

Modeling of the glycinetripeptide cyclization in the Ser65Gly/Tyr66Gly mutant of green fluorescent protein

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Section S1. Computed energy profiles for the chromophore cyclization in the wild-type green fluorescent protein (GFP) and its Ser65Gly/Tyr66Gly mutant.

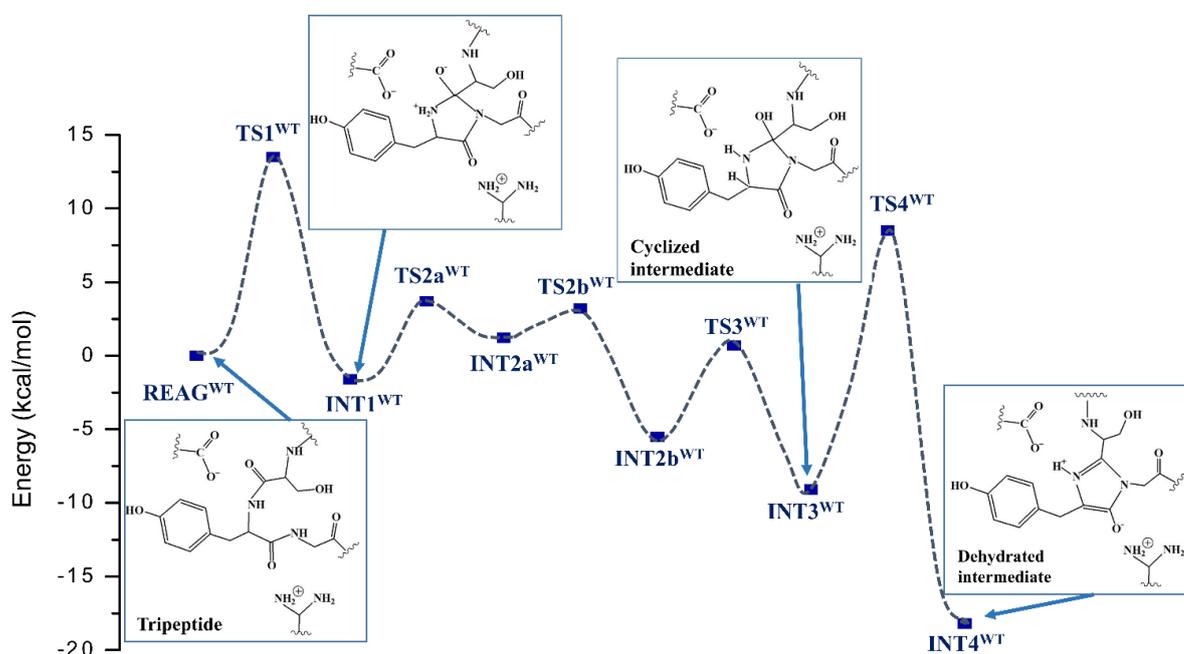


Figure S1 Computed reaction energy profile for the chromophore cyclization and dehydration in the wild-type GFP. Insets illustrate chemical transformations at the elementary steps. This figure is drawn by materials of Ref. 4.

