

Supporting Information

Mechanism of Biocatalytic Friedel-Crafts Acylation by Acyltransferase from *Pseudomonas protegens*

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1. Superposition of structures

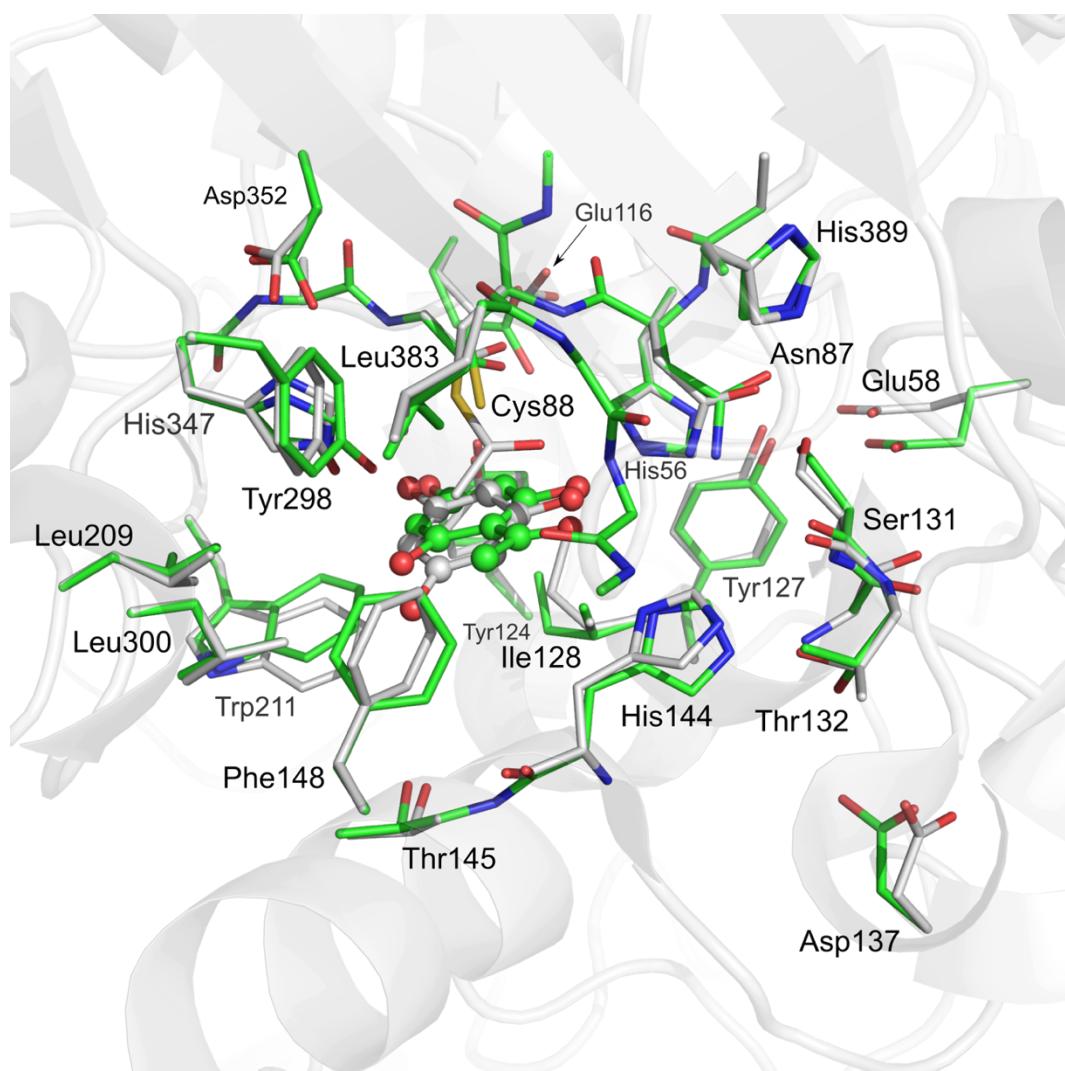


Figure S1. Overlap of the optimized structure of E:S (in green) with the X-ray structure (PDB 5MG5).

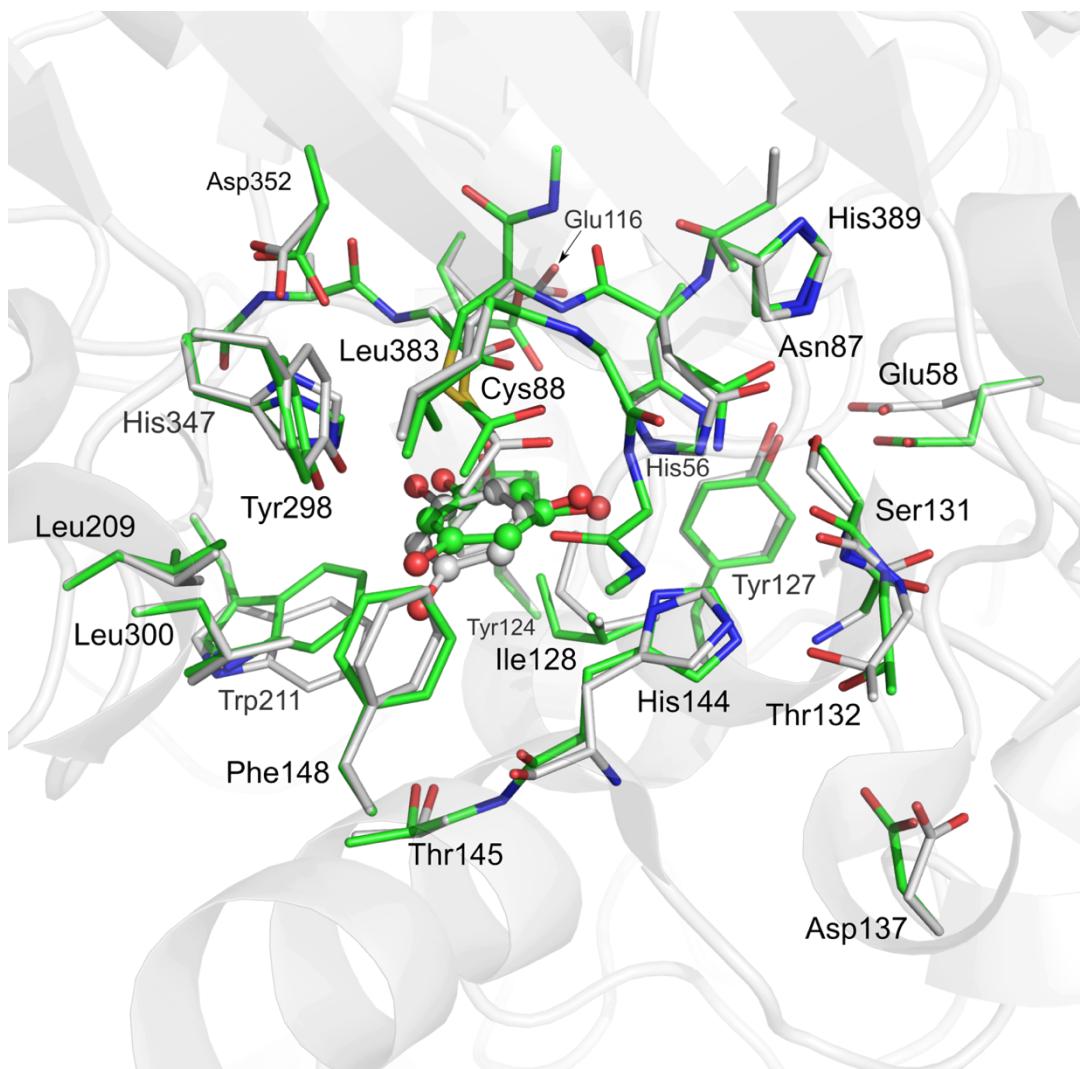


Figure S2. Overlap of the optimized structure of **Int6** (in green) with the X-ray structure (PDB 5MG5).

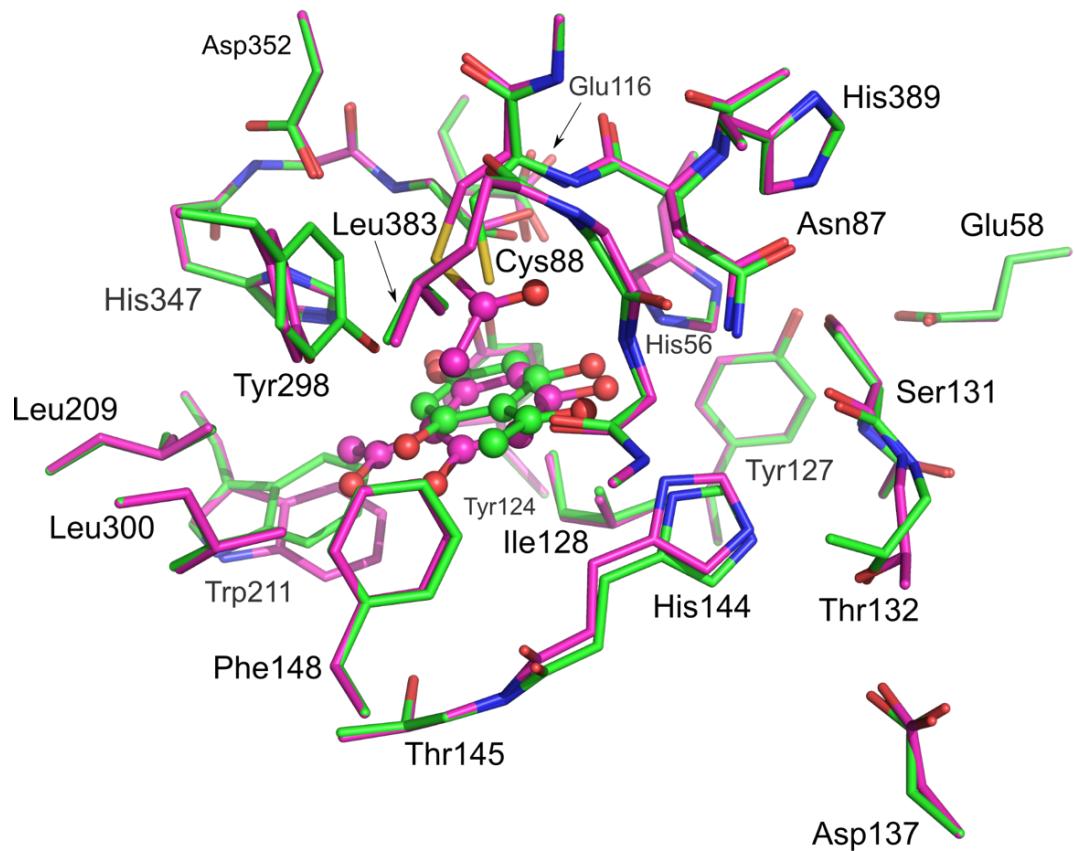


Figure S3. Overlap of the optimized structure of **Int6** (in green) with **Int7** (in purple).

2. Alternative binding mode of Int7

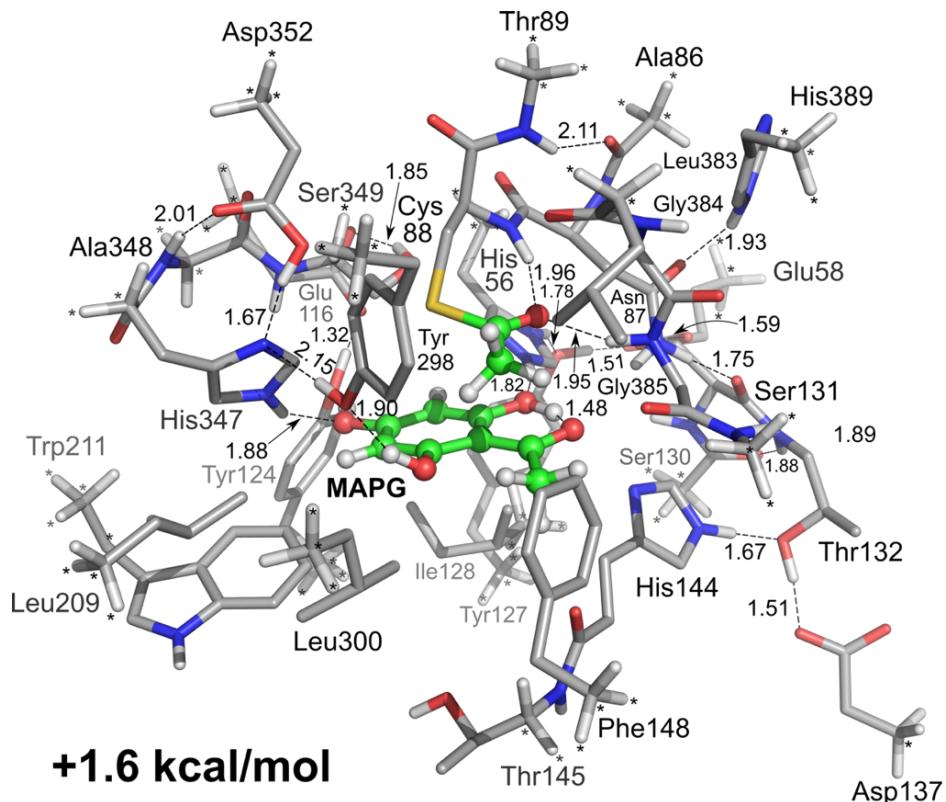


Figure S4. Optimized structure of the intermediate after binding of the second substrate, in which MAPG binds in a different mode compared to that in **Int7** (Figure 5 in the main text) but similar to the first MAPG substrate in E:S (Figure 2 in the main text). Energy relative to **Int7** is given.

Since the binding mode in Figure S4 is only 1.6 kcal/mol higher than **Int7**, we have examined the feasibility of the proposed mechanism for the second half-reaction with this binding mode. The calculations showed that the new structure corresponding to **Int9** (Figure S5) is as high as 29.6 kcal/mol relative to **Int7**. The reason for the high energy is that this structure lacks hydrogen bonds between substrate and a number of active site residues, such as His56, Tyr124 and His347. Moreover, no general base is present to deprotonate the hydroxyl group at the *para* position relative to the carbon where the acetyl group will be added, which has been demonstrated to be important for the formation of a key dienone intermediate in the reaction. This binding mode is thus concluded to be unproductive.

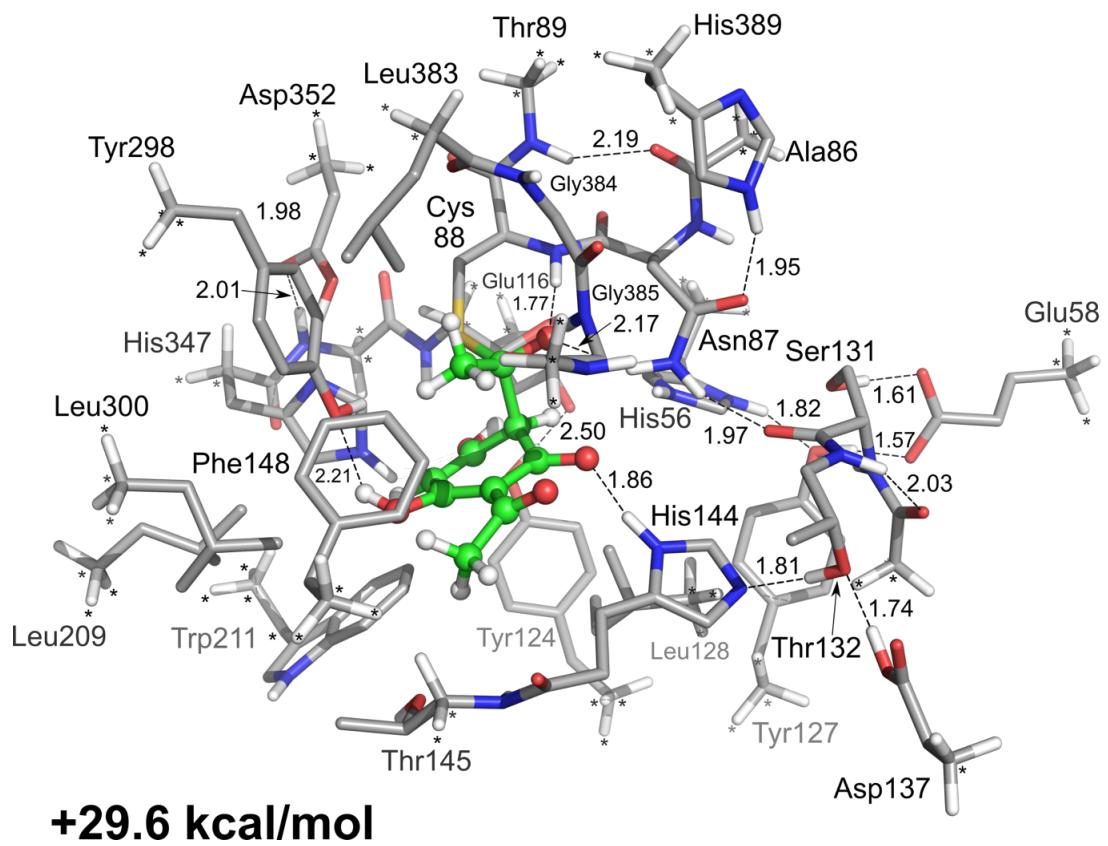


Figure S5. Optimized structure of the intermediate corresponding to **Int9** with the new binding mode of the second MAPG substrate. Energy relative to **Int7** is given.

3. Structures of intermediates and transition states of the second half-reaction

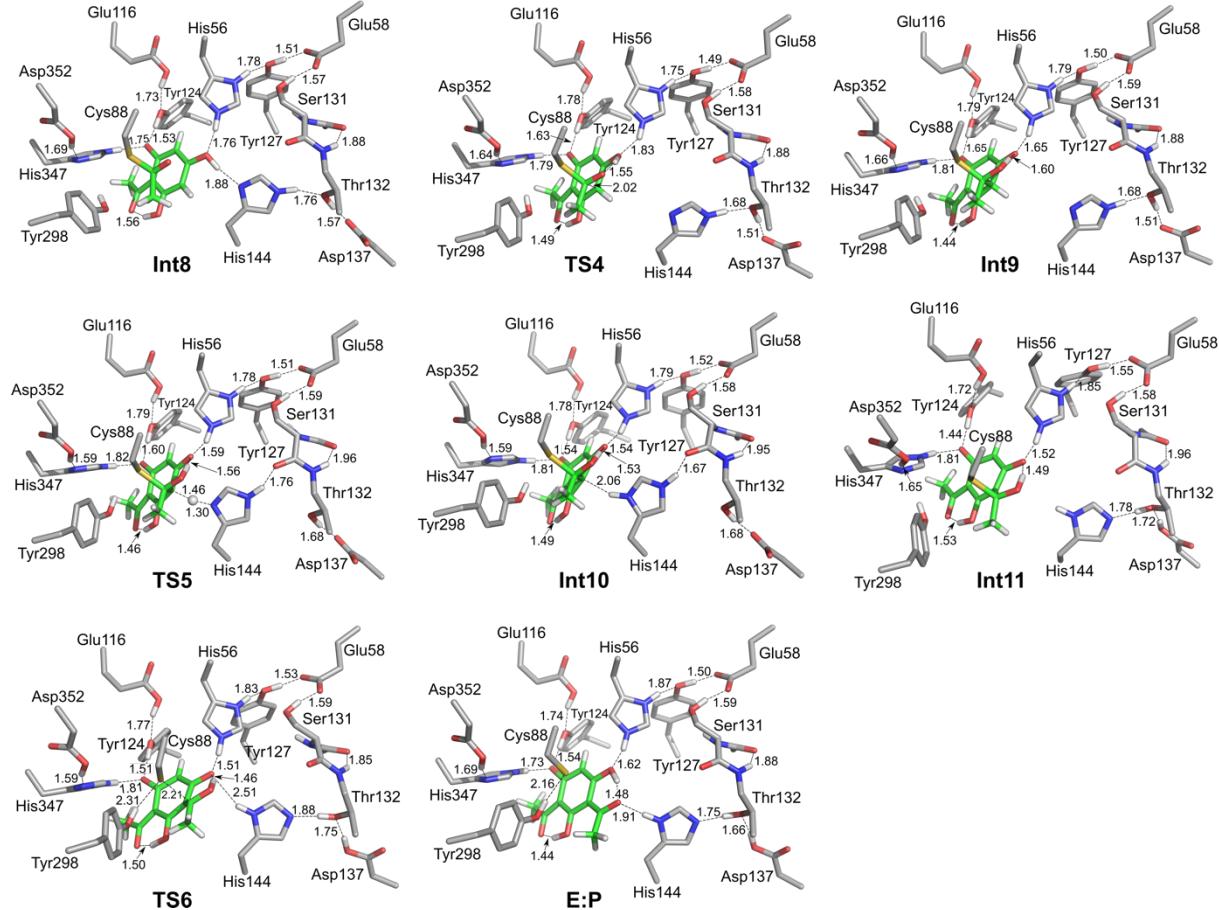
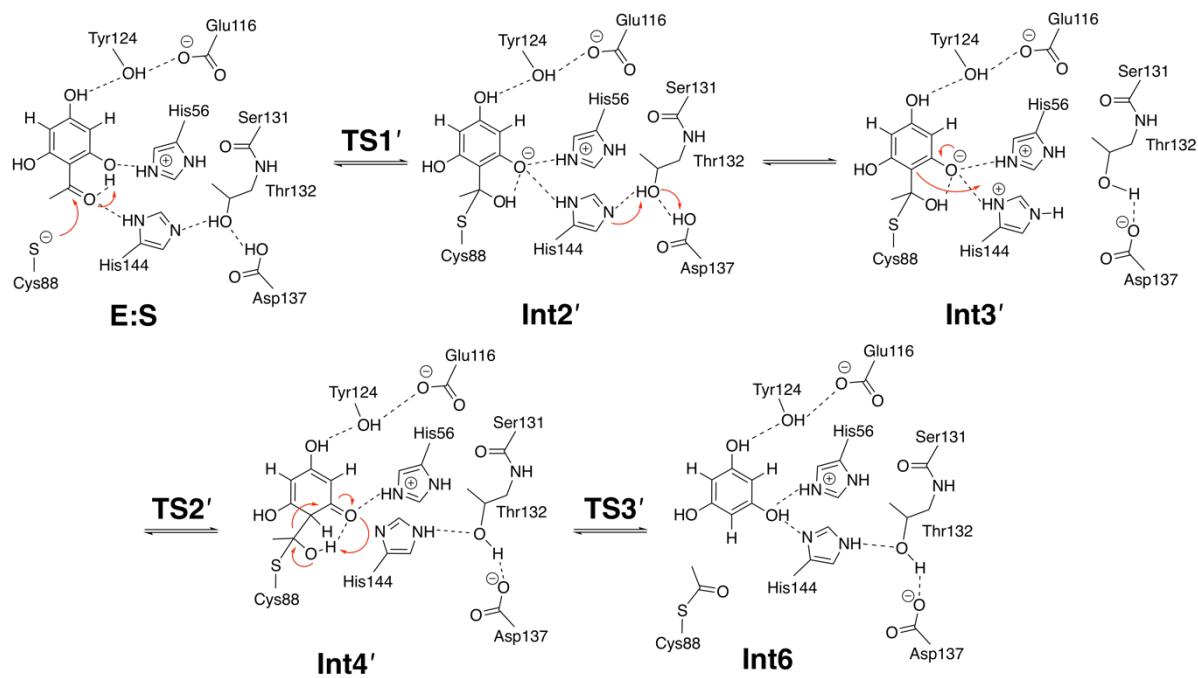


Figure S6. Optimized structures of intermediates and transition states involved in the second half-reaction of the suggested mechanism. For clarity, only a part of the active site model is shown (see **Figure 5** in the main text for full model), and most of nonpolar hydrogens have been omitted. Selected distances are given in Å.

4. Alternative mechanism with the *para*-hydroxyl group being neutral throughout



Scheme S1. An alternative pathway for the first half-reaction with the *para*-hydroxyl group being neutral throughout.

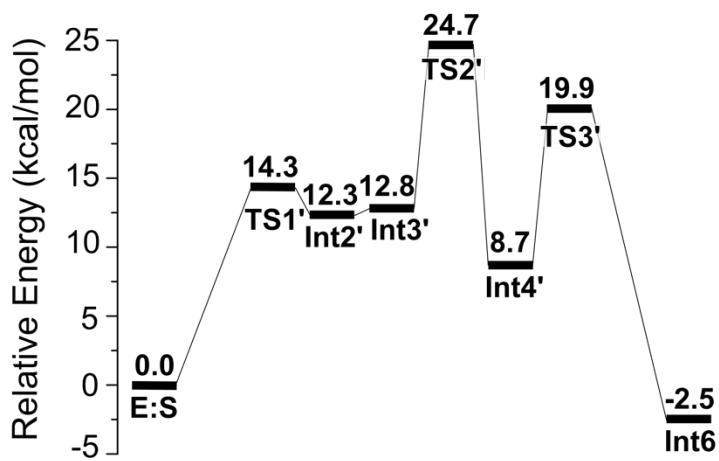


Figure S7. Calculated energy profile for the alternative pathway for the first half-reaction with the *para*-hydroxyl group being neutral throughout.

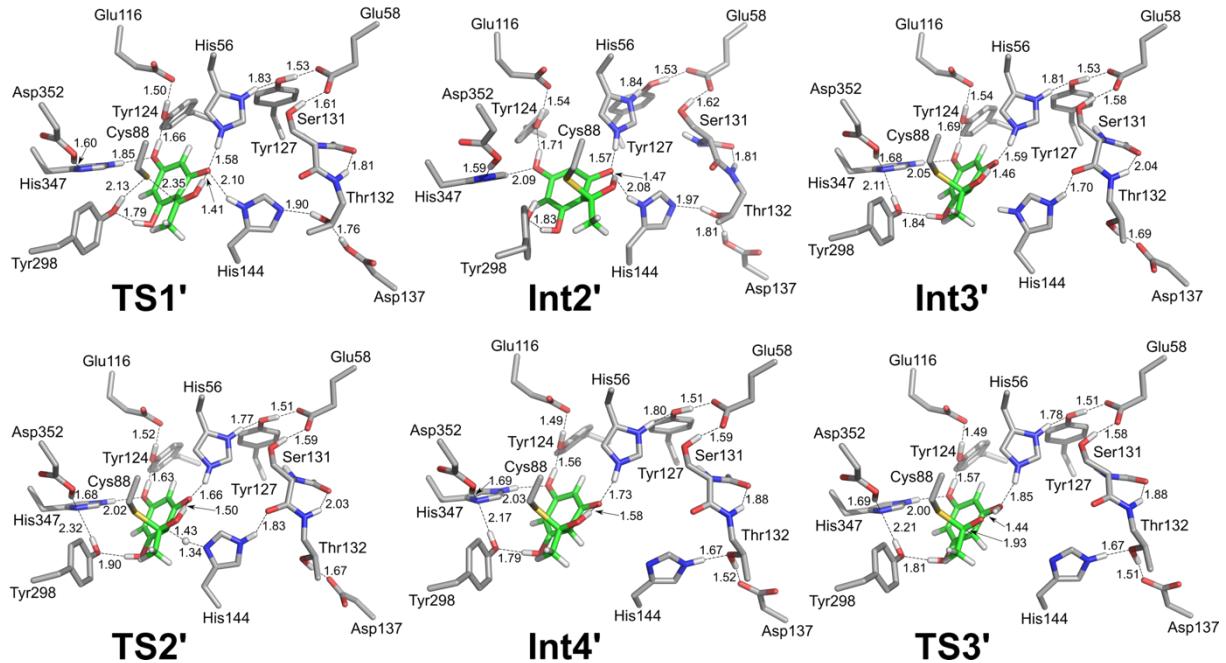


Figure S8. Optimized structures of intermediates and transition states in the alternative pathway for the first half-reaction with the para-hydroxyl group being neutral throughout. For clarity, only a part of the active site model is shown (see **Figure 2** for full model), and most of nonpolar hydrogens have been omitted. Selected distances are given in Å.

5. Absolute energies and energy corrections for intermediates and transition states

Table S1. Calculated absolute energies (au), energy corrections (au) and final relative energies (kcal/mol) for the intermediates and transition states of the proposed mechanism.

BS1=6-31G(d,p), BS2=6-311+G(2d,2p)

| | E _{B3S1} | E _{B3S2} | E _{solvation} | E _{ZPE} | E _{dispersion} | ΔE _{total} |
|--------------|-------------------|-------------------|------------------------|------------------|-------------------------|---------------------|
| E:S | -9236.728537 | -9239.282925 | -9236.928283 | 3.540236 | -0.982674 | 0.0 |
| Int1 | -9236.734729 | -9239.289496 | -9236.928871 | 3.540775 | -0.97756 | -0.3 |
| TS1 | -9236.718722 | -9239.27078 | -9236.908972 | 3.539872 | -0.984428 | 13.4 |
| Int2 | -9236.717208 | -9239.270198 | -9236.907795 | 3.539771 | -0.985527 | 13.4 |
| Int3 | -9236.695835 | -9239.251358 | -9236.905311 | 3.541077 | -0.991091 | 14.2 |
| TS2 | -9236.687459 | -9239.244448 | -9236.895567 | 3.538101 | -0.992587 | 17.6 |
| Int4 | -9236.72748 | -9239.283813 | -9236.932279 | 3.542812 | -0.977543 | -2.1 |
| TS3 | -9236.704356 | -9239.261327 | -9236.907457 | 3.539664 | -0.977611 | 11.1 |
| Int5 | -9236.727068 | -9239.28458 | -9236.928578 | 3.539649 | -0.978083 | -2.5 |
| Int6 | -9236.723800 | -9239.278342 | -9236.931873 | 3.540026 | -0.979552 | -2.5 |
| Int7 | -9389.399315 | -9392.002478 | -9389.602609 | 3.577396 | -0.995827 | -5.0 |
| Int8 | -9389.401134 | -9392.004265 | -9389.600463 | 3.577431 | -0.994536 | -3.6 |
| TS4 | -9389.376498 | -9391.977365 | -9389.578849 | 3.576295 | -0.994243 | 10.7 |
| Int9 | -9389.399092 | -9391.998831 | -9389.60219 | 3.579962 | -0.994546 | -1.0 |
| TS5 | -9389.368051 | -9391.965922 | -9389.575402 | 3.576002 | -1.010048 | 14.5 |
| Int10 | -9389.376369 | -9391.976111 | -9389.585496 | 3.577386 | -1.008227 | 7.9 |
| Int11 | -9389.402747 | -9392.001137 | -9389.594645 | 3.578877 | -0.993519 | 3.9 |
| TS6 | -9389.401269 | -9391.998226 | -9389.590063 | 3.57835 | -0.998516 | 7.4 |
| E:P | -9389.425035 | -9392.023048 | -9389.609833 | 3.580177 | -0.99136 | -4.6 |

6. Experimental details

A. Site directed mutagenesis of *PpATase*

The single mutation (D137N) was introduced with the QuickChange II site-directed mutagenesis kit (Agilent Genomics) according to the standard procedure provided by the supplier without modifications. The primer sequences and plasmids used in this study are listed in Table S2.

