56767

val+05_95			
C	1.82402	-0.40127	-0.05787
C	-0.04918	0.95162	-0.20218
N	0.42244	-0.23109	-0.14203
O	2.54518	0.18957	0.71230

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O	-2.36060	-1.13029	-0.27600
H	2.18688	-1.19075	-0.73942
H	-1.13205	1.07114	-0.21871
H	0.58754	1.84166	-0.24774
H	-1.39245	-1.24783	-0.29195
H	-2.60769	-1.39196	0.62341

val+05_96			
C	0.46871	0.79819	-0.22401
C	1.18876	-0.31646	-0.05942
N	-0.93514	0.80806	-0.33938
O	-1.48252	1.81867	0.54599
O	0.56427	-1.54570	0.04119
H	0.95166	1.75732	-0.37189
H	2.27532	-0.31152	-0.09578
H	-2.03470	2.33754	-0.06085
H	-1.30820	-0.07740	0.00458
H	1.12764	-2.14160	0.55618

val+05_97			
C	0.34798	-0.03459	-0.61531
C	1.02629	-0.96109	0.24998
N	-0.98686	0.10097	-0.51739
O	2.23599	-1.14005	0.28347
O	-1.79825	1.30135	0.57955
H	0.88459	0.65331	-1.25655
H	0.33901	-1.56104	0.89964
H	-1.49363	0.51286	-1.29203
H	-1.49756	-0.65620	-0.07205
H	-1.00767	1.59287	1.06909

val+05_98			
C	1.25491	0.31327	-0.07308
C	-0.59944	1.92796	-0.03851
N	-0.09083	0.63638	-0.00967
O	-1.77877	2.18777	0.01795
O	1.68224	-0.81914	-0.04638
H	1.90237	1.20514	-0.15121
H	0.19432	2.69274	-0.11885
H	-0.75741	-0.12807	0.06352
H	-0.64367	-3.18508	0.21868
H	-0.05303	-2.73628	0.15804

val+05_99			
C	0.40241	0.17003	-0.06611
C	1.30870	-0.79535	0.09589
N	-0.98054	-0.10794	-0.19708
O	-1.76324	0.77938	0.61302
O	0.67256	1.51901	-0.16609
H	2.37526	-0.59013	0.09924
H	0.97869	-1.81806	0.21812
H	-1.39033	1.66973	0.46056
H	-1.27535	0.05416	-1.16318
H	1.57974	1.68896	0.13264

val+05_9			
C	0.50382	-0.21909	-0.96978
C	-0.18026	0.92575	-0.56959
N	0.50025	-1.33423	-0.00140
O	-0.41313	1.97306	-1.16535
O	-0.64024	0.79394	0.78471
H	-0.06096	-2.15889	-0.26838
H	1.43401	-1.68368	0.25355
H	0.06799	-0.92724	0.84626
H	0.83504	-0.44137	-1.96968
H	-1.06622	1.64725	0.96756

val+07_100			
C	-1.03013	0.76867	0.07804
C	0.27292	0.83319	-0.16424
N	0.73164	-1.82501	0.47748
O	1.41238	0.99651	-0.40606
O	-1.81789	1.89010	-0.20580
H	1.56158	-1.60612	1.02647
H	-1.48131	-0.16628	0.38273
H	1.06977	-2.09598	-0.44472
H	0.32051	-2.66059	0.89182

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H	-2.00067	2.34172	0.63458
val+07_101			
C	0.12994	0.39209	0.09385
C	-0.82934	1.30167	0.10816
N	-0.22071	-1.05791	-0.02340
O	-1.52689	-1.34410	-0.10922
O	1.48654	0.49265	0.16835
H	-1.84151	0.92236	0.03122
H	-0.62897	2.36379	0.19093
H	0.33395	-1.39700	-0.84127
H	0.25121	-1.50954	0.79202
H	1.73308	1.42819	0.24245
val+07_102			
C	0.64706	-0.13584	0.00726
C	-0.50405	0.53283	-0.04351
N	0.58078	-1.61657	-0.17576
O	-0.64986	-2.12692	-0.37779
O	-0.67860	1.86858	0.09526
H	1.63905	0.27821	0.16875
H	-1.42145	-0.01982	-0.21281
H	1.23019	-1.83999	-0.95934
H	1.04386	-2.03194	0.66011
H	0.17942	2.29946	0.24313
val+07_103			
C	0.78830	1.11913	-0.62903
C	-0.57090	1.15579	0.05056
N	0.18107	-0.08014	-0.18271
O	-0.25928	-1.05905	-1.15360
O	0.63336	-0.80908	0.95132
H	1.64639	1.37678	-0.00987
H	-1.46622	1.28155	-0.56026
H	-0.72272	1.34055	1.11868
H	0.25656	-0.75333	-1.92877
H	-0.06206	-1.48190	1.08808
val+07_104			
C	0.37134	0.04754	0.10903
C	-0.67556	0.94581	-0.46442
N	-1.01545	-0.00684	0.67811
O	-1.29826	0.44401	1.87434
O	0.76483	-1.07142	-0.60497
H	1.06597	0.43615	0.85049
H	-1.08621	0.69800	-1.44018
H	-0.72822	1.97791	-0.13958
H	-1.50765	-0.84974	0.33389
H	1.04090	-0.79472	-1.49411
val+07_105			
C	0.60335	0.33049	0.35449
C	-0.53528	1.08103	-0.30496
N	-0.74321	-0.28305	0.24099
O	-1.50208	-0.56495	1.23100
O	-0.75532	-1.27853	-0.87299
H	0.86741	0.57141	1.37800
H	1.37129	-0.10564	-0.27425
H	-1.06001	1.84179	0.26177
H	-0.54844	1.15998	-1.38611
H	-1.38970	-1.90334	-0.47175
val+07_106			
C	0.40782	-0.56917	0.45564
C	1.50232	0.13541	0.21910
N	-0.83779	-0.26403	-0.28583
O	-0.81152	0.71021	-1.10548
O	-1.88131	-0.08671	0.88314
H	1.48197	0.92582	-0.52321
H	2.41803	-0.06424	0.76436
H	-1.24936	-1.13637	-0.66241
H	0.28894	-1.37633	1.16831
H	-1.91908	0.88921	0.85677
val+07_107			
C	3.07641	-0.68082	-1.44404
C	-0.08019	0.64201	0.68128

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N	-0.10988	-0.43171	0.00141
O	4.10271	-0.80790	-1.91396
O	-2.77895	-1.00600	0.89293
H	0.78476	1.31400	0.75096
H	-0.97582	0.91961	1.24026
H	-1.89394	-1.12606	0.49033
H	0.78080	-0.60045	-0.47701
H	-3.32791	-0.73176	0.14373

val+07_109

C	-0.94049	0.32763	0.45915
C	0.38972	0.29360	0.47496
N	-1.73803	-0.73437	-0.17478
O	-2.67968	-0.21516	-1.00221
O	1.07085	-0.82032	0.04781
H	0.98034	1.12626	0.84931
H	-1.54441	1.15732	0.79561
H	-2.14584	-1.32887	0.57807
H	-1.06353	-1.35977	-0.65984
H	1.97277	-0.57202	-0.20270

val+07_10

C	0.58763	0.78506	-0.27198
C	-0.55897	1.54183	0.08089
N	0.61063	-0.45309	0.34195
O	-1.41438	1.13276	0.88842
O	0.16918	-1.74894	-0.48199
H	-0.64575	2.54720	-0.37287
H	1.36144	1.04452	-0.97855
H	-0.10854	-0.41761	1.08754
H	1.50546	-0.82502	0.65483
H	-0.51670	-1.34870	-1.05004

val+07_110

C	1.07527	-1.78683	-0.21149
C	-0.22223	1.08834	-0.56871
N	-1.32426	0.09832	0.12302
O	2.18379	-2.02131	-0.32018
O	0.80861	1.06189	0.42987
H	0.14233	0.37195	-1.33634
H	-1.71708	0.58663	0.92655
H	-2.08058	-0.07410	-0.54182
H	-0.93776	-0.80486	0.44992
H	0.81542	1.95105	0.80909

val+07_111

C	0.26762	0.98060	-0.22825
C	-0.93120	1.18910	0.26777
N	0.33848	-1.87094	0.04131
O	1.65719	-2.01495	-0.51450
O	1.34784	0.88113	-0.68464
H	-1.52082	0.35155	0.61058
H	-1.31147	2.20203	0.32540
H	-0.23877	-2.48739	-0.53449
H	0.40470	-2.33106	0.95163
H	1.89344	-1.09137	-0.71411

val+07_112

C	-0.09957	2.39788	0.06369
C	-0.50110	-1.19376	0.08400
N	0.66288	-0.30110	0.07386
O	-1.21419	2.12899	0.29900
O	0.98668	2.76416	-0.17100
H	-0.26626	-2.27026	0.12761
H	-1.13165	-0.94672	0.94381
H	1.24010	-0.47279	0.89539
H	-1.09709	-1.01325	-0.81626
H	1.25459	-0.50565	-0.72950

val+07_113

C	-0.20594	-0.01653	-0.44633
C	0.47581	0.95162	0.33520
N	-0.09062	-1.29094	0.07333
O	0.97238	-2.30991	-0.55813
O	1.06977	0.66788	1.39218
H	-0.71570	0.13151	-1.38637
H	0.42621	1.99776	-0.02183

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H	0.27057	-1.18026	1.03793
H	1.67603	-1.67609	-0.79547
H	-0.88931	-1.91875	0.00560

val+07_114			
C	0.49415	2.10323	0.88994
C	-0.26469	-1.48680	0.30787
N	-0.32511	-0.77709	-0.84152
O	0.00284	-1.02966	1.41179
O	0.29211	2.08597	-0.30926
H	0.75472	3.04914	1.40500
H	-0.48708	-2.56166	0.16012
H	0.42541	1.18592	1.49961
H	-0.55312	-1.23063	-1.71369
H	-0.13834	0.22748	-0.83176

val+07_115			
C	0.44749	0.72639	0.17212
C	-0.93303	0.72435	0.45546
N	1.29975	-0.15017	-0.36199
O	-0.83810	-2.02366	0.13550
O	0.66393	1.82187	0.75843
H	-1.48356	1.34872	-0.25993
H	2.28902	-0.04655	-0.17336
H	-1.64072	-2.24593	-0.36015
H	0.91590	-1.07964	-0.52538
H	-1.10617	-1.26918	0.71090

val+07_117			
C	0.71734	0.93245	-0.13324
C	-0.67129	0.78986	-0.30943
N	0.37653	-2.17759	0.11742
O	0.77512	2.10148	-0.57582
O	1.71799	0.15176	0.16839
H	-1.22214	1.24208	0.52649
H	1.33142	-0.78231	0.30751
H	0.83227	-2.89160	-0.44916
H	-0.02100	-2.64404	0.93109
H	-0.39885	-1.80297	-0.43423

val+07_119			
C	-0.85192	0.10085	0.35409
C	-0.11968	1.35729	-0.00436
N	-0.81524	-0.98752	-0.39731
O	-0.29984	2.23001	-0.82413
O	0.77294	1.03070	0.85145
H	-1.33372	0.02212	1.32158
H	2.74805	-0.27000	-0.14380
H	-0.42138	-0.94250	-1.32994
H	3.24983	-0.71575	-0.46587
H	-0.96663	-1.91251	-0.01379

val+07_11			
C	2.14146	-0.83432	-1.33056
C	-0.66187	1.04257	-0.10440
N	0.11253	0.28140	0.87248
O	-0.87724	0.27316	-1.25972
O	3.08867	-1.21353	-0.82885
H	-1.66663	1.33635	0.23554
H	-0.09444	1.96508	-0.31282
H	-0.45999	-0.46486	1.26439
H	0.41212	0.87655	1.64324
H	-0.00121	-0.05270	-1.53241

val+07_120			
C	0.44372	0.17778	-0.82544
C	-0.77457	0.83038	-0.27346
N	0.79612	-1.13233	-0.04933
O	0.09693	-1.37687	1.05921
O	1.16029	0.49484	-1.73310
H	-0.68259	0.86305	0.81596
H	-1.64498	0.19328	-0.46959
H	-0.90766	1.81412	-0.72393
H	1.83002	-1.05445	0.08712
H	0.70944	-1.87359	-0.78384

val+07_121

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C	-0.02917	1.23017	-0.51227
C	0.29098	-1.24726	-0.22239
N	-0.28081	0.01452	0.31065
O	-1.64882	0.10963	0.15335
O	0.43574	1.17912	-1.61786
H	-0.40708	2.10980	0.01920
H	-0.20110	-2.06173	0.30960
H	1.37415	-1.26521	-0.06737
H	0.05105	-1.28287	-1.28267
H	0.01126	0.13412	1.29587

val+07_122

C	0.45786	0.61985	-0.30135
C	-0.32897	1.41124	0.70249
N	-0.06484	-1.84108	0.28067
O	1.24080	-2.06369	-0.27182
O	-0.59720	1.23997	-0.73507
H	-1.04038	0.90325	1.34449
H	-0.01916	2.41652	0.97251
H	1.46857	-1.14177	-0.52479
H	-0.03224	-2.29243	1.19683
H	-0.69264	-2.41007	-0.29125

val+07_124

C	-0.22629	-0.10970	0.25749
C	0.37837	1.05720	-0.47839
N	-0.03695	-1.28026	-0.20597
O	-0.59082	-2.35083	0.46284
O	1.11222	0.67991	-1.61696
H	-0.81159	0.08649	1.16580
H	-0.43418	1.74900	-0.75941
H	1.02602	1.61261	0.22057
H	-1.07652	-2.01394	1.24608
H	1.03932	-0.28769	-1.69365

val+07_125

C	0.93414	1.26025	0.50175
C	-0.78570	0.59062	0.26538
N	0.58925	0.10571	0.04893
O	-0.80201	-2.30484	-0.51911
O	-0.24500	1.88366	0.76429
H	1.89823	1.73186	0.67601
H	-1.34160	0.06846	1.04427
H	-1.37401	0.73792	-0.64123
H	-0.77888	-2.45183	-1.47621
H	0.01609	-1.80361	-0.34458

val+07_128

C	-1.03001	0.89930	-0.05681
C	0.46075	0.58839	-0.02141
N	0.82542	-0.71075	-0.56943
O	0.40535	-1.70098	0.40480
O	-1.81684	0.27940	-0.73640
H	-1.35775	1.77130	0.55231
H	0.96790	1.37090	-0.60992
H	0.84421	0.66445	1.00128
H	0.18507	-0.88908	-1.34767
H	1.23121	-2.18513	0.56297

val+07_129

C	-0.84272	-0.18558	-1.21239
C	0.06742	-0.20330	-0.06569
N	0.76166	0.98025	0.31417
O	1.01935	0.91665	1.73591
O	-1.35280	-0.29522	0.12807
H	-1.05608	0.75716	-1.71959
H	0.62220	-1.10386	0.18876
H	-0.94635	-1.07252	-1.83810
H	0.12584	1.77415	0.21676
H	1.98248	1.03127	1.77290

val+07_12

C	0.34486	1.72945	2.13304
C	0.14459	-0.77347	-0.43203
N	-0.34281	0.56230	-0.76601
O	0.38955	2.86490	2.09498
O	-0.30096	-1.14752	0.84647

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H	-0.20803	-1.57140	-1.10314
H	1.24480	-0.73809	-0.50072
H	-1.34784	0.53399	-0.93164
H	0.09933	0.90920	-1.61584
H	-0.05610	-0.41605	1.44058

val+07_131

C	-0.14239	-0.13460	-0.67111
C	1.13469	0.20189	-0.10282
N	-1.09954	-0.65097	0.12072
O	2.06479	0.71473	-0.70979
O	-2.32097	0.35751	1.01127
H	1.23922	-0.07989	0.97612
H	-0.40838	0.12969	-1.68687
H	-0.79943	-1.06809	0.99736
H	-1.87026	-1.15029	-0.30728
H	-1.93243	1.23252	0.82940

val+07_132

C	0.07004	-1.59424	-1.19700
C	-1.41618	1.31957	1.32430
N	-0.53294	-0.73896	-0.48072
O	-2.59432	1.31097	1.05449
O	1.39779	-1.79736	-1.11297
H	-0.69001	1.97212	0.79910
H	-1.53319	-0.72214	-0.67914
H	-0.36394	-2.25955	-1.94790
H	-0.98378	0.68407	2.12314
H	1.72934	-1.18089	-0.43221

val+07_134

C	-0.79320	-0.81827	-0.33463
C	0.29922	-0.03739	0.00515
N	-2.00827	-0.12985	0.12528
O	0.17794	1.07934	0.59222
O	1.54093	-0.50441	-0.31609
H	-1.53278	0.73686	0.53715
H	-2.66799	0.15457	-0.60900
H	-2.54611	-0.60730	0.85946
H	-0.86103	-1.78797	-0.79461
H	2.14577	0.18822	0.00108

val+07_135

C	0.35592	0.13449	-0.28718
C	-0.98005	-0.53768	-0.29396
N	1.25615	-0.13238	0.62615
O	1.19622	-0.97596	1.57154
O	-2.02864	0.38662	-0.57535
H	-1.11509	-1.06045	0.66156
H	-1.03466	-1.28762	-1.09233
H	2.13021	0.41503	0.56472
H	0.61408	0.88955	-1.02113
H	-2.08173	0.99802	0.17599

val+07_136

C	0.39028	-0.03272	1.09737
C	1.35085	0.25467	-0.03205
N	-0.85973	-0.60039	0.58972
O	-1.01225	0.75714	0.76334
O	-1.19910	-1.06146	-0.72463
H	2.04784	-0.59125	-0.10073
H	1.94388	1.13125	0.24723
H	0.93534	0.44246	-1.03609
H	-1.43474	-1.17822	1.20663
H	-0.97006	-0.28819	-1.27429

val+07_137

C	0.08125	-1.51850	0.92036
C	-1.40199	0.86106	-0.48149
N	-0.56781	-0.25566	-0.92587
O	0.40777	-0.49384	0.13537
O	1.07035	-1.67314	1.78385
H	-2.16204	1.01523	-1.25480
H	-1.89352	0.68422	0.48621
H	-0.78661	1.76220	-0.41629
H	-1.12678	-1.11460	-0.88231
H	1.78599	-1.00896	1.63517

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val+07_138			
C	0.83050	-0.83061	-0.29010
C	-0.75028	1.20746	0.37028
N	-0.44971	-0.17101	-0.03886
O	-0.15887	-0.32282	-1.39399
O	-1.46662	-1.01309	0.43865
H	1.58214	-0.02024	-0.22110
H	-0.00072	1.85099	-0.08677
H	-0.70909	1.25757	1.45984
H	-1.75067	1.46196	0.01372
H	-0.98228	-1.86990	0.42644

val+07_139			
C	0.70531	-1.81889	-0.73638
C	-0.66614	0.16887	0.52124
N	-0.43773	-1.24411	0.06824
O	-0.67808	-1.36633	-1.31887
O	-0.04695	1.05636	-0.33246
H	1.31676	-0.91183	-0.91831
H	-0.22905	0.27523	1.51811
H	-1.75862	0.29708	0.57180
H	-0.97565	-1.93289	0.59752
H	-0.34334	0.81620	-1.23100

val+07_13			
C	-0.84812	-1.28263	-0.54375
C	0.04170	2.07684	1.59968
N	0.01983	-0.76277	-1.42508
O	0.99352	1.50079	1.11539
O	-0.54819	-0.92424	0.71245
H	-0.93675	1.57970	1.72787
H	0.11412	3.12887	1.93415
H	-0.10310	-0.97566	-2.40411
H	0.82235	-0.16719	-1.18999
H	0.23905	-0.32700	0.78599

val+07_140			
C	2.05360	-1.14180	0.75874
C	-0.63001	0.64951	-0.88075
N	-0.55976	-0.25174	0.27436
O	1.75370	-1.64168	1.77335
O	2.44844	-0.67421	-0.23898
H	-0.23005	0.13392	-1.75947
H	-1.63971	1.01719	-1.12822
H	-0.92077	0.21405	1.10508
H	-1.16276	-1.05878	0.12396
H	0.01112	1.51725	-0.69586

val+07_141			
C	0.60704	-1.28464	-0.03669
C	-1.19948	1.75218	-0.04403
N	-0.35617	-2.14442	0.15498
O	-2.11156	2.54245	-0.07166
O	-1.11269	0.67699	-0.82802
H	1.57294	-1.77109	0.17896
H	-0.34053	1.85917	0.65118
H	-0.27052	0.13876	-0.59642
H	-1.31634	-1.84172	-0.00828
H	-0.26029	-3.11748	0.45458

val+07_142			
C	-0.64739	0.04858	-0.64959
C	1.31275	0.93234	0.32341
N	-1.72695	-0.31818	0.46045
O	2.32498	0.93187	0.97645
O	0.56981	-0.17714	0.11961
H	0.87188	1.81093	-0.18218
H	-0.70561	-0.86553	-1.26382
H	-1.77278	0.45255	1.12878
H	-1.56024	-1.18165	1.00930
H	-2.64124	-0.38266	0.00738

val+07_143			
C	-0.70010	0.31259	0.81594
C	1.56327	0.39567	-0.06597
N	-2.14977	-0.98189	-0.44268

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O	-0.82344	-0.40336	-0.30408
O	0.54609	0.72497	0.92318
H	1.67066	-0.68771	-0.15111
H	1.29621	0.81441	-1.03904
H	2.48174	0.84808	0.30703
H	-2.61160	-0.66524	0.41962
H	-2.55317	-0.41451	-1.19379

val+07_144			
C	1.71665	0.64877	-0.05283
C	-1.79669	-0.33932	0.16178
N	0.48528	-0.12651	-0.29625
O	0.40695	1.14194	-0.83582
O	-0.46746	-0.42167	0.70109
H	1.50689	1.05174	0.95693
H	-2.00748	0.67476	-0.18688
H	-1.93855	-1.06125	-0.65462
H	-2.44937	-0.60180	0.99575
H	0.48256	-0.86996	-1.00265

val+07_145			
C	0.69874	-0.29522	-0.08940
C	1.75487	0.15685	-0.46644
N	-0.52497	-0.81029	0.21668
O	-1.24648	0.02690	1.14350
O	-2.79952	0.35925	-1.10936
H	2.70863	0.54671	-0.73639
H	-1.99066	0.32938	0.57217
H	-2.12641	-0.32536	-1.28337
H	-0.45485	-1.72173	0.66661
H	-2.45335	1.14590	-1.55929

val+07_146			
C	0.40553	-0.31850	-0.04159
C	1.51218	0.14170	-0.19317
N	-0.88526	-0.71315	0.18138
O	-3.52948	0.51034	0.18033
O	2.77215	0.46793	-0.42863
H	-2.59846	0.40837	0.45573
H	-3.55778	1.39186	-0.21959
H	-0.97220	-1.45333	0.87411
H	-1.38990	-0.97820	-0.66156
H	2.91923	1.39497	-0.17300

val+07_148			
C	0.37685	0.25593	0.29745
C	-0.95931	0.94249	0.13620
N	0.45769	-1.01924	-0.19623
O	1.34196	0.74420	0.88333
O	1.75009	-1.56925	-0.22716
H	-1.33904	1.21491	1.12545
H	-0.81996	1.86829	-0.43097
H	-1.70283	0.31766	-0.36799
H	2.25255	-0.87207	0.25807
H	-0.05032	-1.28053	-1.03276

val+07_14			
C	0.54130	2.51474	-0.58404
C	-0.75404	-1.26428	-0.20425
N	-0.44963	-0.05336	0.55537
O	-0.17898	3.24261	-1.07819
O	0.94403	-0.11281	0.92058
H	-1.83862	-1.30122	-0.36041
H	-0.26220	-1.20632	-1.17962
H	-0.42721	-2.18649	0.29826
H	-0.92698	-0.11345	1.45604
H	1.28273	0.70638	0.51815

val+07_150			
C	-0.58570	0.88527	0.42510
C	0.60438	0.92112	-0.51145
N	-0.16383	-0.33264	-0.31020
O	-0.85627	-0.91668	-1.21290
O	0.58421	-1.24467	0.60684
H	-1.53738	1.27289	0.07958
H	-0.40532	0.87300	1.49400
H	0.47737	1.33348	-1.50602

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H	1.60093	0.93339	-0.08485
H	0.29931	-2.08627	0.20150
val+07_151			
C	0.50610	0.53094	0.00294
C	1.31302	-0.50635	0.17011
N	-0.90001	0.36470	-0.36432
O	-1.26649	1.07083	-1.37220
O	-1.67650	0.72123	0.93132
H	0.76699	1.57986	0.05350
H	2.36349	-0.36179	0.39741
H	0.96291	-1.53235	0.08468
H	-2.17550	1.47579	0.56033
H	-1.14482	-0.64106	-0.41817
val+07_152			
C	1.39505	-1.34394	0.04474
C	-1.41733	1.76872	0.55431
N	0.37900	-0.88025	-0.73236
O	2.42281	-1.85301	-0.36498
O	-1.89505	0.65663	0.50402
H	1.19274	-1.18721	1.12425
H	-1.97888	2.62201	0.97974
H	-0.39914	1.98732	0.17964
H	-0.50020	-0.56981	-0.32821
H	0.42710	-1.05537	-1.72764
val+07_153			
C	0.20483	0.49093	-0.33451
C	0.83618	-0.77299	-0.06771
N	-1.12980	0.53892	-0.49548
O	2.03110	-0.93609	0.13739
O	-2.30011	0.80764	0.86951
H	0.74658	1.42710	-0.28502
H	0.13390	-1.64508	-0.09370
H	-1.53688	1.34173	-0.96055
H	-1.66695	0.73638	1.60685
H	-1.59936	-0.33114	-0.72988
val+07_154			
C	0.63005	-0.35615	-0.23292
C	2.03510	-0.88271	-0.13403
N	-2.82049	1.49085	-0.07430
O	0.23206	0.64096	0.33493
O	-3.20009	2.49807	0.48697
H	-0.05559	-0.94767	-0.87736
H	2.01843	-1.90953	0.25440
H	2.48235	-0.93273	-1.13553
H	2.63962	-0.24587	0.51526
H	-1.79534	1.34468	0.15838
val+07_155			
C	0.24816	-1.07225	0.30259
C	-0.53119	1.23447	-0.32659
N	-0.88816	-0.18229	-0.06488
O	1.34393	-0.65254	0.55603
O	-1.51953	-0.37700	1.14708
H	-0.03768	1.32523	-1.29910
H	-1.46217	1.80095	-0.29764
H	0.13297	1.54904	0.47526
H	-1.43968	-0.54955	-0.85931
H	-0.11107	-2.10406	0.37564
val+07_158			
C	1.27026	-1.56886	-0.79034
C	-1.02484	0.90065	0.05472
N	-0.22017	0.10376	1.01098
O	0.77788	-1.19091	-1.82847
O	-0.49188	0.30652	2.17253
H	0.85082	-2.41070	-0.20344
H	2.18654	-1.11233	-0.36459
H	-1.50096	0.19137	-0.63144
H	-1.75103	1.53153	0.57430
H	-0.31801	1.48968	-0.54136
val+07_15			
C	-0.15094	-1.55181	-1.08221

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C	-0.34808	1.87088	1.52275
N	0.65062	-0.64804	-0.68679
O	-0.79781	2.78050	2.17261
O	-0.35942	1.82899	0.18691
H	-1.22430	-1.36330	-1.02405
H	0.11972	0.97728	1.98622
H	0.15873	-2.52215	-1.48451
H	1.63097	-0.92570	-0.78801
H	0.06080	0.98285	-0.12293

val+07_16

C	-0.41831	-0.97577	1.98535
C	-0.15874	-1.38858	0.83517
N	0.12613	-1.65358	-0.53702
O	0.40709	1.48522	0.27608
O	-0.19126	1.02904	-0.97080
H	0.16371	0.73319	0.88767
H	-0.50926	-2.34650	-0.95715
H	1.08595	-1.99458	-0.69076
H	0.01742	-0.73856	-1.04385
H	-1.08043	1.42192	-0.91540

val+07_17

C	0.30838	-0.32032	-0.82874
C	-0.53629	0.52047	0.12165
N	-0.01879	-1.57871	-0.70766
O	-1.22446	-0.18245	1.15193
O	0.30017	1.48180	0.72825
H	-1.32922	0.99707	-0.47756
H	-0.72869	-1.89578	-0.03286
H	0.43743	-2.29413	-1.26389
H	-0.61010	-0.19083	1.90594
H	1.11197	1.48458	0.19022

val+07_18

C	1.76821	1.74241	0.41071
C	-0.92317	-0.50809	-0.33620
N	0.31225	-1.09756	0.17333
O	2.89508	1.60076	0.46343
O	-1.25331	0.64115	0.40082
H	-1.80696	-1.15987	-0.26172
H	-0.75564	-0.28948	-1.40416
H	0.64644	-1.83428	-0.44604
H	0.14616	-1.51608	1.08743
H	-0.45495	1.19854	0.40128

val+07_19

C	0.70798	-0.77178	-0.45195
C	-0.94705	1.98430	0.56013
N	-0.47219	-0.79239	0.02576
O	0.11580	2.41638	0.17594
O	-1.09861	-2.01543	0.13052
H	1.24479	-1.66964	-0.78062
H	-1.11777	1.67345	1.60992
H	-1.82533	1.88613	-0.10836
H	1.18890	0.19820	-0.52843
H	-0.49102	-2.71192	-0.20211

val+07_1

C	0.08137	0.54707	-0.61079
C	-0.65596	1.59793	-0.22954
N	-0.05808	-0.58310	0.37094
O	1.21754	-0.87607	0.89157
O	-0.57957	-1.69927	-0.31206
H	-1.28300	1.65218	0.66923
H	-0.65795	2.49679	-0.84211
H	-0.65610	-0.49797	1.20563
H	1.77188	-0.45594	0.18823
H	-0.35793	-1.43121	-1.23809

val+07_21

C	-0.17821	-1.05349	0.65131
C	-0.79094	1.05815	-0.38120
N	-1.13843	-0.29434	0.05685
O	0.93611	-0.63504	0.93611
O	0.24162	1.09105	-1.33077
H	-1.67578	1.49910	-0.84382