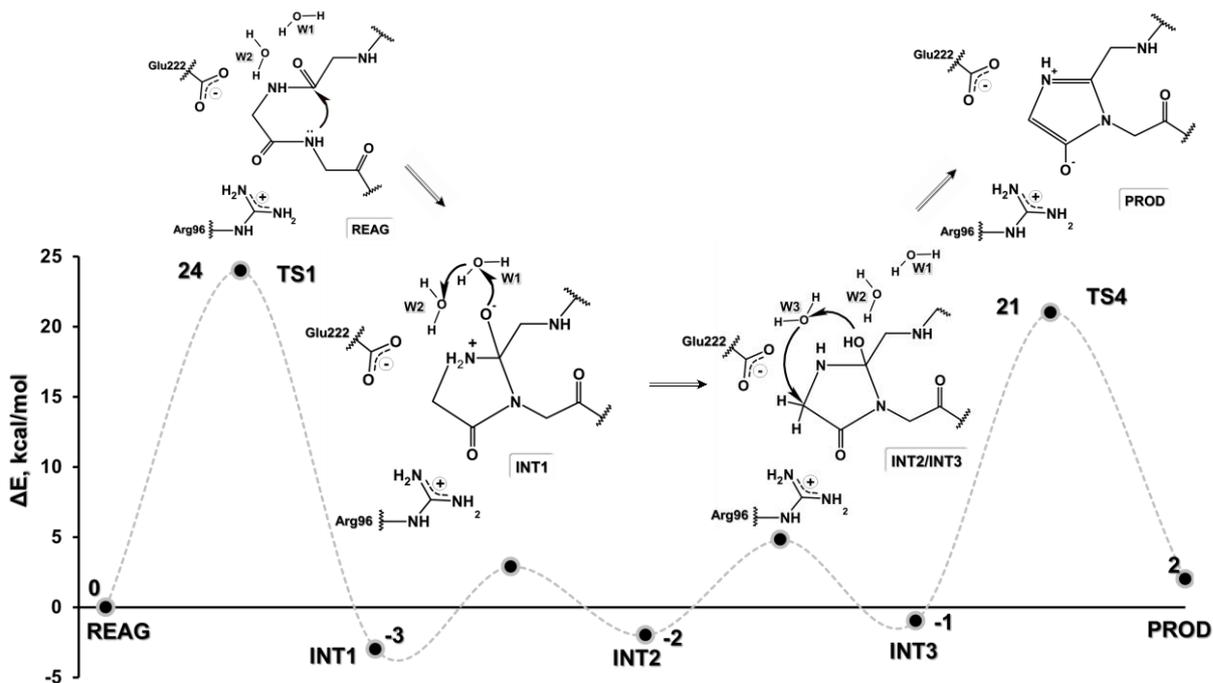


Figure S2 Computed reaction energy profile for the Gly65-Gly66-Gly67 cyclization. Insets illustrate chemical transformations at the elementary steps.

Section S2. Color versions of Figs 1, 3, 4 in the main text.

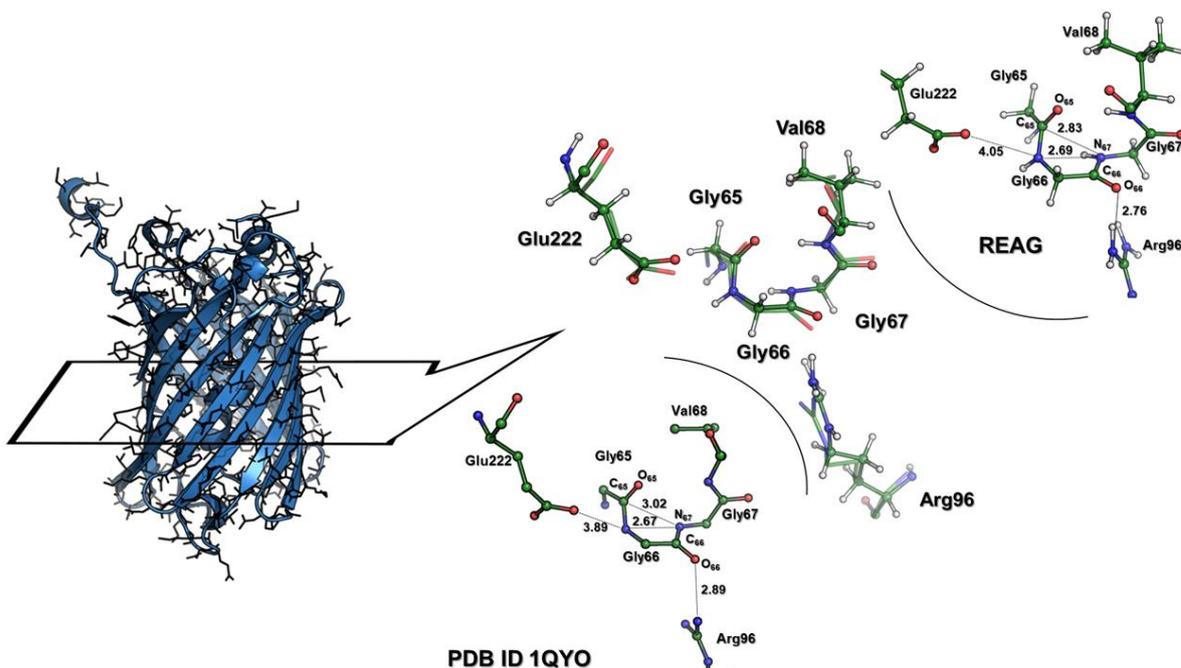


Figure S3 Structural features of the Ser65Gly/Tyr66Gly mutant of GFP. (a) General view of the protein barrel; (b) superposition of the peptide chains from computations (balls and sticks) and from the crystal structure PDB ID 1QYO (sticks); (c) fragment of the crystal

structure showing few distances given in Å; (d) fragment of the computationally derived structure showing the same distances as in panel c.