Table S2. Plasmids and primers used in this study.

| Plasmids | Origin (GenBankID) | Description/Comments |
|----------------------|-----------------------|--|
| pEG332 | Reference [1] | Codon-optimized gene fragments <i>phlA</i> , <i>phlC</i> and <i>phlB</i> based on <i>phlACB</i> from <i>P. protegens</i> DSM19095, assembled by Gibson cloning and overlap-extension PCR. PCR primers: OE1-4ATaseCH-Fow/Rev. |
| pEG332-D137N | this study | Single mutation D137N introduced to pEG332; PCR primers: <i>Pp</i> -D137N-Fow/Rev. |
| Primers | Origin | Sequence (5'→3') |
| Sequencing-Fow | Eurofins | TTGTTCTGTGCGGCCGGTTT |
| Sequencing-Rev | Eurofins | CTTAGATCTCGTCGACTGAGT |
| <i>Pp</i> -D137N-Fow | IDT | TGGCTCGAGCACTGAATGTGAATATAACTAC TTTCTCGG |
| <i>Pp</i> -D137N-Rev | IDT | CCGAGAAAGTAGTTATATTCACATTCACTGC TCGAGCCA |

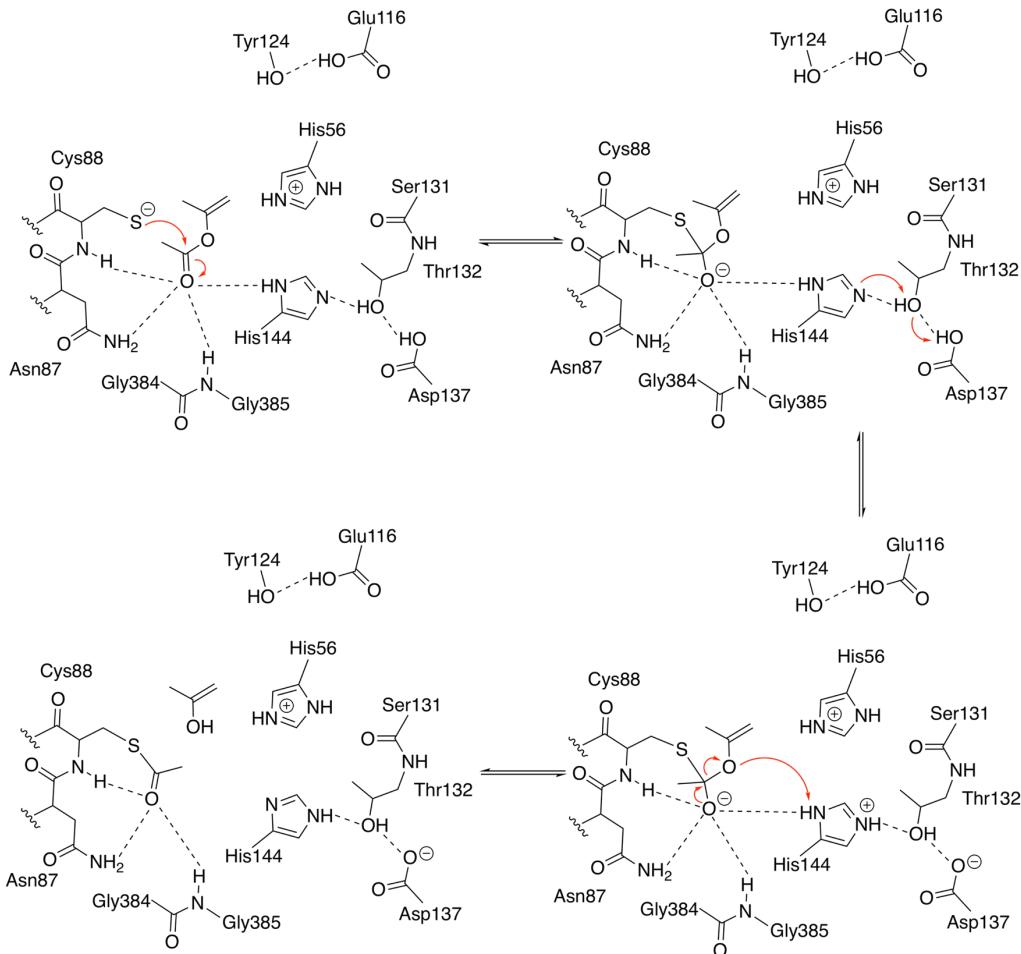
B. Cultivation and expression of the *PpATase* variant

The plasmid (pEG332 or pEG332-*Pp*-D137N) was introduced into chemically competent *E. coli* BL21(DE3) host cells following standard procedures. A single colony, picked from an agar-plate (LB/ampicillin, 100 µg mL⁻¹), was used for inoculation of an overnight-culture (10 mL, LB/Amp, 100 µg mL⁻¹) which was grown at 37 °C and 140 rpm for 15 h. The main culture (1 L) containing LB/Amp (100 µg mL⁻¹) was then inoculated with the overnight culture (10 mL) and shaken in a 5 L-non-baffled flask at 37 °C and 140 rpm until the OD₆₀₀ reached 0.7. The cells were induced with anhydrotetracycline (AHTC, 200 µg L⁻¹) and protein expression was continued for 21 h at 30 °C. The cells were harvested by centrifugation (15 min, 8,000 rpm, 12,028×g), washed with potassium phosphate buffer (50 mM, pH 7.5) and centrifuged again (15 min, 8,000 rpm, 12,028×g). Wet cells were resuspended in potassium phosphate buffer (50 mM, pH 7.5, 7 mL buffer to 1 g wet cells). The suspension was disrupted by ultrasonication (40 % amplitude, 8 min, pulse 1 sec, pause 4 sec) followed by centrifugation (30 min, 14,000 rpm, 23,519×g). The cell-free extract was shock-frozen in liquid nitrogen and stored at -20 °C until direct use for biotransformations.

C. Activity Test

To a solution of resorcinol (**1**, 1.1 mg, 0.01 mmol, 10 mM final concentration) in potassium phosphate buffer (100 mM, pH 7.5, total volume 1 mL) containing imidazole (Im, 100 mM final concentration, added from 1M stock solution prepared in the reaction buffer) donor substrate isopropenyl acetate (IPEA, 10.9 μ L, 100 mM final concentration) was added. The bioacetylation was started by addition of the cell-free extract of recombinant *PpATase* variant (400 μ L). The reaction mixture was shaken for 1.5 h at 35 °C and 750 rpm in an orbital shaker. The reaction was quenched by addition of acetonitrile (1 mL). The precipitated protein was removed by centrifugation (30 min, 14,000 rpm) and the supernatant was subjected to HPLC analysis for determination of conversions. Reaction without enzyme (negative control) and with the wild-type *PpATase* (positive control) were performed. The relative amounts of the C-acetylated (**2**) and O-acetylated (**3**) products and the resorcinol substrate were determined by HPLC according to standard curves with authentic samples. The composition of the product mixture is given in Table S3.

Note here that, for practical reasons, IPEA is used as the acyl donor in the experiments. The deacylation of this donor is expected to follow the same mechanism as in O-acylation enzymes, where the stabilization of the alkoxide intermediate by an oxyanion hole becomes important (see Scheme S2).



Scheme S2. Plausible mechanism for the deacylation of IPEA by *PpATase*.

D. HPLC Method

The conversions of all biotransformations were measured at 25 °C by HPLC using an Agilent liquid chromatograph, equipped with an SPD-M20A diode array detector, Phenomenex Luna® 5µm C18 (2) 100A (250 × 4.6 mm) column. H₂O/MeCN-gradient (+TFA, 0.1 vol%) was used as an eluent. *Method:* 0-15% MeCN (0-5 min), 15-60% MeCN (5-22 min), 60-100% MeCN (22-25 min), 100-0% MeCN (25-30 min), flow rate = 1 mL min⁻¹, sample vol. = 2 µL. Reaction products were quantified at 254 nm from the peak areas on the basis of standard curves with reference compounds.

Table S3. *PpATase*-variant activity test: Friedel-Crafts bioacetylation of **1**.

| | | <i>PpATase</i> or variants KPi-buffer 35 °C, 1.5 h | | |
|----------------------------|----------------|---|--------------|--------------|
| | | IPEA/Im acetone | 2 | 3 |
| 1 (10 mM) | | | | |
| Acetylation IPEA/Im | | | | |
| Entry | Enzyme | 2 [%] | 3 [%] | 1 [%] |
| 1 | <i>PpATase</i> | 44 | 15 | 41 |
| 2 | w/o enzyme | 0 | 32 | 68 |
| 3 | D137N | 0 | 21 | 79 |

References:

- [1] Schmidt, N. G.; Pavkov-Keller, T.; Richter, N.; Wiltschi, B.; Gruber, K.; Kroutil, W. Biocatalytic Friedel-Crafts Acylation and Fries Reaction. *Angew. Chem. Int. Ed.* **2017**, *56*, 7615–7619.

7. Cartesian coordinates

E:S

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -8.78747500 | 1.93667400 | 2.73687600 | C | -4.23292100 | 2.43149400 | -0.93234700 |
| C | -8.93038600 | 0.81365200 | 1.74168400 | C | -4.77650700 | -0.96688100 | -7.33165000 |
| O | -9.92441100 | 0.07887800 | 1.74134700 | C | -3.57586700 | -1.03000100 | -6.40134700 |
| N | -7.84484000 | 0.58249300 | 0.96069300 | C | -2.72777400 | -0.30924500 | -4.20227300 |
| C | -7.91228900 | -0.35989600 | -0.15438000 | C | -1.32224800 | 0.00721700 | -4.78000800 |
| C | -7.62190800 | -1.80020600 | 0.33653100 | C | -2.81341900 | -1.63114000 | -3.40803800 |
| O | -6.64166000 | -2.46391400 | -0.03773900 | C | -4.17469800 | -1.85247200 | -2.77155500 |
| C | -6.92761500 | 0.12949600 | -1.23282800 | C | 1.05738800 | -0.59719800 | -4.77457000 |
| O | -6.92314200 | 1.54046000 | -1.30913600 | C | 1.36258800 | -1.05163700 | -6.20668400 |
| N | -8.54479300 | -2.26575400 | 1.19591700 | C | 1.99725100 | -1.37837800 | -3.82482300 |
| C | -8.62544100 | -3.62114900 | 1.71596700 | C | 0.31473000 | -1.84050600 | 0.99391900 |
| C | -7.76584600 | -3.93794100 | 2.97391300 | C | 0.59061000 | -2.32414700 | -8.13878800 |
| C | -6.40364500 | -4.52776800 | 2.60596400 | C | 1.73025200 | 8.79025500 | -5.19926000 |
| O | -7.66763700 | -2.80084600 | 3.83274300 | C | 2.27427500 | 7.57852500 | -4.42250800 |
| C | -9.98598800 | -5.08425700 | 8.97033400 | C | 1.54075600 | 7.29520800 | -3.10975100 |
| C | -9.02720800 | -4.03223200 | 8.40375600 | C | 0.33764000 | 6.34606000 | -3.23596000 |
| C | -8.83843600 | -4.08209800 | 6.88917500 | C | -1.35797900 | 8.93235300 | 4.83181200 |
| O | -9.34826200 | -4.91647200 | 6.16227600 | C | -0.20963500 | 9.23322800 | 3.84325600 |
| O | -8.03961800 | -3.09671000 | 6.47515300 | C | 0.04427500 | 8.21221900 | 2.76577700 |
| C | -1.68829300 | -2.88889800 | 5.86963700 | C | -0.87147100 | 7.99753400 | 1.72695600 |
| C | -0.43541500 | -3.58559500 | 6.38721400 | C | 1.23514900 | 7.47840800 | 2.75387500 |
| O | -0.12665400 | -4.71702600 | 6.02180800 | C | -0.61963600 | 7.07819200 | 0.71528400 |
| C | -1.68553100 | -2.80235100 | 4.33644600 | C | 1.51164500 | 6.56194000 | 1.74320400 |
| C | -2.99238100 | -2.31836800 | 3.78899100 | C | 0.58041900 | 6.34932300 | 0.72361600 |
| C | -4.24042900 | -2.13631400 | 4.34004700 | C | -5.55739400 | 5.96046300 | 5.08021100 |
| N | -3.13977000 | -1.96427900 | 2.45938600 | C | -5.37574100 | 7.08752400 | 4.03335000 |
| C | -4.43353900 | -1.58445300 | 2.26367000 | C | -5.77346400 | 6.59502100 | 2.65383100 |
| N | -5.13049300 | -1.68272700 | 3.38241700 | C | -7.09501700 | 6.23667900 | 2.35004000 |
| N | 0.30291000 | -2.88103900 | 7.29460400 | C | -4.80582500 | 6.36700700 | 1.66808000 |
| C | 1.63120300 | -3.33595900 | 7.67450500 | C | -7.44213900 | 5.65467000 | 1.13113000 |
| C | 2.43632000 | -2.17755200 | 8.27220300 | C | -5.13268500 | 5.79881500 | 0.43808600 |
| C | 3.90546300 | -2.55265200 | 8.43866200 | C | -6.45468500 | 5.41652100 | 0.15862200 |
| O | 2.27800800 | -0.98935500 | 7.49424100 | C | -3.69541900 | 2.99792900 | 3.53894000 |
| N | -4.44153900 | 3.47340000 | -1.74027500 | C | -2.33777900 | 2.46583300 | 4.03015600 |
| N | -2.94111400 | 2.10786200 | -1.01248700 | C | -1.29554200 | 3.58458600 | 4.19346900 |
| N | -3.69553400 | -0.25203800 | -5.28743900 | C | -1.85555300 | 1.32677300 | 3.12960600 |
| N | -4.16628400 | -2.17394100 | -1.45779400 | C | -0.99516600 | 4.38778900 | 2.92950400 |
| N | -0.32296300 | -0.82404300 | -4.38536800 | C | 3.73497400 | -7.94447200 | 6.46690300 |
| N | 0.42718200 | -1.84115000 | -6.78774000 | C | 4.34594800 | -6.67607500 | 5.83902900 |
| N | 7.00660400 | 3.76101700 | 5.92976800 | C | 3.82841400 | -6.40463000 | 4.44776000 |
| N | 6.05787200 | 1.51260200 | -1.45841600 | C | 4.66524200 | -6.55304400 | 3.33622800 |
| N | 4.80876400 | 2.81081400 | -0.18305000 | C | 2.48666600 | -6.05585300 | 4.24077600 |
| N | 6.89642100 | 4.66993400 | -3.50389600 | C | 4.17926700 | -6.35803700 | 2.04206200 |
| N | 3.51522100 | 4.20171900 | -3.29920600 | C | 1.99646500 | -5.88734800 | 2.94743800 |
| N | 0.24341600 | -5.75332400 | -4.24040600 | C | 2.83828600 | -6.03293700 | 1.84169700 |
| N | -1.35392300 | -4.24969800 | -1.41798400 | C | 11.06268700 | 1.02606100 | 3.67097800 |
| N | -1.71116800 | -7.13883000 | 0.71049600 | C | 9.90688400 | 0.60248500 | 2.74974200 |
| N | -4.82139400 | -5.17499700 | -7.12010300 | C | 8.51798200 | 1.15466500 | 3.12285600 |
| N | -5.12854700 | -4.03825600 | -5.23029500 | C | 8.45145700 | 2.67820700 | 2.96461100 |
| C | -3.65327500 | 4.47837800 | -4.73159800 | C | 7.42065100 | 0.49326400 | 2.27691900 |
| C | -3.08931900 | 4.91463400 | -3.36691500 | C | 8.11027700 | 6.56271500 | 2.62671800 |
| C | -3.24459800 | 3.84978100 | -2.34095800 | C | 7.22947600 | 6.83216000 | 3.84179200 |
| C | -2.30040900 | 2.97192100 | -1.88310100 | C | 6.87193300 | 5.57996400 | 4.59264800 |
| C | | | | C | 7.63115800 | 4.93590100 | 5.53738300 |
| C | | | | C | 5.70756000 | 4.75471400 | 4.37836800 |
| C | | | | C | 5.82923500 | 3.61607400 | 5.22392400 |
| C | | | | C | 4.57239600 | 4.86982700 | 3.55792500 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 4.86993000 | 2.59922900 | 5.25093300 | O | 0.17855200 | 5.68037100 | -4.28077400 |
| C | 3.60736100 | 3.87217800 | 3.59362200 | O | -0.39923000 | 6.23215600 | -2.18989400 |
| C | 3.76089400 | 2.74353800 | 4.42563700 | O | 0.84688600 | 5.42331900 | -0.23229700 |
| C | 8.49804500 | -5.48995900 | -3.46898500 | O | -6.73781700 | 4.83495700 | -1.03383800 |
| C | 6.96182600 | -5.57613900 | -3.40020400 | O | 3.94687100 | -1.83409700 | -0.34454000 |
| C | 6.27889500 | -4.53307000 | -2.53975400 | O | 7.71319000 | 5.58618900 | -1.57503600 |
| C | 5.68455100 | -3.41963800 | -3.14588600 | O | 4.75517400 | 3.96639200 | -5.18423400 |
| C | 6.16897500 | -4.64715100 | -1.14666900 | O | 0.61594400 | 3.60900700 | -2.48513500 |
| C | 4.96394300 | -2.48612500 | -2.41200800 | O | 7.10618300 | 1.97915600 | -4.71197400 |
| C | 5.42336000 | -3.73340400 | -0.39503800 | O | 5.61338000 | 0.51576000 | -3.87876300 |
| C | 4.77997100 | -2.67147300 | -1.03880500 | O | 2.03977200 | -4.68843900 | -5.12633800 |
| C | 9.28233800 | -4.71743400 | 3.07641900 | O | -1.81752800 | -6.13185000 | -2.58550000 |
| C | 7.87564600 | -4.13673400 | 2.86162200 | O | 0.15142000 | -5.93468500 | 0.21353600 |
| C | 7.16575000 | -3.63036500 | 4.13140800 | O | 2.14893800 | 3.44999300 | 0.72418300 |
| C | 7.99014000 | -2.57623200 | 4.88233400 | O | 2.95688900 | -0.98993000 | 2.01276000 |
| C | 5.77124300 | -3.08612400 | 3.78924700 | O | -1.25020300 | 0.22920400 | -0.03682800 |
| C | 8.70844600 | 3.53554400 | -2.38588100 | O | -9.43283400 | 2.24736700 | -1.49706000 |
| C | 7.75060400 | 4.71707900 | -2.44870500 | O | -9.23764800 | 4.49135200 | -1.27879700 |
| C | 8.33264300 | 2.61389900 | -1.19114300 | O | -0.89043200 | -2.09036800 | 0.63818300 |
| C | 6.86236500 | 2.50106900 | -0.91567200 | S | 1.47703900 | -1.28442600 | -2.05145700 |
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| C | 4.83422100 | 1.72196500 | -0.99552200 | H | -2.02281700 | 5.13590500 | -3.44277800 |
| C | 5.65877800 | 5.42774800 | -3.52421200 | H | -1.23908100 | 2.93255700 | -2.10194100 |
| C | 4.58852000 | 4.48688200 | -4.08346700 | H | -5.00387400 | 1.94753800 | -0.36158000 |
| C | 2.73136700 | 3.01970200 | -3.64154800 | H | -3.40543000 | 3.43261600 | -4.93962800 |
| C | 1.63927400 | 2.65184500 | -2.66546200 | H | -5.67267200 | -1.27260600 | -6.77986000 |
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| C | 2.19347100 | -7.08639200 | -4.91546500 | H | -3.29739200 | -2.42696900 | -1.01181700 |
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| C | 3.98156700 | -7.85432700 | -1.52713300 | H | 2.19430400 | 6.67806200 | -5.03743400 |
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| C | 2.47657300 | 1.23687900 | 1.43609300 | H | -2.34285500 | 9.09937400 | 4.38610500 |
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| H | 8.95512800 | -2.96989400 | 5.21686400 | H | 1.54105300 | -2.92153500 | 2.39330500 |
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| H | 8.31158800 | 7.50365300 | 2.10509600 |
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| H | 6.30937800 | 0.90536400 | -8.26564100 |
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Int1

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| N | -5.14806200 | -1.78729300 | 3.39678300 |
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| N | -4.45546500 | 3.52258900 | -1.62618700 |
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|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
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| C | -2.75382700 | -0.15704200 | -4.15875300 | C | 5.68010000 | -3.36632700 | -3.24874000 |
| C | -1.32246900 | 0.28559400 | -4.55876900 | C | 6.16899600 | -4.61938500 | -1.26679800 |
| C | -2.81380300 | -1.51935500 | -3.43370800 | C | 4.93705400 | -2.45827600 | -2.50508500 |
| C | -4.17654900 | -1.79102600 | -2.82101200 | C | 5.40248500 | -3.73124700 | -0.50658400 |
| C | 1.02881400 | -0.46925300 | -4.79174200 | C | 4.74128300 | -2.67116900 | -1.13733900 |
| C | 1.35688500 | -0.88000900 | -6.23593800 | C | 9.30453700 | -4.78759500 | 2.97320200 |
| C | 1.91781300 | -1.33366200 | -3.86519100 | C | 7.89872800 | -4.19959600 | 2.77210900 |
| C | 0.23300200 | -1.84079400 | 0.99712400 | C | 7.27787700 | -3.52591300 | 4.01039300 |
| C | 0.60985300 | -2.15111400 | -8.18503300 | C | 8.10529500 | -2.33138100 | 4.50356500 |
| C | 1.74050800 | 8.89565200 | -4.99753700 | C | 5.82979500 | -3.10162400 | 3.72582300 |
| C | 2.20928500 | 7.60537000 | -4.30507300 | C | 8.72308200 | 3.58571100 | -2.30333100 |
| C | 1.49343800 | 7.23067700 | -3.00374800 | C | 7.76361900 | 4.76722400 | -2.34338000 |
| C | 0.02254700 | 6.87996900 | -3.17786400 | C | 8.34837700 | 2.63663000 | -1.12912400 |
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| C | -0.21223900 | 9.10910200 | 4.02579400 | C | 6.10152800 | 3.29523200 | -0.02376600 |
| C | 0.02717600 | 8.07557200 | 2.95124300 | C | 4.83557800 | 1.78041000 | -1.00530200 |
| C | -0.90180600 | 7.84645000 | 1.92722400 | C | 5.67197300 | 5.49976900 | -3.39844200 |
| C | 1.21410700 | 7.33378700 | 2.93119800 | C | 4.58812600 | 4.60856600 | -4.01153900 |
| C | -0.66403900 | 6.90697600 | 0.92912400 | C | 2.74655600 | 3.09251400 | -3.56945200 |
| C | 1.47568600 | 6.39585300 | 1.93446700 | C | 1.52565000 | 2.86180200 | -2.67984900 |
| C | 0.52946700 | 6.17010800 | 0.93016400 | C | 6.17956000 | 1.73094300 | -7.36868600 |
| C | -5.54389400 | 5.83040700 | 5.21651000 | C | 5.73862500 | 0.82303200 | -6.21118800 |
| C | -5.36683900 | 6.98528400 | 4.20084400 | C | 6.20881200 | 1.27327600 | -4.84954100 |
| C | -5.77055300 | 6.53205500 | 2.81024600 | C | 2.21695300 | -6.98297800 | -5.06922400 |
| C | -7.09341700 | 6.18381800 | 2.50069500 | C | 1.49039200 | -5.64158300 | -4.93941700 |
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| C | -5.13717600 | 5.80001400 | 0.57109400 | C | 2.79668200 | -5.74035800 | -2.14378000 |
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| C | -2.34757600 | 2.33823300 | 4.14054800 | C | -1.22349300 | -5.00359800 | -2.63699100 |
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| C | 3.76015200 | -8.09433800 | 6.29098000 | C | -2.89479300 | -7.80967500 | -6.42007700 |
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| C | 4.75023400 | -6.64565700 | 3.20186400 | C | -4.06041300 | -4.82338200 | -5.10779700 |
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| C | 4.29725800 | -6.43519300 | 1.89824300 | C | 1.73642600 | 2.17476400 | 0.83523600 |
| C | 2.08431700 | -6.01007600 | 2.75017700 | C | 2.53079900 | 1.12678000 | 1.38905300 |
| C | 2.95800200 | -6.12432700 | 1.66570200 | C | 2.07770300 | -0.16725500 | 1.45362100 |
| C | 11.08016100 | 0.94263300 | 3.69605400 | C | 0.42123100 | 1.86221800 | 0.41369700 |
| C | 9.92063700 | 0.54216400 | 2.77011600 | C | -0.03721100 | 0.56440900 | 0.48375900 |
| C | 8.62116900 | 1.34974800 | 2.94694700 | C | 0.75275900 | -0.51504100 | 1.01764200 |
| C | 8.77586800 | 2.78818000 | 2.43874600 | C | -13.21131200 | 4.75764300 | -3.09286900 |
| C | 7.44888100 | 0.66415500 | 2.23126700 | C | -11.72527400 | 4.45117900 | -2.79563800 |
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| C | 7.68061500 | 4.83724100 | 5.67809900 | O | -2.54534900 | -1.53833200 | -6.66090700 |
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| C | 4.63234200 | 4.73995000 | 3.68530100 | O | 2.44030200 | -0.57722800 | -6.73539600 |
| C | 4.95267800 | 2.46369400 | 5.36566000 | O | -0.64638600 | 7.17566900 | -4.14886800 |
| C | 3.69008300 | 3.72097600 | 3.69534000 | O | -0.55022500 | 6.25320400 | -2.14109000 |
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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| O | 7.73017700 | 5.62666700 | -1.46114000 | H | 4.13041300 | -5.96557600 | 6.35462300 |
| O | 4.68824900 | 4.22300600 | -5.17159200 | H | 5.46061200 | -6.89469200 | 5.68283000 |
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| O | 0.19479100 | -5.97767700 | 0.03163200 | H | 3.84064100 | -8.92361400 | 5.58145500 |
| O | 2.23740700 | 3.37218500 | 0.69922200 | H | 10.23956400 | 0.64566400 | 1.72370600 |
| O | 2.91690700 | -1.11806600 | 1.97414400 | H | 9.70459400 | -0.52476400 | 2.91416900 |
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| H | -1.27408300 | 2.93140800 | -2.02906800 | H | 12.03769100 | 0.66884900 | 3.23637800 |
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| H | 0.65400500 | 8.88934600 | -5.09467700 | H | 3.10052100 | -1.61913800 | -1.02914500 |
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| H | -7.87171000 | 6.33135500 | 3.24682100 | H | 10.03006300 | -4.02083700 | 3.26161300 |
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| H | -8.47323900 | 5.37984300 | 1.03513600 | H | 8.82909700 | 2.97692000 | -0.20751700 |
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| H | -0.86732700 | 0.83168800 | 3.56060500 | H | 1.38680700 | 1.78260400 | -2.53504700 |
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| H | -0.29103100 | 3.53614200 | 2.49782800 | H | 6.15577200 | -0.18679700 | -6.33136200 |
| H | -3.60245400 | 3.27627500 | 2.58311200 | H | 7.12325700 | 2.22446600 | -7.12641500 |

