

## Supplementary Information:

### **Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants**

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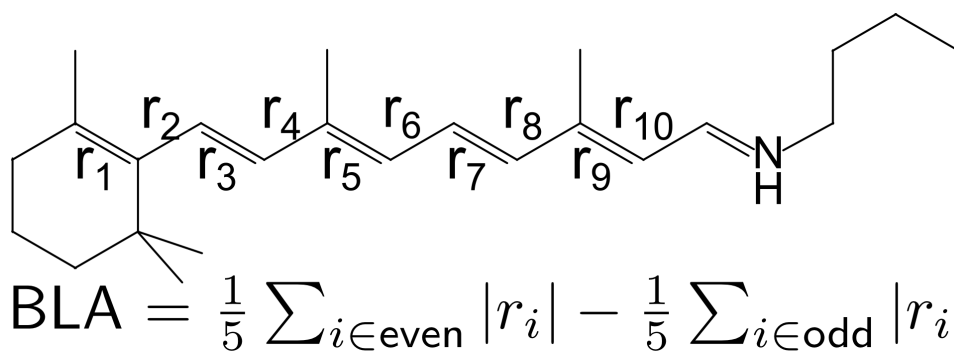
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The definition of bond length alternation (BLA) used in this work.



The QM/MM optimized structure of the retinal chromophore including the Lys296 sidechain (all values are in Å):

	x	y	z
C	13.29400	39.24900	13.64700
C	11.95800	38.96100	14.26400
C	11.82600	37.61400	14.96400
C	11.80300	36.43200	14.01100
N	10.47800	36.10600	13.46600
H	13.72400	38.35400	13.18400
H	14.01600	39.53500	14.41900
H	11.70700	39.72100	15.01300
H	11.16400	39.01800	13.50500
H	12.67600	37.50500	15.64100
H	10.93300	37.57200	15.59500
H	12.45800	36.63100	13.15600
H	12.12200	35.51600	14.51100
H	10.44700	35.16400	13.03600
H	13.28000	40.03000	12.88700
C	-0.45400	32.61600	10.51800
C	-1.54700	31.59100	10.12400
C	-2.94300	32.19400	10.08100
C	-2.94400	33.26000	8.99500
C	-1.81400	34.25600	9.14500
C	-0.67900	33.99500	9.86100
C	0.30800	35.06500	10.04600
C	1.47500	35.07000	10.74900
C	2.41900	36.16600	10.82700
C	3.58800	35.93200	11.50200
C	4.71300	36.81100	11.67900
C	5.88900	36.32100	12.16400
C	7.11600	37.04600	12.42800
C	8.18300	36.32200	12.89500
C	9.42100	36.85200	13.36800
C	0.87700	31.97000	10.09300
C	-0.49100	32.79900	12.04800
C	-2.10000	35.58100	8.46800
C	2.12300	37.46400	10.13400
C	7.20000	38.51200	12.13100
H	-1.31800	31.18700	9.12700
H	-1.48600	30.73600	10.81000
H	-3.70400	31.43400	9.87000
H	-3.19500	32.64400	11.05100
H	-2.90500	32.76700	8.01000
H	-3.89100	33.80200	8.98300

H	0.05000	36.00000	9.56600
H	1.78900	34.19600	11.30600
H	3.71800	34.94000	11.93000
H	4.61400	37.86400	11.43000
H	5.93000	35.25800	12.38400
H	8.09800	35.24100	12.90900
H	1.75500	32.52400	10.40700
H	0.95900	30.97400	10.54000
H	0.91200	31.84500	9.00800
H	0.15400	33.60100	12.40300
H	-1.50600	33.04500	12.35400
H	-0.18500	31.87500	12.55300
H	-2.57000	36.28100	9.17200
H	-1.21300	36.07200	8.05900
H	-2.80000	35.43500	7.63600
H	3.05000	38.00700	9.94800
H	1.64900	37.30000	9.15900
H	1.46000	38.08800	10.74800
H	8.13100	38.95900	12.48400
H	7.16400	38.65500	11.04500
H	6.35800	39.06100	12.55200
H	9.49500	37.88100	13.70000

The structure of the protein surrounding the QM region (all values are in Å):

	x	y	z
N	14.67300	7.86600	20.28900
C	15.38100	9.12100	20.53700
C	14.46200	10.18200	21.14700
O	14.92400	11.08800	21.84800
C	16.02100	9.64800	19.24800
C	16.79700	10.99500	19.37500
C	15.97500	12.30500	19.19600
N	16.38600	13.34800	20.16100
C	15.61400	14.28400	20.74900
N	14.31000	14.41000	20.49100
N	16.14800	15.13900	21.62800
H	15.31600	7.15200	19.96800
H	14.31800	7.49600	21.16500
H	16.17200	8.92400	21.26400
H	15.27000	9.74100	18.46100
H	16.72500	8.89500	18.89300
H	17.34600	11.00200	20.31800
H	17.56900	10.99800	18.60400
H	16.09000	12.68900	18.18200
H	14.91300	12.10900	19.31200
H	17.38000	13.35200	20.35800
H	13.79100	15.15300	20.97100
H	13.81200	13.82100	19.83600
H	15.53400	15.83800	22.06400
H	17.11700	15.13200	21.90900
N	13.16400	10.06500	20.88200
C	12.18800	11.00000	21.43600
C	11.80300	10.65100	22.87800
O	12.03100	9.52800	23.34600
C	10.94400	11.08700	20.54200
C	11.24900	11.26200	19.04000
S	12.20700	12.73600	18.59600
C	11.07100	14.04600	19.11600
H	12.87800	9.23600	20.37900
H	12.63100	11.99900	21.45200
H	10.34200	10.18700	20.66900
H	10.30500	11.90100	20.88200
H	11.79300	10.39600	18.66400
H	10.32400	11.27800	18.46800
H	11.47700	15.01500	18.83100
H	10.10300	13.91700	18.63300
H	10.92400	14.04600	20.19600

N	11.22400	11.62600	23.57600
C	10.80100	11.45300	24.96100
C	9.36900	10.93000	25.00700
O	8.76200	10.83600	26.07300
C	10.93100	12.76800	25.74200
C	9.99200	13.95500	25.34900
C	10.30100	15.17700	26.23000
C	10.03100	14.37800	23.86400
H	11.07500	12.53000	23.15000
H	11.43400	10.71700	25.46200
H	10.77700	12.54900	26.80000
H	11.96800	13.10100	25.67500
H	8.96400	13.66300	25.57200
H	9.60900	15.99600	26.03600
H	10.21900	14.93100	27.28900
H	11.31100	15.55000	26.05400
H	9.44000	15.27900	23.70200
H	11.04800	14.59100	23.53000
H	9.59800	13.62100	23.21100
N	8.83300	10.60300	23.83600
C	7.63000	9.77800	23.74600
C	7.98200	8.39500	23.17200
O	9.12000	8.14100	22.79100
C	6.52500	10.46800	22.92400
C	6.98700	11.00000	21.59400
C	7.21900	12.36300	21.42100
C	7.19500	10.14800	20.51700
C	7.64800	12.86700	20.19500
C	7.62600	10.64500	19.28900
C	7.85700	12.00200	19.12700
H	9.40200	10.67200	23.00600
H	7.20400	9.56700	24.72300
H	5.68400	9.80500	22.73800
H	6.11100	11.28900	23.51000
H	7.06700	13.04800	22.24300
H	7.02000	9.09100	20.62100
H	7.83600	13.92100	20.08600
H	7.82900	9.98900	18.47300
H	8.19300	12.38800	18.17500
N	7.00600	7.50200	23.12300
C	7.23600	6.16200	22.61900
C	7.47100	6.15300	21.11200
O	6.66800	6.68200	20.34000
C	6.07300	5.23200	22.98400

C	6.41300	3.77200	22.79800
C	7.64800	3.35700	23.58600
O	8.54100	2.70500	23.05900
N	7.69000	3.72600	24.86000
H	6.04700	7.76200	23.35800
H	8.14800	5.83200	23.11800
H	5.76400	5.40700	24.01400
H	5.21600	5.50300	22.38100
H	5.58300	3.22000	23.20400
H	6.50700	3.51000	21.74400
H	8.44200	3.50400	25.50500
H	6.84400	4.13900	25.22900
N	8.57500	5.53700	20.70400
C	8.94900	5.47400	19.29800
C	9.10600	4.01800	18.89500
O	9.14100	3.68300	17.70600
C	10.28100	6.19800	19.05400
O	11.32500	5.51500	19.74900
C	10.21000	7.65100	19.56000
H	9.27000	5.25000	21.37800
H	8.17600	5.85500	18.64000
H	10.50400	6.19800	17.98500
H	12.14300	5.97000	19.57500
H	11.07900	8.21100	19.21900
H	9.32700	8.17600	19.20700
H	10.21100	7.69800	20.64500
N	9.19400	3.16000	19.90800
C	9.39900	1.73400	19.71200
C	8.09900	0.99700	19.97300
O	7.44700	1.20700	20.99800
C	10.46900	1.21500	20.67400
O	11.27600	0.24100	20.04600
H	9.04300	3.47700	20.85500
H	9.73000	1.53700	18.68900
H	11.13100	2.02800	20.97600
H	10.05100	0.81400	21.60100
H	11.96000	-0.01000	20.66000
N	7.72800	0.11600	19.05500
C	6.46200	-0.57000	19.18100
C	6.41300	-1.83800	18.35300
O	7.18600	-2.02100	17.40700
C	5.33000	0.36900	18.76900
C	5.32100	0.74400	17.31400
C	4.51500	0.05600	16.41800

C	6.11000	1.78500	16.83200
C	4.48700	0.39500	15.08200
C	6.08900	2.13300	15.49400
C	5.26900	1.42800	14.62400
O	5.22100	1.74400	13.28700
H	8.29000	-0.07500	18.23600
H	6.31100	-0.87000	20.22200
H	4.37600	-0.10100	19.00000
H	5.37300	1.28800	19.34800
H	3.89900	-0.76500	16.75600
H	6.74300	2.34200	17.50800
H	3.84300	-0.15400	14.41100
H	6.70300	2.94800	15.13700
H	4.61200	1.20200	12.79900
N	5.49600	-2.72200	18.71700
C	5.28400	-3.92000	17.92900
C	3.89100	-3.92100	17.30600
O	2.90300	-3.59000	17.95800
C	5.50500	-5.23200	18.75100
O	4.44500	-5.39700	19.69900
C	6.85000	-5.21000	19.48200
H	4.87400	-2.55900	19.50400
H	5.99100	-3.99300	17.10000
H	5.47600	-6.08500	18.07000
H	4.17000	-6.32000	19.68900
H	7.03700	-6.16000	19.98300
H	7.67100	-5.04300	18.78400
H	6.89400	-4.42800	20.24100
N	3.83500	-4.26900	16.02600
C	2.57400	-4.55600	15.36800
C	2.18800	-5.99500	15.65200
O	2.97600	-6.91600	15.42300
C	2.68700	-4.34100	13.86400
C	2.72000	-2.88400	13.42400
C	2.83900	-2.77000	11.91100
C	1.48000	-2.16700	13.94300
H	4.68300	-4.53700	15.54900
H	1.79000	-3.93900	15.78800
H	3.58300	-4.84500	13.49800
H	1.87100	-4.85000	13.35900
H	3.60000	-2.41100	13.86300
H	2.89700	-1.72700	11.59800
H	3.73800	-3.26800	11.54600
H	1.98300	-3.22000	11.40700



H	1.41300	-1.15400	13.54600
H	0.55500	-2.68500	13.68900
H	1.53800	-2.07300	15.01600
N	0.97400	-6.18300	16.15600
C	0.45100	-7.51400	16.40000
C	-0.84200	-7.70100	15.62900
O	-1.43900	-6.72000	15.15800
C	0.19000	-7.71400	17.88800
C	1.35600	-7.32600	18.76800
C	2.36200	-8.44800	18.96200
O	3.37500	-8.19800	19.64700
O	2.14200	-9.56900	18.44200
H	0.35000	-5.38400	16.28400
H	1.13500	-8.29700	16.06700
H	-0.62600	-7.09800	18.22700
H	-0.14800	-8.73300	18.08700
H	1.82700	-6.37100	18.53500
H	0.93500	-7.23800	19.75500
N	-1.26000	-8.96400	15.51400
C	-2.49600	-9.35700	14.83200
C	-2.60700	-8.82900	13.41600
O	-3.54100	-8.08100	13.10800
C	-3.71500	-8.90100	15.62300
C	-3.84100	-9.60100	16.94100
O	-2.96500	-10.37400	17.32400
N	-4.93200	-9.33300	17.65500
H	-0.71500	-9.69500	15.95000
H	-2.50400	-10.44600	14.75300
H	-3.67600	-7.83300	15.81900
H	-4.63700	-9.10900	15.07700
H	-5.07500	-9.77200	18.55300
H	-5.62900	-8.68900	17.30500
N	-1.66300	-9.22900	12.56600
C	-1.55600	-8.71700	11.20200
C	-1.69000	-7.19300	11.17100
O	-2.42100	-6.64700	10.34700
C	-2.59200	-9.38200	10.27500
C	-2.26500	-9.19500	8.79000
O	-1.10100	-9.09400	8.41400
N	-3.29700	-9.14100	7.94700
H	-0.91400	-9.81100	12.91500
H	-0.54500	-8.96600	10.87400
H	-2.60800	-10.45600	10.46100
H	-3.59900	-9.02100	10.49200

H	-3.14200	-9.01300	6.95600
H	-4.24600	-9.22000	8.28700
N	-1.01200	-6.51700	12.09600
C	-0.92900	-5.06100	12.08500
C	-2.15500	-4.30300	12.56700
O	-2.29000	-3.10700	12.33200
H	-0.41400	-7.03000	12.73400
H	-0.12200	-4.77300	12.74800
H	-0.65100	-4.70600	11.09100
N	-3.04500	-4.99400	13.25900
C	-4.28500	-4.39000	13.70900
C	-4.13300	-3.95300	15.15600
O	-4.93300	-3.15900	15.68200
C	-5.44000	-5.38900	13.55900
O	-5.18000	-6.54900	14.31500
H	-2.87300	-5.97300	13.45100
H	-4.55100	-3.50800	13.12300
H	-6.37400	-4.94000	13.90100
H	-5.58500	-5.66000	12.51200
H	-4.56100	-7.09700	13.81900
N	-3.09400	-4.47100	15.79600
C	-2.80600	-4.11400	17.17500
C	-1.41800	-3.50400	17.26400
O	-0.49500	-3.93300	16.57400
C	-2.89200	-5.34000	18.11500
C	-2.49900	-4.96700	19.54100
C	-4.29700	-5.92300	18.09000
H	-2.46700	-5.11900	15.32800
H	-3.50400	-3.36600	17.55700
H	-2.25000	-6.10800	17.71500
H	-2.68300	-5.80000	20.22000
H	-1.44000	-4.73700	19.63600
H	-3.06900	-4.11500	19.91400
H	-4.36600	-6.80000	18.73300
H	-5.03200	-5.19900	18.44400
H	-4.60400	-6.23000	17.09200
N	-1.28600	-2.48100	18.09500
C	0.01100	-1.92600	18.41200
C	0.25300	-2.20800	19.88600
O	-0.57400	-1.89900	20.74000
C	0.06500	-0.40200	18.12700
C	-0.05500	-0.13000	16.63100
C	1.35200	0.21600	18.63300
C	0.01200	1.34500	16.28000

H	-2.06700	-2.19100	18.66600
H	0.80700	-2.38400	17.82900
H	-0.76600	0.08300	18.64200
H	0.76300	-0.60900	16.12000
H	-0.98000	-0.55400	16.23900
H	1.38800	1.28500	18.48300
H	1.47200	0.07100	19.70100
H	2.21800	-0.22200	18.14400
H	-0.35500	1.48300	15.26600
H	-0.62300	1.94400	16.93200
H	1.02800	1.73500	16.31300
N	1.38100	-2.82200	20.18400
C	1.70700	-3.10600	21.56400
C	2.89300	-2.27100	21.94200
O	3.82000	-2.07700	21.15300
C	1.98300	-4.59700	21.77900
S	0.48000	-5.57000	21.61700
H	2.05100	-3.06600	19.45500
H	0.90500	-2.85200	22.26000
H	2.68500	-4.97400	21.06500
H	2.40400	-4.77600	22.77000
H	0.24600	-5.21700	20.34800
N	2.85200	-1.77500	23.16500
C	3.75400	-0.72900	23.58800
C	4.24200	-1.07900	24.98200
O	3.51200	-1.70600	25.74500
C	2.99200	0.62800	23.56100
C	3.66700	1.58900	22.61200
C	2.79200	1.23100	24.93500
C	3.28300	1.32000	21.23200
H	2.11600	-2.03600	23.80700
H	4.61200	-0.69900	22.92000
H	1.97700	0.46700	23.19200
H	3.42100	2.62300	22.85500
H	4.74300	1.46700	22.68500
H	2.21600	2.15200	24.84900
H	2.24600	0.58900	25.62800
H	3.74700	1.49300	25.33500
H	3.80000	2.00000	20.56500
H	3.49600	0.30700	20.92700
H	2.22000	1.51800	21.10200
N	5.48700	-0.70700	25.31300
C	5.90100	-0.89200	26.70900
C	4.97900	-0.08900	27.63600

O	4.72100	1.07700	27.35600
C	7.31800	-0.29500	26.73800
C	7.78900	-0.31800	25.30100
C	6.54300	-0.09200	24.48600
H	5.91600	-1.95400	26.96200
H	7.31200	0.73800	27.07600
H	7.98500	-0.84500	27.40200
H	8.56000	0.42700	25.09700
H	8.20700	-1.29900	25.07000
H	6.65400	-0.53500	23.49600
H	6.33100	0.97100	24.37600
N	4.46300	-0.69300	28.70100
C	3.73700	0.09000	29.68900
C	4.71600	0.90600	30.52100
O	4.93200	0.62400	31.69900
C	2.87000	-0.78800	30.59000
C	1.86900	0.03600	31.40900
O	1.00900	-0.63700	32.16100
N	1.87300	1.26400	31.35000
H	4.69200	-1.65600	28.90000
H	3.07200	0.76900	29.14700
H	2.28900	-1.47400	29.97300
H	3.46800	-1.41300	31.25500
H	1.13400	1.75500	31.84100
H	2.34200	1.78100	30.60500
N	5.31200	1.91400	29.89000
C	6.36100	2.70800	30.51400
C	5.96100	4.15500	30.81700
O	6.80200	4.97900	31.16700
C	7.66500	2.64600	29.68900
C	7.51700	3.18500	28.24300
O	8.48400	3.15400	27.47700
N	6.32600	3.67500	27.87400
H	5.12100	1.98400	28.89200
H	6.62700	2.30200	31.49100
H	8.46300	3.20000	30.18500
H	8.00800	1.61300	29.63400
H	6.11000	3.84300	26.89100
H	5.54300	3.59500	28.49900
N	4.67500	4.45900	30.66900
C	4.17300	5.77900	30.99400
C	4.45000	6.80600	29.91300
O	4.14900	7.98200	30.07400
H	3.99700	3.79000	30.29700

H	3.09300	5.70900	31.12600
H	4.57600	6.13200	31.94500
N	5.02900	6.36400	28.80600
C	5.30100	7.25600	27.69400
C	4.07800	7.31000	26.79800
O	3.31300	6.35500	26.69400
C	6.52300	6.78400	26.89600
C	7.78600	7.63700	27.07900
C	8.99800	7.06100	26.35300
O	9.23800	5.84600	26.37600
N	9.76600	7.93100	25.69500
H	5.22000	5.38200	28.69600
H	5.50700	8.26200	28.06300
H	6.79500	5.77700	27.11500
H	6.30300	6.77800	25.82700
H	7.60000	8.65500	26.75700
H	8.03200	7.69200	28.14000
H	10.54500	7.61600	25.13400
H	9.54100	8.91300	25.74400
N	3.88800	8.44700	26.15600
C	2.77400	8.60300	25.24900
C	3.16300	8.00600	23.92000
O	4.33600	7.95300	23.57700
C	2.43600	10.08000	25.08900
S	1.88600	10.86600	26.62700
H	4.58100	9.19800	26.24900
H	1.88600	8.09300	25.62900
H	3.29500	10.63300	24.70500
H	1.63100	10.19400	24.36500
H	2.95600	10.49900	27.34200
N	2.18400	7.55000	23.16100
C	2.50300	6.95600	21.88900
C	1.57900	7.43400	20.80100
O	0.38900	7.62600	21.02100
C	2.42200	5.42900	21.96700
C	2.45700	4.78000	20.62600
C	1.28300	4.39600	19.99600
C	3.66300	4.61300	19.96700
C	1.31300	3.83600	18.74200
C	3.70400	4.04900	18.71300
C	2.52800	3.65900	18.09900
H	1.21200	7.63500	23.42400
H	3.50900	7.20600	21.54400
H	3.19200	5.01400	22.61100

H	1.48500	5.14500	22.44900
H	0.33000	4.54000	20.48500
H	4.58900	4.93000	20.41800
H	0.39300	3.54700	18.25700
H	4.64900	3.92000	18.20500
H	2.56500	3.22100	17.11300
N	2.12700	7.57600	19.60700
C	1.31600	7.88800	18.45300
C	2.14600	7.68700	17.20500
O	3.30500	8.09200	17.17100
C	0.82900	9.33700	18.51700
S	-0.56900	9.62300	17.42200
H	3.14000	7.50000	19.48200
H	0.46700	7.20100	18.43600
H	0.54400	9.66400	19.51600
H	1.61400	9.99700	18.17300
H	-1.38400	8.74500	18.01700
N	1.56400	7.07500	16.17600
C	2.33700	6.81700	14.96300
C	2.67700	8.09900	14.23400
O	3.76800	8.23400	13.69200
C	1.57900	5.91000	14.00200
C	1.43500	4.45400	14.40800
C	0.33500	3.83100	13.54800
C	2.78600	3.73000	14.24000
H	0.59900	6.74300	16.24600
H	3.27100	6.32700	15.23000
H	0.59000	6.32000	13.82900
H	2.05800	5.93800	13.02000
H	1.13100	4.38800	15.45300
H	0.30200	2.75000	13.66100
H	-0.64900	4.22600	13.80500
H	0.50200	4.02500	12.48800
H	2.67800	2.67200	14.47900
H	3.16000	3.79900	13.21800
H	3.55200	4.12600	14.90600
N	1.72500	9.02900	14.21600
C	1.85600	10.24400	13.44000
C	3.04300	11.07300	13.91500
O	3.65900	11.78700	13.12700
C	0.55500	11.05700	13.49200
H	0.79100	8.76400	14.53400
H	2.02300	9.95800	12.40300
H	0.66400	12.02700	13.00700

H	-0.25900	10.53400	12.99200
H	0.25200	11.24400	14.52300
N	3.36200	10.94600	15.20100
C	4.51400	11.60900	15.82300
C	5.85300	11.12700	15.27300
O	6.83000	11.86800	15.28000
C	4.50700	11.36300	17.33600
C	3.36000	11.99400	18.04000
C	2.50000	12.91900	17.53300
C	2.92300	11.72700	19.37600
N	1.55800	13.25700	18.47300
C	1.80100	12.55400	19.62000
C	3.36700	10.86600	20.39300
C	1.11600	12.55000	20.84300
C	2.68800	10.86400	21.61000
C	1.57200	11.69600	21.82100
H	2.81700	10.30300	15.75900
H	4.45300	12.68000	15.63000
H	4.52200	10.29700	17.55900
H	5.40900	11.77600	17.78700
H	2.53800	13.33200	16.53500
H	0.77700	13.89900	18.33500
H	4.22500	10.22900	20.23600
H	0.26400	13.18000	21.02800
H	3.04300	10.21600	22.39000
H	1.06200	11.68100	22.77200
N	5.89700	9.87500	14.82200
C	7.14400	9.25200	14.37500
C	7.46400	9.58900	12.92400
O	8.58500	9.36400	12.46900
C	7.07200	7.73100	14.52300
C	7.22200	7.07500	15.90200
C	7.62400	8.09100	16.96500
C	5.96200	6.30200	16.29700
H	5.04700	9.32100	14.79600
H	7.99100	9.63900	14.94300
H	6.17700	7.35900	14.02400
H	7.88000	7.30000	13.92800
H	8.02600	6.33900	15.84700
H	7.57700	7.68100	17.96500
H	8.62500	8.49300	16.80300
H	6.90200	8.90400	16.98400
H	6.02800	5.89400	17.30600
H	5.11000	6.96100	16.25000

H	5.77400	5.47100	15.61600
N	6.46600	10.09800	12.20200
C	6.63600	10.51100	10.81500
C	7.83800	11.43200	10.67400
O	8.18000	12.17400	11.59600
C	5.36600	11.18500	10.29500
C	4.10800	10.30900	10.17400
C	2.93500	11.05000	9.49200
C	2.46900	12.33500	10.21000
N	1.35500	12.99100	9.51100
H	5.57900	10.25600	12.66000
H	6.82200	9.61100	10.22500
H	5.16100	12.04700	10.92900
H	5.57800	11.59700	9.30600
H	4.34800	9.42200	9.58600
H	3.82000	9.93900	11.15500
H	3.22300	11.29200	8.46800
H	2.09500	10.35900	9.41000
H	2.12500	12.09900	11.21200
H	3.27800	13.05800	10.31000
H	1.63600	13.31900	8.60300
H	0.57200	12.37000	9.40900
H	1.06200	13.78300	10.06200
N	8.50600	11.35800	9.53100
C	9.77400	12.04700	9.38000
C	9.58900	13.56100	9.35000
O	8.60700	14.07700	8.81000
C	10.50300	11.58000	8.12400
O	9.69100	11.78400	6.98300
H	8.17700	10.80400	8.75300
H	10.40400	11.78700	10.23500
H	11.44000	12.12500	7.99800
H	10.76800	10.52400	8.19700
H	10.28600	11.84700	6.22900
N	10.55200	14.25400	9.94600
C	10.59100	15.70400	9.93600
C	11.07500	16.23900	8.58900
O	10.88500	17.41000	8.26800
C	11.48300	16.19700	11.07600
C	10.89300	15.89100	12.43800
O	9.68600	16.00600	12.63200
N	11.73900	15.48700	13.38400
H	11.30400	13.75800	10.40200
H	9.58300	16.06400	10.09600