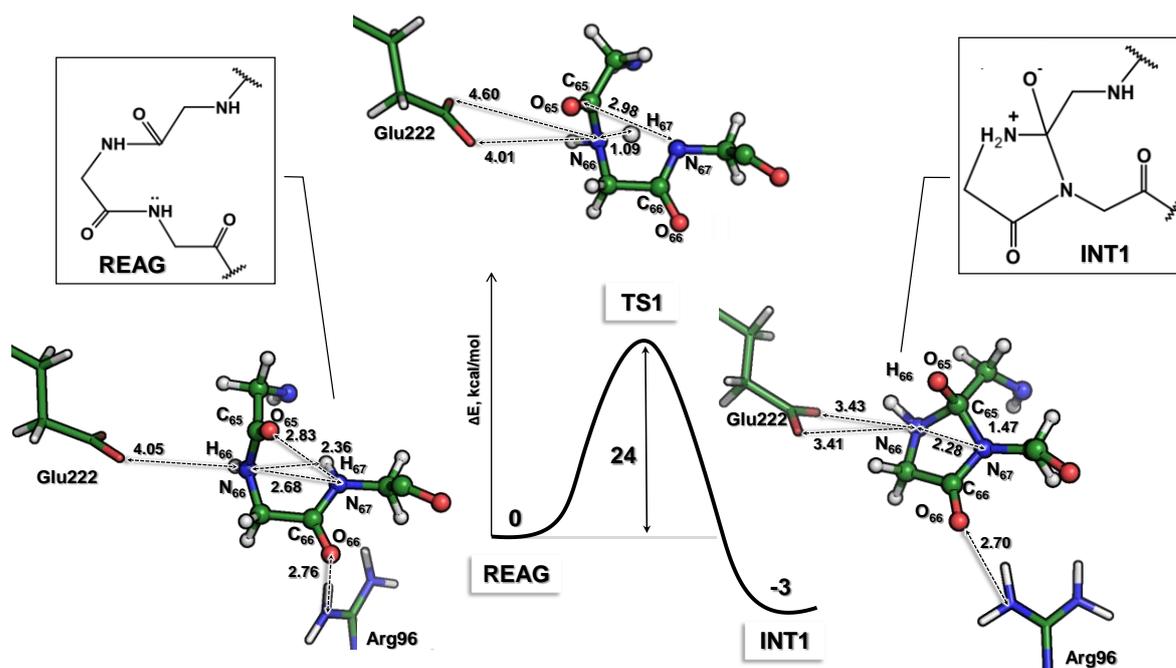


Figure S4 The first step in the Gly65-Gly66-Gly67 cyclization: REAG → TS1 → INT1. Distances between atoms are given in Å.