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|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 1.44121900 | -7.89287000 | -3.25079600 | H | 9.74064300 | 3.96037100 | -2.15492200 |
| H | 2.80759400 | -8.72309500 | -3.97323700 | H | 5.41988100 | 2.49678900 | -7.55552800 |
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| H | 1.79604800 | -5.89830800 | -1.73050400 | H | 0.09248300 | -1.49397000 | -8.89139700 |
| H | 2.75620600 | -4.93309200 | -2.87410400 | H | 0.21896800 | -3.16452600 | -8.31776100 |
| H | 3.44077200 | -5.38899100 | -1.33599600 | H | -4.94627000 | 0.20468900 | -7.69527700 |
| H | 4.12967800 | -8.95656400 | -2.00202500 | H | -4.63604000 | -1.47916200 | -8.21146200 |
| H | 4.49760100 | -7.56651200 | -0.96556400 | H | -3.29360500 | -7.93177700 | -5.40885200 |
| H | 2.86345300 | -8.23663000 | -0.98764800 | H | -1.90691300 | -8.27907400 | -6.46516800 |
| H | 1.69337100 | -7.62372300 | -5.78946400 | H | 3.17963600 | -6.67999900 | -5.49427900 |
| H | -0.98072200 | -3.96931900 | -4.50975600 | H | 8.89113300 | -6.06788100 | -4.38401400 |
| H | 0.41707800 | -3.81719400 | -3.42640000 | H | 8.95198000 | -5.75134400 | -2.63994500 |
| H | -0.14032500 | -6.56167000 | -4.05695800 | H | -1.17649800 | -9.14703900 | 0.06821900 |
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| H | -1.90149800 | -4.13015900 | 0.45255400 | H | 2.70102000 | -7.94276600 | 6.51938700 |
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| H | -5.49897300 | -3.33058400 | -4.60049300 | H | -7.25332200 | 1.35934700 | 0.78695200 |
| H | -6.31026600 | -3.51243100 | -7.02590900 | H | -8.91484100 | -0.32580000 | -0.56527800 |
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| H | 1.36524000 | 4.49513800 | 0.23836500 | H | -0.89339100 | -2.24808400 | 3.99852000 |
| H | 3.53602900 | 1.33424500 | 1.72887300 | H | -1.45987100 | -3.90621500 | 3.89972300 |
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| H | -5.36713100 | 4.91750600 | 4.63750700 | H | -7.86669000 | 1.67995500 | 3.37457800 |
| H | -4.88011400 | 5.89946800 | 6.08487300 | H | -10.96832400 | -5.10676300 | 8.47572400 |
| H | -4.39326400 | 2.07479700 | 3.64084200 | H | -9.68938300 | -6.31439600 | 8.54925600 |
| H | -3.98007500 | 3.73463600 | 4.25725200 | H | -9.67765200 | -3.83325000 | 1.86347600 |
| H | -1.30173100 | 7.76606400 | 5.35988800 | H | -8.35372100 | -4.35306900 | 0.81122500 |
| H | -1.18689600 | 9.50384200 | 5.86654600 | H | -5.88860900 | -0.16144800 | -0.95339400 |
| H | -4.72710900 | 4.69265900 | -4.62693700 | H | -7.12584100 | -0.31373800 | -2.18833600 |
| H | -3.16521600 | 5.18834300 | -5.39602800 | H | 2.19678300 | -3.79343400 | 6.68652600 |
| H | 2.03960900 | 9.81392100 | -4.48106200 | H | -2.54186100 | -3.65373400 | 6.16673100 |
| H | 2.16489700 | 8.91257500 | -6.00674500 | H | 1.61026900 | -4.42138000 | 8.21629400 |
| H | 8.32354400 | 7.45135800 | 2.27574300 | H | -1.81205700 | -2.05379600 | 6.31011300 |
| H | 9.06909900 | 6.03374500 | 3.07006300 | H | 2.95808100 | -1.37697700 | 6.77785000 |
| H | 5.71000800 | 6.40486300 | -4.01345000 | | | | |
| H | 2.39311800 | 3.17634500 | -4.60272800 | | | | |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -8.76459100 | 1.97192100 | 2.88594200 | C | 0.95178000 | -0.79347800 | -4.65185800 |
| C | -8.92209400 | 0.83821000 | 1.90454700 | C | 1.28566100 | -1.29489600 | -6.07239300 |
| O | -9.90650000 | 0.09017500 | 1.94822100 | C | 1.83511000 | -1.54966000 | -3.64469400 |
| N | -7.86317300 | 0.60746500 | 1.08926800 | C | 0.58946800 | -1.81480500 | -0.16564500 |
| C | -7.95474000 | -0.34426000 | -0.01663700 | C | 0.44723800 | -2.39813800 | -8.08748600 |
| C | -7.67024900 | -1.79486700 | 0.44456400 | C | 1.62625600 | 8.74696800 | -5.28162100 |
| O | -6.81010500 | -2.51266500 | -0.08876800 | C | 2.10851100 | 7.48012800 | -4.55277800 |
| C | -6.98393300 | 0.13265200 | -1.11567800 | C | 1.43157600 | 7.15189200 | -3.21660400 |
| O | -6.96631300 | 1.54082400 | -1.20546700 | C | -0.03936100 | 6.77722900 | -3.33456300 |
| N | -8.46868900 | -2.22278400 | 1.43747900 | C | -1.30725800 | 8.99149500 | 4.79381000 |
| C | -8.56399500 | -3.59311700 | 1.91955500 | C | -0.19136700 | 9.24393900 | 3.75046200 |
| C | -7.53933400 | -4.02302500 | 3.00536600 | C | 0.03650200 | 8.15706400 | 2.72479500 |
| C | -6.25750100 | -4.60178100 | 2.40499300 | C | -0.90912200 | 7.86567600 | 1.73179400 |
| O | -7.28551900 | -2.96545800 | 3.92877400 | C | 1.23091500 | 7.42642900 | 2.71674600 |
| C | -9.86323900 | -4.98474900 | 9.20916200 | C | -0.67983600 | 6.87935500 | 0.77732100 |
| C | -8.92509700 | -3.94792300 | 8.57715900 | C | 1.48280700 | 6.44157100 | 1.76302900 |
| C | -8.69572800 | -4.10091900 | 7.07354400 | C | 0.52112600 | 6.15275200 | 0.78909300 |
| O | -9.18835600 | -4.97601600 | 6.38608600 | C | -5.50079300 | 6.02078100 | 5.13748400 |
| O | -7.87885700 | -3.14336200 | 6.62106700 | C | -5.33186500 | 7.13149100 | 4.06956500 |
| C | -1.29035800 | -2.66590800 | 5.46203300 | C | -5.74090000 | 6.61005100 | 2.70382600 |
| C | -0.10422000 | -3.40020400 | 6.08494400 | C | -7.07442400 | 6.30296000 | 2.39771800 |
| O | 0.30300900 | -4.47040000 | 5.64831900 | C | -4.77400800 | 6.29272800 | 1.74175700 |
| C | -1.28944400 | -2.66972800 | 3.91852800 | C | -7.43562700 | 5.68791100 | 1.19882200 |
| C | -2.62204000 | -2.22670700 | 3.38033300 | C | -5.11380500 | 5.68950900 | 0.53242000 |
| C | -3.89453800 | -2.36082200 | 3.89126200 | C | -6.44988600 | 5.36217200 | 0.25017400 |
| N | -2.80312000 | -1.56827200 | 2.17031800 | C | -3.66123400 | 3.04322500 | 3.59843900 |
| C | -4.13946200 | -1.32144000 | 2.02600100 | C | -2.34077600 | 2.52877600 | 4.21512900 |
| N | -4.83111400 | -1.79664800 | 3.04614100 | C | -1.31097300 | 3.64978400 | 4.41829600 |
| N | 0.43023500 | -2.82163600 | 7.21227100 | C | -1.78379500 | 1.33330700 | 3.44410900 |
| C | 1.73184200 | -3.24585000 | 7.71646700 | C | -0.81136300 | 4.30968700 | 3.13749600 |
| C | 2.46076400 | -2.06152700 | 8.36725100 | C | 3.81883800 | -7.86562100 | 6.52424700 |
| C | 3.92571000 | -2.39804900 | 8.63181400 | C | 4.47498200 | -6.62701000 | 5.87734000 |
| O | 2.32348400 | -0.87158100 | 7.59179400 | C | 4.04527700 | -6.34243900 | 4.45728400 |
| N | -4.45818900 | 3.33076800 | -1.66572300 | C | 4.90991100 | -6.59260000 | 3.38449600 |
| N | -2.88458200 | 2.02484800 | -0.94723900 | C | 2.77285300 | -5.82421100 | 4.18965900 |
| N | -3.74143600 | -0.24209700 | -5.21823700 | C | 4.51728100 | -6.31747500 | 2.07286800 |
| N | -4.36950200 | -2.23196300 | -1.43810500 | C | 2.37250200 | -5.55674900 | 2.88098600 |
| N | -0.45570200 | -0.93171500 | -4.32013000 | C | 3.24715200 | -5.79786800 | 1.81878400 |
| N | 0.27240400 | -1.88942600 | -6.74508500 | C | 11.09816500 | 1.07809400 | 3.52341900 |
| N | 7.12503100 | 3.90287500 | 5.91176000 | C | 9.92224500 | 0.64704800 | 2.63257100 |
| N | 5.95743600 | 1.64353500 | -1.61839500 | C | 8.55048000 | 1.22860700 | 3.02156100 |
| N | 4.78359500 | 2.84220100 | -0.18343800 | C | 8.51364500 | 2.75116300 | 2.84267100 |
| N | 6.81765700 | 4.64479600 | -3.62060800 | C | 7.42612000 | 0.57415600 | 2.20668200 |
| N | 3.48180400 | 4.15149800 | -3.36672400 | C | 8.12720200 | 6.60275100 | 2.46776100 |
| N | 0.10004600 | -6.06691400 | -3.91395800 | C | 7.26499400 | 6.88425800 | 3.69333700 |
| N | -1.58490400 | -4.61051100 | -1.11664200 | C | 6.94865000 | 5.64683000 | 4.48383600 |
| N | -1.81882600 | -7.22026900 | 0.72955700 | C | 7.69163100 | 5.10065000 | 5.50040400 |
| N | -4.90582600 | -5.23217200 | -7.03884400 | C | 5.85844400 | 4.73313500 | 4.24168200 |
| N | -5.30601900 | -4.13334100 | -5.14457800 | C | 6.00331800 | 3.64616100 | 5.14832800 |
| C | -3.74700500 | 4.43821100 | -4.68672500 | C | 4.78381700 | 4.72026200 | 3.33614400 |
| C | -3.16981500 | 4.82838300 | -3.31563900 | C | 5.12169000 | 2.56105600 | 5.16065300 |
| C | -3.28923000 | 3.74407400 | -2.29671300 | C | 3.89691200 | 3.65183300 | 3.34975300 |
| C | -2.30684400 | 2.90637300 | -1.83898700 | C | 4.07205300 | 2.57918000 | 4.24927700 |
| C | -4.18452900 | 2.30520400 | -0.84872200 | C | 8.42717700 | -5.51223300 | -3.50890000 |
| C | -4.90830700 | -1.03433700 | -7.21254800 | C | 6.89381400 | -5.60996700 | -3.41532500 |
| C | -3.67023400 | -1.06037300 | -6.31180400 | C | 6.25933500 | -4.50241200 | -2.60906500 |
| C | -2.83854400 | -0.35888000 | -4.06916800 | C | 5.71135300 | -3.39669600 | -3.26950400 |
| C | -1.38381400 | 0.04383800 | -4.42962600 | C | 6.22560100 | -4.51338100 | -1.20857800 |
| C | -2.96197200 | -1.72491700 | -3.35770700 | C | 5.14002700 | -2.34191900 | -2.57034600 |
| C | -4.33886600 | -1.93025900 | -2.74844700 | C | 5.63156000 | -3.47482100 | -0.48781600 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 5.07792200 | -2.38954200 | -1.17446000 | O | 1.58291800 | -4.75529400 | -5.02098000 |
| C | 9.31184100 | -4.67186400 | 3.01562900 | O | -1.91954200 | -6.62293100 | -2.14317100 |
| C | 7.90187300 | -4.09545300 | 2.81055500 | O | -0.74015000 | -5.54261300 | 1.85274800 |
| C | 7.19935900 | -3.58129900 | 4.08071000 | O | 2.13482600 | 3.29079100 | 0.70816400 |
| C | 8.02826100 | -2.52276500 | 4.82024200 | O | 2.85082200 | -1.30623800 | 1.65805400 |
| C | 5.80403400 | -3.03865500 | 3.74047700 | O | -1.41348200 | 0.14159600 | 0.09471800 |
| C | 8.64888100 | 3.52603300 | -2.51982800 | O | -9.48235900 | 2.22793400 | -1.36643600 |
| C | 7.69003100 | 4.70793500 | -2.57930800 | O | -9.27167400 | 4.46994900 | -1.15029400 |
| C | 8.29270100 | 2.61473500 | -1.31219600 | O | -0.66600800 | -2.02821800 | -0.64380500 |
| C | 6.81921300 | 2.52994800 | -0.99384100 | S | 1.76825500 | -0.83551800 | -1.95351300 |
| C | 6.09074500 | 3.27994600 | -0.09267200 | H | -3.63871200 | 5.74973600 | -2.95203200 |
| C | 4.75165200 | 1.85296200 | -1.10704700 | H | -2.10998400 | 5.05100600 | -3.40561400 |
| C | 5.58190500 | 5.40335000 | -3.63265100 | H | -1.25919800 | 2.89718000 | -2.09830500 |
| C | 4.50120000 | 4.48403800 | -4.20506200 | H | -4.91884000 | 1.81168600 | -0.23928500 |
| C | 2.65390700 | 2.99326400 | -3.68002500 | H | -3.51662200 | 3.38912400 | -4.90475800 |
| C | 1.43310600 | 2.85201500 | -2.77320400 | H | -5.78072100 | -1.33616200 | -6.62426400 |
| C | 6.02861900 | 1.50647200 | -7.48485200 | H | -2.80997500 | -2.51914100 | -4.09672700 |
| C | 5.62737700 | 0.64179100 | -6.28517600 | H | -2.18963200 | -1.80229900 | -2.58870900 |
| C | 6.10772300 | 1.17473500 | -4.95774700 | H | -5.27790300 | -2.35667400 | -0.97255900 |
| C | 2.10178500 | -7.12579300 | -4.84164800 | H | -3.51911000 | -2.28501000 | -0.90001300 |
| C | 1.25069500 | -5.86885800 | -4.62897900 | H | -3.14672000 | 0.42781200 | -3.37472700 |
| C | 2.51601900 | -7.81162800 | -3.52048200 | H | -4.66473300 | 0.08818300 | -4.97586600 |
| C | 3.48825600 | -6.99409100 | -2.64682300 | H | 1.51357100 | -2.39289300 | -8.31391500 |
| C | 2.86724700 | -5.72852300 | -2.03975400 | H | -0.67786800 | -1.82331700 | -6.39822200 |
| C | 4.07299600 | -7.87358900 | -1.53536000 | H | 1.96242500 | 6.62012100 | -5.21525400 |
| C | -0.64939400 | -4.96555100 | -3.34191700 | H | 3.18993000 | 7.54554000 | -4.37838700 |
| C | -1.44026900 | -5.47955900 | -2.13450800 | H | 1.49005900 | 7.99783400 | -2.51671500 |
| C | -2.31672900 | -4.92749600 | 0.10819100 | H | 1.95730900 | 6.32000700 | -2.73612100 |
| C | -1.53984300 | -5.91742900 | 1.00145600 | H | 0.53797800 | 8.73655100 | -5.35893400 |
| C | -0.95806100 | -8.33234900 | 1.13390200 | H | -0.39975400 | 10.19564800 | 3.24240700 |
| C | -3.02996200 | -7.99386900 | -6.08606300 | H | 0.74965900 | 9.39582500 | 4.29234700 |
| C | -2.81247500 | -6.50292000 | -6.42568800 | H | 1.98558400 | 7.63068700 | 3.47287600 |
| C | -3.94387000 | -5.57447800 | -6.10602300 | H | -1.84493400 | 8.41951300 | 1.70170700 |
| C | -4.18060600 | -4.90082500 | -4.92628300 | H | 2.40786300 | 5.87664300 | 1.77908200 |
| C | -5.69268100 | -4.36310700 | -6.43025600 | H | -1.41805900 | 6.65940000 | 0.01478900 |
| C | 1.63510100 | 2.08227900 | 0.82598200 | H | 0.07230700 | 5.77051100 | -1.63963600 |
| C | 2.45419400 | 1.01899000 | 1.31050000 | H | -2.30481300 | 9.15093000 | 4.37347300 |
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| C | 0.28710200 | 1.78185100 | 0.50021500 | H | -4.28042800 | 7.43675800 | 4.02558200 |
| C | -0.14860300 | 0.46209600 | 0.43036300 | H | -7.85422600 | 6.53899600 | 3.11938000 |
| C | 0.76733200 | -0.63261100 | 0.65930800 | H | -3.72740200 | 6.51149800 | 1.94174900 |
| C | -13.29458000 | 4.68050400 | -3.01392600 | H | -8.47257100 | 5.46514500 | 0.96838200 |
| C | -11.80303500 | 4.38236600 | -2.73295400 | H | -4.34160600 | 5.47166200 | -0.19638900 |
| C | -11.46685900 | 3.58528300 | -1.46094700 | H | -7.75950100 | 4.56662300 | -1.02359300 |
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| C | 1.32317300 | -3.11588300 | 0.00917900 | H | -2.60254300 | 2.16965200 | 5.22298400 |
| O | -2.68431400 | -1.75600700 | -6.55231400 | H | -1.63562100 | 1.56377700 | 2.38759500 |
| O | -1.13442900 | 1.20606300 | -4.74870500 | H | -0.81512800 | 1.00768500 | 3.84160000 |
| O | -5.37126100 | -1.83209900 | -3.43232600 | H | -2.47645800 | 0.49198600 | 3.51012000 |
| O | 2.43133700 | -1.17447600 | -6.50512000 | H | -1.75778600 | 4.41660800 | 5.06808900 |
| O | -0.73861600 | 7.04604900 | -4.29240200 | H | -0.45354400 | 3.24331500 | 4.97239900 |
| O | -0.57704000 | 6.17042000 | -2.26819000 | H | -1.63306600 | 4.72203600 | 2.54490700 |
| O | 0.72215000 | 5.19288100 | -0.15424500 | H | -0.13713800 | 5.13527900 | 3.36664700 |
| O | -6.74761100 | 4.75129300 | -0.92387600 | H | -0.26621700 | 3.60527800 | 2.50445200 |
| O | 4.47089400 | -1.37869000 | -0.48405000 | H | -3.56273000 | 3.36666300 | 2.55956800 |
| O | 7.66790300 | 5.59121100 | -1.72136900 | H | 4.26873600 | -5.75100100 | 6.50652500 |
| O | 4.59186400 | 4.05720100 | -5.35243500 | H | 5.56305700 | -6.76398000 | 5.89394700 |
| O | 0.27293400 | 3.46395400 | -3.33999800 | H | 5.90398700 | -6.98851900 | 3.58048800 |
| O | 7.00178300 | 2.00969000 | -4.84468400 | H | 2.08488700 | -5.61278900 | 5.00164900 |
| O | 5.51467800 | 0.58879900 | -3.93242800 | H | 5.20399300 | -6.49892500 | 1.25118900 |

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|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 1.37656900 | -5.17318700 | 2.69589900 | H | 3.57278300 | -5.25383000 | -1.35517600 |
| H | 2.94279900 | -5.57639100 | 0.80255700 | H | 4.53671900 | -8.78256700 | -1.93609600 |
| H | 3.88356600 | -8.72640100 | 5.85061500 | H | 4.83283100 | -7.32340400 | -0.97267400 |
| H | 10.12724600 | 0.93944800 | 1.59332200 | H | 3.29548900 | -8.17625100 | -0.82363900 |
| H | 9.86248000 | -0.44939900 | 2.63023200 | H | 1.54182000 | -7.83359800 | -5.46567700 |
| H | 8.37348700 | 1.00376400 | 4.08564400 | H | -1.36090200 | -4.54476600 | -4.06678900 |
| H | 7.50949400 | 3.13921100 | 3.01655100 | H | 0.03930400 | -4.16515800 | -3.05815000 |
| H | 8.80011400 | 3.02206600 | 1.82008800 | H | -0.17786400 | -6.98533900 | -3.59631900 |
| H | 9.18739600 | 3.27250400 | 3.52880900 | H | -3.30641900 | -5.32034200 | -0.14360000 |
| H | 6.44731800 | 0.94443800 | 2.52767500 | H | -2.43029000 | -4.00119300 | 0.67197000 |
| H | 7.52423500 | 0.80118000 | 1.14038100 | H | -1.10997500 | -3.70450800 | -1.12260300 |
| H | 7.43108900 | -0.51543000 | 2.31632200 | H | 0.09802700 | -8.06196900 | 1.01816700 |
| H | 12.04786400 | 0.78825600 | 3.05740600 | H | -2.27041300 | -7.34521700 | -0.17131800 |
| H | 6.32954300 | 7.36566500 | 3.38256500 | H | -2.57984900 | -6.39845000 | -7.49086200 |
| H | 7.77865500 | 7.60894800 | 4.33829100 | H | -1.92424400 | -6.16642100 | -5.87868800 |
| H | 8.59250300 | 5.47037600 | 5.96975700 | H | -3.69078200 | -4.93521600 | -3.96605600 |
| H | 7.51139700 | 3.28134700 | 6.60121800 | H | -5.63664100 | -3.39863100 | -4.51934800 |
| H | 4.65115200 | 5.53654900 | 2.63089800 | H | -6.54948600 | -3.87244200 | -6.87035200 |
| H | 3.07209700 | 3.62736900 | 2.64629600 | H | -3.72146900 | -8.48643500 | -6.77405000 |
| H | 5.25453600 | 1.73323600 | 5.85164200 | H | -11.24883900 | 5.32623100 | -2.68837600 |
| H | 3.37013500 | 1.75212200 | 4.21796200 | H | -11.39703100 | 3.83473600 | -3.59405400 |
| H | 7.63445400 | 5.91807800 | 1.77159000 | H | -11.83718600 | 4.12714800 | -0.58107900 |
| H | 6.46959000 | -5.58791300 | -4.42587400 | H | -11.94098200 | 2.59930900 | -1.48023600 |
| H | 6.63050200 | -6.58814700 | -2.99342900 | H | -13.89432300 | 3.76495700 | -3.05773100 |
| H | 6.65131500 | -5.35617700 | -0.66760800 | H | 1.18998100 | 0.27112000 | -4.62619400 |
| H | 5.73155300 | -3.35705000 | -4.35548100 | H | 1.55652600 | -2.60935900 | -3.64431300 |
| H | 5.57036600 | -3.50975400 | 0.59484800 | H | 2.85598400 | -1.50442400 | -4.02408800 |
| H | 4.76913700 | -1.47007100 | -3.09356000 | H | 1.30401600 | 4.40407700 | 0.20106100 |
| H | 3.68046600 | -1.07990000 | -1.02488200 | H | 3.43667200 | 1.23757300 | 1.71087500 |
| H | 8.75101200 | -4.49569900 | -3.74635900 | H | 3.68693800 | -1.27626000 | 1.14915200 |
| H | 7.95043900 | -3.28047700 | 2.07541100 | H | -0.38179700 | 2.59552600 | 0.24592500 |
| H | 7.26010000 | -4.86402700 | 2.36282900 | H | -1.16615400 | -1.12083500 | -0.47043600 |
| H | 7.07077200 | -4.44304600 | 4.75412000 | H | -5.38104100 | 3.79391300 | -1.66026700 |
| H | 8.21887500 | -1.65775900 | 4.17531800 | H | 5.86603200 | 0.96257100 | -3.03599500 |
| H | 7.49515100 | -2.16045200 | 5.70650600 | H | 2.36848700 | -2.97231500 | 0.25020100 |
| H | 8.99575600 | -2.91393600 | 5.15101600 | H | 0.84264200 | -3.67279300 | 0.82354900 |
| H | 5.87306600 | -2.16711100 | 3.07956400 | H | 1.23684500 | -3.70147500 | -0.90725100 |
| H | 5.27386100 | -2.72006700 | 4.64551700 | H | 3.94104400 | 3.15534200 | 0.32633700 |
| H | 5.18641400 | -3.79284200 | 3.24669700 | H | -0.75821600 | -1.85758300 | -4.06391800 |
| H | 10.03932600 | -3.89454400 | 3.26860200 | H | -13.73205500 | 5.34593000 | -2.26234100 |
| H | 8.67555100 | 1.60698300 | -1.49994000 | H | -13.32929900 | 5.16900700 | -3.99273100 |
| H | 8.78752200 | 2.98468600 | -0.40966100 | H | -5.33285400 | 5.08940700 | 4.58619800 |
| H | 6.38621900 | 4.06838600 | 0.57879900 | H | -4.82377000 | 6.11795600 | 5.99300900 |
| H | 3.85266200 | 1.31096300 | -1.36300800 | H | -4.37432100 | 2.21517000 | 3.66813700 |
| H | 8.59139900 | 2.94363800 | -3.43963700 | H | -3.95181400 | 3.89409400 | 4.22352500 |
| H | 5.37351700 | 5.74112000 | -2.61351000 | H | -1.25694400 | 7.95818800 | 5.15260900 |
| H | 6.85246600 | 3.82604800 | -4.22660600 | H | -1.13446500 | 9.71151700 | 5.60046600 |
| H | 1.25598900 | 1.78902900 | -2.57390500 | H | -4.83491700 | 4.56145900 | -4.67468600 |
| H | 1.60736700 | 3.32778900 | -1.80453700 | H | -3.28506800 | 5.03096700 | -5.48340900 |
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| H | 3.27494600 | 2.08916500 | -3.62104900 | H | 2.03508600 | 8.73070500 | -6.29718800 |
| H | 3.62465100 | 4.33141000 | -2.38092500 | H | 8.31995900 | 7.53817500 | 1.93339300 |
| H | 4.55002300 | 0.45866400 | -6.23283700 | H | 9.07756900 | 6.14688900 | 2.76211700 |
| H | 6.07634700 | -0.35857900 | -6.36570100 | H | 5.61038100 | 6.28786300 | -4.27749000 |
| H | 6.97571900 | 2.01138200 | -7.28235300 | H | 2.28517200 | 3.04324600 | -4.71004900 |
| H | 1.63145200 | -8.07766100 | -2.92569600 | H | 9.66921300 | 3.90292700 | -2.39809200 |
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| H | 4.31550800 | -6.67587600 | -3.29455700 | H | 6.16163100 | 0.83250700 | -8.33664400 |
| H | 1.95659200 | -5.97288800 | -1.47937600 | H | -0.08101500 | -1.76327500 | -8.80825400 |
| H | 2.62440000 | -4.98429500 | -2.79792700 | H | 0.05430200 | -3.41436400 | -8.18228900 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -5.10056100 | -0.02434900 | -7.59102000 | C | -7.69703800 | -1.80459800 | 0.50237700 |
| H | -4.79821600 | -1.72407200 | -8.05660100 | O | -6.88861000 | -2.54888800 | -0.07365100 |
| H | -3.41309000 | -8.08244400 | -5.06524900 | C | -7.01475300 | 0.09972100 | -1.08225800 |
| H | -2.04272200 | -8.46478900 | -6.13060200 | O | -6.99086800 | 1.50599200 | -1.19208300 |
| H | 3.01890300 | -6.85234100 | -5.37373800 | N | -8.43717300 | -2.20238100 | 1.55197100 |
| H | 8.78585900 | -6.19202200 | -4.28846600 | C | -8.52679700 | -3.56675900 | 2.05269900 |
| H | 8.87340000 | -5.81835300 | -2.55684900 | C | -7.44964300 | -3.99811000 | 3.08369500 |
| H | -1.21256500 | -9.11906600 | 0.41581600 | C | -6.19354400 | -4.56628800 | 2.42290000 |
| H | -1.08631200 | -8.68388200 | 2.16368100 | O | -7.15595500 | -2.94502500 | 4.00142800 |
| H | 2.76355800 | -7.70631000 | 6.76382600 | C | -9.83797300 | -4.87334900 | 9.32314900 |
| H | 4.39368600 | -8.10229400 | 7.42559400 | C | -8.91269800 | -3.83428000 | 8.67409200 |
| H | 9.64894800 | -5.16273300 | 2.09652600 | C | -8.65631300 | -4.02268900 | 7.17863400 |
| H | 9.33384200 | -5.42082200 | 3.81405300 | O | -9.12029200 | -4.92350500 | 6.50552200 |
| H | 11.07137300 | 0.57269100 | 4.49414700 | O | -7.84929500 | -3.06045000 | 6.71420000 |
| H | 11.12889900 | 2.16634000 | 3.64776800 | C | -1.21293600 | -2.56992100 | 5.42615500 |
| H | -2.33064400 | 1.25317900 | -0.45285000 | C | -0.04475700 | -3.30142000 | 6.08565900 |
| H | -7.29209500 | 1.41457500 | 0.85465000 | O | 0.38153300 | -4.36830500 | 5.66007800 |
| H | -8.98255900 | -0.31330000 | -0.40038000 | C | -1.18802700 | -2.60577100 | 3.88238400 |
| H | -9.16025000 | -1.54759600 | 1.76901500 | C | -2.51357900 | -2.17434700 | 3.31644100 |
| H | -5.54565000 | -4.85294800 | 3.19601700 | C | -3.79060800 | -2.29926400 | 3.82017600 |
| H | -6.49224800 | -5.51494300 | 1.84715700 | N | -2.68489000 | -1.53881100 | 2.09266000 |
| H | -5.79386200 | -3.89508000 | 1.71672400 | C | -4.02067200 | -1.29405800 | 1.93663600 |
| H | -8.03096600 | -4.80351200 | 3.59962200 | N | -4.72194600 | -1.74967000 | 2.96028900 |
| H | -6.56735100 | -2.39144700 | 3.56591900 | N | 0.45129900 | -2.72583500 | 7.23350200 |
| H | -7.90894800 | 1.88138200 | -1.33393700 | C | 1.74824000 | -3.13402200 | 7.76364300 |
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| H | -0.50006400 | -2.01069300 | 3.53795100 | O | 2.32511800 | -0.75635600 | 7.61591900 |
| H | -1.04963900 | -3.67823100 | 3.56171600 | N | -4.47228100 | 3.26430000 | -1.67906400 |
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| H | -4.54802500 | -0.80167400 | 1.17265000 | N | -4.45320400 | -2.30843400 | -1.43120700 |
| H | -7.72860500 | -3.19970600 | 5.63756400 | N | -0.48849000 | -1.06820200 | -4.24686100 |
| H | 0.25094800 | -1.83230400 | 7.33226500 | N | 0.22930600 | -1.98228900 | -6.70424300 |
| H | 1.96524900 | -1.81631900 | 9.31500700 | N | 7.11368600 | 4.00929600 | 5.85600300 |
| H | 4.44548000 | -2.60954600 | 7.68963600 | N | 5.89929500 | 1.71096100 | -1.66705500 |
| H | 4.42599200 | -1.55813800 | 9.12024700 | N | 4.77365400 | 2.89832900 | -0.18440400 |
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| H | -10.85502000 | -4.94282600 | 8.75091300 | N | -4.93099100 | -5.32832200 | -6.96621200 |
| H | -9.47955500 | -5.99792400 | 9.06218300 | N | -5.36389500 | -4.22290300 | -5.08310800 |
| H | -9.56949600 | -3.68663700 | 2.33850500 | C | -3.79109200 | 4.37488400 | -4.71968900 |
| H | -8.48656600 | -4.27808900 | 1.06816100 | C | -3.21536600 | 4.77203400 | -3.34865500 |
| H | -5.96653000 | -0.18660500 | -0.86640600 | C | -3.31659100 | 3.68378100 | -2.33017200 |
| H | -7.23837000 | -0.35654500 | -2.06258900 | C | -2.32427200 | 2.84761800 | -1.89091700 |
| H | 2.32172900 | -3.62249900 | 6.86823900 | C | -4.17795200 | 2.23617500 | -0.87020500 |
| H | -2.18066600 | -3.19737800 | 5.81837400 | C | -4.95197700 | -1.13276700 | -7.16819700 |
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| H | 2.71365600 | -1.03540000 | 6.72005100 | C | -1.40465400 | -0.08388900 | -4.40269200 |
| | | | | C | -3.02697200 | -1.81916200 | -3.33961300 |
| | | | | C | -4.41113000 | -1.99883700 | -2.73864200 |
| C | -8.77570600 | 2.00061300 | 2.90399800 | C | 0.91910600 | -0.95548000 | -4.57809900 |
| C | -8.93636300 | 0.85115200 | 1.94111300 | C | 1.26188000 | -1.47998800 | -5.99151700 |
| O | -9.91490300 | 0.09637400 | 2.01056800 | C | 1.79249700 | -1.68587000 | -3.54563100 |
| N | -7.88735100 | 0.61208100 | 1.11716700 | C | 0.76111600 | -1.76367400 | -0.45382800 |
| C | -7.98242300 | -0.35883600 | 0.02859300 | C | 0.40271000 | -2.49864300 | -8.04520100 |