H	12.44800	15.69900	10.99400
H	11.70900	17.25400	11.00900
H	11.40400	15.30200	14.31700
H	12.73400	15.46900	13.20700
N	11.69400	15.36300	7.80500
C	12.15400	15.70700	6.47400
C	13.52400	15.14200	6.13900
O	14.09000	14.33300	6.88300
H	11.88300	14.43200	8.14100
H	11.43400	15.31800	5.75300
H	12.20000	16.78600	6.31600
N	14.06900	15.57800	5.01000
C	15.36200	15.09000	4.57000
C	16.48700	15.68000	5.40700
O	16.34800	16.74000	6.02800
C	15.61500	15.35700	3.06600
O	15.94600	16.74100	2.85300
C	14.38700	14.97800	2.24600
H	13.62100	16.34000	4.50500
H	15.37300	14.00500	4.70200
H	16.46500	14.75500	2.73600
H	15.17600	17.25100	3.08600
H	14.59900	15.05600	1.17900
H	14.08900	13.94700	2.44000
H	13.52700	15.61800	2.44800
N	17.60400	14.96700	5.41700
C	18.79800	15.39400	6.11900
C	19.38200	16.65800	5.49700
O	20.02900	17.45600	6.17800
C	19.81200	14.25100	6.10500
C	19.54200	13.26400	4.98700
O	19.16200	13.65700	3.88100
N	19.71000	11.97100	5.27300
H	17.67300	14.14600	4.82200
H	18.55600	15.58700	7.16000
H	20.83800	14.61400	6.02500
H	19.75800	13.72800	7.06100
H	19.71800	11.28600	4.52700
H	20.05300	11.69200	6.18500
N	19.15100	16.82800	4.19700
C	19.57300	18.02600	3.48100
C	18.77700	19.22100	3.98900
O	19.34900	20.26100	4.31300
C	19.37500	17.85300	1.98100

H	18.63100	16.11400	3.70500
H	20.63300	18.20400	3.67500
H	19.68700	18.74700	1.44000
H	19.96900	17.02200	1.60200
H	18.33300	17.66000	1.72300
N	17.45600	19.06000	4.06000
C	16.58000	20.08700	4.62800
C	16.97300	20.35000	6.08000
O	16.97200	21.49000	6.52600
C	15.11300	19.65500	4.53600
C	14.59400	19.50900	3.11500
C	13.20400	18.89300	3.05500
O	12.80200	18.22900	4.03700
O	12.51300	19.07600	2.02800
H	17.05400	18.17900	3.75500
H	16.71300	21.01300	4.06500
H	14.98400	18.72600	5.09100
H	14.48900	20.39400	5.04000
H	14.52200	20.51100	2.68900
H	15.27700	18.99400	2.44700
N	17.32500	19.28200	6.79500
C	17.80000	19.35000	8.17800
C	19.01200	20.25400	8.23800
O	19.08300	21.17200	9.05800
C	18.21500	17.95300	8.66300
C	17.91300	17.62100	10.12400
C	18.33400	18.69900	11.10500
C	17.73200	18.44200	12.49000
N	17.92000	19.59200	13.42900
H	17.18300	18.36500	6.37900
H	16.98400	19.75300	8.78000
H	17.65000	17.22100	8.09800
H	19.26700	17.73300	8.48900
H	16.86700	17.61000	10.13400
H	18.27400	16.63100	10.40500
H	19.42100	18.73900	11.15100
H	17.98300	19.67900	10.79100
H	16.68200	18.20600	12.45500
H	18.21000	17.56300	12.92500
H	17.62000	19.34000	14.35600
H	18.90300	19.80800	13.45800
H	17.40100	20.40100	13.12300
N	19.97200	19.97700	7.36200
C	21.21100	20.74500	7.30800

C	20.95000	22.20100	6.91000
O	21.43500	23.13100	7.56300
C	22.19500	20.08600	6.33800
C	23.59200	20.69300	6.26300
C	24.23500	20.72300	7.64600
C	24.44500	19.91100	5.27400
H	19.86900	19.16500	6.75700
H	21.62900	20.73300	8.31500
H	22.29300	19.03600	6.61700
H	21.76400	20.07600	5.33600
H	23.51000	21.71000	5.88900
H	25.27500	21.04400	7.58100
H	23.74200	21.42900	8.31400
H	24.22600	19.74100	8.12000
H	25.43800	20.35200	5.17600
H	24.57400	18.87400	5.58600
H	23.99500	19.90500	4.28000
N	20.18600	22.39300	5.83700
C	19.77600	23.73300	5.42300
C	19.15000	24.46100	6.60700
O	19.43800	25.63600	6.84700
C	18.79200	23.66600	4.25900
H	19.83200	21.58300	5.32800
H	20.66400	24.28400	5.10800
H	18.48100	24.66500	3.95200
H	19.24200	23.18200	3.39300
H	17.89400	23.10800	4.52100
N	18.31200	23.74600	7.35700
C	17.68100	24.31300	8.54300
C	18.68900	24.69800	9.63400
O	18.61300	25.79600	10.18900
C	16.63400	23.35400	9.09500
H	18.06200	22.80000	7.07600
H	17.16300	25.22700	8.24400
H	16.22700	23.73100	10.03200
H	15.79900	23.22700	8.41000
H	17.02400	22.36600	9.31300
N	19.61700	23.79100	9.94400
C	20.59800	24.02800	11.00200
C	21.57200	25.14600	10.65900
O	21.99000	25.90200	11.53700
C	21.37900	22.75600	11.33600
C	20.60400	21.81300	12.22300
O	20.88600	20.51700	12.09600

N	19.75900	22.23700	13.01400
H	19.58100	22.88500	9.47900
H	20.07300	24.40800	11.87800
H	21.68700	22.24300	10.42400
H	22.29800	22.99800	11.87400
H	19.40300	21.67200	13.76200
H	19.50000	23.21800	13.03100
N	21.93900	25.23900	9.38400
C	22.82900	26.30000	8.92400
C	22.15000	27.64700	9.08000
O	22.70200	28.57000	9.67100
C	23.22200	26.11700	7.44100
C	24.10500	24.87400	7.27300
C	23.92300	27.37500	6.91800
C	24.17600	24.35000	5.85100
H	21.59800	24.55200	8.71200
H	23.73300	26.29900	9.53700
H	22.31300	25.96700	6.85500
H	25.11300	25.09600	7.62700
H	23.76000	24.06000	7.90900
H	24.37800	27.19900	5.94400
H	23.24300	28.21400	6.76400
H	24.72200	27.70100	7.58500
H	24.85600	23.50100	5.79000
H	23.19600	24.02900	5.49700
H	24.54900	25.10100	5.15600
N	20.93800	27.74100	8.55100
C	20.17400	28.97300	8.61600
C	19.94700	29.40000	10.06100
O	20.03300	30.58000	10.37400
C	18.85000	28.82800	7.85700
C	18.97900	28.88500	6.33200
C	17.75300	28.31400	5.64000
C	19.23000	30.32000	5.88200
H	20.52800	26.93800	8.08400
H	20.77200	29.75700	8.15300
H	18.36100	27.90200	8.16600
H	18.17300	29.62600	8.14300
H	19.83200	28.27400	6.03000
H	17.86700	28.33600	4.55600
H	17.58100	27.27700	5.92900
H	16.85400	28.87700	5.89200
H	19.31100	30.37600	4.79600
H	18.41700	30.98400	6.17900

H	20.15500	30.73100	6.28400
N	19.68600	28.44100	10.94400
C	19.49600	28.77000	12.34800
C	20.76100	29.35100	12.96600
O	20.70000	30.34200	13.68900
C	19.01700	27.55300	13.12400
C	17.56600	27.23000	12.84600
C	17.17900	25.85500	13.31600
O	18.02000	24.96700	13.43100
N	15.90000	25.66800	13.59100
H	19.56000	27.48200	10.63300
H	18.72400	29.54000	12.42100
H	19.67200	26.71500	12.88400
H	19.12200	27.70900	14.19500
H	16.93300	27.97800	13.32700
H	17.34400	27.29600	11.78100
H	15.67400	24.73100	13.92100
H	15.34900	26.42800	14.08900
N	21.90400	28.73800	12.67700
C	23.18100	29.25600	13.14600
C	23.41600	30.67400	12.62900
O	23.85500	31.55800	13.37700
C	24.33400	28.33600	12.73500
C	24.61200	27.30500	13.75800
C	24.27400	25.98200	13.71000
C	25.25900	27.51000	15.01900
N	24.68000	25.35100	14.86000
C	25.28600	26.26500	15.68000
C	25.82000	28.62600	15.65300
C	25.85400	26.10300	16.94100
C	26.38700	28.46300	16.90700
C	26.39900	27.21000	17.53700
H	21.89400	27.91200	12.08800
H	23.15000	29.31900	14.23500
H	24.13500	27.85800	11.77600
H	25.25900	28.89900	12.60100
H	23.79900	25.49100	12.88100
H	24.54900	24.36000	15.04300
H	25.81300	29.59200	15.17000
H	25.86300	25.14300	17.43700
H	26.82500	29.31400	17.40900
H	26.84400	27.11500	18.51700
N	23.10400	30.88100	11.35300
C	23.23600	32.19100	10.72500

C	22.39000	33.25500	11.42800
O	22.89900	34.30400	11.81000
C	22.85700	32.13700	9.23500
C	23.94400	31.41500	8.44300
C	22.63400	33.54400	8.68300
C	23.63600	31.27500	6.97300
H	22.78300	30.09600	10.79100
H	24.27900	32.50400	10.81300
H	21.92500	31.59100	9.11100
H	24.89400	31.93900	8.55300
H	24.11600	30.42400	8.85700
H	22.49000	33.54800	7.60500
H	21.71900	34.00500	9.05300
H	23.47600	34.20500	8.89400
H	24.34100	30.58800	6.50500
H	22.63600	30.87100	6.81000
H	23.72200	32.21700	6.43200
N	21.10400	32.98000	11.61100
C	20.23700	33.96000	12.24600
C	20.63500	34.14300	13.69200
O	20.52500	35.23800	14.23300
C	18.76400	33.55100	12.21600
O	18.55400	32.52000	13.17300
C	18.39700	33.03600	10.87500
H	20.71100	32.11800	11.23900
H	20.32300	34.88200	11.68200
H	18.14200	34.41000	12.47700
H	19.16000	31.80800	12.99900
H	17.40700	33.39800	10.59700
H	19.08600	33.32500	10.08300
H	18.30300	31.96400	10.89100
N	21.07300	33.06100	14.32100
C	21.62500	33.15400	15.65800
C	22.82800	34.07800	15.61400
O	22.96100	34.98800	16.44000
C	22.07100	31.78600	16.16100
C	23.02200	31.85600	17.32400
C	24.38100	31.65900	17.13900
C	22.56100	32.14200	18.59900
C	25.25800	31.72900	18.20800
C	23.43100	32.20100	19.67100
C	24.78000	32.00000	19.47500
H	21.09000	32.16000	13.85300
H	20.88200	33.57000	16.34100

H	21.17800	31.24800	16.45100
H	22.52900	31.18800	15.38300
H	24.76600	31.45100	16.15100
H	21.50600	32.30000	18.76700
H	26.31600	31.57400	18.05100
H	23.05000	32.37700	20.66500
H	25.46100	32.04500	20.31300
N	23.70000	33.83000	14.64100
C	24.93800	34.58300	14.51500
C	24.66900	36.07200	14.34100
O	25.22100	36.88600	15.08300
C	25.79000	34.04900	13.37500
H	23.57300	33.01300	14.04200
H	25.49800	34.45100	15.44300
H	26.73100	34.59700	13.31300
H	26.04500	33.00100	13.53000
H	25.30700	34.13900	12.40500
N	23.81900	36.44600	13.38700
C	23.54400	37.87200	13.25600
C	22.61000	38.43400	14.32900
O	22.68300	39.61600	14.62300
C	23.19300	38.33900	11.82900
C	22.02500	37.89800	10.95200
C	22.47900	36.80700	10.00300
C	20.85000	37.44800	11.76800
H	23.38300	35.75400	12.77700
H	24.49000	38.37100	13.40300
H	23.07600	39.42200	11.91400
H	24.10500	38.25500	11.23500
H	21.69900	38.74300	10.34200
H	21.66200	36.18200	9.65900
H	22.93000	37.25000	9.11500
H	23.25000	36.17700	10.43400
H	19.98800	37.16200	11.18700
H	21.15100	36.64100	12.41600
H	20.57000	38.28300	12.39800
N	21.77200	37.59900	14.94300
C	21.02400	38.06400	16.11200
C	21.99200	38.44800	17.22400
O	21.79000	39.44200	17.92100
C	20.04300	37.01300	16.61500
O	19.11200	36.69400	15.60100
H	21.68600	36.63000	14.65200
H	20.45600	38.95500	15.83600

H	20.55300	36.10600	16.94200
H	19.49600	37.39500	17.47900
H	19.59400	36.13400	14.97600
N	23.04600	37.65600	17.38000
C	24.11700	37.99200	18.30400
C	24.83800	39.24300	17.81900
O	25.07100	40.16700	18.59900
C	25.08900	36.82600	18.44200
H	23.12700	36.80600	16.82500
H	23.68500	38.19200	19.28700
H	25.85100	37.04900	19.19000
H	24.57200	35.92200	18.76600
H	25.60900	36.59300	17.51600
N	25.17800	39.27200	16.52900
C	25.83500	40.43500	15.92600
C	24.98400	41.69300	16.04800
O	25.49800	42.75700	16.38800
C	26.17800	40.19400	14.45200
C	27.20000	39.11800	14.06700
C	27.69900	39.34800	12.64400
C	28.36800	39.04500	15.05000
H	25.04100	38.43400	15.96700
H	26.75400	40.62700	16.48200
H	25.28300	40.16200	13.84100
H	26.63100	41.13300	14.12700
H	26.75200	38.14200	14.03000
H	28.37800	38.55400	12.33100
H	26.87100	39.36300	11.93400
H	28.23400	40.29400	12.55100
H	29.11800	38.32800	14.71400
H	28.86300	40.01000	15.16000
H	28.04200	38.71500	16.03700
N	23.68800	41.56700	15.76000
C	22.74500	42.67700	15.91000
C	22.69200	43.13500	17.36800
O	22.76900	44.32700	17.65400
C	21.33300	42.28600	15.44000
S	21.13600	41.88100	13.66900
H	23.33000	40.67900	15.39200
H	23.09300	43.51300	15.30000
H	20.96400	41.43800	16.01900
H	20.64700	43.10900	15.64900
H	21.93100	40.79900	13.74400
N	22.56300	42.18000	18.28600



C	22.55300	42.47600	19.71600
C	23.83900	43.16700	20.15600
O	23.79900	44.17100	20.86900
C	22.36200	41.20000	20.53200
C	20.98900	40.92700	21.14600
C	21.08700	39.77500	22.13900
C	20.42700	42.17000	21.81400
H	22.47800	41.20700	18.00200
H	21.75400	43.19500	19.88100
H	22.71300	40.32900	19.98500
H	23.04300	41.22700	21.38600
H	20.32500	40.61000	20.35200
H	20.10500	39.44700	22.47700
H	21.57200	38.94800	21.64200
H	21.68000	40.03500	23.01700
H	19.56600	41.91500	22.43300
H	21.15900	42.65300	22.46300
H	20.06200	42.90400	21.09800
N	24.97600	42.61800	19.73800
C	26.27400	43.21100	20.03700
C	26.30100	44.66000	19.55500
O	26.74700	45.56700	20.26400
C	27.38800	42.42300	19.33800
C	28.54700	42.04000	20.24200
S	28.40400	40.35000	20.86100
C	29.04900	39.41100	19.47600
H	24.94400	41.74300	19.21200
H	26.40500	43.19100	21.12100
H	27.01900	41.53600	18.83600
H	27.80800	43.00500	18.51400
H	29.48800	42.11800	19.69500
H	28.63700	42.73100	21.08100
H	29.03300	38.34500	19.70200
H	28.44700	39.57600	18.58200
H	30.07800	39.69900	19.25800
N	25.78300	44.85300	18.34700
C	25.85100	46.12200	17.63300
C	24.86700	47.17900	18.15800
O	25.23200	48.34700	18.29800
C	25.69000	45.84800	16.12800
C	24.93900	46.90300	15.37200
C	25.61200	47.94900	14.76300
C	23.56700	46.82100	15.22200
C	24.92000	48.91000	14.04700

C	22.87700	47.78000	14.51300
C	23.55100	48.81800	13.92300
H	25.44200	44.04300	17.83800
H	26.84900	46.54300	17.77300
H	26.65500	45.64700	15.66100
H	25.08100	44.96900	15.96700
H	26.68700	48.02800	14.85200
H	23.01500	46.00800	15.67100
H	25.45300	49.72500	13.57800
H	21.80300	47.70800	14.41000
H	23.02900	49.55300	13.33400
N	23.63700	46.76500	18.46000
C	22.61100	47.67700	18.97600
C	22.75700	47.81200	20.50000
O	22.84100	46.82200	21.22600
C	21.22200	47.18900	18.52300
C	20.09200	48.20000	18.53900
C	20.38000	49.57700	18.53900
C	18.75500	47.76700	18.57500
C	19.33600	50.51700	18.55800
C	17.70900	48.70700	18.59200
C	17.99900	50.08300	18.58100
O	16.98700	50.99800	18.59500
H	23.39400	45.78400	18.32500
H	22.82700	48.62600	18.49400
H	21.28700	46.83700	17.49200
H	20.93100	46.31800	19.11300
H	21.37700	49.97200	18.61700
H	18.52100	46.71200	18.59100
H	19.47400	51.54200	18.88000
H	16.68500	48.41900	18.65900
H	16.15400	50.56300	18.48100
N	22.78300	49.05900	20.96200
C	22.91500	49.38100	22.37500
C	24.34300	49.16900	22.88000
O	25.11100	48.44400	22.25100
H	22.77800	49.82400	20.30400
H	22.62700	50.42300	22.51600
H	22.22700	48.77900	22.97100
N	24.65300	49.81100	24.00300
C	25.96700	49.72500	24.62800
C	27.05800	49.74800	23.54500
O	28.09600	49.09900	23.66700
C	26.01800	48.48300	25.53800

C	25.82400	48.70500	27.02500
C	26.89700	49.16000	27.81400
C	24.58200	48.43700	27.62600
C	26.72300	49.36400	29.19400
C	24.40500	48.64100	29.00500
C	25.47600	49.10800	29.79000
O	25.30800	49.31000	31.12900
H	23.95400	50.38400	24.45400
H	26.11900	50.61900	25.23300
H	25.30800	47.72700	25.19800
H	26.97800	47.97200	25.46100
H	27.85900	49.36100	27.36300
H	23.75200	48.07900	27.03100
H	27.55600	49.71900	29.78400
H	23.44500	48.43900	29.45900
H	26.09800	49.62200	31.56100
N	26.79500	50.51100	22.48800
C	27.71700	50.65100	21.36900
C	27.16200	51.69500	20.38900
O	25.95600	51.93500	20.32800
C	28.01600	49.28500	20.71300
C	28.97600	49.25900	19.51200
C	30.17900	50.18200	19.63600
O	30.54900	50.84400	18.54400
N	30.77400	50.31200	20.70000
H	25.91700	51.00700	22.42500
H	28.62000	51.07600	21.80800
H	28.43700	48.57400	21.41700
H	27.07400	48.83500	20.39600
H	29.34000	48.24200	19.36400
H	28.42600	49.49000	18.60400
H	31.58900	50.90600	20.76100
H	30.51400	49.76300	21.50800
N	28.06900	52.30300	19.62900
C	27.76400	53.33300	18.39300
C	27.09000	54.70600	18.33300
O	27.68000	55.61300	18.92500
C	26.93000	52.48000	17.41100
O	27.69100	51.33000	17.02900
C	26.51300	53.24000	16.14600
H	29.04500	52.09100	19.78800
H	28.74100	53.51000	17.93800
H	26.01600	52.10400	17.87200
H	28.04100	50.95000	17.82600

H	26.66200	52.55600	15.30900
H	25.44100	53.41400	16.01100
H	27.13900	54.07700	15.82300
N	25.86600	54.81800	17.82600
C	25.07700	56.04000	17.91600
C	24.33100	56.07800	19.26000
O	24.51500	55.21000	20.11400
C	24.14400	56.12000	16.69800
C	23.45700	57.42800	16.44700
C	22.13200	57.58400	16.22600
C	24.04100	58.76400	16.39000
N	21.86000	58.92400	16.03000
C	25.34100	59.28600	16.54400
C	23.00000	59.69600	16.11800
C	25.59500	60.66400	16.42200
C	23.23700	61.07300	15.99500
C	24.54600	61.55900	16.14700
H	25.41900	53.99800	17.44500
H	25.75200	56.89200	17.90400
H	24.72000	55.91500	15.79500
H	23.39100	55.33300	16.75900
H	21.39400	56.80000	16.26600
H	20.92100	59.29700	15.94600
H	26.17400	58.62600	16.72900
H	26.60400	61.03700	16.53200
H	22.41500	61.72900	15.75500
H	24.75100	62.61400	16.04100
N	23.48800	57.09200	19.43600
C	22.70800	57.26900	20.65100
C	21.42000	56.44000	20.55600
O	21.17400	55.75900	19.56000
C	22.44900	58.76500	20.85500
C	21.66900	59.07600	22.13600
C	22.07900	58.23300	23.35000
C	21.15800	58.35400	24.57200
N	21.29300	57.22600	25.51000
H	23.31400	57.72000	18.66300
H	23.32100	56.89000	21.46700
H	23.40900	59.28100	20.90100
H	21.92600	59.17900	19.99200
H	21.80600	60.13100	22.37700
H	20.59700	58.99400	21.94700
H	22.24100	57.17400	23.19300
H	23.07300	58.57100	23.64900

H	21.52400	59.21900	25.12700
H	20.14500	58.67800	24.34200
H	20.93300	57.49000	26.41000
H	20.71200	56.47600	25.16400
H	22.24400	56.92300	25.61900
N	20.61100	56.51300	21.60900
C	19.34600	55.81000	21.72300
C	18.61600	56.21900	23.01300
O	19.23700	56.64800	23.98400
C	19.67100	54.31200	21.66300
O	18.46500	53.55700	21.49700
H	20.85300	57.13600	22.36500
H	18.73200	56.09500	20.86600
H	20.33200	53.99000	20.86200
H	20.15400	54.00000	22.59100
H	18.22500	53.58700	20.57700
N	17.29400	56.07500	22.99100
C	16.42100	56.40400	24.10500
C	15.50600	55.19700	24.34300
O	15.31100	54.79300	25.49200
C	15.65100	57.72000	23.85100
O	14.83600	58.01100	24.99100
C	14.75900	57.67300	22.60400
H	16.88900	55.64300	22.17600
H	17.00600	56.52900	25.01900
H	16.37400	58.53000	23.73900
H	14.19500	57.31600	25.10300
H	14.33800	58.66000	22.41000
H	15.32100	57.40000	21.71000
H	13.91300	56.99400	22.69900
N	14.97500	54.66500	23.24500
C	14.07900	53.50900	23.28000
C	14.22300	52.69400	21.99300
O	13.28200	52.59800	21.19900
S	11.86000	53.11300	24.94800
C	12.63200	53.96300	23.54000
H	12.76300	53.50900	25.85400
H	15.17200	55.06200	22.34000
H	14.39600	52.84500	24.08800
H	11.96400	53.86900	22.68500
H	12.60400	55.02600	23.78200
N	15.41000	52.11600	21.79600
C	15.64600	51.15800	20.72700
C	15.41900	49.75800	21.27300

O	15.97700	48.76300	20.78500
H	16.16400	52.28600	22.45000
H	15.07600	51.40100	19.82900
H	16.72200	51.31200	20.72500
N	14.57800	49.69600	22.30200
C	14.35600	48.49000	23.08800
C	13.70100	47.36900	22.27900
O	13.97900	46.19300	22.49300
C	10.75800	47.00200	23.82400
C	8.57100	48.68900	23.17000
C	9.49800	46.48700	23.57900
C	8.41800	47.32900	23.26000
C	13.48400	48.83100	24.29800
C	12.07800	49.25300	23.93200
C	11.62800	50.52600	23.70900
C	10.94400	48.38900	23.75000
N	10.28700	50.50900	23.39900
C	9.84300	49.21000	23.41900
H	14.13500	50.55000	22.59600
H	15.32400	48.13000	23.44400
H	13.42200	47.97300	24.96900
H	13.95100	49.62800	24.87800
H	12.36700	51.27100	23.52300
H	9.76300	51.31900	23.08100
H	11.58000	46.34600	24.07000
H	7.75000	49.34500	22.93500
H	9.34200	45.41800	23.63000
H	7.44700	46.89600	23.07000
N	12.82900	47.75500	21.35700
C	12.09100	46.81200	20.53100
C	12.99700	45.80100	19.85600
O	12.79900	44.58000	19.96400
C	11.30200	47.55700	19.45900
C	11.57200	49.05500	19.44200
C	10.30100	49.83000	19.57700
O	10.25900	51.00700	19.17400
O	9.32600	49.23800	20.08000
H	11.40200	46.27700	21.18400
H	11.53700	47.18200	18.46100
H	10.26100	47.24800	19.54700
H	12.32400	49.54400	20.05500
H	11.93000	49.26500	18.43400
H	12.57900	48.73000	21.30200
N	14.00200	46.31100	19.16100