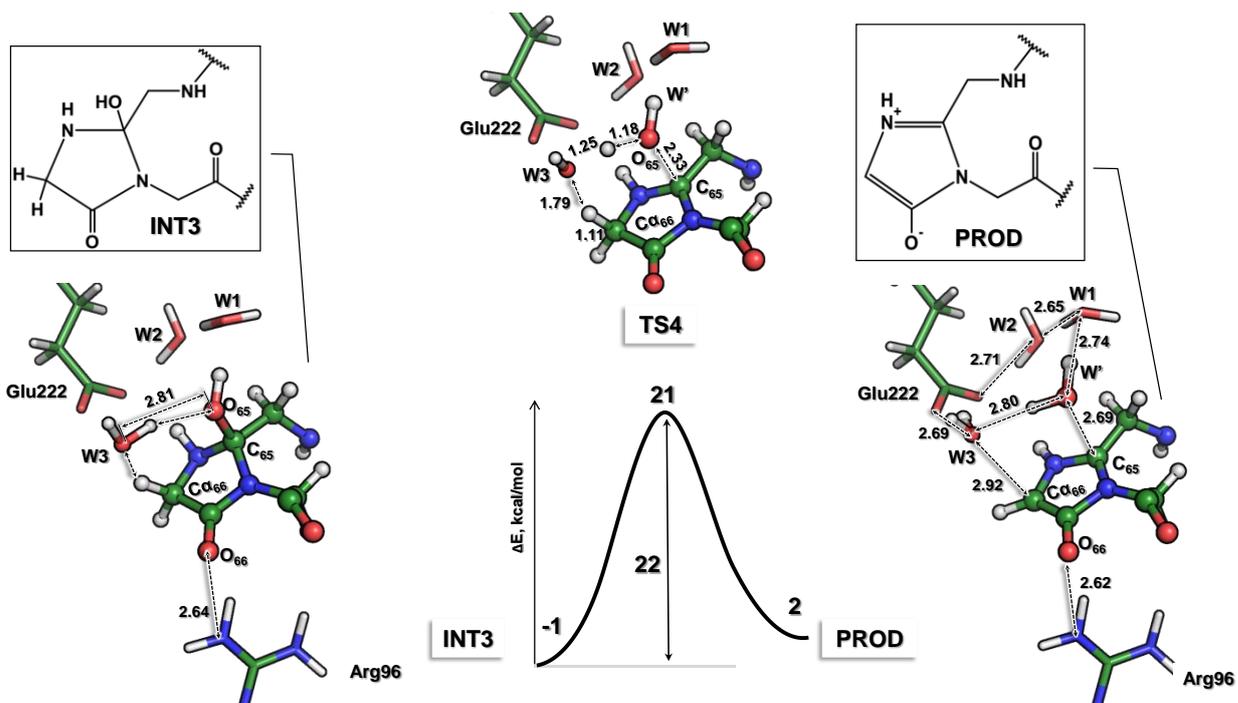


Figure S5 Dehydration step: $\text{INT3} \rightarrow \text{TS4} \rightarrow \text{PROD}$. Distances between atoms are given in Å.

Section S3. Cartesian coordinates of the stationary points along the reaction pathway shown in Figs 3, 4 in the main text or in Figs S4, S5 in the Supplementary Materials.

REAG

N 24.3350 27.6310 35.5670
H 24.5960 28.5450 35.2390
C 25.3090 26.5690 35.4410
H 24.8620 25.6680 35.0160
H 26.1040 26.8930 34.7660
C 25.9490 26.1960 36.7600
O 25.8750 25.0540 37.2450
N 26.5280 27.2130 37.4140
H 26.6680 28.0790 36.9100
C 26.7760 27.1310 38.8290
H 27.3940 26.2690 39.0900
H 27.3210 28.0060 39.1750
C 25.4970 26.9700 39.6180
O 25.5250 26.7450 40.8410
N 24.3460 26.9850 38.9490
H 24.2790 27.4880 38.0790
C 23.1330 26.7420 39.6640
H 23.0250 27.4050 40.5210
H 22.3030 26.9050 38.9930
C 23.1210 25.3290 40.1580
O 22.4430 24.9700 41.1320
N 21.1290 33.5070 46.2020
H 20.2420 33.6940 45.7490
C 22.2450 34.4000 45.8390
H 22.9350 34.4430 46.6840
C 23.0540 33.9720 44.5930
H 22.4540 34.1050 43.6910
H 23.9110 34.6450 44.5290
C 23.6170 32.5460 44.5180
H 24.0660 32.2520 45.4670
H 22.8210 31.8380 44.2800
C 24.7050 32.4400 43.3980
H 24.2440 32.8510 42.4980
H 25.4910 33.1250 43.7190
N 25.3250 31.0910 43.1020
H 26.0250 30.7970 43.7590
C 25.0690 30.2470 42.0870
N 24.0070 30.3920 41.3260
H 23.9050 29.7950 40.5190
H 23.2650 31.0300 41.5860
N 25.9370 29.2620 41.8950
H 25.6900 28.4270 41.3620
H 26.7680 29.1300 42.4540
C 21.7640 35.8130 45.5860
O 20.9150 36.0410 44.7240