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H	-0.52980	1.63182	0.51619
H	-1.92888	-0.76649	-0.36293
H	-0.50333	-2.08777	0.87178
H	1.03472	0.78151	-0.85782

val+07_22

C	-0.03937	-1.08157	-0.18476
C	-1.32516	0.96797	-0.41552
N	-1.19995	-0.44001	-0.14943
O	-0.42231	1.69011	-0.72709
O	2.17377	0.71224	0.64494
H	1.65571	0.01501	0.18750
H	-2.37234	1.30320	-0.29640
H	-2.10191	-0.86987	0.09028
H	-0.26327	-2.13160	0.08066
H	1.87252	1.51081	0.18691

val+07_23

C	-0.89117	-0.31246	0.99795
C	-0.34425	0.83841	0.20817
N	-0.55776	-1.45983	0.46211
O	0.42369	0.56801	-0.99264
O	1.76071	0.16178	-0.56568
H	-1.19453	1.42634	-0.16580
H	0.24171	1.48858	0.87006
H	0.01813	-1.55353	-0.38203
H	2.27935	0.90290	-0.92676
H	-0.86318	-2.32948	0.88484

val+07_24

C	2.21180	1.29295	0.27600
C	-1.33072	0.48464	-0.07620
N	0.32813	-1.65952	-0.02837
O	2.48635	2.39579	0.29734
O	-0.66075	1.36138	-0.57709
H	-2.01393	-0.15310	-0.66960
H	-1.34358	0.28976	1.01286
H	0.42587	-2.06899	-0.95630
H	1.07004	-0.96556	0.05903
H	0.53688	-2.40196	0.63803

val+07_25

C	1.74367	0.09710	-2.25487
C	-0.51029	1.29126	0.66525
N	0.45271	-1.33057	0.18175
O	1.40863	1.18423	-2.19976
O	-1.14958	1.12844	1.67932
H	-0.95698	1.19847	-0.34435
H	0.56177	1.57084	0.67317
H	0.01416	-1.98338	-0.46616
H	-0.05647	-1.40767	1.06122
H	1.39068	-1.68932	0.35413

val+07_26

C	0.32763	0.43328	0.13372
C	-0.39802	-0.88870	0.18829
N	0.62763	0.89944	-1.15801
O	-0.01193	1.36583	1.14742
O	1.32461	0.65637	1.07883
H	-1.38261	-0.80868	-0.28673
H	0.17775	-1.65665	-0.33676
H	-0.53216	-1.17930	1.23113
H	-0.15837	0.82944	-1.79651
H	0.97797	1.85278	-1.12897

val+07_27

C	-0.72235	1.05280	0.35492
C	-0.17244	-1.29988	-0.29569
N	-1.04085	-0.21216	0.21410
O	0.26400	1.71881	0.13361
O	1.74059	0.88584	-0.63562
H	-0.58169	-1.68517	-1.23499
H	0.82060	-0.87524	-0.45398
H	-0.14079	-2.10312	0.44705
H	-1.98172	-0.45796	0.49132
H	2.34864	1.35359	-0.03681

val+07_28
C 1.01398 1.90913 1.40357
C -0.29413 -1.16275 0.27714
N -0.16981 0.65173 -1.22886
O 0.46398 2.55850 2.15817
O -0.81821 0.10509 -0.08221
H -0.42185 -1.89725 -0.53459
H 0.77377 -1.10172 0.53904
H -0.86211 -1.49413 1.15165
H -0.24826 -0.05896 -1.96546
H 0.82565 0.70735 -0.98715

val+07_29
C 0.91260 0.05974 0.94582
C -1.08193 -0.66192 -0.30103
N -0.05694 0.29173 0.10407
O -0.16118 1.52579 -0.47439
O -1.23602 1.62302 -1.34015
H 1.60561 0.86263 1.15707
H -2.05509 -0.23074 -0.06206
H -1.03178 -0.76939 -1.38549
H -0.89777 -1.59977 0.22283
H 0.99100 -0.91650 1.39912

val+07_2
C -1.34170 -0.28477 -0.38473
C -0.74460 0.98334 -0.06223
N -0.77579 -1.39993 -0.04070
O 0.26042 1.45480 -0.61567
O 1.88816 -0.61261 0.43153
H -1.35821 1.60816 0.62173
H -1.17410 -2.28541 -0.34530
H 0.15721 -1.43636 0.40856
H 1.57925 0.19523 -0.03484
H 2.51997 -1.02034 -0.17994

val+07_31
C -0.00377 -0.93010 -0.39609
C 0.78372 0.25421 -0.23393
N -1.37787 -0.59294 0.13807
O 0.16733 1.48629 -0.55271
O 0.56342 1.22608 0.87773
H 1.84000 0.18649 -0.49321
H 0.37589 -1.83089 0.08274
H -1.54081 0.36607 -0.20645
H -2.09952 -1.20669 -0.24061
H -1.48579 -0.54764 1.16576

val+07_32
C 0.76288 -1.41420 0.17956
C -0.39694 2.14068 -0.29146
N -0.67145 -1.35694 0.22648
O -0.67588 1.36759 -1.18353
O 0.21608 -0.62823 1.20351
H 1.21267 -2.35946 0.48546
H -0.35026 3.23339 -0.47143
H -0.17416 1.79231 0.73158
H 1.29561 -0.87434 -0.60657
H -0.94325 -0.59489 -0.41020

val+07_36
C 0.25219 0.72170 0.15475
C 0.00005 1.99114 0.01671
N 0.09909 -0.25844 -0.79801
O -0.16204 3.15614 0.13062
O -1.38302 -0.78358 -1.12632
H 0.36774 -0.04437 -1.76388
H 0.52024 -1.14687 -0.51927
H 1.52571 -1.85060 1.55862
H 1.32146 -1.13089 1.55297
H -1.83624 -0.42584 -0.33779

val+07_38
C -0.35644 0.29483 -0.46331
C -0.16494 1.17949 0.49526
N 0.82013 -0.69305 -0.41261
O -0.70552 2.27928 1.06478

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O	0.62156	1.64847	1.53852
H	-1.75345	-1.75937	-0.50211
H	1.34262	-0.63778	-1.29153
H	0.43615	-1.64331	-0.36878
H	1.50518	-0.60141	0.35749
H	-1.81878	-2.50465	-0.43622

val+07_39

C	-0.73317	1.27576	-0.07177
C	0.56938	1.33097	0.15659
N	0.20689	-1.90625	0.18959
O	-1.55800	0.26672	0.38144
O	1.74757	1.31625	0.28213
H	-1.20897	2.10883	-0.57808
H	0.11368	-2.43208	-0.67794
H	-1.03894	-0.58022	0.32688
H	0.15600	-2.57911	0.95279
H	1.14947	-1.51786	0.19877

val+07_3

C	-0.37577	-1.13195	-0.32494
C	-0.42659	0.18747	-0.08775
N	1.06165	-1.55562	0.12826
O	-1.49090	0.97221	-0.47723
O	0.57756	0.95502	0.55535
H	1.49845	-2.09013	-0.62446
H	0.99014	-2.18574	0.92960
H	1.66809	-0.75704	0.39008
H	-1.93851	1.29205	0.32517
H	0.62868	1.79774	0.07212

val+07_40

C	-2.34972	0.58449	-1.55941
C	0.97015	0.73510	0.61001
N	-0.15361	-0.16410	0.35498
O	-1.93395	-0.24030	-2.23116
O	0.34426	-1.26629	-0.42887
H	0.63552	1.49505	1.32550
H	1.24751	1.23266	-0.32374
H	-0.41630	-0.60848	1.23581
H	1.85575	0.22134	1.01126
H	-0.21041	-1.22166	-1.22659

val+07_41

C	-0.50487	1.39997	-0.39268
C	0.46694	2.10834	0.13685
N	0.38275	-1.20054	0.42864
O	-1.40942	0.84014	-0.89606
O	-0.71146	-1.90383	-0.18521
H	0.46092	3.18563	0.02138
H	1.25724	1.60964	0.67853
H	0.35038	-1.50114	1.40504
H	1.21315	-1.64649	0.03326
H	-1.22192	-1.17522	-0.58166

val+07_42

C	-1.23776	-0.39374	-1.22019
C	-1.09402	-0.21900	0.26798
N	1.60494	0.61016	1.51445
O	-1.28385	-1.42283	-0.16534
O	1.70751	0.04089	0.17862
H	0.59620	0.56255	1.68805
H	2.01720	-0.11975	2.09970
H	-0.34707	-0.44460	-1.83661
H	-2.19482	-0.22266	-1.70338
H	2.14148	0.76027	-0.30547

val+07_44

C	0.38381	0.94990	-0.03888
C	-0.96757	1.31984	0.18265
N	0.50336	-0.32992	-0.54642
O	-1.92516	0.57405	-0.09630
O	0.89961	-1.53170	0.43063
H	1.27278	1.51496	0.19730
H	-1.14130	2.33428	0.58884
H	-0.44654	-0.60843	-0.85328
H	1.22656	-0.51349	-1.23938

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H	0.45644	-1.22550	1.24494
val+07_45			
C	-1.10357	1.62206	2.14027
C	-0.80597	-1.42925	-0.51265
N	-0.37831	1.70198	1.21841
O	0.07669	-1.19463	-1.31397
O	1.17384	1.39315	-0.99657
H	-1.33132	-2.40203	-0.51605
H	2.11748	1.28991	-0.80115
H	-1.12224	-0.69585	0.24948
H	0.24896	1.70992	0.39341
H	0.86764	0.49614	-1.25526
val+07_46			
C	-1.02784	0.82731	0.96163
C	-0.00234	0.28711	-0.06980
N	-0.33579	-1.07092	-0.48239
O	-2.09114	0.09317	0.91742
O	1.28514	0.36851	0.50203
H	-0.09458	0.93636	-0.95851
H	-1.93414	-0.66594	0.25123
H	-0.05454	-1.27144	-1.43761
H	0.14350	-1.73111	0.12869
H	1.18562	0.97685	1.25941
val+07_47			
C	0.23516	0.79955	-0.53362
C	-1.05691	0.80910	-0.20359
N	-0.96600	-1.32980	0.73996
O	-1.77337	-0.16502	0.45486
O	0.80028	1.93131	-1.09820
H	-1.70033	1.65701	-0.41514
H	-1.52547	-2.08510	0.33874
H	-1.06754	-1.42517	1.75269
H	0.88578	-0.04172	-0.31992
H	1.48011	1.64524	-1.72578
val+07_48			
C	-1.20959	0.23601	0.39449
C	0.11455	-0.30819	-0.13857
N	0.13120	-1.75820	-0.04711
O	-1.93953	-0.38604	1.12465
O	-1.50939	1.51129	0.04272
H	0.90629	0.20460	0.44093
H	1.07209	-2.09824	0.12896
H	0.24395	0.01278	-1.18389
H	-0.45600	-2.03304	0.73892
H	-0.84517	1.85203	-0.57971
val+07_49			
C	-3.09854	0.11942	-1.48723
C	-0.41412	0.04074	-0.03520
N	0.08809	1.13440	-0.59786
O	-2.76170	1.06758	-2.02915
O	0.51947	-0.44695	0.81961
H	2.88667	-0.00338	1.78442
H	1.01727	1.50567	-0.39253
H	-0.47891	1.63244	-1.26900
H	3.55889	0.07949	2.09217
H	0.13727	-1.24090	1.21975
val+07_4			
C	0.01173	-1.00771	-0.68255
C	-1.19950	0.96888	0.17071
N	-1.07371	-0.30919	-0.12704
O	1.24773	-0.35611	-0.42115
O	-0.18982	1.84633	0.02652
H	-2.16898	1.38751	0.40148
H	-1.93627	-0.84325	-0.08912
H	-0.00418	-2.05517	-0.37766
H	1.55481	-0.56645	0.48444
H	0.60137	1.31716	-0.24192
val+07_51			
C	-0.31133	0.97315	0.72740
C	0.66211	-1.11220	0.32715

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N	0.13955	-1.70580	-0.85402
O	0.76383	0.35402	0.27226
O	-0.05741	2.27894	0.54786
H	1.68848	-1.44230	0.49491
H	0.02995	-1.35975	1.18127
H	-0.81779	-1.40028	-1.01429
H	0.69213	-1.45776	-1.67119
H	-0.83671	2.74289	0.89075

val+07_52

C	-0.04165	1.58047	0.45428
C	1.24154	1.97485	0.37449
N	-0.21054	0.27944	-0.18622
O	-0.52410	-0.82378	0.79535
O	-0.85160	-1.97864	0.01077
H	-0.98953	1.96140	0.83915
H	1.38515	2.98480	0.79111
H	-0.95910	0.16887	-0.88336
H	0.74697	0.12697	-0.56570
H	-0.01814	-2.48640	0.06015

val+07_53

C	-1.25541	2.37551	-0.28646
C	0.13761	0.50456	-0.16854
N	-0.69867	-0.28319	-0.66021
O	-0.07517	1.91664	0.05975
O	1.45758	-2.24145	-0.36884
H	-1.17058	3.45396	-0.01957
H	1.13709	0.22616	0.14917
H	-1.56655	0.23220	-0.88160
H	0.59458	-1.93020	-0.70032
H	1.22233	-2.79229	0.39252

val+07_54

C	-0.64082	1.69714	-0.68616
C	0.12460	-0.53204	-0.12527
N	0.14729	-0.11056	1.19895
O	-0.08265	0.63753	-1.16898
O	-0.94412	-1.37299	-0.34192
H	-0.75553	2.35201	-1.58921
H	1.08912	-0.92524	-0.46095
H	-0.62749	0.54268	1.34363
H	1.00982	0.38740	1.40179
H	-1.02180	-1.51542	-1.29956

val+07_55

C	-0.16699	0.06790	-0.19874
C	1.05689	-0.29227	0.23664
N	1.28150	-1.76149	0.00625
O	-0.54898	1.30145	-0.08597
O	-2.00316	1.43171	-0.66953
H	1.90561	0.19927	0.70359
H	1.41579	-2.32506	0.85706
H	2.04751	-1.99361	-0.64096
H	0.37370	-2.01049	-0.43152
H	-2.10138	2.38769	-0.50023

val+07_56

C	-1.08229	0.22320	0.01595
C	1.31449	0.46594	0.26656
N	1.10168	-1.06352	0.08544
O	-0.05659	1.00170	-0.09335
O	-2.21804	0.89419	-0.16881
H	1.87725	0.76765	-0.62833
H	0.03007	-1.12849	0.20637
H	1.58813	-1.56832	0.82382
H	1.33186	-1.49698	-0.82053
H	-2.01407	1.84473	-0.32794

val+07_57

C	1.30712	1.95919	-0.91264
C	0.31400	1.87286	-0.06650
N	0.67800	0.53692	0.41224
O	-1.30293	-1.51068	0.99816
O	-0.62202	-1.98128	-0.20020
H	-0.54119	2.41466	0.31335
H	1.50289	0.47217	0.99851

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H	-0.82330	-0.66130	1.12671
H	0.60555	-0.23718	-0.24542
H	-1.36550	-1.98425	-0.82912

val+07_58

C	0.67795	0.03383	-0.12901
C	-0.12733	1.19854	-0.04443
N	-0.07115	-1.11271	-0.31300
O	-1.36634	1.17192	-0.16723
O	-0.37151	-2.06734	0.93418
H	0.40531	2.15717	0.10247
H	0.29734	-1.84328	-0.91912
H	-1.02294	-0.79683	-0.57427
H	1.74787	-0.04221	-0.00712
H	-0.43379	-1.39311	1.63762

val+07_60

C	0.61587	-0.54769	-0.35427
C	-0.37050	0.38827	-0.01586
N	0.16871	-1.85338	0.16929
O	-1.33402	0.09275	0.73333
O	-0.28316	1.67315	-0.47231
H	0.82003	-2.31711	0.81051
H	-0.69327	-1.49445	0.70489
H	-0.13317	-2.54418	-0.52949
H	1.27708	-0.55007	-1.20768
H	0.54653	1.76490	-0.96922

val+07_61

C	-0.64971	1.06331	-0.04516
C	0.63814	0.60122	-0.22334
N	0.74634	-0.71650	0.28752
O	-0.82562	2.32851	-0.52894
O	0.79512	-1.85243	-0.71655
H	1.53980	1.00727	-0.67676
H	-0.13109	-0.83908	0.82390
H	1.57965	-0.95053	0.83296
H	-1.74274	2.56802	-0.33407
H	0.21752	-1.47530	-1.41056

val+07_62

C	-0.04746	0.79672	-0.38510
C	0.74566	1.13853	0.61805
N	-0.86158	-0.44486	-0.42682
O	-0.73929	-1.08190	-1.53611
O	-0.49137	-1.29496	0.80840
H	-0.17627	1.34465	-1.31099
H	1.33384	2.04859	0.55184
H	-1.83992	-0.24315	-0.14907
H	0.83581	0.52200	1.50370
H	-0.00772	-1.99171	0.32230

val+07_63

C	-0.36433	0.11911	0.12447
C	0.90399	0.26549	0.54453
N	-0.75842	-1.29263	0.00622
O	-1.43958	0.93204	-0.24026
O	1.24575	1.62525	0.64599
H	-1.53382	-1.57662	0.62538
H	-1.01208	-1.59051	-0.94888
H	0.13792	-1.72585	0.30723
H	-1.09316	1.83406	-0.13575
H	2.16153	1.64445	0.95028

val+07_64

C	0.46420	1.33207	0.07526
C	0.48224	2.50109	0.38609
N	0.53845	0.04358	-0.34405
O	0.55549	-0.87699	0.79225
O	-1.54631	-1.85280	-0.82503
H	0.44144	3.52465	0.67743
H	-1.21562	-2.55231	-1.40876
H	-0.28444	-0.26696	-0.87201
H	1.46836	-1.20947	0.76918
H	-1.01500	-1.94677	-0.01235

val+07_66

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C	-0.79653	0.56705	-0.93796
C	-0.92111	-0.81198	-0.31458
N	0.40758	-1.36075	-0.24365
O	-0.08662	1.45364	-0.65665
O	1.05798	1.04556	0.92693
H	-1.58807	-1.43721	-0.91331
H	-1.43155	-0.58144	0.64270
H	0.95955	-0.76998	0.39490
H	1.85399	1.46263	0.55196
H	0.38306	-2.33731	0.03357

val+07_69

C	-1.95001	2.02477	0.19901
C	0.36201	-1.14730	-0.14500
N	0.33480	0.24845	0.39099
O	-1.30977	2.13941	-0.75718
O	-0.63768	0.42854	1.31858
H	-0.61791	-1.33006	-0.58516
H	1.15955	-1.26211	-0.88791
H	0.51156	-1.81220	0.70541
H	0.19264	0.90109	-0.41334
H	1.27330	0.47081	0.76739

val+07_6

C	0.47615	-1.19592	0.09424
C	-0.32910	1.14435	0.18400
N	-0.50783	-0.26130	-0.13132
O	1.65600	-0.93063	0.22808
O	-1.81964	-0.73673	0.08046
H	-0.70932	1.36908	1.18752
H	-0.85286	1.76564	-0.54924
H	0.05832	-2.21825	0.09126
H	0.74239	1.34666	0.14075
H	-2.22411	-0.72939	-0.80485

val+07_71

C	-0.70041	0.84817	-0.17748
C	-0.95312	-0.41111	0.16609
N	0.07816	-1.39235	0.35670
O	-0.63867	1.97413	-0.48366
O	2.13787	0.47748	-0.12596
H	-2.01037	-0.63745	0.30502
H	2.29593	0.49222	-1.08148
H	-0.08370	-2.20532	-0.23523
H	0.09564	-1.71990	1.32161
H	1.64238	-0.35827	0.02499

val+07_72

C	-1.01324	0.58370	1.27678
C	-0.28234	1.21488	0.18356
N	0.35615	-1.68676	-0.47761
O	-1.21016	-0.67847	1.35922
O	0.95067	1.17317	0.05514
H	-0.89266	1.96380	-0.37075
H	1.01317	-0.90135	-0.41854
H	0.09632	-1.80504	-1.45579
H	-0.74476	-1.20523	0.57513
H	0.83885	-2.53460	-0.18326

val+07_74

C	1.61220	0.95061	-0.62425
C	0.56029	0.49105	0.05601
N	-2.02400	-1.57173	0.23115
O	1.95944	1.87502	0.37988
O	0.80006	1.36997	1.13191
H	-2.68833	-1.53473	-0.54090
H	-1.78503	-2.55482	0.35433
H	-2.54399	-1.30056	1.06481
H	2.17553	0.85095	-1.53789
H	-0.26927	-0.21145	0.05105

val+07_75

C	-0.84637	-1.35845	-0.30146
C	-1.30254	-0.14182	0.23833
N	1.79455	0.35430	0.11972
O	-2.43893	-0.56542	0.54645
O	-0.77666	1.00970	0.55343

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H	-1.19207	-1.48346	-1.33662
H	2.30983	0.53803	-0.73959
H	1.62259	-0.65265	0.16822
H	0.21496	0.95479	0.31915
H	2.40734	0.59339	0.89807

val+07_78

C	1.28653	1.00507	-0.26332
C	-1.07198	0.82727	-0.24588
N	-0.19793	-1.55110	0.46116
O	0.13719	1.49374	0.15094
O	-1.32241	0.59780	-1.38488
H	2.00579	1.77481	0.11441
H	-1.72024	0.74549	0.62892
H	-0.70370	-2.18061	-0.16014
H	0.62533	-1.22692	-0.05332
H	0.13650	-2.11235	1.24352

val+07_79

C	-1.16992	2.09696	0.03112
C	1.07931	-1.76894	-0.23714
N	0.43314	-0.68029	-0.15824
O	0.15193	2.06891	-0.10264
O	-1.91036	1.13548	0.09716
H	-1.52679	3.13804	0.07665
H	2.16522	-1.73758	-0.34764
H	0.61930	-2.76288	-0.20199
H	-0.58039	-0.79927	-0.05637
H	0.44688	1.11007	-0.14120

val+07_80

C	0.36445	0.74374	-0.50481
C	1.35170	0.09381	0.09819
N	-1.60193	-1.00177	0.39343
O	-0.43550	1.39100	-1.07455
O	2.63674	0.64673	0.05899
H	1.14036	-0.78274	0.69615
H	3.14644	0.15980	-0.60939
H	-2.09621	-0.34971	1.00070
H	-1.76816	-1.93284	0.77334
H	-2.07999	-0.96451	-0.50555

val+07_81

C	-0.89468	-0.81583	-0.75101
C	-1.52204	0.48267	-0.24440
N	2.09911	0.16398	0.38989
O	-1.59403	-1.63334	-1.31150
O	-0.88908	1.34648	0.32442
H	-2.61066	0.56768	-0.44244
H	1.36891	0.85212	0.57520
H	2.51667	-0.06596	1.29084
H	2.82307	0.64539	-0.14214
H	0.19144	-0.93119	-0.56866

val+07_82

C	2.32782	0.71222	-0.81190
C	0.65463	-0.16819	-0.21067
N	-0.26729	0.21349	0.74640
O	1.01376	0.86953	-1.14680
O	2.09011	-0.22163	0.13932
H	0.36207	-1.09552	-0.70512
H	-2.86275	1.02735	-0.17968
H	0.03713	0.98570	1.33100
H	-0.65578	-0.54790	1.29040
H	-3.57999	1.17194	-0.31333

val+07_84

C	-0.01385	1.60535	0.18724
C	0.31049	-2.08822	0.41440
N	-0.43583	1.00308	-0.94751
O	0.42289	1.03082	1.17635
O	-0.15298	-1.95080	-0.70162
H	-0.10017	2.70868	0.14442
H	0.53551	-3.09784	0.81188
H	0.52033	-1.22006	1.06258
H	-0.78386	1.55054	-1.72051
H	-0.40502	-0.01516	-1.02713

val+07_85
C 0.54342 -1.41221 -0.13114
C 0.50178 -0.10024 -0.28322
N -0.68498 0.67300 -0.39071
O 1.34075 -2.46596 0.14729
O -0.20010 -2.53772 -0.02467
H 1.43935 0.44467 -0.25618
H -1.52412 0.10672 -0.30267
H -1.56834 3.34760 1.60167
H -1.33017 2.75289 1.22101
H -0.73109 1.17455 -1.27548

val+07_86
C -0.46103 0.73405 -0.93254
C 0.39565 -0.44778 -0.50824
N 0.81443 -0.26347 0.93033
O -1.16782 0.69737 -1.91436
O 1.49973 0.88319 1.10209
H -0.36746 1.62342 -0.28198
H 1.33285 -0.44340 -1.07146
H -0.13705 -1.39449 -0.66378
H -0.04905 -0.31655 1.51374
H 1.35585 -1.10824 1.20410

val+07_87
C 0.92350 1.72714 0.79881
C -0.28056 -1.22781 0.36424
N 0.50501 -0.28590 -0.43350
O -0.34265 1.96672 1.20700
O 0.30180 2.60461 -0.02094
H -0.48234 -2.19060 -0.13034
H -1.23785 -0.76261 0.61855
H 1.42644 -0.65672 -0.65076
H 0.04212 -0.06371 -1.31242
H 0.25094 -1.42721 1.29997

val+07_88
C 1.11520 0.00747 0.30576
C -0.98644 -0.87225 -0.62336
N -0.21826 0.12182 -0.27117
O 0.25996 2.34901 -0.02639
O -0.66198 1.40372 -0.43970
H 1.80996 0.54135 -0.34413
H 1.35511 -1.05181 0.39677
H -0.63192 -1.88246 -0.48747
H -1.95696 -0.64152 -1.04094
H 1.10995 0.52188 1.26774

val+07_89
C 1.59958 0.17095 0.35663
C -1.75476 0.37309 -1.22752
N 0.69698 -0.59042 1.01546
O 1.36708 0.84945 -0.63571
O -1.96597 -0.38577 -0.30087
H 2.60930 0.12710 0.80956
H -2.57000 0.65571 -1.92285
H -0.27091 -0.63103 0.69043
H 0.96985 -1.12253 1.82834
H -0.75345 0.80165 -1.40527

val+07_8
C 0.60207 -0.29890 0.11255
C -1.56719 0.83871 -0.01742
N -0.74898 -0.21241 0.03750
O 1.25113 0.86659 -0.28068
O 1.06496 -1.48101 -0.47690
H -1.13600 1.82572 -0.06743
H -2.62409 0.67140 0.12163
H -1.18186 -1.13125 0.06294
H 1.74799 1.20569 0.47848
H 1.77818 -1.82224 0.08232

val+07_90
C -0.23478 -0.83280 0.27594
C -0.89843 -1.96158 0.35274
N 0.43777 0.19641 0.29057

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O	1.54030	2.73326	-0.45001
O	2.37384	2.24312	0.63925
H	-0.53205	-2.85055	-0.14872
H	-1.82947	-2.01740	0.90593
H	1.90209	1.40205	0.83636
H	1.16374	3.52672	-0.03023
H	0.28130	0.88548	-0.45372

val+07_91			
C	-0.39928	0.57039	-0.38120
C	-0.63743	1.87858	-0.48221
N	0.64889	-2.36512	0.13657
O	0.50304	2.22192	0.27010
O	0.76567	0.77779	0.38152
H	-1.30869	2.61850	-0.88638
H	1.19632	-2.92051	-0.51964
H	1.30983	-1.73910	0.59597
H	0.32646	-3.01172	0.85539
H	-0.72091	-0.42784	-0.63163

val+07_92			
C	-0.33293	-0.39265	0.58420
C	0.50167	0.83001	0.16190
N	-0.41425	-1.36883	-0.51291
O	0.88739	1.66140	0.94780
O	0.72776	0.89028	-1.15921
H	-1.33814	-0.02449	0.81671
H	0.30731	0.07163	-1.52581
H	-1.31543	-1.83727	-0.53661
H	0.08732	-0.78468	1.51760
H	0.29741	-2.08939	-0.41698

val+07_93			
C	-1.01628	0.52517	0.56519
C	0.36364	0.51564	-0.11729
N	0.83380	-0.86366	-0.31707
O	-1.51290	1.52645	1.02172
O	-1.61505	-0.67545	0.57302
H	0.23809	1.00043	-1.09157
H	1.03747	1.14961	0.47049
H	-0.96123	-1.28710	0.14897
H	1.35545	-0.96399	-1.18307
H	1.44732	-1.15589	0.43991

val+07_94			
C	-0.64436	1.09873	0.58923
C	0.77075	1.17057	0.00203
N	-0.11481	-1.32684	-0.41528
O	-0.86632	0.99100	1.77205
O	1.77162	1.12403	0.67741
H	-1.45318	1.19055	-0.16854
H	0.79593	1.30422	-1.10182
H	-1.02751	-1.77927	-0.43592
H	0.33969	-1.61771	0.44923
H	0.43079	-1.71578	-1.18289

val+07_95			
C	1.06330	-0.93712	0.82295
C	1.50350	-0.61514	-0.38304
N	-1.48724	0.83693	-0.17061
O	0.68603	-0.37335	-1.46806
O	0.65357	-1.12523	1.91878
H	2.57305	-0.61456	-0.56417
H	-0.12119	0.09666	-1.12567
H	-1.44021	0.55124	0.80690
H	-2.40510	0.56142	-0.51623
H	-1.45792	1.85516	-0.18164

val+07_97			
C	-1.09645	0.70361	-0.35839
C	0.19488	0.77323	-0.04454
N	0.94709	-0.40422	0.41739
O	2.10936	-0.54514	-0.26838
O	-1.82341	-0.43337	-0.10127
H	-1.62587	1.54509	-0.79879
H	0.82533	1.63655	-0.19794
H	0.30897	-1.21917	0.31779

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H	1.09336	-0.31476	1.44553
H	-2.59936	-0.45932	-0.68020
val+07_98			
C	-0.85018	0.97462	-0.29295
C	0.50402	0.56052	-0.51600
N	0.77458	-0.60302	0.06595
O	1.83730	-1.24824	0.07610
O	-1.04722	2.14736	-0.90606
H	1.31058	1.03775	-1.06885
H	0.18017	-3.24366	1.79312
H	0.78123	-2.98320	1.43795
H	-0.04453	-0.99392	0.57290
H	-1.96856	2.40829	-0.74245
val+07_99			
C	-1.00155	0.71978	0.52531
C	0.27096	0.81105	-0.03283
N	0.86224	-0.46610	-0.48126
O	-1.71485	1.57272	1.04466
O	-1.50829	-0.61949	0.41618
H	0.93328	1.65673	0.03923
H	1.65103	-0.81969	0.08391
H	0.08760	-1.14613	-0.38947
H	1.17667	-0.47110	-1.46097
H	-2.40119	-0.55957	0.79324
val+07_9			
C	-0.48688	1.16628	0.49894
C	-0.25502	2.50208	-0.30341
N	0.20104	1.17662	-0.58414
O	0.17348	-1.53229	1.23503
O	0.60084	-1.64606	-0.15436
H	-1.05882	2.90210	-0.91871
H	0.46689	3.22406	0.07422
H	-0.23739	-0.62857	1.21213
H	0.75575	0.54197	-1.15285
H	-0.00200	-2.34539	-0.46034