C	14.88700	45.43500	18.41600
C	15.88900	44.65000	19.27800
O	16.29700	43.55000	18.90600
C	15.53200	46.18400	17.24500
C	14.48600	46.56400	16.18300
C	13.39600	45.48300	15.99100
O	12.19100	45.81400	16.09200
O	13.73900	44.30200	15.73100
H	14.31900	44.57600	18.07000
H	16.10800	47.03600	17.50700
H	16.24300	45.50800	16.76700
H	14.02400	47.48000	16.53700
H	14.96800	46.79800	15.23600
H	14.14600	47.30900	19.15100
N	16.27500	45.18300	20.43000
C	17.08600	44.36700	21.30900
C	16.17500	43.30200	21.92500
O	16.60400	42.18600	22.18000
C	17.89400	45.17500	22.37700
C	17.09600	45.36300	23.66800
C	18.44000	46.49500	21.79400
C	17.52200	44.41500	24.78300
H	16.98500	44.64100	25.70500
H	17.31800	43.37400	24.53800
H	18.58800	44.50400	24.99700
H	15.93200	46.08400	20.73400
H	17.84800	43.85000	20.72000
H	18.77300	44.57600	22.62200
H	17.31500	46.36300	24.04400
H	16.02000	45.39000	23.55300
H	19.10000	46.99200	22.50500
H	19.02600	46.30600	20.89600
H	17.64900	47.19400	21.54700
N	14.90900	43.64500	22.13400
C	13.97700	42.67200	22.67400
C	13.76900	41.49100	21.73200
O	13.78100	40.35800	22.18900
C	12.62800	43.29500	23.03900
C	11.70500	42.33300	23.76500
C	10.67600	41.68500	23.08900
C	11.88900	42.05200	25.11700
C	9.82800	40.79200	23.74800
C	11.05100	41.16200	25.78800
C	10.02400	40.54500	25.09700

O	9.19300	39.68300	25.74500
H	14.59300	44.60000	21.97600
H	14.41200	42.28600	23.59900
H	12.78600	44.15400	23.69100
H	12.12000	43.67900	22.15900
H	10.53900	41.85500	22.03000
H	12.68900	42.53200	25.66300
H	9.03700	40.29900	23.22400
H	11.20500	40.96100	26.83900
H	8.48600	39.37100	25.19300
N	13.57100	41.73600	20.43500
C	13.34700	40.59900	19.55100
C	14.63500	39.84000	19.31600
O	14.61500	38.60900	19.20300
C	12.61300	40.91700	18.20300
C	11.83300	42.20100	18.28400
C	13.55300	40.86000	17.00300
H	13.47700	42.68800	20.09100
H	12.67100	39.91300	20.06700
H	11.89000	40.11900	18.04600
H	11.10300	42.25000	17.47900
H	11.28000	42.30800	19.21800
H	12.48700	43.05700	18.14100
H	13.01800	41.16400	16.10200
H	14.39100	41.55200	17.10000
H	13.93300	39.85900	16.78900
N	15.75400	40.56100	19.27700
C	17.04700	39.89500	19.11800
C	17.33700	39.03300	20.34100
O	17.92500	37.96100	20.22200
C	18.17500	40.90300	18.86000
H	15.71400	41.57300	19.33300
H	16.99400	39.24600	18.24200
H	19.09900	40.38500	18.60500
H	17.93600	41.54300	18.01100
H	18.34600	41.54800	19.72200
N	16.89800	39.48700	21.51300
C	17.07700	38.69500	22.72900
C	16.19400	37.45200	22.67300
O	16.64500	36.34400	22.95700
C	16.76800	39.51400	24.00400
O	17.52100	40.73100	23.98500
C	17.14200	38.73200	25.25200
H	16.46700	40.40300	21.57200



H	18.11600	38.36300	22.77800
H	15.70900	39.77600	24.04500
H	17.19800	41.27900	23.25800
H	16.99500	39.33700	26.14700
H	16.53200	37.83700	25.37800
H	18.18700	38.42100	25.23400
N	14.93400	37.63500	22.29000
C	14.04100	36.49800	22.14400
C	14.60700	35.56200	21.08200
O	14.56700	34.34600	21.23600
C	12.61200	36.93300	21.73200
C	11.98200	37.83400	22.79900
C	11.72900	35.71500	21.42600
C	12.01600	37.27600	24.20600
H	11.39000	37.87600	24.86700
H	11.64700	36.25300	24.25300
H	13.02200	37.29300	24.62600
H	14.58100	38.56800	22.09700
H	14.00800	35.94200	23.08200
H	12.67300	37.51800	20.81300
H	12.40400	38.80900	22.86100
H	10.94800	38.02800	22.51900
H	10.68500	36.00000	21.32500
H	12.00300	35.23100	20.49000
H	11.78300	34.96700	22.21700
N	15.15500	36.13900	20.01600
C	15.58800	35.35100	18.86500
C	16.74300	34.43700	19.22600
O	16.73100	33.25600	18.90500
C	15.96200	36.24500	17.67500
C	15.17100	35.94500	16.39800
C	15.75300	36.62300	15.15800
O	16.05400	37.83300	15.22400
O	15.91400	35.94700	14.11500
H	15.07600	37.15000	19.90100
H	14.74600	34.71600	18.57700
H	15.92200	37.30000	17.88600
H	17.01700	36.10600	17.42700
H	15.17900	34.86900	16.21900
H	14.13000	36.20500	16.56100
H	16.23800	36.51300	13.41400
N	17.73700	34.96700	19.91700
C	18.86900	34.12900	20.25200
C	18.54900	33.23200	21.44800

O	19.12100	32.15800	21.59000
C	20.14700	34.95100	20.43000
C	20.26400	35.68600	21.72400
S	21.90800	36.40500	21.81300
C	22.93600	34.95400	21.62400
H	20.26600	35.64200	19.59400
H	19.51400	36.47300	21.80200
H	20.14700	35.03700	22.59200
H	23.93000	35.15400	22.02400
H	22.52300	34.09900	22.15900
H	23.06100	34.71700	20.56900
H	17.72600	35.95400	20.15900
H	19.08800	33.46500	19.41100
H	20.94500	34.22200	20.32400
N	17.61000	33.65600	22.28600
C	17.06900	32.75700	23.30100
C	16.43800	31.54100	22.61700
O	16.62600	30.39700	23.04200
C	15.99800	33.44800	24.17900
C	16.64800	34.25400	25.30100
C	15.04300	32.41900	24.78600
C	15.63600	34.83000	26.27300
H	16.11000	35.58900	26.89600
H	14.80800	35.31400	25.75300
H	15.23600	34.08400	26.96000
H	17.18200	34.56900	22.16600
H	17.88300	32.39300	23.93200
H	15.39600	34.11900	23.57500
H	17.33500	33.61900	25.86300
H	17.27000	35.04900	24.89700
H	14.30400	32.86600	25.44700
H	14.40100	31.92300	24.05700
H	15.57100	31.65700	25.36200
N	15.70200	31.79700	21.54100
C	15.01800	30.72900	20.84300
C	15.97300	29.71200	20.19400
O	15.68800	28.50300	20.17400
C	14.00900	31.30500	19.84500
C	14.29200	31.05600	18.38700
C	12.99400	30.73300	17.68800
C	13.12100	30.78900	16.17700
N	11.84100	30.33400	15.54500
H	11.58600	29.41300	15.85400
H	11.12800	31.02500	15.75400

H	15.51600	32.76200	21.27600
H	14.44400	30.18100	21.58800
H	13.05700	30.84000	20.10600
H	13.82600	32.36600	19.99800
H	14.70700	31.97000	17.96300
H	14.97800	30.27900	18.08200
H	12.66300	29.74300	18.00000
H	12.21900	31.43400	18.00000
H	13.36100	31.79400	15.83300
H	13.92400	30.14900	15.81900
H	11.96900	30.34400	14.54400
N	17.10900	30.18600	19.68900
C	18.13500	29.32300	19.08600
C	18.80500	28.46800	20.14000
O	19.19700	27.33600	19.88300
C	22.55400	27.80200	17.00700
C	19.21700	30.14200	18.37000
C	20.39300	29.31400	17.89000
C	21.51300	29.12700	18.69400
C	20.37700	28.72200	16.63700
C	22.58600	28.37700	18.25800
C	21.44800	27.96800	16.19600
H	17.23900	31.19000	19.68800
H	17.67400	28.69500	18.33100
H	18.78000	30.66800	17.52000
H	19.59500	30.91700	19.03800
H	21.55600	29.57600	19.67500
H	19.51500	28.85800	16.00100
H	23.44600	28.23600	18.89600
H	21.42100	27.49300	15.22600
H	23.35100	27.16800	16.70100
N	18.95400	29.04400	21.32900
C	19.46900	28.29600	22.46500
C	18.55300	27.10400	22.68800
O	19.00600	25.98300	22.89200
C	19.55300	29.16600	23.74100
C	20.99700	29.62200	23.97400
C	19.02800	28.42200	24.97500
C	21.53800	30.54500	22.89700
H	22.60600	30.70900	23.04000
H	21.40800	30.15100	21.89100
H	21.06500	31.52300	22.95100
H	18.64300	29.99800	21.47000
H	20.45400	27.89900	22.20800

H	18.95600	30.06700	23.62900
H	21.07200	30.13900	24.93200
H	21.64500	28.74800	24.05900
H	19.20600	29.02600	25.86500
H	17.95000	28.26400	24.97100
H	19.54000	27.47500	25.15600
N	17.25400	27.33400	22.59000
C	16.30100	26.25000	22.76200
C	16.35000	25.29800	21.57600
O	16.36300	24.08900	21.74700
C	14.87900	26.78600	22.92600
C	14.79400	27.64100	24.18600
C	13.89400	25.63500	22.98800
C	13.61100	28.58200	24.19600
H	13.62900	29.20900	25.08800
H	13.61100	29.24600	23.33600
H	12.66300	28.04500	24.19900
H	16.92300	28.27600	22.41800
H	16.56200	25.68500	23.66100
H	14.61200	27.40300	22.07100
H	14.77500	27.00600	25.07300
H	15.67700	28.26700	24.30200
H	12.89800	25.98500	23.25700
H	13.76400	25.12600	22.03200
H	14.18200	24.89400	23.73400
N	16.37900	25.85800	20.37300
C	16.40100	25.06300	19.15500
C	17.62000	24.15700	19.12700
O	17.52200	22.97000	18.82600
C	16.42400	25.98200	17.94000
C	15.20500	25.88300	17.06000
C	14.99900	27.13100	16.23800
O	14.76800	27.02100	15.01400
O	15.06400	28.23000	16.82200
H	15.50500	24.44400	19.14900
H	16.53400	26.99600	18.29400
H	17.29800	25.82100	17.30500
H	15.29300	25.02100	16.40900
H	14.31300	25.72400	17.65800
H	16.27600	26.87100	20.29700
N	18.77400	24.72600	19.44900
C	20.00300	23.96700	19.40000
C	19.93000	22.73500	20.29800
O	20.40300	21.65300	19.93200

C	21.18500	24.84100	19.79500
C	22.46100	24.05200	19.91300
C	23.09500	23.55100	18.78000
C	23.02600	23.79400	21.15000
C	24.26200	22.82100	18.87700
C	24.19300	23.06900	21.26000
C	24.80900	22.58400	20.12200
O	25.97300	21.85900	20.23600
H	18.81700	25.72400	19.66800
H	20.15100	23.62600	18.37300
H	21.32800	25.63300	19.05900
H	20.98400	25.34200	20.74400
H	22.67400	23.73900	17.80200
H	22.54300	24.17100	22.03000
H	24.73300	22.44700	17.97800
H	24.62500	22.88300	22.23200
H	26.31600	21.57000	19.39600
N	19.31700	22.89400	21.46500
C	19.24900	21.80900	22.43700
C	17.96100	21.00300	22.38700
O	17.97700	19.81300	22.64000
C	23.40800	23.78000	24.61100
C	19.44500	22.34800	23.85400
C	20.83000	22.84700	24.12200
C	21.08500	24.20500	24.21600
C	21.88000	21.95600	24.27300
C	22.36200	24.67400	24.45600
C	23.16700	22.41100	24.51900
H	18.94500	23.80300	21.70800
H	20.05500	21.09200	22.26700
H	18.72000	23.13800	24.06000
H	19.24100	21.56400	24.58600
H	20.28300	24.90200	24.26600
H	21.70300	20.89200	24.20200
H	22.53600	25.73600	24.56200
H	23.97900	21.70700	24.63800
H	24.40700	24.14300	24.80900
N	16.83900	21.63800	22.07200
C	15.56800	20.96900	22.29300
C	14.53900	21.16700	21.19900
O	13.34700	21.00300	21.46100
C	14.96400	21.44100	23.62100
C	15.72200	20.98700	24.83000
N	15.97600	19.74800	25.30900

C	16.31900	21.86600	25.70800
C	16.71600	19.89900	26.45700
N	16.90900	21.18700	26.67600
H	15.65800	19.88200	22.33600
H	14.91400	22.53100	23.62400
H	13.94100	21.12200	23.78200
H	15.62200	18.86500	24.88400
H	16.35600	22.94700	25.70200
H	17.06700	19.09200	27.08800
H	16.82200	22.64000	21.85300
H	17.40900	21.57700	27.46700
N	14.99100	21.49700	19.98800
C	14.09700	21.93400	18.91500
C	12.85400	21.06900	18.75500
O	11.76400	21.56900	18.46700
C	14.82400	21.99200	17.57200
C	13.90400	22.41300	16.43000
C	14.62400	22.62200	15.11900
O	15.82300	22.97700	15.14700
O	13.98500	22.43000	14.05900
H	13.75300	22.93700	19.17400
H	15.59700	22.74200	17.61100
H	15.30100	21.04000	17.33700
H	13.13600	21.66400	16.23200
H	13.39000	23.34100	16.68400
H	15.99000	21.58900	19.85000
N	13.02300	19.76900	18.96500
C	11.95600	18.83000	18.68700
C	11.45700	18.20700	19.95600
O	10.62000	17.32200	19.92500
C	13.55400	19.44300	13.98400
C	12.43400	17.76400	17.70400
C	12.83100	18.33000	16.39600
C	11.86700	18.71800	15.48500
C	14.16200	18.54000	16.09500
C	12.22400	19.26200	14.28200
C	14.52300	19.09100	14.88900
H	13.93600	19.42200	19.21800
H	11.08300	19.30400	18.23800
H	13.26300	17.19700	18.13200
H	11.64900	17.03300	17.51500
H	10.82000	18.57800	15.71100
H	14.93000	18.28500	16.81200
H	11.46600	19.60300	13.59500

H	15.55700	19.30700	14.68600
H	13.78500	20.04600	13.12100
N	11.97500	18.67600	21.07900
C	11.43800	18.25600	22.35900
C	10.17100	19.03000	22.69600
O	10.05000	20.22400	22.43000
C	12.48100	18.40200	23.45900
C	13.71300	17.55700	23.19600
O	13.68800	16.73500	22.25400
O	14.70300	17.70600	23.93200
H	12.75000	19.44300	23.58000
H	12.05600	18.08600	24.41300
H	12.55400	19.51300	21.04300
H	11.18100	17.19400	22.31400
N	9.21700	18.30100	23.24300
C	8.01000	18.85200	23.80700
C	8.44400	19.85200	24.86200
O	9.25500	19.51900	25.71000
C	7.23300	17.69400	24.43500
C	5.83900	17.98300	24.86500
C	4.94600	18.28200	23.70700
O	4.54200	17.33400	23.00200
O	4.64800	19.47800	23.50400
H	7.48300	19.25300	22.99700
H	7.19600	16.86400	23.72600
H	7.77700	17.30300	25.29500
H	5.43600	17.12000	25.39900
H	5.81900	18.81000	25.57600
H	9.40300	17.32400	23.40700
N	7.90000	21.08400	24.82100
C	6.89700	21.55800	23.86200
C	7.40200	22.55000	22.82100
O	6.57100	23.26900	22.26900
C	5.92100	22.29900	24.76500
C	6.85100	22.98100	25.72800
C	7.95400	21.96600	25.99900
H	6.36300	20.83800	23.29200
H	5.23600	22.99000	24.27100
H	5.29900	21.57700	25.29500
H	7.26900	23.88400	25.28000
H	6.34300	23.28800	26.64300
H	7.74100	21.40200	26.90900
H	8.93200	22.43700	26.10500
N	8.70600	22.62400	22.57200

C	9.19600	23.41100	21.43700
C	8.46900	22.92300	20.18600
O	8.03000	23.70600	19.35300
C	10.70700	23.27000	21.28600
H	9.32200	21.91300	22.95300
H	8.94900	24.46200	21.60300
H	11.07000	23.85400	20.44000
H	11.23200	23.61700	22.17600
H	11.00200	22.23700	21.10400
N	8.34900	21.61000	20.06900
C	7.32900	21.04800	19.21700
C	6.28600	20.43000	20.12600
O	6.61300	19.75500	21.09900
C	7.88800	20.00400	18.24400
C	6.74900	19.31300	17.52500
C	8.84200	20.68700	17.24300
H	8.71200	21.02900	20.81600
H	6.83400	21.80700	18.61200
H	8.45000	19.25400	18.80300
H	7.14800	18.67400	16.73700
H	6.16500	18.65300	18.16700
H	6.06900	20.02600	17.05600
H	9.37300	19.95800	16.63500
H	8.29400	21.34300	16.56700
H	9.56700	21.30700	17.74700
N	5.02500	20.70800	19.84300
C	3.95300	20.05700	20.57200
C	3.43900	18.87200	19.77900
O	2.89100	19.03000	18.68500
C	2.77900	21.01600	20.84400
C	3.24200	22.22700	21.65900
C	1.61300	20.26000	21.51200
C	2.15000	23.29500	21.81700
H	2.52500	24.15000	22.37900
H	1.78500	23.64500	20.85100
H	1.29500	22.92800	22.38200
H	4.78700	21.32000	19.05900
H	4.30400	19.63300	21.45200
H	2.41800	21.38900	19.89200
H	3.58700	21.90200	22.64100
H	4.10300	22.68300	21.17900
H	0.78300	20.92000	21.75400
H	1.17300	19.49300	20.87700
H	1.93600	19.78200	22.43800



N	3.64800	17.67800	20.32200
C	3.08100	16.46000	19.74100
C	1.78600	16.21300	20.48500
O	1.80000	15.88400	21.67200
C	4.02300	15.27500	19.93500
C	5.41200	15.53300	19.41700
C	5.81200	15.05900	18.16500
C	6.31500	16.27600	20.16400
C	7.08200	15.31200	17.68900
C	7.58000	16.53600	19.70000
C	7.96100	16.06000	18.46600
O	9.22400	16.31400	18.01900
H	4.04600	17.60700	21.26800
H	2.92400	16.56500	18.67200
H	4.10800	15.00100	20.98800
H	3.64000	14.40100	19.43300
H	5.12900	14.47200	17.56800
H	6.03100	16.66300	21.13100
H	7.39200	14.92000	16.73200
H	8.24000	17.12700	20.31600
H	9.75700	16.69500	18.72400
N	0.66800	16.39000	19.79700
C	-0.61400	16.31200	20.45800
C	-1.40900	15.07100	20.09600
O	-1.07300	14.33000	19.16100
C	-1.43000	17.58100	20.20400
O	-1.64200	17.77800	18.82600
H	-0.92100	18.45400	20.61200
H	-2.31500	18.47200	18.74700
H	0.68800	16.63200	18.80900
H	-0.50700	16.27300	21.54400
H	-2.40000	17.54300	20.70300
N	-2.49100	14.87800	20.84000
C	-3.28200	13.65100	20.77300
C	-4.03200	13.49000	19.46100
O	-4.61500	12.44000	19.21400
C	-4.26500	13.58300	21.95000
O	-5.21400	14.64500	21.89900
H	-3.72000	13.63300	22.89300
H	-5.89800	14.42200	21.25600
H	-2.76100	15.55000	21.54400
H	-2.59900	12.80300	20.85800
H	-4.79800	12.63000	21.95500
N	-4.03900	14.51300	18.62300

C	-4.64700	14.36400	17.30300
C	-3.58600	14.06600	16.27500
O	-3.85100	14.01600	15.07900
C	-5.51000	15.58300	16.90100
C	-4.72100	16.89400	16.82500
O	-3.49000	16.91000	16.86300
N	-5.44600	18.00400	16.69000
H	-3.53100	15.36200	18.83800
H	-5.33700	13.52000	17.25800
H	-5.99200	15.40300	15.94000
H	-6.31700	15.70000	17.62500
H	-4.97800	18.90700	16.64600
H	-6.45300	17.96900	16.67000
N	-2.36100	13.89300	16.75300
C	-1.26100	13.51000	15.88400
C	-0.42100	14.66700	15.38400
O	0.67600	14.46300	14.85100
H	-2.16200	14.03300	17.74100
H	-0.60900	12.85300	16.46100
H	-1.59400	12.91500	15.03200
N	-0.93500	15.87800	15.57100
C	-0.24700	17.08600	15.14000
C	1.10400	17.25300	15.78700
O	1.32800	16.83500	16.91700
C	-1.09900	18.33800	15.40600
C	-2.15700	18.55700	14.34500
O	-2.23200	17.81300	13.37100
N	-2.98500	19.57800	14.52900
H	-1.80600	15.98500	16.08200
H	-0.05500	16.98300	14.06900
H	-1.54200	18.32500	16.39500
H	-0.47000	19.22900	15.38500
H	-3.72800	19.80700	13.86400
H	-2.86900	20.15500	15.34600
N	2.01300	17.84200	15.02800
C	3.24900	18.36200	15.56700
C	3.17400	19.84400	15.30800
O	3.22600	20.29100	14.16700
C	4.46900	17.79000	14.85500
C	4.56200	16.28600	14.78500
C	5.89200	15.95700	14.11600
C	5.90300	14.59500	13.47600
N	7.21300	14.38900	12.79800
H	7.31300	15.01100	12.01300

H	7.97600	14.59100	13.42500
H	1.72700	18.21700	14.13400
H	3.38100	18.12700	16.61600
H	4.50600	18.16900	13.83200
H	5.36000	18.18400	15.34300
H	4.49400	15.83900	15.77600
H	3.72800	15.89300	14.20200
H	6.10400	16.68700	13.33200
H	6.70100	16.05700	14.84000
H	5.75300	13.83400	14.23200
H	5.09800	14.48700	12.74700
H	7.34700	13.43800	12.46400
N	3.04000	20.60300	16.38100
C	2.82400	22.02900	16.27900
C	4.04400	22.71600	16.84900
O	4.45500	22.43900	17.98100
C	1.58200	22.41500	17.04800
O	0.46900	21.73500	16.46900
C	1.34200	23.92600	17.00100
H	2.98700	20.16700	17.29900
H	2.68300	22.35600	15.24600
H	1.65200	22.11400	18.08800
H	0.39300	20.89700	16.95100
H	0.40800	24.19800	17.47700
H	2.12300	24.49300	17.50800
H	1.28400	24.26800	15.97100
N	4.65600	23.56800	16.03600
C	5.93300	24.16900	16.40400
C	5.68000	25.36900	17.31300
O	5.67800	26.52700	16.88100
C	6.77700	24.52200	15.16000
C	8.19000	24.90200	15.56100
C	6.83100	23.33300	14.22900
H	4.28500	23.74700	15.10200
H	6.51900	23.43900	16.96700
H	6.32200	25.35800	14.62300
H	8.77700	25.20200	14.69300
H	8.22700	25.72300	16.27500
H	8.67700	24.04000	16.00500
H	7.50300	23.52600	13.39600
H	7.18500	22.43400	14.73400
H	5.86100	23.10800	13.78700
N	5.44800	25.06600	18.58500
C	5.04100	26.07200	19.54200

C	6.19600	27.03100	19.80300
O	5.98100	28.18200	20.15600
C	2.56200	27.99200	21.44300
C	3.26500	29.15600	23.93500
C	1.88900	29.08500	21.94200
C	2.24500	29.66100	23.17300
C	4.55500	25.42200	20.82700
C	4.51600	26.35700	22.00100
C	5.33300	26.33600	23.08100
C	3.62200	27.45600	22.19200
N	5.00800	27.35300	23.94200
C	3.95300	28.05100	23.42500
H	5.43100	24.08800	18.84800
H	4.22300	26.66500	19.13800
H	3.55500	25.05200	20.63600
H	5.18100	24.57900	21.05200
H	6.12700	25.61600	23.22500
H	5.48400	27.53000	24.82200
H	2.27900	27.55500	20.49700
H	3.53200	29.60300	24.88200
H	1.07700	29.51600	21.37400
H	1.69700	30.52100	23.53100
N	7.41900	26.57200	19.57200
C	8.57400	27.45200	19.67200
C	8.37900	28.63600	18.74200
O	8.67900	29.77100	19.08500
C	9.83600	26.72200	19.24600
C	11.14400	26.99300	19.99700
C	12.30900	26.84300	19.04800
C	11.15100	28.33200	20.65600
H	12.12800	28.51500	21.10600
H	10.98900	29.14400	19.94900
H	10.44200	28.42200	21.47700
H	7.53700	25.59700	19.31000
H	8.60200	27.77700	20.71100
H	9.67500	25.65000	19.33700
H	10.00200	26.83900	18.17200
H	11.25000	26.25100	20.79000
H	13.26300	26.99800	19.55400
H	12.32000	25.83500	18.63100
H	12.25900	27.54100	18.21300
N	7.89700	28.33300	17.54700
C	7.72200	29.32000	16.50700
C	6.59100	30.28700	16.91000