N 31.2170 23.5080 30.9140
H 30.7890 22.5900 30.9460
C 31.9440 23.9590 32.0960
H 32.7300 24.6410 31.7700
C 30.9600 24.6990 33.0530
H 30.4730 25.4300 32.4060
H 30.2240 23.9390 33.3180
C 31.4930 25.3910 34.3250
H 31.9520 24.6610 34.9910
H 32.2330 26.1380 34.0560
C 30.4030 26.0820 35.1370
O 29.9970 27.2010 34.7340
O 29.9650 25.4840 36.1590
C 32.6550 22.8040 32.8010
O 32.1160 21.7020 32.9150

TS1

N 24.3870 27.1540 35.5230
H 24.8590 27.9610 35.1370
C 25.1230 25.9410 35.6940
H 24.4340 25.2210 36.1490
H 25.4670 25.5200 34.7430
C 26.3350 26.0160 36.5860
O 27.0710 25.0880 36.7910
N 26.4200 27.2390 37.3970
H 27.0300 27.8880 36.8860
C 26.7730 27.0310 38.8160
H 27.3550 26.1210 38.9260
H 27.3790 27.8560 39.1850
C 25.4310 26.9500 39.5290
O 25.3890 26.8850 40.7840
N 24.4310 26.9530 38.6810
H 25.3700 27.5200 37.5150
C 23.1420 26.8740 39.3330
H 22.9950 27.6670 40.0580
H 22.3660 26.9540 38.5810
C 23.0560 25.5410 40.0240
O 22.5150 25.2830 41.1030
N 31.2170 23.5080 30.9140
H 30.7890 22.5900 30.9460
C 31.9490 23.9610 32.0940
H 32.7420 24.6330 31.7670
C 30.9680 24.7180 33.0230
H 30.7300 25.6090 32.4400
H 30.0820 24.0810 33.0410
C 31.3310 25.1310 34.4650
H 31.4410 24.2690 35.1240
H 32.2790 25.6730 34.4620
C 30.3540 26.0810 35.1380
O 29.9970 27.1000 34.5070
O 30.0370 25.8510 36.3450
C 32.6550 22.8040 32.8010

O 32.1160 21.7020 32.9150

INT1

N 23.8310 27.5920 35.6270

H 24.2500 28.4620 35.3370

C 24.6120 26.3900 35.6130

H 23.9010 25.5620 35.6320

H 25.2100 26.3270 34.6950

C 25.5790 26.1230 36.7680

O 25.8250 24.8250 36.9170

N 26.9190 26.8450 36.5160

H 27.4570 26.2500 35.8350

C 27.5050 26.9930 37.8580

H 28.1670 26.1610 38.0530

H 28.1120 27.8900 37.9270

C 26.3060 26.9970 38.7780

O 26.3460 27.1550 39.9890

N 25.2030 26.7930 38.0240

H 26.7680 27.7540 36.0780

C 23.8800 26.7480 38.6170

H 23.6220 27.6900 39.0750

H 23.1470 26.5820 37.8260

C 23.7280 25.6200 39.5980

O 23.0380 25.6830 40.6280

N 21.1790 33.4410 46.1770

H 20.3090 33.6120 45.6870

C 22.3010 34.3410 45.8430

H 22.9590 34.3970 46.7120

C 23.1630 33.9040 44.6340

H 22.6080 34.0850 43.7130

H 24.0500 34.5410 44.6250

C 23.6650 32.4500 44.5500

H 24.0610 32.1250 45.5130

H 22.8290 31.8010 44.2850

C 24.7750 32.2810 43.4590

H 24.3810 32.7830 42.5730

H 25.6110 32.8710 43.8370

N 25.2800 30.9010 43.0970

H 26.0250 30.5560 43.6740

C 24.9590 30.1770 42.0070

N 23.9710 30.5650 41.2260

H 23.6640 29.8710 40.5590

H 23.2610 31.1680 41.6150

N 25.6450 29.0700 41.7620

H 25.5450 28.5760 40.8740

H 26.4860 28.8070 42.2640

C 21.8050 35.7470 45.5720

O 20.9460 35.9550 44.7140

N 31.2170 23.5080 30.9140

H 30.7890 22.5900 30.9460

C 31.9130 23.9570 32.1200

H 32.6840 24.6700 31.8240

C 30.8950 24.6440 33.0780
H 30.5560 25.5080 32.5040
H 30.0690 23.9340 33.1400
C 31.3170 25.0790 34.4980
H 31.5470 24.2210 35.1260
H 32.2100 25.7000 34.4220
C 30.3190 25.9170 35.2910
O 29.8260 26.9320 34.7040
O 30.0970 25.6020 36.4760
C 32.6550 22.8040 32.8010
O 32.1160 21.7020 32.9150