Coordinates and thermochemical properties for the all C₂H₅NO₂ water phase structures

Filename	dfH	S(scaled)S(UNscaled)		G	Cv(UNscaled)
Units	kJ/mol	J/molK	J/molK	Hartree	J/molK
val+03_10:	-353.3	310.9	308.7	-284.080661	79.1
val+03_12:	-356.9	318.9	316.5	-284.082938	81.2
val+03_13:	74.8	315.7	313.2	-283.918144	84.9
val+03_14:	-12.5	320.4	318.1	-283.951937	81.2
val+03_15:	-40.6	322.8	320.1	-283.962894	89.3
val+03_16:	-110.2	321.4	319.0	-283.989241	83.4
val+03_17:	-60.1	318.2	315.6	-283.969813	87.2
val+03_18:	-145.3	318.2	315.8	-284.002267	83.8
val+03_19:	-27.5	321.8	319.6	-283.957781	79.1
val+03_1:	-132.6	315.6	313.1	-283.997120	83.7
val+03_20:	-169.1	314.3	312.2	-284.010885	77.5
val+03_21:	-38.2	323.7	321.4	-283.962085	80.5
val+03_22:	-311.9	316.9	314.8	-284.065559	75.6
val+03_24:	-52.2	323.5	321.1	-283.967403	82.5
val+03_25:	-153.6	329.8	327.5	-284.006725	82.0
val+03_27:	-102.6	317.3	314.9	-283.985869	82.8
val+03_28:	-350.4	307.3	305.2	-284.079121	76.4
val+03_29:	102.0	326.9	324.4	-283.909053	85.0
val+03_2:	-30.8	307.5	305.1	-283.957436	83.0
val+03_30:	85.9	319.7	317.4	-283.914345	80.1
val+03_31:	-55.3	316.3	314.1	-283.967739	76.9
val+03_32:	-174.6	319.9	317.7	-284.013605	78.7
val+03_33:	-384.4	316.1	314.0	-284.093091	76.8
val+03_34:	-329.4	319.0	316.7	-284.072455	81.7
val+03_35:	-256.2	315.0	312.7	-284.044127	81.9
val+03_36:	-447.0	318.2	316.0	-284.117178	78.6
val+03_37:	-417.7	318.6	316.2	-284.106054	81.5
val+03_38:	-404.2	313.4	311.2	-284.100331	77.9
val+03_39:	-221.1	325.2	322.9	-284.031918	80.7
val+03_3:	-164.3	312.8	310.3	-284.008885	84.9
val+03_40:	-149.4	311.0	308.8	-284.002998	79.2
val+03_41:	-121.5	324.4	322.2	-283.993875	77.8
val+03_42:	-154.0	316.1	313.9	-284.005314	77.6

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val+03_43:	-367.5	314.6	312.4	-284.086458	76.1
val+03_44:	-190.1	317.3	315.0	-284.019212	78.2
val+03_45:	-214.7	314.8	312.7	-284.028296	75.6
val+03_46:	-252.4	318.7	316.4	-284.043079	80.2
val+03_47:	-430.6	314.7	312.4	-284.110510	79.5
val+03_48:	-104.9	320.2	318.0	-283.987083	77.9
val+03_49:	-78.2	316.3	314.1	-283.976458	76.2
val+03_4:	-308.1	311.0	308.5	-284.063425	85.5
val+03_50:	15.3	307.1	305.0	-283.939834	75.6
val+03_51:	-89.6	301.3	299.2	-283.979098	73.8
val+03_52:	-108.1	310.7	308.6	-283.987238	74.1
val+03_53:	-105.7	303.2	301.3	-283.985476	69.3
val+03_54:	-122.6	302.7	300.9	-283.991864	69.2
val+03_55:	-256.2	296.7	294.9	-284.042043	67.9
val+03_56:	-272.3	302.6	300.4	-284.048862	78.1
val+03_57:	-31.5	305.0	302.7	-283.957411	78.5
val+03_58:	-129.4	306.0	303.8	-283.994811	76.8
val+03_59:	140.8	306.7	304.5	-283.891973	77.3
val+03_5:	-306.3	316.6	314.0	-284.063377	87.5
val+03_60:	1.1	299.4	297.5	-283.944355	70.2
val+03_61:	-75.8	297.7	295.8	-283.973469	69.2
val+03_62:	-94.8	306.3	304.3	-283.981669	72.9
val+03_63:	-270.4	304.3	302.0	-284.048334	79.2
val+03_64:	-170.7	302.2	300.0	-284.010105	77.6
val+03_65:	-244.2	303.2	301.0	-284.038218	77.6
val+03_66:	-99.6	312.1	309.8	-283.984158	81.1
val+03_67:	-266.2	296.8	294.6	-284.045867	76.9
val+03_68:	111.1	299.1	297.2	-283.902438	70.7
val+03_69:	22.7	307.5	305.6	-283.937032	70.0
val+03_6:	-320.8	313.0	310.7	-284.068502	79.9
val+03_70:	-40.5	307.7	305.6	-283.961154	74.9
val+03_71:	-91.4	310.4	308.4	-283.980838	72.3
val+03_72:	-26.1	299.9	298.0	-283.954777	72.0
val+03_73:	-31.5	307.7	305.7	-283.957736	74.1
val+03_74:	-70.9	311.3	309.3	-283.973150	74.1
val+03_75:	-262.0	294.0	292.2	-284.043948	68.1
val+03_76:	30.6	296.9	295.1	-283.932838	67.5
val+03_77:	-35.7	295.3	293.8	-283.957903	62.5
val+03_78:	-34.7	295.9	294.2	-283.957595	63.5
val+03_79:	-131.9	289.5	287.9	-283.993879	61.4
val+03_7:	-182.7	318.3	316.0	-284.016497	80.6
val+03_80:	202.3	308.3	306.2	-283.868737	75.4
val+03_81:	147.3	297.4	295.5	-283.888425	70.1
val+03_82:	27.4	308.6	306.5	-283.935388	74.6
val+03_83:	44.2	299.8	298.0	-283.928000	69.4
val+03_84:	-100.2	304.3	302.0	-283.983500	79.8
val+03_8:	-321.4	313.1	310.9	-284.068721	78.2
val+03_9:	-308.4	306.2	304.0	-284.063009	78.4
val+05_100:	-438.5	321.6	319.3	-284.114319	80.4
val+05_103:	-224.2	305.4	303.2	-284.030832	76.3
val+05_105:	-168.5	307.4	305.1	-284.009846	78.8
val+05_106:	-321.7	383.5	380.6	-284.076837	94.7
val+05_107:	-172.8	388.1	385.3	-284.020674	93.6
val+05_108:	-151.1	305.2	303.1	-284.002998	74.8
val+05_109:	-152.3	316.9	314.7	-284.004753	76.0
val+05_10:	-233.0	367.1	364.3	-284.041191	93.5
val+05_110:	-273.1	360.0	357.0	-284.055677	99.4
val+05_112:	-24.4	301.2	299.4	-283.954273	68.4
val+05_113:	-22.0	310.4	308.1	-283.954414	78.9
val+05_114:	22.5	296.3	294.5	-283.935869	66.7
val+05_115:	-26.5	293.3	291.6	-283.954163	64.2
val+05_116:	0.5	320.9	318.6	-283.947011	78.6
val+05_117:	-414.8	313.9	311.6	-284.104427	81.4
val+05_118:	-411.3	307.1	305.1	-284.102304	71.4
val+05_119:	-294.2	426.5	422.9	-284.071248	113.8
val+05_11:	-220.2	357.3	354.4	-284.035226	95.3
val+05_120:	-436.5	371.4	368.8	-284.119191	88.9
val+05_122:	-349.1	353.4	350.7	-284.083876	90.8
val+05_123:	-289.1	359.9	356.7	-284.061744	101.4
val+05_125:	-353.5	362.8	360.3	-284.086603	84.1
val+05_127:	-107.3	320.6	318.5	-283.988062	77.0
val+05_128:	-363.5	363.4	360.7	-284.090479	90.1
val+05_129:	-9.6	317.3	315.1	-283.950460	77.8
val+05_12:	-414.8	314.0	311.7	-284.104422	81.4
val+05_130:	-251.7	375.3	372.4	-284.049247	97.3
val+05_131:	-293.4	443.9	440.2	-284.072924	114.3
val+05_132:	-289.0	382.7	379.6	-284.064324	99.4

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val+05_133:	-121.2	307.5	305.3	-283.991865	75.4
val+05_134:	-256.2	314.5	312.1	-284.044051	81.7
val+05_135:	-121.0	315.6	313.6	-283.992698	72.6
val+05_136:	-122.9	309.8	307.8	-283.992746	72.0
val+05_137:	80.8	313.4	310.9	-283.915592	84.0
val+05_139:	64.3	385.3	382.0	-283.930037	104.1
val+05_13:	-271.5	303.0	300.9	-284.048609	76.0
val+05_140:	-22.6	348.6	345.6	-283.958946	97.4
val+05_141:	-163.7	345.1	342.2	-284.012300	93.0
val+05_143:	83.9	367.4	364.2	-283.920532	103.3
val+05_144:	-33.4	333.8	331.2	-283.961385	87.5
val+05_145:	-202.1	313.1	310.9	-284.023302	78.6
val+05_146:	92.8	322.9	320.3	-283.912113	88.5
val+05_147:	-89.0	314.7	312.2	-283.980405	84.2
val+05_148:	-171.5	314.5	312.2	-284.011807	80.9
val+05_149:	-20.0	315.7	313.3	-283.954253	81.9
val+05_150:	-194.0	306.7	304.4	-284.019499	80.5
val+05_152:	-45.4	328.2	325.4	-283.965353	91.8
val+05_153:	-15.2	318.7	316.2	-283.952751	84.2
val+05_154:	-50.9	316.8	314.5	-283.966116	79.9
val+05_155:	72.1	317.4	315.0	-283.919344	82.2
val+05_156:	-201.6	308.6	306.4	-284.022614	79.4
val+05_157:	197.5	327.2	324.5	-283.872684	89.1
val+05_158:	148.6	320.2	317.8	-283.890541	83.1
val+05_159:	111.7	320.6	318.3	-283.904626	79.9
val+05_15:	-256.2	315.5	313.2	-284.044192	81.9
val+05_160:	-8.3	323.9	321.6	-283.950706	80.6
val+05_161:	-35.2	335.8	333.2	-283.962332	89.1
val+05_162:	237.9	329.7	327.2	-283.857622	85.9
val+05_16:	-447.1	318.3	316.1	-284.117192	78.6
val+05_17:	223.9	304.4	302.1	-283.860081	80.4
val+05_18:	183.9	307.8	305.5	-283.875668	79.9
val+05_19:	80.9	297.9	296.0	-283.913800	71.1
val+05_1:	210.4	369.9	367.0	-283.872639	95.4
val+05_20:	-158.5	306.6	304.5	-284.005977	76.2
val+05_21:	177.9	298.8	296.8	-283.876929	72.8
val+05_22:	-185.1	319.8	317.4	-284.017597	82.0
val+05_23:	-245.6	355.8	353.3	-284.044716	87.1
val+05_24:	111.4	307.3	305.2	-283.903247	75.1
val+05_27:	-151.1	304.8	302.8	-284.002952	74.7
val+05_28:	-71.8	307.2	304.8	-283.973007	81.2
val+05_29:	24.7	303.0	300.9	-283.935777	75.1
val+05_2:	-85.6	321.0	318.6	-283.979823	82.2
val+05_30:	138.9	309.0	306.8	-283.892962	77.5
val+05_31:	113.3	319.9	317.3	-283.903961	85.3
val+05_32:	152.7	321.3	318.8	-283.889094	85.8
val+05_33:	287.8	300.3	298.2	-283.835239	74.8
val+05_34:	-86.2	350.8	348.1	-283.983460	90.6
val+05_35:	136.9	299.8	297.8	-283.892673	72.8
val+05_36:	79.3	312.3	310.2	-283.916036	74.0
val+05_37:	-197.4	353.2	350.4	-284.026056	92.6
val+05_38:	70.7	316.3	313.9	-283.919753	84.5
val+05_39:	-144.5	363.0	359.7	-284.007038	103.1
val+05_40:	22.6	312.1	309.8	-283.937610	81.2
val+05_41:	-156.3	308.9	306.5	-284.005405	83.1
val+05_42:	77.3	303.9	301.6	-283.915831	81.0
val+05_43:	230.6	301.1	298.7	-283.857139	81.6
val+05_44:	-92.4	303.8	301.3	-283.980452	83.4
val+05_45:	-303.7	314.3	311.7	-284.062122	87.5
val+05_46:	-240.9	308.7	306.4	-284.037584	79.4
val+05_47:	-101.2	312.2	309.9	-283.984778	81.3
val+05_48:	-262.2	304.3	302.1	-284.045215	78.5
val+05_49:	-47.0	339.9	337.0	-283.967259	94.7
val+05_4:	-104.8	361.0	357.8	-283.991697	102.9
val+05_50:	-224.4	387.9	384.6	-284.040312	105.3
val+05_51:	-127.9	313.1	310.6	-283.995026	85.2
val+05_52:	-55.7	304.1	302.0	-283.966526	75.2
val+05_53:	-30.8	317.1	314.9	-283.958517	77.8
val+05_54:	-127.1	310.9	308.7	-283.994483	77.2
val+05_55:	-57.5	311.9	309.4	-283.968090	84.8
val+05_56:	-121.6	305.3	303.0	-283.991737	78.4
val+05_58:	-296.5	322.5	320.1	-284.060324	82.6
val+05_5:	-251.2	327.2	324.6	-284.043602	88.3
val+05_61:	-123.7	308.1	306.0	-283.992877	75.8
val+05_62:	278.2	311.7	309.5	-283.840199	76.5
val+05_63:	-99.0	315.5	313.1	-283.984308	81.7
val+05_64:	135.9	315.8	313.5	-283.894869	80.5

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val+05_65:	-430.5	315.2	312.9	-284.110550	79.4
val+05_67:	-110.4	376.0	373.3	-283.995526	90.1
val+05_69:	-97.9	333.2	330.7	-283.985887	85.2
val+05_6:	-228.2	309.9	307.7	-284.032890	78.9
val+05_70:	234.1	310.3	308.2	-283.856832	76.6
val+05_71:	150.9	315.9	313.6	-283.889185	79.9
val+05_72:	-55.8	304.5	302.4	-283.966587	75.3
val+05_73:	-339.5	402.8	400.0	-284.085825	95.0
val+05_74:	-349.1	353.0	350.2	-284.083814	90.8
val+05_76:	-120.2	310.7	308.7	-283.991845	72.1
val+05_77:	-152.0	322.0	319.7	-284.005229	78.6
val+05_78:	-413.0	315.2	313.0	-284.103868	77.3
val+05_79:	-359.8	319.8	317.6	-284.084119	76.9
val+05_7:	-307.0	318.2	315.9	-284.063824	80.8
val+05_80:	-290.4	352.3	349.5	-284.061389	94.6
val+05_81:	-290.4	352.7	349.8	-284.061434	94.6
val+05_83:	-213.3	317.3	315.2	-284.028041	74.2
val+05_84:	239.6	309.5	307.4	-283.854671	74.7
val+05_85:	-39.5	376.8	374.3	-283.968628	85.6
val+05_86:	178.8	314.5	312.3	-283.878400	77.9
val+05_88:	-100.2	304.4	302.1	-283.983522	79.8
val+05_8:	-111.5	380.2	377.1	-283.996428	99.5
val+05_90:	-42.1	304.5	302.4	-283.961381	75.4
val+05_91:	67.3	298.2	296.1	-283.919009	76.6
val+05_92:	-168.3	317.4	315.2	-284.010898	77.5
val+05_93:	-113.5	324.5	322.0	-283.990846	85.0
val+05_94:	18.5	315.0	312.6	-283.939503	82.0
val+05_95:	-311.0	365.9	363.0	-284.070793	96.5
val+05_96:	-141.8	321.0	318.5	-284.001252	83.8
val+05_97:	-91.8	327.4	324.9	-283.982912	85.9
val+05_98:	-347.1	361.2	357.9	-284.083989	102.5
val+05_99:	-162.9	312.2	309.7	-284.008254	84.2
val+05_9:	-306.9	317.1	314.8	-284.063677	80.6
val+07_100:	-251.1	326.4	323.8	-284.043493	88.2
val+07_101:	122.7	319.4	317.4	-283.900332	74.7
val+07_102:	-89.2	308.8	306.5	-283.979812	78.7
val+07_103:	67.3	297.8	295.7	-283.918966	76.5
val+07_104:	-47.6	296.9	294.9	-283.962618	73.6
val+07_105:	67.2	298.3	296.2	-283.919051	76.6
val+07_106:	22.5	312.7	310.3	-283.937705	81.4
val+07_109:	-80.9	314.9	312.7	-283.977353	77.4
val+07_10:	-145.2	315.9	313.6	-284.001949	80.2
val+07_110:	-330.1	372.7	369.9	-284.078840	92.7
val+07_111:	-120.6	367.9	364.8	-283.998493	100.8
val+07_113:	-96.6	307.7	305.7	-283.982521	73.9
val+07_114:	-349.1	353.8	351.1	-284.083927	90.9
val+07_115:	-254.1	311.7	309.2	-284.042949	84.8
val+07_116:	-303.4	313.3	310.7	-284.061905	86.7
val+07_117:	-107.6	344.6	341.8	-283.990881	92.6
val+07_118:	-294.1	429.5	425.8	-284.071560	113.8
val+07_119:	-289.0	378.9	375.9	-284.063869	99.1
val+07_11:	-191.2	314.1	311.8	-284.019278	80.1
val+07_120:	-152.2	318.5	316.4	-284.004898	77.1
val+07_121:	-121.2	307.1	305.0	-283.991824	75.3
val+07_122:	110.0	307.5	305.3	-283.903811	77.4
val+07_123:	0.5	323.1	320.9	-283.947275	78.8
val+07_124:	-24.3	301.3	299.5	-283.954264	68.6
val+07_125:	147.2	296.6	294.6	-283.888402	72.4
val+07_126:	-292.7	446.7	443.1	-284.073000	113.8
val+07_128:	-175.3	317.6	315.4	-284.013620	78.8
val+07_129:	-92.9	304.2	302.1	-283.980717	74.5
val+07_130:	-251.5	367.8	364.8	-284.048355	97.3
val+07_131:	-92.4	329.1	326.6	-283.983337	86.2
val+07_134:	-307.1	320.2	317.8	-284.064099	81.0
val+07_135:	-108.5	308.4	306.5	-283.987116	70.3
val+07_136:	-256.2	315.9	313.5	-284.044239	81.9
val+07_137:	-44.9	320.2	318.0	-283.964234	78.3
val+07_138:	209.0	300.5	298.3	-283.865315	78.8
val+07_139:	111.7	303.0	300.9	-283.902626	74.3
val+07_13:	-167.3	374.1	371.3	-284.016992	92.3
val+07_140:	-209.6	317.6	315.4	-284.026665	78.6
val+07_141:	-353.0	358.2	355.8	-284.085914	84.3
val+07_143:	-13.5	324.7	322.4	-283.952777	81.5
val+07_144:	-193.8	320.4	318.2	-284.020978	77.5
val+07_145:	-44.5	377.8	374.4	-283.970634	107.3
val+07_146:	-166.8	381.0	377.5	-284.017558	109.5
val+07_148:	-120.6	368.0	364.9	-283.998500	100.8

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val+07_149:	-204.2	332.1	329.6	-284.026268	84.4
val+07_14:	-181.3	377.9	375.0	-284.022722	93.4
val+07_150:	67.2	298.1	295.9	-283.919014	76.6
val+07_151:	18.5	314.8	312.4	-283.939469	82.0
val+07_152:	-384.9	313.5	311.3	-284.092951	76.3
val+07_153:	-108.9	319.3	317.3	-283.988511	73.6
val+07_154:	-23.7	310.6	308.4	-283.955086	79.2
val+07_155:	-123.7	308.4	306.3	-283.992902	75.9
val+07_158:	-63.1	394.3	391.5	-283.979574	93.3
val+07_15:	-189.9	383.7	381.1	-284.026687	89.8
val+07_17:	-242.7	308.4	306.1	-284.038231	78.4
val+07_18:	-321.7	385.0	382.1	-284.077015	94.7
val+07_19:	222.0	320.8	318.2	-283.862664	89.3
val+07_1:	-47.0	340.1	337.2	-283.967304	94.7
val+07_21:	-389.4	311.8	309.7	-284.094508	75.2
val+07_22:	-175.0	347.5	344.6	-284.016879	94.2
val+07_23:	-30.7	318.5	316.3	-283.958648	77.8
val+07_24:	-294.1	430.1	426.5	-284.071624	113.8
val+07_25:	-296.0	452.4	448.7	-284.074907	116.0
val+07_26:	-114.8	400.7	397.6	-283.999992	98.5
val+07_27:	143.2	316.2	314.0	-283.892127	77.2
val+07_29:	180.2	315.2	312.9	-283.877951	81.6
val+07_2:	-225.2	381.9	378.6	-284.039905	105.1
val+07_30:	-339.5	407.6	404.7	-284.086360	95.0
val+07_31:	129.1	313.2	310.9	-283.897181	79.6
val+07_32:	-27.4	316.3	314.1	-283.957122	78.4
val+07_36:	-313.6	423.1	419.6	-284.078259	110.9
val+07_39:	-285.3	531.5	526.6	-284.079780	145.3
val+07_3:	-128.0	313.8	311.3	-283.995142	85.3
val+07_41:	-273.2	361.1	358.0	-284.055826	99.5
val+07_42:	136.8	389.6	386.7	-283.902902	93.5
val+07_44:	-85.6	322.2	319.9	-283.979969	82.4
val+07_46:	-139.0	307.5	305.3	-283.998637	79.5
val+07_47:	128.0	302.9	300.9	-283.896404	71.7
val+07_48:	-304.9	376.0	372.7	-284.069587	104.2
val+07_49:	19.5	320.2	317.8	-283.939697	81.6
val+07_4:	-389.5	311.8	309.7	-284.094533	75.3
val+07_50:	-323.4	394.9	392.2	-284.078811	89.1
val+07_51:	-124.0	316.7	314.4	-283.993985	81.8
val+07_52:	350.6	324.7	322.2	-283.814103	84.1
val+07_53:	-62.4	376.9	373.9	-283.977348	99.4
val+07_54:	-125.8	397.9	395.0	-284.003874	96.4
val+07_56:	19.5	323.8	321.4	-283.940114	81.9
val+07_57:	260.7	388.0	384.9	-283.855538	100.0
val+07_58:	-94.0	319.3	317.0	-283.982846	81.4
val+07_59:	311.3	396.3	392.6	-283.837217	116.1
val+07_60:	11.8	349.1	346.1	-283.945912	95.1
val+07_61:	61.7	315.2	312.7	-283.923084	83.9
val+07_62:	22.6	311.9	309.5	-283.937583	81.2
val+07_63:	-82.6	320.3	317.7	-283.978611	86.9
val+07_64:	-44.1	364.8	361.4	-283.968986	107.0
val+07_65:	-166.7	379.9	376.4	-284.017405	109.4
val+07_67:	-295.1	452.9	449.2	-284.074593	115.8
val+07_69:	-127.5	337.1	334.6	-283.997623	84.8
val+07_6:	12.1	314.8	312.1	-283.941908	89.4
val+07_73:	-251.6	369.1	366.1	-284.048532	97.3
val+07_74:	64.1	371.4	368.5	-283.928521	93.9
val+07_75:	-251.6	376.1	373.3	-284.049316	94.8
val+07_76:	-30.8	315.7	313.5	-283.958340	77.8
val+07_78:	-158.6	316.1	313.9	-284.007098	78.0
val+07_81:	-289.0	376.8	373.7	-284.063630	99.1
val+07_83:	-55.8	304.2	302.1	-283.966571	75.3
val+07_84:	-347.6	379.9	377.2	-284.086312	91.9
val+07_85:	136.4	378.8	375.3	-283.901843	109.9
val+07_86:	-172.2	320.9	318.7	-284.012817	79.2
val+07_87:	222.0	308.5	306.3	-283.861244	77.2
val+07_88:	180.2	316.8	314.5	-283.878139	81.7
val+07_89:	-349.1	353.5	350.8	-284.083873	90.9
val+07_8:	-149.9	317.5	314.9	-284.003924	88.6
val+07_90:	5.5	378.3	375.2	-283.951650	99.9
val+07_91:	64.1	373.6	370.7	-283.928784	93.9
val+07_92:	-290.1	362.9	359.7	-284.062464	102.3
val+07_93:	-411.4	304.5	302.5	-284.102025	71.3
val+07_95:	-251.6	365.8	362.9	-284.048161	97.3
val+07_98:	-76.7	310.7	308.5	-283.975260	76.6
val+07_9:	212.3	379.4	376.5	-283.872987	95.0

val+03_10			
C	0.16008	0.12114	-0.31727
C	-1.33528	-0.01587	-0.10275
N	0.67214	1.28392	-0.33041
O	0.87616	-1.01366	-0.48614
O	-1.94299	1.24373	0.06675
H	-1.76660	-0.54392	-0.96788
H	-1.50693	-0.65299	0.77916
H	1.68272	1.25772	-0.48231
H	0.29976	-1.79677	-0.43992
H	-1.20527	1.88429	-0.01092

val+03_12			
C	0.43177	-0.34981	0.12132
C	-1.88180	-0.63519	-0.04278
N	-0.52438	-1.16856	-0.02610
O	0.39824	1.00093	0.27346
O	1.70519	-0.79361	0.14283
H	-2.05467	0.05882	-0.88008
H	-2.14701	-0.11300	0.89009
H	-2.58833	-1.46146	-0.15945
H	-0.52156	1.31533	0.25766
H	2.29676	-0.03115	0.26294

val+03_13			
C	-0.05135	-0.98890	0.16905
C	1.26009	-1.12456	-0.05096
N	-0.86858	0.04557	-0.32413
O	-0.24489	1.18626	-0.72391
O	0.27942	1.95000	0.47296
H	-0.62270	-1.72434	0.72944
H	1.83046	-0.40733	-0.63284
H	1.78656	-1.98605	0.34233
H	-1.68243	0.26133	0.24894
H	1.13723	1.50182	0.60193

val+03_14			
C	0.18732	-0.72818	-0.26816
C	1.48633	-1.01983	-0.23122
N	-1.72206	0.47371	0.26287
O	-0.39805	0.07338	0.68292
O	-1.61996	1.79258	-0.25472
H	-0.50627	-1.10878	-1.01374
H	2.14447	-0.61335	0.53039
H	1.90567	-1.69525	-0.96780
H	-2.14070	0.65160	1.17750
H	-1.65454	1.65572	-1.21735

val+03_15			
C	-0.23768	0.46149	-0.14357
C	1.10676	0.37423	-0.01736
N	-1.03916	1.46958	0.33564
O	1.75321	-0.68232	-0.58453
O	2.21550	-1.64347	0.51172
H	-0.76316	-0.34248	-0.65318
H	1.71832	1.11875	0.49232
H	-1.89898	1.63849	-0.17060
H	-0.57933	2.32657	0.62043
H	1.37502	-2.11503	0.66704

val+03_16			
C	0.26101	0.08339	0.41542
C	1.46167	-0.10410	-0.14229
N	-1.67096	1.27581	-0.01941
O	-0.28716	1.34809	0.44284
O	2.18774	-1.26382	-0.12644
H	-0.31633	-0.70228	0.90091
H	1.99112	0.70031	-0.64262
H	-1.61063	1.58301	-0.99516
H	-2.09172	2.06422	0.47647
H	1.68196	-1.95403	0.33538

val+03_17			
C	-0.16917	0.45786	0.16333
C	1.13218	0.25025	-0.07462
N	-0.84535	1.67700	0.21150

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O	-1.10016	-0.52123	0.48902
O	-0.52357	-1.83681	0.42552
H	1.76131	1.08378	-0.36370
H	1.57771	-0.72615	0.04551
H	-1.73706	1.65829	-0.27735
H	-0.27633	2.44485	-0.12839
H	-0.62616	-2.04794	-0.52393

val+03_18			
C	0.14757	-0.08728	0.12590
C	1.47222	-0.15949	-0.05174
N	-1.58785	1.39802	-0.36073
O	-0.44483	1.07757	0.50261
O	-0.74331	-1.11168	0.06969
H	2.06736	0.74409	-0.02871
H	1.97287	-1.11162	-0.18779
H	-2.39022	1.23047	0.25079
H	-1.50401	2.41515	-0.41065
H	-0.30040	-1.89443	-0.29767

val+03_19			
C	0.97241	-0.54126	0.14583
C	-1.30573	-0.80760	-0.22253
N	0.03233	-0.51580	-0.70785
O	-2.26378	0.00715	-0.87105
O	-2.06044	1.36826	-0.40264
H	0.82569	-0.75265	1.21404
H	1.99541	-0.34757	-0.18018
H	-1.40275	-0.71204	0.86950
H	-1.58827	-1.82074	-0.53419
H	-1.37908	1.67655	-1.03122

val+03_1			
C	-0.12274	-0.41135	-0.01681
C	1.19463	-0.51803	-0.21647
N	-0.84939	0.80552	0.12187
O	1.90725	-1.69575	-0.25176
O	-0.10613	1.90965	-0.42036
H	-0.75201	-1.28585	0.13950
H	1.83477	0.34096	-0.37255
H	-1.69703	0.76307	-0.44569
H	1.29971	-2.43974	-0.10436
H	-0.00426	2.49561	0.34772

val+03_20			
C	1.69154	-0.12824	0.15393
C	-1.70330	-0.54669	-0.26652
N	0.57777	-0.18879	-0.46129
O	-0.44644	-0.64482	0.39239
O	-2.18720	0.76288	-0.34627
H	2.55369	0.18958	-0.42463
H	1.80752	-0.37959	1.20869
H	-2.35421	-1.20003	0.32469
H	-1.61207	-0.90819	-1.29305
H	-2.39669	1.05898	0.55517

val+03_21			
C	0.69892	-0.58927	-0.12708
C	-0.78468	-0.64794	0.16688
N	1.50882	-1.57050	-0.17986
O	-1.25835	0.50090	0.86530
O	-1.30149	1.59043	-0.10391
H	1.09325	0.41062	-0.33440
H	-1.35538	-0.77607	-0.76301
H	-1.02030	-1.48451	0.83485
H	1.02109	-2.45156	0.03042
H	-0.67807	2.21570	0.31001

val+03_22			
C	0.67909	-0.24575	-0.00924
C	-1.65686	-0.56556	-0.35805
N	1.89135	-0.42901	-0.33287
O	-0.29762	-0.90339	-0.67668
O	-2.18332	0.38590	-1.22766
H	0.31451	0.40431	0.79583
H	-1.71158	-0.25041	-0.69137
H	-2.22182	-1.48483	-0.50927