O	6.75800	31.50600	16.86000
N	7.91400	25.62900	11.55000
C	7.38700	28.60200	15.20100
C	6.91700	29.51500	14.08500
C	6.45500	28.71900	12.88200
N	7.37200	27.64500	12.52500
C	7.01800	26.56400	11.82900
N	5.76300	26.41400	11.41300
H	7.52500	27.40400	17.39200
H	8.64300	29.89300	16.37900
H	8.26400	28.03400	14.89300
H	6.59000	27.88700	15.32400
H	6.06300	30.12000	14.38700
H	7.70400	30.21400	13.80300
H	5.48500	28.28600	13.13000
H	6.28600	29.35200	12.02300
H	8.34500	27.83100	12.70700
H	5.49700	25.63400	10.83000
H	5.04700	27.14200	11.47400
H	7.71700	24.84900	10.92300
H	8.86500	25.66300	11.87100
N	5.46400	29.72100	17.34700
C	4.27200	30.49600	17.65300
C	4.46800	31.28900	18.92600
O	4.02700	32.42200	19.00600
C	3.02100	29.60500	17.73400
C	2.80400	28.81700	16.45600
C	2.55400	29.46100	15.24700
C	2.88500	27.43400	16.45000
C	2.36900	28.73800	14.07400
C	2.71600	26.71700	15.29000
C	2.44800	27.36700	14.10800
O	2.28700	26.62600	12.96000
H	5.39300	28.71100	17.32000
H	4.12200	31.21400	16.84300
H	3.09100	28.92600	18.58500
H	2.17200	30.25000	17.93000
H	2.48700	30.53700	15.22000
H	3.07400	26.89400	17.36100
H	2.17500	29.25100	13.14300
H	2.81400	25.64400	15.30500
H	2.55000	27.11200	12.15900
N	5.15400	30.69600	19.89900
C	5.52700	31.41100	21.10900

C	6.50600	32.56700	20.80200
O	6.28000	33.68700	21.25300
C	6.20100	30.46600	22.12300
H	5.48200	29.73400	19.79500
H	4.61800	31.80700	21.56500
H	6.36900	30.97100	23.07500
H	5.58900	29.59600	22.31200
H	7.16700	30.11100	21.76100
N	7.55400	32.32800	19.98800
C	8.45700	33.35400	19.45600
C	7.74100	34.47400	18.68700
O	8.09200	35.63600	18.84400
C	9.86200	32.82800	19.08800
C	10.65800	33.75500	18.17500
C	10.43100	33.50800	16.65700
O	10.02900	32.33200	16.31400
O	10.70900	34.43900	15.88700
H	8.69600	33.90600	20.37100
H	10.39100	32.57000	20.01300
H	9.71400	31.90900	18.51000
H	10.50600	34.81400	18.37900
H	11.72900	33.59300	18.34700
H	7.65700	31.37800	19.63400
N	6.65700	34.17000	17.97200
C	5.95900	35.18100	17.20000
C	5.08900	35.99200	18.17700
O	5.06600	37.20600	18.03300
C	3.29600	33.02700	14.13100
C	5.03300	31.79500	12.26800
C	2.79600	32.19200	13.14300
C	3.66100	31.57400	12.22400
C	4.86200	34.66300	16.23700
C	5.47300	34.02200	15.07900
C	6.77700	33.82600	14.70200
C	4.67700	33.23500	14.20000
N	6.83300	33.01500	13.58500
C	5.55000	32.62200	13.26600
H	6.45000	33.18100	17.84200
H	6.64800	35.85000	16.67100
H	4.24200	33.93800	16.77700
H	4.19200	35.47100	15.92000
H	7.69600	34.16200	15.16100
H	7.72800	32.57500	13.31800
H	2.63400	33.51400	14.83600

H	5.67500	31.34100	11.53000
H	1.73400	31.99700	13.09100
H	3.24900	30.92100	11.46900
N	4.47900	35.36100	19.18900
C	3.77400	36.05700	20.27300
C	4.66200	37.06300	20.99000
O	4.20800	38.12300	21.41600
C	3.29100	35.04900	21.29900
C	1.81800	34.67100	21.37300
C	0.96200	35.40300	20.32500
C	1.65100	33.14000	21.33900
H	0.61600	32.85800	21.53400
H	1.91400	32.73000	20.36500
H	2.26700	32.64800	22.09300
H	4.53200	34.34300	19.22400
H	2.99200	36.66500	19.82400
H	3.87000	34.13500	21.19200
H	3.55500	35.36600	22.31200
H	1.44600	34.99500	22.34700
H	-0.06100	35.02600	20.32600
H	0.89700	36.47200	20.53300
H	1.35000	35.27700	19.32400
N	5.92400	36.68500	21.15500
C	6.88800	37.46100	21.88900
C	7.43700	38.58900	21.01600
O	7.70900	39.68300	21.49800
C	8.03000	36.54500	22.34600
C	7.73300	35.61900	23.51100
C	8.81000	34.54000	23.61900
C	7.62800	36.41400	24.79500
H	7.45100	35.75200	25.64400
H	8.54700	36.96400	25.00300
H	6.80400	37.12600	24.78200
H	6.19500	35.76900	20.81100
H	6.41700	37.89100	22.76900
H	8.36200	35.95300	21.49400
H	8.89100	37.15500	22.61700
H	6.77800	35.12200	23.34000
H	8.60200	33.85900	24.44400
H	8.86100	33.93800	22.71200
H	9.79600	34.97100	23.78700
N	7.59100	38.32300	19.72300
C	8.30600	39.27200	18.86400
C	7.42500	40.14700	17.96700

O	7.69700	41.31900	17.81800
C	9.33900	38.55900	17.98300
O	8.67200	37.62900	17.12200
C	10.35100	37.83900	18.83600
H	7.40300	37.38300	19.38300
H	8.89100	39.97500	19.46300
H	9.84900	39.29000	17.35300
H	8.37700	36.89700	17.66400
H	11.13600	37.39100	18.22600
H	10.83400	38.52500	19.53100
H	9.91300	37.04300	19.43200
N	6.39600	39.56700	17.35200
C	5.52100	40.31100	16.44100
C	4.87500	41.57200	17.01700
O	4.80400	42.58700	16.31800
C	4.42900	39.40500	15.85700
S	5.09600	38.02300	14.92900
H	3.81800	39.97800	15.16000
H	5.55600	37.38300	16.00800
H	6.15100	38.60200	17.56200
H	6.14900	40.63300	15.60900
H	3.76100	39.03400	16.62700
N	4.37100	41.50900	18.27000
C	3.73200	42.73400	18.74500
C	4.80300	43.78500	18.91600
O	4.54200	44.94900	18.66100
C	3.15800	42.32500	20.10600
C	2.97500	40.83100	20.00500
C	4.17200	40.39300	19.21500
H	2.93700	43.05200	18.06700
H	3.84300	42.54700	20.92800
H	2.22100	42.84000	20.32000
H	2.90100	40.34900	20.97900
H	2.06200	40.60400	19.45100
H	3.97400	39.44200	18.73200
H	5.05200	40.28700	19.84900
N	5.99700	43.35300	19.31200
C	7.10400	44.26100	19.53500
C	7.62400	44.84900	18.23400
O	7.99400	46.02200	18.18100
C	8.24300	43.58400	20.29000
C	9.43200	44.53800	20.39600
C	7.75900	43.15300	21.66100
H	6.15200	42.36600	19.45400



H	6.74300	45.09200	20.14200
H	8.58500	42.69800	19.75600
H	10.16200	44.15500	21.10600
H	9.97100	44.65800	19.45500
H	9.12600	45.52300	20.75100
H	8.55700	42.78500	22.28800
H	7.30300	43.98600	22.19800
H	7.01300	42.36200	21.59300
N	7.64300	44.03900	17.18400
C	7.88400	44.55900	15.83800
C	6.80100	45.57000	15.44200
O	7.08500	46.65200	14.91300
C	7.94000	43.41900	14.80500
C	9.27800	42.68200	14.91200
C	7.80800	43.95200	13.40600
C	9.31000	41.39000	14.07400
H	10.33700	41.06100	14.00300
H	8.72000	40.60100	14.54200
H	8.97600	41.48500	13.04400
H	7.42900	43.05300	17.30900
H	8.84100	45.08600	15.83500
H	7.12500	42.71900	14.98400
H	10.09100	43.34200	14.60400
H	9.47800	42.42000	15.95000
H	8.03300	43.24100	12.62000
H	6.79300	44.27800	13.17800
H	8.46400	44.79500	13.24000
N	5.55200	45.22600	15.72500
C	4.45400	46.12100	15.39200
C	4.50700	47.40600	16.20600
O	4.11300	48.47300	15.72800
C	3.12300	45.41800	15.59700
C	2.89000	44.41700	14.48200
C	1.52300	43.77800	14.64100
C	3.03100	45.10400	13.12200
H	2.57700	44.48700	12.34700
H	2.50300	46.05600	13.11200
H	4.06400	45.24100	12.80200
H	5.34200	44.30600	16.10900
H	4.59100	46.46500	14.37700
H	3.09100	44.92200	16.56400
H	2.31100	46.14900	15.60000
H	3.64200	43.64200	14.52400
H	1.37200	43.03200	13.86100

H	1.44600	43.27900	15.60700
H	0.71700	44.50800	14.57200
N	4.99700	47.29200	17.43600
C	5.17600	48.45300	18.27300
C	6.25500	49.33500	17.65400
O	6.11300	50.56100	17.59200
C	5.56100	48.05600	19.69800
C	4.34100	47.43800	20.38700
C	6.10100	49.28900	20.45600
C	4.59600	46.83400	21.75200
H	3.68100	46.39300	22.14800
H	5.34300	46.04300	21.70300
H	4.93400	47.57300	22.47700
H	5.15100	46.36300	17.82600
H	4.24500	49.02500	18.30000
H	6.36200	47.32000	19.66800
H	3.61900	48.24200	20.52700
H	3.80300	46.73700	19.78100
H	6.27600	49.04000	21.49500
H	7.03200	49.69500	20.07900
H	5.37100	50.09900	20.45000
N	7.32300	48.69100	17.19000
C	8.37700	49.38300	16.48300
C	7.78200	50.05900	15.25100
O	8.05400	51.22700	14.98800
C	9.48500	48.41000	16.07300
C	10.67300	49.07500	15.43600
N	11.96100	48.60900	15.59200
C	10.77100	50.17200	14.64400
C	12.79600	49.38500	14.92800
N	12.09700	50.34400	14.34400
H	7.40500	47.69000	17.35300
H	8.78900	50.14800	17.14200
H	9.83200	47.88900	16.96400
H	9.15000	47.63900	15.39500
H	12.15800	47.65200	15.94000
H	10.10500	50.89200	14.22600
H	13.85800	49.21900	14.80600
H	12.42200	51.10400	13.71400
N	6.97700	49.31400	14.49900
C	6.40900	49.83000	13.26200
C	5.55000	51.04100	13.58800
O	5.46200	51.98800	12.82300
C	5.56600	48.75100	12.59100

C	4.56400	49.18100	11.53000
C	5.24600	49.99800	10.44000
C	3.87900	47.95600	10.94200
H	3.22000	48.25700	10.13100
H	4.59300	47.23700	10.53900
H	3.26400	47.45700	11.68300
H	6.83800	48.32900	14.73700
H	7.21100	50.13100	12.58900
H	6.23100	47.98800	12.18500
H	4.98300	48.25400	13.35600
H	3.77800	49.79000	11.97700
H	4.59200	50.11900	9.57600
H	5.53200	51.00100	10.72500
H	6.15400	49.50200	10.10500
N	4.94700	51.00600	14.76200
C	4.01900	52.03300	15.16200
C	4.76300	53.27500	15.57100
O	4.16800	54.32100	15.79800
C	3.15100	51.53500	16.30300
O	2.35200	50.47300	15.83300
H	2.51000	52.34200	16.65400
H	2.93600	49.72700	15.66800
H	5.06300	50.18900	15.35100
H	3.37100	52.30000	14.32400
H	3.73500	51.21200	17.16300
N	6.07400	53.15200	15.66000
C	6.89000	54.29400	15.97900
C	8.18100	54.23400	15.18100
O	9.26400	54.23100	15.74600
C	7.16200	54.32600	17.48200
C	7.81400	55.61500	17.93000
O	7.83900	56.60700	17.19300
N	8.36000	55.60400	19.13800
H	6.53400	52.28100	15.41100
H	6.39500	55.21800	15.67600
H	6.21400	54.27100	18.01300
H	7.75400	53.46300	17.79400
H	8.75700	56.44800	19.52500
H	8.29800	54.78100	19.72300
N	8.06000	54.16900	13.86000
C	9.23900	54.01900	13.00300
C	10.32300	55.07700	13.23900
O	11.50800	54.76100	13.18100
C	8.83700	53.99300	11.52600

C	8.20300	52.67000	11.13300
C	7.71200	52.67500	9.70400
C	9.24900	51.58800	11.35200
H	8.99400	50.69300	10.78400
H	10.25000	51.88800	11.03600
H	9.28200	51.25700	12.38100
H	7.13600	54.21900	13.43700
H	9.72400	53.09500	13.30600
H	8.14600	54.81300	11.32100
H	9.69600	54.17600	10.88700
H	7.37300	52.47500	11.77700
H	7.38400	51.68400	9.39300
H	6.85500	53.33500	9.59500
H	8.48700	52.99800	9.00800
N	9.91300	56.32000	13.50400
C	10.86200	57.41300	13.73100
C	11.57000	57.27100	15.08200
O	12.68900	57.74500	15.24800
C	10.19200	58.81100	13.68700
O	9.25200	58.91900	14.75800
C	9.48900	59.04700	12.36900
H	8.92000	56.51300	13.57800
H	11.62300	57.37000	12.95100
H	10.94600	59.58000	13.78800
H	8.51800	58.32300	14.57700
H	9.11700	60.06900	12.29100
H	10.20500	58.89000	11.57500
H	8.65200	58.36800	12.20500
N	10.91300	56.62500	16.04200
C	11.45900	56.47000	17.37800
C	11.27200	57.70400	18.24100
O	11.54900	57.68200	19.43800
H	9.99100	56.24600	15.85200
H	10.95700	55.62900	17.85600
H	12.51900	56.21300	17.34200
N	10.77400	58.77500	17.63400
C	10.69200	60.06900	18.28800
C	9.61800	60.10300	19.33700
O	9.80700	60.60600	20.44800
C	10.36000	61.15000	17.25800
C	11.43700	61.30800	16.20200
C	11.15200	62.52000	15.31100
C	12.76900	61.43100	16.92600
H	13.54200	61.78300	16.24400

H	12.73200	62.14800	17.74800
H	13.13600	60.47600	17.30100
H	10.49700	58.70500	16.66200
H	11.61800	60.27700	18.82500
H	9.40800	60.94000	16.76700
H	10.22400	62.10500	17.77100
H	11.49500	60.41500	15.59200
H	11.97500	62.67700	14.61600
H	10.24900	62.36500	14.72100
H	11.03600	63.43600	15.89100
N	8.47900	59.55000	18.96900
C	7.24100	59.95000	19.59000
C	6.93000	59.25400	20.91000
O	7.49500	58.21000	21.23600
C	6.10500	59.76100	18.59200
H	8.44600	59.05600	18.08700
H	7.29000	61.02200	19.80300
H	5.12000	59.90400	19.02100
H	6.18800	60.51700	17.81100
H	6.20200	58.81600	18.07400
N	6.06300	59.89300	21.68600
C	5.17400	59.18000	22.58300
C	3.94400	58.95000	21.71000
O	2.85700	59.47200	21.97200
C	4.83800	60.02200	23.81100
C	4.15700	59.20500	24.91200
O	4.82400	58.62400	25.76200
N	2.83200	59.15300	24.91800
H	5.73300	60.79000	21.35800
H	5.59400	58.22100	22.89700
H	5.76300	60.41600	24.23300
H	4.24000	60.90100	23.56300
H	2.33700	58.63600	25.63200
H	2.31000	59.59100	24.16800
N	4.16900	58.16900	20.65200
C	3.28100	58.01000	19.49600
C	1.93700	57.43800	19.85600
O	0.88100	58.04400	19.64100
C	3.94400	57.02500	18.50900
C	3.14900	56.83700	17.21400
O	3.58900	57.38800	16.17700
O	2.10800	56.12700	17.22100
H	4.95200	57.29800	18.24600
H	4.08300	56.03900	18.95500

H	5.08500	57.74800	20.58700
H	3.12500	58.97400	19.01000
N	2.03400	56.25100	20.42900
C	1.00700	55.22900	20.40300
C	-0.44900	55.68300	20.49400
O	-0.86600	56.36000	21.43300
C	1.38500	54.16400	21.42200
C	2.86600	53.84900	21.33800
C	3.71600	54.09100	22.41300
C	3.42300	53.35300	20.15700
C	5.08100	53.81100	22.32600
C	4.78200	53.07100	20.06000
C	5.60500	53.29600	21.14900
O	6.95300	53.01600	21.06000
H	2.96700	55.91500	20.61500
H	1.12600	54.77100	19.41900
H	1.13500	54.50200	22.42900
H	0.80900	53.25300	21.25000
H	3.32300	54.49300	23.33600
H	2.79600	53.17500	19.29500
H	5.72400	53.99600	23.17500
H	5.17500	52.66000	19.14100
H	7.16900	52.38500	20.38100
N	-1.19700	55.30400	19.46400
C	-2.57700	55.72300	19.28100
C	-3.52200	54.52400	19.23800
O	-3.12600	53.40500	19.57400
C	-2.71300	56.60400	18.02400
C	-2.33700	55.87600	16.72100
O	-1.21300	55.15900	16.71800
N	-3.05200	55.98800	15.72600
H	-0.77500	54.79200	18.69100
H	-2.91700	56.32400	20.12600
H	-3.71900	57.02000	17.94800
H	-2.05400	57.46800	18.12100
H	-2.73900	55.60000	14.84900
H	-3.84500	56.61300	15.72500
N	-4.77300	54.76000	18.85100
C	-5.75200	53.67900	18.77200
C	-5.35700	52.68900	17.67600
O	-5.52400	51.47300	17.83500
C	-7.16100	54.22800	18.52900
C	-8.23000	53.52200	19.38400
C	-9.66900	53.84800	18.95100

C	-10.73000	53.44600	19.99000
N	-10.64500	52.02100	20.34900
H	-9.77000	51.80600	20.79100
H	-11.38000	51.79600	20.99700
H	-5.06400	55.70200	18.63400
H	-5.73600	53.15000	19.72800
H	-7.20100	55.29300	18.76100
H	-7.42800	54.15700	17.47200
H	-8.07600	52.44300	19.33000
H	-8.08100	53.80400	20.42800
H	-9.76000	54.92100	18.77600
H	-9.88200	53.37200	17.99300
H	-10.61500	54.04500	20.89400
H	-11.72700	53.65900	19.60200
H	-10.76100	51.44000	19.53800
N	-4.81700	53.22400	16.57900
C	-4.35300	52.40600	15.45900
C	-3.40300	51.31200	15.94100
O	-3.56500	50.13200	15.62800
N	-3.71300	55.32100	9.99500
C	-3.63000	53.27800	14.43200
C	-2.88800	52.49100	13.37100
C	-3.72000	52.32200	12.11600
N	-3.40700	53.33200	11.11000
C	-4.07800	54.46800	10.94600
N	-5.11300	54.75000	11.72500
H	-4.70800	54.22600	16.53100
H	-5.21800	51.93200	14.99100
H	-4.25900	54.07000	14.03500
H	-2.81300	53.74800	14.96200
H	-1.99900	53.06700	13.10800
H	-2.46700	51.52800	13.65400
H	-3.44200	51.37100	11.66100
H	-4.78800	52.23900	12.32200
H	-2.58200	53.14100	10.55700
H	-5.62900	55.61400	11.64000
H	-5.44100	54.11400	12.43100
H	-2.79300	55.30400	9.57400
H	-4.00700	56.29300	10.01300
N	-2.41900	51.73300	16.72200
C	-1.39600	50.84900	17.23300
C	-1.99800	49.70400	18.03300
O	-1.58900	48.55700	17.88900
C	-0.44100	51.62100	18.12400

O	0.08700	52.72100	17.37900
C	0.68600	50.72100	18.56500
H	-2.31100	52.71800	16.92300
H	-0.85300	50.43500	16.38000
H	-0.94700	52.02600	19.00200
H	0.53400	52.37300	16.61600
H	1.56900	51.28600	18.86000
H	0.39200	50.15300	19.44600
H	0.98100	49.99300	17.81300
N	-2.97300	50.03000	18.87400
C	-3.67300	49.02800	19.65400
C	-4.37200	48.00200	18.75500
O	-4.29300	46.80400	18.99200
C	-4.64900	49.72200	20.59900
C	-3.88800	50.51900	21.64400
S	-2.37200	49.60900	22.06600
C	-1.63900	50.73400	23.21700
H	-5.23500	48.95700	21.11100
H	-3.61100	51.49700	21.25300
H	-4.49900	50.68700	22.53200
H	-0.69200	50.33700	23.58400
H	-1.44500	51.69600	22.74200
H	-2.29700	50.89600	24.07100
H	-3.28000	50.99200	18.92100
H	-2.96100	48.34000	20.10200
H	-5.37000	50.35000	20.07900
N	-5.01600	48.48400	17.69800
C	-5.62800	47.61000	16.72100
C	-4.58400	46.72300	16.06700
O	-4.82700	45.53900	15.86300
H	-5.03400	49.48800	17.54800
H	-6.40000	46.99900	17.19100
H	-6.11600	48.21200	15.95400
N	-3.42900	47.29500	15.73100
C	-2.33300	46.52700	15.13500
C	-1.95300	45.36700	16.03900
O	-1.85800	44.22300	15.60600
C	-1.10300	47.40700	14.94000
C	-0.79300	47.95200	13.55700
C	0.54100	48.71400	13.60700
C	-0.76100	46.81700	12.54100
H	-0.37300	47.17000	11.58700
H	-0.10200	46.01300	12.86700
H	-1.74100	46.39600	12.32900



H	-3.30500	48.28800	15.91200
H	-2.69200	46.10500	14.19900
H	-1.14800	48.26500	15.59700
H	-0.20500	46.87300	15.26100
H	-1.57100	48.66200	13.28200
H	0.84800	49.03500	12.61200
H	0.45600	49.60700	14.22600
H	1.35000	48.10300	14.00800
N	-1.76800	45.69100	17.31200
C	-1.35200	44.72800	18.31500
C	-2.39600	43.63800	18.53200
O	-2.06400	42.45900	18.60900
C	-1.03700	45.44200	19.63600
C	0.40300	45.94700	19.81200
C	1.13400	46.07600	18.49100
C	0.43600	47.27200	20.54500
H	1.45300	47.62500	20.70200
H	-0.10600	48.04100	19.99800
H	-0.03000	47.18600	21.52700
H	-1.84600	46.66900	17.57900
H	-0.48800	44.17600	17.94800
H	-1.74400	46.26200	19.76800
H	-1.24100	44.77900	20.48000
H	0.95300	45.21800	20.40900
H	2.08000	46.59300	18.60800
H	1.38500	45.11100	18.05500
H	0.58200	46.66900	17.76200
N	-3.65600	44.03700	18.62800
C	-4.71300	43.09700	18.95100
C	-4.99100	42.19600	17.75900
O	-5.21300	40.98400	17.91400
C	-6.00100	43.85600	19.39300
C	-7.18700	42.90000	19.56800
C	-5.72800	44.58700	20.68000
H	-3.86800	45.03200	18.60000
H	-4.39200	42.45900	19.77800
H	-6.26000	44.58900	18.62600
H	-8.05200	43.43400	19.96100
H	-7.51300	42.44400	18.63300
H	-6.95600	42.10400	20.27600
H	-6.53500	45.28200	20.91100
H	-5.65300	43.88900	21.51400
H	-4.80100	45.15500	20.68200
N	-4.96900	42.77900	16.56400

C	-5.24200	41.98400	15.38900
C	-4.11500	40.97800	15.22100
O	-4.37400	39.82400	14.96500
C	-5.43200	42.83700	14.14200
O	-4.25800	43.55300	13.82000
H	-6.25500	43.52600	14.32600
H	-4.12400	44.19100	14.51900
H	-4.79100	43.77500	16.47600
H	-6.18900	41.47400	15.55500
H	-5.71900	42.20800	13.30000
N	-2.87800	41.40400	15.44200
C	-1.74700	40.49500	15.27500
C	-1.63400	39.39100	16.31400
O	-1.31500	38.26100	15.96800
C	-0.43900	41.24700	15.24600
C	0.75400	40.31800	15.17900
O	0.92900	39.65900	14.13400
O	1.51300	40.24000	16.17600
H	-0.44200	41.91000	14.38200
H	-0.35600	41.88000	16.13200
H	-2.70000	42.38900	15.61200
H	-1.78700	40.08800	14.27400
N	-1.86400	39.71700	17.58200
C	-1.89500	38.68100	18.60400
C	-2.99900	37.70200	18.18800
O	-2.83600	36.49400	18.26600
C	-2.21000	39.25400	20.00400
C	-1.06300	40.10700	20.52500
C	-2.48100	38.14200	21.00700
C	-1.55000	41.30600	21.39500
H	-0.74400	42.02300	21.55200
H	-2.39200	41.83900	20.96000
H	-1.87400	40.95900	22.37600
H	-2.03800	40.68500	17.84100
H	-0.93800	38.15500	18.62200
H	-3.10800	39.86900	19.92400
H	-0.32800	39.50800	21.06500
H	-0.51100	40.53500	19.68700
H	-2.55300	38.53900	22.02000
H	-3.42300	37.62500	20.82200
H	-1.68500	37.39600	21.00500
N	-4.11000	38.25800	17.72000
C	-5.23200	37.46900	17.25700
C	-4.83600	36.53700	16.13600