INT3

N 23.9260 27.6970 35.8140
H 24.2990 28.6070 35.6070
C 24.8170 26.5810 35.7930
H 24.1850 25.6990 35.6740
H 25.4980 26.6620 34.9380
C 25.6970 26.3530 37.0220
O 25.9390 24.9200 37.0990
N 26.9250 27.0870 37.0360
H 28.4450 26.0590 34.1100
C 27.3870 27.0790 38.4150
H 28.0430 26.2480 38.6670
H 27.9380 27.9760 38.6920
C 26.1000 26.9490 39.1810
O 25.9350 26.9830 40.3970
N 25.1180 26.7330 38.2850
H 27.6040 26.7180 36.3780
C 23.7400 26.6890 38.7230
H 23.4540 27.6250 39.1860
H 23.0880 26.5340 37.8610
C 23.5320 25.5320 39.6610
O 22.7800 25.5260 40.6440
N 21.1610 33.4620 46.1890
H 20.2860 33.6340 45.7080
C 22.2730 34.3750 45.8670
H 22.9320 34.4260 46.7360
C 23.1290 33.9680 44.6490
H 22.5660 34.1440 43.7320
H 24.0040 34.6210 44.6390
C 23.6530 32.5270 44.5580
H 24.0520 32.1950 45.5180
H 22.8360 31.8610 44.2770
C 24.7720 32.4030 43.4720
H 24.3670 32.8910 42.5850
H 25.5880 33.0190 43.8540
N 25.3200 31.0380 43.1140
H 26.0360 30.6900 43.7250
C 25.0110 30.2850 42.0440
N 24.0170 30.6290 41.2480
H 23.7480 29.9220 40.5800

H 23.2820 31.2120 41.6230
N 25.7230 29.1940 41.8310
H 25.5540 28.5990 41.0200
H 26.5570 28.9410 42.3470
C 21.7690 35.7790 45.6120
O 20.8920 35.9910 44.7730
O 25.8880 23.8880 34.6590
H 25.1410 24.1980 34.1360
H 25.8720 24.5000 36.1900
O 27.7480 25.4600 33.7570
H 28.1620 24.9780 33.0300
H 26.6590 24.4290 34.3240
O 27.9800 24.2120 38.8930
H 27.4160 24.3790 38.1120
H 28.0660 23.2550 38.9710
N 31.2170 23.5080 30.9140
H 30.7890 22.5900 30.9460
C 31.9180 23.9570 32.1190
H 32.6890 24.6680 31.8220
C 30.9080 24.6400 33.0880
H 30.0840 23.9270 33.1550
C 31.3470 25.0720 34.5040
H 31.6410 24.2180 35.1110
H 32.2060 25.7370 34.4070
C 30.3450 25.8420 35.3570
O 29.7590 26.8460 34.8130
O 30.1900 25.5010 36.5380
C 32.6550 22.8040 32.8010
O 32.1160 21.7020 32.9150

TS4

N 24.0990 27.7830 35.6400
H 24.4260 28.7080 35.4200
C 25.0730 26.7470 35.8200
H 24.5580 25.7860 35.8090
H 25.8160 26.7610 35.0180
C 25.7880 26.8520 37.1240
O 26.1400 24.5570 37.3060
N 27.0570 27.1410 37.2710
H 28.3480 26.2440 34.1270
C 27.4300 27.0430 38.6620
H 27.9020 26.0600 38.8420
H 28.1020 27.8280 39.0110
C 26.1030 26.9620 39.3300
O 25.8270 26.9090 40.5140
N 25.1680 26.8510 38.3250
H 27.7320 27.0330 36.5230
C 23.7630 26.7470 38.6600
H 23.4200 27.6570 39.1340
H 23.1840 26.5900 37.7510
C 23.5650 25.5540 39.5610
O 22.7870 25.5580 40.5280