Int2

| | | | |
|---|-------------|-------------|------------|
| C | -8.77570600 | 2.00061300 | 2.90399800 |
| C | -8.93636300 | 0.85115200 | 1.94111300 |
| O | -9.91490300 | 0.09637400 | 2.01056800 |
| N | -7.88735100 | 0.61208100 | 1.11716700 |
| C | -7.98242300 | -0.35883600 | 0.02859300 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 1.57208100 | 8.68481900 | -5.39207000 | C | 5.80301900 | -2.97756500 | 3.76855700 |
| C | 2.06538700 | 7.43274900 | -4.64441300 | C | 8.61540000 | 3.51178300 | -2.58877800 |
| C | 1.39972800 | 7.12578000 | -3.29680100 | C | 7.65614400 | 4.69345200 | -2.66046100 |
| C | -0.06386500 | 6.71816700 | -3.40254700 | C | 8.26449700 | 2.61761600 | -1.36680800 |
| C | -1.32396600 | 9.05802700 | 4.69024000 | C | 6.79224300 | 2.55544800 | -1.02933400 |
| C | -0.21130200 | 9.29825300 | 3.63978000 | C | 6.09281500 | 3.29886600 | -0.09839400 |
| C | 0.02401200 | 8.19693800 | 2.63067300 | C | 4.70634600 | 1.93860100 | -1.13440500 |
| C | -0.91570900 | 7.88660500 | 1.63776200 | C | 5.53994800 | 5.37038000 | -3.71382200 |
| C | 1.22276100 | 7.47296000 | 2.63571700 | C | 4.46242100 | 4.43681200 | -4.26821600 |
| C | -0.67638200 | 6.89023100 | 0.69596400 | C | 2.61616300 | 2.95472600 | -3.71810900 |
| C | 1.48427700 | 6.47844200 | 1.69484700 | C | 1.38806900 | 2.83850100 | -2.81601300 |
| C | 0.52952200 | 6.17068800 | 0.71895100 | C | 5.97923500 | 1.42345500 | -7.51559200 |
| C | -5.51080100 | 6.08477000 | 5.08920000 | C | 5.58864400 | 0.57538800 | -6.30099200 |
| C | -5.34640400 | 7.17957100 | 4.00367700 | C | 6.05825400 | 1.14626700 | -4.98575400 |
| C | -5.75629000 | 6.63477100 | 2.64718500 | C | 2.07801300 | -7.17983900 | -4.74313000 |
| C | -7.09064600 | 6.32675800 | 2.34584300 | C | 1.24392000 | -5.91342500 | -4.50609800 |
| C | -4.78955000 | 6.29447700 | 1.69260100 | C | 2.48428900 | -7.90492900 | -3.44110400 |
| C | -7.45305800 | 5.68883400 | 1.15924600 | C | 3.50565600 | -7.14766300 | -2.57018700 |
| C | -5.13038300 | 5.66710000 | 0.49588600 | C | 2.96494800 | -5.83934200 | -1.97957100 |
| C | -6.46744000 | 5.33927200 | 0.21902500 | C | 4.02414700 | -8.05453000 | -1.44797800 |
| C | -3.67165100 | 3.09027100 | 3.58288900 | C | -0.66405200 | -4.99219200 | -3.23985500 |
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| C | -1.30546200 | 3.69484900 | 4.35769400 | C | -2.28894900 | -4.90074400 | 0.22543600 |
| C | -1.80354700 | 1.38047400 | 3.38934900 | C | -1.50656300 | -5.89637600 | 1.10677400 |
| C | -0.82590700 | 4.34937500 | 3.06637000 | C | -0.95715200 | -8.31224900 | 1.25942900 |
| C | 3.83910100 | -7.76553500 | 6.62498500 | C | -3.05680700 | -8.07339600 | -5.95650300 |
| C | 4.49706200 | -6.53747500 | 5.95810200 | C | -2.84263600 | -6.58725400 | -6.31678000 |
| C | 4.08918800 | -6.27537600 | 4.52632700 | C | -3.98082000 | -5.66069300 | -6.01796200 |
| C | 4.96248900 | -6.56413600 | 3.46990300 | C | -4.23712400 | -4.98293400 | -4.84476400 |
| C | 2.83487200 | -5.72863800 | 4.23149900 | C | -5.73079900 | -4.46048600 | -6.37308100 |
| C | 4.59685500 | -6.29660900 | 2.14866100 | C | 1.62432300 | 2.09041100 | 0.79282000 |
| C | 2.46240000 | -5.46561200 | 2.91339300 | C | 2.44330400 | 1.03742200 | 1.28601800 |
| C | 3.34646900 | -5.74338600 | 1.86825200 | C | 2.04564000 | -0.28382000 | 1.14890400 |
| C | 11.09089700 | 1.15030700 | 3.47813900 | C | 0.28848200 | 1.76929700 | 0.43963400 |
| C | 9.91463800 | 0.70221800 | 2.59645900 | C | -0.11991700 | 0.43774600 | 0.33302500 |
| C | 8.53953200 | 1.27321500 | 2.98848500 | C | 0.81331900 | -0.63624100 | 0.54169000 |
| C | 8.48988600 | 2.79477700 | 2.80504000 | C | -13.33273300 | 4.62258700 | -3.01414700 |
| C | 7.41755800 | 0.60608700 | 2.18048600 | C | -11.83893500 | 4.33070400 | -2.73598100 |
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| C | 7.24787300 | 6.95144900 | 3.58543200 | C | -9.96632100 | 3.36584600 | -1.30598600 |
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| C | 7.68003100 | 5.19873300 | 5.42100100 | O | -2.71822600 | -1.83700400 | -6.52474200 |
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| C | 5.98920900 | 3.73959900 | 5.10103000 | O | -5.43798800 | -1.88076700 | -3.42849900 |
| C | 4.76599700 | 4.77995100 | 3.27167400 | O | 2.42565000 | -1.42523200 | -6.38745200 |
| C | 5.10550000 | 2.65664700 | 5.13734900 | O | -0.77096600 | 6.96672200 | -4.36051100 |
| C | 3.87620400 | 3.71430500 | 3.30938400 | O | -0.58467500 | 6.10689800 | -2.33162400 |
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| C | 8.40542400 | -5.53757900 | -3.45588300 | O | -6.76578200 | 4.70549800 | -0.94260100 |
| C | 6.87249200 | -5.62632700 | -3.35149200 | O | 4.64761800 | -1.26866500 | -0.45219700 |
| C | 6.26425800 | -4.49552800 | -2.55871600 | O | 7.63792400 | 5.58828700 | -1.81500100 |
| C | 5.72501100 | -3.39314900 | -3.23090200 | O | 4.55648800 | 3.98484400 | -5.40597400 |
| C | 6.26338400 | -4.47781000 | -1.15794900 | O | 0.22958900 | 3.40776600 | -3.42563900 |
| C | 5.20209400 | -2.30669600 | -2.54115600 | O | 6.97203700 | 1.96165000 | -4.89116000 |
| C | 5.71836700 | -3.40782600 | -0.44601400 | O | 5.43436800 | 0.61796700 | -3.94750700 |
| C | 5.18519300 | -2.32072800 | -1.14387300 | O | 1.58459100 | -4.80065100 | -4.89543600 |
| C | 9.31308900 | -4.60902700 | 3.05351700 | O | -1.94958600 | -6.61355700 | -2.01385300 |
| C | 7.90170000 | -4.03770900 | 2.84586500 | O | -0.67591700 | -5.52862200 | 1.93070300 |
| C | 7.20009800 | -3.51328800 | 4.11214200 | O | 2.11279300 | 3.31409400 | 0.69198900 |
| C | 8.02766400 | -2.44575900 | 4.84009100 | O | 2.86875400 | -1.29794600 | 1.58513400 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| O | -1.37864000 | 0.09856200 | -0.02546800 | H | 8.36876900 | 1.05050200 | 4.05396800 |
| O | -9.50980900 | 2.19182300 | -1.35830900 | H | 7.48353000 | 3.17563600 | 2.98175900 |
| O | -9.29656400 | 4.43562700 | -1.16615900 | H | 8.77104600 | 3.06496600 | 1.78068300 |
| O | -0.51918800 | -2.01776400 | -0.95138900 | H | 9.16191300 | 3.32330200 | 3.48724500 |
| S | 1.83766500 | -0.82380000 | -1.92807300 | H | 6.43690700 | 0.96952600 | 2.50383200 |
| H | -3.69869800 | 5.68501300 | -2.98274800 | H | 7.50924100 | 0.82975800 | 1.11295300 |
| H | -2.15902200 | 5.01105000 | -3.44067100 | H | 7.43191700 | -0.48303300 | 2.29399800 |
| H | -1.28167700 | 2.84565800 | -2.16687600 | H | 12.04014900 | 0.85678100 | 3.01336600 |
| H | -4.89842800 | 1.74003400 | -0.24627100 | H | 6.31064800 | 7.42725000 | 3.27141100 |
| H | -3.56335000 | 3.32336400 | -4.92961500 | H | 7.76288800 | 7.68596700 | 4.21808600 |
| H | -5.81764300 | -1.42821300 | -6.56727400 | H | 8.58152600 | 5.57733300 | 5.88203500 |
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| H | -5.36509800 | -2.41496400 | -0.96728500 | H | 3.04835200 | 3.67682700 | 2.60926100 |
| H | -3.60736600 | -2.36305000 | -0.88611200 | H | 5.23863600 | 1.84259200 | 5.84451700 |
| H | -3.15850000 | 0.33877600 | -3.34564500 | H | 3.34795600 | 1.83417900 | 4.21712000 |
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| H | 1.46896000 | -2.49595400 | -8.27214500 | H | 6.43874500 | -5.61917700 | -4.35807700 |
| H | -0.72080500 | -1.90303300 | -6.35852900 | H | 6.60519600 | -6.59344700 | -2.90748600 |
| H | 1.91900600 | 6.56011000 | -5.29008300 | H | 6.67774400 | -5.32138700 | -0.60959600 |
| H | 3.14771400 | 7.50782000 | -4.47926100 | H | 5.71672100 | -3.37915700 | -4.31758800 |
| H | 1.44216700 | 7.99180100 | -2.62073600 | H | 5.68182600 | -3.41632200 | 0.63794700 |
| H | 1.94390200 | 6.31943900 | -2.79416000 | H | 4.83973500 | -1.43749000 | -3.07647900 |
| H | 0.48341800 | 8.66822400 | -5.46287400 | H | 3.87416300 | -0.94464500 | -0.97546100 |
| H | -0.42588300 | 10.24047800 | 3.11673900 | H | 8.73056000 | -4.52501800 | -3.70832200 |
| H | 0.72952700 | 9.46476400 | 4.17779900 | H | 7.94790900 | -3.22945200 | 2.10307900 |
| H | 1.97355100 | 7.69099700 | 3.39199300 | H | 7.26066600 | -4.81188700 | 2.40715100 |
| H | -1.85526300 | 8.43358800 | 1.59755200 | H | 7.07429700 | -4.36909000 | 4.79345000 |
| H | 2.41253300 | 5.91938500 | 1.72139000 | H | 8.21477700 | -1.58640900 | 4.18657000 |
| H | -1.41204100 | 6.65577900 | -0.06477700 | H | 7.49546200 | -2.07639900 | 5.72397400 |
| H | 0.07117600 | 5.73777200 | -1.68856900 | H | 8.99685100 | -2.83134500 | 5.17252700 |
| H | -2.32316300 | 9.20993300 | 4.27104200 | H | 5.87013800 | -2.10998500 | 3.10208300 |
| H | -5.92290400 | 8.07651800 | 4.26456000 | H | 5.27171800 | -2.65460100 | 4.67127700 |
| H | -4.29576900 | 7.48656600 | 3.95323900 | H | 5.18752600 | -3.73640000 | 3.27944200 |
| H | -7.87020500 | 6.58047500 | 3.06181600 | H | 10.04025000 | -3.82733600 | 3.29376300 |
| H | -3.74233500 | 6.51389100 | 1.88881100 | H | 8.63899800 | 1.60452600 | -1.54131200 |
| H | -8.49062400 | 5.46561900 | 0.93198800 | H | 8.76203200 | 3.00040300 | -0.47114300 |
| H | -4.35848300 | 5.42938100 | -0.22712700 | H | 6.41598300 | 4.05925800 | 0.59233300 |
| H | -7.77749300 | 4.52624600 | -1.04075000 | H | 3.78877400 | 1.43204500 | -1.39143100 |
| H | -6.53737600 | 6.05708400 | 5.47010700 | H | 8.55449000 | 2.91690400 | -3.50024400 |
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| H | -1.66137000 | 1.61663600 | 2.33251800 | H | 6.81403000 | 3.79085400 | -4.29402900 |
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| H | -2.50356800 | 0.54507800 | 3.45565000 | H | 1.54396900 | 3.36054600 | -1.86848200 |
| H | -1.73969900 | 4.46454700 | 5.01268400 | H | -0.13001000 | 2.74575200 | -4.04152700 |
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| H | -0.15274100 | 5.17939800 | 3.28217900 | H | 4.51506000 | 0.37358100 | -6.24635800 |
| H | -0.28526500 | 3.64411700 | 2.43045400 | H | 6.05840000 | -0.41695800 | -6.36106900 |
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| H | 5.58522100 | -6.67165400 | 5.99107000 | H | 2.91893800 | -8.87306500 | -3.72178500 |
| H | 5.94312000 | -6.98255600 | 3.68629200 | H | 4.35462200 | -6.89278200 | -3.21844100 |
| H | 2.14028600 | -5.48976100 | 5.02971700 | H | 2.04953600 | -6.02273100 | -1.40435500 |
| H | 5.29068000 | -6.50817300 | 1.33970900 | H | 2.75177300 | -5.09798900 | -2.74944700 |
| H | 1.48150800 | -5.05447000 | 2.70751100 | H | 3.70357400 | -5.39025300 | -1.31267500 |
| H | 3.06386800 | -5.52431600 | 0.84522500 | H | 4.43116700 | -8.99464900 | -1.83823600 |
| H | 3.90240600 | -8.63663100 | 5.96444500 | H | 4.81265700 | -7.55219500 | -0.87917900 |
| H | 10.11186500 | 0.98910800 | 1.55412700 | H | 3.22188000 | -8.30049800 | -0.74193500 |
| H | 9.86525500 | -0.39476600 | 2.60237600 | H | 1.50007000 | -7.86371000 | -5.37768400 |

| | | | | | | | |
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| H | -1.37841700 | -4.59675600 | -3.97645700 | H | 8.76241400 | -6.22701800 | -4.22770800 |
| H | 0.01520400 | -4.18069600 | -2.97267500 | H | 8.85578100 | -5.83022500 | -2.50154700 |
| H | -0.19836500 | -7.01771100 | -3.47666200 | H | -1.21294700 | -9.10889300 | 0.55282400 |
| H | -3.28500100 | -5.28638200 | -0.01270600 | H | -1.08091800 | -8.65030400 | 2.29426200 |
| H | -2.38962900 | -3.97284100 | 0.78982600 | H | 2.78444700 | -7.60492700 | 6.86642900 |
| H | -1.08171200 | -3.69107200 | -1.04101000 | H | 4.41776900 | -7.98921200 | 7.52721600 |
| H | 0.09914100 | -8.04535200 | 1.13702500 | H | 9.64762800 | -5.11147000 | 2.13974400 |
| H | -2.28426500 | -7.32634100 | -0.03526100 | H | 9.33944800 | -5.34727000 | 3.86172700 |
| H | -2.60400200 | -6.49734500 | -7.38192600 | H | 11.06866800 | 0.65780200 | 4.45558900 |
| H | -1.95913100 | -6.23886600 | -5.76914000 | H | 11.12012500 | 2.24016200 | 3.58790800 |
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| H | -5.70607100 | -3.48358000 | -4.46991600 | H | -7.31393300 | 1.41324300 | 0.86825400 |
| H | -6.58344600 | -3.97584200 | -6.82764800 | H | -9.01173100 | -0.33470700 | -0.35255400 |
| H | -3.74976200 | -8.57591900 | -6.63572500 | H | -9.12104300 | -1.52324200 | 1.89077800 |
| H | -11.28657500 | 5.27620400 | -2.70490600 | H | -5.45003200 | -4.82548400 | 3.18155500 |
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| H | -13.93080500 | 3.70537900 | -3.04339000 | H | -6.48173200 | -2.35254200 | 3.59322400 |
| H | 1.16720300 | 0.10801600 | -4.58068000 | H | -7.93242400 | 1.84706700 | -1.32447700 |
| H | 1.46722700 | -2.72376000 | -3.43569600 | H | -9.31021800 | -2.82048800 | 8.80369400 |
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| H | 3.40803700 | 1.26337600 | 1.72517800 | H | -0.94408700 | -3.62203700 | 3.55151000 |
| H | 3.74985000 | -1.18692500 | 1.18250300 | H | -4.10637300 | -2.75544700 | 4.74656000 |
| H | -0.39437800 | 2.57442600 | 0.19349800 | H | -1.97326100 | -1.11972400 | 1.48344700 |
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| H | -5.39742100 | 3.72144800 | -1.66261700 | H | -7.67537300 | -3.14352200 | 5.73930100 |
| H | 5.79158100 | 1.01538900 | -3.05912300 | H | 0.25908500 | -1.73855100 | 7.35081100 |
| H | 2.46756600 | -2.96736600 | 0.13389300 | H | 1.95022300 | -1.68138200 | 9.34608800 |
| H | 0.88934700 | -3.60045900 | 0.62975400 | H | 4.45747400 | -2.47805700 | 7.76487800 |
| H | 1.39528900 | -3.71256100 | -1.07016200 | H | 4.41114100 | -1.40788000 | 9.18086000 |
| H | 3.93759700 | 3.21026300 | 0.33907700 | H | 4.01580300 | -3.13281900 | 9.34935500 |
| H | -0.80137500 | -1.97597400 | -3.94429700 | H | -9.95795000 | -4.66113900 | 10.38947700 |
| H | -13.76822300 | 5.29707200 | -2.26953200 | H | -9.60767700 | 1.91580100 | 3.60771500 |
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| H | -1.14945100 | 9.78901600 | 5.48660400 | H | -5.99778600 | -0.22062800 | -0.83213200 |
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| H | -3.33323000 | 4.95783200 | -5.52590900 | H | 2.35244800 | -3.51592100 | 6.92793000 |
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| H | 9.05827700 | 6.20497500 | 2.65724000 | H | 2.71984100 | -0.93144000 | 6.74847400 |
| H | 5.56440100 | 6.24629700 | -4.37045300 | | | | |
| H | 2.24346900 | 2.99036900 | -4.74730200 | | | | |
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| H | 5.21463800 | 2.17908200 | -7.72291100 | | | | |
| H | 6.11026500 | 0.73846900 | -8.35885800 | | | | |
| H | -0.12939800 | -1.87433500 | -8.77232900 | | | | |
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| H | -3.43593200 | -8.14907600 | -4.93316200 | | | | |
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| H | 2.99260400 | -6.91184200 | -5.28230100 | | | | |

Int3

| | | | |
|---|-------------|-------------|-------------|
| C | -8.91398400 | 1.69596400 | 2.99635200 |
| C | -8.88779900 | 0.61285200 | 1.94716400 |
| O | -9.63948500 | -0.36426200 | 1.99143700 |
| N | -7.85442100 | 0.69409900 | 1.06572300 |
| C | -7.71968800 | -0.32842300 | 0.04501000 |
| C | -6.99161900 | -1.53361100 | 0.67917100 |
| O | -5.74417200 | -1.66773100 | 0.55953400 |
| C | -6.94946000 | 0.26886800 | -1.16471000 |
| O | -7.06835500 | 1.66977200 | -1.22725100 |
| N | -7.74869100 | -2.39718400 | 1.34735100 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -7.28978700 | -3.69944500 | 1.83854000 | C | -0.46924100 | 9.09598000 | 4.17028500 |
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| C | -7.38615300 | -5.52115000 | 3.54445000 | C | -1.06884900 | 7.82157800 | 2.04541000 |
| O | -6.69273400 | -3.26392300 | 4.12721000 | C | 1.01786700 | 7.34074200 | 3.11982200 |
| C | -9.86684400 | -5.54379700 | 9.01736600 | C | -0.77745500 | 6.89356300 | 1.04936800 |
| C | -9.12598800 | -4.34850000 | 8.39680500 | C | 1.33114600 | 6.41395500 | 2.12691400 |
| C | -8.42846900 | -4.61376000 | 7.02474000 | C | 0.42892900 | 6.17764600 | 1.08455200 |
| O | -8.45306200 | -5.78381700 | 6.58264600 | C | -5.72362700 | 5.70690500 | 5.41445000 |
| O | -7.89589400 | -3.58152900 | 6.50351700 | C | -5.57667800 | 6.87650300 | 4.40969700 |
| C | -1.09367600 | -4.15777400 | 5.07511400 | C | -5.97398100 | 6.42743000 | 3.01649800 |
| C | 0.03074400 | -4.50047600 | 6.05146500 | C | -7.29391300 | 6.07040200 | 2.70556000 |
| O | 0.51981100 | -5.62282300 | 6.15049500 | C | -5.00622100 | 6.23377500 | 2.02374600 |
| C | -0.58772200 | -3.28468000 | 3.91294700 | C | -7.63971100 | 5.52040300 | 1.47180600 |
| C | -1.68484000 | -2.74469800 | 3.05315800 | C | -5.33153400 | 5.69790000 | 0.77918800 |
| C | -3.05547200 | -2.85335100 | 3.09527500 | C | -6.65140500 | 5.31466500 | 0.49323300 |
| N | -1.40312100 | -1.93005700 | 1.96445800 | C | -3.83081400 | 2.83344200 | 3.74710600 |
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| N | 0.46528800 | -3.45447800 | 6.81085900 | C | -1.94255200 | 1.23135300 | 3.23215300 |
| C | 1.68983900 | -3.52133200 | 7.58582400 | C | -1.10381300 | 4.26889700 | 3.25611700 |
| C | 1.86817600 | -2.21492600 | 8.36172300 | C | 3.86180500 | -8.04565100 | 6.19414800 |
| C | 3.22072400 | -2.14967500 | 9.06181100 | C | 4.46171900 | -6.76548500 | 5.57613400 |
| O | 1.66331600 | -1.08912600 | 7.50192800 | C | 4.06250100 | -6.51413800 | 4.13923900 |
| N | -4.60316500 | 3.38274600 | -1.41562600 | C | 5.01945400 | -6.54791100 | 3.11784300 |
| N | -2.96857800 | 2.05132700 | -0.91814800 | C | 2.72848000 | -6.25005900 | 3.79913600 |
| N | -3.78713200 | -0.11337600 | -5.21750700 | C | 4.66180000 | -6.29908000 | 1.79062400 |
| N | -4.08342300 | -2.29993100 | -1.55603800 | C | 2.36554600 | -6.01029700 | 2.47383300 |
| N | -0.39989100 | -0.77455200 | -4.28054200 | C | 3.33402200 | -6.02296600 | 1.46674300 |
| N | 0.22252800 | -1.58724000 | -6.79668600 | C | 10.96294800 | 1.15571600 | 3.56908700 |
| N | 7.04136900 | 3.80970500 | 6.09682600 | C | 9.81233700 | 0.73383900 | 2.64372300 |
| N | 5.79186500 | 1.79331200 | -1.43867100 | C | 8.41575400 | 1.25600900 | 3.02688000 |
| N | 4.60516800 | 3.03853300 | -0.04828700 | C | 8.33876900 | 2.78433000 | 2.93411800 |
| N | 6.60341300 | 4.94668900 | -3.40899200 | C | 7.34167000 | 0.61775400 | 2.13668400 |
| N | 3.27093500 | 4.37635600 | -3.17387700 | C | 7.88526300 | 6.66267900 | 2.75439200 |
| N | 0.12875800 | -5.83650000 | -4.11000700 | C | 7.02025300 | 6.87490700 | 3.99196600 |
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| N | -1.76802200 | -7.23979600 | 0.43105400 | C | 7.54158400 | 5.05168200 | 5.73338700 |
| N | -4.91371300 | -4.96283200 | -7.24003000 | C | 5.72114000 | 4.64173800 | 4.47040700 |
| N | -5.36466700 | -4.02187900 | -5.27386900 | C | 5.92851500 | 3.52712700 | 5.33050200 |
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| C | -4.26072600 | 2.30441700 | -0.69767000 | C | 8.40291200 | -5.17825500 | -3.73469900 |
| C | -5.02267300 | -0.80154500 | -7.22636300 | C | 6.86770300 | -5.20040900 | -3.60626800 |
| C | -3.75020300 | -0.84270700 | -6.37501300 | C | 6.36738500 | -4.12533800 | -2.66626800 |
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| C | 1.24408900 | -0.98518100 | -6.14970500 | C | 9.28517600 | -4.60044100 | 2.81816000 |
| C | 1.93913200 | -1.36813300 | -3.78843200 | C | 7.87620000 | -4.01964700 | 2.64697200 |
| C | 0.94034400 | -1.69156300 | -0.87960800 | C | 7.18920400 | -3.53945200 | 3.93816300 |
| C | 0.35590300 | -2.02390200 | -8.16622300 | C | 8.02021700 | -2.48859500 | 4.68592900 |
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| C | 1.86649800 | 7.74103100 | -4.20349300 | C | 8.45492500 | 3.81223700 | -2.36038100 |
| C | 1.21310300 | 7.35146500 | -2.87077400 | C | 7.47352000 | 4.97630600 | -2.36538400 |
| C | -0.21717700 | 6.84878300 | -3.01547000 | C | 8.11872600 | 2.84360900 | -1.19279700 |
| C | -1.58792200 | 8.76908100 | 5.19263600 | C | 6.64598800 | 2.72566300 | -0.85829800 |

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|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 5.90741700 | 3.49545800 | 0.01710500 | H | -3.99949800 | 5.84174100 | -2.69885900 |
| C | 4.57831300 | 2.01983600 | -0.93205400 | H | -2.40038900 | 5.28978900 | -3.13968800 |
| C | 5.35021200 | 5.67654000 | -3.38836300 | H | -1.45078700 | 3.00461500 | -2.14184300 |
| C | 4.29572100 | 4.74595500 | -3.98797200 | H | -4.92856500 | 1.75599800 | -0.05880100 |
| C | 2.46872700 | 3.21518600 | -3.53502000 | H | -3.69420200 | 3.54350500 | -4.70458200 |
| C | 1.21520900 | 3.02228600 | -2.67978400 | H | -5.87320400 | -1.14541600 | -6.63083000 |
| C | 5.86307300 | 1.95703700 | -7.40419200 | H | -2.92185100 | -2.47730500 | -4.48555500 |
| C | 5.47522600 | 1.04294100 | -6.23918000 | H | -2.11975600 | -2.05658500 | -2.96465800 |
| C | 5.91591600 | 1.56589700 | -4.89840000 | H | -4.86789100 | -2.22378900 | -0.90442500 |
| C | 2.10677800 | -6.85408800 | -5.12723900 | H | -3.15440500 | -2.32275000 | -1.16841900 |
| C | 1.30193600 | -5.60262400 | -4.76938800 | H | -3.11508800 | 0.33638900 | -3.32686500 |
| C | 2.48299100 | -7.73583300 | -3.91836000 | H | -4.69625100 | 0.20362600 | -4.91195900 |
| C | 3.54924300 | -7.14367900 | -2.97832400 | H | 1.41619700 | -1.99577100 | -8.42083800 |
| C | 3.11849700 | -5.82713300 | -2.32151600 | H | -0.70556800 | -1.59596600 | -6.39070400 |
| C | 3.93404700 | -8.16985600 | -1.90542000 | H | 1.75006400 | 6.89457000 | -4.88875300 |
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| C | -1.42684200 | -5.32436000 | -2.32632500 | H | 1.18631500 | 8.20142900 | -2.17406400 |
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| C | -1.52612900 | -5.95659900 | 0.79565400 | H | 0.24057200 | 8.96828300 | -4.95653300 |
| C | -0.91756000 | -8.37284900 | 0.79509300 | H | -0.70463800 | 10.05841200 | 3.69604000 |
| C | -3.01005100 | -7.76533400 | -6.40049500 | H | 0.45861400 | 9.26054100 | 4.73082800 |
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| C | 2.39320000 | 0.98273900 | 1.27081600 | H | -2.58636300 | 8.92798800 | 4.77492200 |
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| C | 0.28228100 | 1.75456700 | 0.35297400 | H | -4.53205200 | 7.20655500 | 4.38495000 |
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| O | -1.22055400 | 1.22611100 | -5.00074800 | H | -0.97989900 | 0.81919600 | 3.55524600 |
| O | -5.35849000 | -1.85735900 | -3.38244100 | H | -2.65752700 | 0.40495100 | 3.15965200 |
| O | 2.36021600 | -0.79059900 | -6.63304100 | H | -1.85032000 | 4.05794500 | 5.26375900 |
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| O | 0.69897600 | 5.27583900 | 0.09819700 | H | -0.45334600 | 5.09556200 | 3.54139700 |
| O | -6.92913300 | 4.75945400 | -0.71370900 | H | -0.58110900 | 3.69436900 | 2.48670800 |
| O | 5.39471000 | -0.99471800 | -0.05417800 | H | -3.80276700 | 3.22235400 | 2.72422900 |
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| O | 1.68435300 | -4.46455300 | -5.02637200 | H | 1.32558000 | -5.82656900 | 2.22608000 |
| O | -1.95626600 | -6.44313200 | -2.39921200 | H | 3.05414300 | -5.81692600 | 0.44063100 |
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| O | -9.61371600 | 2.17719500 | -1.36055100 | H | 7.31842900 | 3.13247200 | 3.09825800 |
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| | | | | | | | |
|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 7.48338500 | 0.90371200 | 1.08967300 | H | -1.00777400 | -3.63212200 | -1.22963300 |
| H | 7.36711700 | -0.47482400 | 2.18352000 | H | 0.13981100 | -8.09960800 | 0.69188600 |
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| H | 7.50971700 | 7.59858700 | 4.65617800 | H | -1.93486900 | -5.92673600 | -6.13065500 |
| H | 8.42486200 | 5.44847500 | 6.21386300 | H | -3.76372800 | -4.90551700 | -4.12801700 |
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| H | 7.23016100 | -4.77378300 | 2.18280700 | H | -0.86278600 | -1.08527200 | -1.25665000 |
| H | 7.07779000 | -4.41511500 | 4.59628300 | H | -5.54563500 | 3.80795300 | -1.35984900 |
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| H | 8.99555700 | -2.87763700 | 4.99489000 | H | 0.97402800 | -3.57938600 | 0.16187500 |
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| H | 3.86910900 | -5.49156900 | -1.60325500 | H | -5.23529900 | 0.21967600 | -7.56150600 |
| H | 4.26816500 | -9.11557200 | -2.34736300 | H | -4.90162400 | -1.45259700 | -8.09964000 |
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| H | 0.02485700 | -3.96083300 | -3.21323900 | H | 8.85731800 | -5.51580200 | -2.79760800 |
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| H | 4.44273400 | -8.30930800 | 7.08402000 | C | -9.06832900 | -4.37540000 | 8.48143300 |
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| H | 10.94800100 | 0.60891500 | 4.51735800 | O | -7.93597500 | -3.57251500 | 6.54590300 |
| H | 10.97335900 | 2.23807800 | 3.73978500 | C | -0.78796900 | -4.16295400 | 4.89428100 |
| H | -2.33824200 | 1.24528700 | -0.61900700 | C | 0.29207900 | -4.46019400 | 5.93026200 |
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| H | -8.72178400 | -0.64627500 | -0.26046000 | C | -0.31983400 | -3.20190700 | 3.78205500 |
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| H | -8.04233000 | 1.92378000 | -1.34735700 | C | 1.76875300 | -3.43802700 | 7.60987900 |
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| H | -2.56667000 | -0.87396100 | 0.53234700 | N | -4.12040200 | -2.46266100 | -1.54247000 |
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| H | 0.15171500 | -2.51540100 | 6.60073900 | N | 0.20027600 | -1.62602600 | -6.78256900 |
| H | 1.06292700 | -2.13431100 | 9.10062600 | N | 7.00707400 | 3.94157800 | 6.03054400 |
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| H | 3.33995000 | -2.97705400 | 9.76877400 | N | 6.52497800 | 5.00874700 | -3.47185400 |
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| C | -8.92115400 | 1.60954600 | 3.03024100 | C | 1.22272700 | -1.03924700 | -6.12176800 |
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| O | -9.63898900 | -0.45332300 | 2.02173000 | C | 0.92567600 | -1.67688100 | -0.88064800 |
| N | -7.84404100 | 0.60365900 | 1.11119800 | C | 0.34371300 | -2.07927300 | -8.14677500 |
| C | -7.70184700 | -0.41395300 | 0.08548200 | C | 1.19162100 | 8.99207400 | -4.95742600 |
| C | -6.97146100 | -1.62689600 | 0.70667100 | C | 1.74013600 | 7.72856900 | -4.27122700 |
| O | -5.72810700 | -1.76991600 | 0.57823700 | C | 1.09601500 | 7.34079200 | -2.93452400 |
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| C | -9.75480000 | -5.59493700 | 9.11099800 | | | | |