O	-5.14000	35.33800	16.22200
H	-4.16500	39.26700	17.64200
H	-5.59400	36.87000	18.09500
H	-6.04800	38.11600	17.01700
N	-4.12400	37.03500	15.11600
C	-3.78500	36.13500	14.01600
C	-2.89800	34.99400	14.49000
O	-3.07100	33.86200	14.06200
C	-3.23900	36.82700	12.71600
O	-1.87400	36.47400	12.47200
C	-3.36300	38.27200	12.78100
H	-3.90200	38.02700	15.06700
H	-4.72800	35.68500	13.72700
H	-3.72500	36.42900	11.85300
H	-1.82300	35.55700	12.22600
H	-2.74700	38.72600	12.01000
H	-4.32000	38.65100	12.61600
H	-2.91300	38.60100	13.69200
N	-1.98800	35.28800	15.41200
C	-1.10300	34.26000	15.93100
C	-1.89100	33.23100	16.74200
O	-1.68600	32.03200	16.58800
C	0.01100	34.84500	16.80200
C	0.82900	35.87500	16.01600
C	0.90500	33.72000	17.30100
C	1.79000	36.72100	16.89700
H	2.37200	37.38300	16.26000
H	1.23700	37.34300	17.60100
H	2.48100	36.10700	17.45700
H	-1.87200	36.25000	15.72100
H	-0.64600	33.74900	15.08000
H	-0.43300	35.35300	17.66000
H	1.42500	35.34900	15.26900
H	0.21500	36.54700	15.42800
H	1.88100	34.05000	17.64600
H	0.45400	33.18200	18.13600
H	1.10600	32.98900	16.51700
N	-2.81300	33.70400	17.57600
C	-3.64100	32.80300	18.34500
C	-4.47400	31.87800	17.45900
O	-4.49100	30.68000	17.68500
C	-4.54100	33.57000	19.31400
C	-5.57400	32.64000	19.92200
C	-3.70000	34.19000	20.38900

H	-2.94100	34.71000	17.67600
H	-2.97600	32.16300	18.93100
H	-5.06600	34.36300	18.77900
H	-6.08300	33.13000	20.75300
H	-6.36600	32.36300	19.22500
H	-5.12600	31.72800	20.31900
H	-4.29400	34.85900	21.01200
H	-3.27200	33.43000	21.04400
H	-2.86500	34.77000	20.00500
N	-5.13900	32.44100	16.44600
C	-5.91100	31.65300	15.48200
C	-5.03400	30.71200	14.66200
O	-5.40800	29.56500	14.40900
C	-8.71500	32.25300	17.13700
C	-9.86900	34.77100	17.72100
C	-9.60100	32.41400	18.18400
C	-10.17300	33.66300	18.46400
C	-6.68900	32.55900	14.53200
C	-7.52400	33.58100	15.22800
C	-7.64100	34.89400	14.90100
C	-8.38300	33.37100	16.36100
N	-8.49600	35.52400	15.76800
C	-8.96800	34.61200	16.66900
H	-5.09600	33.45400	16.33200
H	-6.58100	31.00000	16.02700
H	-6.00900	33.04900	13.84300
H	-7.38300	31.94900	13.97300
H	-7.13300	35.39600	14.09900
H	-8.73900	36.50900	15.70300
H	-8.31300	31.27300	16.97100
H	-10.31300	35.73200	17.94100
H	-9.85900	31.56300	18.79800
H	-10.86700	33.75500	19.28800
N	-3.86500	31.19700	14.24300
C	-2.97400	30.35600	13.46300
C	-2.42400	29.21400	14.29500
O	-2.32200	28.09600	13.82200
H	-3.60400	32.16700	14.41600
H	-3.46900	29.98800	12.56200
H	-2.13900	30.95200	13.15400
N	-2.06200	29.51700	15.53900
C	-1.54900	28.52600	16.45500
C	-2.63200	27.50000	16.71200
O	-2.39000	26.28500	16.66500

C	-1.15100	29.15700	17.79600
O	-0.18400	30.19000	17.57100
C	-0.55800	28.09800	18.72400
H	-2.12100	30.48200	15.85700
H	-0.68400	28.03600	16.00000
H	-2.01100	29.61800	18.28600
H	-0.63900	30.91700	17.13500
H	-0.17400	28.55800	19.63400
H	-1.28900	27.35400	19.04100
H	0.27100	27.57100	18.25000
N	-3.83100	27.99800	16.98200
C	-4.99200	27.13500	17.14800
C	-5.22500	26.30400	15.88200
O	-5.52400	25.11100	15.96100
C	-6.24700	27.94600	17.45000
O	-6.06000	28.65300	18.68200
C	-7.45700	27.02200	17.56300
H	-3.96600	29.00400	17.01800
H	-4.79500	26.44900	17.97500
H	-6.44100	28.67500	16.66300
H	-5.45000	29.37200	18.50500
H	-8.33200	27.58200	17.89100
H	-7.73300	26.55000	16.62200
H	-7.29000	26.22900	18.29300
N	-5.07900	26.93500	14.72100
C	-5.23200	26.23200	13.44900
C	-4.18500	25.12400	13.33100
O	-4.49100	23.98500	12.95100
C	-5.11800	27.20400	12.28600
H	-4.90600	27.93900	14.69800
H	-6.22300	25.78000	13.43400
H	-5.31400	26.70700	11.33800
H	-5.83700	28.00800	12.39100
H	-4.13800	27.66400	12.20700
N	-2.95000	25.45800	13.67100
C	-1.87300	24.48300	13.63900
C	-2.16900	23.28500	14.56000
O	-1.89500	22.14700	14.21700
C	-0.56200	25.15300	14.02900
H	-2.73600	26.42800	13.90800
H	-1.79300	24.10800	12.62000
H	0.26400	24.44900	13.92200
H	-0.33400	25.99900	13.38700
H	-0.56300	25.50700	15.05800

N	-2.73400	23.57300	15.72600
C	-3.05100	22.57400	16.73100
C	-4.24900	21.73200	16.31100
O	-4.44900	20.64000	16.81400
C	-3.36200	23.28000	18.05200
C	-2.13400	23.83200	18.78400
C	-2.55900	24.58400	20.00300
C	-1.19400	22.71500	19.17600
H	-0.26400	23.11900	19.57500
H	-1.62600	22.10000	19.96600
H	-0.92100	22.03800	18.38500
H	-2.84600	24.55500	15.96700
H	-2.22300	21.87500	16.81300
H	-4.07700	24.08300	17.87700
H	-3.87500	22.59100	18.72600
H	-1.60500	24.51500	18.12800
H	-1.69800	24.99100	20.53400
H	-3.20000	25.42700	19.74100
H	-3.11000	23.95300	20.70100
N	-5.03600	22.25900	15.38000
C	-6.24800	21.60900	14.91200
C	-6.04100	20.78300	13.64600
O	-4.92200	20.63100	13.15200
C	-7.33300	22.65500	14.65100
O	-7.65200	23.33300	15.84300
H	-8.18400	22.17900	14.20100
H	-6.89000	23.87200	16.06400
H	-4.77000	23.14500	14.96700
H	-6.63100	20.92100	15.66900
H	-6.97500	23.39100	13.93400
N	-7.15600	20.27500	13.13000
C	-7.18700	19.40700	11.96600
C	-8.40900	19.78500	11.15500
O	-9.31300	20.43800	11.66700
C	-7.30000	17.92200	12.38800
C	-6.24200	17.45800	13.39300
C	-5.57100	16.15100	12.96300
C	-4.57100	16.38300	11.83000
N	-3.74700	15.17000	11.53700
H	-3.19800	14.93200	12.34600
H	-4.33000	14.38800	11.29400
H	-8.04300	20.39600	13.61200
H	-6.29900	19.55600	11.34700
H	-8.28400	17.74000	12.82600

H	-7.28000	17.30200	11.49100
H	-5.45500	18.18700	13.55900
H	-6.72500	17.31900	14.35900
H	-5.02500	15.77900	13.82500
H	-6.30900	15.39000	12.70500
H	-5.12400	16.61000	10.91800
H	-3.95900	17.26000	11.98300
H	-3.12300	15.35800	10.77200
N	-8.42300	19.36700	9.89300
C	-9.56800	19.52500	9.01300
C	-10.27100	20.87100	8.99100
O	-9.64200	21.92400	8.89300
H	-7.62500	18.86200	9.53600
H	-9.23500	19.32000	7.99500
H	-10.28000	18.73400	9.25500
N	-11.59600	20.80800	9.08500
C	-12.46300	21.96900	9.00600
C	-12.13300	22.99900	10.07500
O	-12.10100	24.19900	9.79200
C	-13.93700	21.54700	9.12400
C	-14.46400	20.98000	10.43600
C	-14.11000	19.68100	10.86200
C	-15.36600	21.74200	11.20900
C	-14.64400	19.15700	12.05600
C	-15.91400	21.20900	12.39000
C	-15.54900	19.92000	12.81900
O	-16.07300	19.42000	13.97200
H	-12.03100	19.90300	9.17300
H	-12.31200	22.43200	8.02800
H	-14.55000	22.41200	8.86300
H	-14.15700	20.81900	8.34200
H	-13.43900	19.07000	10.27600
H	-15.65500	22.73500	10.89500
H	-14.35900	18.16200	12.37000
H	-16.60800	21.80000	12.97100
H	-15.76400	18.54200	14.17200
N	-11.89700	22.55500	11.30600
C	-11.65300	23.54200	12.34500
C	-10.28300	24.22100	12.18300
O	-10.14800	25.42000	12.40200
C	-11.94500	23.01900	13.76600
C	-12.33500	21.56500	13.73400
C	-10.79400	23.31900	14.71900
H	-11.91300	21.57000	11.52500

H	-12.37900	24.34800	12.22000
H	-12.81000	23.56800	14.14400
H	-12.55500	21.21000	14.74100
H	-13.23800	21.40100	13.15300
H	-11.54000	20.92800	13.34500
H	-11.10600	23.08900	15.73800
H	-10.00400	22.63500	14.51400
H	-10.46000	24.33700	14.75800
N	-9.29100	23.47100	11.72700
C	-8.04800	24.09700	11.33300
C	-8.28400	25.15500	10.25800
O	-7.77400	26.27400	10.36300
N	-2.60700	20.87000	11.76700
C	-7.04800	23.07200	10.83100
C	-5.92000	23.72200	10.03500
C	-4.92100	22.70200	9.60700
N	-4.14100	22.22900	10.74000
C	-3.26700	21.23400	10.67900
N	-3.05400	20.60900	9.52800
H	-9.45600	22.48900	11.52900
H	-7.62500	24.60900	12.19500
H	-6.63900	22.53400	11.67800
H	-7.53600	22.33600	10.19700
H	-6.26800	24.16800	9.10200
H	-5.43500	24.51900	10.59700
H	-5.42600	21.85700	9.13700
H	-4.33700	23.17000	8.83100
H	-4.27600	22.73800	11.61900
H	-2.39200	19.85400	9.42900
H	-3.42500	20.99300	8.67300
H	-1.96500	20.09200	11.78900
H	-2.76100	21.31700	12.67100
N	-9.05700	24.80200	9.23100
C	-9.42200	25.74800	8.18100
C	-10.08600	27.00700	8.74400
O	-9.70700	28.13500	8.38000
C	-10.34800	25.11300	7.10900
C	-10.77000	26.15900	6.07800
C	-9.65600	23.94200	6.42200
H	-9.42500	23.85600	9.18700
H	-8.49600	26.06100	7.69300
H	-11.25200	24.73300	7.57800
H	-11.24600	25.68400	5.22000
H	-11.50500	26.85700	6.47600



H	-9.92100	26.73100	5.70200
H	-10.37900	23.29500	5.92400
H	-8.96200	24.30000	5.66000
H	-9.06000	23.32800	7.08700
N	-11.04900	26.81000	9.64700
C	-11.76500	27.92700	10.26400
C	-10.79500	28.87500	10.96200
O	-10.82700	30.09000	10.74600
C	-12.80100	27.47000	11.31400
C	-13.86900	26.56000	10.69100
C	-13.45600	28.68400	11.97400
C	-14.37200	27.04800	9.36300
H	-15.25700	26.48400	9.06700
H	-14.65800	28.10000	9.39000
H	-13.63900	26.90800	8.56800
H	-11.34100	25.85800	9.85900
H	-12.24200	28.50800	9.47300
H	-12.31100	26.90100	12.10500
H	-13.61900	25.52100	10.68300
H	-14.72600	26.55100	11.36500
H	-14.31500	28.39300	12.57800
H	-12.78500	29.19200	12.66400
H	-13.80600	29.41300	11.24200
N	-9.93700	28.31300	11.80400
C	-9.03500	29.13400	12.58600
C	-8.00300	29.83400	11.71600
O	-7.75200	31.02100	11.89000
C	-11.15600	27.91500	16.98000
C	-8.42000	28.32800	13.71900
C	-9.35000	28.16700	14.86500
C	-9.71000	29.27800	15.62800
C	-9.92600	26.93300	15.15100
C	-10.60000	29.15500	16.69000
C	-10.82300	26.80400	16.20900
H	-9.96400	27.30700	11.95500
H	-9.62500	29.93700	13.03200
H	-8.05100	27.36500	13.36600
H	-7.57100	28.85800	14.11900
H	-9.31500	30.24900	15.37300
H	-9.59300	26.09200	14.58000
H	-10.87900	30.02300	17.27000
H	-11.24900	25.83900	16.44400
H	-11.85200	27.81400	17.80100
N	-7.45800	29.10900	10.74500

C	-6.56200	29.72200	9.78900
C	-7.26000	30.89800	9.11900
O	-6.65700	31.96100	8.93800
C	-3.66700	30.62000	5.72100
C	-6.07200	28.72800	8.73300
C	-5.22900	29.36900	7.66600
C	-3.84700	29.43600	7.80400
C	-5.81800	29.94100	6.54600
C	-3.06700	30.04600	6.83300
C	-5.04200	30.56400	5.57300
H	-7.71900	28.13200	10.62500
H	-5.69400	30.10300	10.33200
H	-5.49700	27.93400	9.21000
H	-6.92100	28.23500	8.25600
H	-3.36500	29.01600	8.67600
H	-6.89100	29.90900	6.41800
H	-1.99500	30.09600	6.95100
H	-5.51200	31.01100	4.70900
H	-3.05600	31.11500	4.98000
N	-8.52600	30.70600	8.75600
C	-9.28500	31.76600	8.10000
C	-9.54700	32.93400	9.04700
O	-9.48400	34.08900	8.64400
C	-10.58800	31.23300	7.49700
C	-10.39100	30.42600	6.20800
C	-11.68000	29.70800	5.77700
C	-9.85900	31.31400	5.09000
H	-9.85500	30.77600	4.14100
H	-10.47300	32.20500	4.95400
H	-8.83100	31.63300	5.25400
H	-8.96400	29.79700	8.88400
H	-8.66400	32.17500	7.30600
H	-11.10900	30.62500	8.23600
H	-11.26300	32.06400	7.28300
H	-9.64300	29.65400	6.38700
H	-11.50500	29.05900	4.91800
H	-12.07100	29.08900	6.58500
H	-12.45900	30.42000	5.50400
N	-9.82700	32.62700	10.30500
C	-9.93000	33.66800	11.31400
C	-8.59400	34.39400	11.46500
O	-8.55800	35.60800	11.57700
C	-10.36300	33.07700	12.65900
C	-11.81000	32.58000	12.66300

S	-12.14200	31.55500	14.11700
C	-11.83100	32.75100	15.43500
H	-10.25100	33.84800	13.42300
H	-12.49800	33.42600	12.65100
H	-12.03600	31.99400	11.77500
H	-12.03100	32.30200	16.40800
H	-10.79800	33.07100	15.41600
H	-12.46800	33.62800	15.32400
H	-9.94200	31.64900	10.56500
H	-10.67700	34.40000	10.99800
H	-9.69100	32.27300	12.95000
N	-7.49700	33.64400	11.46600
C	-6.18500	34.25000	11.55600
C	-5.96300	35.12000	10.34700
O	-5.40300	36.21000	10.43900
H	-7.58500	32.62600	11.44000
H	-6.10100	34.85900	12.43900
H	-5.42300	33.47300	11.60200
N	-6.44100	34.64000	9.20700
C	-6.28900	35.36600	7.96300
C	-7.04200	36.68600	8.01700
O	-6.52200	37.73100	7.61000
C	-6.78700	34.52500	6.80100
C	-6.68600	35.26300	5.47400
C	-5.22400	35.55700	5.19000
C	-7.32900	34.46500	4.34300
H	-7.26500	35.00000	3.39500
H	-6.84400	33.49700	4.21200
H	-8.38600	34.28100	4.54100
H	-6.78700	33.68100	9.18100
H	-5.22700	35.57900	7.84500
H	-6.23100	33.58700	6.75300
H	-7.82600	34.25400	6.94100
H	-7.23200	36.20500	5.49000
H	-5.09900	35.93000	4.17300
H	-4.81500	36.33100	5.83900
H	-4.60100	34.66600	5.28500
N	-8.25300	36.66300	8.55800
C	-9.02500	37.90300	8.63300
C	-8.36400	38.92900	9.54100
O	-8.34600	40.12600	9.25700
C	-10.45800	37.62000	9.08100
S	-11.38700	36.70600	7.83000
H	-10.98600	38.55700	9.26600

H	-10.62700	35.60100	7.89400
H	-8.66200	35.77600	8.84100
H	-9.07100	38.34800	7.63600
H	-10.47200	37.06300	10.01900
N	-7.82400	38.44800	10.64700
C	-7.12100	39.31300	11.56200
C	-5.85600	39.82100	10.87100
O	-5.47100	40.96600	11.02500
C	-6.75000	38.52300	12.80600
C	-7.73700	38.58800	13.93000
C	-9.04200	38.14700	13.76600
C	-7.35100	39.06500	15.17000
C	-9.93200	38.19200	14.81000
C	-8.22000	39.11900	16.21100
C	-9.51400	38.67300	16.03400
O	-10.38800	38.72300	17.09100
H	-7.88300	37.45400	10.84400
H	-7.73700	40.17300	11.83600
H	-6.36200	37.51900	12.63000
H	-6.00400	39.13700	13.27700
H	-9.37200	37.75700	12.81400
H	-6.38700	39.39300	15.39400
H	-10.94600	37.84500	14.67200
H	-7.89100	39.50500	17.16600
H	-9.99000	39.06500	17.88500
N	-5.22600	38.94800	10.09500
C	-3.97900	39.27300	9.43300
C	-4.18200	40.35600	8.40100
O	-3.38400	41.28000	8.29100
H	-5.55500	37.98600	10.04900
H	-3.23300	39.61600	10.14700
H	-3.58300	38.37900	8.95200
N	-5.25800	40.22800	7.63500
C	-5.60000	41.21300	6.63000
C	-5.77100	42.56800	7.29700
O	-5.23000	43.58400	6.83100
C	-6.89800	40.82000	5.89400
C	-6.62100	39.63400	4.95300
C	-7.49000	42.03800	5.14700
C	-7.85100	38.94400	4.41200
H	-7.57100	38.08800	3.79700
H	-8.48100	38.57200	5.22000
H	-8.45400	39.60400	3.79000
H	-5.83600	39.39400	7.72900

H	-4.78100	41.29100	5.91200
H	-7.63600	40.50100	6.63200
H	-6.01000	39.97600	4.11600
H	-6.01100	38.88300	5.45300
H	-8.31200	41.73900	4.49800
H	-7.91600	42.79100	5.81100
H	-6.74600	42.52000	4.51200
N	-6.51800	42.56600	8.39900
C	-6.71500	43.75900	9.21400
C	-5.35800	44.35000	9.62500
O	-5.13000	45.54700	9.51600
C	-7.55100	43.40400	10.45100
C	-7.87600	44.59300	11.32300
C	-9.06600	45.28600	11.16700
C	-6.98700	45.03100	12.29900
C	-9.36400	46.37100	11.95900
C	-7.27700	46.11600	13.10300
C	-8.47000	46.78400	12.92400
O	-8.77100	47.87400	13.71000
H	-6.91400	41.68800	8.71500
H	-7.25200	44.49800	8.61600
H	-8.48500	42.93500	10.13900
H	-7.06000	42.67900	11.08700
H	-9.77700	44.97600	10.41400
H	-6.02400	44.56100	12.38200
H	-10.30100	46.89000	11.81200
H	-6.56200	46.44900	13.84000
H	-9.61500	48.25900	13.50200
N	-4.45900	43.49200	10.08600
C	-3.10700	43.90400	10.44300
C	-2.31400	44.48600	9.28500
O	-1.65400	45.50700	9.44500
C	-2.33600	42.73200	11.02800
O	-3.07000	42.24500	12.14800
C	-0.94400	43.16200	11.47900
H	-4.70800	42.51800	10.25000
H	-3.19600	44.68100	11.20600
H	-2.22100	41.91700	10.31800
H	-3.41900	42.94600	12.72000
H	-0.44100	42.33800	11.98700
H	-0.28700	43.44800	10.65700
H	-0.99000	43.98900	12.18500
N	-2.37200	43.84100	8.12500
C	-1.62300	44.31200	6.96900

C	-2.12500	45.67100	6.53300
O	-1.33300	46.55800	6.20300
C	1.41100	40.38500	5.73000
C	-1.71800	43.33000	5.79500
C	-0.62100	42.29900	5.77300
C	-0.02000	41.87600	6.94900
C	-0.18000	41.76300	4.57200
C	0.98500	40.92100	6.93100
C	0.82900	40.80500	4.54800
H	-2.89200	42.96500	8.06700
H	-0.57900	44.45400	7.25300
H	-2.68600	42.82700	5.78200
H	-1.65600	43.87000	4.84700
H	-0.33100	42.24900	7.91300
H	-0.62500	42.08100	3.63900
H	1.41500	40.59300	7.86400
H	1.16000	40.38800	3.60700
H	2.15700	39.64300	5.74600
N	-3.44200	45.83100	6.52700
C	-4.02600	47.09600	6.11600
C	-3.59500	48.16600	7.09200
O	-3.15900	49.22700	6.66700
C	-6.95800	45.51500	2.24500
C	-5.55200	47.02600	6.01700
C	-6.04500	46.50100	4.69600
C	-5.47700	45.36500	4.12900
C	-7.07700	47.13600	4.01900
C	-5.92600	44.87300	2.91000
C	-7.53500	46.64900	2.80000
H	-4.05000	45.05800	6.79000
H	-3.62700	47.37600	5.13800
H	-5.96500	46.41700	6.82300
H	-5.97500	48.02300	6.15600
H	-4.68300	44.82500	4.61800
H	-7.54100	48.02000	4.43600
H	-5.47600	43.98700	2.48500
H	-8.34100	47.15300	2.28400
H	-7.31300	45.13400	1.29800
N	-3.68900	47.87000	8.39100
C	-3.27600	48.82000	9.40300
C	-1.80100	49.18200	9.24300
O	-1.44200	50.35700	9.23600
C	-3.57400	48.29600	10.80500
C	-4.87100	48.85300	11.37200

O	-5.82700	49.09500	10.63100
N	-4.90300	49.07300	12.69500
H	-4.06600	46.97100	8.67900
H	-3.82000	49.75100	9.23900
H	-3.59100	47.20700	10.83900
H	-2.77700	48.60000	11.47900
H	-5.76200	49.39800	13.11500
H	-4.11600	48.86100	13.29100
N	-0.96300	48.16400	9.08700
C	0.47300	48.34600	8.94900
C	0.75800	49.21700	7.74600
O	1.70100	49.98700	7.74200
C	1.16300	46.97400	8.77600
H	-1.32200	47.21000	9.11800
H	0.85800	48.84100	9.84300
H	2.21900	47.08600	8.53000
H	1.09700	46.37800	9.68700
H	0.71300	46.39900	7.96800
N	-0.05300	49.04700	6.70900
C	0.12100	49.76500	5.45900
C	-0.10200	51.25700	5.67500
O	0.68700	52.07700	5.19700
C	-0.83900	49.21400	4.38700
H	-0.77100	48.33000	6.76300
H	1.14600	49.64900	5.10500
H	-0.63800	49.69000	3.42700
H	-0.70400	48.14300	4.24100
H	-1.88600	49.40200	4.61100
N	-1.16000	51.60600	6.40900
C	-1.44400	53.01400	6.69500
C	-0.27800	53.59900	7.46700
O	0.15000	54.73100	7.20600
C	-2.71600	53.18600	7.52500
C	-3.74700	52.07800	7.37500
C	-4.66400	52.28000	6.17600
C	-6.13900	52.27700	6.60500
N	-6.32300	51.99900	8.06800
H	-5.92200	51.10900	8.31200
H	-5.90900	52.71600	8.63700
H	-1.75900	50.87600	6.77900
H	-1.56200	53.54000	5.74600
H	-2.39800	53.09600	8.56600
H	-3.17100	54.13300	7.55800
H	-3.27200	51.15500	7.50400