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H	2.48621	0.12549	0.28479
H	-1.87017	1.26566	-0.96022
val+03_24			
C	-0.06996	-0.15952	-0.11932
C	-2.37929	-0.16024	0.09117
N	-1.12881	-0.82612	-0.24787
O	1.12165	-0.77944	-0.41691
O	2.18285	0.20099	-0.32004
H	0.05299	0.87782	0.20558
H	-2.25300	0.88341	0.41605
H	-3.04508	-0.17628	-0.77921
H	-2.88024	-0.71539	0.89245
H	2.63761	-0.11123	0.48600
val+03_25			
C	0.10580	-0.30708	0.20101
C	-2.24173	-0.26487	0.15429
N	1.21716	-0.66870	0.71615
O	-1.03423	-0.66568	0.82003
O	2.28711	-0.17999	-0.08063
H	0.02927	0.28245	-0.71520
H	-2.28566	0.82407	0.04627
H	-3.05984	-0.60221	0.79078
H	-2.32148	-0.73969	-0.82934
H	3.06299	-0.51740	0.39415
val+03_27			
C	0.22530	0.82699	0.13431
C	-1.23120	0.53564	-0.05026
N	0.73786	1.98104	-0.00926
O	1.07224	-0.21181	0.47551
O	0.36477	-1.45885	0.71657
H	-1.73048	1.45999	-0.34313
H	-1.67399	0.15564	0.87502
H	-1.38435	-0.22561	-0.82114
H	1.74759	1.95518	0.17096
H	0.63496	-1.96702	-0.07258
val+03_28			
C	0.52542	-0.27685	-0.33822
C	-1.82801	-0.55513	-0.32931
N	0.58688	0.80967	0.32444
O	-0.52965	-1.02285	-0.71563
O	1.63461	-0.88942	-0.79967
H	-2.03253	0.42910	-0.76313
H	-2.53239	-1.28553	-0.72620
H	-1.91748	-0.51028	0.76098
H	-0.33074	1.15021	0.60411
H	2.38669	-0.33922	-0.51888
val+03_29			
C	0.25443	-0.93504	0.21277
C	1.41622	-1.13666	-0.41078
N	-1.51572	1.29972	-0.40910
O	0.04256	0.19807	0.94815
O	-1.40325	0.59527	0.78389
H	-0.55789	-1.65850	0.24389
H	2.19200	-0.37755	-0.42403
H	1.62473	-2.09478	-0.87427
H	-2.23749	0.82530	-0.95067
H	-1.83309	2.23558	-0.15735
val+03_2			
C	0.35578	-0.90554	-0.18451
C	1.68854	-0.97434	-0.17804
N	-0.40100	0.24825	-0.52850
O	-1.47691	0.32677	0.41504
O	0.35867	1.42723	-0.43228
H	-0.28388	-1.75937	0.01085
H	2.31531	-0.11871	-0.40200
H	2.17628	-1.92052	0.02802
H	-2.18455	0.74916	-0.10279
H	0.73897	1.43317	0.47429
val+03_30			
C	1.82249	0.42505	0.10843

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C	-2.14815	-0.47223	0.16284
N	0.74256	-0.06962	-0.35541
O	-1.46146	0.24426	-0.86255
O	-0.30263	0.85702	-0.25716
H	1.90030	1.43235	0.51877
H	2.69942	-0.21381	0.07910
H	-2.45493	0.19556	0.97492
H	-3.03056	-0.87894	-0.33975
H	-1.53223	-1.29034	0.55151

val+03_31

C	1.67483	0.55788	-0.12379
C	-1.52656	-0.01320	-0.02943
N	2.08824	-0.62597	0.02297
O	0.46830	1.12163	0.20434
O	-0.39649	0.13436	0.83309
H	2.28281	1.35103	-0.56146
H	-2.05109	0.93910	-0.15360
H	-2.16540	-0.72479	0.50124
H	-1.23517	-0.42235	-1.00195
H	1.35944	-1.20020	0.45758

val+03_32

C	0.84321	-1.30334	-0.03648
C	-0.54371	-0.69537	0.02784
N	-0.54246	0.46768	0.90615
O	1.25140	-1.96285	-0.96950
O	0.13537	1.52342	0.18007
H	1.46830	-1.11783	0.86268
H	-0.89861	-0.48970	-0.99219
H	-1.21571	-1.44165	0.47762
H	-1.50201	0.80649	0.98504
H	0.80111	1.82604	0.81908

val+03_33

C	0.74012	-1.04162	0.20958
C	-1.47057	0.04038	-0.04929
N	-0.07323	-0.13471	-0.39205
O	1.95002	-1.12423	0.03851
O	-1.69416	0.87203	1.07413
H	0.18357	-1.73126	0.87083
H	-1.98779	0.41611	-0.93795
H	-1.88323	-0.93553	0.21535
H	0.37963	0.56299	-0.97360
H	-1.49656	1.78663	0.81399

val+03_34

C	1.15781	-0.87798	0.22633
C	-0.28525	-0.50600	-0.11530
N	-0.40905	0.89515	-0.40337
O	2.10164	-0.12288	0.15128
O	-1.03443	-1.00933	1.00101
H	1.27394	-1.92541	0.56942
H	-0.55783	-1.06666	-1.02249
H	-1.36812	1.11830	-0.66184
H	-0.18419	1.44172	0.42655
H	-1.96131	-1.08600	0.72331

val+03_35

C	0.11992	1.01065	-0.07911
C	-1.38772	0.96262	0.01246
N	0.76566	-0.20580	-0.16877
O	0.78317	2.04195	-0.02456
O	0.03520	-1.30678	-0.65340
H	-1.75397	1.96203	0.25145
H	-1.81402	0.63572	-0.94186
H	-1.71802	0.25148	0.77557
H	1.70525	-0.17892	-0.55622
H	-0.00078	-1.92155	0.10074

val+03_36

C	0.68368	-0.09483	0.01524
C	-1.46138	1.17186	0.22095
N	-0.00974	1.05754	0.16445
O	1.89882	-0.17599	-0.12734
O	-0.12919	-1.18607	0.05864
H	-1.71209	2.19092	0.52118

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H	-1.93110	0.96423	-0.74816
H	-1.86862	0.47979	0.96186
H	0.54056	1.89614	0.04963
H	0.45764	-1.95710	-0.03284

val+03_37

C	0.10039	0.03003	-0.01472
C	-1.42156	-0.04450	0.15881
N	0.75376	-1.13154	-0.20097
O	0.65470	1.13329	0.02104
O	-1.93241	1.25416	0.35219
H	-1.86334	-0.51294	-0.73331
H	-1.65693	-0.69096	1.01706
H	1.75815	-1.12675	-0.31839
H	0.27727	-2.02241	-0.22153
H	-1.13703	1.82653	0.30562

val+03_38

C	1.06425	-0.01217	0.17588
C	-0.41454	0.22087	-0.09241
N	-0.74848	1.63233	0.06127
O	1.88795	0.86938	0.27937
O	1.45460	-1.30548	0.25554
H	-1.00124	-0.37064	0.62222
H	-0.62418	-0.20528	-1.09088
H	-1.70366	1.77739	-0.26117
H	-0.15279	2.17691	-0.56059
H	0.69409	-1.90621	0.16098

val+03_39

C	0.73878	-1.01703	0.05654
C	-1.42141	0.25739	0.17825
N	0.00510	0.11819	-0.03686
O	1.93993	-1.10951	-0.16566
O	0.63216	1.26185	-0.53665
H	0.11228	-1.86403	0.38699
H	-1.61792	0.99958	0.95889
H	-1.91714	0.56646	-0.74760
H	-1.82162	-0.70853	0.49457
H	1.09905	1.65223	0.22652

val+03_3

C	-0.13063	-0.47216	-0.06985
C	1.18925	-0.62007	-0.24269
N	-0.82515	0.74667	0.08785
O	-1.04534	-1.47911	0.05827
O	-0.09124	1.84525	-0.43834
H	1.82736	0.24562	-0.34881
H	1.63471	-1.60824	-0.27597
H	-1.70931	0.71403	-0.42031
H	-0.58258	-2.32915	-0.01632
H	0.04942	2.40916	0.34048

val+03_40

C	-0.08016	-0.73020	0.27193
C	1.33687	-0.73403	-0.30230
N	-0.29789	0.60571	0.92126
O	-1.30027	1.15977	0.51639
O	-1.04112	-1.02833	-0.68587
H	-0.13480	-1.41649	1.13597
H	1.55225	-1.72598	-0.70793
H	1.41665	0.00241	-1.10772
H	2.06957	-0.50280	0.47604
H	-1.70298	-0.30505	-0.61918

val+03_41

C	-0.03913	-0.71550	0.40338
C	-1.35859	-0.47280	-0.34856
N	1.03696	-0.92177	-0.59341
O	1.88091	-0.04785	-0.58854
O	-1.33940	0.72815	-1.10367
H	-0.11896	-1.65444	0.96554
H	0.21598	0.11630	1.07013
H	-2.17926	-0.48873	0.38083
H	-1.52618	-1.28320	-1.06416
H	-1.34693	1.47184	-0.47972

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val+03_42			
C	1.13911	-1.03960	-0.23193
C	-0.31880	-1.12873	0.16671
N	-0.95597	1.05129	-0.31587
O	1.81469	-0.03579	-0.12833
O	-0.82146	0.05690	0.73353
H	1.56306	-1.98134	-0.64166
H	-0.90040	-1.44488	-0.71358
H	-0.42208	-1.91225	0.93041
H	-1.76836	1.58256	0.00207
H	-0.15200	1.66515	-0.16534

val+03_43			
C	-0.99775	1.15854	-0.06946
C	-0.41676	-1.14002	-0.20866
N	0.89180	-1.11908	0.36735
O	-1.00536	1.13080	1.14387
O	-0.72838	0.13437	-0.87935
H	-1.22259	2.05443	-0.66741
H	-1.22222	-1.31478	0.50899
H	-0.47544	-1.86251	-1.02134
H	0.86281	-0.99340	1.37355
H	1.41419	-1.96133	0.15237

val+03_44			
C	1.58864	-0.39699	0.08704
C	-1.74659	-0.31473	0.05463
N	0.47061	0.38013	0.01908
O	2.67178	0.00231	0.49056
O	-0.58626	-0.09319	-0.76319
H	1.38187	-1.43565	-0.22289
H	-2.08190	0.61899	0.51998
H	-2.51078	-0.68115	-0.63428
H	-1.54369	-1.06371	0.82712
H	0.56262	1.39339	0.00885

val+03_45			
C	1.14268	-1.13043	0.13597
C	-1.16543	1.25634	-0.06898
N	-0.01505	0.79525	0.71208
O	1.87664	-1.83449	-0.51259
O	0.89777	0.14815	-0.22662
H	0.60828	-1.41730	1.05383
H	-0.88585	1.85184	-0.94743
H	-1.77469	1.86947	0.60264
H	-1.75410	0.39212	-0.38699
H	0.53316	1.60955	0.99228

val+03_46			
C	0.62831	0.97155	0.31925
C	-0.85546	0.80820	0.11509
N	0.71322	-1.38939	0.08801
O	1.18946	2.03194	0.49854
O	1.42087	-0.13946	0.30626
H	-1.31240	1.79767	0.15674
H	-1.06640	0.33663	-0.84845
H	-1.28522	0.16287	0.88592
H	1.21520	-1.78199	-0.71097
H	1.01232	-1.94692	0.89061

val+03_47			
C	0.51019	0.15549	0.08216
C	-1.82302	-0.12177	-0.12821
N	1.71812	-0.37403	-0.26673
O	0.34786	1.11000	0.82775
O	-0.49918	-0.55725	-0.47614
H	-1.98763	0.91057	-0.44727
H	-2.49805	-0.79312	-0.65918
H	-1.98476	-0.19770	0.95017
H	2.52641	0.20911	-0.10330
H	1.76307	-0.99470	-1.06336

val+03_48			
C	-0.58169	-1.11813	-0.21479
C	0.85209	-1.31538	0.24735
N	-1.43608	1.06377	-0.03736
O	-1.53638	2.12948	-0.55445

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O	-0.73187	0.17455	-0.85885
H	-1.29053	-1.16530	0.61709
H	-0.87143	-1.85386	-0.96957
H	0.96480	-2.31702	0.67633
H	1.11965	-0.57920	1.01232
H	1.55035	-1.21981	-0.59027
val+03_49			
C	-0.42018	-1.15221	-0.03145
C	-1.01232	1.13820	0.02639
N	0.94931	-1.27946	0.57476
O	1.67149	-0.33143	0.35569
O	-0.66996	-0.00570	-0.76218
H	-1.10842	-1.30224	0.81676
H	-0.49864	-2.02620	-0.69120
H	-0.17538	1.46218	0.65304
H	-1.88370	0.92662	0.66033
H	-1.26461	1.93325	-0.67805
val+03_4			
C	-0.26416	0.01090	0.13402
C	1.07266	-0.11999	0.05809
N	-0.98316	1.20498	0.21243
O	-1.07707	-1.08109	0.23110
O	1.60513	-1.40944	0.22911
H	1.76183	0.71486	-0.01617
H	-1.81697	1.18053	-0.37043
H	-0.41907	2.01097	-0.03945
H	-0.47068	-1.84724	0.21322
H	2.01539	-1.68329	-0.60831
val+03_50			
C	0.56365	-0.16627	0.04066
C	-0.12419	1.14389	-0.02589
N	1.05288	0.83491	-0.87621
O	0.04149	-1.27448	-0.65379
O	-0.85016	-1.96410	0.26846
H	1.14414	-0.43890	0.92011
H	-1.05841	1.22873	-0.57512
H	-0.00421	1.83060	0.80884
H	1.90283	1.26167	-0.50977
H	-1.70054	-1.52866	0.06539
val+03_51			
C	0.93713	-0.08653	-0.32955
C	0.38395	1.25478	-0.17520
N	0.12338	-1.26129	-0.38510
O	1.12282	0.62723	0.90461
O	-1.05823	-1.10284	0.41698
H	1.85008	-0.24294	-0.90491
H	-0.68209	1.36441	0.00974
H	0.87632	2.10535	-0.64556
H	0.62497	-2.03350	0.05618
H	-1.77103	-1.20137	-0.23559
val+03_52			
C	0.56048	0.54335	0.40043
C	-0.41282	-0.45906	-0.16885
N	0.11890	1.81659	0.90612
O	0.84401	1.66055	-0.40198
O	-0.92867	-1.21388	0.92038
H	1.40860	0.11577	0.93753
H	-1.20149	0.08210	-0.71415
H	0.11962	-1.09627	-0.88981
H	-0.85950	1.93955	0.61327
H	-1.40142	-1.97630	0.55236
val+03_53			
C	-0.07233	-0.27727	-0.13103
C	-0.78065	1.03622	0.18187
N	1.01373	0.52693	-0.77601
O	0.29702	1.78646	-0.43629
O	-0.80048	-1.07217	-1.02200
H	0.28171	-0.86113	0.72586
H	-0.89669	1.28296	1.24272
H	-1.73318	1.16205	-0.34388
H	1.83062	0.54059	-0.15617

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H	-0.30906	-1.89755	-1.16678
val+03_54			
C	0.20661	-0.36025	0.10062
C	-0.60007	0.92433	-0.03352
N	0.61455	1.69043	0.39186
O	1.32240	0.40317	0.64299
O	-0.34199	-1.27213	0.99044
H	0.50972	-0.84971	-0.83382
H	-0.98721	1.17229	-1.02446
H	-1.39643	0.99615	0.71212
H	1.07308	2.03978	-0.45553
H	0.11546	-2.12295	0.89260
val+03_55			
C	0.21494	-0.81880	0.04334
C	0.46825	1.15722	-0.28888
N	-0.24333	0.37978	0.74192
O	1.00743	-0.04497	-0.87938
O	-0.83664	-1.51404	-0.54136
H	0.85165	-1.49781	0.62469
H	-0.16765	1.72902	-0.97798
H	1.26306	1.80017	0.10631
H	-1.25665	0.46355	0.68275
H	-0.56335	-2.43412	-0.69132
val+03_56			
C	0.40566	-0.62291	-0.33744
C	-0.26526	0.66773	-0.29809
N	-0.27466	-1.83996	-0.56148
O	0.23310	0.11952	0.92829
O	0.39389	1.76456	-0.82518
H	1.44219	-0.64072	-0.66847
H	-1.35478	0.72734	-0.34851
H	0.20699	-2.61795	-0.11529
H	-1.22399	-1.81155	-0.19643
H	-0.02874	2.56875	-0.48041
val+03_57			
C	0.65456	-0.06818	-0.27306
C	-0.32144	-1.12360	0.17090
N	0.26098	1.28668	-0.58607
O	1.05783	0.91819	0.65332
O	-1.07888	1.48013	-0.21661
H	1.45144	-0.42800	-0.92907
H	-1.09108	-0.70583	0.82006
H	0.22420	-1.90251	0.71408
H	-0.79287	-1.58945	-0.70147
H	-1.17913	2.44618	-0.28428
val+03_58			
C	0.68624	-0.57790	-0.01890
C	-0.79935	1.36876	0.14281
N	0.48539	0.81925	-0.29386
O	1.23852	0.26971	0.92713
O	-0.33184	-1.37484	0.45058
H	1.37734	-1.08827	-0.69248
H	-0.62882	2.36617	0.55585
H	-1.32674	0.74411	0.86859
H	-1.40929	1.46911	-0.76271
H	-0.45715	-2.11231	-0.16822
val+03_59			
C	-1.56559	0.61282	0.08652
C	-0.62361	-0.52268	-0.05518
N	-0.33805	0.57680	0.90772
O	0.56414	1.53170	0.28327
O	1.86568	1.28563	0.83873
H	-2.48462	0.52131	0.65799
H	-1.58312	1.34641	-0.71496
H	-0.00685	-0.55242	-0.94857
H	-0.82821	-1.47943	0.41655
H	2.22413	0.62305	0.21613
val+03_5			
C	0.70434	0.01293	0.11204
C	-0.63409	-0.03075	0.12955

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N	-1.47156	1.11964	0.22772
O	1.38640	1.19265	0.21873
O	1.55893	-1.06197	0.08231
H	-1.14263	-0.98910	0.16079
H	-2.18107	1.10956	-0.50425
H	-0.91716	1.96305	0.09326
H	2.20842	1.11097	-0.29605
H	1.08302	-1.83248	-0.26821

val+03_60

C	-0.71910	-0.73646	0.20514
C	-1.62402	0.42843	-0.18470
N	0.35594	0.26521	0.49688
O	-0.47585	1.31611	-0.17221
O	1.44086	-0.02416	-0.35533
H	-0.43335	-1.37630	-0.63262
H	-0.97805	-1.33726	1.07927
H	-2.10090	0.38332	-1.16861
H	-2.36241	0.71091	0.57337
H	2.18978	0.42121	0.07870

val+03_61

C	1.07981	0.97662	-0.06888
C	0.96160	-1.02937	-0.08942
N	0.18196	0.03019	-0.77309
O	1.98994	-0.08700	0.26508
O	-1.15160	0.10342	-0.25783
H	0.59631	1.42463	0.81084
H	1.54177	1.74508	-0.69832
H	1.33076	-1.83376	-0.73502
H	0.42776	-1.43527	0.78154
H	-1.69391	0.14505	-1.06229

val+03_62

C	-0.47531	1.56511	-0.26021
C	0.39448	-0.59874	0.42974
N	0.61308	0.64147	-0.34804
O	0.60908	1.79499	0.61337
O	-0.09856	-1.58723	-0.43681
H	-1.40653	1.24214	0.20865
H	-0.58318	2.26420	-1.08903
H	-0.34955	-0.45360	1.22110
H	1.35675	-0.87142	0.87866
H	0.62084	-1.84432	-1.03673

val+03_63

C	0.00905	-0.07364	0.29153
C	-0.42741	1.31594	0.34498
N	-0.91284	-1.15851	0.35068
O	0.05187	0.73611	-0.90347
O	1.24161	-0.36079	0.84740
H	-1.49057	1.55574	0.36878
H	0.23061	2.06090	0.79071
H	-0.53692	-1.96855	-0.14366
H	-1.77624	-0.90294	-0.12462
H	1.64285	-1.09676	0.35316

val+03_64

C	0.24973	-0.04867	0.31805
C	-0.89266	-0.96903	-0.03731
N	0.04052	1.25194	0.87152
O	0.48572	1.02791	-0.55897
O	1.36726	-0.66229	0.84272
H	-1.73033	-0.39878	-0.44575
H	-0.57015	-1.69292	-0.79465
H	-1.22581	-1.52053	0.84713
H	-0.95705	1.48032	0.78010
H	1.47658	-1.52766	0.41585

val+03_65

C	-0.62934	0.40393	-0.16082
C	-0.01955	-0.91181	0.12115
N	0.52221	-0.08669	-0.94997
O	-0.43561	1.39626	0.79725
O	-0.58967	-2.10515	-0.33124
H	-1.55881	0.46358	-0.72556
H	0.56205	-0.99722	1.04086

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H	1.37668	0.37195	-0.63135
H	-0.50461	2.25814	0.35367
H	-1.21326	-2.40488	0.35090

val+03_66

C	-0.53974	-0.32586	0.07010
C	-1.09036	1.05099	-0.00930
N	0.09617	0.63629	-0.81163
O	-1.12074	-1.40145	-0.59871
O	1.31917	1.08999	-0.18618
H	0.03406	-0.57874	0.96206
H	-1.97236	1.25555	-0.61018
H	-0.90201	1.71640	0.82815
H	-1.93707	-1.63214	-0.12504
H	1.69836	1.65668	-0.87885

val+03_67

C	0.02883	-0.24718	-0.08914
C	-0.44969	1.11904	0.18089
N	0.41596	0.79710	-1.00917
O	0.95709	-0.75900	0.81206
O	-0.77162	-1.21659	-0.68132
H	-1.47073	1.39295	-0.07020
H	-0.00061	1.66470	1.00692
H	1.37736	1.07234	-0.80620
H	1.44291	-1.46493	0.34910
H	-1.26018	-1.65932	0.03386

val+03_68

C	0.37409	-0.00082	0.27145
C	-0.43745	-1.17980	-0.19161
N	-0.33527	1.20639	0.73589
O	1.00832	0.74980	-0.80856
O	0.63793	1.97812	-0.03970
H	1.13396	-0.27896	1.01078
H	-1.18012	-0.87530	-0.93538
H	0.22312	-1.93095	-0.63711
H	-0.94542	-1.64056	0.66231
H	-1.19196	1.28469	0.17164

val+03_69

C	0.41464	-0.14078	-0.26558
C	-0.50020	-1.21209	0.26923
N	0.56867	1.79322	0.34666
O	1.19819	0.52791	0.74092
O	-0.25367	1.07968	-0.63695
H	1.05035	-0.50832	-1.08258
H	-1.14682	-1.58062	-0.53474
H	0.09437	-2.05352	0.64178
H	-1.11843	-0.81684	1.08049
H	-0.09350	1.97446	1.11698

val+03_6

C	1.36821	-0.08559	-0.20847
C	-0.10607	0.06145	0.14091
N	1.87339	-0.90557	-1.03754
O	-0.50318	1.41675	0.07073
O	-0.83193	-0.76868	-0.72823
H	2.02427	0.61312	0.31959
H	-0.26491	-0.21499	1.19166
H	1.11712	-1.47831	-1.43549
H	-0.35556	1.71461	-0.84426
H	-1.75213	-0.79400	-0.41990

val+03_70

C	0.96628	0.26517	-0.11404
C	-1.40858	-0.28996	0.16397
N	-0.00003	-0.68655	0.15723
O	0.68953	1.42703	-0.89043
O	0.93477	1.46412	0.60410
H	1.95478	-0.16024	-0.28407
H	-1.52888	0.57927	0.81387
H	-1.99933	-1.11246	0.57360
H	-1.79095	-0.03824	-0.83375
H	0.18142	-1.56303	-0.31857

val+03_71

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C	0.70036	0.45409	0.09686
C	-1.05435	-1.09356	-0.16824
N	0.51590	1.88607	0.09338
O	0.00276	-0.33808	-0.77697
O	1.72829	1.16523	-0.48552
H	0.89027	-0.00006	1.07241
H	-1.85781	-0.43767	0.18593
H	-1.44010	-1.75537	-0.94426
H	-0.67635	-1.69357	0.66838
H	-0.03257	2.08531	-0.75406

val+03_72

C	0.43235	0.03381	-0.14404
C	-0.45414	1.28198	-0.09035
N	-0.02879	-1.22591	-0.58064
O	1.21206	0.71637	-1.20154
O	0.52255	2.00266	-0.87897
H	1.05721	-0.09643	0.74554
H	-1.40429	1.16840	-0.62852
H	-0.61869	1.75099	0.88365
H	-0.12422	-1.89979	0.17095
H	-0.88745	-1.18228	-1.12216

val+03_73

C	0.84512	0.64043	-0.40000
C	0.00658	-0.23911	0.49910
N	-0.89149	-1.14689	-0.21679
O	0.24737	1.80921	-0.89515
O	1.35370	1.83341	0.12715
H	1.50286	0.13265	-1.11087
H	-0.57895	0.41461	1.15387
H	0.67887	-0.83182	1.13088
H	-0.35428	-1.77897	-0.80924
H	-1.49418	-0.61312	-0.84216

val+03_74

C	0.89828	0.26487	-0.08490
C	0.62108	1.70630	-0.09285
N	-0.67572	-1.36327	-0.49149
O	1.56365	1.08739	0.83310
O	0.01137	-0.61333	0.54341
H	1.50008	-0.20895	-0.86107
H	-0.29623	2.06194	0.37198
H	1.07315	2.35831	-0.83854
H	-0.65821	-2.31459	-0.12073
H	-1.64715	-1.05767	-0.39962

val+03_75

C	0.44856	-0.43207	0.10629
C	0.41997	1.54201	-0.14743
N	-0.52636	-1.42598	-0.03196
O	0.69875	0.45511	-1.02568
O	0.01802	0.67434	0.91635
H	1.38434	-0.88129	0.46303
H	-0.38711	2.19824	-0.49871
H	1.31563	2.12799	0.10300
H	-0.15926	-2.28405	-0.43291
H	-1.32815	-1.10280	-0.56838

val+03_76

C	0.14768	-0.63565	-0.18483
C	-1.11325	0.24798	0.12566
N	1.21418	0.22342	0.28676
O	-0.70473	1.58046	0.00409
O	0.93402	1.43673	-0.18371
H	0.25344	-0.77971	-1.26168
H	0.14759	-1.59576	0.33360
H	-1.47214	0.03106	1.14150
H	-1.90237	0.02549	-0.60356
H	1.25909	0.24309	1.31206

val+03_77

C	-0.88645	-0.00513	-0.07224
C	0.34264	-0.86332	0.31224
N	0.93514	1.33961	0.25506
O	-0.48765	1.33770	0.27172
O	1.27119	0.09584	0.85564

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H	-1.11102	-0.07758	-1.14277
H	-1.78158	-0.23452	0.50902
H	0.77532	-1.36358	-0.56220
H	0.14044	-1.59667	1.09496
H	1.17948	1.21744	-0.74124

val+03_78

C	-0.30899	1.17187	-0.35388
C	0.42234	-0.93565	-0.15754
N	-0.63643	-0.17396	-0.81034
O	1.10275	1.24821	-0.52819
O	1.59022	-0.14976	-0.38490
H	-0.75258	1.94076	-0.99411
H	-0.56980	1.35773	0.70242
H	0.58755	-1.90368	-0.64091
H	0.26671	-1.07250	0.92653
H	-1.55166	-0.45973	-0.46389

val+03_79

C	0.14996	-1.05092	-0.11230
C	0.91502	1.09459	-0.07824
N	-0.95017	-0.07941	0.02972
O	1.26083	-0.23752	-0.46298
O	-0.22463	0.98439	0.73731
H	0.36346	-1.60064	0.81657
H	-0.07563	-1.74765	-0.92465
H	0.71142	1.68559	-0.98273
H	1.71067	1.54732	0.52012
H	-1.60214	-0.40096	0.74837

val+03_7

C	0.64981	0.53372	-0.08961
C	-0.82347	0.51700	-0.41534
N	1.37724	-0.46505	0.23657
O	-1.36039	1.82835	-0.52420
O	0.62061	-1.65742	0.24932
H	1.17082	1.48902	-0.13767
H	-1.35986	-0.09178	0.32610
H	-0.97771	0.03537	-1.38862
H	-1.38349	2.21059	0.36752
H	1.26916	-2.31819	0.54183

val+03_80

C	-0.13164	-0.12969	0.37604
C	0.14763	-1.42153	-0.38746
N	-0.38467	0.95889	-0.59122
O	-0.05049	2.21601	0.01515
O	0.86755	1.57837	-0.93138
H	-1.05710	-0.20840	0.95767
H	0.69109	0.15279	1.03962
H	-0.67326	-1.66375	-1.06953
H	1.07364	-1.34315	-0.96581
H	0.25744	-2.24514	0.32404

val+03_81

C	-0.65218	1.06722	0.12308
C	0.29492	-1.18639	0.17994
N	0.01492	0.03905	0.93590
O	0.60686	1.65589	-0.27592
O	1.22110	0.89322	0.85152
H	-1.23726	0.70207	-0.72637
H	-1.23244	1.75642	0.74528
H	-0.63798	-1.75826	0.14078
H	0.65119	-0.98933	-0.83990
H	1.03825	-1.76950	0.72829

val+03_82

C	1.05292	-1.40304	0.24761
C	-1.06193	1.39918	-0.10537
N	0.29493	-0.42809	-0.48738
O	1.68790	-0.16228	0.08183
O	-0.64362	0.12042	0.39075
H	1.43989	-2.24034	-0.33399
H	0.70381	-1.63987	1.25274
H	-0.24654	2.12656	-0.03081
H	-1.40027	1.31947	-1.14309
H	-1.88979	1.70099	0.53841

val+03_83
C -0.12559 1.39167 0.04470
C -0.02962 -1.66998 0.14055
N 0.50305 -0.45456 -0.46561
O -0.64833 0.39953 -0.83845
O 0.81414 0.49123 0.63106
H -0.86549 1.77647 0.75700
H 0.36581 2.21320 -0.49562
H -0.79663 -1.45568 0.89156
H 0.81579 -2.20011 0.58961
H -0.44044 -2.27828 -0.67099

val+03_84
C 0.04215 0.18108 0.20571
C -1.25323 -0.55222 -0.03248
N 1.19108 -0.61782 0.24775
O -0.04195 1.32407 1.05247
O 0.20702 1.41473 -0.43762
H -2.06830 0.16849 -0.11353
H -1.19058 -1.13831 -0.95394
H -1.46172 -1.23508 0.79767
H 1.98992 -0.10995 0.61785
H 1.05372 -1.47919 0.76761

val+03_8
C 0.46051 -0.30295 -0.04638
C -1.83478 -0.44156 -0.25666
N -0.50401 -0.56133 -0.82682
O 1.73156 -0.39638 -0.49160
O -2.64403 0.43921 -1.01598
H 0.35405 -0.00169 1.00394
H -1.80716 -0.13100 0.80375
H -2.33334 -1.41469 -0.31455
H 2.33944 -0.15132 0.22482
H -2.22954 1.31652 -0.96991

val+03_9
C -0.63720 -0.81891 0.08333
C 1.57544 -0.21203 -0.36330
N 0.64257 -1.04802 -0.57058
O -0.83804 0.45091 0.65809
O -1.60231 -1.08692 -0.90310
H -0.70721 -1.51955 0.92550
H 1.46863 0.67609 0.26800
H 2.54547 -0.38017 -0.83337
H -0.92083 1.08462 -0.07764
H -2.47001 -1.00832 -0.47243

val+05_100
C 1.07780 -0.14184 0.31735
C -0.95777 1.15037 -0.10286
N -0.21903 -0.10535 -0.09388
O 1.67655 0.80585 0.80223
O 1.71337 -1.34117 0.19159
H -0.76370 1.68749 0.82728
H -0.67236 1.79339 -0.94488
H -2.02450 0.92825 -0.17092
H -0.58549 -0.85853 -0.65993
H 1.11782 -2.03707 -0.13397

val+05_103
C 0.22123 0.31558 -0.21496
C -1.25716 0.25951 -0.10708
N 1.01629 -0.72082 -0.21826
O 2.32755 -0.54537 -0.31854
O 0.84605 1.48629 -0.31761
H -1.59303 0.80154 0.78400
H -1.71858 0.73434 -0.97998
H -1.60444 -0.77469 -0.04307
H 0.64749 -1.66867 -0.14438
H 1.80500 1.18478 -0.36942

val+05_105
C 0.63606 -0.48705 -0.24863
C -0.98001 1.21057 0.26910
N 0.02101 0.59796 -0.61972