| | | | | | | | |
|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 1.25673400 | 6.45151200 | 2.07002300 | C | 1.16967500 | 3.02785800 | -2.69581300 |
| C | 0.34418300 | 6.19264500 | 1.04414300 | C | 5.80354800 | 1.97654600 | -7.44108000 |
| C | -5.77071700 | 5.67894600 | 5.40257500 | C | 5.43481900 | 1.06231900 | -6.26922000 |
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| C | -7.36293800 | 6.00447600 | 2.70721300 | C | 1.33838200 | -5.62201900 | -4.74011300 |
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| C | -5.41599900 | 5.68401600 | 0.75633300 | C | 3.17193200 | -5.77165500 | -2.30475600 |
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| C | 4.26154300 | -6.47453500 | 4.14645700 | C | -3.93371600 | -5.46601800 | -6.24788500 |
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| C | 2.95452600 | -6.21691000 | 3.70936400 | C | -5.70156400 | -4.27040300 | -6.52059600 |
| C | 5.01117700 | -6.37489500 | 1.83450100 | C | 1.51897900 | 2.05234700 | 0.80800500 |
| C | 2.68007600 | -6.02881800 | 2.35477300 | C | 2.33884600 | 0.95814000 | 1.25741400 |
| C | 3.71082500 | -6.09723500 | 1.41439000 | C | 1.97930100 | -0.33990900 | 1.00229400 |
| C | 10.96342500 | 1.32436600 | 3.51401500 | C | 0.24194200 | 1.75722400 | 0.27953900 |
| C | 9.81283300 | 0.87928700 | 2.59862300 | C | -0.12198700 | 0.45076600 | -0.02820400 |
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| C | 8.31681600 | 2.91435300 | 2.87692100 | C | -13.57693300 | 4.37804700 | -2.74292700 |
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| C | 7.81265400 | 6.78563300 | 2.67155300 | C | -11.67516500 | 3.33741500 | -1.23631700 |
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| C | 6.70864200 | 5.72135000 | 4.66830000 | C | 1.59244900 | -3.01875800 | -0.61289000 |
| C | 7.49301300 | 5.18678400 | 5.65989200 | O | -2.75774100 | -1.54068400 | -6.67336600 |
| C | 5.67381200 | 4.75190500 | 4.40382900 | O | -1.28578000 | 1.24410800 | -4.80912600 |
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| C | 4.59327300 | 4.70442300 | 3.50735400 | O | 2.35220300 | -0.87301500 | -6.58260000 |
| C | 5.08373400 | 2.50574700 | 5.24819800 | O | -1.06953000 | 7.12961300 | -3.99717000 |
| C | 3.77289100 | 3.58384400 | 3.49069900 | O | -0.82006300 | 6.14667400 | -2.03154800 |
| C | 4.02419000 | 2.49191600 | 4.34788500 | O | 0.61433800 | 5.28673600 | 0.05594100 |
| C | 8.45020000 | -5.09760600 | -3.72893900 | O | -7.00910100 | 4.71230600 | -0.72005700 |
| C | 6.91612900 | -5.11997200 | -3.59013700 | O | 5.27891700 | -1.05179600 | 0.06980600 |
| C | 6.40807100 | -4.06955900 | -2.62282200 | O | 7.32986400 | 5.88588000 | -1.52133200 |
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| C | 5.66682900 | -1.78281400 | -2.20737600 | O | 6.79080000 | 2.39604700 | -4.77888800 |
| C | 5.89405900 | -3.31817600 | -0.35479800 | O | 5.23756700 | 1.01875900 | -3.91761600 |
| C | 5.60811000 | -2.03935700 | -0.83632400 | O | 1.69214000 | -4.47965500 | -5.02080700 |
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| C | 8.04810400 | -2.35210900 | 4.67150500 | O | 2.78736000 | -1.37311500 | 1.37008300 |
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| C | 8.39201400 | 3.90640300 | -2.42068000 | O | -9.63944200 | 2.06410800 | -1.32838700 |
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| C | 6.61239100 | 2.79031900 | -0.90423000 | S | 2.02585600 | -0.62888800 | -2.06018900 |
| C | 5.87069100 | 3.53138000 | -0.00702200 | H | -4.07935400 | 5.80035500 | -2.73979300 |
| C | 4.56456500 | 2.03547900 | -0.95896700 | H | -2.48004700 | 5.24290300 | -3.16835100 |
| C | 5.26212900 | 5.72019800 | -3.45152000 | H | -1.52586300 | 2.97571000 | -2.12742600 |
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| C | 2.41135000 | 3.22165400 | -3.56580800 | H | -3.75676100 | 3.46257600 | -4.69997500 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -5.88898500 | -1.26760000 | -6.58930900 | H | 8.37335800 | 5.59516300 | 6.13594600 |
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| H | -4.90262500 | -2.38472500 | -0.88627100 | H | 2.93727800 | 3.53739200 | 2.80145300 |
| H | -3.19568600 | -2.50805900 | -1.14564900 | H | 5.27788100 | 1.66282700 | 5.90543800 |
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| H | 1.62320100 | 6.87909700 | -4.95279900 | H | 6.53899800 | -5.29972000 | -0.85860900 |
| H | 2.81974500 | 7.84073100 | -4.10895000 | H | 6.10392400 | -2.57303600 | -4.14446500 |
| H | 1.09037300 | 8.18618800 | -2.23173700 | H | 5.80367600 | -3.52541900 | 0.70399700 |
| H | 1.68318600 | 6.55004900 | -2.45658100 | H | 5.39912000 | -0.81036100 | -2.59800100 |
| H | 0.10404100 | 8.94005200 | -5.02326700 | H | 5.34752600 | -0.18658800 | -0.37054800 |
| H | -0.80868000 | 10.07957400 | 3.62984200 | H | 8.79640200 | -4.07861000 | -3.93046200 |
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| H | -8.73336900 | 5.16316100 | 1.25379600 | H | 8.56559800 | 3.29311900 | -0.33532000 |
| H | -4.65219500 | 5.58166300 | -0.00603400 | H | 6.14958800 | 4.35062000 | 0.63351400 |
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| H | -6.79266500 | 5.59686700 | 5.78723100 | H | 8.35217200 | 3.35919800 | -3.36244000 |
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| H | 8.95442100 | 3.42741900 | 3.60230600 | H | -3.15500700 | -5.33003700 | -0.26982300 |
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| H | 7.47219100 | 0.99595100 | 1.05844300 | H | -0.96290900 | -3.64703700 | -1.21913300 |
| H | 7.36964300 | -0.36430300 | 2.17814200 | H | 0.24342800 | -8.08449700 | 0.75786900 |
| H | 11.92420100 | 1.08545800 | 3.04141900 | H | -2.18821600 | -7.35471900 | -0.34747400 |
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| H | -3.75087700 | -5.00896100 | -4.05488500 | H | -2.42697300 | 1.24459500 | -0.59248800 |
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| H | 3.26876600 | 1.17579100 | 1.77156300 | H | 0.40909400 | -3.71052900 | 3.14443600 |
| H | 3.72088700 | -1.14358900 | 1.19623600 | H | -3.41612900 | -3.42367300 | 3.79069800 |
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| H | -0.87258400 | -1.12628900 | -1.31721600 | H | -2.59519300 | -0.96802800 | 0.45924800 |
| H | -5.62154700 | 3.79240200 | -1.35306100 | H | -7.13315800 | -3.40666100 | 5.09350300 |
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| H | -1.51940200 | 9.48777100 | 5.96835500 | H | -5.865556500 | -0.01891500 | -0.98823000 |
| H | -5.13006100 | 4.58552600 | -4.45889100 | H | -7.24769300 | -0.32102400 | -2.03335300 |
| H | -3.60160500 | 5.13184400 | -5.25999600 | H | 2.67719600 | -3.55316500 | 6.99482600 |
| H | 1.47229200 | 9.91883700 | -4.44543800 | H | -1.09101500 | -5.11238900 | 4.45029700 |
| H | 1.59328600 | 9.02461200 | -5.97568500 | H | 1.76682600 | -4.28615300 | 8.30308600 |
| H | 7.97202800 | 7.74480900 | 2.16925700 | H | -1.65174700 | -3.73127500 | 5.41399800 |
| H | 8.77898900 | 6.35008400 | 2.94387900 | H | 2.38961400 | -0.98298400 | 6.90037300 |
| H | 5.25829200 | 6.62709600 | -4.06505600 | | | | |
| H | 2.03362500 | 3.29588500 | -4.59102900 | | | | |
| H | 9.39885000 | 4.31287200 | -2.28601000 | | | | |
| H | 5.01608500 | 2.71815900 | -7.60976200 | C | -8.75566800 | 2.03946200 | 2.92933500 |
| H | 5.95147500 | 1.33726500 | -8.31687900 | C | -8.92063800 | 1.01805800 | 1.82936700 |
| H | -0.20948800 | -1.43720200 | -8.84114600 | O | -9.91807200 | 0.29383500 | 1.76568900 |
| H | -0.01808600 | -3.10400700 | -8.27447800 | N | -7.85781400 | 0.87937400 | 0.99537600 |
| H | -5.27258100 | 0.09824500 | -7.53308400 | C | -7.95979400 | 0.05670700 | -0.20679900 |
| H | -4.92025900 | -1.57379500 | -8.05994500 | C | -7.69013100 | -1.43094900 | 0.11287900 |
| H | -3.31398300 | -7.98587200 | -5.30262800 | O | -6.71707900 | -2.04343100 | -0.36891400 |
| H | -1.94006800 | -8.28710200 | -6.38947100 | C | -6.95339800 | 0.60980200 | -1.23457700 |
| H | 3.07364300 | -6.54194500 | -5.60705300 | O | -6.88032300 | 2.01959600 | -1.18587300 |
| H | 8.82476800 | -5.73765200 | -4.53470600 | N | -8.58194700 | -2.01960000 | 0.91785900 |
| H | 8.91312300 | -5.42214800 | -2.79142100 | C | -8.49819100 | -3.42391400 | 1.29875800 |
| H | -1.04198100 | -9.14304600 | 0.12497100 | C | -8.86853600 | -3.70325400 | 2.75804700 |
| H | -0.91690700 | -8.76528000 | 1.88642700 | C | -8.83229300 | -5.21185100 | 3.01792500 |
| H | 2.93314900 | -7.82773200 | 6.49432500 | O | -7.98100900 | -2.99805800 | 3.60334700 |
| H | 4.57957800 | -8.19467500 | 7.13191800 | C | -10.15369300 | -5.32859700 | 8.70231100 |
| H | 9.70117800 | -4.90553900 | 1.87734100 | C | -9.01578300 | -4.50108100 | 8.09597400 |
| H | 9.40688700 | -5.23331200 | 3.58671700 | C | -9.08813600 | -4.32400400 | 6.55554600 |
| H | 10.95974000 | 0.78476000 | 4.46650700 | O | -10.06960600 | -4.80383900 | 5.95270000 |
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| | | | | C | -1.79552900 | -3.90766500 | 5.62683600 |

Int4

| | | | |
|---|--------------|-------------|-------------|
| C | -8.75566800 | 2.03946200 | 2.92933500 |
| C | -8.92063800 | 1.01805800 | 1.82936700 |
| O | -9.91807200 | 0.29383500 | 1.76568900 |
| N | -7.85781400 | 0.87937400 | 0.99537600 |
| C | -7.95979400 | 0.05670700 | -0.20679900 |
| C | -7.69013100 | -1.43094900 | 0.11287900 |
| O | -6.71707900 | -2.04343100 | -0.36891400 |
| C | -6.95339800 | 0.60980200 | -1.23457700 |
| O | -6.88032300 | 2.01959600 | -1.18587300 |
| N | -8.58194700 | -2.01960000 | 0.91785900 |
| C | -8.49819100 | -3.42391400 | 1.29875800 |
| C | -8.86853600 | -3.70325400 | 2.75804700 |
| C | -8.83229300 | -5.21185100 | 3.01792500 |
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| O | -10.06960600 | -4.80383900 | 5.95270000 |
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| C | -1.79552900 | -3.90766500 | 5.62683600 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -0.50065500 | -4.40882900 | 6.24382100 | C | -6.90943700 | 6.35534600 | 2.77702500 |
| O | -0.11190800 | -5.57015300 | 6.11869300 | C | -4.59657100 | 6.36239200 | 2.16750400 |
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| C | -3.17795900 | -3.73214600 | 3.51882100 | C | -4.92129900 | 5.87893600 | 0.90071300 |
| C | -4.41535700 | -3.67801100 | 4.12964600 | C | -6.25647300 | 5.60388800 | 0.56491700 |
| N | -3.30821000 | -3.38328400 | 2.18472600 | C | -3.63852700 | 2.90952800 | 3.79610600 |
| C | -4.60303000 | -3.13174000 | 2.01193300 | C | -2.30647000 | 2.26288800 | 4.22195300 |
| N | -5.30843500 | -3.29550000 | 3.15752700 | C | -1.23175800 | 3.30229300 | 4.57536400 |
| N | 0.19915200 | -3.49772300 | 6.98178100 | C | -1.83319400 | 1.26066800 | 3.16104200 |
| C | 1.50845600 | -3.81685700 | 7.51918200 | C | -0.83869400 | 4.22702200 | 3.42801600 |
| C | 2.07534500 | -2.61430500 | 8.27145400 | C | 3.48895500 | -8.39516000 | 6.01836200 |
| C | 3.51530600 | -2.85525500 | 8.71386700 | C | 4.13300200 | -7.11537100 | 5.44564000 |
| O | 1.96105300 | -1.42504900 | 7.48344300 | C | 3.61153500 | -6.72063600 | 4.08052100 |
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| N | -2.82012000 | 2.11388300 | -0.90503900 | C | 2.29876000 | -6.25207000 | 3.91982200 |
| N | -3.58750300 | 0.36528000 | -5.30323200 | C | 3.94466800 | -6.49414600 | 1.67956900 |
| N | -4.31727800 | -1.68399000 | -1.65821300 | C | 1.81704100 | -5.91901100 | 2.65345500 |
| N | -0.28808100 | -0.44228600 | -4.34300100 | C | 2.63541800 | -6.03791500 | 1.52715800 |
| N | 0.37084200 | -1.34767600 | -6.82201700 | C | 11.06040700 | 0.53400900 | 3.79984700 |
| N | 7.11212600 | 3.24030300 | 6.25164300 | C | 9.89641900 | 0.20302500 | 2.85370100 |
| N | 6.02203600 | 1.58103300 | -1.27636400 | C | 8.53507200 | 0.81096500 | 3.23759300 |
| N | 4.87718900 | 2.84683800 | 0.12592900 | C | 8.56240700 | 2.34242800 | 3.16645500 |
| N | 7.00880800 | 4.74512300 | -3.12114900 | C | 7.42256900 | 0.25952800 | 2.33615300 |
| N | 3.66412900 | 4.31059100 | -2.96664600 | C | 8.26067500 | 6.20404000 | 3.11095000 |
| N | 0.01203300 | -5.51941500 | -4.56504200 | C | 7.38534900 | 6.41908400 | 4.34077600 |
| N | -1.71229200 | -4.19616200 | -1.73865300 | C | 7.01012200 | 5.12558900 | 5.00765300 |
| N | -1.93662400 | -7.08666100 | 0.34059000 | C | 7.71061800 | 4.46236000 | 5.98414800 |
| N | -4.92112600 | -4.49889600 | -7.45428900 | C | 5.90946900 | 4.26597500 | 4.64511500 |
| N | -5.30764400 | -3.53884500 | -5.48306600 | C | 6.00700200 | 3.08862300 | 5.43968800 |
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| C | -3.14871400 | 3.99258600 | -2.04327500 | C | 3.94615400 | 3.32905700 | 3.60713400 |
| C | -2.21106400 | 3.04897200 | -1.71945300 | C | 4.07663500 | 2.16470900 | 4.39294400 |
| C | -4.09632700 | 2.46296600 | -0.72598000 | C | 8.33131100 | -5.44229400 | -3.74029800 |
| C | -4.81014400 | -0.32436100 | -7.30435900 | C | 6.79344800 | -5.38423900 | -3.63532300 |
| C | -3.55391100 | -0.41059400 | -6.43189100 | C | 6.33191300 | -4.32709200 | -2.65340300 |
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| C | -1.22879400 | 0.52268500 | -4.49093700 | C | 6.16123600 | -4.59418300 | -1.28877800 |
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| C | -4.27476700 | -1.43916000 | -2.97500200 | C | 5.83126400 | -3.58630500 | -0.38001600 |
| C | 1.10115500 | -0.27963300 | -4.72753600 | C | 5.68578400 | -2.27574600 | -0.83582300 |
| C | 1.38783700 | -0.73774500 | -6.17462700 | C | 9.12612100 | -5.10961900 | 2.84077500 |
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| C | 0.52027500 | -1.77239800 | -8.19678600 | C | 7.90369200 | -3.01780400 | 4.75543000 |
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| C | 2.38325100 | 7.76713000 | -3.91401200 | C | 8.78576000 | 3.49136100 | -2.07997300 |
| C | 1.66388300 | 7.37448300 | -2.61888300 | C | 7.85870500 | 4.69902000 | -2.06214300 |
| C | 0.18223300 | 7.06984300 | -2.79390600 | C | 8.38204700 | 2.50177700 | -0.95081000 |
| C | -1.14337900 | 8.68399900 | 5.46400900 | C | 6.90846800 | 2.44641700 | -0.64771300 |
| C | 0.00334500 | 8.98391500 | 4.46636900 | C | 6.19857900 | 3.22808000 | 0.23824000 |
| C | 0.22523200 | 7.97650500 | 3.36089900 | C | 4.81340800 | 1.85843200 | -0.79246200 |
| C | -0.70728400 | 7.79366700 | 2.33036600 | C | 5.78886800 | 5.52989200 | -3.09934300 |
| C | 1.39836700 | 7.21361200 | 3.31803500 | C | 4.71103600 | 4.66803700 | -3.75536100 |
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| C | 1.64115700 | 6.29848800 | 2.29383500 | C | 1.51535500 | 3.12541700 | -2.53785200 |
| C | 0.68907800 | 6.11784800 | 1.28932600 | C | 6.19516200 | 1.91573700 | -7.22213200 |
| C | -5.42225700 | 5.81722700 | 5.52317700 | C | 5.73543500 | 0.98500400 | -6.09741000 |
| C | -5.19255700 | 7.00201700 | 4.54982300 | C | 6.17242900 | 1.43829400 | -4.73154700 |
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| C | 1.31413900 | -5.43625800 | -4.94723000 | H | -2.98658700 | 0.85963200 | -3.40817200 |
| C | 2.20485200 | -7.71130000 | -4.08290500 | H | -4.50740100 | 0.67840600 | -5.02466800 |
| C | 3.26157900 | -7.28851400 | -3.04503500 | H | 1.58578300 | -1.78600100 | -8.42782600 |
| C | 2.92109300 | -5.97351500 | -2.33462100 | H | -0.57386800 | -1.28854100 | -6.45486000 |
| C | 3.44391200 | -8.41023500 | -2.01407900 | H | 2.22237900 | 6.96104700 | -4.63818300 |
| C | -0.69000100 | -4.40169700 | -3.96360600 | H | 3.46210200 | 7.78323600 | -3.71328500 |
| C | -1.55133100 | -4.96860900 | -2.83680300 | H | 1.73760200 | 8.16905800 | -1.86262100 |
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| C | -1.32306000 | -5.96527800 | -0.11594600 | H | 0.86944900 | 9.12716500 | -4.65301600 |
| C | -1.20534800 | -8.32618200 | 0.53827400 | H | -0.16658800 | 9.97720700 | 4.02940100 |
| C | -3.14309800 | -7.39838200 | -6.66724800 | H | 0.93574000 | 9.06529300 | 5.03732900 |
| C | -2.88868500 | -5.89636000 | -6.91826400 | H | 2.14237700 | 7.33508200 | 4.10151000 |
| C | -3.99027500 | -4.95458000 | -6.53807700 | H | -1.62695600 | 8.37364100 | 2.32726800 |
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| C | -5.68287200 | -3.64966400 | -6.78787200 | H | -1.21889900 | 6.73580300 | 0.51958000 |
| C | 1.73969100 | 1.87275700 | 0.82034900 | H | 0.23346100 | 5.93696200 | -1.19019200 |
| C | 2.59210100 | 0.74643700 | 1.18428900 | H | -2.12663400 | 8.90364400 | 5.03817600 |
| C | 2.21787600 | -0.53109800 | 0.94282100 | H | -5.74831200 | 7.88886200 | 4.88073400 |
| C | 0.42345800 | 1.62186600 | 0.37188200 | H | -4.13190400 | 7.27818200 | 4.55775700 |
| C | -0.02561500 | 0.33442400 | 0.11386800 | H | -7.69998200 | 6.53772400 | 3.50216400 |
| C | 0.90690000 | -0.87107100 | 0.28873300 | H | -3.55123900 | 6.54465500 | 2.40759900 |
| C | -13.10783900 | 5.30349000 | -2.82215700 | H | -8.29091800 | 5.67786800 | 1.25140800 |
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| C | -9.77766700 | 3.92623300 | -1.16637600 | H | -6.45717000 | 5.78986800 | 5.87889400 |
| C | 1.74913900 | -2.98112800 | -1.02372600 | H | -2.50741300 | 1.69647900 | 5.14315500 |
| O | -2.57840100 | -1.10231700 | -6.72237600 | H | -1.68762700 | 1.74833200 | 2.19328400 |
| O | -0.96792800 | 1.67732600 | -4.83212800 | H | -0.87749900 | 0.80139700 | 3.43834100 |
| O | -5.29858000 | -1.31712200 | -3.67137800 | H | -2.56206900 | 0.45539600 | 3.01976900 |
| O | 2.51626400 | -0.57098300 | -6.63910200 | H | -1.60201800 | 3.90946300 | 5.41344200 |
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| O | -0.39744300 | 6.40457600 | -1.78226800 | H | -1.70781900 | 4.74246100 | 3.01026700 |
| O | 0.87564100 | 5.22507800 | 0.26647000 | H | -0.14036800 | 4.99263500 | 3.76726600 |
| O | -6.54108000 | 5.10580800 | -0.66445800 | H | -0.35533500 | 3.68045200 | 2.61290700 |
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| H | -3.44266100 | 6.05858200 | -2.51325900 | H | 7.57878600 | 0.56245000 | 1.29574600 |
| H | -1.91915900 | 5.36877500 | -3.00517900 | H | 7.38319300 | -0.83348400 | 2.35732100 |
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| H | -3.34127800 | 3.87732500 | -4.66417300 | H | 7.91249200 | 7.06296800 | 5.05578400 |
| H | -5.67751300 | -0.64929300 | -6.72383700 | H | 8.60451200 | 4.76189600 | 6.51283100 |
| H | -2.79265400 | -2.02119800 | -4.39393600 | H | 7.44814600 | 2.55718500 | 6.90873500 |
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| H | -5.23499200 | -1.79039600 | -1.19889000 | H | 3.12559100 | 3.39769900 | 2.90306700 |
| H | -3.47287200 | -1.76706300 | -1.11260900 | H | 5.20055500 | 1.13265100 | 5.92627600 |

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|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 3.35213800 | 1.36537000 | 4.27288000 | H | -11.22570700 | 4.43118100 | -3.40853500 |
| H | 7.76056600 | 5.58699900 | 2.35920000 | H | -11.62959300 | 4.72096600 | -0.39080300 |
| H | 6.36546600 | -5.16627700 | -4.62033900 | H | -11.80635000 | 3.19902900 | -1.29323000 |
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| H | 6.29357100 | -5.60913300 | -0.92153000 | H | 1.33364400 | 0.78651500 | -4.69452200 |
| H | 6.20394300 | -2.77669800 | -4.14367100 | H | 1.83889900 | -2.12651200 | -3.82797400 |
| H | 5.69407900 | -3.80793300 | 0.67123500 | H | 3.06530000 | -0.94746800 | -4.24474300 |
| H | 5.62559500 | -0.99091400 | -2.56837400 | H | 1.38525700 | 4.40509800 | 0.54954100 |
| H | 5.59314400 | -0.41107000 | -0.33241000 | H | 3.54478200 | 0.95874900 | 1.65549300 |
| H | 8.73823800 | -4.43784100 | -3.89524400 | H | 3.92596700 | -1.39768000 | 1.11140100 |
| H | 7.81995700 | -3.62355700 | 1.97771300 | H | -0.21755900 | 2.47118200 | 0.17079400 |
| H | 7.07679800 | -5.19765600 | 2.17007800 | H | -0.75095200 | -1.07649100 | -1.32783000 |
| H | 6.88814900 | -4.90104200 | 4.58618400 | H | -5.22567800 | 4.09277900 | -1.35542800 |
| H | 8.12497700 | -2.12680600 | 4.15711000 | H | 5.83345200 | 1.15909500 | -2.85517200 |
| H | 7.37710000 | -2.68619500 | 5.65729700 | H | 2.75701800 | -2.94645500 | -0.62299600 |
| H | 8.85661000 | -3.45508900 | 5.06934500 | H | 1.13277300 | -3.64808300 | -0.41368400 |
| H | 5.77407200 | -2.51982600 | 3.00560600 | H | 1.79127600 | -3.40182700 | -2.03007400 |
| H | 5.15486400 | -3.10034100 | 4.55731600 | H | 4.04672500 | 3.14996700 | 0.65220500 |
| H | 5.02733500 | -4.12483100 | 3.12494100 | H | -0.53793600 | -1.32135600 | -3.91798100 |
| H | 9.87266500 | -4.37585200 | 3.16003700 | H | -13.55128400 | 5.92083200 | -2.03387700 |
| H | 8.73594800 | 1.49895700 | -1.20685000 | H | -13.11259200 | 5.86345600 | -3.76273600 |
| H | 8.87110600 | 2.78995400 | -0.01593700 | H | -5.27031300 | 4.92442000 | 4.90724700 |
| H | 6.51755300 | 4.01368000 | 0.90142800 | H | -4.75754100 | 5.83180300 | 6.39374500 |
| H | 3.89933200 | 1.36341100 | -1.08197000 | H | -4.37522400 | 2.09933100 | 3.79361000 |
| H | 8.73406700 | 2.98300200 | -3.04269600 | H | -3.91652800 | 3.72004900 | 4.47802700 |
| H | 5.56851700 | 5.79708200 | -2.06219700 | H | -1.12778500 | 7.62608800 | 5.74611800 |
| H | 7.04500400 | 3.98944400 | -3.80247200 | H | -0.96500500 | 9.33753600 | 6.32429400 |
| H | 1.26771200 | 2.07266600 | -2.37672800 | H | -4.62736500 | 5.06522900 | -4.35890800 |
| H | 1.65696600 | 3.57248200 | -1.55119900 | H | -3.05153500 | 5.54841700 | -5.10693500 |
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| H | 3.75703600 | 4.46556200 | -1.97171800 | H | 8.48822700 | 7.17035600 | 2.65029500 |
| H | 4.65527200 | 0.81316700 | -6.10426300 | H | 9.19300100 | 5.70077100 | 3.38518700 |
| H | 6.18322100 | -0.01241200 | -6.21749400 | H | 5.85288300 | 6.45817100 | -3.67649200 |
| H | 7.15359100 | 2.37274000 | -6.96701900 | H | 2.44781900 | 3.35067400 | -4.39829500 |
| H | 1.24598500 | -7.85608500 | -3.56538700 | H | 9.81242600 | 3.82774900 | -1.90832500 |
| H | 2.48487500 | -8.69612700 | -4.47871100 | H | 5.45733000 | 2.70953000 | -7.37711400 |
| H | 4.21343700 | -7.15490100 | -3.58032400 | H | 6.32426700 | 1.30265700 | -8.11938300 |
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| H | 2.96482500 | -5.12541400 | -3.01737700 | H | 0.10096200 | -2.76784700 | -8.37235500 |
| H | 3.63497600 | -5.77516900 | -1.53071300 | H | -4.96839700 | 0.71566200 | -7.61025600 |
| H | 3.70021400 | -9.36523700 | -2.48756000 | H | -4.70475400 | -0.95323200 | -8.19566300 |
| H | 4.23552500 | -8.16106900 | -1.29987900 | H | -3.54599400 | -7.55156200 | -5.66240300 |
| H | 2.52232500 | -8.55338800 | -1.43786100 | H | -2.16855700 | -7.89345800 | -6.73261900 |
| H | 1.36520200 | -7.29020400 | -6.02633500 | H | 2.92187400 | -6.48558400 | -5.78087700 |
| H | -1.33518600 | -3.89535800 | -4.69480800 | H | 8.68499200 | -6.07264600 | -4.56302400 |
| H | 0.03812300 | -3.67935100 | -3.59526500 | H | 8.75296300 | -5.83000300 | -2.80724000 |
| H | -0.43695700 | -6.41494000 | -4.41492700 | H | -1.46965800 | -9.05089200 | -0.24048900 |
| H | -3.26190600 | -5.18540900 | -0.74011100 | H | -1.36162600 | -8.74914800 | 1.53644500 |
| H | -2.31774800 | -4.09193800 | 0.27659800 | H | 2.43331800 | -8.22320800 | 6.25517400 |
| H | -1.08269500 | -3.40267600 | -1.61898900 | H | 4.04023800 | -8.71217200 | 6.91026200 |
| H | -0.14595800 | -8.08353600 | 0.43929500 | H | 9.46570800 | -5.54098000 | 1.89316400 |
| H | -2.94046700 | -7.13126000 | 0.25113100 | H | 9.11419200 | -5.91552000 | 3.58198800 |
| H | -2.66243100 | -5.73785400 | -7.97837000 | H | 11.00321600 | -0.04044900 | 4.72999400 |
| H | -1.98666800 | -5.61486900 | -6.36379000 | H | 11.11894400 | 1.60884500 | 4.00482200 |
| H | -3.74975000 | -4.50549000 | -4.35006700 | H | -2.30897700 | 1.27046800 | -0.54985800 |
| H | -5.61384700 | -2.83783100 | -4.80802200 | H | -7.27904300 | 1.70183900 | 0.85521400 |
| H | -6.51344700 | -3.09247900 | -7.19801300 | H | -8.98087700 | 0.14929400 | -0.59603800 |
| H | -3.83460600 | -7.83096400 | -7.39513200 | H | -9.31541600 | -1.42265500 | 1.30424700 |
| H | -11.05557000 | 5.91397800 | -2.49137900 | H | -9.19301300 | -5.40292000 | 4.03187100 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -9.47219000 | -5.74999300 | 2.30705200 | N | -3.29730400 | -3.26473500 | 2.18006300 |
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| H | -9.89853800 | -3.34857200 | 2.93399700 | N | -5.29770600 | -3.23160800 | 3.15744600 |
| H | -6.33951800 | -3.16431700 | 3.29808000 | N | 0.20828300 | -3.47535800 | 6.99110800 |
| H | -7.81046800 | 2.39524100 | -1.31122800 | C | 1.51948200 | -3.80441500 | 7.51961600 |
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| H | -1.06432100 | -3.52310500 | 3.61780000 | O | 1.97898200 | -1.41298700 | 7.48603900 |
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| H | -4.74969900 | -3.86721100 | 5.13814200 | N | -2.87863200 | 2.11222700 | -0.88409700 |
| H | 0.38027700 | -1.60456100 | 0.91339200 | N | -3.58856700 | 0.36437600 | -5.31343600 |
| H | -5.07955100 | -2.83055800 | 1.08903600 | N | -4.36042300 | -1.80203000 | -1.72254500 |
| H | -8.12644400 | -3.29217700 | 4.59125400 | N | -0.27624600 | -0.42721100 | -4.32971100 |
| H | -0.01211900 | -2.51334300 | 6.88916000 | N | 0.37167300 | -1.35223300 | -6.82021200 |
| H | 1.44728900 | -2.41440600 | 9.14733700 | N | 7.11643500 | 3.26739200 | 6.24804500 |
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| H | 3.58626000 | -3.72623800 | 9.37356700 | N | 6.99146700 | 4.75526400 | -3.13513300 |
| H | -10.06374300 | -5.40149500 | 9.79386000 | N | 3.64149300 | 4.32375500 | -2.97151700 |
| H | -9.60804600 | 1.90615500 | 3.59942000 | N | 0.03685000 | -5.50159000 | -4.53859100 |
| H | -8.75716000 | 3.09401500 | 2.63086100 | N | -1.70356000 | -4.17900500 | -1.71251900 |
| H | -7.85802600 | 1.81336800 | 3.51147400 | N | -1.92561000 | -7.08790600 | 0.34665800 |
| H | -11.12146900 | -4.88276000 | 8.45654000 | N | -4.93658900 | -4.54228100 | -7.44246000 |
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| H | 2.19633500 | -4.10143100 | 6.70568300 | C | -4.14814400 | 2.49046100 | -0.70658900 |
| H | -2.60333900 | -4.48314100 | 6.09308500 | C | -4.81810900 | -0.33960600 | -7.30196700 |
| H | 1.44063500 | -4.68908000 | 8.17787700 | C | -3.55791400 | -0.42139100 | -6.43514300 |
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| | | | | C | -2.88139700 | -1.27690400 | -3.58200500 |
| | | | | C | -4.28224800 | -1.44900000 | -3.01392500 |
| | | | | C | 1.10451800 | -0.24535300 | -4.74110400 |

TS3

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|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -8.76088900 | 2.02675600 | 2.93267800 | C | 1.37379600 | -0.69487700 | -6.19525000 |
| C | -8.92875300 | 0.99798000 | 1.83883900 | C | 2.09053800 | -1.02643800 | -3.85815300 |
| O | -9.92591200 | 0.27305100 | 1.78312800 | C | 1.03918900 | -1.72556100 | -1.29342600 |
| N | -7.86767500 | 0.85176800 | 1.00325700 | C | 0.51443400 | -1.77749000 | -8.19764500 |
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| C | -7.71075400 | -1.46160100 | 0.10966200 | C | 2.36895300 | 7.77365100 | -3.92352200 |
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| C | -6.96184900 | 0.57861500 | -1.22503100 | C | 0.17937500 | 7.03944900 | -2.80863000 |
| O | -6.88896700 | 1.98913000 | -1.17804100 | C | -1.15981200 | 8.68911300 | 5.45448700 |
| N | -8.57395300 | -2.04217800 | 0.95032600 | C | -0.01366200 | 8.98869800 | 4.45519600 |
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| O | -7.97031200 | -3.00796900 | 3.62603800 | C | -0.48922500 | 6.88309000 | 1.29156100 |
| C | -10.13848000 | -5.33894300 | 8.71459700 | C | 1.62750500 | 6.29186000 | 2.29694000 |
| C | -8.98682200 | -4.52977600 | 8.10978400 | C | 0.68348800 | 6.11637200 | 1.28341100 |
| C | -9.06014600 | -4.34249000 | 6.57101200 | C | -5.43246600 | 5.81356800 | 5.52022600 |
| O | -10.03703700 | -4.82551200 | 5.96358400 | C | -5.20841500 | 6.99802000 | 4.54547900 |
| O | -8.07738700 | -3.69156000 | 6.07574100 | C | -5.59507300 | 6.60216100 | 3.13225900 |
| C | -1.77708300 | -3.85002600 | 5.61084600 | C | -6.92540300 | 6.33223100 | 2.77930100 |
| C | -0.48582800 | -4.36672000 | 6.22376200 | C | -4.61626300 | 6.37562900 | 2.15753400 |
| O | -0.09780800 | -5.52491600 | 6.07203600 | C | -7.27162900 | 5.83819900 | 1.52264900 |
| C | -1.82556600 | -4.02476400 | 4.08316100 | C | -4.94134900 | 5.89424200 | 0.88991900 |
| C | -3.15972000 | -3.64418900 | 3.50567900 | C | -6.27405500 | 5.60115100 | 0.56014800 |