H	-4.14900	52.17400	8.37300
H	-4.45000	53.20400	5.65000
H	-4.48000	51.49300	5.44300
H	-6.70300	53.01700	6.06100
H	-6.56000	51.37800	6.15100
H	-7.30700	51.94900	8.28200
N	0.23200	52.81600	8.41700
C	1.35000	53.25600	9.23200
C	2.57200	53.50500	8.35000
O	3.22400	54.54900	8.45400
C	1.65900	52.24100	10.32700
C	2.83600	52.70700	11.15900
C	0.41500	52.03100	11.21400
H	-0.14900	51.88600	8.55700
H	1.07400	54.20400	9.70100
H	1.92400	51.28400	9.88000
H	3.00000	52.00700	11.97600
H	3.77400	52.75800	10.60700
H	2.64500	53.67700	11.61500
H	0.52200	51.14000	11.82900
H	0.28900	52.87400	11.89400
H	-0.52000	51.95100	10.67700
N	2.85600	52.56100	7.45800
C	3.97700	52.71800	6.54000
C	3.79500	53.91900	5.63200
O	4.73000	54.68500	5.42000
C	4.18900	51.46200	5.69700
C	4.99500	50.41100	6.40300
C	6.33500	50.62800	6.69800
C	4.42000	49.18800	6.77000
C	7.07400	49.66300	7.34800
C	5.15100	48.23200	7.41300
C	6.47800	48.47200	7.70300
O	7.21100	47.51300	8.34600
H	2.32700	51.69100	7.45700
H	4.87500	52.90800	7.13200
H	3.23500	51.05200	5.36200
H	4.73800	51.70300	4.78400
H	6.81200	51.55600	6.42000
H	3.40300	48.96000	6.50500
H	8.11300	49.84500	7.57900
H	4.67900	47.30100	7.68900
H	6.67600	46.75500	8.56400
N	2.59100	54.06400	5.08700



C	2.24500	55.21600	4.26500
C	2.46800	56.50800	5.05100
O	3.12900	57.43300	4.57300
C	0.78900	55.10500	3.75700
C	0.71500	54.02000	2.67300
C	0.30100	56.42000	3.20100
C	-0.69300	53.51500	2.35000
H	-0.65800	52.71800	1.60700
H	-1.18200	53.11500	3.23900
H	-1.32300	54.30900	1.95000
H	1.86800	53.37000	5.27700
H	2.92100	55.24000	3.40700
H	0.14500	54.83400	4.59300
H	1.18900	54.37500	1.75700
H	1.30500	53.15300	2.96800
H	-0.76500	56.36600	2.98600
H	0.45700	57.31500	3.78800
H	0.79300	56.63100	2.25100
N	1.93800	56.55500	6.27000
C	2.10800	57.72300	7.12800
C	3.58200	57.97300	7.44400
O	4.03400	59.11300	7.43000
C	1.31600	57.57000	8.43100
C	-0.19900	57.65600	8.26800
C	-0.94400	57.65400	9.60100
O	-0.29400	57.81700	10.66000
O	-2.18300	57.49300	9.58800
H	1.73200	58.59700	6.59200
H	1.57200	56.62800	8.91600
H	1.63600	58.35600	9.11900
H	-0.37700	58.66700	7.94400
H	-0.58800	56.87600	7.63400
H	1.37000	55.77800	6.61200
N	4.32900	56.90700	7.71900
C	5.71700	57.06600	8.11600
C	6.52300	57.63500	6.96000
O	7.36300	58.52300	7.15000
C	6.29800	55.76200	8.57600
H	3.89600	55.98500	7.76300
H	5.76200	57.76100	8.95600
H	7.35000	55.87500	8.84100
H	5.78700	55.38600	9.46000
H	6.23700	54.99500	7.80300
N	6.25000	57.11700	5.76700

C	6.91400	57.56100	4.55400
C	6.81600	59.08500	4.41000
O	7.79600	59.75100	4.10000
C	6.28800	56.87900	3.34100
C	6.87900	57.32200	2.02400
C	6.32400	58.38300	1.30000
C	7.98800	56.68000	1.50000
C	6.87400	58.78700	0.07700
C	8.53900	57.07000	0.28800
C	7.98400	58.12000	-0.42000
O	8.55900	58.48300	-1.61700
H	5.56200	56.36900	5.70600
H	7.96900	57.28800	4.61800
H	6.39900	55.79700	3.42800
H	5.21700	57.06200	3.30200
H	5.48500	58.92600	1.69600
H	8.43700	55.85600	2.03700
H	6.43900	59.61700	-0.46100
H	9.40100	56.54200	-0.09400
H	9.29200	57.92900	-1.86200
N	5.63000	59.62100	4.66600
C	5.38800	61.05000	4.52400
C	5.77700	61.84000	5.76600
O	5.79400	63.06500	5.74200
C	3.92300	61.31200	4.16300
C	3.54900	60.82100	2.79900
N	3.18400	59.51400	2.55400
C	3.51200	61.45400	1.60300
C	2.92500	59.36700	1.26600
N	3.11600	60.52700	0.66600
H	5.98800	61.44100	3.70100
H	3.25300	60.87900	4.90800
H	3.72700	62.38600	4.17700
H	3.10700	58.76600	3.25000
H	3.73600	62.48200	1.34900
H	2.61000	58.44900	0.78700
H	4.86900	59.01800	4.95300
N	6.08300	61.13500	6.84800
C	6.47800	61.77900	8.08900
C	7.98900	62.00500	8.13300
O	8.46100	63.03600	8.60700
C	6.04700	60.94100	9.30900
O	4.61500	60.90100	9.37700
C	6.60500	61.54400	10.61000

H	6.07700	60.12300	6.80200
H	5.98000	62.74100	8.18400
H	6.41800	59.92100	9.22100
H	4.31300	60.37700	8.63000
H	6.16900	61.04900	11.47800
H	7.68400	61.42300	10.71100
H	6.37400	62.60400	10.69200
N	8.74000	61.03300	7.63000
C	10.18600	61.08800	7.70400
C	10.72800	62.05300	6.63500
O	10.02500	62.34600	5.65900
C	10.79500	59.66600	7.58500
C	10.24600	58.75400	8.69200
C	10.53300	59.08100	6.21000
H	8.30800	60.19700	7.24600
H	10.43500	61.46200	8.69700
H	11.86400	59.73100	7.71800
H	9.16500	58.76400	8.80300
H	10.55700	57.71900	8.54900
H	10.67700	59.08800	9.62500
H	10.95600	58.08400	6.13300
H	9.48000	59.02400	5.95200
H	11.04400	59.66700	5.45300
N	11.96100	62.57200	6.83200
C	12.59700	63.50500	5.88400
C	12.63500	62.96300	4.46500
O	12.67400	61.74900	4.28800
C	14.03100	63.65000	6.42400
C	13.92000	63.36500	7.86900
C	12.79100	62.36600	8.03500
H	12.06400	64.45600	5.92500
H	14.70000	62.91500	5.97300
H	14.45000	64.63700	6.22500
H	14.85700	63.01300	8.30400
H	13.65500	64.28600	8.38900
H	12.27900	62.51000	8.98200
H	13.20500	61.36400	7.99900
N	12.66300	63.86100	3.48000
C	12.49400	63.50600	2.07400
C	13.53900	62.56000	1.48800
O	13.29000	61.90800	0.47300
C	12.40000	64.76100	1.20800
C	13.70200	65.60300	1.23400
C	13.51000	67.12300	1.10800

C	14.79700	67.86000	1.51800
N	14.64600	69.32300	1.51000
H	13.85300	69.62100	2.04800
H	15.48300	69.69400	1.94500
H	12.65700	64.84100	3.72000
H	11.53000	63.01400	2.00200
H	12.14900	64.50100	0.17800
H	11.56100	65.35900	1.56600
H	14.23100	65.42200	2.17000
H	14.38100	65.25100	0.45600
H	13.21900	67.38100	0.08900
H	12.69400	67.44100	1.75900
H	15.08000	67.55900	2.52700
H	15.62600	67.58300	0.86500
H	14.57600	69.68200	0.57400
N	14.70100	62.46400	2.10700
C	15.77200	61.70700	1.47700
C	15.80100	60.19800	1.65900
O	14.84000	59.48000	1.36600
H	14.84700	62.89100	3.01000
H	15.81200	61.91100	0.40500
H	16.70100	62.13200	1.85900
N	16.94200	59.72500	2.14800
C	17.18500	58.31600	2.39100
C	16.17500	57.71300	3.37500
O	15.84800	56.53400	3.28500
N	19.04000	54.29800	2.79800
C	18.61800	53.17600	2.19400
N	18.22300	53.18100	0.91200
N	18.59700	52.02700	2.87900
C	18.61700	58.11300	2.90300
C	19.02300	56.69500	3.36300
C	19.06900	55.65300	2.23600
H	18.77800	58.78200	3.75000
H	20.01800	56.75900	3.80600
H	18.37800	56.35200	4.17100
H	18.20400	55.77200	1.59100
H	19.95300	55.78600	1.61100
H	19.43800	54.25300	3.72600
H	17.92800	52.34100	0.43500
H	18.28300	54.00500	0.32600
H	18.31200	51.15900	2.44800
H	18.89500	51.95600	3.83800
H	17.63700	60.38900	2.45700

H	17.05500	57.78200	1.45700
H	19.31800	58.44100	2.13400
N	15.67200	58.52200	4.30600
C	14.73100	58.01900	5.30700
C	13.50300	57.40400	4.65600
O	12.94500	56.44500	5.16500
C	14.31600	59.12700	6.27700
S	15.62100	59.60300	7.43700
H	13.50800	58.73800	6.89100
H	14.86300	60.40900	8.18600
H	15.95300	59.50100	4.32100
H	15.22500	57.23100	5.87900
H	13.93600	60.00400	5.75400
N	13.10100	57.95000	3.51400
C	11.92200	57.45600	2.81300
C	12.23800	56.21000	1.99500
O	11.36500	55.37000	1.77400
N	7.76600	63.39600	3.10900
C	11.30200	58.56400	1.94900
C	10.74300	59.71100	2.78200
C	10.00800	60.73800	1.94100
N	9.31100	61.72600	2.76200
C	8.36000	62.53100	2.30000
N	7.99800	62.46700	1.02400
H	13.63300	58.71200	3.11000
H	11.16300	57.16100	3.54200
H	12.04200	58.94800	1.24500
H	10.50900	58.15000	1.34100
H	10.07200	59.28600	3.52000
H	11.57000	60.13200	3.30300
H	10.67100	61.21900	1.23000
H	9.25700	60.21200	1.35100
H	9.54600	61.72300	3.75500
H	7.24100	63.02400	0.66100
H	8.53000	61.99700	0.27000
H	7.06000	64.04300	2.78900
H	8.01900	63.44500	4.08600
N	13.49200	56.08500	1.56500
C	13.95500	54.86600	0.91600
C	13.87800	53.67900	1.86700
O	13.41500	52.61500	1.47500
C	15.39300	55.00900	0.40600
C	15.58000	55.99100	-0.73700
C	17.05100	56.19200	-1.08400

O	17.70500	55.12300	-1.53500
N	17.59300	57.29100	-0.94200
H	16.06200	55.24900	1.22700
H	15.72300	54.03100	0.05000
H	15.05300	55.64000	-1.62500
H	15.13600	56.95300	-0.47800
H	18.55900	57.41600	-1.20800
H	17.05400	58.09900	-0.66800
H	14.17200	56.77300	1.86000
H	13.30500	54.65700	0.06300
N	14.34400	53.84500	3.10600
C	14.34900	52.70900	4.03200
C	12.96000	52.38900	4.57700
O	12.64700	51.22800	4.77500
C	15.44400	52.78500	5.16200
C	16.20600	54.07500	5.09800
C	14.85400	52.53300	6.55500
H	14.76000	54.72800	3.38300
H	14.63400	51.82300	3.45800
H	16.16400	51.98700	4.97500
H	16.99500	54.09500	5.85000
H	16.69400	54.21400	4.13500
H	15.55900	54.92800	5.29800
H	15.64900	52.60700	7.29700
H	14.09500	53.26900	6.82000
H	14.44500	51.53500	6.67000
N	12.12300	53.40700	4.78400
C	10.71900	53.15300	5.08900
C	10.11200	52.28100	3.98300
O	9.44800	51.27200	4.25100
C	9.90600	54.45100	5.22100
C	8.41000	54.12800	5.30600
C	10.36400	55.23900	6.43500
H	12.44800	54.36200	4.69000
H	10.66500	52.59800	6.02900
H	10.07000	55.07000	4.33800
H	7.84900	55.00300	5.62400
H	7.97700	53.82100	4.35300
H	8.21100	53.35000	6.04300
H	9.92200	56.23200	6.44200
H	10.02300	54.74700	7.34700
H	11.43900	55.31900	6.54100
N	10.36900	52.66600	2.73700
C	9.91300	51.89300	1.58900

C	10.47900	50.47800	1.65000
O	9.74700	49.50000	1.50600
C	10.29800	52.58000	0.26400
O	9.67300	53.86800	0.20700
C	9.84400	51.75100	-0.94100
H	10.91900	53.50000	2.57700
H	8.82400	51.81700	1.64400
H	11.37100	52.73000	0.18300
H	10.14800	54.44400	0.80800
H	9.96600	52.31500	-1.86600
H	10.43500	50.84300	-1.05900
H	8.79300	51.46700	-0.86600
N	11.77900	50.37400	1.89600
C	12.41300	49.07800	2.05600
C	11.83000	48.27900	3.21400
O	11.66900	47.05300	3.13600
H	12.35100	51.21300	1.95800
H	12.32500	48.50500	1.13100
H	13.47800	49.22700	2.23600
N	11.52200	48.96600	4.30500
C	10.96100	48.28600	5.45600
C	9.58700	47.73200	5.12000
O	9.25200	46.61900	5.51500
C	10.89900	49.22400	6.65600
C	12.27400	49.56400	7.18400
S	12.23000	50.56100	8.68000
C	11.51100	49.32700	9.75900
H	10.30800	48.74000	7.43000
H	12.71400	48.61500	7.49000
H	13.00400	49.91700	6.48800
H	11.57800	49.65100	10.79700
H	10.45400	49.20100	9.53600
H	12.01700	48.36600	9.67100
H	11.77300	49.95400	4.38200
H	11.60300	47.44600	5.72500
H	10.36400	50.13800	6.40300
N	8.81000	48.51300	4.37900
C	7.47600	48.12200	3.97200
C	7.59900	46.84600	3.16900
O	6.94700	45.84400	3.47800
C	6.79300	49.23300	3.15400
H	9.14700	49.44300	4.13900
H	6.88200	47.92400	4.86600
H	5.76700	48.95400	2.91500

H	6.75300	50.16400	3.71900
H	7.30200	49.43600	2.21300
N	8.47800	46.87200	2.17100
C	8.72300	45.69400	1.34500
C	9.14100	44.50400	2.17900
O	8.53000	43.42900	2.09000
C	7.88900	44.71600	-2.14400
C	7.05400	46.78800	-3.89100
C	7.08600	44.45300	-3.24800
C	6.67700	45.48500	-4.10600
C	9.74800	45.98800	0.25100
C	9.10100	46.65900	-0.90600
C	9.11400	47.99300	-1.20000
C	8.28800	46.03600	-1.90300
N	8.37600	48.23500	-2.32900
C	7.86100	47.05100	-2.78500
H	8.99000	47.73100	1.99200
H	7.77600	45.41700	0.87500
H	10.56200	46.60500	0.63300
H	10.20700	45.07000	-0.12000
H	9.66400	48.73300	-0.65200
H	8.25500	49.15400	-2.74800
H	8.20400	43.91800	-1.48700
H	6.73400	47.57700	-4.55700
H	6.77200	43.43800	-3.44700
H	6.05200	45.25000	-4.95600
N	10.17300	44.70400	2.99500
C	10.64200	43.67400	3.90900
C	9.48400	43.11200	4.72300
O	9.30400	41.92200	4.82700
C	11.68000	44.24800	4.86200
C	13.11900	43.89300	4.53900
C	14.05200	44.45600	5.59900
C	13.25600	42.38000	4.42200
H	14.30400	42.08600	4.48200
H	12.73600	41.87100	5.23300
H	12.89900	41.98100	3.47400
H	10.61800	45.62100	3.02800
H	11.01600	42.86200	3.29100
H	11.56700	45.32400	4.95700
H	11.50700	43.87500	5.87500
H	13.38100	44.34800	3.58200
H	15.09400	44.41500	5.28200
H	13.81400	45.48800	5.84200



H	13.94900	43.86800	6.50400
N	8.69900	44.00500	5.28600
C	7.59800	43.64100	6.13900
C	6.50800	42.84000	5.41300
O	6.11700	41.75300	5.86300
C	3.76200	44.29400	9.41900
C	7.01300	44.93000	6.73700
C	5.87800	44.70300	7.66800
C	6.10700	44.53000	9.02900
C	4.57700	44.67600	7.19200
C	5.06400	44.34200	9.90200
C	3.52200	44.47300	8.06100
H	8.90700	45.00000	5.18000
H	7.98400	43.03000	6.95800
H	7.81600	45.41100	7.28500
H	6.69800	45.63200	5.96700
H	7.11700	44.53700	9.41500
H	4.38000	44.82200	6.14100
H	5.25900	44.20100	10.95500
H	2.51100	44.44300	7.68200
H	2.93900	44.12000	10.09600
N	5.99300	43.36700	4.30300
C	4.82100	42.72600	3.69100
C	5.15400	41.40900	2.99000
O	4.32900	40.49300	2.93300
C	2.10200	46.87400	4.89800
C	4.05300	43.68300	2.77800
C	3.36700	44.80300	3.51900
C	3.80200	46.13000	3.38300
C	2.29700	44.53600	4.35700
C	3.17000	47.15900	4.06300
C	1.66300	45.55500	5.04200
H	6.32600	44.27100	3.96600
H	4.12900	42.45200	4.49200
H	4.72200	44.09000	2.01800
H	3.28300	43.13500	2.23200
H	4.62700	46.36500	2.72800
H	1.95300	43.52100	4.49100
H	3.52200	48.17600	3.96000
H	0.84600	45.32600	5.70600
H	1.63400	47.64100	5.47700
N	6.37400	41.30400	2.48200
C	6.79800	40.07900	1.82300
C	7.04300	39.01000	2.88300

O	6.43900	37.93400	2.86000
C	8.06700	40.32600	0.98300
C	8.69900	39.01400	0.54700
C	7.72600	41.19800	-0.21900
H	7.02600	42.08000	2.56000
H	6.00800	39.71800	1.15900
H	8.80700	40.85400	1.58700
H	9.49200	39.19400	-0.18000
H	9.17000	38.47100	1.36800
H	7.97200	38.35300	0.07300
H	8.61900	41.42900	-0.80100
H	7.01800	40.70300	-0.88400
H	7.28500	42.14900	0.07900
N	7.91800	39.34300	3.82500
C	8.23100	38.49300	4.95900
C	6.97100	38.06200	5.72400
O	6.75200	36.88500	5.95500
C	9.16000	39.25800	5.91100
O	10.03600	38.39000	6.59700
H	8.66300	39.96500	6.57500
H	9.54400	37.81000	7.16600
H	8.32700	40.27000	3.81500
H	8.74000	37.60900	4.56700
H	9.89300	39.78900	5.31500
N	6.14700	39.02500	6.12300
C	4.99200	38.70900	6.95100
C	3.95600	37.94500	6.14900
O	3.29800	37.04200	6.67400
C	3.25300	40.65900	10.55400
C	5.37600	41.64500	12.14900
C	3.05100	41.02600	11.87500
C	4.11000	41.51300	12.66000
C	4.37300	39.98000	7.53400
C	5.10000	40.51000	8.72000
C	6.42700	40.84500	8.79900
C	4.53800	40.78400	10.00900
N	6.72000	41.29100	10.06000
C	5.57900	41.27700	10.82000
H	6.32900	40.00900	5.92500
H	5.34200	38.16500	7.81600
H	4.16400	40.75300	6.79800
H	3.39600	39.69900	7.92100
H	7.12900	40.78400	7.98500
H	7.61300	41.75800	10.28200

H	2.43000	40.29700	9.95900
H	6.18600	41.98500	12.77000
H	2.06700	40.93000	12.31000
H	3.92600	41.74400	13.69600
N	3.82200	38.30800	4.87200
C	2.91100	37.61700	3.97800
C	3.33200	36.17600	3.73900
O	2.50300	35.32900	3.45500
H	4.39400	39.05300	4.49200
H	1.89700	37.64000	4.38200
H	2.88600	38.14100	3.02300
N	4.62500	35.89100	3.85100
C	5.10500	34.53300	3.60900
C	4.67400	33.55900	4.70400
O	4.57200	32.36600	4.45900
C	6.62800	34.50900	3.41700
C	7.09200	34.91500	2.01200
S	6.36500	33.89200	0.69900
C	6.81700	32.25000	1.27200
H	7.01600	33.51600	3.64100
H	6.82900	35.93500	1.76800
H	8.17900	34.85200	1.95100
H	6.58700	31.51100	0.50400
H	7.88400	32.19300	1.49100
H	6.26100	31.97300	2.16700
H	5.29000	36.62600	4.06700
H	4.62700	34.16300	2.70300
H	7.08000	35.17400	4.14900
N	4.38800	34.06100	5.90100
C	4.01100	33.16900	7.00800
C	2.72200	32.40000	6.75200
O	2.69400	31.17300	6.91100
C	7.76900	35.15800	9.77700
C	3.94100	33.91800	8.35400
C	5.27400	34.35800	8.85800
C	6.08400	33.48300	9.55700
C	5.72900	35.64300	8.62200
C	7.31500	33.87500	10.02400
C	6.96800	36.04300	9.08000
H	4.46400	35.05700	6.06900
H	4.80200	32.42100	7.10400
H	3.27500	34.77800	8.29000
H	3.50600	33.26800	9.11600
H	5.74300	32.47000	9.68900

H	5.07400	36.27400	8.07400
H	7.94200	33.17700	10.54900
H	7.31200	37.05000	8.89800
H	8.74000	35.46700	10.14000
N	1.63700	33.10800	6.37100
C	0.47100	32.29400	6.01200
C	0.75000	31.37000	4.82900
O	0.16600	30.28900	4.77900
C	-0.59900	33.33700	5.65200
C	0.15100	34.60700	5.40700
C	1.32500	34.54600	6.33500
H	0.09900	31.67500	6.82200
H	-1.22800	33.05200	4.80600
H	-1.26000	33.47800	6.50200
H	0.45100	34.61000	4.36400
H	-0.46000	35.49600	5.56700
H	1.07100	34.89200	7.33600
H	2.13800	35.13900	5.95800
N	1.62900	31.77200	3.91100
C	1.94700	30.92200	2.75900
C	2.63100	29.64800	3.26200
O	2.24500	28.52600	2.91400
C	2.89200	31.62900	1.74000
C	2.32500	32.97200	1.28300
C	3.13300	30.74900	0.53200
C	0.98600	32.86800	0.62200
H	0.64200	33.86000	0.32700
H	1.01300	32.26500	-0.28500
H	0.22000	32.46100	1.28200
H	2.10100	32.66000	4.01000
H	1.01800	30.62700	2.26900
H	3.86300	31.82300	2.18800
H	2.18600	33.57900	2.14900
H	3.03400	33.49300	0.63800
H	3.65200	31.29400	-0.25700
H	3.76400	29.89500	0.77800
H	2.20700	30.35400	0.11300
N	3.65300	29.84500	4.08900
C	4.38200	28.76100	4.72200
C	3.46400	27.84200	5.52300
O	3.60700	26.62300	5.47800
C	5.47400	29.34300	5.61900
C	6.61000	29.97300	4.80600
C	7.86000	30.13000	5.64400

C	6.90300	29.13300	3.57000
H	7.84000	29.45200	3.11100
H	7.01700	28.07500	3.80700
H	6.15100	29.25700	2.79100
H	3.93500	30.80200	4.30800
H	4.75600	28.09600	3.94700
H	5.07100	30.05500	6.34000
H	5.89100	28.52700	6.21100
H	6.36000	30.96300	4.45800
H	8.62600	30.69500	5.11300
H	7.64600	30.64900	6.57700
H	8.27400	29.15800	5.91500
N	2.51900	28.42600	6.25700
C	1.55900	27.63400	7.03200
C	0.75700	26.75500	6.07500
O	0.64000	25.53900	6.27700
C	-2.00100	26.64800	10.60000
C	0.63300	28.56800	7.81400
C	-0.27700	27.87900	8.78400
C	-0.14400	28.10800	10.14100
C	-1.30000	27.03500	8.34200
C	-1.00000	27.49200	11.05000
C	-2.15300	26.42000	9.24000
H	2.48400	29.44000	6.31500
H	2.14900	27.03600	7.67700
H	1.23900	29.28700	8.36300
H	0.02300	29.16100	7.13600
H	0.66100	28.71900	10.51800
H	-1.49100	26.87200	7.29400
H	-0.82600	27.65800	12.09700
H	-2.93400	25.76300	8.88400
H	-2.65400	26.14900	11.28900
N	0.21100	27.37700	5.03300
C	-0.49500	26.64800	3.98400
C	0.36800	25.52200	3.37900
O	-0.11600	24.42000	3.15500
C	-0.99200	27.60700	2.88700
C	-2.17600	28.43100	3.39900
C	-1.40600	26.83900	1.64900
C	-2.54900	29.63200	2.48500
H	-3.38000	30.19600	2.90600
H	-1.70700	30.31700	2.37700
H	-2.86200	29.32200	1.49000
H	0.34400	28.38000	4.92200