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O	0.22796	1.20183	-1.75151
O	1.54532	-1.02761	-1.08002
H	0.41863	-0.94362	0.70722
H	-0.65343	2.23084	0.48102
H	-1.92866	1.24031	-0.27108
H	-1.08871	0.64626	1.19695
H	1.91081	-1.82350	-0.66173

val+05_106			
C	2.57529	-0.36246	1.23182
C	-0.77175	-0.26607	-0.15362
N	-1.67705	-1.32711	0.23256
O	2.61167	-1.05252	0.32616
O	-0.29295	0.33932	1.04866
H	0.05634	-0.71894	-0.71763
H	-1.23028	0.51136	-0.78816
H	-2.59701	-0.94453	0.44434
H	-1.79945	-1.97263	-0.54448
H	0.04811	1.21748	0.81545

val+05_107			
C	2.02348	-1.52882	-1.48878
C	-0.47307	0.71503	0.44524
N	-0.42316	-0.73787	0.57463
O	2.06704	-0.46784	-1.89972
O	-1.04838	-1.34533	-0.56475
H	-0.06424	1.15134	1.36294
H	-1.49347	1.10801	0.29551
H	0.14891	1.02046	-0.40056
H	-0.98661	-1.01758	1.38020
H	-1.94599	-0.96030	-0.63491

val+05_108			
C	0.88993	-1.28099	-0.31740
C	-1.16107	-0.12449	0.35663
N	0.09870	-0.26548	-0.46804
O	0.24114	0.68648	-1.31917
O	-1.32210	1.21492	0.67537
H	0.66541	-2.01122	0.44747
H	1.74716	-1.36759	-0.97207
H	-1.96432	-0.51843	-0.28044
H	-1.06715	-0.71719	1.26677
H	-1.05470	1.67899	-0.14791

val+05_109			
C	0.39687	-0.09923	-0.28922
C	-0.91848	0.03496	0.41321
N	0.90895	-1.27602	-0.50526
O	0.41096	-2.40451	-0.14886
O	-1.49606	1.31924	0.22173
H	0.95617	0.76211	-0.63465
H	-1.58200	-0.78042	0.08865
H	-0.78584	-0.08379	1.49670
H	1.80371	-1.30981	-1.01255
H	-1.74858	1.38887	-0.71295

val+05_10			
C	-1.19966	0.36225	0.05468
C	-2.51180	0.96125	0.11132
N	-0.31171	-0.50223	-0.16771
O	-1.20838	1.60235	0.55065
O	2.57354	-0.30469	0.25227
H	-3.18550	0.73300	0.93279
H	-2.94692	1.41730	-0.77381
H	1.59838	-0.35234	0.14156
H	-0.72066	-1.34903	-0.56457
H	2.87951	-0.02605	-0.62390

val+05_110			
C	1.42503	-1.28701	-0.08301
C	0.51663	-0.36915	0.19751
N	-0.78844	-0.35307	-0.42168
O	2.22219	-2.10891	-0.34436
O	-1.52954	1.99806	1.01664
H	0.76014	0.40122	0.92265
H	-0.73578	-0.25967	-1.43405
H	-1.43806	1.19314	0.45139

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H	-1.32536	-1.19316	-0.21525
H	-1.16269	2.70075	0.45865
val+05_112			
C	0.42916	-0.04233	0.18956
C	-0.17273	1.22728	-0.19027
N	-0.36180	-1.29185	0.05042
O	-0.97976	-1.60000	1.23091
O	0.84271	0.57588	-1.00775
H	1.14837	-0.14975	0.99653
H	-1.17095	1.24429	-0.62480
H	0.14991	2.14129	0.30271
H	0.28386	-2.03710	-0.26802
H	-1.02046	-1.16180	-0.73939
val+05_113			
C	0.50829	0.00839	0.07952
C	-0.38704	-1.21643	0.11472
N	-0.35165	1.30215	0.04311
O	-1.50675	1.36714	-0.32858
O	1.06144	0.37547	-1.07289
H	1.13506	0.08367	0.98720
H	-0.94513	-1.27442	1.05500
H	0.25096	-2.10228	0.03627
H	-1.07987	-1.20679	-0.73023
H	0.24678	2.13981	-0.09913
val+05_114			
C	0.01605	-0.69635	-0.07845
C	1.04786	0.41802	0.04069
N	-1.11890	0.31274	-0.04694
O	-2.05183	0.25763	-0.87603
O	0.10287	1.45254	-0.27381
H	-0.03549	-1.15456	-1.06549
H	-0.08009	-1.44501	0.71073
H	1.86950	0.37101	-0.68244
H	1.46536	0.52226	1.05129
H	-1.38782	0.60070	0.90695
val+05_115			
C	-0.99609	0.38643	0.17849
C	1.00051	0.43912	-0.24508
N	0.02792	-0.73493	-0.05568
O	0.25416	-1.63385	0.89677
O	-0.08308	1.36651	-0.31660
H	-1.92043	0.31887	-0.39897
H	-1.16691	0.43464	1.25758
H	1.61355	0.41291	-1.14834
H	1.59154	0.50735	0.67258
H	-0.15656	-1.16354	-0.97975
val+05_116			
C	-0.12674	1.32614	0.02099
C	-0.41523	-1.27894	0.09516
N	0.26303	-0.10646	-0.51065
O	1.31787	-0.28933	-1.08016
O	0.29807	1.12355	1.24396
H	-1.21466	1.43087	-0.16253
H	0.44045	1.99951	-0.64836
H	-1.22826	-0.93488	0.72829
H	0.31230	-1.86499	0.65767
H	-0.78792	-1.86865	-0.74738
val+05_117			
C	-0.44345	-0.06158	0.29750
C	0.68536	0.84401	-0.20829
N	-0.11526	-1.36694	0.39460
O	-1.54073	0.41102	0.59630
O	1.84345	0.15116	-0.65824
H	0.26769	1.50405	-0.97783
H	0.99665	1.47635	0.63023
H	-0.77762	-2.03289	0.76721
H	0.82757	-1.66219	0.18155
H	1.68306	-0.13489	-1.57164
val+05_118			
C	0.55882	0.86631	0.32186

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C	-0.57479	-0.14691	-0.04598
N	0.07491	-1.50171	-0.10564
O	0.22070	2.05751	0.40970
O	1.69509	0.32733	0.48681
H	-1.35759	-0.15366	0.71257
H	-1.01722	0.08841	-1.01393
H	-0.29715	-2.17009	0.57181
H	1.07565	-1.23364	0.14460
H	0.04318	-1.93585	-1.03021

val+05_119

C	2.04825	0.33585	-1.06707
C	-1.48848	1.04560	-0.25465
N	-0.61225	-1.34460	0.51887
O	2.61489	1.18256	-1.57243
O	-0.56267	1.82736	-0.14715
H	-1.67822	0.47381	-1.17996
H	-2.24246	0.90900	0.54107
H	-0.86387	-2.25754	0.14006
H	-0.48786	-1.48175	1.52157
H	0.31167	-1.12638	0.14669

val+05_11

C	-0.49626	1.12440	-0.06873
C	-0.37854	2.54979	0.09370
N	-1.11125	0.08998	-0.42034
O	0.67614	1.53144	0.48000
O	0.50818	-2.43248	0.04699
H	-0.83431	3.05121	0.94428
H	-0.09006	3.18209	-0.74274
H	0.04809	-3.06332	-0.53003
H	-0.55057	-0.75833	-0.23829
H	1.33008	-2.24507	-0.43454

val+05_120

C	-0.19672	2.35831	0.63269
C	-0.03121	-1.23991	0.23537
N	0.37195	-0.08067	-0.57116
O	-0.69467	1.85205	1.56326
O	0.27688	2.96899	-0.24638
H	-1.10754	-1.18599	0.42911
H	0.48029	-1.20017	1.20270
H	0.18299	-2.21880	-0.22217
H	-0.08660	-0.12612	-1.48035
H	1.36983	-0.13849	-0.77067

val+05_122

C	0.31225	-1.42898	-0.30348
C	-0.64266	2.23767	-0.51206
N	0.75222	-0.70401	0.74116
O	-0.33977	-0.99135	-1.25227
O	-0.02690	2.17818	0.53665
H	0.59629	-2.49463	-0.23710
H	-1.06677	3.19275	-0.87103
H	-0.79782	1.34263	-1.13773
H	1.28305	-1.14204	1.48079
H	0.55421	0.29667	0.79697

val+05_123

C	-0.09472	1.02160	0.33832
C	-0.44060	-0.25017	-0.47771
N	-1.41026	-0.16147	-1.30691
O	-0.83550	1.99309	0.06753
O	0.85852	0.88239	1.12877
H	0.09549	-1.18987	-0.37644
H	2.32420	-1.94144	1.82504
H	-1.86515	0.75976	-1.34288
H	1.97802	-1.30451	1.65316
H	-1.73393	-0.92177	-1.90080

val+05_125

C	-1.59129	1.63193	0.20884
C	1.14359	-2.02958	0.26650
N	0.07197	-1.35751	0.13389
O	-2.47146	0.86811	-0.14229
O	-0.33477	1.30995	0.47555
H	-1.75104	2.71328	0.34774

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H	2.05959	-1.51461	0.55891
H	1.20958	-3.10846	0.10408
H	-0.19875	0.30684	0.34319
H	-0.72533	-1.93666	-0.14220

val+05_127

C	0.58103	0.28665	-0.14144
C	-1.73565	-0.09781	-0.13996
N	1.78193	-0.20135	-0.24433
O	2.88340	0.35357	0.15793
O	-0.44137	-0.38155	-0.70116
H	0.43333	1.23970	0.35603
H	-1.94145	0.97741	-0.17253
H	-2.45391	-0.62938	-0.76362
H	-1.79565	-0.45891	0.89156
H	1.84725	-1.11635	-0.71347

val+05_128

C	1.54964	-1.62327	-0.90501
C	-1.46307	1.22007	0.14512
N	0.36085	-1.75625	-0.72911
O	2.70713	-1.61523	-1.15135
O	-1.44576	-0.13093	0.62816
H	-0.48195	1.70009	0.24208
H	-1.73334	1.17075	-0.91149
H	-2.21282	1.81543	0.67817
H	-0.29502	-1.14394	-0.20854
H	-1.19774	-0.11152	1.56666

val+05_129

C	1.96040	-0.42391	0.12387
C	-1.57422	-0.30573	0.17447
N	0.75679	-0.15994	-0.29075
O	0.38189	0.39868	-1.33667
O	-0.25050	-0.60096	0.63575
H	2.08215	-0.92168	1.07270
H	2.77778	-0.12533	-0.51430
H	-1.73204	0.76968	0.06223
H	-2.20554	-0.69674	0.97413
H	-1.79762	-0.81668	-0.76523

val+05_12

C	0.33854	0.79744	0.17500
C	0.72532	-0.68575	0.14576
N	-0.49310	1.18100	-0.81617
O	0.78890	1.54595	1.04308
O	0.02118	-1.46297	-0.81524
H	0.61828	-1.08109	1.16292
H	1.78767	-0.74036	-0.11552
H	-0.77034	0.51323	-1.52235
H	-0.76219	2.15055	-0.90910
H	-0.83538	-1.70780	-0.43028

val+05_130

C	1.61501	0.29771	-0.77405
C	0.89072	-0.28298	0.16982
N	-2.51682	-0.13272	0.01110
O	2.27902	0.79738	-1.61237
O	-0.03214	-1.26453	-0.14427
H	1.07569	0.00335	1.20430
H	-2.62209	0.67513	-0.60169
H	-0.95235	-0.84857	-0.08879
H	-3.25331	-0.78721	-0.25111
H	-2.74413	0.19033	0.95097

val+05_131

C	1.28181	-0.17666	0.40285
C	-0.33985	2.77003	0.52671
N	-1.13848	-1.19414	0.15292
O	1.47932	0.62584	-0.49058
O	-1.19699	2.62003	-0.20786
H	1.58763	-1.23470	0.32416
H	0.85715	0.11739	1.37812
H	-1.69237	-0.36357	-0.05334
H	-1.22969	-1.79862	-0.66306
H	-1.62323	-1.67269	0.91197

val+05_132
C 0.69647 -0.22845 0.06343
C 1.99029 -1.03409 0.05144
N -2.34328 0.98611 -0.55165
O 0.52211 0.65962 0.87272
O 2.17051 -1.92209 -0.75296
H 2.73058 -0.74455 0.82126
H -1.61107 1.20873 0.12411
H -2.54212 1.86266 -1.03442
H -3.17626 0.79328 0.00506
H -0.05513 -0.50311 -0.69749

val+05_133
C 1.07977 -0.63901 0.46149
C -0.66101 1.03096 -0.26341
N -0.30624 -0.38246 0.00996
O 1.81204 0.23927 0.84039
O -0.83054 -0.87268 1.20365
H 1.28583 -1.71324 0.44575
H -0.20658 1.34788 -1.20515
H -1.74827 1.07780 -0.32052
H -0.29274 1.62738 0.56841
H -0.57206 -0.96970 -0.79338

val+05_134
C -0.11115 -0.76988 0.11880
C 1.37223 -0.49432 0.03319
N -0.94085 0.33199 0.07189
O -0.59905 -1.88476 0.27841
O -0.44523 1.50711 -0.52291
H 1.91075 -1.41888 0.24580
H 1.67368 0.28406 0.74068
H 1.63379 -0.14017 -0.96949
H -1.90223 0.14872 -0.20332
H -0.41853 2.15194 0.20605

val+05_135
C -0.38073 -0.29592 0.01297
C 1.08509 -0.67655 -0.02867
N -0.61553 1.19600 -0.08989
O -1.78739 1.56832 -0.08167
O 0.35196 1.94745 -0.17294
H -0.95746 -0.71884 -0.81307
H -0.87143 -0.58365 0.94611
H 1.15822 -1.76579 0.05049
H 1.63726 -0.23231 0.80309
H 1.55172 -0.36671 -0.96701

val+05_136
C 1.02377 -0.58980 -0.07846
C -0.47162 -0.36177 -0.04303
N -0.75643 1.10229 0.02246
O 1.81296 0.26671 -0.41883
O -0.51072 1.61307 1.26768
H 1.35427 -1.61271 0.18272
H -0.93069 -0.80838 0.84069
H -0.91415 -0.80939 -0.94470
H -1.73191 1.25249 -0.28396
H -0.16159 1.54668 -0.69897

val+05_137
C 0.05187 -0.08335 0.00353
C 1.28505 -0.43633 -0.30476
N -1.02635 -1.09022 -0.21845
O -0.67735 1.01652 0.50489
O -2.11045 -0.62348 -1.03815
H 2.00697 0.36001 -0.05721
H -1.45047 -1.43460 0.65326
H -0.57628 -1.86598 -0.71372
H -0.10279 1.79438 0.42719
H -2.16939 0.31315 -0.74687

val+05_139
C 0.34455 -1.31804 -0.15091
C 1.53389 -1.41910 0.04101
N -1.00434 -1.15538 -0.29774
O -2.31215 0.79750 1.33936

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O	-2.85223	1.48510	0.17568
H	2.58486	-1.52456	0.18712
H	-1.25914	-0.69459	-1.17046
H	-1.81307	0.07100	0.88604
H	-1.52180	-2.02976	-0.21970
H	-2.25656	2.25443	0.12639

val+05_13			
C	0.04128	-0.16917	0.29404
C	1.06074	0.97878	0.12344
N	0.60558	-1.31827	0.14013
O	2.27318	0.47051	-0.13725
O	-1.24182	-0.05342	0.55974
H	0.60157	1.63074	-0.66662
H	0.95114	1.57899	1.06546
H	1.63181	-1.09110	-0.06097
H	0.15045	-2.22016	0.20195
H	-1.48244	0.88901	0.64209

val+05_140			
C	0.83787	-0.43748	0.30981
C	1.51469	0.55241	0.12485
N	-2.21662	-0.51403	-0.26096
O	0.11214	-1.49740	0.50821
O	-1.95886	0.85019	-0.63989
H	2.13422	1.40520	-0.02916
H	-0.86063	-1.25466	0.23973
H	-2.64524	-0.94298	-1.08296
H	-2.94700	-0.45978	0.45112
H	-1.00038	0.94553	-0.48265

val+05_141			
C	-0.49500	-0.45936	0.13955
C	-0.11163	-1.67355	0.31408
N	-1.87498	-0.01378	-0.09432
O	0.45992	-2.71461	0.49650
O	-0.32762	2.31049	0.09158
H	0.05360	1.39585	0.20274
H	-1.84203	1.02144	-0.13165
H	-2.27753	-0.34109	-0.98091
H	-2.53620	-0.27503	0.64706
H	-0.07642	2.54905	-0.81572

val+05_143			
C	1.15287	0.18473	0.19372
C	1.89670	1.12339	0.36924
N	-2.74337	0.04422	-0.06560
O	0.39731	-0.84272	-0.06362
O	-0.56259	-1.04041	1.05805
H	2.55285	1.95093	0.51333
H	-3.07629	-0.47703	-0.87604
H	-2.57496	0.99803	-0.38394
H	-3.52446	0.09212	0.58803
H	-1.40326	-0.63255	0.62161

val+05_144			
C	-0.45348	0.75847	-0.19332
C	-1.43186	-0.37140	-0.24381
N	0.78199	0.44386	-0.12016
O	-2.76532	0.08889	-0.45601
O	1.33805	-0.91148	-0.19801
H	-1.35902	-0.93857	0.70167
H	-1.19662	-1.07723	-1.05074
H	1.54977	1.10753	-0.10197
H	-2.79203	0.98726	-0.08718
H	1.50501	-1.14733	0.73413

val+05_145			
C	1.48084	-0.33376	-0.41671
C	-0.84358	0.43198	0.39632
N	0.61940	0.43379	0.27770
O	0.91784	-1.33869	-1.10601
O	-1.45364	1.47859	-0.32536
H	-1.23767	-0.55041	0.11166
H	-1.09809	0.59820	1.44443
H	1.06505	1.20343	0.76299
H	-0.06036	-1.41227	-1.04533

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H	-1.32739	1.30684	-1.27287
val+05_146			
C	-0.79172	0.27757	-0.06509
C	-1.65935	-0.94366	0.04000
N	0.44161	0.11707	0.17565
O	1.40249	1.14984	0.11900
O	1.15393	-1.02291	0.62444
H	-2.30701	-0.82758	0.91920
H	-2.33150	-0.98469	-0.82442
H	-1.12193	-1.89576	0.12914
H	0.88081	1.87253	-0.28497
H	1.87027	-1.13042	-0.03266
val+05_147			
C	0.49855	-0.92722	0.30784
C	-1.16991	0.87582	0.22405
N	0.17207	0.33870	0.16916
O	1.86003	-1.01923	0.19200
O	1.11233	1.39309	-0.06055
H	-1.24770	1.60307	1.03819
H	-1.41358	1.36846	-0.72237
H	-1.85068	0.04348	0.39908
H	2.09886	-1.95182	0.29401
H	1.96334	0.91005	-0.07561
val+05_148			
C	1.75481	-1.22815	0.19112
C	-0.33810	-0.00271	0.02282
N	0.97441	-0.41654	-0.48082
O	-0.33677	1.30572	0.51371
O	-1.21393	-0.15892	-1.05777
H	2.67354	-1.33515	-0.42216
H	-0.56237	-0.64929	0.87455
H	1.19477	0.00419	-1.39139
H	-0.23437	1.90861	-0.24471
H	-2.09140	0.13966	-0.76495
val+05_149			
C	0.86472	1.26413	-0.14523
C	-1.20116	-0.01661	-0.21085
N	0.26510	0.14735	-0.01052
O	-1.73373	1.17850	-0.67995
O	0.84443	-1.06994	0.49325
H	1.92907	1.15729	0.09687
H	-1.61700	-0.31797	0.75939
H	-1.34767	-0.83287	-0.92961
H	-0.96902	1.80993	-0.62420
H	0.93766	-1.64052	-0.29435
val+05_150			
C	0.66098	-0.97273	0.79890
C	-0.60285	-0.71850	-0.01504
N	1.54582	-0.05039	0.52875
O	-0.74444	0.57122	-0.62014
O	-1.70362	-0.99645	0.81939
H	-0.55695	-1.40717	-0.87381
H	1.36592	0.73277	-0.11202
H	2.46774	-0.06850	0.95310
H	-0.95746	1.19110	0.10039
H	-2.50055	-0.91965	0.26808
val+05_152			
C	1.38240	0.81645	-0.60654
C	-0.99974	1.16650	-0.12857
N	0.38105	1.62219	-0.44337
O	1.66772	-0.33968	-0.61035
O	0.15189	-1.65156	-0.28608
H	-1.29935	1.60120	0.82810
H	-1.67036	1.50829	-0.92064
H	-0.96496	0.07241	-0.08009
H	0.56229	2.61625	-0.52057
H	0.42105	-1.73933	0.64562
val+05_153			
C	0.60577	1.37968	-0.97028
C	-1.23294	-0.06307	-0.11152

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N	1.54719	0.59888	-0.47421
O	-0.67839	1.09586	-0.80711
O	1.46826	-0.69918	0.17225
H	-0.94246	-0.05597	0.94014
H	-2.31400	0.05490	-0.20083
H	-0.90973	-0.99008	-0.58412
H	2.51114	0.81998	-0.68851
H	1.58666	-0.49651	1.11869

val+05_154			
C	1.68347	0.35323	-0.23462
C	-1.53880	-0.62252	-0.00227
N	0.42843	0.67452	0.03877
O	-0.44104	-0.16507	0.80757
O	1.99939	-0.88132	0.17301
H	-2.15636	0.22091	-0.33092
H	-2.12375	-1.27279	0.65180
H	-1.18225	-1.18389	-0.87165
H	0.05808	1.60841	-0.09351
H	1.23504	-1.29598	0.63881

val+05_155			
C	0.11201	-1.39002	-0.43514
C	-1.19859	-0.96283	0.15867
N	1.07192	-0.55004	-0.14615
O	-1.25324	0.26872	0.92149
O	-1.28768	1.37374	-0.02850
H	-1.96878	-0.93407	-0.62223
H	-1.50315	-1.72726	0.88790
H	0.93885	0.29876	0.41325
H	2.02138	-0.71222	-0.46502
H	-2.23612	1.60142	-0.00066

val+05_156			
C	0.99705	-0.34542	-0.92382
C	-1.21529	-0.55943	0.15553
N	1.41059	0.07372	0.27310
O	-0.34276	-0.55865	-0.99752
O	-1.30050	0.67576	0.81040
H	-2.17937	-0.88895	-0.24117
H	-0.83778	-1.27397	0.89211
H	2.39932	0.25185	0.38587
H	0.81265	0.36433	1.04613
H	-1.71672	1.31516	0.20828

val+05_157			
C	0.95784	1.27270	1.15338
C	-1.19472	0.69107	0.03816
N	0.18493	0.61402	0.46636
O	0.69962	-0.88218	-0.31930
O	2.04191	-1.01330	0.04912
H	1.97827	0.87432	1.24383
H	-1.22529	0.70559	-1.05344
H	-1.64037	1.60025	0.44314
H	-1.72902	-0.18955	0.40121
H	1.99673	-1.55793	0.85964

val+05_158			
C	0.75093	1.24393	0.21120
C	-1.22161	-1.29503	0.07130
N	0.68187	-0.00561	0.42638
O	-0.39633	-0.61614	1.04170
O	1.63151	-1.07599	0.20953
H	1.74055	1.46840	-0.21377
H	-1.61250	-0.57531	-0.65520
H	-2.03571	-1.72454	0.65619
H	-0.65742	-2.08418	-0.43170
H	2.25851	-0.69982	-0.43701

val+05_159			
C	1.00386	-1.70937	0.16327
C	-1.13903	-0.57735	0.01039
N	0.23787	-0.81078	-0.41297
O	-1.29432	0.62361	0.73696
O	-1.16561	1.71220	-0.22699
H	1.98196	-1.64791	-0.35964
H	-1.80021	-0.57608	-0.86173

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H	-1.40423	-1.36887	0.71356
H	0.52966	-0.20030	-1.18230
H	-0.35237	2.13946	0.10166

val+05_15

C	0.55504	0.33902	-0.16887
C	-0.80155	0.96261	0.06455
N	0.57730	-1.03079	-0.33478
O	1.59993	0.97505	-0.26975
O	-0.49374	-1.77757	0.19012
H	-0.70145	2.04711	0.00215
H	-1.17877	0.68673	1.05496
H	-1.53287	0.61223	-0.66992
H	1.47123	-1.48244	-0.16015
H	-0.92261	-2.16534	-0.59330

val+05_160

C	1.79072	0.19261	0.01056
C	-1.57526	-0.36792	-0.01576
N	0.74753	-0.31138	-0.52213
O	-0.32916	-1.03319	0.17683
O	-1.71489	0.79848	0.74169
H	1.72124	0.05710	1.10279
H	-2.31425	-1.08475	0.34734
H	-1.72990	-0.17773	-1.08737
H	0.56361	-0.35502	-1.52371
H	-1.26225	1.52340	0.28105

val+05_161

C	1.46206	-0.97438	0.19514
C	-1.88150	-0.30414	0.01244
N	1.79373	0.29028	0.22675
O	0.42080	-1.46017	-0.19119
O	-0.78159	-0.13793	-0.82151
H	-2.67620	0.37563	-0.34631
H	-2.29849	-1.32639	-0.01553
H	-1.68674	-0.04494	1.06804
H	1.08459	0.95175	-0.09622
H	2.68204	0.60937	0.58479

val+05_162

C	2.64165	-0.31737	0.22043
C	-1.44436	0.21962	-0.40430
N	1.67154	0.33422	-0.22810
O	-0.50231	1.29759	-0.34335
O	0.50190	0.95148	0.60806
H	2.59037	-0.46345	1.30774
H	-1.90917	0.05678	0.57280
H	-2.19446	0.55246	-1.12707
H	-0.96923	-0.70197	-0.75692
H	1.45155	0.62914	-1.17999

val+05_16

C	0.23367	0.63390	0.17683
C	-0.52833	-1.73687	-0.04092
N	0.39398	-0.69309	0.38732
O	1.05706	1.49887	0.45499
O	-0.97792	0.91803	-0.37525
H	-1.54477	-1.50290	0.28438
H	-0.52985	-1.86695	-1.12997
H	-0.22108	-2.67548	0.42391
H	1.31221	-0.95860	0.71230
H	-1.00768	1.88678	-0.46379

val+05_17

C	0.29204	1.36975	0.25741
C	-0.87630	-0.97113	-0.11880
N	0.28264	-0.05424	-0.10721
O	0.36388	0.79033	-1.20871
O	1.47762	-0.73174	0.19201
H	-0.78890	1.58531	0.37085
H	-1.75716	-0.38411	-0.37196
H	-0.96668	-1.40742	0.87643
H	-0.70717	-1.74916	-0.86727
H	1.59953	-1.36530	-0.54444

val+05_18

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C	1.04610	0.90515	1.03385
C	0.53224	-0.15883	0.17389
N	-0.16368	1.16331	0.06627
O	-0.17350	-1.15820	0.84545
O	-0.91336	-1.95449	-0.14072
H	1.91197	1.37029	0.54958
H	0.92299	-0.50752	-0.78345
H	-1.07774	1.26038	0.49981
H	-0.08734	1.64902	-0.82701
H	-1.81278	-1.59412	-0.02547

val+05_19

C	-0.25896	0.58768	0.78115
C	0.21508	-0.62254	0.00029
N	0.45961	1.41648	-0.30455
O	0.98405	0.25590	-0.96685
O	-0.77917	-1.36534	-0.62186
H	-1.32952	0.72513	0.59145
H	0.96171	-1.29960	0.43913
H	-0.09651	1.98470	-0.95763
H	1.25385	1.98072	0.01040
H	-0.41524	-2.22922	-0.88482

val+05_1

C	-0.20727	2.29288	0.84575
C	0.60763	2.25273	-0.13580
N	0.37219	0.92318	0.55311
O	-1.06430	-1.13927	-0.54900
O	-0.42775	-2.28063	0.09597
H	-0.92867	2.71443	1.52481
H	1.15780	2.61146	-0.98895
H	-0.53151	-0.38399	-0.14436
H	1.14583	0.73495	1.20285
H	-1.08604	-2.49264	0.78124

val+05_20

C	0.28815	0.95349	-0.27013
C	1.01519	-1.31656	0.09977
N	-1.14830	0.52966	0.10352
O	1.13413	-0.04823	0.43071
O	0.13677	-1.80305	-0.60625
H	0.44944	1.82372	0.38148
H	1.81120	-1.91587	0.56574
H	-1.36936	0.42945	1.10721
H	-1.80592	1.20318	-0.29463
H	-1.30801	-0.38529	-0.33722

val+05_21

C	0.40752	0.12526	-0.70927
C	-0.16400	1.25891	0.02515
N	1.00612	0.47943	0.52982
O	-0.90134	-1.42121	0.69625
O	-0.35569	-1.15860	-0.65882
H	0.96048	0.13517	-1.64298
H	-1.11647	1.08408	0.51729
H	0.04498	2.27434	-0.29826
H	0.62663	-0.20247	1.20506
H	-1.15482	-1.06401	-1.21665

val+05_22

C	-0.28480	0.20255	0.37087
C	0.73502	1.25374	0.03031
N	-0.04412	-1.00435	0.04048
O	1.92582	0.72440	-0.52211
O	-1.09573	-1.86842	0.38051
H	-1.21412	0.50116	0.86044
H	0.26122	1.97969	-0.65342
H	0.99813	1.81208	0.93873
H	1.68688	-0.12756	-0.92745
H	-0.76850	-2.73499	0.08773

val+05_23

C	0.81252	0.88897	-0.33283
C	-0.94048	1.49016	-0.10544
N	-0.23009	0.20249	-0.01275
O	0.33791	2.15507	-0.46677
O	-0.91792	-2.58004	0.53963