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|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| C | -3.64426700 | 2.90777300 | 3.79447700 | C | -0.65508900 | -4.38296600 | -3.92664600 |
| C | -2.30969200 | 2.26462100 | 4.21627300 | C | -1.52480900 | -4.95339700 | -2.80746800 |
| C | -1.23889800 | 3.30775000 | 4.57011200 | C | -2.23871600 | -4.81271000 | -0.51743300 |
| C | -1.83451300 | 1.27001800 | 3.14955200 | C | -1.31165700 | -5.96162700 | -0.09798100 |
| C | -0.85632500 | 4.23977900 | 3.42512600 | C | -1.19149600 | -8.32667200 | 0.54543300 |
| C | 3.50783000 | -8.37896500 | 6.02365500 | C | -3.13600400 | -7.40976600 | -6.65912100 |
| C | 4.15218200 | -7.09876700 | 5.45113200 | C | -2.88215300 | -5.90529600 | -6.90051500 |
| C | 3.63671200 | -6.70674400 | 4.08308900 | C | -3.98935100 | -4.96670300 | -6.52771200 |
| C | 4.44937700 | -6.83956500 | 2.95031500 | C | -4.20868900 | -4.35345200 | -5.31197200 |
| C | 2.33005700 | -6.22323300 | 3.91883100 | C | -5.69964200 | -3.68636900 | -6.78693800 |
| C | 3.97351700 | -6.49964200 | 1.68105200 | C | 1.79120000 | 1.88230800 | 0.83327600 |
| C | 1.85306800 | -5.89125000 | 2.65044100 | C | 2.63856700 | 0.78489800 | 1.20352600 |
| C | 2.67021600 | -6.02743300 | 1.52550100 | C | 2.21010100 | -0.51755700 | 1.08988500 |
| C | 11.05973100 | 0.56272900 | 3.78833700 | C | 0.46375900 | 1.59549300 | 0.38833900 |
| C | 9.89458800 | 0.22844600 | 2.84408300 | C | 0.04306700 | 0.29441500 | 0.28531600 |
| C | 8.53425600 | 0.84046000 | 3.22580700 | C | 0.90226300 | -0.83403300 | 0.56352300 |
| C | 8.56473600 | 2.37175900 | 3.14738600 | C | -13.12411700 | 5.27550100 | -2.81845000 |
| C | 7.41904200 | 0.28757400 | 2.32834200 | C | -11.63754600 | 4.95297600 | -2.54204800 |
| C | 8.24753100 | 6.22619000 | 3.09606900 | C | -11.30631600 | 4.14315600 | -1.27772100 |
| C | 7.37306300 | 6.44087600 | 4.32648800 | C | -9.78567600 | 3.90637600 | -1.16642600 |
| C | 7.00461200 | 5.14736600 | 4.99699900 | C | 1.72344300 | -3.03851500 | -0.98450200 |
| C | 7.70418800 | 4.49493400 | 5.98136500 | O | -2.58461500 | -1.11598200 | -6.72509800 |
| C | 5.91628200 | 4.27480800 | 4.62805600 | O | -0.98253900 | 1.64399900 | -4.96663900 |
| C | 6.02029000 | 3.10089000 | 5.42664700 | O | -5.29203500 | -1.25390700 | -3.71435000 |
| C | 4.87316300 | 4.36423400 | 3.69083100 | O | 2.48628900 | -0.48723500 | -6.68206500 |
| C | 5.13346300 | 2.02770000 | 5.29776800 | O | -0.49358400 | 7.39146000 | -3.75588200 |
| C | 3.97850400 | 3.30868800 | 3.56878500 | O | -0.39091500 | 6.35816900 | -1.80266000 |
| C | 4.11589100 | 2.14777700 | 4.35857700 | O | 0.87131200 | 5.22282500 | 0.26294600 |
| C | 8.33695300 | -5.42673300 | -3.74377700 | O | -6.55846600 | 5.10321700 | -0.67022100 |
| C | 6.79874100 | -5.37360300 | -3.63614000 | O | 5.39355800 | -1.29537600 | 0.10570600 |
| C | 6.33136500 | -4.32399100 | -2.64833500 | O | 7.82281800 | 5.52382300 | -1.15088400 |
| C | 6.10586200 | -3.01012800 | -3.07481300 | O | 4.80666000 | 4.30747300 | -4.92587600 |
| C | 6.16120900 | -4.59880800 | -1.28505200 | O | 0.38276700 | 3.70988800 | -3.16373800 |
| C | 5.76947100 | -1.99760900 | -2.18114200 | O | 7.11675700 | 2.18000200 | -4.53218000 |
| C | 5.81768300 | -3.59928700 | -0.37188600 | O | 5.45734600 | 0.87629000 | -3.76381900 |
| C | 5.65711800 | -2.28841700 | -0.82137200 | O | 1.95693400 | -4.36600900 | -4.95613800 |
| C | 9.13646600 | -5.08584200 | 2.83667100 | O | -2.01930300 | -6.07850800 | -2.92742300 |
| C | 7.74767300 | -4.45676500 | 2.66154600 | O | -0.08785700 | -5.84225100 | -0.16424800 |
| C | 7.05551400 | -3.98972500 | 3.95526600 | O | 2.24010300 | 3.09659200 | 0.86547100 |
| C | 7.90728000 | -2.98898800 | 4.74687700 | O | 2.98226300 | -1.57003200 | 1.43972300 |
| C | 5.67604700 | -3.39501900 | 3.63816500 | O | -1.18946200 | -0.00496900 | -0.20820200 |
| C | 8.77475800 | 3.50834200 | -2.09416200 | O | -9.36503000 | 2.73420400 | -1.35002500 |
| C | 7.84631600 | 4.71515500 | -2.07945000 | O | -9.07736700 | 4.93747100 | -0.93374500 |
| C | 8.37324700 | 2.52000300 | -0.96204700 | O | -0.17647500 | -1.78218400 | -1.72545900 |
| C | 6.89925900 | 2.45928900 | -0.66830400 | S | 2.18122800 | -0.49388800 | -2.10765000 |
| C | 6.17581600 | 3.25362000 | 0.19516500 | H | -3.41835600 | 6.04848900 | -2.51835300 |
| C | 4.80951000 | 1.86040100 | -0.82692400 | H | -1.91586600 | 5.32437900 | -3.02565200 |
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| C | 2.78538800 | 3.21885400 | -3.37684400 | H | -3.36042100 | 3.86956100 | -4.67535000 |
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| C | 6.18237500 | 1.92322000 | -7.23100900 | H | -2.73836500 | -2.01527200 | -4.37556600 |
| C | 5.72141800 | 0.99184800 | -6.10747700 | H | -2.14326300 | -1.46076400 | -2.80300800 |
| C | 6.16443300 | 1.43842700 | -4.74155100 | H | -5.28814500 | -1.90998800 | -1.28632100 |
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| C | 1.34159300 | -5.43187700 | -4.91319400 | H | -2.97741700 | 0.87612700 | -3.42855800 |
| C | 2.20742900 | -7.73950200 | -4.10225800 | H | -4.51274000 | 0.65719600 | -5.02686900 |
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| | | | | | | | |
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| H | 2.15137400 | 6.51010600 | -2.18124000 | H | 5.58952800 | -0.99641700 | -2.54781000 |
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| H | 0.91838300 | 9.07357900 | 5.02620200 | H | 7.82417000 | -3.60536700 | 1.97214500 |
| H | 2.11892900 | 7.32661200 | 4.10807300 | H | 7.08649100 | -5.18132900 | 2.17018900 |
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| H | -4.16045400 | 5.74842500 | 0.15164700 | H | 6.48438400 | 4.05341700 | 0.84624900 |
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| H | 6.44187100 | 0.66596900 | 2.64603800 | H | -2.30324900 | -4.08638500 | 0.30304600 |
| H | 7.56853600 | 0.59459100 | 1.28808300 | H | -1.09201200 | -3.36501100 | -1.60120500 |
| H | 7.38322300 | -0.80570900 | 2.34623800 | H | -0.13275500 | -8.08137600 | 0.44549000 |
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| H | 7.45529200 | 2.58909500 | 6.90862500 | H | -5.62497300 | -2.83503800 | -4.82589200 |
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| H | 5.23656100 | 1.13396400 | 5.90630500 | H | -11.07223000 | 5.89050600 | -2.49195600 |
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| H | 7.74802600 | 5.60668800 | 2.34598800 | H | -11.63898100 | 4.69534000 | -0.39005400 |
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| H | 1.89913700 | -2.10229300 | -3.91906500 | H | -8.93787400 | -3.52886800 | 8.55875300 |
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| H | 1.39613500 | 4.40389500 | 0.53803900 | H | -1.04774800 | -3.41154400 | 3.61164300 |
| H | 3.62572700 | 0.99718400 | 1.59531700 | H | -1.57616400 | -5.06818200 | 3.85117300 |
| H | 3.91772300 | -1.38523600 | 1.20810200 | H | -4.72683100 | -3.84111400 | 5.12282700 |
| H | -0.17599600 | 2.42083500 | 0.10323900 | H | 0.42388600 | -1.72726400 | 0.95458600 |
| H | -1.02111200 | -0.76995100 | -0.84604500 | H | -5.07948500 | -2.71421800 | 1.10067400 |
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| H | 2.62764300 | -2.90839300 | -0.39634700 | H | 1.48394700 | -2.40619400 | 9.15279400 |
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| H | 4.01387500 | 3.17123800 | 0.58441600 | H | 3.62093400 | -3.72723600 | 9.34561600 |
| H | -0.46879500 | -1.21146500 | -3.71988100 | H | -10.03996800 | -5.42933700 | 9.80409500 |
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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 2.39270811 | -2.18213827 | 8.31491002 | C | 3.82623800 | -7.93914900 | 6.45028700 |
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| C | -0.42659700 | 9.14103200 | 3.97473900 | C | 5.96374600 | 3.47341400 | -0.03065900 |
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| C | -1.12753700 | 7.78742100 | 1.92996300 | C | 5.50521800 | 5.56837600 | -3.40141200 |
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| C | -0.88469200 | 6.82431100 | 0.95491700 | C | 2.61805100 | 3.11341200 | -3.53853600 |
| C | 1.28236200 | 6.39402900 | 1.92925300 | C | 1.37534600 | 2.89598800 | -2.67586400 |
| C | 0.32575800 | 6.11315600 | 0.94899000 | C | 6.06525200 | 1.76175700 | -7.32831500 |
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| C | 0.24160900 | 1.64001200 | 0.49302000 | H | -4.47026900 | 7.28189900 | 4.18844100 |
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| H | -3.55822300 | 3.43969500 | -4.86974400 | H | 7.60252807 | 7.55833600 | 4.69152639 |
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| H | 1.89157700 | 6.76088400 | -4.99752300 | H | 6.20153700 | -5.53851600 | -0.69538300 |
| H | 3.08076400 | 7.69372400 | -4.11179400 | H | 6.67189300 | -2.62184900 | -3.80680400 |
| H | 1.30804600 | 8.09194100 | -2.29737600 | H | 5.44716100 | -3.76164500 | 0.85568200 |
| H | 1.82831900 | 6.43025100 | -2.51134300 | H | 5.97474300 | -0.85455600 | -2.25776500 |
| H | 0.43061300 | 8.85786100 | -5.12735300 | H | 5.46019500 | -0.33862000 | -0.11405400 |
| H | -0.63338500 | 10.09978200 | 3.47967100 | H | 8.89795500 | -4.29193000 | -3.67696000 |

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| H | 7.92870100 | -3.18611600 | 2.18314900 | H | -0.44602200 | 2.40065200 | 0.14492400 |
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| H | 7.03804200 | -4.51546300 | 4.78107700 | H | -5.47489829 | 3.75039413 | -1.63000259 |
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| H | 5.76963800 | -2.25639500 | 3.13688700 | H | 2.78087000 | -3.61518100 | -0.97077000 |
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| H | 5.14520500 | -3.90789900 | 3.29264300 | H | -0.34893000 | -1.37981500 | -3.71673200 |
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| H | 6.21318500 | 4.34112800 | 0.55588700 | H | -5.03465100 | 5.91233500 | 6.09758100 |
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| H | 4.55030200 | 0.69737500 | -6.15618400 | H | 8.90515900 | 6.23188700 | 3.05351200 |
| H | 6.08176300 | -0.12786800 | -6.24593100 | H | 5.52775600 | 6.46669400 | -4.02712600 |
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| H | 0.33004000 | -1.64731300 | 1.44731300 | N | -3.60800100 | -0.16039300 | -5.33091600 |
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| H | 2.61296272 | -1.22846734 | 6.62131485 | C | -1.20883100 | 0.08751700 | -4.82020500 |
| | | | | C | -2.71348300 | -1.52761700 | -3.44439800 |
| | | | | C | -4.07633900 | -1.71091900 | -2.80127600 |
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| C | -8.85282700 | 1.95511000 | 2.79970900 | C | 1.34681100 | -0.97116700 | -6.26273200 |
| C | -8.95115800 | 0.84457700 | 1.78036000 | C | 2.21511900 | -1.28174600 | -4.03946200 |
| O | -9.87355500 | 0.02550800 | 1.80677300 | C | 1.40678800 | -2.21800800 | -1.55378100 |
| N | -7.89821000 | 0.73560600 | 0.92468300 | C | 0.52111400 | -2.35044600 | -8.06199100 |
| C | -7.96394400 | -0.19746200 | -0.19754500 | C | 1.62206000 | 8.79027500 | -5.20881800 |
| C | -7.53858300 | -1.61242400 | 0.24884500 | C | 2.16544800 | 7.59647800 | -4.40737700 |
| O | -6.49613700 | -2.14727100 | -0.17276500 | C | 1.41250300 | 7.34855000 | -3.09706700 |
| C | -7.04689000 | 0.33968900 | -1.31911300 | C | 0.28440500 | 6.30557300 | -3.18597000 |
| O | -7.03379500 | 1.74962600 | -1.35333600 | C | -1.44707600 | 8.99570100 | 4.82703300 |
| N | -8.35561700 | -2.22939800 | 1.11221500 | C | -0.31473900 | 9.26594000 | 3.80941700 |
| C | -8.09831900 | -3.58362300 | 1.58816000 | C | -0.07725900 | 8.20609900 | 2.76066200 |
| C | -8.36278300 | -3.81213100 | 3.07686200 | C | -1.00889400 | 7.95063100 | 1.74444500 |
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| O | -7.51504000 | -2.97749800 | 3.84740100 | C | -0.76743800 | 7.00171500 | 0.75615700 |
| C | -10.01111100 | -5.02339500 | 9.08803100 | C | 1.38108400 | 6.52994200 | 1.76101100 |
| C | -9.28846900 | -3.87426700 | 8.36790700 | C | 0.43623000 | 6.27997300 | 0.76444800 |
| C | -8.82656300 | -4.18029700 | 6.91223100 | C | -5.63415500 | 6.00914900 | 5.10613000 |
| O | -9.01231300 | -5.33593400 | 6.47758700 | C | -5.43250700 | 7.12460400 | 4.04770600 |
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| O | 0.15060700 | -4.53228400 | 5.76552000 | C | -7.46806200 | 5.72024500 | 1.11250700 |
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| C | -4.01729700 | -2.75474300 | 3.96225700 | C | -3.76340600 | 3.04247300 | 3.58349600 |
| N | -2.97857700 | -1.78682600 | 2.21762900 | C | -2.44219700 | 2.52734200 | 4.19140300 |
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| C | 1.59654600 | -3.23910300 | 7.75591100 | C | 3.71602700 | -7.84780000 | 6.57899700 |
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|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 4.22981600 | -6.43851000 | 2.10651100 | C | 1.45302300 | 1.86537000 | 0.77660600 |
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| C | 2.95012700 | -5.92580000 | 1.88926000 | C | 1.90390300 | -0.37382300 | 1.54714400 |
| C | 11.00263900 | 1.13016100 | 3.70100600 | C | 0.13268000 | 1.51071700 | 0.48553100 |
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| C | 8.46541700 | 1.28100800 | 3.12313000 | C | 0.57650300 | -0.74382800 | 1.29667900 |
| C | 8.43756900 | 2.80374900 | 2.94353200 | C | -13.31304400 | 4.66425200 | -3.15287200 |
| C | 7.37150500 | 0.62863200 | 2.26515500 | C | -11.82318900 | 4.40632400 | -2.84638900 |
| C | 8.02621000 | 6.64712500 | 2.62101500 | C | -11.48792200 | 3.72639000 | -1.50965600 |
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| C | 7.46207400 | 5.04745000 | 5.57371400 | O | -2.63037800 | -1.76812300 | -6.60665200 |
| C | 5.66516300 | 4.78679600 | 4.23884000 | O | -1.04827000 | 0.95162100 | -5.66859500 |
| C | 5.75638000 | 3.65222500 | 5.09412600 | O | -5.11836400 | -1.76633300 | -3.47403800 |
| C | 4.60991300 | 4.85043700 | 3.31213400 | O | 2.37521800 | -0.67592300 | -6.87182800 |
| C | 4.84384100 | 2.59416900 | 5.03473400 | O | 0.25879800 | 5.51748400 | -4.16509300 |
| C | 3.69153800 | 3.80934300 | 3.25876800 | O | -0.50231900 | 6.24304600 | -2.18555500 |
| C | 3.81414100 | 2.68785000 | 4.10606800 | O | 0.69803500 | 5.32194400 | -0.16656400 |
| C | 8.44990900 | -5.44967300 | -3.38486100 | O | -6.74020700 | 4.83268500 | -1.01753500 |
| C | 6.91532300 | -5.40242200 | -3.25699500 | O | 5.23378400 | -1.29575600 | 0.35723700 |
| C | 6.44989900 | -4.32875900 | -2.28994900 | O | 7.60969500 | 5.61865700 | -1.54820500 |
| C | 6.40674300 | -2.98898300 | -2.69648300 | O | 4.72743300 | 3.87540900 | -5.09371300 |
| C | 6.07333600 | -4.61188900 | -0.97119600 | O | 0.52798300 | 3.55386100 | -2.40554600 |
| C | 6.01516100 | -1.97368100 | -1.83051700 | O | 7.06052500 | 1.95911100 | -4.67945100 |
| C | 5.65851900 | -3.60978100 | -0.08819900 | O | 5.41028300 | 0.68893700 | -3.83283100 |
| C | 5.63968600 | -2.28349700 | -0.52130100 | O | 1.94820800 | -4.67433100 | -4.61812000 |
| C | 9.24397900 | -4.62466300 | 3.15322600 | O | -1.92400800 | -6.46893100 | -2.45227000 |
| C | 7.82915200 | -4.06847900 | 2.93288800 | O | 0.04018300 | -5.78214300 | 0.41368100 |
| C | 7.11667900 | -3.53685500 | 4.19004500 | O | 1.94420900 | 3.12016400 | 0.57396500 |
| C | 7.91652200 | -2.43163800 | 4.89181400 | O | 2.75600200 | -1.33053400 | 2.03484100 |
| C | 5.70533400 | -3.04660300 | 3.83582000 | O | -1.60610600 | -0.12265800 | 0.48914700 |
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| C | 6.78617200 | 2.57253100 | -0.85700000 | S | 2.51103100 | -0.98159800 | -2.24310700 |
| C | 6.04046000 | 3.40267800 | -0.04754300 | H | -3.60066900 | 5.70369800 | -2.90967500 |
| C | 4.73247900 | 1.84366100 | -0.89788700 | H | -2.08020200 | 4.99403500 | -3.39136700 |
| C | 5.56717700 | 5.45606900 | -3.51632500 | H | -1.30154800 | 2.76535400 | -2.06556900 |
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| C | 2.64913600 | 3.03563900 | -3.60972400 | H | -3.52327600 | 3.41744600 | -4.95493700 |
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| C | 6.10311000 | 1.21676500 | -4.84687100 | H | -4.98210400 | -1.94822100 | -0.98655500 |
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| C | 1.40318600 | -5.77534900 | -4.54367100 | H | -2.84573600 | 0.62362200 | -3.59715400 |
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| C | 3.43230100 | -7.42782600 | -2.55154700 | H | 1.57968400 | -2.35368300 | -8.32627300 |
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| C | -0.71128300 | -4.82912000 | -3.71969900 | H | 3.23133700 | 7.76950800 | -4.20686700 |
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| C | -2.11874300 | -4.91262800 | -0.19785500 | H | 2.08674100 | 6.94919800 | -2.32595100 |
| C | -1.17370600 | -5.98189700 | 0.37621200 | H | 0.53125900 | 8.75582500 | -5.29002800 |
| C | -0.98684900 | -8.31646000 | 1.12367700 | H | -0.51039800 | 10.23094200 | 3.32186300 |
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|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 0.17222400 | 5.53789600 | -1.01857500 | H | 8.89851100 | -2.78197300 | 5.22503700 |
| H | -2.43793900 | 9.15365500 | 4.39101700 | H | 5.74889600 | -2.22839300 | 3.10791300 |
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| H | -4.34670300 | 5.54067800 | -0.22825400 | H | 6.31575100 | 4.27731900 | 0.51633000 |
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| H | -1.79717700 | 1.54819400 | 2.37062000 | H | 6.86665200 | 3.92052300 | -4.12509700 |
| H | -0.94875100 | 0.97516000 | 3.80338800 | H | 1.16219300 | 1.67343100 | -3.00442600 |
| H | -2.61984300 | 0.47438800 | 3.49452300 | H | 2.01470600 | 2.41858200 | -1.66710300 |
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| H | -1.71029400 | 4.67663800 | 2.44123700 | H | 3.27143500 | 4.69125900 | -2.39592100 |
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| H | 5.68623500 | -7.05034300 | 3.57444000 | H | 4.36013400 | -7.20824600 | -3.09963100 |
| H | 1.95494500 | -5.56545600 | 5.11602200 | H | 1.98964500 | -6.27727600 | -1.38905200 |
| H | 4.86848000 | -6.68305600 | 1.26198100 | H | 2.90020100 | -5.31307900 | -2.56924000 |
| H | 1.14440100 | -5.21771100 | 2.81542900 | H | 3.68028400 | -5.84990500 | -1.08857000 |
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| H | 3.78917600 | -8.71077400 | 5.90876800 | H | 4.50382800 | -8.16435700 | -0.80052700 |
| H | 10.08487600 | 0.98059800 | 1.74754000 | H | 2.84190600 | -8.74217200 | -0.91950700 |
| H | 9.78695100 | -0.40067700 | 2.78505500 | H | 1.55051300 | -7.66695700 | -5.51766500 |
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| H | 8.76310000 | 3.07432600 | 1.93250100 | H | -0.30242300 | -6.84596500 | -4.06972800 |
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| H | 6.38280400 | 1.00927800 | 2.54282500 | H | -2.16617400 | -4.06762300 | 0.49534200 |
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| H | 7.35944200 | -0.45993200 | 2.37426600 | H | 0.06476400 | -8.04721700 | 1.00798400 |
| H | 11.96176700 | 0.84664700 | 3.25111900 | H | -2.73749800 | -7.24453500 | 0.58694900 |
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| H | 5.34287600 | -3.85447400 | 0.91932600 | H | 3.18619000 | -1.06798000 | -4.48645400 |
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| H | 7.20039800 | -4.85476800 | 2.49775500 | H | -1.99181700 | -0.77137200 | 1.16751400 |
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| H | 1.21525500 | -3.77453500 | -0.09775700 | H | 4.31148700 | -2.62594000 | 7.76065500 |
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| H | 3.91569300 | 3.28931900 | 0.37470600 | H | 3.86242100 | -3.26101400 | 9.35128000 |
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| H | 0.13278700 | -3.36849800 | -8.16408100 | N | -7.91800000 | 0.84435600 | 0.92991300 |
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| H | -4.72708400 | -1.69586700 | -8.09902800 | C | -7.58389700 | -1.55570000 | 0.44079200 |
| H | -3.35910200 | -8.05772300 | -5.10717000 | O | -6.56611100 | -2.14094200 | 0.02561600 |
| H | -1.97325700 | -8.43216300 | -6.15538500 | C | -7.10920300 | 0.26420500 | -1.28549900 |
| H | 3.07194900 | -6.80360800 | -5.32601700 | O | -7.10262200 | 1.66690300 | -1.43475800 |
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| N | 5.90779500 | 1.27885300 | -1.65564900 | C | 8.47853727 | 1.15312540 | 2.74992424 |
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| | | | | | | | |
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| C | 2.18851000 | 0.88178800 | 1.72090700 | H | -5.88890000 | 8.36291100 | 3.70130900 |
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| C | 2.05500900 | -2.83829500 | -0.16473500 | H | -4.37994800 | 5.60379100 | -0.71990300 |
| O | -2.84768300 | -2.35028200 | -6.48297900 | H | -7.80205900 | 4.60699900 | -1.42676200 |
| O | -1.20421900 | 0.35785600 | -5.82171400 | H | -6.53721000 | 6.41716700 | 5.00425500 |
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| H | 6.21393500 | 4.31219300 | -0.37955200 | H | -4.82742800 | 6.56849200 | 5.46016300 |
| H | 3.79687400 | 0.99532500 | -1.37149500 | H | -4.47434324 | 2.59391221 | 3.47102964 |
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| H | 6.76036100 | 3.41988300 | -4.66325200 | H | -1.11755700 | 10.09325300 | 4.75809200 |
| H | 1.33181700 | 1.36386400 | -2.80396200 | H | -4.93524300 | 4.17772100 | -5.05153800 |
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| H | 0.06338900 | 3.84398700 | -3.27839700 | H | 1.86551900 | 9.22317300 | -5.63071700 |
| H | 3.24435300 | 1.78967400 | -3.91634200 | H | 1.94888700 | 8.15675300 | -7.04893000 |
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| H | 4.10409900 | -7.22468800 | -2.67873900 | H | 6.00627000 | 0.09293700 | -8.49152100 |
| H | 1.71338500 | -6.32874700 | -0.97256500 | H | -0.25698700 | -2.48685900 | -8.70997900 |
| H | 2.48234400 | -5.42117800 | -2.29401500 | H | -0.12765900 | -4.08447000 | -7.95709100 |
| H | 3.37137300 | -5.73075700 | -0.81277200 | H | -5.25494400 | -0.62106900 | -7.59584200 |
| H | 4.07676200 | -9.33292500 | -1.31129500 | H | -4.96764900 | -2.35434200 | -7.92844400 |
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| H | -0.11049200 | -1.67303000 | 1.81058700 | H | -4.87022300 | -1.23628100 | 1.28787100 |
| H | 3.10715600 | -0.90074100 | 2.98249900 | H | -7.77017200 | -2.62138500 | 5.16025200 |
| H | -5.46601500 | 3.77603500 | -1.93089800 | H | 0.16542600 | -1.29244600 | 7.44424200 |
| H | 5.68223600 | 0.60956100 | -3.24643200 | H | 2.00257100 | -1.09167000 | 9.29159500 |
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| H | 1.29077800 | -3.24649600 | 0.49515100 | H | 4.46042800 | -0.92941000 | 8.99132700 |
| H | 2.72519800 | -3.64804900 | -0.47141200 | H | 4.01674000 | -2.61357100 | 9.34755000 |

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|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -10.16381700 | -3.85890400 | 10.58727700 | N | 5.95106000 | 1.29453300 | -1.71012300 |
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| H | -1.72709600 | -1.37511700 | 6.22651300 | C | -4.34973400 | 2.27666300 | -0.93840500 |
| H | 2.67470600 | -0.63172000 | 6.59862800 | C | -5.05603400 | -1.58062800 | -7.12308500 |
| H | 4.80556000 | 2.69253000 | 1.74014500 | C | -3.76032600 | -1.52578600 | -6.29011600 |
| H | 3.29495100 | 3.39226500 | 2.34844300 | C | -2.78371900 | -0.59246600 | -4.19274800 |
| H | 4.49541000 | 2.69631500 | 3.46965200 | C | -1.35056600 | -0.21703600 | -4.65304300 |
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| | | | | C | -4.23944500 | -2.04232300 | -2.71660800 |
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| C | -8.81283500 | 2.10986300 | 2.78466100 | C | 1.14984200 | -1.49022400 | -6.25992900 |
| C | -8.93694500 | 0.92504600 | 1.85620300 | C | 2.06109100 | -1.68029000 | -4.03299300 |
| O | -9.85944600 | 0.11313800 | 1.96632800 | C | 1.36024300 | -2.35124500 | -1.42068800 |
| N | -7.90138800 | 0.74520700 | 0.99163900 | C | 0.29371800 | -2.98988100 | -7.96041400 |
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| O | -7.40761300 | -2.71776800 | 4.17897100 | C | -0.74449600 | 6.82973200 | 0.27118900 |
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| N | 6.89679700 | 4.31079000 | 5.51890400 | | | | |

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|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 8.50137068 | 1.05354438 | 2.75717039 | C | 2.33758100 | 1.09111100 | 1.48078000 |
| C | 8.17330690 | 2.54815093 | 2.69288726 | C | -13.41358900 | 4.39305200 | -3.23958000 |
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| C | 7.64487500 | 5.16572700 | 4.72479700 | O | -2.80029000 | -2.26794200 | -6.49542900 |
| C | 5.46571000 | 5.60318300 | 4.35091400 | O | -1.15742500 | 0.82252700 | -5.28326000 |
| C | 5.55418400 | 4.55034300 | 5.30482400 | O | -5.28091000 | -2.04325000 | -3.39381400 |
| C | 4.19161300 | 6.05775300 | 3.96733100 | O | 2.17118600 | -1.23301400 | -6.89656100 |
| C | 4.42191500 | 3.95891900 | 5.87494400 | O | -0.86552100 | 6.64656400 | -4.82000500 |
| C | 3.06342300 | 5.47368600 | 4.52905900 | O | -0.67277000 | 5.91171900 | -2.74256200 |
| C | 3.17828600 | 4.43547300 | 5.47542500 | O | 0.66462900 | 5.10715000 | -0.57160600 |
| C | 8.33123800 | -5.76213400 | -3.26363400 | O | -6.81680200 | 4.74772800 | -1.28622700 |
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| C | 6.34022700 | -4.63235600 | -2.18197200 | O | 7.53994300 | 5.42500100 | -2.23160100 |
| C | 6.32466500 | -3.29449700 | -2.59642200 | O | 4.47209300 | 3.59007400 | -5.68175300 |
| C | 5.95927000 | -4.90518100 | -0.86288300 | O | 0.13385600 | 3.09484900 | -3.58918100 |
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| C | 4.70807100 | 1.54911900 | -1.30603400 | O | 4.29441200 | 0.56779000 | 2.68882300 |
| C | 5.45276100 | 5.11238100 | -4.11260100 | C | 4.09222783 | 2.86561881 | 2.22790236 |
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| C | 2.73225100 | -6.16501700 | -1.58351500 | H | -3.07313800 | 0.25041100 | -3.55630100 |
| C | 3.67139900 | -8.42261500 | -0.99212500 | H | -4.64138100 | -0.19317000 | -5.05330200 |
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| H | -3.61583900 | 3.49086500 | 2.30492000 | H | 6.81857700 | 1.47233100 | -7.52196700 |
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| H | 7.26763839 | -4.75597565 | 2.51336794 | H | 3.39526000 | -0.70002800 | 2.61408100 |
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| H | 8.84383470 | -2.62995270 | 5.26537557 | H | 1.17599400 | -3.50651500 | 0.37243400 |
| H | 5.70232250 | -2.17458859 | 3.09694123 | H | 2.69047800 | -3.69526700 | -0.53649400 |