N 21.1470 33.4890 46.2080
H 20.2640 33.6800 45.7490
C 22.2560 34.4090 45.8990
H 22.9090 34.4550 46.7720
C 23.1190 34.0130 44.6800
H 22.5610 34.1990 43.7620
H 23.9940 34.6670 44.6810
C 23.6450 32.5740 44.5750
H 24.0390 32.2300 45.5320
H 22.8300 31.9110 44.2800
C 24.7700 32.4630 43.4930
H 24.3660 32.9530 42.6060
H 25.5800 33.0820 43.8820
N 25.3300 31.1040 43.1330
H 26.0360 30.7550 43.7560
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N 24.0330 30.6790 41.2660
H 23.7560 29.9580 40.6170
H 23.2960 31.2620 41.6380
N 25.7360 29.2490 41.8670
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H 26.5610 28.9800 42.3910
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C 31.3970 25.1820 34.4560
H 31.7250 24.3630 35.0930
H 32.2310 25.8700 34.3180
C 30.3710 25.9480 35.2790
O 29.7850 26.9390 34.7010
O 30.1900 25.6410 36.4610
C 32.6550 22.8040 32.8010
O 32.1160 21.7020 32.9150
O 25.9010 23.7910 34.5780
H 25.1150 24.1650 34.1660
H 26.0700 24.0500 36.4760
O 27.5800 25.7310 33.7860
H 27.9560 25.2000 33.0700
H 26.6020 24.4600 34.3850
O 28.0830 24.2870 38.7120
H 27.1430 24.3600 37.8910
H 28.0410 23.3980 39.0780

PROD

N 23.8990 27.8210 35.4860
H 24.2370 28.7510 35.3100

C 24.8660 26.7930 35.7360
H 24.3360 25.8370 35.7320
H 25.6150 26.7750 34.9380
C 25.5730 26.9400 37.0280
O 25.8890 24.2680 37.0490
N 26.8750 27.1120 37.1860
H 28.3400 25.9980 34.1600
C 27.2150 27.0930 38.5260
H 28.9400 24.6920 37.4760
H 28.2220 27.2610 38.8580
C 26.0450 26.8960 39.2360
O 25.7400 26.7920 40.4630
N 25.0420 26.8180 38.2470
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C 23.6530 26.7560 38.6370
H 23.3420 27.6730 39.1180
H 23.0350 26.6100 37.7500
C 23.4780 25.5770 39.5530
O 22.7780 25.5670 40.5760
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C 22.3120 34.3050 45.7970
H 22.9900 34.3600 46.6510
C 23.1480 33.8700 44.5700
H 22.5680 34.0350 43.6610
H 24.0220 34.5240 44.5350
C 23.6780 32.4280 44.4880
H 24.0970 32.1150 45.4450
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H 24.3550 32.7470 42.4920
H 25.5970 32.9130 43.7360
N 25.3280 30.9140 43.0470
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C 24.9910 30.1200 42.0060
N 23.9440 30.4280 41.2650
H 23.6770 29.7530 40.5650
H 23.2190 31.0120 41.6540
N 25.7270 29.0510 41.7890
H 25.5240 28.3260 41.0670
H 26.5960 28.8650 42.2770
C 21.8150 35.7150 45.5380
O 20.9510 35.9300 44.6860
N 31.2170 23.5080 30.9140
H 30.7890 22.5900 30.9460
C 31.9210 23.9530 32.1150
H 32.6900 24.6690 31.8230
C 30.9120 24.6190 33.0950
H 30.5400 25.4770 32.5310
H 30.1020 23.8920 33.1760
C 31.3740 25.0510 34.5010
H 31.7030 24.2030 35.0960

H 32.2100 25.7430 34.3920
C 30.3610 25.7770 35.3620
O 29.7450 26.7660 34.8490
O 30.2430 25.4150 36.5530
C 32.6550 22.8040 32.8010
O 32.1160 21.7020 32.9150
O 25.7940 23.6800 34.3710
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H 25.9020 23.8900 36.1430
O 27.6710 25.4310 33.7270
H 28.1450 24.9660 33.0260
H 26.5220 24.3190 34.1660
O 28.4080 24.4390 38.2630
H 26.7910 24.2700 37.4240
H 28.6700 23.5330 38.4870