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H	1.85677	0.63141	-0.48576
H	-1.66121	1.56589	-0.92071
H	-1.32573	1.87737	0.83878
H	-0.67965	-1.64126	0.37897
H	-1.11014	-2.91237	-0.35001

val+05_24

C	0.15811	1.76682	0.83386
C	-0.44500	-0.56803	-0.30239
N	0.47950	0.36529	0.40478
O	0.95882	1.39874	-0.43010
O	-1.21944	-1.27305	0.61418
H	-0.87189	1.88989	0.43323
H	-1.08948	0.07668	-0.90074
H	0.16282	-1.21194	-0.94649
H	1.23809	-0.09488	0.91264
H	-0.74794	-2.07982	0.87741

val+05_27

C	-1.14709	-1.00845	0.12719
C	-0.02408	1.16207	-0.03005
N	-0.03656	-0.34015	0.13983
O	1.07155	1.50098	-0.80886
O	1.13777	-0.82548	0.33027
H	-1.10902	-2.07393	0.31222
H	-2.07323	-0.48258	-0.05821
H	-0.94439	1.47978	-0.52046
H	0.02861	1.56362	0.99077
H	1.77914	0.90484	-0.47990

val+05_28

C	0.69484	0.84994	-0.36827
C	0.73461	-0.62969	-0.17849
N	-0.76112	1.26100	0.12281
O	1.26310	0.17063	0.84563
O	-0.44699	-1.33177	0.12384
H	1.45657	-1.24370	-0.72376
H	-0.67987	2.01216	0.80964
H	-1.28588	0.47632	0.53883
H	-1.28745	1.62881	-0.67246
H	-0.22801	-2.03699	0.75595

val+05_29

C	0.60447	0.85775	-0.24372
C	-0.82444	1.15262	-0.45004
N	-0.29811	0.69954	0.87874
O	1.26962	-0.23136	-0.84658
O	0.33216	-1.32915	-1.02879
H	1.35696	1.64093	-0.16936
H	-1.40293	0.44028	-1.03042
H	-1.17690	2.18082	-0.48213
H	-0.51733	-0.29187	0.98957
H	0.73180	-1.99286	-0.43606

val+05_2

C	-0.35218	0.37038	0.27473
C	0.72516	1.25601	0.42709
N	0.03013	-0.91776	-0.08469
O	1.92388	0.94512	0.21772
O	0.12303	-1.91659	1.11819
H	-1.39556	0.56799	0.46632
H	0.46073	2.29239	0.71321
H	-0.58419	-1.40635	-0.73674
H	1.00559	-0.85164	-0.41817
H	0.43052	-2.74916	0.70333

val+05_30

C	0.63089	1.00022	-0.00862
C	-0.75973	1.45057	0.23387
N	-0.29506	0.14250	0.76368
O	-0.69478	-0.90972	-0.15687
O	-1.93955	-1.42702	0.33855
H	1.46281	1.38866	0.57133
H	0.87677	0.65480	-1.00894
H	-1.45715	1.40480	-0.59642
H	-0.97904	2.18414	1.00439
H	-1.63127	-2.03364	1.04013

val+05_31			
C	-0.21051	-0.38350	0.05552
C	1.09217	-0.18035	-0.10033
N	-0.97425	-1.51751	0.18433
O	-2.36769	0.59094	-0.56774
O	-1.03467	0.85706	0.04882
H	1.50170	0.82155	-0.13125
H	1.76600	-1.02706	-0.15957
H	-1.95183	-1.26025	0.00910
H	-0.83936	-2.02038	1.05623
H	-1.27216	1.07350	0.97457

val+05_32			
C	-1.29926	0.85007	-0.48326
C	-0.00645	0.83211	-0.10873
N	-1.99556	-0.39717	0.11299
O	0.54959	-0.09642	0.78303
O	1.76995	-0.68509	0.17610
H	0.69986	1.60171	-0.41704
H	-2.69621	-0.11084	0.80122
H	-2.50861	-0.88594	-0.62367
H	-1.36058	-1.06584	0.57379
H	1.37334	-1.33011	-0.44064

val+05_33			
C	-0.87739	1.77547	0.00037
C	0.57583	1.24158	0.07042
N	0.08535	-0.10947	-0.38068
O	-1.13837	0.38153	-0.79787
O	0.00159	-1.02336	0.71928
H	-1.32428	1.50798	0.97676
H	1.24737	1.59488	-0.72028
H	1.11785	1.17648	1.01710
H	0.57527	-0.59642	-1.14670
H	-0.68261	-1.66356	0.43551

val+05_34			
C	-1.84218	0.44675	0.04180
C	-0.07723	-0.40310	0.14489
N	-0.95637	0.13523	-0.88045
O	-1.21136	-0.10758	1.07184
O	2.24770	1.21714	0.86737
H	-2.68878	1.11998	0.08335
H	0.04060	-1.49054	0.07498
H	-0.83970	0.41209	-1.84667
H	1.47325	0.64758	0.59084
H	2.12596	1.29155	1.82635

val+05_35			
C	-1.22988	1.18040	-0.87006
C	-0.07120	0.63064	-0.05190
N	-0.81210	-0.74315	-0.01334
O	-1.75295	-0.30932	-0.98708
O	1.12110	0.49760	-0.76115
H	-1.93373	1.61166	-0.13308
H	0.11530	0.97776	0.97046
H	-0.27389	-1.55778	-0.33801
H	-1.28050	-0.96710	0.87478
H	1.83526	0.26649	-0.14122

val+05_36			
C	-0.71181	0.63822	-0.86756
C	0.24614	-0.00608	0.10872
N	-0.04755	-1.46436	0.03236
O	-1.32226	-1.69467	0.48056
O	-0.93338	1.86150	-0.43500
H	0.12008	0.28065	1.15728
H	1.27582	0.20870	-0.21857
H	0.06970	-1.74188	-0.95740
H	0.66363	-1.99426	0.56134
H	-1.50968	2.32128	-1.07402

val+05_37			
C	0.90987	0.54951	-0.46007
C	-2.04690	1.32346	0.92810
N	2.09290	0.37924	-1.05081

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O	-1.91136	0.14004	1.18685
O	0.53993	-0.63376	0.07754
H	-2.94267	1.87729	1.25900
H	2.59185	-0.51240	-1.06606
H	2.53725	1.15849	-1.51348
H	-1.27949	1.87050	0.35758
H	-0.33119	-0.48087	0.50555

val+05_38			
C	-0.87120	1.04859	0.17349
C	0.39764	0.52845	0.21851
N	0.42085	-0.85508	-0.11868
O	-0.87618	2.39878	0.47924
O	0.62594	-1.74764	1.06685
H	1.37190	0.95066	0.45703
H	-0.52095	-1.05287	-0.49001
H	1.15342	-1.13019	-0.77990
H	-1.79536	2.69117	0.40203
H	0.66284	-2.65099	0.69024

val+05_39			
C	-1.23303	1.78305	0.00785
C	-0.24288	1.09679	0.12039
N	0.41829	-2.14803	-0.25974
O	-2.35955	2.49263	0.10940
O	0.87796	0.41804	0.17156
H	-0.14142	-2.31094	-1.09613
H	1.28752	-2.66583	-0.38590
H	-0.07602	-2.59278	0.51307
H	-2.59131	2.85065	-0.76531
H	0.68974	-0.59079	0.00141

val+05_40			
C	-0.19313	0.69906	0.13013
C	1.06292	1.10861	0.05041
N	-0.59185	-0.60277	-0.45188
O	0.30969	-1.28468	-1.05340
O	-1.22611	-1.34891	0.77211
H	-1.01895	1.21731	0.60123
H	1.36135	2.05380	0.48957
H	-1.47351	-0.49597	-0.98025
H	1.80572	0.50191	-0.45506
H	-0.41113	-1.76157	1.12034

val+05_41			
C	-0.31989	0.75615	-0.18444
C	-1.48073	1.41753	-0.24598
N	-0.09020	-0.48370	0.44998
O	0.82670	1.24395	-0.74993
O	-1.25553	-1.11607	0.93359
H	-1.51224	2.40767	-0.68305
H	-2.39112	0.98898	0.14979
H	0.40568	-1.13028	-0.16623
H	1.58727	0.95225	-0.21630
H	-1.84364	-1.24488	0.16128

val+05_42			
C	0.17311	-0.17014	-0.85023
C	-0.89386	0.46126	-0.06116
N	-0.16629	-0.77418	0.44098
O	-0.79008	1.59391	0.73221
O	-0.73094	-2.10096	0.43646
H	1.15437	0.30945	-0.81795
H	-1.94482	0.25969	-0.26626
H	0.36223	-0.67504	1.30818
H	0.10310	1.96216	0.61959
H	-0.59560	-2.33305	-0.50702

val+05_43			
C	0.29391	0.61033	1.07395
C	-0.40387	1.18361	-0.15807
N	0.00519	-0.21601	-0.09102
O	0.92367	-0.61326	-1.08155
O	-0.96588	-1.25298	0.04426
H	1.36702	0.82119	1.06777
H	-1.48235	1.33514	-0.13457
H	0.11067	1.72477	-0.95456

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H	1.49355	-1.26187	-0.62175
H	-0.99901	-1.32692	1.02164
val+05_44			
C	-0.02541	-0.34018	-0.39341
C	0.52136	0.77928	-1.14011
N	-0.45010	1.04631	0.09278
O	0.60447	-1.09359	0.59466
O	-1.04597	-1.08146	-0.94995
H	1.52498	1.01590	-0.76300
H	-1.38242	1.38698	-0.12512
H	-0.11894	1.31010	1.01903
H	1.53635	-0.82488	0.63234
H	-1.40491	-1.65946	-0.25282
val+05_45			
C	-0.12291	0.50813	0.44685
C	-0.21583	-0.80322	0.16182
N	-1.17306	1.28929	0.92817
O	1.04058	1.22721	0.38279
O	-1.44502	-1.45419	0.31427
H	0.65113	-1.41313	-0.08227
H	-2.05630	0.79941	0.82175
H	-1.21378	2.20014	0.47729
H	1.72163	0.68026	-0.04185
H	-1.74092	-1.75260	-0.56211
val+05_46			
C	0.58235	-0.39494	0.38644
C	-0.75255	0.24633	0.44415
N	-0.21815	-0.18792	-0.84330
O	0.82845	-1.67379	0.87880
O	-0.97671	1.61166	0.62361
H	1.48986	0.20239	0.42872
H	-1.56653	-0.31889	0.89752
H	-0.64920	-1.05403	-1.16968
H	-0.00280	-2.06789	1.19078
H	-0.42512	2.07547	-0.02923
val+05_47			
C	0.54426	0.05123	0.27785
C	-0.52487	0.84589	-0.37387
N	-0.62539	-0.64102	-0.24407
O	1.79053	-0.23229	-0.26540
O	-1.48796	-1.01504	0.85541
H	0.61108	0.10706	1.36052
H	-1.16844	1.43730	0.27190
H	-0.43351	1.18960	-1.40197
H	1.70453	-0.26422	-1.23265
H	-2.20903	-1.47980	0.39797
val+05_48			
C	-0.00788	0.00494	0.01549
C	-1.28458	0.65460	-0.35720
N	-1.01053	0.15028	1.03254
O	1.14099	0.75448	0.24956
O	0.22918	-1.30898	-0.38834
H	-1.98067	0.09323	-0.97515
H	-1.34285	1.73707	-0.43653
H	-1.47703	-0.74776	1.16349
H	1.47024	1.07469	-0.60694
H	0.53693	-1.29695	-1.31023
val+05_49			
C	0.91864	-0.34173	0.38684
C	2.20028	-0.56253	0.40901
N	-0.32890	-0.13865	0.34454
O	-2.90191	-0.35230	-0.55328
O	-1.04746	0.59520	1.16853
H	2.89463	0.08633	-0.12275
H	2.61942	-1.40217	0.96145
H	-0.89684	-0.57993	-0.40466
H	-2.55747	0.15936	0.21967
H	-3.02619	0.32290	-1.23905
val+05_4			
C	0.33877	1.51021	0.01631

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C	-0.74813	2.24583	0.52778
N	0.71651	0.26970	-0.22459
O	0.91465	2.60512	-0.30471
O	-0.86926	-1.92842	0.68712
H	-0.54273	2.51295	1.57578
H	1.56318	0.10604	-0.75619
H	0.15843	-0.53341	0.09766
H	-0.35694	-2.39153	1.36974
H	-0.92658	-2.57319	-0.03680

val+05_50

C	-0.03414	-0.07650	0.37334
C	1.24589	0.03820	0.08905
N	-1.25671	-0.14396	0.56121
O	2.04741	-1.07358	-0.10503
O	-3.47487	0.01569	-1.38396
H	1.70842	1.02208	0.08728
H	-1.52938	-0.26433	1.54492
H	-2.71527	-0.05362	-0.76772
H	2.68717	-0.85489	-0.80219
H	-3.72882	0.94832	-1.31440

val+05_51

C	-1.03546	0.35864	-0.04235
C	0.27596	0.08534	0.01469
N	-1.76770	-0.98628	-0.14731
O	1.25184	1.06398	0.05380
O	0.87451	-1.16552	0.08015
H	-2.43455	-0.96946	-0.92228
H	-2.32311	-1.17128	0.69230
H	-1.14176	-1.79626	-0.28421
H	0.77259	1.89817	-0.09397
H	1.70168	-1.13234	-0.43162

val+05_52

C	0.65376	-0.60145	0.11607
C	-0.66154	-0.29261	0.78758
N	1.44166	0.33874	-0.22902
O	-0.77879	1.90589	0.03997
O	-0.77625	1.05242	1.22122
H	0.85301	-1.66502	-0.06488
H	-0.76338	-0.88911	1.70323
H	-1.48871	-0.56670	0.11515
H	0.17401	1.81560	-0.20829
H	2.28413	-0.02284	-0.68253

val+05_53

C	-0.62814	-0.14072	-0.01621
C	-0.01473	1.04877	-0.01371
N	0.11754	-1.37536	0.06850
O	1.30903	1.35293	0.04501
O	2.21037	0.21581	-0.13223
H	-1.71413	-0.16279	-0.07331
H	-0.57692	1.97846	-0.03909
H	-0.11661	-2.00210	-0.70129
H	1.59057	-0.57785	-0.00094
H	-0.10618	-1.87676	0.92829

val+05_54

C	-0.79986	1.27448	-0.22291
C	0.50280	0.98144	-0.11570
N	0.17484	-1.33603	0.13162
O	-1.86562	0.41848	-0.18756
O	1.12411	-0.24624	0.05727
H	-1.08961	2.31223	-0.35551
H	1.25432	1.76085	-0.16014
H	0.49081	-1.97730	-0.59787
H	0.39877	-1.78742	1.02014
H	-1.46047	-0.47380	-0.06213

val+05_55

C	-0.01432	0.03453	0.22999
C	-1.26741	0.43862	-0.00455
N	0.54147	-1.24082	0.05531
O	0.90777	0.94358	0.70368
O	2.10156	0.94713	-0.17347
H	-2.06101	-0.27790	-0.18544

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H	-1.51076	1.49410	0.00503
H	-0.08558	-1.89494	-0.40132
H	2.19833	-0.01855	-0.33167
H	0.90125	-1.64314	0.91954

val+05_56

C	0.37369	0.41409	-0.08137
C	0.02874	1.71665	-0.02285
N	-0.38701	-1.79823	-0.07159
O	-0.85857	-0.48369	-0.00241
O	1.44453	-0.24679	-0.18401
H	-1.00830	2.01365	0.06916
H	0.79938	2.47618	-0.06738
H	-0.77773	-2.26758	-0.89350
H	0.68428	-1.62000	-0.15508
H	-0.64031	-2.30679	0.78034

val+05_58

C	0.37680	0.88712	0.18803
C	0.70088	-0.40335	-0.18490
N	-0.32426	-1.45334	-0.02905
O	-0.94957	0.99478	0.67051
O	1.07464	1.92028	0.15144
H	1.65432	-0.72393	-0.57034
H	-0.06605	-2.20136	0.62642
H	-1.05252	1.93507	0.89319
H	-1.16978	-1.00320	0.34465
H	-0.59027	-1.91576	-0.90714

val+05_5

C	0.50406	-0.22353	0.16876
C	-0.63671	0.21896	-0.41867
N	0.55052	-1.85774	0.07873
O	1.49842	0.23491	0.74614
O	-0.87755	1.59617	-0.52802
H	-1.36909	-0.44228	-0.87258
H	0.59828	-2.23453	1.02879
H	1.41700	-2.12957	-0.39295
H	-0.23584	-2.29642	-0.40634
H	-1.38608	1.87573	0.25133

val+05_61

C	-0.10561	1.22566	-0.51299
C	-0.34810	-1.22958	0.04825
N	0.53224	-0.04601	-0.12172
O	0.36412	1.94464	-1.35685
O	1.01121	0.45937	1.07798
H	-0.98311	1.41329	0.11516
H	-1.18562	-0.93017	0.67859
H	0.24425	-1.99139	0.55627
H	-0.69197	-1.58261	-0.92703
H	1.29089	-0.25711	-0.78645

val+05_62

C	0.72912	1.43453	-0.67213
C	-0.96984	-1.22933	-0.02386
N	0.95105	0.09422	-0.09108
O	1.62432	1.08216	0.58865
O	0.05103	-0.58497	0.76411
H	-0.22036	1.72192	-0.18024
H	-1.55228	-0.49293	-0.58628
H	-0.53708	-1.97470	-0.70029
H	-1.60306	-1.72575	0.71184
H	1.57070	-0.58307	-0.54801

val+05_63

C	0.15198	0.09046	-0.11100
C	0.40306	-1.36972	0.05612
N	-1.02640	0.62469	-0.34105
O	1.16997	0.88538	-0.02037
O	0.82065	2.27191	-0.19237
H	-0.16615	-1.75619	0.90781
H	1.46701	-1.54250	0.22531
H	0.08530	-1.91434	-0.83880
H	-1.87521	0.08546	-0.42744
H	-0.96822	1.64725	-0.41931

val+05_64			
C	0.49786	1.05662	-0.69739
C	-0.10786	-1.42298	-0.33847
N	0.21605	-0.15636	0.36439
O	-0.82650	1.54292	-0.92337
O	0.09267	2.19773	0.05753
H	-1.05541	-1.28898	-0.86143
H	0.68630	-1.62080	-1.05950
H	-0.18672	-2.24402	0.37533
H	-0.53864	0.11748	1.00523
H	1.06685	-0.26941	0.92098

val+05_65			
C	0.56419	-0.46168	-0.17224
C	-0.96652	1.30671	0.13752
N	0.90707	-1.70953	0.25968
O	-0.48178	0.01756	0.54524
O	1.08996	0.13139	-1.10239
H	-0.18300	2.06292	0.23179
H	-1.32011	1.27836	-0.89638
H	-1.79218	1.53267	0.81248
H	1.80764	-2.05509	-0.03977
H	0.58803	-2.01171	1.17006

val+05_67			
C	-1.31633	1.37387	-1.76400
C	-0.17728	1.13772	-0.18679
N	0.72908	-1.86068	0.77461
O	0.02977	1.33395	-1.60104
O	-1.59474	1.20587	-0.44709
H	0.18022	1.97858	0.40985
H	0.15298	0.15135	0.16952
H	0.28573	-2.16410	1.64178
H	1.73150	-1.96841	0.92997
H	0.48406	-2.56875	0.08239

val+05_69			
C	-0.58568	-1.76223	0.11524
C	1.05547	1.96476	-0.39022
N	-0.12021	-0.56163	-0.01300
O	1.80986	1.15169	-0.91251
O	-0.64468	0.53262	0.40535
H	-0.00934	-2.57707	-0.30072
H	-1.52653	-1.90889	0.62940
H	0.27720	2.49582	-0.96427
H	1.19037	2.30591	0.65027
H	0.78394	-0.42799	-0.50844

val+05_6			
C	0.12366	-0.11435	-0.16331
C	1.16167	0.77892	-0.13956
N	0.60733	-1.50275	0.02757
O	2.37291	0.44291	0.12517
O	-1.16271	0.04247	-0.62377
H	0.89977	1.83295	-0.34646
H	0.22662	-1.99531	0.84285
H	1.63142	-1.31196	0.17509
H	0.47891	-2.11187	-0.78900
H	-1.77378	0.08309	0.13292

val+05_70			
C	1.01031	0.77821	-0.02253
C	-0.83541	-1.12468	0.31971
N	0.32759	-0.48807	-0.46391
O	0.19195	1.74433	0.51044
O	1.17483	0.92877	1.33288
H	1.82266	1.09550	-0.67849
H	-0.41177	-1.23294	1.33121
H	-1.55594	-0.29449	0.39699
H	0.01068	-0.32083	-1.42435
H	1.06681	-1.19111	-0.56135

val+05_71			
C	1.12769	-0.43933	0.15058
C	-1.34090	-0.50589	0.01494
N	-0.03572	0.10162	0.26446
O	-0.16643	1.41074	0.67549

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O	1.07537	1.99162	0.92545
H	1.96202	0.20422	0.39843
H	1.19348	-1.46732	-0.17432
H	-1.87142	0.10557	-0.71662
H	-1.19079	-1.51380	-0.36871
H	-1.89901	-0.53294	0.95249

val+05_72

C	-0.86271	-0.37302	0.32501
C	0.41764	-1.13174	0.07734
N	-0.85638	0.89829	0.41220
O	1.58532	-0.34262	0.23273
O	1.57857	0.67758	-0.80791
H	-1.76891	-0.98741	0.39526
H	0.52547	-1.93557	0.81686
H	0.38033	-1.59659	-0.91967
H	-1.79653	1.27038	0.56722
H	0.85590	1.24879	-0.44885

val+05_73

C	1.37534	0.00704	0.28789
C	-2.08747	0.83004	-0.04008
N	0.52722	-1.01247	0.01128
O	1.92920	0.70835	-0.54999
O	-1.71573	1.97276	-0.19649
H	1.50490	0.16241	1.37424
H	-2.32501	0.16398	-0.89166
H	-2.22134	0.38427	0.96418
H	0.40796	-1.31432	-0.94798
H	0.20383	-1.62906	0.74420

val+05_74

C	-1.46844	-0.68599	-0.03359
C	1.79163	1.25662	-0.20054
N	-0.38140	-1.47377	-0.12411
O	-1.45739	0.54514	-0.00109
O	2.16278	0.09791	-0.24527
H	-2.41201	-1.25909	0.01093
H	0.72134	1.51400	-0.13077
H	2.51721	2.08947	-0.22826
H	0.55293	-1.06347	-0.17193
H	-0.47813	-2.47922	-0.14467

val+05_76

C	-0.59030	0.92364	-0.24615
C	-0.53994	-0.48525	0.31962
N	0.88443	-0.90840	0.23079
O	-1.35025	1.77372	0.16729
O	1.67080	0.08474	0.76467
H	0.07362	1.10936	-1.11198
H	-1.19970	-1.16523	-0.23639
H	-0.81169	-0.47478	1.37496
H	1.11471	-1.09879	-0.75948
H	1.00402	-1.81471	0.71056

val+05_77

C	-1.18680	0.23255	0.02234
C	0.23224	0.76427	0.12423
N	1.16262	-1.35068	0.05605
O	-2.08032	0.54916	0.78006
O	1.15335	-0.04480	-0.57934
H	-1.35827	-0.45655	-0.83118
H	0.50462	0.89033	1.18081
H	0.27249	1.74935	-0.36042
H	2.07632	-1.38951	0.51656
H	1.24134	-1.98362	-0.74171

val+05_78

C	0.51755	0.47160	-0.69470
C	-0.00513	-0.44336	0.39336
N	0.38765	-1.82508	0.13484
O	0.94739	0.10950	-1.77072
O	0.40940	1.76967	-0.34136
H	0.71798	2.30359	-1.09877
H	-1.09399	-0.26470	0.45070
H	0.40767	-0.11213	1.35271
H	-0.07937	-2.42694	0.81082

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H	0.03215	-2.09974	-0.77978
val+05_79			
C	-1.28004	0.74911	0.77154
C	0.89949	0.22485	-0.02044
N	0.64396	-1.10277	-0.49815
O	0.00564	0.55470	1.08990
O	-2.12817	0.95316	1.60980
H	-1.48673	0.71788	-0.31086
H	0.74057	0.94707	-0.82557
H	1.88739	0.38462	0.41933
H	1.22717	-1.79440	-0.03539
H	0.80350	-1.17152	-1.49846
val+05_7			
C	0.73526	0.32304	-0.05277
C	-0.26717	-0.61761	-0.16947
N	0.24368	-1.98478	0.00744
O	1.95321	0.06457	0.16575
O	0.34334	1.64262	-0.19389
H	-1.32231	-0.48425	-0.33612
H	-0.13501	-2.48948	0.81731
H	1.25995	-1.83508	0.16478
H	0.13117	-2.59977	-0.80666
H	1.16618	2.15046	-0.08587
val+05_80			
C	1.11646	0.05166	-0.30310
C	0.03556	1.13132	-0.27650
N	-1.04830	-1.04459	0.57700
O	2.06096	0.05250	0.46045
O	0.05377	2.05610	0.51074
H	1.00497	-0.69334	-1.11448
H	-0.72690	1.04009	-1.07403
H	-1.75520	-0.57745	1.14330
H	-0.57329	-1.70793	1.18769
H	-1.54342	-1.58987	-0.12727
val+05_81			
C	-0.80421	-0.86417	-0.10528
C	-1.01156	0.64937	-0.12184
N	1.50238	0.23536	0.25934
O	-0.91530	-1.55046	-1.10117
O	-1.29878	1.25920	-1.13221
H	-0.60961	-1.29229	0.89703
H	-0.94527	1.13487	0.87091
H	2.03123	-0.51440	-0.18425
H	1.79909	0.27310	1.23352
H	1.80283	1.10571	-0.17755
val+05_83			
C	-0.40537	1.53519	-0.13659
C	0.00562	-1.78951	-0.02769
N	0.52371	-0.57141	-0.65495
O	0.59406	1.85822	0.46967
O	-0.60781	0.35381	-0.73439
H	-1.28869	2.16745	-0.29480
H	-0.44864	-1.62065	0.95757
H	0.85874	-2.46705	0.07923
H	-0.72778	-2.25519	-0.69066
H	1.15695	-0.10127	-0.00067
val+05_84			
C	-0.60635	0.68156	-0.02693
C	0.79663	0.97335	0.38381
N	0.49282	-0.20484	-0.45149
O	0.56912	-1.49057	0.15508
O	-0.45841	-2.27626	-0.45722
H	-1.27183	0.18962	0.67204
H	-1.06339	1.26334	-0.81953
H	1.35897	1.75663	-0.11244
H	1.11488	0.69885	1.38303
H	0.74155	-0.23198	-1.44445
val+05_85			
C	-0.95491	1.22691	-0.43194
C	0.80192	-1.99669	0.32285

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N	0.20494	0.84268	0.32676
O	0.15780	0.78523	-1.17035
O	0.62103	-2.70049	1.29356
H	-1.80198	0.54430	-0.37988
H	-1.20285	2.28385	-0.52902
H	1.78020	-1.52764	0.10591
H	0.00987	-1.79186	-0.42022
H	0.75207	1.69181	0.51262

val+05_86			
C	0.32274	-1.06567	-0.78578
C	0.62901	0.32312	-0.19899
N	-0.70859	1.03623	-0.16416
O	1.54727	-1.83981	-0.62524
O	0.40975	-2.03557	0.30931
H	1.25704	0.89207	-0.88961
H	1.05107	0.35526	0.81177
H	-0.65101	2.05638	-0.21911
H	-1.23542	0.66709	-0.97318
H	-1.24177	0.79639	0.67689

val+05_88			
C	0.29035	-0.17905	0.44662
C	-0.58315	0.89458	-0.15066
N	0.41838	-1.34756	-0.31374
O	1.40432	0.28279	1.20597
O	0.19732	-0.38454	1.82926
H	-0.14989	1.25979	-1.08762
H	-1.57900	0.49514	-0.36335
H	-0.66620	1.72622	0.55065
H	1.17163	-1.93866	0.02727
H	0.54164	-1.16180	-1.30441

val+05_8			
C	0.36278	1.84775	0.12408
C	-0.65247	1.43802	-0.60050
N	0.92257	-1.42704	0.14300
O	1.26885	2.22414	0.77102
O	-0.43590	-1.77724	-0.17549
H	-0.87121	0.37443	-0.64446
H	-1.25409	2.16386	-1.13503
H	1.37183	-2.28836	0.46289
H	1.37637	-1.18397	-0.74034
H	-0.40891	-2.44849	-0.88248

val+05_90			
C	-0.10050	-0.24957	-0.45881
C	-0.80627	1.01680	-0.12920
N	0.59535	0.79968	0.38579
O	1.62021	1.51263	-0.08102
O	-0.43529	-1.45359	0.11452
H	0.40634	-0.33121	-1.41587
H	-1.59433	1.00268	0.61931
H	-0.85293	1.80070	-0.87614
H	0.60918	0.53774	1.38199
H	-1.33207	-1.40656	0.48413

val+05_91			
C	-0.60646	1.15153	-0.46507
C	0.60503	1.00037	0.42420
N	-0.03908	-0.19285	-0.17129
O	0.49972	-0.95464	-1.06024
O	-0.81815	-0.88942	0.87687
H	-1.56364	1.36615	-0.00471
H	-0.46453	1.45319	-1.49656
H	0.48290	1.11725	1.49500
H	1.58722	1.19493	0.00975
H	-1.23170	-1.58911	0.33385

val+05_92			
C	0.74860	1.17888	-0.29365
C	-0.71502	0.85542	-0.06040
N	-0.95915	-0.55583	-0.31873
O	1.34122	2.07643	0.26721
O	-0.32671	-1.33768	0.70208
H	-1.30491	1.42959	-0.79026
H	-1.00706	1.19572	0.94685