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| H | 3.73927200 | 3.08313900 | -0.26084700 | H | -10.09213000 | -4.04660300 | 10.59117700 |
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| H | -5.25552100 | -0.60001000 | -7.56882400 | O | -9.92222700 | 0.37937300 | 1.87928500 |
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| H | -2.15748300 | -8.91237500 | -5.56067400 | C | -7.73709900 | -1.48391500 | 0.30571900 |
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| H | 8.68354200 | -6.49360400 | -3.99823300 | C | -7.04485700 | 0.43101400 | -1.22944600 |
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| N | 5.95871200 | 1.41299700 | -1.65910200 | C | 8.53005800 | 0.76583200 | 2.88780000 |
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| C | 0.12881300 | 6.69259400 | -3.46537200 | C | 8.31031200 | 2.38126700 | -1.43715900 |
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| C | 0.26928900 | 8.19773700 | 2.56948200 | C | 4.75180600 | 1.71878400 | -1.19548200 |
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| C | 1.44600500 | 7.44003500 | 2.62140400 | C | 4.56345900 | 4.29609000 | -4.34435300 |
| C | -0.40061900 | 6.89982700 | 0.61902600 | C | 2.67427300 | 2.86867500 | -3.79051000 |
| C | 1.71153700 | 6.42923300 | 1.69686800 | C | 1.42389400 | 2.80485300 | -2.90697100 |
| C | 0.77984500 | 6.15008000 | 0.69526000 | C | 5.99479800 | 1.23935600 | -7.58412300 |
| C | -5.36649800 | 6.23519900 | 5.00917000 | C | 5.56010700 | 0.40151800 | -6.37719500 |
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| C | -5.58964300 | 6.83506900 | 2.57312700 | C | 1.85931800 | -7.24904800 | -4.79743600 |
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| C | -6.33589500 | 5.63582700 | 0.10804200 | C | 3.42900700 | -8.59607800 | -1.45071800 |
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| C | -0.83198100 | 4.49520200 | 2.97635000 | C | -1.20733700 | -8.28774900 | 1.20593900 |
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| C | 2.47264900 | 0.78035100 | 1.41433500 | H | -5.71209100 | 8.24845700 | 4.21619700 |
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| H | -1.11624500 | 6.67936700 | -0.16414800 | H | 7.41044800 | -2.30247400 | 5.67526300 |
| H | 0.29173800 | 5.69575000 | -1.77843100 | H | 8.89224500 | -3.09267200 | 5.11895000 |
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| H | 5.18257100 | -2.81361100 | 4.64445900 | H | 3.98324600 | 3.13341800 | 0.13945700 |
| H | 5.04315300 | -3.94042300 | 3.29267600 | H | -0.58016100 | -1.63075800 | -3.66975800 |
| H | 9.90140500 | -4.09488900 | 3.23478600 | H | -13.65877200 | 5.65538000 | -2.35587800 |
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| H | 3.83782000 | 1.18979900 | -1.42249800 | H | -4.34321600 | 2.38051700 | 3.59326700 |
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| H | 6.95621000 | 1.71844800 | -7.38758800 | H | 2.30240900 | 2.91273800 | -4.81960700 |
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| H | 2.80501600 | -5.41318500 | -2.67160100 | H | -0.10596300 | -3.53709200 | -8.18654500 |
| H | 3.51709400 | -5.92952800 | -1.15535400 | H | -5.17020800 | -0.00767200 | -7.62850200 |
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| H | -9.91621800 | -4.54680200 | 10.35473600 | N | 5.97700900 | 1.36794600 | -1.57328000 |
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| H | -9.92759300 | -5.64045200 | 8.95115800 | N | -1.80754800 | -4.34260600 | -1.42860300 |
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| H | 5.03943000 | 2.47478900 | 2.10538200 | C | -3.71049300 | -0.93598100 | -6.39942000 |
| H | 3.46723700 | 3.08198600 | 2.64279700 | C | -2.82057100 | -0.25347800 | -4.18227400 |
| H | 4.52826800 | 2.17028200 | 3.76083700 | C | -1.35648000 | 0.11694000 | -4.53485700 |
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| C | -8.73403500 | 2.26678200 | 2.83124000 | C | 1.23844600 | -1.30564900 | -6.17563800 |
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| O | -9.93161800 | 0.44364100 | 1.83387100 | C | 1.05729000 | -1.72131100 | -1.02977600 |
| N | -7.88121900 | 0.94445600 | 0.98264700 | C | 0.32592100 | -2.45305700 | -8.12480800 |
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| O | -6.93157900 | 1.90384800 | -1.29603500 | C | -1.05535500 | 9.05512300 | 4.69627700 |
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| C | -8.79507300 | -4.94376200 | 3.52574500 | C | 1.46949900 | 7.40579000 | 2.67189300 |
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| C | -10.04904700 | -4.61702400 | 9.19152300 | C | 1.71147500 | 6.39802100 | 1.73727500 |
| C | -8.92694800 | -3.82546700 | 8.51204500 | C | 0.75610800 | 6.12431200 | 0.75679100 |
| C | -9.02517700 | -3.75494100 | 6.96460300 | C | -5.34124000 | 6.22166300 | 5.05838100 |
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| C | -4.38392800 | -3.28388000 | 4.38904600 | C | -3.59850200 | 3.17871600 | 3.53433800 |
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| C | 2.20869500 | -2.00862500 | 8.31352500 | C | 4.16923900 | -6.71846300 | 5.83300700 |
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| N | 7.04046300 | 3.77438100 | 5.90622700 | | | | |

| | | | | | | | |
|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 8.53156600 | 0.69103300 | 2.91791400 | C | 2.50709600 | 0.72303800 | 1.31661900 |
| C | 8.32177200 | 2.20872400 | 2.91895700 | C | -13.17960000 | 5.08675000 | -3.08119300 |
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| C | 7.01425500 | 5.50413900 | 4.44980000 | C | 1.74949000 | -3.05358300 | -0.79980000 |
| C | 7.81639800 | 4.67428500 | 5.19336400 | O | -2.73779000 | -1.64375500 | -6.65940200 |
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| C | 4.55522900 | 3.38840100 | 6.13088700 | O | -0.55976600 | 7.08029300 | -4.33009800 |
| C | 3.24697400 | 4.93658800 | 4.77366100 | O | -0.38823100 | 6.17295300 | -2.31958100 |
| C | 3.32736200 | 3.86954600 | 5.69154700 | O | 0.94348100 | 5.14366100 | -0.18390400 |
| C | 8.20572500 | -5.79577000 | -3.53345900 | O | -6.59220600 | 5.04713100 | -1.03052400 |
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| C | 5.57857900 | -2.30912700 | -2.22868600 | O | 7.01084300 | 1.73617500 | -4.88462200 |
| C | 5.70524500 | -3.75553700 | -0.29604400 | O | 5.37164400 | 0.48510800 | -3.99315100 |
| C | 5.49961300 | -2.48620000 | -0.84472100 | O | 1.73564500 | -4.78668900 | -4.82170400 |
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| C | 7.72634900 | -4.34040200 | 2.78941600 | O | -0.17476600 | -5.85626400 | 0.22953500 |
| C | 7.04753600 | -3.80820500 | 4.06460600 | O | -1.18743200 | 0.09828400 | -0.54768900 |
| C | 7.91861300 | -2.78383300 | 4.80285100 | O | 2.27262800 | 3.02980200 | 0.70714400 |
| C | 5.67324700 | -3.21166600 | 3.73029600 | O | 2.60641000 | -1.62355800 | 1.61903500 |
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| C | 8.33197300 | 2.34294600 | -1.38060300 | O | -0.19898400 | -1.99587600 | -1.60838100 |
| C | 6.85661700 | 2.31664400 | -1.06857100 | S | 2.08001500 | -0.61800900 | -2.15225500 |
| C | 6.14022000 | 3.20929400 | -0.29956600 | C | 3.60951100 | 0.86703900 | 2.25774000 |
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| C | 5.58898000 | 0.43432600 | -6.34343100 | H | -3.44233300 | 3.47417600 | -4.95940300 |
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| C | 3.38595600 | -8.53397600 | -1.48827500 | H | -4.64350000 | 0.23957500 | -5.05184900 |
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| C | -3.06633300 | -6.44682600 | -6.45631800 | H | 0.77326100 | 8.68786800 | -5.45507700 |
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| C | 0.47184600 | 1.62123400 | 0.18517600 | H | 2.62156800 | 5.80851000 | 1.78183400 |
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| H | -5.67228600 | 8.24014000 | 4.26837900 | H | 5.16670800 | -2.85976200 | 4.63669600 |
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| H | -8.29993700 | 5.78436900 | 0.86606800 | H | 8.83916800 | 2.70171100 | -0.48037500 |
| H | -4.16837500 | 5.68997600 | -0.28994300 | H | 6.45284600 | 4.09715300 | 0.22402400 |
| H | -7.61824600 | 4.90018000 | -1.13201200 | H | 3.85754400 | 1.15061200 | -1.32842700 |
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| H | -3.56318900 | 3.52122300 | 2.49493200 | H | 6.99339600 | 1.74623100 | -7.34501900 |
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| | | | | | | | |
|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 3.99896800 | 3.13807400 | 0.16697000 | H | -9.94209200 | -4.61404700 | 10.28393800 |
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| H | -4.33769100 | 2.37422200 | 3.60897800 | H | -9.19312700 | -3.94869700 | 1.07238000 |
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| H | -0.85898600 | 9.77373600 | 5.49892200 | H | -7.28659800 | 0.04067100 | -2.19438100 |
| H | -4.72935400 | 4.68903500 | -4.74629000 | H | 2.24799800 | -3.61905200 | 6.87302100 |
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| H | 2.33849300 | 2.94457800 | -4.77716600 | H | 4.44004900 | 2.06129500 | 3.78666300 |
| H | 9.75307700 | 3.57891600 | -2.46756900 | | | | |
| H | 5.29123400 | 2.05687200 | -7.74971700 | | | | |
| H | 6.14003000 | 0.59188400 | -8.39413100 | | | | |
| H | -0.18248500 | -1.80632400 | -8.84799500 | C | -8.79648800 | 2.09125600 | 2.96503800 |
| H | -0.09954800 | -3.45741600 | -8.21325900 | C | -8.85666600 | 0.90737200 | 2.03245500 |
| H | -5.14323500 | 0.09848500 | -7.63766500 | O | -9.68266500 | 0.00188700 | 2.17265600 |
| H | -4.89555400 | -1.61255000 | -8.09422500 | N | -7.83818800 | 0.83318800 | 1.13350900 |
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| H | 2.75605700 | -6.97293900 | -5.38845800 | O | -5.99752400 | -1.81510100 | 0.60286400 |
| H | 8.54196700 | -6.49096900 | -4.30961100 | C | -7.00727800 | 0.21426400 | -1.07084600 |
| H | 8.64272200 | -6.11079500 | -2.58010100 | O | -7.08861900 | 1.60836600 | -1.25659000 |
| H | -1.54116900 | -9.07239000 | 0.41597300 | N | -7.97885000 | -2.19112500 | 1.64784000 |
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| H | -9.03744100 | 0.10704200 | -0.53024200 | C | -1.09852400 | -2.79581700 | 5.47597900 |
| H | -9.32897300 | -1.30543100 | 1.52454600 | C | 0.02581300 | -3.33946500 | 6.34821400 |
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| H | -9.88795100 | -3.10740200 | 3.30620900 | C | -3.16139200 | -2.48154800 | 3.19395100 |
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| H | -1.04092200 | -3.15306800 | 3.81128800 | C | 1.88592000 | -2.71670000 | 7.81003000 |
| H | -1.58364300 | -4.77653500 | 4.19656600 | C | 2.47161500 | -1.41746300 | 8.37211500 |
| H | -4.69755600 | -3.41375100 | 5.41339600 | C | 3.92695900 | -1.59829200 | 8.79155800 |
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| H | 4.26809500 | -2.52172200 | 7.86871500 | N | -4.42999400 | -2.85466100 | -1.40287900 |
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| H | 3.72496500 | -3.06097700 | 9.46531400 | N | -0.00501200 | -2.37181600 | -6.65064000 |
| | | | | N | 7.05641700 | 4.41784200 | 5.45742300 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| N | 5.78556200 | 1.53222200 | -1.96496800 | C | 8.50113700 | 1.17509600 | 2.64268700 |
| N | 4.64313500 | 2.81548500 | -0.57734100 | C | 8.22011600 | 2.67838000 | 2.55348000 |
| N | 6.55657600 | 4.41074400 | -4.19627200 | C | 7.45917600 | 0.39080100 | 1.83138900 |
| N | 3.24254300 | 3.90164500 | -3.80090000 | C | 8.03489900 | 6.78721900 | 1.70074300 |
| N | -0.07002500 | -6.30662200 | -3.56039400 | C | 7.20860200 | 7.14700800 | 2.93057300 |
| N | -1.69413900 | -4.63676800 | -0.85481300 | C | 6.87797300 | 6.02974000 | 3.88116900 |
| N | -1.83952600 | -7.16889200 | 1.26587500 | C | 7.75385000 | 5.28886600 | 4.63516400 |
| N | -5.15846300 | -5.71916500 | -6.59956800 | C | 5.55327000 | 5.58744200 | 4.25246900 |
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| C | -4.03561600 | 4.06200000 | -4.91276600 | C | 4.25539100 | 5.96345800 | 3.86420700 |
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| C | -3.02522600 | -0.83770200 | -4.01195800 | C | 5.60929500 | -3.51930400 | -3.06808300 |
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| C | 1.05803600 | -1.84562500 | -6.00079300 | C | 9.32986500 | -4.41547000 | 2.98312600 |
| C | 1.72680100 | -1.82675000 | -3.57511100 | C | 7.90368900 | -3.87616300 | 2.79637100 |
| C | 0.75832100 | -1.80965800 | -0.68511200 | C | 7.23395000 | -3.31902200 | 4.06583800 |
| C | 0.10881100 | -2.96559100 | -7.96707300 | C | 8.07816700 | -2.22990300 | 4.74008300 |
| C | 1.28033700 | 8.35275500 | -5.96983900 | C | 5.82528700 | -2.79846400 | 3.74844400 |
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| C | 1.25235000 | 6.92339800 | -3.77320200 | C | 7.45028100 | 4.54392200 | -3.18019600 |
| C | -0.19282500 | 6.44690600 | -3.78233500 | C | 8.11723100 | 2.54948600 | -1.80011200 |
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| C | -0.24723500 | 9.46401900 | 3.06960000 | C | 5.94865900 | 3.26924900 | -0.55848700 |
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| C | -6.60124300 | 5.44102600 | -0.00075100 | C | 3.89595900 | -8.21065100 | -1.16109200 |
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| C | 11.08290200 | 1.36676800 | 3.03933500 | C | 0.56916300 | -0.73389500 | 0.41649500 |
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| C | 2.23766400 | 0.87547100 | 1.42798900 | H | -5.93431700 | 8.26629100 | 3.95670100 |
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| C | 1.43649900 | -3.10623200 | -0.28491800 | H | -4.53531100 | 5.66098300 | -0.58050100 |
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| O | -1.36361000 | 0.70301300 | -4.83450200 | H | -6.51317300 | 6.29017000 | 5.24209900 |
| O | -5.57524500 | -2.09194000 | -3.20835700 | H | -2.45848300 | 2.31930500 | 4.92784700 |
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| O | -6.92948400 | 4.78090800 | -1.14009200 | H | -0.33186400 | 3.40764900 | 4.43221900 |
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| O | 4.27964500 | 3.69117400 | -5.81666200 | H | -0.48583300 | 3.90091100 | 1.98869700 |
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| S | 1.83011700 | -0.88540500 | -2.00435700 | H | 7.21770500 | 2.91917500 | 2.91823900 |
| C | 3.35058200 | 1.03898400 | 2.34568200 | H | 8.28291500 | 3.01855300 | 1.51330800 |
| O | 3.84538600 | 0.03990100 | 2.94041700 | H | 8.93090500 | 3.26822800 | 3.13846100 |
| C | 3.97489000 | 2.36951600 | 2.66605700 | H | 6.45065100 | 0.52646900 | 2.23235900 |
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| H | -2.43076200 | 4.93483900 | -3.73559200 | H | 7.67061000 | -0.68315200 | 1.83709000 |
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| H | -0.94249500 | -2.25547200 | -6.28246300 | H | 6.45187700 | -6.74296000 | -2.85515300 |
| H | 1.67861700 | 6.24282200 | -5.75437700 | H | 6.58635300 | -5.55276300 | -0.54051500 |
| H | 2.92329700 | 7.26638200 | -5.07081800 | H | 5.58632400 | -3.45839400 | -4.15310500 |
| H | 1.28302600 | 7.84057600 | -3.16774100 | H | 5.60932200 | -3.69636000 | 0.79344800 |
| H | 1.86010900 | 6.18335700 | -3.24258100 | H | 4.71628100 | -1.58026100 | -2.83155100 |
| H | 0.19072100 | 8.31477000 | -5.99945100 | H | 3.92027400 | -1.04692700 | -0.71202900 |
| H | -0.49708000 | 10.35359600 | 2.47629200 | H | 8.57663400 | -4.71220600 | -3.75144400 |
| H | 0.69122600 | 9.70334000 | 3.58321700 | H | 7.90884700 | -3.09786900 | 2.02158100 |
| H | 1.94723500 | 7.85870700 | 3.00291400 | H | 7.26505200 | -4.67881400 | 2.40881500 |
| H | -1.81542400 | 8.45614700 | 1.02992100 | H | 7.13299500 | -4.15630500 | 4.77409200 |
| H | 2.45702600 | 5.98094000 | 1.46749400 | H | 8.25105000 | -1.39501300 | 4.05299700 |
| H | -1.30484400 | 6.58022400 | -0.49841900 | H | 7.56500500 | -1.82975000 | 5.62177600 |
| H | 0.08838400 | 5.53954500 | -2.05385700 | H | 9.05401400 | -2.60576400 | 5.06449600 |
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| | | | | | | | |
|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 5.32267400 | -2.44589400 | 4.65650800 | H | 3.83281300 | 3.11182800 | -0.01146900 |
| H | 5.20045100 | -3.58059500 | 3.31099700 | H | -0.88619400 | -2.26402700 | -3.84920700 |
| H | 10.05401000 | -3.61445700 | 3.16025400 | H | -13.95900700 | 5.06770400 | -2.24686000 |
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| H | 6.25594600 | 4.11501600 | 0.03393900 | H | -4.79672200 | 6.46577800 | 5.65470800 |
| H | 3.69260300 | 1.20724700 | -1.62817700 | H | -4.38665800 | 2.41517300 | 3.59012400 |
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| H | 2.65564800 | -5.29936600 | -2.58652800 | H | -0.27855800 | -3.98899700 | -7.97912100 |
| H | 3.62885900 | -5.53304400 | -1.15377000 | H | -5.44074200 | -0.59821800 | -7.46083800 |
| H | 4.27969700 | -9.17523700 | -1.51315200 | H | -5.13871500 | -2.32405500 | -7.81798000 |
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| H | 3.09957700 | -8.40886000 | -0.43368300 | H | -2.26912600 | -8.89922900 | -5.52185800 |
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| H | 0.08099500 | -7.97808200 | 1.50705600 | H | 9.64264200 | -4.96628900 | 2.08978400 |
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| H | -0.98983100 | -1.25878700 | -1.24255300 | H | 0.19906500 | -2.25269300 | 3.80495700 |
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| H | 1.36427500 | 4.37648100 | -0.05159800 | H | -3.80793700 | -2.88542100 | 3.95921400 |
| H | -0.44513900 | -1.32318700 | 1.28987100 | H | -2.80247000 | -0.96902800 | 0.34077000 |
| H | 3.05325300 | -1.06505300 | 2.41232800 | H | -7.17221300 | -2.79690100 | 5.40102300 |
| H | -5.58170800 | 3.77700000 | -1.72511800 | H | 0.38559700 | -1.47149200 | 7.08907800 |
| H | 5.63817100 | 0.74539900 | -3.34238700 | H | 1.87440600 | -1.10273200 | 9.23624400 |
| H | 2.43419800 | -2.93433600 | 0.10743200 | H | 4.54125400 | -1.88675000 | 7.93004600 |
| H | 0.84150400 | -3.61779700 | 0.47847400 | H | 4.32213100 | -0.66420300 | 9.19853800 |
| H | 1.50796800 | -3.75036100 | -1.16380800 | H | 4.02621200 | -2.38120400 | 9.55059400 |

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|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -9.96676400 | -4.06847800 | 10.76872400 | N | 5.80005100 | 1.49528700 | -1.95729300 |
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| H | -8.85197000 | 3.09164800 | 2.52082200 | N | 6.60050800 | 4.37211800 | -4.17891900 |
| H | -7.86479900 | 1.97930600 | 3.52672900 | N | 3.28010900 | 3.88962700 | -3.79316100 |
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| H | -8.98220500 | -5.28288400 | 9.90988000 | N | -1.70713900 | -4.64825400 | -0.84668900 |
| H | -8.18110200 | -4.25434900 | 1.75355400 | N | -1.89603000 | -7.16910200 | 1.19726400 |
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| H | -5.95548900 | -0.04133200 | -0.91295500 | N | -5.64082100 | -4.55662500 | -4.76510000 |
| H | -7.34173000 | -0.35114800 | -1.94921400 | C | -3.99113800 | 4.10485500 | -4.92606100 |
| H | 2.55455200 | -3.10302700 | 7.02390100 | C | -3.43130000 | 4.69019300 | -3.61292200 |
| H | -1.97574600 | -3.42873500 | 5.64466400 | C | -3.48053900 | 3.70901400 | -2.49540900 |
| H | 1.88402500 | -3.48712600 | 8.58864400 | C | -2.46528000 | 2.89789100 | -2.07167800 |
| H | -1.37358900 | -1.77464600 | 5.75956300 | C | -4.26582600 | 2.34288500 | -0.92128700 |
| H | 2.83479000 | -0.56163700 | 6.64581900 | C | -5.21954100 | -1.52003000 | -7.05346200 |
| H | 4.80375700 | 2.54471600 | 1.97294500 | C | -3.93287600 | -1.48461100 | -6.22871100 |
| H | 3.28127400 | 3.20109400 | 2.57876700 | C | -3.00964500 | -0.80096900 | -4.04008400 |
| H | 4.39336600 | 2.31209600 | 3.67026700 | C | -1.56438000 | -0.40932100 | -4.43877500 |
| | | | | C | -3.15476200 | -2.19458600 | -3.39380400 |
| | | | | C | -4.48419500 | -2.32694400 | -2.67276600 |
| | | | | C | 0.77523300 | -1.22902800 | -4.63058700 |

Int10

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -8.78875100 | 2.14566500 | 2.93229400 | C | 1.06184500 | -1.83352900 | -6.02645900 |
| C | -8.85234000 | 0.96202500 | 2.00160300 | C | 1.71433100 | -1.87859000 | -3.59996400 |
| O | -9.67443400 | 0.05354300 | 2.14966900 | C | 0.74317900 | -1.81906500 | -0.64043000 |
| N | -7.83833700 | 0.88600300 | 1.09838800 | C | 0.11002400 | -2.94375200 | -7.98994900 |
| C | -7.82061900 | -0.20605500 | 0.13997200 | C | 1.35924500 | 8.35954700 | -5.95513000 |
| C | -7.19537700 | -1.43921400 | 0.82513300 | C | 1.90645900 | 7.15938000 | -5.15941300 |
| O | -5.99285000 | -1.75005300 | 0.60589000 | C | 1.31947400 | 6.92442400 | -3.76047600 |
| C | -7.01230800 | 0.24825100 | -1.10361600 | C | -0.12526300 | 6.44645300 | -3.77343200 |
| O | -7.07777500 | 1.64214900 | -1.28863000 | C | -1.28588400 | 9.26714800 | 4.16176300 |
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| C | -7.59736600 | -3.41821700 | 2.24193000 | C | 0.08020600 | 8.29203200 | 2.15367800 |
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| C | -7.64920700 | -5.03066000 | 4.14241900 | C | 1.27433400 | 7.56537000 | 2.25129900 |
| O | -6.80305600 | -2.76655400 | 4.42095300 | C | -0.54409100 | 6.87393500 | 0.27206000 |
| C | -9.70140100 | -4.37999600 | 9.72586200 | C | 1.57132800 | 6.51427400 | 1.38342100 |
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| C | -8.36581700 | -3.72298900 | 7.56157000 | C | -5.46565600 | 6.33012600 | 4.81883100 |
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| C | -1.25396600 | -2.79621000 | 5.61507100 | C | -7.10907700 | 6.43399000 | 2.13864700 |
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| O | 0.24820500 | -4.52610900 | 6.36212900 | C | -7.50379300 | 5.76920300 | 0.97850000 |
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| C | 1.84419800 | -2.75557500 | 7.79273700 | C | 3.90044800 | -7.44532700 | 6.84706300 |
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| N | -0.00401800 | -2.35630900 | -6.67354400 | C | 9.92870600 | 0.74655200 | 2.19477400 |
| N | 7.08064200 | 4.36083800 | 5.49088800 | | | | |

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|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 8.50252300 | 1.10136000 | 2.65358600 | C | 2.27494600 | 0.92396000 | 1.44469800 |
| C | 8.23338200 | 2.60712200 | 2.57265900 | C | -13.48728300 | 4.46669200 | -3.00168900 |
| C | 7.45707900 | 0.33115300 | 1.83347100 | C | -11.98588600 | 4.20486500 | -2.74697000 |
| C | 8.08030500 | 6.72110000 | 1.72964200 | C | -11.59967200 | 3.52260100 | -1.42394700 |
| C | 7.25318200 | 7.08325500 | 2.95822500 | C | -10.06912400 | 3.34894700 | -1.33187900 |
| C | 6.91482100 | 5.97195200 | 3.91241500 | C | 1.40494600 | -3.12414400 | -0.24240700 |
| C | 7.78502800 | 5.21176300 | 4.65318900 | O | -2.94450500 | -2.16353000 | -6.50868700 |
| C | 5.58603000 | 5.56300200 | 4.30706200 | O | -1.33209600 | 0.71958600 | -4.86712500 |
| C | 5.72683600 | 4.54929500 | 5.29598400 | O | -5.56520200 | -2.05855900 | -3.21680500 |
| C | 4.29157100 | 5.96722800 | 3.93650300 | O | 2.21019700 | -1.81312500 | -6.46638000 |
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| C | 3.19361700 | 5.37406700 | 4.54680800 | O | -0.55732300 | 5.81589100 | -2.67004900 |
| C | 3.36014900 | 4.37855700 | 5.53067800 | O | 0.90695400 | 5.13560600 | -0.48392800 |
| C | 8.21943700 | -5.75996200 | -3.44582600 | O | -6.88166200 | 4.79429300 | -1.14754800 |
| C | 6.68937400 | -5.82279900 | -3.30369100 | O | 4.58011500 | -1.54935000 | -0.19635800 |
| C | 6.11849500 | -4.69973000 | -2.47154700 | O | 7.48307600 | 5.42557100 | -2.35303600 |
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| C | 5.62491000 | -3.67467500 | -0.31488600 | O | 5.26802200 | 0.28928600 | -4.18583500 |
| C | 5.08545500 | -2.55656900 | -0.96153800 | O | 1.40922900 | -5.06860200 | -4.71729400 |
| C | 9.28902600 | -4.49468100 | 2.98166200 | O | -2.13359500 | -6.70077800 | -1.74851800 |
| C | 7.86823100 | -3.94099600 | 2.79387900 | O | -0.66551600 | -5.42430900 | 2.02472600 |
| C | 7.20271400 | -3.37884100 | 4.06372200 | O | -1.24273100 | 0.21075700 | -0.68960100 |
| C | 8.05952900 | -2.30216300 | 4.74217000 | O | 2.16010500 | 3.19814300 | 0.64849000 |
| C | 5.80157400 | -2.83786300 | 3.74617900 | O | 2.37527800 | -1.44030700 | 1.81901300 |
| C | 8.46003200 | 3.32523800 | -3.05608900 | O | -9.60830800 | 2.17939800 | -1.42930200 |
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| C | 8.14137800 | 2.49343900 | -1.78381800 | O | -0.53133200 | -2.12555500 | -1.17318500 |
| C | 6.67681000 | 2.42166800 | -1.41765700 | S | 1.81763700 | -0.94756600 | -2.02584900 |
| C | 5.97132600 | 3.22563800 | -0.54462900 | C | 3.39091100 | 1.08981100 | 2.35030500 |
| C | 4.61066400 | 1.73315600 | -1.42109100 | O | 3.92858100 | 0.09351300 | 2.91517700 |
| C | 5.36312200 | 5.12701400 | -4.20397400 | C | 3.97541900 | 2.43308900 | 2.70117000 |
| C | 4.26911500 | 4.17259600 | -4.68565000 | H | -3.97227800 | 5.60703700 | -3.35293100 |
| C | 2.43730800 | 2.72217300 | -4.00992200 | H | -2.38895200 | 4.97346000 | -3.74021200 |
| C | 1.21797600 | 2.66526200 | -3.08541800 | H | -1.44721300 | 2.84923800 | -2.42821000 |
| C | 5.70316200 | 0.98549000 | -7.80345900 | H | -4.94559300 | 1.87641100 | -0.23196000 |
| C | 5.33569500 | 0.19387100 | -6.54314400 | H | -3.73596800 | 3.04613700 | -5.02865600 |
| C | 5.83831300 | 0.81002800 | -5.26195800 | H | -6.06065400 | -1.78018500 | -6.40434500 |
| C | 1.86018700 | -7.45060000 | -4.48884500 | H | -3.10418400 | -2.95431100 | -4.17973600 |
| C | 1.05125500 | -6.16357500 | -4.29331800 | H | -2.34529600 | -2.36849100 | -2.68452300 |
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| C | 3.33606500 | -7.35681700 | -2.34762700 | H | -3.49272300 | -2.91975000 | -0.99355300 |
| C | 2.82727100 | -6.01839000 | -1.79899800 | H | -3.28153700 | -0.03517800 | -3.30714000 |
| C | 3.86105900 | -8.22826200 | -1.20065900 | H | -4.86845300 | -0.33341600 | -4.85297700 |
| C | -0.83915600 | -5.16448500 | -3.07095100 | H | 1.16718300 | -2.96306600 | -8.25711100 |
| C | -1.61411400 | -5.57979200 | -1.82116300 | H | -0.94016700 | -2.24200200 | -6.30239700 |
| C | -2.39911700 | -4.93562100 | 0.40556700 | H | 1.74520500 | 6.24658400 | -5.74292400 |
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| C | -1.02745100 | -8.25950900 | 1.63733100 | H | 1.34814100 | 7.84138700 | -3.15460200 |
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| C | -0.10616400 | 0.46444100 | -0.05298600 | H | -1.75394400 | 8.46851000 | 1.03333900 |
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| H | -5.88830300 | 8.29235700 | 3.94194100 | H | 5.30088100 | -2.48709400 | 4.65616000 |
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| H | 10.05824200 | 1.10780100 | 1.16460300 | H | 3.06777700 | -8.43514400 | -0.47210500 |
| H | 10.01243200 | -0.34693200 | 2.14067100 | H | 1.25794800 | -8.15179200 | -5.08050000 |
| H | 8.40571500 | 0.79404300 | 3.70691100 | H | -1.56156300 | -4.79859500 | -3.81496700 |
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| H | 6.31399800 | 7.54114600 | 2.62610900 | H | -2.89894900 | -6.88328700 | -7.03958200 |
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| H | 5.55161100 | -3.51713700 | -4.18033100 | H | 1.43540900 | -2.92031400 | -3.42413000 |
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| H | 4.70689200 | -1.61903800 | -2.86787600 | H | -1.00682500 | -1.22540300 | -1.14896200 |
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| H | 8.24384900 | -1.46812300 | 4.05716700 | H | 5.65491700 | 0.71906700 | -3.33484900 |
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| H | 9.02980600 | -2.69100700 | 5.06800800 | H | 0.82157300 | -3.61028600 | 0.54736200 |
| H | 5.84627900 | -1.98998500 | 3.05569100 | H | 1.43325500 | -3.78430900 | -1.11215000 |