H	-1.35900	26.16600	4.44700
H	-0.19400	28.29000	2.60500
H	-3.04900	27.79100	3.53600
H	-1.94900	28.82200	4.38900
H	-1.86400	27.48500	0.90400
H	-0.57300	26.37300	1.12200
H	-2.13800	26.07600	1.89700
N	1.65400	25.79300	3.16600
C	2.56100	24.80500	2.58500
C	3.05100	23.74600	3.58800
O	3.40100	22.63700	3.19700
C	3.77800	25.50400	1.97500
C	3.52000	26.45400	0.81500
C	4.82200	27.14600	0.39800
C	2.90000	25.68100	-0.33800
H	2.81000	26.31400	-1.22100
H	3.50300	24.81900	-0.61900
H	1.89300	25.33300	-0.11000
H	1.99100	26.73800	3.33700
H	2.02900	24.26700	1.80400
H	4.29800	26.04600	2.76600
H	4.48300	24.74500	1.63800
H	2.80300	27.21900	1.08200
H	4.65600	27.83000	-0.43500
H	5.23600	27.72900	1.22100
H	5.57900	26.42400	0.08900
N	3.08900	24.10100	4.87200
C	3.69800	23.24800	5.88200
C	2.88100	22.04500	6.32800
O	1.80200	21.79400	5.80600
H	2.84200	25.05300	5.13900
H	4.67800	22.92400	5.54400
H	3.86000	23.87200	6.73800
N	3.40700	21.28600	7.29900
C	2.66900	20.19800	7.95000
C	1.31600	20.67000	8.49800
O	0.34900	19.91300	8.45800
C	3.59400	19.79200	9.10100
C	4.97000	20.16700	8.62300
C	4.79200	21.40200	7.79800
H	2.53800	19.38000	7.23900
H	3.37300	20.35400	10.01200
H	3.51100	18.73200	9.34400
H	5.66200	20.33900	9.44700

H	5.37800	19.36700	8.00300
H	5.53000	21.43800	7.00100
H	4.95700	22.28500	8.40800
N	1.25300	21.90100	9.00000
C	-0.01700	22.50300	9.43200
C	-0.98500	22.72500	8.27200
O	-2.13700	23.05400	8.48900
C	0.19900	23.87000	10.08900
C	1.58900	24.15100	10.62500
C	2.57100	24.57100	9.55200
O	2.74200	25.78600	9.32000
O	3.18900	23.67900	8.95200
H	-0.47800	21.83400	10.16000
H	-0.02600	24.68500	9.39800
H	-0.52400	23.98500	10.89000
H	1.50400	24.96000	11.34400
H	1.95500	23.28400	11.17300
H	2.08800	22.50900	8.96900
N	-0.51000	22.59400	7.04100
C	-1.34300	22.88700	5.89500
C	-1.55900	21.70300	4.98700
O	-2.25600	20.75800	5.34200
H	0.46100	22.34400	6.88000
H	-2.32400	23.29600	6.13800
H	-0.84600	23.68500	5.35700
N	-0.95000	21.75600	3.80900
C	-1.06900	20.68300	2.83400
C	0.23500	19.89700	2.71000
O	0.45600	19.17000	1.73200
C	-5.28800	23.29200	1.67600
C	-1.50700	21.25100	1.48900
C	-2.82700	21.96300	1.54800
C	-4.01200	21.24500	1.66700
C	-2.88900	23.35100	1.50300
C	-5.23800	21.89800	1.72900
C	-4.11400	24.01500	1.56200
H	-0.45000	22.60400	3.54900
H	-1.82000	19.94700	3.12400
H	-0.74200	21.92600	1.10100
H	-1.59500	20.45100	0.75200
H	-3.98800	20.16500	1.71000
H	-1.97600	23.92000	1.40800
H	-6.15200	21.32700	1.81900
H	-4.15400	25.09400	1.51700

H	-6.23900	23.80400	1.72300
N	1.08900	20.05600	3.71900
C	2.30400	19.27600	3.85100
C	3.15500	19.14300	2.60600
O	3.71200	18.07300	2.35200
H	0.89000	20.74000	4.44400
H	2.92900	19.71100	4.62900
H	2.03400	18.28000	4.20400
N	3.26300	20.20900	1.81900
C	4.18500	20.16700	0.68800
C	5.59700	20.35200	1.22100
O	6.55400	19.81200	0.67600
C	3.84200	21.19100	-0.42500
C	2.49400	21.83100	-0.16900
C	4.93900	22.24200	-0.56900
H	2.88200	21.09800	2.12500
H	4.13900	19.18300	0.21400
H	3.78200	20.65200	-1.37200
H	2.22800	22.50000	-0.98800
H	1.69700	21.08900	-0.10500
H	2.48300	22.42900	0.73700
H	4.66100	22.94000	-1.35900
H	5.07200	22.85000	0.32500
H	5.90000	21.84100	-0.89400
N	5.70800	21.10900	2.30800
C	6.96100	21.24600	3.02900
C	6.95300	20.28900	4.21800
O	5.96500	20.16100	4.93200
C	7.16000	22.68300	3.52500
C	7.36000	23.83600	2.53000
C	7.38000	25.17400	3.26900
C	8.63700	23.66000	1.69600
H	8.77400	24.49700	1.01000
H	9.52400	23.60300	2.32800
H	8.59800	22.75500	1.08900
H	4.86900	21.51500	2.71300
H	7.81300	21.00000	2.39300
H	6.31100	22.93600	4.15400
H	8.01400	22.69000	4.20500
H	6.51500	23.84400	1.84500
H	7.42800	26.00500	2.56500
H	6.48200	25.31400	3.87300
H	8.24400	25.25300	3.92900
N	8.07100	19.61200	4.40500



C	8.34500	18.84400	5.59800
C	8.56000	19.82700	6.74800
O	8.63100	21.03900	6.52300
C	9.65000	18.10500	5.36200
O	10.68200	19.07000	5.22800
H	9.59500	17.52000	4.44300
H	11.44700	18.66100	4.77800
H	8.87700	19.80200	3.82700
H	7.53100	18.15000	5.81700
H	9.84600	17.38800	6.14900
N	8.69800	19.34000	7.97700
C	8.93800	20.29100	9.06000
C	10.30000	20.96800	8.94300
O	10.43600	22.12500	9.28500
C	8.70000	19.70700	10.47800
C	7.89100	18.42800	10.40500
C	10.00200	19.54400	11.25300
H	8.72100	18.34100	8.15100
H	8.18400	21.07600	8.96300
H	8.10200	20.42800	11.03800
H	7.71200	18.02300	11.40100
H	6.91600	18.58300	9.94800
H	8.39200	17.66500	9.83200
H	9.82700	18.96500	12.16000
H	10.75700	19.01900	10.68100
H	10.41600	20.50000	11.57700
N	11.29600	20.25000	8.43300
C	12.58800	20.85800	8.15900
C	12.41700	21.92000	7.07900
O	12.93000	23.02600	7.20500
C	13.60700	19.80700	7.71400
C	14.01600	18.84500	8.80400
C	14.30800	17.51200	8.51200
C	14.12600	19.26800	10.12200
C	14.68500	16.62400	9.50700
C	14.50700	18.39400	11.11800
C	14.78100	17.07100	10.81200
O	15.15400	16.20700	11.81800
H	11.13400	19.27500	8.18800
H	12.93200	21.39300	9.04100
H	13.22900	19.25100	6.85400
H	14.51400	20.31400	7.39000
H	14.27800	17.19600	7.48700
H	13.97100	20.29300	10.41500

H	14.91200	15.60000	9.24500
H	14.71200	18.70900	12.10400
H	15.37600	15.33900	11.50300
N	11.69000	21.57100	6.02400
C	11.40200	22.49900	4.94900
C	10.72700	23.74200	5.49100
O	11.07400	24.86200	5.12100
H	11.28500	20.63400	5.96000
H	12.32500	22.76300	4.43000
H	10.74700	22.01500	4.22400
N	9.76300	23.54200	6.38700
C	9.04700	24.64700	7.01000
C	10.01100	25.49600	7.83200
O	9.97900	26.72500	7.78700
C	7.95200	24.09700	7.91500
O	7.33700	25.11800	8.67000
H	8.35100	23.37100	8.61700
H	6.51300	25.37500	8.22400
H	9.48500	22.58600	6.61000
H	8.59700	25.27200	6.23800
H	7.18800	23.58200	7.33100
N	10.86600	24.81500	8.58900
C	11.88200	25.46700	9.39300
C	12.79600	26.33900	8.52300
O	13.01600	27.51100	8.82900
C	12.70100	24.42800	10.15900
O	11.86100	23.80700	11.13300
C	13.91100	25.08100	10.85500
H	10.79300	23.80300	8.66200
H	11.37800	26.12300	10.10600
H	13.08700	23.65100	9.50900
H	12.41100	23.28900	11.71200
H	14.40900	24.36400	11.50800
H	14.67000	25.43900	10.15900
H	13.60800	25.92500	11.47700
N	13.30200	25.76300	7.43500
C	14.09100	26.50200	6.45000
C	13.38700	27.77200	5.98300
O	13.95400	28.86700	6.03100
C	14.40500	25.62300	5.21600
C	14.95600	26.46900	4.05500
C	15.37500	24.51700	5.59800
H	13.08300	24.78400	7.24800
H	15.02700	26.80100	6.92700

H	13.49600	25.14400	4.86000
H	15.38100	25.82600	3.28300
H	14.18700	27.05800	3.55400
H	15.74400	27.14500	4.37500
H	15.51500	23.81600	4.77500
H	16.34900	24.93600	5.84200
H	15.04800	23.93900	6.45500
N	12.14600	27.61500	5.53800
C	11.35800	28.74100	5.08500
C	11.17100	29.79400	6.15400
O	11.33800	30.98600	5.90300
H	11.73500	26.68500	5.52700
H	11.82500	29.18600	4.20500
H	10.37900	28.37800	4.77000
N	10.80800	29.35300	7.35100
C	10.52700	30.27700	8.43700
C	11.78400	31.01900	8.86400
O	11.72900	32.17400	9.25400
C	9.90500	29.53800	9.62100
C	8.44200	29.26800	9.44400
N	7.96200	28.11100	8.86000
C	7.35200	30.01700	9.74100
C	6.64400	28.15500	8.82300
N	6.24600	29.29700	9.35800
H	9.79000	31.00300	8.10100
H	10.44300	28.61800	9.85200
H	9.98500	30.16100	10.51500
H	8.52700	27.32200	8.54100
H	7.33600	31.00600	10.16200
H	5.97800	27.40300	8.52100
H	10.62900	28.36000	7.49800
N	12.92100	30.34600	8.76900
C	14.17300	30.94400	9.17900
C	14.55200	32.06000	8.20800
O	15.06700	33.09100	8.60800
C	15.28600	29.88700	9.27100
O	14.83100	28.79400	10.07300
C	16.48700	30.46200	9.92800
H	12.90400	29.38400	8.44700
H	14.02800	31.37500	10.17200
H	15.54600	29.50300	8.28200
H	14.11400	28.34600	9.61100
H	17.20000	29.68100	10.18000
H	16.98200	31.18300	9.27800

H	16.22700	30.96400	10.86100
N	14.27000	31.85700	6.93200
C	14.49700	32.89700	5.94500
C	13.61400	34.10200	6.22300
O	14.08600	35.24400	6.25000
C	14.25300	32.38500	4.51100
C	15.36300	31.40300	4.11700
C	14.20900	33.55500	3.53300
C	14.94700	30.32700	3.12100
H	15.77100	29.64000	2.92600
H	14.11100	29.73800	3.49700
H	14.64500	30.76300	2.16900
H	13.82700	30.99100	6.64300
H	15.53600	33.22800	6.02000
H	13.29200	31.87100	4.47200
H	16.23300	31.94400	3.74100
H	15.72400	30.87500	5.00000
H	14.23800	33.19500	2.50500
H	13.29300	34.14300	3.60800
H	15.06100	34.22500	3.66000
N	12.32900	33.87300	6.44200
C	11.46900	35.02500	6.65100
C	11.56300	35.59600	8.10900
O	11.26600	36.77900	8.30600
C	10.02300	34.76500	6.21500
C	9.35000	33.74600	7.12700
C	9.99600	34.28600	4.76800
C	7.93200	33.45600	6.69700
H	7.45600	32.77900	7.40200
H	7.33200	34.36300	6.65000
H	7.88000	32.96400	5.72900
H	11.94000	32.93600	6.41100
H	11.78400	35.83000	5.98300
H	9.47100	35.70400	6.28100
H	9.91800	32.82400	7.08700
H	9.37900	34.06400	8.16300
H	9.00400	34.27600	4.34900
H	10.58600	34.94600	4.13100
H	10.40300	33.28000	4.65900
N	12.06500	34.84300	9.11800
C	12.49600	35.38400	10.41800
C	13.73400	36.26500	10.26300
O	13.79400	37.31700	10.88300
C	13.11000	34.42800	11.45400

C	12.07000	33.41500	11.94900
O	12.56400	32.34200	12.33900
O	10.86200	33.78400	12.01900
H	13.94700	33.85900	11.02500
H	13.49200	34.95800	12.33700
H	12.14100	33.83700	8.95000
H	11.68700	35.97900	10.85100
N	14.63600	35.91400	9.34100
C	15.78400	36.72900	8.96300
C	15.32300	38.06900	8.43100
O	15.79200	39.12500	8.85500
C	16.56000	35.99900	7.87400
C	18.05100	35.74000	8.02000
C	18.53100	36.07500	9.41200
C	18.33400	34.28500	7.66000
H	19.38900	34.04000	7.78700
H	17.75000	33.58500	8.25600
H	18.08900	34.09100	6.61500
H	14.55500	35.00300	8.89600
H	16.30700	36.88900	9.88700
H	16.08800	35.04200	7.69100
H	16.43600	36.48200	6.90200
H	18.59500	36.37900	7.32200
H	19.56200	35.75300	9.52200
H	18.50300	37.15200	9.57600
H	17.96300	35.58300	10.19800
N	14.37400	38.00200	7.50500
C	13.84300	39.17300	6.85000
C	13.02600	40.00500	7.81800
O	13.22500	41.19600	7.92400
C	12.96400	38.76700	5.67900
C	13.66200	38.00300	4.56800
S	12.45600	37.59400	3.28300
C	13.53900	37.07700	1.95000
H	12.41900	39.61900	5.27300
H	14.41900	38.65100	4.12500
H	14.18900	37.11900	4.89600
H	12.95300	36.75900	1.08700
H	14.18700	37.89800	1.64100
H	14.16600	36.24300	2.26500
H	14.04900	37.08300	7.22400
H	14.66900	39.77100	6.46500
H	12.24100	38.06100	6.05700
N	12.10700	39.36800	8.53100

C	11.16200	40.10100	9.36000
C	11.73900	40.54800	10.72100
O	11.29000	41.56200	11.23900
C	9.92300	39.24500	9.65900
O	10.27900	38.02600	10.28600
H	9.30400	39.05800	8.79000
H	10.67900	37.47100	9.60900
H	11.93100	38.37800	8.36700
H	10.81700	40.98000	8.81000
H	9.28400	39.82700	10.32100
N	12.72000	39.87400	11.32800
C	13.27400	40.34300	12.58100
C	14.58800	41.05800	12.30600
O	14.72700	42.23900	12.61600
H	12.66500	41.14000	13.02800
H	13.04300	38.99000	10.93600
H	13.28800	39.56200	13.34200
N	15.54300	40.38000	11.66600
C	16.92700	40.84900	11.68800
C	17.09400	42.00100	10.70600
O	17.53200	43.07900	11.09500
C	17.88000	39.70500	11.38500
C	17.63100	38.51400	12.28400
O	16.76500	37.67700	12.00800
N	18.36600	38.44900	13.39100
H	15.35600	39.44900	11.28800
H	17.19300	41.22100	12.68100
H	17.79400	39.37400	10.35100
H	18.91100	40.04500	11.49300
H	18.23200	37.73100	14.10000
H	19.03900	39.17200	13.58800
N	16.69300	41.77700	9.45600
C	16.86200	42.75900	8.39100
C	15.95400	43.96000	8.59400
O	16.38100	45.10400	8.47300
C	16.60800	42.11200	7.02800
S	17.83700	40.82700	6.63400
H	16.67200	42.86900	6.24600
H	17.47000	39.99300	7.61600
H	16.30500	40.86300	9.22700
H	17.89300	43.11800	8.40800
H	15.60400	41.69900	6.97000
N	14.70100	43.69000	8.92800
C	13.74900	44.74700	9.17500

C	14.18800	45.61100	10.35200
O	14.11900	46.84000	10.29100
C	11.03400	45.69500	12.03500
C	8.98300	47.41100	11.12600
C	10.29300	46.47300	12.91600
C	9.28800	47.32200	12.45500
C	12.38800	44.15100	9.47000
C	11.29700	45.15700	9.50800
C	10.59100	45.64300	8.44400
C	10.75400	45.78100	10.67200
N	9.64400	46.54000	8.87900
C	9.72000	46.63800	10.24300
H	14.38000	42.72900	8.94700
H	13.67900	45.38000	8.28900
H	12.12300	43.43100	8.69600
H	12.40100	43.60600	10.41100
H	10.74800	45.34700	7.41800
H	8.91000	46.98400	8.31300
H	11.80700	45.03600	12.40200
H	8.19900	48.06800	10.77600
H	10.50200	46.40100	13.97400
H	8.72300	47.91100	13.15600
N	14.63700	44.96100	11.42000
C	15.00400	45.66300	12.63800
C	16.24600	46.50000	12.40300
O	16.41700	47.56100	13.00600
H	14.66800	43.95000	11.42300
H	14.17800	46.29100	12.97700
H	15.20300	44.93400	13.42300
N	17.10000	46.00600	11.51100
C	18.31600	46.69600	11.11300
C	17.99500	47.97700	10.37100
O	18.55000	49.03800	10.67100
C	19.16500	45.79600	10.21600
C	20.49300	45.44700	10.86900
C	21.30500	46.71500	11.08600
C	20.21400	44.77800	12.18400
H	21.16400	44.51400	12.64800
H	19.68800	45.37100	12.92900
H	19.66700	43.84800	12.04900
H	16.91000	45.09500	11.10900
H	18.81600	47.02100	12.02200
H	18.64100	44.88800	9.93700
H	19.38500	46.26500	9.25400

H	21.04600	44.76700	10.21900
H	22.31300	46.46300	11.42000
H	21.41400	47.28000	10.16000
H	20.89900	47.39000	11.83800
N	17.10600	47.85700	9.39000
C	16.60100	49.00000	8.65300
C	15.93500	49.95400	9.61600
O	16.13500	51.16100	9.55200
C	15.58100	48.55600	7.60300
C	16.13800	48.01500	6.29300
C	15.04800	48.03500	5.23300
C	17.32900	48.84100	5.84800
H	17.60000	48.59600	4.82000
H	17.12300	49.91200	5.87900
H	18.21900	48.63500	6.44300
H	16.72600	46.93700	9.18300
H	17.43700	49.55100	8.23000
H	14.86900	47.84700	8.02500
H	14.99900	49.43800	7.34600
H	16.46200	46.98400	6.44600
H	15.34700	47.47600	4.34600
H	14.11900	47.60500	5.59900
H	14.81700	49.05400	4.91700
N	15.14500	49.39100	10.51700
C	14.37300	50.18500	11.44300
C	15.30600	50.94600	12.35000
O	15.04200	52.09100	12.71200
H	14.94800	48.39200	10.45200
H	13.75300	50.89100	10.89700
H	13.71900	49.53700	12.02500
N	16.40400	50.29800	12.71500
C	17.37400	50.91700	13.59200
C	18.05500	52.01100	12.78800
O	18.21600	53.13400	13.25700
C	18.40200	49.88500	14.07500
C	19.49200	50.47500	14.91400
N	19.29000	50.87900	16.21900
C	20.78200	50.76500	14.62500
C	20.41600	51.37300	16.70300
N	21.33700	51.31200	15.75800
H	16.87500	51.35900	14.45700
H	17.90900	49.10500	14.65600
H	18.87000	49.38200	13.23000
H	18.41900	50.88600	16.74000



H	21.31900	50.65500	13.69700
H	20.60900	52.12200	17.46100
H	16.52000	49.32200	12.45600
N	18.45200	51.65400	11.57100
C	19.06300	52.58800	10.63500
C	18.16700	53.81500	10.41600
O	18.62400	54.95900	10.49200
C	19.34400	51.87000	9.30900
C	20.02200	52.73100	8.26900
C	19.64800	52.66700	6.92400
C	21.03200	53.61300	8.63100
C	20.27100	53.45200	5.97700
C	21.65900	54.40600	7.69500
C	21.28000	54.32800	6.36800
O	21.92000	55.13600	5.44400
H	18.30100	50.69500	11.26200
H	19.99500	52.91400	11.09800
H	19.98600	51.00700	9.48700
H	18.43000	51.48300	8.87400
H	18.86600	51.98800	6.61500
H	21.36500	53.69600	9.65400
H	19.99900	53.36000	4.94400
H	22.43900	55.08300	8.01300
H	22.60200	55.67400	5.83100
N	16.88100	53.57300	10.17400
C	15.94000	54.66500	9.99600
C	15.98200	55.59700	11.19400
O	15.96500	56.81400	11.04400
C	14.52200	54.13100	9.81900
C	13.45600	55.22100	9.83200
C	13.71400	56.22600	8.70300
C	12.07500	54.58500	9.70700
H	11.29300	55.34400	9.73600
H	11.97200	54.03500	8.77100
H	11.89500	53.88000	10.51700
H	16.55900	52.60900	10.05300
H	16.24000	55.21800	9.10400
H	14.44700	53.54000	8.91800
H	14.30100	53.43500	10.62600
H	13.43500	55.75600	10.78200
H	12.89300	56.93900	8.62900
H	14.61900	56.81400	8.84600
H	13.79300	55.72600	7.73700
N	16.05500	55.02000	12.38800

C	15.97000	55.82900	13.59600
C	17.21600	56.66000	13.80700
O	17.13000	57.82100	14.19200
N	12.82900	51.74200	17.68800
C	15.67400	54.96200	14.81200
C	14.25200	54.47500	14.81100
C	13.96300	53.62700	16.00000
N	12.53400	53.48400	16.22300
C	12.01700	52.57400	17.04000
N	10.70200	52.48300	17.20200
H	16.10900	54.01100	12.45400
H	15.14200	56.53500	13.48400
H	16.36600	54.12100	14.86100
H	15.84000	55.54400	15.72100
H	13.59200	55.33900	14.81000
H	14.03700	53.94800	13.89400
H	14.42700	52.65100	15.85300
H	14.39500	54.06500	16.90100
H	11.92300	54.09600	15.69000
H	10.35700	51.89200	18.00800
H	10.04500	53.10500	16.72100
H	12.40100	51.18900	18.42500
H	13.82600	51.84300	17.65300
N	18.36600	56.05000	13.54700
C	19.63700	56.74500	13.58200
C	19.57100	57.93400	12.61700
O	19.97300	59.05500	12.96400
C	20.78800	55.79400	13.19700
C	22.07900	56.56600	12.87400
C	21.01900	54.76000	14.30400
H	18.34700	55.07700	13.25300
H	19.79600	57.13500	14.58800
H	20.50400	55.25000	12.29600
H	22.93200	55.89000	12.82000
H	22.02700	57.06700	11.90700
H	22.31200	57.32300	13.62000
H	21.53700	53.89100	13.89700
H	21.64400	55.12400	15.11000
H	20.09000	54.38900	14.73700
N	19.03000	57.68500	11.42500
C	18.92800	58.71400	10.39600
C	18.02600	59.84900	10.84300
O	18.34100	61.02400	10.63000
C	18.42000	58.13400	9.07200

C	19.38800	57.31300	8.21500
C	18.64000	56.67900	7.05600
C	20.51600	58.18100	7.70100
H	21.16700	57.61700	7.03200
H	20.14200	59.04100	7.14300
H	21.14800	58.55200	8.50700
H	18.72300	56.74100	11.20300
H	19.92000	59.14200	10.24900
H	17.51600	57.55500	9.24900
H	18.10300	58.96800	8.44800
H	19.81900	56.51600	8.82000
H	19.31300	56.14500	6.39000
H	17.90000	55.96200	7.41200
H	18.11500	57.42700	6.46000
N	16.91400	59.49500	11.47300
C	15.96600	60.49200	11.95300
C	16.59000	61.36000	13.04500
O	16.45600	62.57700	13.03400
C	14.69900	59.83200	12.50200
C	13.99400	59.04600	11.39500
C	13.77000	60.87900	13.10800
C	13.40200	59.89500	10.32100
H	13.04700	59.25500	9.51700
H	12.54900	60.47200	10.68000
H	14.11900	60.58400	9.88500
H	16.67800	58.50800	11.54600
H	15.72500	61.16600	11.13100
H	14.96800	59.12500	13.28800
H	14.67200	58.49900	10.78800
H	13.26200	58.34800	11.79600
H	12.78800	60.46100	13.29600
H	14.12800	61.24700	14.06900
H	13.63800	61.73900	12.45100
N	17.27100	60.70600	13.97800
C	17.93500	61.35500	15.09500
C	18.99900	62.33800	14.58100
O	19.02600	63.50500	14.96400
C	18.57700	60.27600	15.97100
C	19.04500	60.76900	17.30200
N	20.21500	60.59500	17.95800
C	18.25500	61.54100	18.13200
C	20.11400	61.25500	19.15700
N	18.92000	61.82000	19.23400
H	17.17500	61.89800	15.65800