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H	-1.95991	-0.74818	-0.25874
H	1.24343	0.53437	-1.04966
H	-0.70720	-1.05462	1.55861

val+05_93

C	0.98712	-0.21586	1.09082
C	-0.43666	0.06499	0.25136
N	-0.50673	-1.27204	-0.47634
O	1.43243	0.78159	1.64262
O	-0.33301	1.12185	-0.64896
H	-1.31504	0.12365	0.90188
H	-1.36117	-1.81628	-0.34520
H	-0.33345	-1.15921	-1.47858
H	0.33143	-1.75039	-0.02041
H	-1.21691	1.37310	-0.96648

val+05_94

C	0.61865	0.19017	-0.26058
C	1.40169	-0.82149	0.08572
N	-0.59677	0.51590	0.48685
O	-0.67690	1.75855	0.84025
O	-1.75801	0.09525	-0.43223
H	0.78378	0.89987	-1.06128
H	2.31846	-1.01736	-0.45973
H	1.16643	-1.48083	0.91704
H	-0.74922	-0.16116	1.25313
H	-2.05981	0.99219	-0.67924

val+05_95

C	1.73860	-0.49956	-0.01158
C	0.00424	1.04537	-0.23498
N	0.38147	-0.16781	-0.15380
O	2.43891	-0.14004	0.91202
O	-2.32431	-1.25696	-0.32633
H	2.08468	-1.19465	-0.79446
H	-1.06328	1.25342	-0.29355
H	0.69990	1.88870	-0.26291
H	-1.35009	-1.18581	-0.28146
H	-2.58600	-1.28184	0.60686

val+05_96

C	0.49047	0.79613	-0.19234
C	1.15582	-0.35300	-0.02123
N	-0.91036	0.87135	-0.37418
O	-1.46120	1.83854	0.56420
O	0.48528	-1.55354	0.04383
H	1.02381	1.73429	-0.29584
H	2.24092	-0.38837	0.00477
H	-1.96160	2.43014	-0.02160
H	-1.33233	-0.01679	-0.10041
H	1.08500	-2.23165	0.38941

val+05_97

C	0.33216	-0.04673	-0.61635
C	0.98394	-0.95615	0.26913
N	-1.00327	0.13171	-0.51860
O	2.19783	-1.18070	0.29403
O	-1.66942	1.42554	0.50077
H	0.87361	0.59516	-1.29936
H	0.29590	-1.50683	0.95220
H	-1.48900	0.49638	-1.33262
H	-1.53396	-0.60900	-0.06479
H	-0.93790	1.45903	1.14399

val+05_98

C	1.18310	0.28916	-0.01548
C	-0.50749	2.05809	-0.01790
N	-0.12764	0.72676	-0.01708
O	-1.66564	2.42305	-0.01983
O	1.50293	-0.88366	-0.01502
H	1.91275	1.11416	-0.01479
H	0.34975	2.74994	-0.01658
H	-0.86459	0.02518	-0.01815
H	-0.55100	-3.50750	0.08914
H	-0.12146	-2.90048	0.06619

val+05_99

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C	0.47822	0.28188	0.15141
C	1.27550	-0.74916	-0.17036
N	-0.91751	0.17654	0.29077
O	-1.60196	1.12924	-0.55071
O	0.89368	1.53064	0.50212
H	2.35369	-0.68253	-0.06771
H	0.85585	-1.69016	-0.50627
H	-2.03977	1.70690	0.09574
H	-1.23239	-0.73719	-0.02734
H	1.84258	1.60363	0.30935

val+05_9

C	-0.41895	-0.59654	-0.23791
C	-0.20790	0.76494	-0.30906
N	0.83563	-1.33478	-0.03264
O	0.91637	1.33350	-0.20636
O	-1.33703	1.54002	-0.50799
H	1.54820	-0.57927	0.00091
H	0.88984	-1.86553	0.84440
H	1.08841	-1.98161	-0.78870
H	-1.33331	-1.15807	-0.32463
H	-1.00096	2.45283	-0.53013

val+07_100

C	-0.90919	0.43940	-0.09175
C	0.36189	0.24635	0.34342
N	0.69247	-1.35672	0.32171
O	1.32505	0.91120	0.74684
O	-1.41030	1.74164	-0.23127
H	1.50716	-1.51186	-0.27769
H	-1.56122	-0.37123	-0.40393
H	-0.06868	-1.95926	-0.00015
H	0.95963	-1.64547	1.26623
H	-1.85801	1.98216	0.59689

val+07_101

C	-0.09200	0.85966	1.39754
C	-0.61953	0.71035	-0.05786
N	-0.39675	-0.71544	-0.42589
O	-0.75974	-1.51579	0.63677
O	1.21845	0.91364	1.40586
H	-1.69579	0.87974	-0.08492
H	-0.11725	1.38121	-0.77286
H	-0.92207	-0.94005	-1.28766
H	0.59445	-0.85097	-0.68597
H	1.67752	0.86986	0.52809

val+07_102

C	-0.10753	0.14144	1.18755
C	0.29480	0.04214	-0.07043
N	0.20105	-1.25790	-0.79731
O	-0.30217	-2.30448	-0.09189
O	0.82409	0.95209	-0.92287
H	-0.04924	1.07363	1.73682
H	-0.50074	-0.75322	1.65130
H	-0.34859	-1.05605	-1.65439
H	1.15768	-1.44331	-1.15497
H	0.89705	1.81367	-0.47851

val+07_103

C	0.72056	0.79894	-0.72339
C	-0.62260	0.97319	-0.05500
N	-0.01468	-0.37739	-0.20501
O	-0.51648	-1.31311	-0.93541
O	0.62340	-0.82425	1.05334
H	1.61435	1.07562	-0.17582
H	-1.50165	1.11122	-0.67410
H	-0.65170	1.36366	0.95536
H	0.77377	0.81402	-1.80566
H	-0.00047	-1.53161	1.31010

val+07_104

C	0.34832	0.07306	-0.01248
C	-0.60792	1.13136	-0.41232
N	-1.08541	0.01426	0.48301
O	-1.40077	0.23777	1.75911
O	0.73758	-0.80344	-0.99677

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H	1.02191	0.25245	0.82219
H	-0.98513	1.11534	-1.43028
H	-0.58634	2.08549	0.10041
H	-1.63428	-0.68809	-0.03251
H	1.12373	-1.59151	-0.57777

val+07_105

C	0.56892	0.29094	0.34495
C	-0.52603	1.10392	-0.30409
N	-0.81405	-0.24764	0.22835
O	-1.57554	-0.49496	1.23823
O	-0.93060	-1.19290	-0.90453
H	0.85025	0.51340	1.36798
H	1.30981	-0.18057	-0.28980
H	-1.00575	1.88902	0.26844
H	-0.53459	1.19718	-1.38409
H	-1.03440	-2.02919	-0.40923

val+07_106

C	0.41837	-0.59136	0.33588
C	1.46980	0.20270	0.21066
N	-0.86890	-0.23285	-0.30153
O	-0.90905	0.84416	-0.99310
O	-1.86546	-0.23498	0.90864
H	1.40188	1.11427	-0.37214
H	2.40881	-0.05052	0.68969
H	-1.26986	-1.06093	-0.77215
H	0.36846	-1.52405	0.88379
H	-1.75404	0.69736	1.18066

val+07_109

C	-0.94976	0.30612	0.47330
C	0.38334	0.28973	0.47645
N	-1.73184	-0.73708	-0.19795
O	-2.66132	-0.21039	-1.06887
O	1.07886	-0.75301	-0.06103
H	0.95596	1.10097	0.91629
H	-1.55144	1.09803	0.89381
H	-2.18129	-1.32936	0.52112
H	-1.06081	-1.36421	-0.67351
H	2.02000	-0.52649	-0.11422

val+07_110

C	0.48802	0.65243	-0.49997
C	-0.09881	1.56910	0.28503
N	0.53550	-0.69185	-0.01295
O	-0.63114	1.29446	1.50085
O	-0.09304	-1.58272	-0.98653
H	0.90015	0.90802	-1.47315
H	-0.18326	2.61703	0.01528
H	-0.49022	0.33172	1.62796
H	1.49510	-1.03487	-0.00735
H	-0.93230	-1.80532	-0.55096

val+07_111

C	1.90623	-1.09920	1.21418
C	-0.81566	0.91130	-0.19867
N	-0.84191	-0.46911	-0.66580
O	2.06847	-2.19355	1.47430
O	0.50636	1.41437	-0.21148
H	-1.39314	1.61297	-0.81796
H	-1.24607	0.91994	0.81446
H	-1.74215	-0.89470	-0.44935
H	-0.74020	-0.49602	-1.67964
H	1.04155	0.76511	0.27986

val+07_111

C	0.34576	0.92280	0.29619
C	-0.92731	1.18627	0.10656
N	0.27532	-1.81585	-0.35435
O	1.68016	-2.05879	-0.14194
O	1.50046	0.78678	0.49158
H	-1.60177	0.40098	-0.20347
H	-1.28159	2.19855	0.26709
H	-0.18992	-2.50047	0.24457
H	1.99748	-1.17736	0.12520
H	0.10841	-2.13420	-1.31073

val+07_113			
C	-0.38703	-0.01180	-0.30750
C	0.55857	0.83684	0.21541
N	-0.09370	-1.41789	-0.07984
O	1.25337	-1.82522	-0.45402
O	1.61915	0.43546	0.81384
H	-1.19798	0.21206	-0.98296
H	0.38305	1.92024	0.09304
H	-0.17292	-1.67362	0.91164
H	1.73819	-1.08359	0.03605
H	-0.71151	-2.03618	-0.60955

val+07_114			
C	0.30840	2.16553	0.92521
C	-0.31026	-1.52074	0.26744
N	-0.02976	-0.82308	-0.84835
O	-0.36912	-1.05407	1.40565
O	0.45641	2.07568	-0.27997
H	0.42541	3.13435	1.44351
H	-0.49123	-2.59264	0.07009
H	0.05337	1.28539	1.53917
H	-0.00031	-1.28438	-1.74677
H	0.15799	0.17985	-0.79788

val+07_115			
C	0.32421	0.58645	0.27047
C	-0.94099	0.51428	-0.22261
N	0.97689	-0.88613	0.25136
O	-1.46643	-0.69153	-0.73716
O	1.07957	1.46955	0.70798
H	-1.55142	1.40607	-0.32561
H	1.84422	-0.87394	-0.28991
H	-2.16570	-0.99900	-0.13573
H	0.30342	-1.53758	-0.16900
H	1.21074	-1.18199	1.20181

val+07_116			
C	0.72763	-0.10657	-0.05873
C	-0.49797	0.37653	0.19183
N	1.02305	-1.43478	-0.39680
O	-1.56247	-0.50289	0.38954
O	1.81554	0.72934	-0.01261
H	-0.68019	1.43965	0.31965
H	2.44767	0.41633	-0.68374
H	0.17809	-2.00026	-0.38032
H	-2.26402	-0.27589	-0.24228
H	1.71368	-1.84827	0.22816

val+07_117			
C	0.70931	1.00152	-0.06123
C	-0.46544	1.27906	0.66340
N	0.38643	-2.26882	0.04668
O	0.98587	2.23387	-0.17306
O	1.43976	0.01140	-0.42879
H	-1.30409	1.45715	-0.02542
H	0.96078	-0.95840	-0.21534
H	1.10949	-2.98824	0.06732
H	-0.09733	-2.30602	0.94399
H	-0.28738	-2.54241	-0.66854

val+07_118			
C	-2.41930	0.89458	-0.08797
C	1.17795	0.65622	-0.81993
N	0.19873	-1.36829	0.59830
O	-2.93084	1.84201	-0.45427
O	0.58241	1.66046	-0.47830
H	2.14621	0.36331	-0.37600
H	0.47333	-1.40400	1.57962
H	-0.72210	-0.93078	0.57854
H	0.82787	0.00961	-1.64356
H	0.06055	-2.33691	0.31026

val+07_119			
C	0.22653	1.58711	0.67753
C	-1.05979	0.86050	0.29353
N	0.81290	-1.84730	-0.89731

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O	-2.13858	1.37658	0.49826
O	1.32147	1.09900	0.48947
H	0.08124	2.58312	1.13698
H	1.25761	-1.02157	-0.49413
H	1.21903	-1.95010	-1.82771
H	1.16706	-2.63924	-0.36018
H	-0.92505	-0.13542	-0.16852

val+07_11

C	1.08746	0.15391	-1.78887
C	-0.21001	1.06321	0.09402
N	0.39399	0.42091	1.21759
O	0.74646	1.18316	-1.04859
O	0.47168	-0.95156	-1.32510
H	-1.09483	0.56161	-0.30324
H	-0.43759	2.10442	0.31734
H	0.10767	-0.54863	1.30374
H	0.19134	0.90736	2.08430
H	0.73723	-1.68470	-1.90429

val+07_120

C	0.51551	0.18366	-0.70439
C	-0.85591	0.70602	-0.39556
N	0.81970	-1.12359	-0.04855
O	1.03659	-0.70627	1.25474
O	1.38144	0.70934	-1.35845
H	-1.22569	0.29882	0.54546
H	-1.53179	0.41343	-1.20955
H	-0.82861	1.79678	-0.35193
H	1.65909	-1.52736	-0.49330
H	0.05637	-1.81463	-0.13486

val+07_121

C	-0.04029	1.22608	-0.51722
C	0.29731	-1.25089	-0.21207
N	-0.27946	0.01545	0.29999
O	-1.65738	0.11770	0.12285
O	0.36456	1.17422	-1.65063
H	-0.33624	2.11901	0.04112
H	-0.18019	-2.06064	0.33922
H	1.37801	-1.25373	-0.05097
H	0.06026	-1.31389	-1.27176
H	-0.01037	0.14699	1.28556

val+07_122

C	0.54822	0.18741	-0.03476
C	-0.43391	1.06542	0.66339
N	0.16338	-1.28788	0.30201
O	0.94173	-2.12724	-0.54383
O	-0.61219	0.73507	-0.71908
H	-1.20696	0.67064	1.32831
H	-0.15063	2.09648	0.88075
H	1.56781	-1.43954	-0.88521
H	0.39369	-1.53378	1.27020
H	-0.81934	-1.52479	0.11092

val+07_123

C	0.40141	-0.99808	-0.21422
C	-0.28373	1.42540	0.52734
N	-0.61818	0.07964	-0.23098
O	-1.76702	-0.22659	-0.46848
O	-0.20025	0.88259	1.71601
H	1.32318	-0.61367	0.21335
H	0.01832	-1.84723	0.35268
H	-1.15096	2.06578	0.27995
H	0.63383	1.82101	0.04756
H	0.53740	-1.28724	-1.26051

val+07_124

C	-0.47049	0.05786	-0.15513
C	0.36722	1.25076	-0.27640
N	0.11983	-1.28077	0.10159
O	-0.66295	-2.27940	-0.40608
O	-0.19494	0.56704	-1.43131
H	-1.50174	0.07030	0.18771
H	-0.06193	2.22592	-0.05795
H	1.44854	1.17274	-0.18162

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H	0.26364	-1.36677	1.12507
H	1.07243	-1.27490	-0.30748
val+07_125			
C	0.99691	0.73101	-0.39329
C	-0.86790	0.51719	0.48472
N	0.09566	-0.47371	-0.09616
O	-0.31626	-1.11668	-1.32523
O	-0.19123	1.61305	-0.04060
H	1.63799	0.73103	0.51159
H	-0.81439	0.42653	1.57946
H	-1.89374	0.37300	0.12480
H	0.44800	-1.20548	0.52593
H	-0.98455	-1.77775	-1.05170
val+07_126			
C	-0.03868	-2.53069	1.77713
C	0.27827	2.37255	-0.22875
N	-0.12947	-0.17800	-0.84366
O	-0.01521	-3.32728	2.58749
O	1.45243	2.60356	-0.01151
H	-0.17396	2.48859	-1.22997
H	-0.43306	2.10761	0.57373
H	-0.09525	-0.80914	-0.04302
H	-0.97834	-0.41717	-1.35590
H	0.64506	-0.44933	-1.44864
val+07_128			
C	-1.01775	0.89504	-0.01704
C	0.46650	0.57939	0.02250
N	0.85211	-0.68327	-0.59355
O	0.32658	-1.74571	0.24518
O	-1.82021	0.26167	-0.67323
H	-1.33291	1.77950	0.57515
H	0.98511	1.39627	-0.50395
H	0.82447	0.60171	1.05755
H	0.29619	-0.78464	-1.44539
H	1.13522	-2.21216	0.51248
val+07_129			
C	-0.87027	-0.12563	-1.20715
C	0.04863	-0.20818	-0.07143
N	0.82693	0.91886	0.30544
O	1.01599	0.88098	1.73951
O	-1.38067	-0.19761	0.14174
H	-1.02259	0.82932	-1.71073
H	0.53110	-1.14998	0.17959
H	-1.04047	-1.00534	-1.82654
H	0.28864	1.77207	0.14655
H	1.98371	0.88451	1.82381
val+07_130			
C	-0.02256	2.28229	0.69192
C	-0.72140	1.39533	0.00079
N	0.54968	-1.74622	-0.40080
O	0.57969	3.08327	1.31558
O	-1.11268	0.19709	0.57098
H	-1.01781	1.65699	-1.01411
H	1.29800	-1.35789	-0.97386
H	-0.50186	-0.52611	0.21506
H	1.00475	-2.28099	0.33830
H	0.06419	-2.42456	-0.98686
val+07_131			
C	-0.16730	-0.16477	-0.66414
C	1.11027	0.16316	-0.11865
N	-1.14066	-0.62647	0.14929
O	2.06229	0.61718	-0.76034
O	-2.31270	0.49330	0.89188
H	1.21841	-0.05492	0.96912
H	-0.43133	0.03821	-1.69419
H	-0.84880	-1.02997	1.03700
H	-1.89507	-1.15707	-0.27560
H	-1.72981	1.27385	0.92261
val+07_134			
C	-0.77906	-0.81757	-0.18036

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C	0.32501	-0.01598	0.02325
N	-2.03403	-0.09278	0.06667
O	0.28783	1.19918	0.36947
O	1.55381	-0.61971	-0.17808
H	-1.70641	0.85902	0.32505
H	-2.65543	-0.00944	-0.74625
H	-2.60168	-0.45741	0.84051
H	-0.83557	-1.85563	-0.45980
H	2.20004	0.08412	0.00554

val+07_135

C	-0.50513	-0.56020	0.58818
C	-1.25909	-0.56664	-0.52341
N	0.74419	0.22928	0.63975
O	1.18650	0.72550	-0.59154
O	-0.97766	0.07935	-1.65847
H	-0.75497	-1.08384	1.50066
H	-2.18276	-1.14284	-0.53939
H	1.48624	-0.35484	1.05109
H	0.62107	1.01177	1.30080
H	-0.04599	0.49206	-1.43767

val+07_136

C	0.02185	0.22265	0.81314
C	1.23779	0.41443	-0.06354
N	-1.01311	-0.51168	0.27065
O	-0.11096	0.71781	1.92830
O	-0.71159	-1.40742	-0.77204
H	1.76914	-0.53522	-0.18654
H	1.89739	1.14233	0.41099
H	0.95754	0.76082	-1.06288
H	-1.66283	-0.91817	0.93867
H	-1.19293	-1.05226	-1.54026

val+07_137

C	1.12740	-1.04374	0.25612
C	-1.32929	0.85472	-0.55155
N	-0.94932	-0.55594	-0.66860
O	-0.16595	-0.87553	0.52889
O	1.71370	-1.31336	1.41341
H	-2.05028	1.05229	-1.35121
H	-1.78290	1.10844	0.41549
H	-0.44515	1.47675	-0.71383
H	-1.78022	-1.12287	-0.49073
H	1.06860	-1.32276	2.16222

val+07_138

C	0.84152	-0.81675	-0.26871
C	-0.75165	1.20542	0.36196
N	-0.44916	-0.17701	-0.04715
O	-0.13116	-0.33239	-1.40061
O	-1.47776	-1.01731	0.40095
H	1.57442	0.00605	-0.18585
H	0.00516	1.84835	-0.08259
H	-0.71776	1.24843	1.45109
H	-1.74734	1.46102	-0.00407
H	-1.00188	-1.87552	0.45308

val+07_139

C	0.59065	-1.86194	-0.80329
C	-0.58172	0.16307	0.53655
N	-0.46844	-1.25889	0.06246
O	-0.80764	-1.38879	-1.30336
O	0.07219	1.02638	-0.32201
H	1.21612	-0.97957	-1.03691
H	-0.10157	0.20955	1.51625
H	-1.65581	0.36506	0.62743
H	-0.99497	-1.91380	0.64454
H	-0.38232	0.97862	-1.18175

val+07_13

C	0.10155	-0.15196	0.14172
C	-0.24361	2.29471	1.17235
N	-0.08351	-0.63440	-1.07923
O	-0.00007	2.31602	2.36680
O	0.50084	-1.06202	1.03286
H	-1.26260	2.13408	0.77658

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H	0.51214	2.54700	0.40702
H	-0.38815	-0.01243	-1.81620
H	0.05219	-1.61246	-1.35443
H	0.60563	-1.97184	0.66513

val+07_140

C	1.54063	-0.52051	-0.14297
C	-0.45126	0.73018	-0.06041
N	-1.61362	0.07775	-0.55212
O	0.50618	-0.17500	0.60364
O	2.24485	-1.36922	0.62043
H	0.08797	1.21753	-0.87423
H	-0.71977	1.44987	0.71396
H	-2.11472	-0.40247	0.19187
H	-1.37390	-0.61041	-1.26272
H	3.01743	-1.63401	0.09474

val+07_141

C	0.96807	-1.65919	-0.44973
C	-1.69895	1.51101	0.34094
N	-0.19339	-1.50640	0.04684
O	-2.32344	2.55270	0.31492
O	-1.89198	0.52084	-0.51837
H	1.62869	-2.49413	-0.20363
H	-0.91366	1.30968	1.09240
H	1.33974	-0.92321	-1.16357
H	-1.26155	-0.24953	-0.30800
H	-0.44113	-2.25156	0.70280

val+07_143

C	-0.47971	-0.06049	1.17512
C	1.50567	0.49361	-0.14189
N	-2.30689	-0.65388	-0.10810
O	-0.91209	-0.23162	-0.07823
O	0.78422	0.31678	1.11845
H	1.53661	-0.44765	-0.69348
H	1.02360	1.26359	-0.74680
H	2.50932	0.80349	0.14638
H	-2.69902	0.00045	-0.78945
H	-2.24180	-1.54127	-0.61288

val+07_144

C	1.02695	0.96383	-0.14255
C	-1.85746	-0.48529	0.16928
N	0.41639	-0.24946	-0.23449
O	0.65462	1.90360	0.54272
O	-0.53541	-0.59713	0.72116
H	1.89410	1.00656	-0.82725
H	-2.07196	0.54819	-0.12081
H	-1.98134	-1.15038	-0.69244
H	-2.52608	-0.79316	0.97628
H	0.91899	-1.05005	-0.60540

val+07_145

C	0.93472	-0.31457	0.04516
C	2.01275	0.18077	-0.20151
N	-0.28858	-0.87797	0.21355
O	-1.18820	-0.00776	0.92649
O	-3.05355	0.47374	-1.03727
H	2.97276	0.61183	-0.37371
H	-1.87735	0.18085	0.24074
H	-2.99407	-0.29274	-1.63084
H	-0.25042	-1.74867	0.74052
H	-2.70206	1.20692	-1.56842

val+07_146

C	0.19521	-0.01966	-0.61457
C	1.32163	0.16962	-0.21909
N	-1.12814	-0.18799	-0.93353
O	-2.89684	0.59265	1.29699
O	2.60944	0.31421	0.04072
H	-1.42832	0.39353	-1.71401
H	-3.05634	-0.25092	1.74657
H	-2.29835	0.34217	0.55905
H	-1.37093	-1.15663	-1.13401
H	2.72864	0.65501	0.94587

val+07_148			
C	0.21265	1.31422	0.64217
C	-0.98790	1.66088	0.23639
N	0.27777	-1.26302	-0.48375
O	1.29663	1.09806	1.05255
O	1.59344	-1.60374	-0.00389
H	-1.36637	2.64179	0.50221
H	-1.58028	0.97400	-0.35092
H	-0.31858	-2.01520	-0.13381
H	1.84607	-0.79551	0.47781
H	0.33428	-1.40910	-1.49337

val+07_149			
C	-0.30721	0.64397	-0.04065
C	1.12399	0.34724	0.47411
N	-1.15419	-0.77188	-0.27864
O	-0.92093	1.62285	-0.29905
O	1.87109	1.38923	0.68083
H	-2.00810	-0.75823	0.28622
H	-1.43458	-0.83716	-1.26127
H	-0.61191	-1.60532	-0.03676
H	0.86752	-0.33280	1.35346
H	1.44731	-0.41970	-0.30566

val+07_14			
C	0.60073	2.93716	-0.57339
C	-0.72727	-1.49966	-0.17767
N	-0.67545	-0.26919	0.61154
O	0.48522	3.95690	-1.05889
O	0.72198	0.07444	0.78166
H	-1.76528	-1.85132	-0.18263
H	-0.42728	-1.28012	-1.20694
H	-0.08121	-2.29846	0.21578
H	-0.96752	-0.49937	1.56246
H	0.76648	0.95543	0.36997

val+07_150			
C	-0.56223	0.82620	0.44131
C	0.63137	0.94714	-0.47620
N	0.21641	-0.37746	0.03987
O	-0.46269	-1.12164	-1.04447
O	0.90138	-1.09600	0.86154
H	-1.55472	0.90552	0.01378
H	-0.44414	1.07462	1.48987
H	0.46066	1.11631	-1.53329
H	1.57776	1.27768	-0.06461
H	-0.74609	-1.91345	-0.54620

val+07_151			
C	0.46205	0.49711	0.23009
C	1.33041	-0.48104	0.01640
N	-0.98269	0.27272	0.16740
O	-1.43988	0.96251	-1.13067
O	-1.62533	0.70461	1.20470
H	0.68425	1.51890	0.51065
H	2.39557	-0.29905	0.10909
H	1.01870	-1.48760	-0.25004
H	-1.90296	1.71970	-0.71972
H	-1.19092	-0.70607	-0.09231

val+07_152			
C	1.28767	-0.73797	-0.11861
C	-0.65023	0.79028	0.17359
N	0.21728	-0.06312	-0.61189
O	1.98836	-1.51126	-0.75999
O	-1.91368	0.21700	0.44278
H	1.47874	-0.50364	0.94515
H	-0.85713	1.70588	-0.38404
H	-0.10951	1.04904	1.09199
H	-1.77485	-0.54527	1.02900
H	-0.04056	-0.25584	-1.57447

val+07_153			
C	-0.12504	0.45474	0.34543
C	0.71845	-0.69719	-0.16331
N	-1.49614	0.53371	-0.25554
O	1.80423	-0.95882	0.30885

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O	-2.19255	1.61010	0.21798
H	0.35401	1.41135	0.11734
H	0.30139	-1.29128	-1.00303
H	-1.39482	0.56012	-1.28537
H	-0.26510	0.39275	1.42711
H	-1.98493	-0.35807	-0.06257

val+07_154

C	-0.03805	-0.31861	0.27133
C	1.30900	-0.37967	-0.42632
N	-0.84582	0.92460	-0.15448
O	-0.08113	0.11087	1.53029
O	-2.04352	0.94525	-0.35813
H	-0.69292	-1.16396	-0.00155
H	1.89631	-1.18010	0.03711
H	1.20224	-0.59786	-1.49411
H	1.85440	0.56048	-0.29224
H	-0.39442	1.79890	0.18391

val+07_155

C	0.30998	-1.00293	0.41525
C	-0.64618	1.25876	-0.20012
N	-0.73903	-0.22174	-0.26831
O	0.82957	-1.96149	-0.09536
O	-1.76209	-0.74418	0.50918
H	0.17293	1.61191	-0.83119
H	-1.60453	1.64952	-0.54392
H	-0.48810	1.53195	0.84332
H	-0.79886	-0.53110	-1.24936
H	0.46191	-0.61869	1.42963

val+07_158

C	1.39771	-1.67763	-0.69026
C	-1.13639	1.01828	0.02035
N	-0.30166	0.09131	0.80999
O	1.26688	-1.49237	-1.88181
O	-0.43952	0.19780	2.00943
H	0.78771	-2.41457	-0.13470
H	2.15437	-1.14171	-0.08685
H	-1.74953	0.40179	-0.64735
H	-1.74666	1.65697	0.66390
H	-0.45431	1.60084	-0.60981

val+07_15

C	0.23439	-2.47647	0.57788
C	0.04422	1.98331	0.27041
N	-0.06958	-1.72906	-0.45785
O	0.66898	1.19333	-0.40286
O	0.41202	3.26588	0.35459
H	-0.53773	-2.04454	-1.31253
H	-0.85201	1.71775	0.85061
H	-0.12110	-3.50154	0.32423
H	0.16103	-0.73198	-0.45992
H	-0.19993	3.75281	0.93545

val+07_17

C	-0.27092	-0.61589	-0.51640
C	-0.56744	0.57418	0.43911
N	-0.24810	-1.73339	0.10309
O	-0.84472	0.14485	1.63302
O	0.75463	1.26673	0.34377
H	-1.30871	1.24610	-0.05339
H	-0.03806	-0.55050	-1.57563
H	0.01696	-2.63038	-0.28998
H	-0.49334	-1.56169	1.11327
H	0.71010	1.88169	-0.40956

val+07_18

C	1.09257	2.39866	1.43336
C	-0.38730	-0.50924	-0.13233
N	0.54405	-1.47126	-0.68144
O	1.14605	1.58454	2.22842
O	-0.08567	0.75567	-0.72431
H	-0.23442	-0.47622	0.95597
H	-1.44795	-0.74870	-0.31977
H	0.22223	-1.79190	-1.59309
H	0.58460	-2.29099	-0.07992