H	17.85700	59.48600	16.18000
H	19.39900	59.79500	15.44700
H	17.24500	61.89900	17.99100
H	20.88600	61.32000	19.91100
H	17.33700	59.69400	13.89700
H	18.58500	62.37400	20.01400
N	19.85400	61.85100	13.69100
C	20.87700	62.67000	13.07500
C	20.23200	63.87700	12.39500
O	20.73100	65.00900	12.48500
C	21.70700	61.83400	12.08700
C	22.74800	60.93500	12.76800
C	23.48400	59.99500	11.80600
O	23.32600	60.13700	10.56800
O	24.22200	59.10700	12.30200
H	21.53700	63.05100	13.85600
H	21.04600	61.23700	11.45800
H	22.23900	62.50200	11.40700
H	23.48400	61.54900	13.28800
H	22.25300	60.31700	13.51500
H	19.78800	60.87100	13.42100
N	19.10800	63.63400	11.73300
C	18.35800	64.71600	11.12200
C	17.86200	65.69100	12.19800
O	18.10400	66.89600	12.12500
C	17.18100	64.15600	10.32800
C	16.40300	65.20500	9.61400
N	16.52700	65.70900	8.36500
C	15.37200	65.89700	10.21300
C	15.56300	66.68100	8.22700
N	14.88100	66.77300	9.35400
H	19.01600	65.25400	10.43600
H	17.53500	63.43900	9.58700
H	16.47400	63.61600	10.94500
H	17.10600	65.34900	7.61300
H	14.96500	65.80400	11.20600
H	15.17200	67.06800	7.30700
H	18.74600	62.68700	11.68500
N	17.17400	65.15000	13.20000
C	16.67900	65.93800	14.33100
C	17.80200	66.75000	15.00300
O	17.61600	67.89200	15.41100
C	15.98300	65.01200	15.36500
C	14.46600	65.04000	15.17700

C	16.33100	65.39900	16.79300
C	14.03300	64.83500	13.77000
H	12.96400	64.63800	13.76000
H	14.18700	65.72500	13.16700
H	14.50700	63.98600	13.29000
H	16.98100	64.14700	13.18900
H	15.98200	66.67600	13.94800
H	16.32300	63.98800	15.22600
H	14.01400	64.26900	15.80200
H	14.06100	65.99000	15.52700
H	15.74900	64.78700	17.48200
H	17.36800	65.19500	17.06100
H	16.07800	66.43300	17.03500
N	18.97400	66.14400	15.10800
C	20.09500	66.77000	15.77000
C	20.56800	67.95500	14.92800
O	20.62200	69.09400	15.39700
C	21.21000	65.73600	15.94900
C	21.58700	65.28300	17.36600
C	20.52200	65.58200	18.41200
C	21.92100	63.81300	17.35400
H	22.22100	63.45500	18.33900
H	21.07800	63.20700	17.01800
H	22.76100	63.65400	16.68300
H	19.03600	65.15800	14.84700
H	19.75400	67.20100	16.70800
H	21.01500	64.87100	15.32100
H	22.13900	66.11200	15.51400
H	22.48400	65.82500	17.67000
H	20.76600	65.09800	19.35900
H	20.44700	66.64600	18.63700
H	19.54200	65.21100	18.11000
N	20.87500	67.68000	13.66700
C	21.38300	68.69400	12.75500
C	20.39300	69.82700	12.43000
O	20.74500	71.00100	12.51500
C	21.86700	68.04400	11.45500
C	23.03700	67.11400	11.75500
C	22.23900	69.10900	10.43100
C	23.48900	66.30700	10.57000
H	24.22800	65.56600	10.87500
H	22.65600	65.76700	10.11800
H	23.95800	66.91900	9.80000
H	20.75200	66.73200	13.31700

H	22.24400	69.16400	13.23600
H	21.05000	67.45200	11.03600
H	23.88100	67.69500	12.13000
H	22.79700	66.41700	12.55600
H	22.66400	68.66900	9.53100
H	21.39100	69.68500	10.06500
H	22.97700	69.80800	10.82600
N	19.16200	69.48600	12.06500
C	18.20700	70.50600	11.63000
C	17.19700	70.90100	12.69900
O	16.42800	71.84100	12.51000
C	17.46000	70.05100	10.37200
C	18.35500	69.49000	9.31300
N	18.57200	68.21500	8.91400
C	19.16600	70.28200	8.52500
C	19.50000	68.25700	7.90100
N	19.84300	69.51700	7.68800
H	18.71800	71.42600	11.34100
H	16.72000	69.28800	10.62400
H	16.89600	70.88700	9.97100
H	18.07400	67.38800	9.23500
H	19.28400	71.35800	8.53100
H	19.86100	67.40300	7.34300
H	18.88300	68.50500	12.03200
N	17.20000	70.19800	13.82200
C	16.15100	70.37700	14.80700
C	14.95900	69.52400	14.42100
O	14.97500	68.83800	13.39300
H	17.80300	69.39000	13.91800
H	16.51500	70.08600	15.79200
H	15.84600	71.42100	14.89900
N	13.92300	69.56100	15.24900
C	12.66800	68.89600	14.93100
C	11.70900	69.93200	14.36600
O	11.11300	70.70700	15.11600
C	12.06600	68.26600	16.18400
C	10.88400	67.36100	15.87600
O	10.85300	66.23100	16.40700
O	9.98400	67.77500	15.11700
H	12.82800	67.66700	16.68300
H	11.76000	69.01700	16.91300
H	13.94800	70.17400	16.05100
H	12.80800	68.09300	14.20200
N	11.56200	69.94600	13.04600

C	10.67700	70.90400	12.40300
C	9.61800	70.19100	11.56700
O	9.94100	69.36700	10.71300
C	11.46200	71.89600	11.52100
C	12.68800	72.41800	12.26900
C	10.56400	73.05000	11.07700
C	13.65700	73.15100	11.38200
H	14.51300	73.50200	11.95700
H	14.03500	72.50600	10.58800
H	13.21400	74.03200	10.91900
H	12.07100	69.28400	12.45000
H	10.14200	71.50600	13.13900
H	11.81400	71.36600	10.63300
H	12.38100	73.05500	13.09900
H	13.28300	71.61700	12.70400
H	11.08600	73.72900	10.40500
H	9.69000	72.70800	10.52300
H	10.20700	73.63100	11.92700
N	8.35400	70.51600	11.82300
C	7.23800	69.85800	11.15900
C	6.49600	70.78100	10.20200
O	6.31500	71.96600	10.48100
N	8.48500	64.46300	14.73600
C	6.25000	69.30800	12.18900
C	6.87900	68.42600	13.24000
C	7.72100	67.34200	12.60500
N	8.27300	66.45900	13.62300
C	7.92600	65.18600	13.77700
N	7.04200	64.63200	12.95900
H	8.14800	71.25400	12.48100
H	7.62900	69.03500	10.66000
H	5.73000	70.12700	12.68900
H	5.48400	68.77700	11.63100
H	7.49900	69.02400	13.90900
H	6.10400	67.98800	13.86900
H	7.17800	66.82500	11.82500
H	8.59500	67.75100	12.11900
H	8.98200	66.92200	14.24700
H	6.79100	63.66200	13.08700
H	6.62900	65.05500	12.11700
H	8.28000	63.47600	14.85800
H	9.20600	64.88200	15.32500
N	6.07500	70.22400	9.07000
C	5.15500	70.90200	8.16900

C	4.00400	69.94500	7.92000
O	4.22000	68.80500	7.50800
C	5.83900	71.28300	6.85300
C	6.88200	72.40200	7.09000
C	7.49300	73.02400	5.82300
C	8.58500	74.05400	6.17400
N	9.29000	74.53200	4.97500
H	8.63800	74.89700	4.30200
H	9.91200	75.28700	5.23300
H	6.29800	69.25100	8.88600
H	4.74000	71.80800	8.61800
H	6.30700	70.41200	6.39000
H	5.08900	71.64100	6.14600
H	6.42300	73.20000	7.67600
H	7.68700	72.00600	7.71200
H	7.90400	72.24300	5.18400
H	6.70600	73.50500	5.24000
H	8.14300	74.90800	6.69000
H	9.31700	73.62200	6.85900
H	9.83400	73.80500	4.54500
N	2.78600	70.40200	8.19100
C	1.61200	69.54100	8.09700
C	1.30900	69.16300	6.65500
O	1.18200	70.03200	5.78800
C	0.36300	70.19300	8.73700
O	0.61100	70.43000	10.12800
C	-0.86400	69.28200	8.59800
H	2.65500	71.33600	8.55000
H	1.83000	68.63000	8.66000
H	0.14800	71.15000	8.25900
H	0.96600	69.64500	10.56000
H	-1.70500	69.66100	9.18000
H	-1.21800	69.19300	7.57000
H	-0.63200	68.28200	8.96300
N	1.20800	67.85900	6.40800
C	0.83500	67.34200	5.09700
C	-0.45700	66.52600	5.19200
O	-0.71400	65.85100	6.19600
C	1.95800	66.48900	4.47200
O	2.26100	65.39200	5.33600
C	3.21800	67.32300	4.26700
H	1.34200	67.17700	7.15100
H	0.63200	68.15700	4.39900
H	1.62700	66.09100	3.51100



H	2.86200	65.70800	6.00700
H	4.00400	66.73500	3.79200
H	3.01900	68.17700	3.62000
H	3.62000	67.71100	5.20200
N	-1.26800	66.60100	4.14100
C	-2.59900	66.00600	4.14500
C	-2.61600	64.62600	3.49200
O	-2.10400	64.44600	2.38700
C	-3.59300	66.93800	3.44500
C	-5.06400	66.48300	3.52600
C	-6.05300	67.57400	3.09200
C	-7.51500	67.13300	3.25400
N	-8.44400	68.19700	2.84200
H	-8.31500	68.43400	1.87400
H	-9.39300	67.89000	2.96600
H	-0.98600	67.12000	3.32300
H	-2.95100	65.89900	5.17400
H	-3.51500	67.92000	3.91300
H	-3.31200	67.07900	2.40000
H	-5.21500	65.59400	2.91200
H	-5.29100	66.18500	4.54900
H	-5.87800	68.47100	3.68800
H	-5.85700	67.84600	2.05400
H	-7.71100	66.24000	2.65800
H	-7.71400	66.87000	4.29200
H	-8.31100	69.02200	3.39900
N	-3.21300	63.65900	4.18600
C	-3.31000	62.29000	3.68900
C	-4.35600	61.57200	4.53800
O	-4.07500	61.22400	5.68700
C	-1.93000	61.57900	3.64800
C	-1.78400	60.11800	3.15500
C	-1.93000	59.10800	4.29100
C	-2.78800	59.81900	2.04200
H	-2.56400	58.88800	1.51800
H	-3.80600	59.72800	2.41700
H	-2.78100	60.60200	1.28200
H	-3.53600	63.81000	5.14300
H	-3.69000	62.34300	2.66600
H	-1.33800	62.14600	2.93000
H	-1.38900	61.78900	4.57700
H	-0.83900	60.16800	2.54700
H	-1.43300	58.64600	3.32700
H	-0.93300	59.75000	4.28300

H	-2.43500	60.04800	4.75500
N	-5.53000	61.37400	3.94600
C	-6.64400	60.70400	4.61100
C	-6.14700	59.38600	5.21900
O	-6.22000	59.17100	6.42600
C	-7.83500	60.53500	3.64700
C	-9.07800	59.84700	4.20800
O	-9.18300	59.78000	5.53400
N	-9.92200	59.34200	3.47800
H	-5.65400	61.69800	2.99800
H	-7.03300	61.34600	5.38400
H	-8.13400	61.51200	3.26600
H	-7.51000	59.96900	2.77400
H	-10.37600	58.62000	4.05200
H	-9.83000	59.26400	2.47600
N	-5.63900	58.51500	4.35200
C	-5.11700	57.20900	4.75400
C	-6.25000	56.41400	5.42300
O	-7.28600	56.14200	4.81400
C	-3.83700	57.34400	5.62700
C	-2.71300	58.07300	4.86200
C	-3.36800	55.97000	6.13800
C	-1.37100	58.29400	5.57900
H	-5.60400	58.76200	3.37600
H	-4.92100	56.64600	3.84000
H	-4.02900	57.83700	6.54400
H	-2.24900	57.05000	4.65400
H	-3.05700	57.45400	3.91700
H	-2.29100	55.83700	6.25100
H	-3.70700	55.93000	7.16800
H	-3.72500	55.15000	5.52400
H	-0.57800	57.53900	5.50700
H	-1.01600	59.16600	6.20700
H	-1.80500	57.96300	6.51200
N	-6.02500	56.05000	6.68200
C	-7.06800	55.36100	7.50000
C	-8.52800	56.09200	7.62700
O	-9.53000	55.39600	7.77900
H	-5.16900	56.35900	7.12200
H	-7.37800	54.41700	7.12600
H	-6.67600	55.20100	8.50400
N	-8.52900	57.41900	7.53900
C	-9.74200	58.21900	7.61400
C	-10.09700	58.85000	6.26700

O	-10.04100	58.17200	5.24300
H	-7.67000	57.89900	7.28400
H	-10.60400	57.65000	7.96600
H	-9.57100	58.99900	8.35700
N	-10.44900	60.13100	6.31200
C	-10.82300	60.91500	5.14700
C	-10.10400	62.26500	5.25200
O	-10.18900	63.07800	4.32800
C	-12.35700	61.04200	5.01900
O	-12.66700	61.79200	3.83900
C	-13.01500	61.72500	6.22500
H	-10.51000	60.57600	7.21000
H	-10.85300	61.08700	4.08400
H	-12.78700	60.04600	4.89800
H	-12.13600	62.58700	3.84900
H	-14.09700	61.77800	6.09600
H	-12.83500	61.16700	7.14400
H	-12.65500	62.74200	6.37900
N	-9.42000	62.46200	6.37600
C	-8.67700	63.67300	6.65900
C	-7.63100	63.40400	7.75000
O	-7.74600	63.87700	8.88000
C	-9.63100	64.81700	7.04100
C	-8.99300	66.19200	7.29700
C	-9.94900	67.32000	7.67500
O	-10.58200	67.88200	6.75300
O	-10.03200	67.59800	8.88900
H	-9.29200	61.67000	6.98900
H	-8.13000	63.97100	5.76100
H	-10.37300	64.95000	6.25300
H	-10.20100	64.53200	7.92600
H	-8.23700	66.14200	8.07900
H	-8.44600	66.49900	6.40700
N	-6.61000	62.63400	7.38200
C	-5.52200	62.27400	8.29000
C	-4.32400	63.17900	7.99900
O	-3.84700	63.25000	6.86500
C	-5.19900	60.75400	8.22700
C	-4.11300	60.37000	9.25300
C	-4.79800	60.33200	6.80200
C	-4.02200	61.18500	10.55300
H	-3.56400	60.55200	11.31400
H	-3.36200	62.03800	10.50700
H	-4.99000	61.46600	10.96500

H	-6.48800	62.37600	6.41600
H	-5.85600	62.48500	9.30400
H	-6.09600	60.23500	8.59900
H	-4.25000	59.32200	9.52800
H	-3.06300	60.45600	8.95200
H	-4.51000	59.42300	7.37700
H	-5.62300	60.93800	6.89700
H	-3.74700	60.12200	7.23200
N	-3.83500	63.86200	9.03200
C	-2.69600	64.76500	8.88100
C	-1.41500	64.19600	9.49600
O	-1.42900	63.62400	10.58700
C	-4.55300	67.03500	7.60600
O	-3.66400	67.69700	7.02900
O	-5.58800	66.59200	7.06400
C	-3.00800	66.14600	9.47000
C	-4.37800	66.76100	9.09900
H	-4.49600	67.70900	9.62600
H	-4.22000	63.72900	9.95400
H	-2.49600	64.94500	7.82400
H	-2.95200	66.09500	10.55800
H	-2.22000	66.83300	9.17300
H	-5.19000	66.12500	9.45300
N	-0.31400	64.36900	8.77200
C	1.00000	63.89300	9.18300
C	1.93200	65.08500	9.40100
O	1.98400	66.00200	8.57300
C	1.59300	62.93800	8.10800
C	3.08500	63.14600	7.93900
C	1.26600	61.47500	8.43100
H	1.72700	61.15600	9.36600
H	0.19000	61.32500	8.52400
H	-0.36900	64.89000	7.90000
H	0.94900	63.35200	10.13000
H	1.14300	63.17000	7.14000
H	3.48500	62.34900	7.31600
H	3.33700	64.06600	7.41400
H	3.63500	63.11700	8.87800
H	1.62000	60.80900	7.64400
N	2.65000	65.08700	10.52200
C	3.63900	66.13400	10.78000
C	4.99700	65.74100	10.19200
O	5.80400	65.08000	10.84800
C	3.77100	66.43500	12.28100

C	2.48100	66.87200	12.98400
C	1.71000	67.94900	12.22800
O	2.27300	69.04000	11.97100
O	0.53200	67.69400	11.88800
H	4.14000	65.54800	12.79800
H	4.52400	67.18600	12.45700
H	1.83200	66.00500	13.11600
H	2.70800	67.23400	13.98800
H	2.59000	64.30800	11.16100
H	3.35200	67.06800	10.29000
N	5.23600	66.16100	8.95300
C	6.44800	65.82300	8.21000
C	7.70400	66.48700	8.77100
O	7.69100	67.67400	9.08000
C	6.31300	66.26000	6.74000
O	5.12900	65.68500	6.17500
C	7.52600	65.83300	5.92400
H	5.28500	64.74400	6.06200
H	7.31700	65.90200	4.85600
H	8.36800	66.49700	6.09800
H	7.84000	64.81000	6.13800
H	4.53300	66.69000	8.45000
H	6.57400	64.74800	8.25200
H	6.21300	67.34500	6.67500
N	8.79000	65.72300	8.88500
C	10.08400	66.29500	9.23100
C	10.68700	67.02700	8.03500
O	10.67300	66.52100	6.91100
C	11.04300	65.22800	9.74900
C	10.75800	64.79300	11.18700
C	11.49100	63.52000	11.52800
C	11.12500	65.90600	12.15500
H	10.91800	65.61000	13.18400
H	12.18600	66.13500	12.08900
H	10.59500	66.83900	11.99200
H	8.73800	64.72500	8.68000
H	9.92500	67.02800	10.01400
H	10.99300	64.37200	9.07800
H	12.07300	65.58800	9.69400
H	9.69000	64.59200	11.29100
H	11.31100	63.23600	12.56200
H	11.14200	62.69000	10.91500
H	12.56700	63.62300	11.38500
N	11.20400	68.22500	8.30000

C	11.77800	69.11400	7.28600
C	13.13400	69.62600	7.81000
O	13.43900	69.46800	8.99400
C	10.78100	70.27300	6.96100
C	11.34100	71.25600	5.95100
C	9.47600	69.70000	6.43000
H	9.64400	69.03700	5.58100
H	8.94200	69.13500	7.19300
H	11.19100	68.56500	9.25800
H	11.99100	68.55800	6.37100
H	10.56100	70.82300	7.87800
H	10.56600	71.92800	5.59100
H	12.10100	71.89300	6.38400
H	11.75500	70.75300	5.07600
H	8.79600	70.47900	6.10500
N	13.94900	70.21100	6.93300
C	15.28500	70.67300	7.28700
C	15.32700	72.16200	7.63600
O	16.19500	72.61000	8.39200
C	16.24400	70.39400	6.13000
C	16.05000	69.01600	5.51300
C	17.14500	68.65000	4.53700
O	17.07900	69.09500	3.37000
O	18.07100	67.91300	4.93900
H	16.10700	71.13800	5.34300
H	17.27300	70.51300	6.47200
H	16.20300	68.33000	6.32100
H	15.06800	68.85000	5.06900
H	13.65000	70.31300	5.97600
H	15.65500	70.11300	8.14700
N	14.39200	72.92700	7.08200
C	14.42700	74.38000	7.21700
C	13.03300	74.97900	7.33400
O	12.03300	74.30600	7.07800
C	15.16600	75.00500	6.02900
C	14.47000	74.86600	4.66600
O	14.40700	73.72600	4.15800
O	13.99800	75.90400	4.15600
H	13.68500	72.52700	6.48300
H	14.94600	74.66600	8.13400
H	15.33600	76.06500	6.22400
H	16.16400	74.57300	5.95000
N	12.97700	76.25000	7.72300
C	11.71200	76.96100	7.85300

C	11.34700	77.64900	6.54400
O	10.50500	77.16000	5.79100
O	9.97300	76.50300	10.54500
O	11.41400	76.09200	12.17500
C	11.78700	77.98400	8.98700
C	12.18100	77.42200	10.37500
C	11.09700	76.60500	11.08200
H	13.83300	76.75500	7.89900
H	10.91100	76.26200	8.10100
H	11.89700	78.56900	6.34600
H	12.51100	78.75700	8.72400
H	10.83300	78.50700	9.07000
H	13.09200	76.82600	10.30900
H	12.42500	78.26200	11.02800
O	4.96300	7.87000	19.43100
H	5.74900	7.33700	19.79300
H	4.94800	7.79900	18.43000
O	-6.62100	39.54700	19.62200
H	-6.09500	40.08800	18.95200
H	-6.03000	39.33300	20.40200
O	5.72700	10.36800	26.62500
H	6.71400	10.53400	26.52700
H	5.31900	11.15200	27.09900
O	-3.19800	19.85500	18.88900
H	-3.78500	20.07600	18.09800
H	-2.60600	20.64100	19.08100
O	12.62000	52.36500	12.63300
H	12.22400	53.29100	12.69700
H	13.62700	52.44700	12.57600
O	0.38700	19.59800	18.01900
H	-0.30400	18.89700	18.24000
H	1.29600	19.25200	18.28700
O	9.14800	42.77100	10.20400
H	9.94700	42.41400	10.70500
H	9.26100	43.76000	10.07800
O	2.67200	3.37900	27.23100
H	2.33900	2.63400	26.64500
H	2.34900	4.25800	26.86000
O	0.37100	21.24400	13.77800
H	0.78700	21.38600	14.68400
H	-0.58900	21.55300	13.82800
O	4.92700	3.47300	25.67300
H	4.09900	3.81400	26.13100
H	5.04500	2.50700	25.92300

O	2.40200	3.44600	29.42900
H	2.57800	3.38200	28.41900
H	1.53800	3.93500	29.56500
O	7.44700	61.25100	14.41900
H	8.17000	60.56100	14.54000
H	6.56800	60.77900	14.32300
O	-1.01000	6.07600	16.34500
H	-1.01300	5.13900	15.98800
H	-1.77200	6.17500	16.99000
O	3.72200	29.94500	9.22300
H	4.71600	29.75300	9.24900
H	3.48200	30.32400	8.32400
O	5.00000	25.73700	7.56900
H	4.53100	26.02100	6.72400
H	4.29300	25.54600	8.26800
O	3.32400	24.02300	13.27000
H	2.95600	24.96100	13.19600
H	3.29300	23.59700	12.36400
O	11.96800	60.89700	-0.97400
H	12.58600	61.35700	-0.30700
H	12.52000	60.29700	-1.55600
O	5.66300	40.25500	22.77700
H	5.02200	39.61400	22.34000
H	6.55300	40.19800	22.30400
O	9.46900	31.99600	13.56300
H	10.05100	32.56200	12.99200
H	9.66600	32.25300	14.50000
O	-0.90700	8.19400	14.19000
H	-1.01700	7.51100	14.92200
H	-1.81000	8.40800	13.81100
O	13.21500	68.40200	11.39700
H	13.46400	68.64300	10.44900
H	14.03300	68.47700	11.98000
O	16.45400	61.35800	4.53000
H	17.12100	62.09900	4.42700
H	16.34000	61.16600	5.50800
O	3.72700	55.90500	10.91800
H	3.60400	55.44700	10.03000
H	2.96600	56.54200	11.06300
O	10.73400	23.72400	17.27700
H	11.17900	22.89000	17.63000
H	9.80700	23.77700	17.65300
O	6.88700	57.32000	14.15700
H	6.36600	56.71100	13.54800



H	6.34200	57.48200	14.98400
O	19.81100	61.83400	8.62900
H	19.19600	61.57500	9.38600
H	20.72700	61.47500	8.81900
O	9.06800	61.71700	-1.22900
H	8.63500	60.92800	-1.67600
H	10.06700	61.57400	-1.23000
O	10.42000	1.15500	28.15500
H	9.77700	1.88400	27.89000
H	10.85100	0.79000	27.32600
O	15.19500	58.77500	16.36100
H	15.89500	58.57000	15.67100
H	14.29500	58.50600	16.00000
O	3.26200	27.76200	10.83100
H	3.03200	26.99400	10.19900
H	3.37700	28.60200	10.28000
O	5.31600	54.87700	12.62100
H	4.68700	55.31700	11.95600
H	5.20300	53.87900	12.55900
O	7.79200	16.08000	7.91000
H	8.15500	15.20600	8.27700
H	6.84600	15.93200	7.61600
O	1.48800	14.65900	12.42300
H	1.20300	14.51300	13.38200
H	1.99800	15.51900	12.36900
O	-9.48000	19.76500	15.19800
H	-10.17000	19.07800	14.96100
H	-9.78900	20.26500	16.01000
O	-7.45500	14.06600	20.28900
H	-7.62800	13.24000	19.74700
H	-8.32300	14.55400	20.41700
O	9.02300	23.09500	11.27800
H	9.60400	22.82100	10.50000
H	9.61800	23.29400	12.05900
O	1.75500	-7.97100	13.01600
H	2.28900	-7.72000	13.83100
H	2.37100	-8.39100	12.34500
O	11.81200	12.13400	5.00400
H	12.79000	11.97700	5.16500
H	11.63200	12.05900	4.02000
O	2.58700	2.87900	33.19200
H	3.23800	3.58700	32.91000
H	2.62300	2.12200	32.52700
O	0.70800	2.24300	34.87600

H	1.45700	2.52400	34.25000
H	0.82100	2.73000	35.74600
O	-0.71900	0.60300	33.74800
H	-0.09700	0.07000	33.15800
H	-0.16700	1.29400	34.25400
O	17.82900	19.95900	18.91400
H	17.76000	20.93600	18.68500
H	18.74400	19.78000	19.28300
O	17.11100	11.71700	4.67100
H	16.83100	10.75600	4.72700
H	18.07100	11.79200	4.96500