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H	-0.86007	1.32693	-0.59800
val+07_19			
C	0.71571	-0.37293	-0.89016
C	-0.85109	1.18208	0.29898
N	-0.16118	-0.02832	0.02693
O	0.17525	0.75618	1.20304
O	-1.36008	-1.22501	0.82814
H	1.59104	-0.92580	-0.57222
H	-1.86800	1.06953	0.65507
H	-0.60251	2.03679	-0.32480
H	0.33816	-0.44187	-1.90336
H	-0.67180	-1.85336	1.10919
val+07_1			
C	-0.58434	1.07808	-0.37147
C	-1.26509	2.17137	-0.55345
N	0.07015	0.01471	-0.17095
O	1.14518	-2.07720	1.22361
O	0.75626	-0.67974	-1.05462
H	-2.31905	2.14184	-0.82588
H	-0.80204	3.15056	-0.44086
H	0.10285	-0.39694	0.78197
H	0.48524	-2.78828	1.24272
H	1.23302	-1.86400	0.26194
val+07_21			
C	-0.41872	-1.04904	0.70268
C	-0.63443	1.06974	-0.46897
N	-1.16621	-0.22885	-0.06609
O	0.70324	-0.75521	1.12070
O	0.55371	0.96669	-1.22187
H	-1.38047	1.56089	-1.09404
H	-0.47259	1.66631	0.43709
H	-2.02129	-0.58030	-0.47754
H	-0.90382	-2.01300	0.93073
H	1.20769	0.58727	-0.60699
val+07_22			
C	-0.03188	-1.02156	0.10616
C	-1.37474	0.94959	-0.34506
N	-1.20128	-0.46151	-0.15455
O	-0.48577	1.75851	-0.28647
O	2.34096	0.73286	0.30732
H	1.61366	0.05865	0.26005
H	-2.42517	1.20467	-0.55255
H	-2.07866	-0.98338	-0.24346
H	-0.21912	-2.10451	0.19770
H	1.83970	1.54297	0.12796
val+07_23			
C	-0.30238	0.21188	0.73848
C	-0.30956	1.08677	-0.27429
N	0.37896	-1.05817	0.63567
O	0.24593	1.00383	-1.51191
O	0.79653	-0.30569	-1.85654
H	-0.79649	2.05429	-0.18591
H	-0.81922	0.48018	1.65715
H	0.79710	-0.78733	-0.96220
H	1.13563	-1.12162	1.31687
H	-0.25380	-1.83345	0.83286
val+07_24			
C	2.27589	1.24699	0.34725
C	-1.30816	0.49839	-0.05786
N	0.28649	-1.62402	-0.11653
O	2.54413	2.34990	0.41848
O	-0.71118	1.41680	-0.58713
H	-2.01295	-0.14654	-0.61261
H	-1.24163	0.29274	1.02491
H	0.40279	-2.07426	-1.02397
H	1.09831	-1.01917	0.00506
H	0.37641	-2.36543	0.57809
val+07_25			
C	2.43079	0.06775	-2.04078
C	-0.85857	1.66642	0.64618

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N	0.84873	-1.79297	0.11199
O	1.64938	0.89180	-1.95467
O	-1.00813	0.60472	1.21482
H	-1.44087	2.56308	0.92822
H	-0.13700	1.79417	-0.18015
H	0.32751	-2.17562	-0.67717
H	0.26555	-1.03623	0.47713
H	0.82092	-2.52372	0.82411

val+07_26

C	-0.36688	-0.79900	-0.17261
C	-0.59940	-2.22010	-0.40054
N	-0.18084	0.33032	0.00771
O	0.27824	3.13778	0.47550
O	1.52462	3.30528	-0.25523
H	-1.52651	-2.36045	-0.96368
H	0.23134	-2.64677	-0.96986
H	-0.68123	-2.74294	0.55665
H	0.10809	2.18167	0.31567
H	2.16506	3.31799	0.47878

val+07_27

C	-0.64849	1.06681	-0.58037
C	-0.09780	-1.36950	-0.42190
N	-0.19309	-0.07961	0.31761
O	0.29384	1.92356	-0.54470
O	1.48255	1.69045	0.26215
H	-1.06170	-1.59441	-0.87981
H	0.66717	-1.26829	-1.19206
H	0.18433	-2.15423	0.28043
H	-0.85060	-0.16179	1.09779
H	0.75779	0.32451	0.64475

val+07_29

C	0.93042	0.02775	0.90001
C	-1.09649	-0.65682	-0.29524
N	-0.05536	0.28661	0.10519
O	-0.15402	1.55682	-0.42268
O	-1.26357	1.70845	-1.27428
H	1.63758	0.81835	1.11626
H	-2.06007	-0.24301	0.00002
H	-1.07513	-0.74394	-1.38103
H	-0.89337	-1.60759	0.19425
H	1.01851	-0.96204	1.32330

val+07_2

C	-0.47417	0.05421	-0.33144
C	-0.58478	1.32437	0.00027
N	-0.28783	-1.16142	-0.48508
O	0.33177	2.26851	-0.42516
O	1.35303	-3.04102	1.09393
H	-1.39824	1.63987	0.64870
H	-0.77304	-1.56421	-1.29632
H	0.80026	-2.39566	0.60443
H	-0.15677	3.08101	-0.63606
H	2.20036	-3.00357	0.62513

val+07_30

C	-1.93612	0.43786	-0.36718
C	1.60612	-0.02275	-0.11021
N	0.82165	-0.87491	0.59247
O	-1.68380	1.51727	-0.85674
O	2.03668	1.04479	0.30883
H	-1.97224	-0.49027	-0.96923
H	1.80669	-0.38466	-1.13477
H	0.65241	-0.69969	1.57542
H	-2.15544	0.31451	0.71070
H	0.60704	-1.79507	0.23302

val+07_31

C	-0.06957	-0.71320	-0.62545
C	0.82992	0.23624	-0.07603
N	-1.43545	-0.52166	-0.02795
O	0.39853	1.56471	0.08834
O	0.73035	0.80234	1.34482
H	1.88039	0.12216	-0.34602
H	0.22795	-1.75706	-0.55703

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H	-2.16894	-0.95126	-0.59472
H	-1.55280	-0.85929	0.93836
H	-1.61778	0.48791	-0.00302

val+07_32

C	-0.29311	-1.53182	0.32476
C	-0.42205	0.77307	-0.05031
N	0.31198	-0.47902	-0.04345
O	0.44867	1.82546	0.32833
O	1.46748	1.92433	-0.70406
H	0.24147	-2.48280	0.32298
H	-0.81246	0.95298	-1.05973
H	-1.23662	0.82045	0.68531
H	-1.34104	-1.55416	0.65103
H	1.91100	1.05742	-0.59148

val+07_36

C	-0.50630	0.08560	1.50057
C	1.93541	1.48729	-1.50536
N	-0.69434	-0.82139	0.62842
O	1.34371	2.29707	-0.96499
O	-0.03075	-0.58088	-2.16448
H	-1.12770	-1.65322	1.04067
H	-0.26944	-0.68515	-1.21206
H	-0.77295	-0.00931	2.55758
H	-0.04873	1.02741	1.19273
H	0.87631	-0.91903	-2.20469

val+07_39

C	-1.31172	1.25486	1.25258
C	0.25222	2.70210	-1.53441
N	-0.36963	-1.42059	-0.41400
O	-1.49292	0.88772	2.31442
O	0.38857	1.66161	-1.97535
H	-0.10666	-0.61804	-0.98492
H	1.84864	-1.72571	2.22938
H	-1.32442	-1.64780	-0.69234
H	0.20203	-2.19420	-0.75313
H	1.31779	-1.61695	1.71818

val+07_3

C	1.03839	-0.23514	-0.46721
C	-0.11568	0.41191	-0.24922
N	1.00589	-1.50623	0.39237
O	-1.19266	-0.01929	0.51346
O	-0.41343	1.63926	-0.81155
H	0.20976	-1.54798	1.04898
H	0.96162	-2.34705	-0.18986
H	1.86743	-1.59060	0.93650
H	-1.58136	0.75675	0.95381
H	0.41283	1.92235	-1.24108

val+07_41

C	-0.49766	2.23175	-0.02201
C	0.00605	1.02468	0.16683
N	-0.35293	-0.10471	-0.65933
O	-0.95655	3.29790	-0.20105
O	1.33550	-1.84732	0.84335
H	0.71810	0.87691	0.97294
H	-0.09634	0.03210	-1.63510
H	-1.35003	-0.30719	-0.62624
H	0.71608	-1.38773	0.22621
H	0.76147	-2.09989	1.58250

val+07_42

C	-0.81955	-0.44948	0.38259
C	-1.93406	-1.35661	0.81109
N	2.30898	0.63371	-0.10597
O	-2.01428	-0.07044	0.07332
O	2.15332	1.48247	-1.27724
H	-2.19433	-2.21870	0.20595
H	-2.32087	-1.29920	1.82311
H	2.79325	-0.18749	-0.47688
H	1.35094	0.31425	0.07604
H	2.58640	2.30279	-0.99422

val+07_44

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C	0.35407	1.03227	-0.02327
C	-0.97521	1.46999	0.07821
N	0.47602	-0.31714	-0.33530
O	-1.97289	0.73769	-0.13467
O	0.70990	-1.24486	0.90667
H	1.24854	1.60189	0.17645
H	-1.11298	2.54043	0.32535
H	-0.44474	-0.62156	-0.69023
H	1.24802	-0.57015	-0.95258
H	0.73127	-2.14453	0.51947

val+07_46

C	-1.42610	1.01190	0.85038
C	-0.08848	0.44827	0.11219
N	-0.39069	-0.98594	-0.28441
O	-2.33950	0.16464	0.69907
O	0.98566	0.50766	0.99889
H	0.08367	1.00703	-0.81373
H	-1.45019	-0.99656	-0.03971
H	-0.22754	-1.22715	-1.26257
H	0.10964	-1.64712	0.31283
H	1.81744	0.46717	0.49916

val+07_47

C	-0.19141	0.33034	-0.65608
C	-1.22833	1.22691	0.00212
N	-0.58342	-0.75962	0.40048
O	-1.75498	-0.06180	0.77995
O	1.11323	0.76581	-0.55250
H	-2.05146	1.46116	-0.69183
H	-0.80720	-1.70277	0.06601
H	0.08985	-0.82036	1.17521
H	-0.31276	-0.13437	-1.64173
H	1.03817	1.49010	0.10837

val+07_48

C	-1.23298	0.90912	0.54295
C	-0.07772	0.00555	0.18162
N	-0.15289	-1.25869	0.27639
O	-2.30339	0.49883	0.94298
O	-0.92333	2.20094	0.36608
H	0.83861	0.48215	-0.16818
H	1.77331	-3.67044	-1.41394
H	1.37872	-3.16179	-1.04038
H	-1.09061	-1.51151	0.62100
H	-1.70132	2.73882	0.61289

val+07_49

C	-0.64625	1.18394	0.45092
C	0.04712	-0.86906	-0.63008
N	0.63178	1.69497	-0.24339
O	-0.45188	-0.30022	0.43213
O	-0.01410	-2.19895	-0.47609
H	1.52870	1.56367	0.25127
H	0.70798	1.15787	-1.11925
H	0.53089	2.68691	-0.46357
H	-0.44923	1.39028	1.51242
H	-0.43061	-2.42091	0.39064

val+07_4

C	0.22425	-0.65910	-0.63942
C	-1.17367	1.06321	0.35515
N	-1.07576	-0.16558	-0.19594
O	1.16765	-0.74036	0.40616
O	-0.21652	1.82896	0.48523
H	-2.19468	1.32791	0.67795
H	-1.87008	-0.79078	-0.15291
H	0.08485	-1.66437	-1.03760
H	1.31439	0.18191	0.68421
H	0.58279	0.00020	-1.43912

val+07_50

C	0.50291	1.82217	0.22155
C	-1.74475	-1.81498	0.35754
N	-1.29149	-1.00622	-0.51392
O	-0.00552	2.86653	0.56806
O	1.82907	1.62542	0.10937

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H	-0.04256	0.90363	-0.04494
H	-1.54734	-1.61973	1.41437
H	-2.33074	-2.71321	0.13337
H	-1.55156	-1.31282	-1.45791
H	2.27408	2.46161	0.35431

val+07_51

C	0.16948	0.67953	0.63645
C	0.69520	-1.86100	-0.02319
N	0.06865	-0.50335	-0.34723
O	0.73438	0.56227	1.68138
O	-0.41316	1.80761	0.23019
H	1.74381	-1.59976	0.19176
H	0.25482	-2.10509	0.95673
H	-0.92771	-0.65514	-0.53405
H	0.45728	-0.18824	-1.24186
H	-0.82996	1.73406	-0.64808

val+07_52

C	-0.01632	1.40761	0.32460
C	1.07034	2.19215	0.39299
N	0.23641	0.12452	-0.34462
O	0.28568	-1.09127	0.53149
O	-1.06544	-1.40069	0.85396
H	-1.06500	1.48126	0.61615
H	0.78955	3.15405	0.86343
H	-0.41334	-0.13740	-1.09697
H	1.20703	0.19813	-0.69065
H	-1.24991	-2.14036	0.23962

val+07_53

C	-1.54441	2.17691	-0.20090
C	0.42971	0.92783	-0.25403
N	-0.14574	-0.17292	-0.39747
O	-0.23291	2.20215	-0.14396
O	1.06883	-2.85970	-0.57598
H	-1.80226	3.25282	-0.09549
H	1.50145	1.08169	-0.19188
H	-1.16747	-0.02041	-0.42388
H	0.68556	-1.95845	-0.53982
H	0.99004	-3.16802	0.33931

val+07_54

C	-0.07895	1.65158	-0.70348
C	-0.01509	-1.59354	-0.76578
N	0.10487	1.20900	0.56239
O	0.77631	2.20330	-1.38623
O	-0.88518	-2.14433	0.05408
H	-1.10177	1.45741	-1.07114
H	0.93681	-1.67910	-0.18362
H	-0.65712	0.81463	1.09585
H	0.98825	1.36699	1.03078
H	-1.76971	-2.12544	-0.36055

val+07_56

C	-1.17078	0.29538	0.19010
C	1.24402	0.45078	0.29382
N	1.10635	-1.07232	0.09918
O	-0.09631	0.95469	-0.14331
O	-2.24538	1.00827	-0.17454
H	1.85433	0.75557	-0.56802
H	0.22561	-1.33414	0.56615
H	1.88514	-1.54985	0.55517
H	1.03284	-1.42553	-0.86818
H	-1.96331	1.85724	-0.59118

val+07_57

C	1.92460	1.66884	-0.08459
C	0.67785	2.05539	0.04685
N	0.55410	0.78471	-0.62933
O	-1.60770	-1.79619	1.39700
O	-0.21901	-1.66233	0.99954
H	-0.08334	2.74956	0.36902
H	0.27926	-0.05213	-0.11318
H	-2.03993	-1.16560	0.79072
H	0.36950	0.75674	-1.62748
H	-0.10273	-2.45789	0.44656

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val+07_58
C 0.63516 -0.02204 -0.18776
C -0.01407 1.20110 0.02641
N -0.24904 -1.10693 -0.30448
O -1.26258 1.33657 0.09157
O -0.38166 -2.04434 0.89389
H 0.64678 2.08522 0.11118
H -0.05012 -1.79092 -1.03607
H -1.19316 -0.69617 -0.40899
H 1.69447 -0.20538 -0.28018
H -0.09038 -1.45111 1.61452

val+07_59
C 1.68537 0.21813 -0.59574
C 0.41611 0.01691 -0.56228
N 1.05533 -1.25436 -0.38072
O -0.86631 0.35058 -0.55534
O -0.97583 1.80747 -0.46522
H 2.58868 0.68432 -0.24733
H -0.39526 -3.42474 1.77115
H -0.04945 -2.92920 1.33448
H 1.09162 -1.73580 -1.28915
H -1.25005 1.89620 0.46974

val+07_60
C 1.34684 0.25447 -0.82735
C 0.37788 0.80572 -0.06447
N -0.15244 -2.18447 0.01980
O 0.25498 0.16096 1.06715
O -0.45596 1.87446 -0.26961
H -0.13004 -1.29429 0.64921
H -1.10186 -2.47094 -0.22356
H 0.34118 -2.96549 0.45433
H 0.35517 -1.86196 -0.81938
H -0.22165 2.29374 -1.11691

val+07_61
C -0.68942 1.04196 -0.01582
C 0.59348 0.60458 -0.23539
N 0.80145 -0.71291 0.27446
O -0.88606 2.31096 -0.52756
O 0.84017 -1.81375 -0.73140
H 1.45944 1.03580 -0.73430
H -0.00039 -0.90738 0.89173
H 1.68483 -0.87822 0.76391
H -1.79813 2.55329 -0.31302
H 0.16203 -1.49982 -1.36362

val+07_62
C -0.30532 0.77064 0.03780
C 0.94018 1.20402 0.15014
N -0.58118 -0.57067 -0.52520
O 0.41939 -1.26510 -0.92089
O -1.40808 -1.26010 0.61375
H -1.20650 1.29569 0.32878
H 1.14600 2.17931 0.57645
H -1.35926 -0.51383 -1.20290
H 1.76691 0.58700 -0.18308
H -0.66044 -1.63307 1.12134

val+07_63
C -0.25223 0.17100 0.05055
C 0.99079 0.27699 0.56411
N -0.77130 -1.22992 -0.00960
O -1.18622 1.05239 -0.49588
O 1.42386 1.62106 0.59970
H -1.60747 -1.39286 0.56579
H -1.00503 -1.54153 -0.96022
H -0.00322 -1.80813 0.35161
H -1.65239 1.49782 0.23246
H 2.31102 1.58798 0.98068

val+07_64
C 0.18076 1.44035 0.49739
C 0.29147 2.60185 0.17041
N -0.03694 0.13730 0.80889

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O	1.01081	-0.71615	0.30978
O	-0.45217	-2.24109	-1.45201
H	0.42347	3.62831	-0.08659
H	-1.30659	-1.78086	-1.49074
H	-0.08722	-0.02272	1.81354
H	0.52156	-1.27953	-0.34135
H	-0.65636	-3.07136	-0.99133

val+07_65

C	0.19483	0.62690	-0.45987
C	-0.21422	1.71739	-0.13648
N	0.60284	-0.66000	-0.70239
O	-0.58617	2.97163	0.05161
O	-0.17052	-2.50014	1.47169
H	0.07441	-1.87556	0.75377
H	0.17921	-1.06305	-1.53638
H	1.61482	-0.75196	-0.77182
H	-1.05884	3.05338	0.89978
H	0.66113	-2.61578	1.95558

val+07_67

C	-2.29253	-0.11127	0.90998
C	0.61586	1.85876	-0.47849
N	0.46871	-1.85071	0.21099
O	-2.97749	-0.92732	1.30980
O	1.51151	1.06080	-0.66881
H	0.73972	2.93303	-0.71103
H	-0.36188	1.55428	-0.06642
H	1.20125	-2.29806	0.76307
H	0.85818	-0.95156	-0.08101
H	0.40446	-2.40735	-0.64178

val+07_69

C	-1.13028	2.34998	1.10134
C	0.55843	-1.08409	0.11053
N	-0.34851	-0.01696	-0.40710
O	-0.15651	2.61206	0.53875
O	-1.45701	0.16280	0.37759
H	-0.01705	-2.00843	0.15034
H	1.42509	-1.18937	-0.54747
H	0.86236	-0.78560	1.11344
H	-0.61063	-0.24783	-1.37659
H	0.19262	0.86883	-0.46802

val+07_6

C	0.21777	-0.87877	-0.22226
C	-0.81948	1.26509	0.32527
N	-0.77517	-0.04491	0.13402
O	1.41027	-0.30915	-0.60342
O	-2.01591	-0.69084	0.32518
H	-1.76597	1.76568	0.19135
H	0.12195	1.78937	0.38376
H	0.19848	-1.87551	0.20647
H	1.95843	-0.12002	0.18193
H	-2.04037	-1.34744	-0.40141

val+07_73

C	0.31615	2.12237	-0.87297
C	-0.52728	1.22395	-0.38895
N	0.67842	-1.78114	0.69131
O	-0.38189	0.73108	0.89549
O	1.05338	2.94162	-1.29562
H	-1.36402	0.91887	-1.01599
H	0.79941	-2.22353	1.60189
H	0.01078	-0.19830	0.82419
H	1.59635	-1.78541	0.24790
H	0.09399	-2.41191	0.14366

val+07_74

C	1.58982	0.87990	-0.64318
C	0.53873	0.50164	0.08612
N	-1.99978	-1.53062	0.27416
O	1.97297	1.88009	0.27823
O	0.81267	1.46486	1.08651
H	-2.63323	-1.45108	-0.52150
H	-1.73459	-2.51493	0.31207
H	-2.57994	-1.37463	1.09863

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H	2.13828	0.69281	-1.55224
H	-0.30801	-0.18373	0.14730
val+07_75			
C	-0.75008	-0.96443	-0.09787
C	-1.90628	-0.36530	0.53294
N	2.11600	0.65622	-0.04444
O	-1.85488	-0.09670	-0.76724
O	-2.62598	-0.11275	1.45975
H	-0.79100	-2.00323	-0.41691
H	0.22690	-0.46744	-0.07108
H	2.94430	0.07789	0.09722
H	2.15105	1.36429	0.68904
H	2.28267	1.15986	-0.91571
val+07_76			
C	-0.55915	-0.66977	0.11372
C	-0.66591	0.61409	-0.24889
N	0.71607	-1.34898	0.12198
O	0.28661	1.48978	-0.66640
O	1.58626	0.89033	-0.96350
H	-1.46014	-1.19875	0.41623
H	-1.61876	1.13587	-0.21967
H	0.68336	-2.20334	-0.43414
H	0.97201	-1.62960	1.06876
H	1.50924	-0.02554	-0.53150
val+07_78			
C	0.60092	0.37282	0.38020
C	-1.62502	1.02204	-0.11120
N	0.80100	-1.15884	0.21097
O	-0.46211	0.61867	-0.62234
O	-2.59439	1.27685	-0.79605
H	1.48644	0.74951	-0.15454
H	-1.59312	1.10109	0.98947
H	0.86427	-1.50498	-0.75917
H	1.65971	-1.43330	0.69554
H	0.03740	-1.67065	0.65853
val+07_81			
C	-1.11302	-0.81499	-0.42356
C	-1.50455	0.40077	0.41211
N	2.24082	0.21240	-0.35193
O	-1.95601	-1.61355	-0.77512
O	-0.68676	1.21798	0.78072
H	-2.58210	0.47556	0.65194
H	2.69696	0.86775	-0.98722
H	-0.03770	-0.89851	-0.66874
H	1.50098	0.74565	0.10682
H	2.93007	0.01894	0.37516
val+07_83			
C	0.60554	0.67340	-0.27197
C	-0.85789	0.32305	-0.38076
N	1.47681	-0.23507	-0.07352
O	-0.67688	-1.72004	0.71412
O	-1.10116	-1.06702	-0.51770
H	0.84162	1.74198	-0.34996
H	-1.28316	0.77003	-1.28851
H	-1.39876	0.73950	0.48271
H	2.42017	0.15509	-0.00889
H	0.30109	-1.63623	0.59539
val+07_84			
C	-0.12364	1.97842	0.37670
C	-0.05299	-2.46620	0.01828
N	0.18033	1.12399	-0.61985
O	0.27413	3.13712	0.47344
O	-0.79146	-1.70550	-0.57530
H	-0.79215	1.52073	1.12968
H	-0.28989	-3.54000	0.11623
H	0.88692	-2.12587	0.48744
H	-0.18232	0.17171	-0.63836
H	0.78855	1.43200	-1.36816
val+07_85			
C	0.51048	-1.46456	0.15842

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C	0.33060	-0.30670	-0.45066
N	-0.77876	0.55880	-0.28348
O	1.40122	-2.46098	0.39013
O	-0.00472	-2.36374	1.03523
H	1.13010	0.04682	-1.09285
H	-1.16119	0.84044	-1.18350
H	-1.11492	3.85237	0.84769
H	-1.52913	0.13148	0.25322
H	-0.99718	3.14936	0.63172

val+07_86

C	-0.46732	0.69234	-0.92504
C	0.24415	-0.58809	-0.51404
N	0.66751	-0.62396	0.88226
O	-0.38508	1.19250	-2.02743
O	1.43775	0.58098	1.12278
H	-1.10421	1.14702	-0.13440
H	1.10696	-0.74763	-1.16758
H	-0.45367	-1.42602	-0.66184
H	-0.15130	-0.49427	1.47954
H	2.32132	0.23123	1.32364

val+07_87

C	0.56712	0.80137	0.68558
C	-0.45018	-1.35481	0.40778
N	0.32029	-0.22501	-0.32512
O	-0.53846	1.55147	1.00462
O	0.66908	2.11609	0.25966
H	-0.28259	-2.22396	-0.24422
H	-1.49874	-1.06099	0.25753
H	1.22422	-0.58828	-0.64180
H	-0.11840	0.22630	-1.14352
H	1.21408	0.44172	1.48009

val+07_88

C	1.09568	0.04618	0.36288
C	-1.09982	-0.82552	-0.28895
N	-0.20025	0.10230	-0.30938
O	0.59806	2.17484	-0.98091
O	-0.46437	1.25368	-1.02084
H	1.15694	0.88743	1.05252
H	1.87346	0.15980	-0.39139
H	-0.90805	-1.73089	0.26782
H	-2.02080	-0.66061	-0.83348
H	1.16374	-0.91002	0.87883

val+07_89

C	1.69167	0.07617	0.11974
C	-1.91764	0.36617	-1.01789
N	0.81841	-0.48460	0.97617
O	1.39593	0.64186	-0.93352
O	-2.01336	-0.22637	0.04142
H	2.74082	-0.01635	0.45345
H	-2.81304	0.61212	-1.61679
H	-0.18389	-0.46581	0.77940
H	1.14541	-0.93197	1.82102
H	-0.93659	0.67699	-1.41480

val+07_8

C	0.57128	-0.34721	0.35297
C	-1.49977	0.85677	-0.11381
N	-0.72347	-0.22918	-0.01126
O	1.27231	0.83122	0.44252
O	1.20788	-1.41952	-0.27322
H	-1.08266	1.81171	0.16760
H	-2.56395	0.70542	-0.21557
H	-1.15744	-1.12468	-0.22208
H	1.37728	1.21865	-0.45727
H	1.78475	-1.84090	0.38310

val+07_90

C	-0.23725	-0.81895	-0.03955
C	-1.16559	-1.60951	0.43687
N	0.60030	0.00382	-0.42209
O	0.96817	2.71908	0.40604
O	2.41940	2.77311	0.32031
H	-0.96362	-2.23817	1.29781

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H	-2.13937	-1.66274	-0.03868
H	2.65989	2.70713	1.26199
H	0.81049	1.77992	0.13471
H	1.25187	-0.32899	-1.13930

val+07_91

C	0.08299	0.76628	-0.07570
C	-0.84830	1.71690	-0.16916
N	0.66160	-2.44094	-0.01647
O	0.09456	2.76470	-0.07338
O	1.12613	1.71716	0.03010
H	-1.90524	1.90034	-0.27590
H	1.03768	-2.76165	0.87591
H	0.26591	-0.30908	-0.05782
H	-0.16920	-3.00982	-0.18019
H	1.33777	-2.74099	-0.71890

val+07_92

C	-1.08153	0.30090	-0.13870
C	0.31727	0.92199	0.10771
N	-1.32543	-0.82631	0.41440
O	0.48179	2.03466	-0.42290
O	1.05821	0.19540	0.81157
H	-1.84705	0.77900	-0.74395
H	2.12164	-1.67486	-0.53554
H	-2.20497	-1.33142	0.33182
H	2.43974	-2.22981	-0.91665
H	-0.55157	-1.21355	0.96896

val+07_93

C	-0.98092	0.48292	0.85386
C	0.15695	0.57122	-0.21618
N	0.68769	-0.82594	-0.38054
O	-1.54823	1.54921	1.14028
O	-1.17886	-0.68952	1.29586
H	-0.22771	0.92922	-1.17117
H	0.96081	1.22897	0.11456
H	0.57503	-1.20529	-1.32262
H	1.66810	-0.92885	-0.11200
H	0.05743	-1.34072	0.30825

val+07_95

C	1.47062	-1.74209	0.35966
C	1.40231	-0.53653	-0.18319
N	-1.57570	1.13244	-0.11948
O	0.50924	-0.26524	-1.20437
O	1.54860	-2.82317	0.82707
H	2.10105	0.22183	0.16757
H	-2.09898	0.58969	0.56670
H	-1.27590	1.98219	0.35737
H	-2.25012	1.42492	-0.82597
H	-0.26331	0.25196	-0.80615

val+07_98

C	-0.85719	0.28196	0.06956
C	0.45415	0.04752	0.14034
N	0.99738	-1.29972	-0.06454
O	1.90131	-1.35358	-1.09934
O	-1.47605	1.48172	0.19772
H	1.22519	0.79251	0.29265
H	-1.57824	-0.51112	-0.11149
H	1.42747	-1.61131	0.82308
H	0.20255	-1.94848	-0.20449
H	-0.81917	2.17699	0.37624

val+07_9

C	1.29420	2.46624	0.43760
C	0.03476	2.56162	-0.52244
N	0.58114	1.43224	0.16314
O	-0.89574	-1.63349	-0.37318
O	0.21416	-1.41459	0.53750
H	-0.89507	2.98421	-0.14419
H	0.18646	2.62347	-1.59917
H	0.46945	0.42218	0.33050
H	-0.62460	-2.47740	-0.78109
H	-0.20686	-1.60367	1.39784