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| H | 3.84947500 | 3.08889300 | -0.00478700 | H | -10.04919600 | -4.01052900 | 10.69931000 |
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| H | 1.73940600 | 8.27638100 | -6.97883100 | H | -1.46645900 | -1.75105800 | 5.86156700 |
| H | 8.25711600 | 7.61920200 | 1.12988600 | H | 2.82023000 | -0.59915600 | 6.61108700 |
| H | 9.03916700 | 6.28444200 | 2.02613500 | H | 4.81217900 | 2.64084800 | 2.02657400 |
| H | 5.37265600 | 5.96732400 | -4.90595400 | H | 3.26360500 | 3.24917100 | 2.61400400 |
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| H | 4.93464400 | 1.73124600 | -8.03125800 | | | | |
| H | 5.81229600 | 0.25697600 | -8.61274400 | | | | |
| H | -0.43910800 | -2.35764500 | -8.73495500 | C | -8.79849400 | 2.14739000 | 2.78837000 |
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| H | -5.42337000 | -0.53706000 | -7.49220600 | O | -9.83128500 | 0.23441200 | 1.76593900 |
| H | -5.13305200 | -2.26398500 | -7.85374400 | N | -7.86903700 | 0.98070600 | 0.87972400 |
| H | -3.65821200 | -8.41423500 | -4.49251700 | C | -7.92768200 | 0.04689000 | -0.23745300 |
| H | -2.31852800 | -8.86707600 | -5.56950100 | C | -7.49371000 | -1.34401300 | 0.26238700 |
| H | 2.76127300 | -7.21367700 | -5.06438500 | O | -6.33585600 | -1.76882000 | 0.12285000 |
| H | 8.55635000 | -6.48997200 | -4.18903800 | C | -7.00373400 | 0.57284500 | -1.35901900 |
| H | 8.69298900 | -6.00345300 | -2.48889800 | O | -6.97092800 | 1.98055100 | -1.38697800 |
| H | -1.30160300 | -9.09144400 | 0.97986900 | N | -8.45741000 | -2.05801800 | 0.87132400 |
| H | -1.12589100 | -8.54256700 | 2.69109700 | C | -8.22808100 | -3.39907900 | 1.38348400 |
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| N | 5.91634100 | 1.39718100 | -1.59926800 | C | 8.48534600 | 0.77834300 | 2.87880800 |
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| N | 6.83628900 | 4.44555100 | -3.74294400 | C | 7.48251500 | 0.08360900 | 1.95152900 |
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| C | -5.005559900 | -1.02944800 | -7.28233900 | C | 6.70008000 | -5.73852400 | -3.42404400 |
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| C | -2.76611900 | -0.39131500 | -4.22302900 | C | 5.95935900 | -3.35846900 | -3.06257900 |
| C | -1.32113600 | -0.05756600 | -4.68281900 | C | 6.10393900 | -4.77981500 | -1.13906800 |
| C | -2.93296200 | -1.74810400 | -3.50232900 | C | 5.66571400 | -2.26876600 | -2.25136000 |
| C | -4.18763000 | -1.75577800 | -2.65296300 | C | 5.79592200 | -3.70299000 | -0.30892100 |
| C | 1.02419000 | -0.82396400 | -4.79585200 | C | 5.62176400 | -2.42918500 | -0.86225200 |
| C | 1.24448200 | -1.33031500 | -6.23235300 | C | 9.13961600 | -4.86011800 | 2.97891000 |
| C | 1.97119600 | -1.60362700 | -3.86813600 | C | 7.74373500 | -4.25182200 | 2.78740100 |
| C | 1.00777000 | -1.76244200 | -0.93265400 | C | 7.07393600 | -3.71309300 | 4.06521900 |
| C | 0.32108700 | -2.50929200 | -8.14529000 | C | 7.95635100 | -2.69474300 | 4.79901900 |
| C | 1.72589400 | 8.63455500 | -5.44193600 | C | 5.70215000 | -3.10452700 | 3.74084900 |
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| C | 0.11781300 | 6.63010300 | -3.43758300 | C | 8.26761200 | 2.40532400 | -1.41611400 |
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| C | 0.19048200 | 8.16101900 | 2.59614900 | C | 4.70468500 | 1.69119300 | -1.12786700 |
| C | -0.69559600 | 7.88781300 | 1.54595800 | C | 5.61344000 | 5.22682000 | -3.76223000 |
| C | 1.36357200 | 7.39855900 | 2.66780700 | C | 4.52046100 | 4.31570600 | -4.32215900 |
| C | -0.42709700 | 6.89393400 | 0.60897600 | C | 2.63758500 | 2.87627000 | -3.78747700 |
| C | 1.65321500 | 6.40130900 | 1.73730400 | C | 1.36778000 | 2.80093900 | -2.93654000 |
| C | 0.75289900 | 6.13831800 | 0.69742800 | C | 5.98047400 | 1.28624400 | -7.57822300 |
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| C | -5.64534900 | 6.76944600 | 2.56943400 | C | 1.87985800 | -7.23973500 | -4.85509100 |
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| C | -6.36331000 | 5.58402000 | 0.09322900 | C | 3.64658200 | -8.55354900 | -1.59926700 |
| C | -3.67416500 | 3.12154100 | 3.49023400 | C | -0.70899500 | -4.90331600 | -3.31672000 |
| C | -2.32857700 | 2.51950100 | 3.94124000 | C | -1.51292000 | -5.38195500 | -2.10944500 |
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| C | -0.88433100 | 4.40575600 | 2.93317100 | C | -1.20299400 | -8.32889800 | 1.13104500 |
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| C | 4.13716900 | -6.27012600 | 2.07606600 | C | 0.05937700 | 0.43387100 | -0.12483700 |
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| C | 2.87782800 | -5.70243400 | 1.88554800 | C | 1.69186500 | 2.02101100 | 0.78494000 |
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| | | | | | | | |
|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 2.43001100 | 0.91310200 | 1.36058000 | H | -5.79036300 | 8.16940900 | 4.22205500 |
| C | -13.27351200 | 4.89268500 | -3.13690100 | H | -4.17890100 | 7.53680900 | 3.91748300 |
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| C | 1.63305700 | -3.10223800 | -0.58767200 | H | -4.25444000 | 5.66696000 | -0.34934400 |
| O | -2.79943600 | -1.83716100 | -6.65865800 | H | -7.67477600 | 4.83713300 | -1.18320800 |
| O | -1.10126600 | 0.98543100 | -5.29775800 | H | -6.48210400 | 6.14699300 | 5.37529200 |
| O | -5.31474800 | -1.95626500 | -3.13114300 | H | -2.50628400 | 2.04269000 | 4.91732900 |
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| O | -0.60618100 | 6.89091900 | -4.37872100 | H | -0.93979400 | 0.95602800 | 3.28577100 |
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| O | 0.99942400 | 5.17509200 | -0.23212300 | H | -1.59737500 | 4.26249900 | 4.96040400 |
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| O | 0.22847800 | 3.26574400 | -3.66328500 | H | -3.64489100 | 3.45991300 | 2.44941500 |
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| O | -0.94433700 | -5.57015500 | 1.93660300 | H | 4.78570600 | -6.45138300 | 1.22364800 |
| O | -1.09373100 | 0.18135700 | -0.74329500 | H | 1.06400600 | -5.04764900 | 2.83481700 |
| O | 2.20463300 | 3.23330400 | 0.77471400 | H | 2.54139700 | -5.44207300 | 0.88880800 |
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| S | 2.14011200 | -0.84568000 | -2.21536200 | H | 7.24653100 | 2.54821600 | 3.17515700 |
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| C | 3.90384500 | 2.40614200 | 2.88234400 | H | 6.45052200 | 0.25180000 | 2.26811500 |
| H | -3.72539800 | 5.78544900 | -3.09589900 | H | 7.58398400 | 0.45765800 | 0.92657700 |
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| H | -4.58781600 | 0.22574000 | -5.09189400 | H | 7.67808200 | 5.74646300 | 1.63919300 |
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| H | 3.30275300 | 7.45414300 | -4.54230100 | H | 6.00229000 | -3.21393400 | -4.13949600 |
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| H | 0.63707600 | 8.62959500 | -5.50864500 | H | 5.48306700 | -0.55220100 | -0.50810400 |
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| H | -1.61411300 | 8.46335200 | 1.45465200 | H | 6.91659900 | -4.57118700 | 4.73801800 |
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|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 5.19746300 | -2.76887100 | 4.65459400 | H | 3.90542100 | 3.13457300 | 0.16745500 |
| H | 5.04695100 | -3.82976900 | 3.25165200 | H | -0.52095400 | -1.63761700 | -3.63190500 |
| H | 9.88621300 | -4.09844600 | 3.22469000 | H | -13.72311800 | 5.56539100 | -2.39880600 |
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| H | 6.35218900 | 4.11537500 | 0.22157400 | H | -4.77375300 | 6.24121700 | 5.85624800 |
| H | 3.80316000 | 1.12786600 | -1.32424400 | H | -4.40400700 | 2.30881600 | 3.56765500 |
| H | 8.57578500 | 2.70491800 | -3.54731500 | H | -3.94742100 | 3.98387400 | 4.10743300 |
| H | 5.41273200 | 5.57839400 | -2.74631100 | H | -1.17050700 | 8.00092300 | 4.99897600 |
| H | 6.85852100 | 3.62724500 | -4.34891100 | H | -1.01234000 | 9.75544700 | 5.43054000 |
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| H | 1.44537600 | 3.42801800 | -2.04509800 | H | -3.25945000 | 5.01722300 | -5.60970600 |
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| H | 3.22346200 | 1.95275100 | -3.70004100 | H | 2.13453900 | 8.60067200 | -6.45742300 |
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| H | 4.47229800 | 0.27219900 | -6.33762400 | H | 9.12478500 | 5.95835500 | 2.62542600 |
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| H | 6.93893400 | 1.77092300 | -7.37973600 | H | 2.26923000 | 2.92423700 | -4.81764800 |
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| H | 1.89129100 | -6.32307500 | -1.46334400 | H | -0.19440600 | -1.87127600 | -8.87121600 |
| H | 2.75242700 | -5.38505400 | -2.70146400 | H | -0.09271000 | -3.51882500 | -8.23003600 |
| H | 3.59612100 | -5.88855600 | -1.25376100 | H | -5.17756300 | -0.01952100 | -7.67047700 |
| H | 3.98506000 | -9.49322200 | -2.05121800 | H | -4.90979200 | -1.72929900 | -8.12033300 |
| H | 4.44581500 | -8.17961800 | -0.95119300 | H | -3.65339800 | -8.08668600 | -5.07033900 |
| H | 2.78691700 | -8.77980200 | -0.95646900 | H | -2.29119400 | -8.50656400 | -6.13232200 |
| H | 1.24731300 | -7.82513200 | -5.53482900 | H | 2.80212600 | -6.99002500 | -5.39039500 |
| H | -1.40337300 | -4.43752900 | -4.02978800 | H | 8.58156900 | -6.43683100 | -4.31083300 |
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|---|--------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -10.05492500 | -4.55621000 | 10.25530900 | N | 5.94056800 | 1.37419600 | -1.85592900 |
| H | -9.64987500 | 2.03902500 | 3.46294600 | N | 4.72419100 | 2.71445200 | -0.58948200 |
| H | -8.81260600 | 3.17305600 | 2.40316100 | N | 6.76529700 | 4.30751400 | -4.07332100 |
| H | -7.88853800 | 1.97602700 | 3.37106000 | N | 3.43495800 | 3.85643000 | -3.74823900 |
| H | -11.06276800 | -4.70249800 | 8.79870000 | N | -0.03438400 | -6.33866000 | -3.59261800 |
| H | -9.64613700 | -5.73017600 | 8.98596000 | N | -1.67400800 | -4.69135200 | -0.87740300 |
| H | -8.77877300 | -4.12011800 | 0.76417700 | N | -1.91370700 | -7.17839100 | 1.13557100 |
| H | -7.16316300 | -3.60966800 | 1.26707300 | N | -5.07289900 | -5.67310800 | -6.71880800 |
| H | -5.98702600 | 0.22326800 | -1.17577000 | N | -5.44005600 | -4.43952700 | -4.90218100 |
| H | -7.32377400 | 0.13387000 | -2.31252300 | C | -3.81196600 | 4.12352100 | -5.00366100 |
| H | 2.22469500 | -3.60494600 | 6.84355500 | C | -3.23355300 | 4.64291600 | -3.67399800 |
| H | -2.57713100 | -3.82838800 | 6.33245400 | C | -3.33841000 | 3.64829900 | -2.56835500 |
| H | 1.54261900 | -4.05194100 | 8.39696300 | C | -2.35023000 | 2.84101400 | -2.07213800 |
| H | -1.83987200 | -2.27500100 | 5.95641600 | C | -4.21152900 | 2.31057900 | -1.01518800 |
| H | 2.58074500 | -1.01909700 | 6.61071600 | C | -5.04539900 | -1.49088700 | -7.15642500 |
| H | 4.75326600 | 2.81559000 | 2.32586700 | C | -3.77306200 | -1.45559400 | -6.30469700 |
| H | 3.10497900 | 3.14160600 | 2.85636300 | C | -2.86626500 | -0.63307800 | -4.14237800 |
| H | 4.24455100 | 2.23287300 | 3.90314900 | C | -1.41017100 | -0.27210400 | -4.52930700 |
| | | | | C | -3.00416100 | -1.97383900 | -3.39110900 |
| | | | | C | -4.35763000 | -2.09311400 | -2.72132700 |
| | | | | C | 0.90940800 | -1.17228300 | -4.67143900 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -8.75849000 | 2.19474300 | 2.76954900 | C | 1.21248200 | -1.79390500 | -6.05354800 |
| C | -8.90923900 | 1.00800600 | 1.84915800 | C | 1.77492200 | -1.85756400 | -3.59943400 |
| O | -9.84260800 | 0.20808200 | 1.98336300 | C | 0.59523500 | -1.84380400 | -0.32525200 |
| N | -7.89325400 | 0.81007000 | 0.97327800 | C | 0.28869100 | -2.95377400 | -8.00269800 |
| C | -7.99655900 | -0.19459900 | -0.08123700 | C | 1.58693300 | 8.33858100 | -5.93727800 |
| C | -7.62875800 | -1.59793600 | 0.43737400 | C | 2.08527700 | 7.12304400 | -5.13408200 |
| O | -6.69926000 | -2.25334400 | -0.05961300 | C | 1.45538500 | 6.89305600 | -3.75364700 |
| C | -7.05756800 | 0.24338900 | -1.22997200 | C | -0.01317200 | 6.49491400 | -3.79639100 |
| O | -7.02963200 | 1.64643500 | -1.36480900 | C | -1.22464900 | 9.25906200 | 4.13351500 |
| N | -8.37498700 | -2.08862200 | 1.44123300 | C | -0.11378400 | 9.43622600 | 3.06757800 |
| C | -8.08944500 | -3.40129800 | 1.99514000 | C | 0.12796400 | 8.27182100 | 2.13379500 |
| C | -8.22762900 | -3.50431300 | 3.51692300 | C | -0.80031100 | 7.90081100 | 1.15170500 |
| C | -7.78879900 | -4.89950900 | 3.96804900 | C | 1.32161500 | 7.54250100 | 2.20386500 |
| O | -7.48995400 | -2.48835000 | 4.19878800 | C | -0.55322800 | 6.84327100 | 0.28135300 |
| C | -9.83599000 | -4.32862800 | 9.54114900 | C | 1.59095000 | 6.48310300 | 1.33735500 |
| C | -8.77922800 | -3.40504600 | 8.92437500 | C | 0.64730300 | 6.12188900 | 0.36939300 |
| C | -8.74155300 | -3.41635900 | 7.39914100 | C | -5.43692300 | 6.35284700 | 4.71635800 |
| O | -9.52464100 | -4.04158300 | 6.70565900 | C | -5.26085500 | 7.40052900 | 3.58878300 |
| O | -7.74649500 | -2.65823200 | 6.93171500 | C | -5.69036100 | 6.81647400 | 2.25688400 |
| C | -1.30519500 | -2.49040700 | 5.56962600 | C | -7.03012000 | 6.50427800 | 1.98647500 |
| C | -0.13286000 | -3.15160900 | 6.28750000 | C | -4.73945200 | 6.44908700 | 1.29726500 |
| O | 0.22645600 | -4.29622700 | 6.03274500 | C | -7.41285900 | 5.83698100 | 0.82366900 |
| C | -1.28875800 | -2.70743100 | 4.04110100 | C | -5.10082200 | 5.79303000 | 0.12216500 |
| C | -2.64119400 | -2.42815500 | 3.45188700 | C | -6.44304100 | 5.46278900 | -0.12347700 |
| C | -3.89833800 | -2.76897900 | 3.89833000 | C | -3.63875000 | 3.26637100 | 3.35261900 |
| N | -2.87271100 | -1.72513600 | 2.27707200 | C | -2.30885700 | 2.73609000 | 3.93141000 |
| C | -4.22533300 | -1.66209800 | 2.08137400 | C | -1.24979500 | 3.83712800 | 4.09041700 |
| N | -4.87383600 | -2.29100700 | 3.04675200 | C | -1.80727700 | 1.53032400 | 3.13310500 |
| N | 0.45047600 | -2.40866300 | 7.28139300 | C | -0.80534000 | 4.49492300 | 2.78823000 |
| C | 1.75279000 | -2.78928100 | 7.80801100 | C | 3.79003900 | -7.49353800 | 6.89375400 |
| C | 2.47205400 | -1.55378800 | 8.36651200 | C | 4.43977300 | -6.29967300 | 6.16177900 |
| C | 3.93498100 | -1.85930000 | 8.67336900 | C | 3.99671500 | -6.10412900 | 4.73031200 |
| O | 2.33902800 | -0.43478800 | 7.48890600 | C | 4.84492600 | -6.44790600 | 3.67037800 |
| N | -4.49736600 | 3.28158500 | -1.89332400 | C | 2.73530400 | -5.57148600 | 4.43757500 |
| N | -2.91361600 | 2.02311300 | -1.11520900 | C | 4.45033600 | -6.24801900 | 2.34616200 |
| N | -3.78847000 | -0.54866500 | -5.27964900 | C | 2.33426500 | -5.37704900 | 3.11590600 |
| N | -4.33103900 | -2.27676100 | -1.39145900 | C | 3.19439200 | -5.70829900 | 2.06660300 |
| N | -0.49614500 | -1.24635700 | -4.32539300 | C | 11.10261100 | 1.17471100 | 3.23787100 |
| N | 0.15915300 | -2.35666300 | -6.69255800 | C | 9.96755300 | 0.65407200 | 2.34331500 |
| N | 7.02749300 | 4.27112700 | 5.57703500 | | | | |

| | | | | | | | |
|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 8.53235300 | 1.02318900 | 2.75804000 | C | 2.37451000 | 0.96840000 | 1.43781000 |
| C | 8.27649900 | 2.53017300 | 2.65781900 | C | -13.33676400 | 4.55462200 | -3.24226900 |
| C | 7.50718800 | 0.25496200 | 1.91238300 | C | -11.84674000 | 4.28605900 | -2.94844300 |
| C | 8.16247400 | 6.64496400 | 1.86029300 | C | -11.50595600 | 3.63552300 | -1.59835000 |
| C | 7.31727100 | 7.01224300 | 3.07470700 | C | -9.98185500 | 3.44420700 | -1.46973300 |
| C | 6.93349700 | 5.90056100 | 4.01105100 | C | 1.29475000 | -3.14364000 | -0.02167300 |
| C | 7.76929500 | 5.11107500 | 4.76022900 | O | -2.80300800 | -2.18002000 | -6.52507100 |
| C | 5.58692100 | 5.52023300 | 4.37378900 | O | -1.14250200 | 0.85499900 | -4.94444100 |
| C | 5.68265300 | 4.49311300 | 5.35392600 | O | -5.41639100 | -2.01959300 | -3.36775100 |
| C | 4.31048100 | 5.95487100 | 3.97621400 | O | 2.36148900 | -1.76596000 | -6.49152800 |
| C | 4.55419200 | 3.91071800 | 5.93999700 | O | -0.75367900 | 6.72506100 | -4.73234000 |
| C | 3.18595300 | 5.37646200 | 4.55107700 | O | -0.50282000 | 5.91465600 | -2.69046600 |
| C | 3.30790100 | 4.36621100 | 5.52610200 | O | 0.86602800 | 5.09524800 | -0.49987200 |
| C | 8.29767500 | -5.83341300 | -3.32198000 | O | -6.76364500 | 4.80234500 | -1.26424100 |
| C | 6.76568300 | -5.90966700 | -3.21354600 | O | 4.47087700 | -1.61920700 | -0.27706700 |
| C | 6.15755300 | -4.77938600 | -2.42127800 | O | 7.63908900 | 5.36921100 | -2.24786600 |
| C | 5.59812900 | -3.68333300 | -3.08696400 | O | 4.50233600 | 3.64878200 | -5.74973900 |
| C | 6.16721000 | -4.76125500 | -1.01985300 | O | 0.21059600 | 3.18100000 | -3.66494200 |
| C | 5.05479100 | -2.61016600 | -2.39133200 | O | 6.89952800 | 1.59558300 | -5.11550600 |
| C | 5.60399400 | -3.70571100 | -0.30388300 | O | 5.46470300 | 0.18516300 | -4.10836400 |
| C | 5.03393900 | -2.62671000 | -0.99189400 | O | 1.46018400 | -5.10809900 | -4.77236300 |
| C | 9.26622800 | -4.58051200 | 3.12395100 | O | -2.04261300 | -6.76090800 | -1.77128500 |
| C | 7.85328900 | -4.01585700 | 2.90738200 | O | -0.79645000 | -5.44165900 | 2.12198600 |
| C | 7.16535700 | -3.44847500 | 4.16289100 | O | -1.37472200 | 0.17801700 | -0.19231600 |
| C | 8.01515500 | -2.37732100 | 4.85888800 | O | 2.20308100 | 3.20976900 | 0.57289400 |
| C | 5.77558200 | -2.89675700 | 3.81515600 | O | 2.53130700 | -1.38929100 | 1.83542900 |
| C | 8.60365100 | 3.25257300 | -2.92066300 | O | -9.53794800 | 2.26511300 | -1.51810400 |
| C | 7.64942200 | 4.43236800 | -3.04768000 | O | -9.29833400 | 4.50908300 | -1.37045000 |
| C | 8.25231000 | 2.42036000 | -1.65565200 | O | -0.67367700 | -2.08145700 | -0.81314000 |
| C | 6.77731300 | 2.34852300 | -1.33703300 | S | 1.76303500 | -0.96925900 | -1.98994100 |
| C | 6.02357300 | 3.18779700 | -0.54193700 | C | 3.53351300 | 1.16610600 | 2.27602600 |
| C | 4.72629700 | 1.61578600 | -1.37989200 | O | 4.13731800 | 0.18614400 | 2.80161900 |
| C | 5.53574300 | 5.07509000 | -4.12029800 | C | 4.07560600 | 2.52764600 | 2.63040300 |
| C | 4.43933600 | 4.13446600 | -4.62466500 | H | -3.71968000 | 5.58449700 | -3.39443900 |
| C | 2.58936400 | 2.69200500 | -3.97845300 | H | -2.17691500 | 4.87247200 | -3.78754800 |
| C | 1.37501700 | 2.62884200 | -3.05240300 | H | -1.30890200 | 2.80414600 | -2.35548400 |
| C | 5.90673000 | 0.93344600 | -7.71677200 | H | -4.93415000 | 1.85980500 | -0.36007500 |
| C | 5.51506000 | 0.14356600 | -6.46287500 | H | -3.57946300 | 3.06141700 | -5.13445800 |
| C | 6.01995800 | 0.74044200 | -5.17261400 | H | -5.89749100 | -1.74727900 | -6.52034500 |
| C | 1.94457500 | -7.47582000 | -4.47538700 | H | -2.90664800 | -2.79177400 | -4.11200500 |
| C | 1.11550500 | -6.19562700 | -4.32123700 | H | -2.21329300 | -2.05732300 | -2.64359400 |
| C | 2.35904800 | -8.10485500 | -3.12653400 | H | -5.22142600 | -2.30879800 | -0.88024300 |
| C | 3.36624000 | -7.27377400 | -2.30770400 | H | -3.45436600 | -2.31358900 | -0.89657000 |
| C | 2.79414300 | -5.95392000 | -1.77394900 | H | -3.15338000 | 0.18086700 | -3.47000800 |
| C | 3.92682900 | -8.10667500 | -1.14902400 | H | -4.69840400 | -0.18538700 | -5.03278300 |
| C | -0.76783300 | -5.19675200 | -3.08405400 | H | 1.34978000 | -2.98064600 | -8.25345000 |
| C | -1.55083800 | -5.62485300 | -1.83988700 | H | -0.78155400 | -2.23826300 | -6.33493900 |
| C | -2.39875500 | -4.92878900 | 0.36836300 | H | 1.91649300 | 6.21821100 | -5.72791600 |
| C | -1.61671000 | -5.86358900 | 1.31361300 | H | 3.17194600 | 7.19632200 | -5.00031400 |
| C | -1.05377600 | -8.26745400 | 1.59969200 | H | 1.52280600 | 7.79385100 | -3.12677400 |
| C | -3.20804400 | -8.37835000 | -5.60261900 | H | 2.01021300 | 6.10950100 | -3.22699800 |
| C | -2.98162600 | -6.91522700 | -6.04135500 | H | 0.49754800 | 8.32654700 | -5.99484200 |
| C | -4.10246500 | -5.95787500 | -5.77528100 | H | -0.33368500 | 10.34011200 | 2.48339100 |
| C | -4.31867700 | -5.20036000 | -4.64360500 | H | 0.82640800 | 9.64246300 | 3.59250800 |
| C | -5.84417100 | -4.75538700 | -6.16410500 | H | 2.06177800 | 7.81249900 | 2.95352100 |
| C | -0.14198300 | 0.46581400 | 0.22156700 | H | -1.73606000 | 8.44806400 | 1.06229700 |
| C | 0.34036500 | 1.77223100 | 0.31136900 | H | 2.51227000 | 5.91644300 | 1.42094700 |
| C | 1.65514600 | 2.03950000 | 0.76114800 | H | -1.27956500 | 6.56198700 | -0.47208600 |
| C | 0.71619300 | -0.65210900 | 0.53169900 | H | 0.17325400 | 5.56765400 | -2.06367700 |
| C | 1.88152200 | -0.37223700 | 1.27900900 | H | -2.22439400 | 9.39887800 | 3.71186400 |

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|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| H | -5.81831100 | 8.31716600 | 3.82132400 | H | 5.25509700 | -2.55021000 | 4.71582700 |
| H | -4.20515700 | 7.68612500 | 3.52055300 | H | 5.14767600 | -3.65859400 | 3.34675900 |
| H | -7.79692300 | 6.77904100 | 2.70830600 | H | 9.99922000 | -3.79170100 | 3.31854000 |
| H | -3.68890400 | 6.67044000 | 1.47263200 | H | 8.63064400 | 1.40187400 | -1.78360700 |
| H | -8.45397000 | 5.60906400 | 0.61946500 | H | 8.76115800 | 2.84145300 | -0.78301000 |
| H | -4.34205300 | 5.53516500 | -0.60768700 | H | 6.29565600 | 4.07103100 | 0.01189300 |
| H | -7.77454500 | 4.60942600 | -1.32184500 | H | 3.84081000 | 1.02867200 | -1.57856200 |
| H | -6.46089500 | 6.35609200 | 5.10472400 | H | 8.53755500 | 2.61363200 | -3.80166100 |
| H | -2.53855500 | 2.38228500 | 4.94857500 | H | 5.34170600 | 5.47831400 | -3.12247500 |
| H | -1.65376700 | 1.78029800 | 2.08165800 | H | 6.78730400 | 3.45027500 | -4.62417300 |
| H | -0.85069200 | 1.15570800 | 3.51520800 | H | 1.20241400 | 1.58958400 | -2.75339600 |
| H | -2.53453000 | 0.71393900 | 3.18086900 | H | 1.55355400 | 3.19366700 | -2.13279500 |
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| H | -1.65234800 | 4.90551100 | 2.23100600 | H | 3.60975500 | 4.08015600 | -2.77652900 |
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| H | -3.57289100 | 3.52944300 | 2.29343500 | H | 6.85971100 | 1.44264100 | -7.55710100 |
| H | 4.24034400 | -5.38517000 | 6.73569300 | H | 1.47473200 | -8.31234800 | -2.50850300 |
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| H | 2.05761300 | -5.29718900 | 5.24022300 | H | 1.88845100 | -6.13495100 | -1.18203800 |
| H | 5.12627500 | -6.49805800 | 1.53373900 | H | 2.55598500 | -5.25487400 | -2.57521500 |
| H | 1.34982800 | -4.97662100 | 2.90704100 | H | 3.52639700 | -5.45522000 | -1.13601800 |
| H | 2.89130000 | -5.53849600 | 1.04029300 | H | 4.35584900 | -9.05349700 | -1.49754600 |
| H | 3.84169300 | -8.39538700 | 6.27493900 | H | 4.70856800 | -7.55187100 | -0.62213600 |
| H | 10.12974400 | 1.00962200 | 1.31588600 | H | 3.14318500 | -8.33939900 | -0.41779900 |
| H | 10.04303000 | -0.44035800 | 2.29582200 | H | 1.36376300 | -8.20314700 | -5.05674200 |
| H | 8.40246700 | 0.72450200 | 3.81054800 | H | -1.48179600 | -4.81377400 | -3.82719400 |
| H | 7.27072800 | 2.78561800 | 3.00144400 | H | -0.07008600 | -4.38791200 | -2.85414100 |
| H | 8.36230000 | 2.86486900 | 1.61744000 | H | -0.32322600 | -7.23381900 | -3.22260500 |
| H | 8.98544600 | 3.11206500 | 3.25369700 | H | -3.38970900 | -5.33517000 | 0.14538900 |
| H | 6.48690500 | 0.41118700 | 2.27287200 | H | -2.51121500 | -3.97063300 | 0.87496800 |
| H | 7.54179100 | 0.57666400 | 0.86569200 | H | -1.19367700 | -3.79061800 | -0.95641300 |
| H | 7.70185100 | -0.82263600 | 1.93007200 | H | 0.00203300 | -8.01122100 | 1.45427600 |
| H | 12.06415800 | 0.86889900 | 2.80441800 | H | -2.37826800 | -7.35840800 | 0.25087400 |
| H | 6.39510200 | 7.49233600 | 2.72638900 | H | -2.75674200 | -6.88371500 | -7.11287600 |
| H | 7.84554100 | 7.79190800 | 3.64239300 | H | -2.08630300 | -6.55063600 | -5.52470900 |
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| H | 7.40431900 | 3.49920500 | 6.10120000 | H | -5.74897300 | -3.65403100 | -4.32944900 |
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| H | 7.65747600 | 5.91954800 | 1.21559600 | H | -11.84811900 | 4.28342000 | -0.78176400 |
| H | 6.33263500 | -5.90379400 | -4.22078400 | H | -11.99619800 | 2.66226800 | -1.49889100 |
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| H | 6.60416800 | -5.59718400 | -0.47638100 | H | 1.17541100 | -0.11572900 | -4.73934000 |
| H | 5.58688500 | -3.66447100 | -4.17384800 | H | 1.46210300 | -2.89992700 | -3.47888200 |
| H | 5.57168100 | -3.71038700 | 0.77966700 | H | 2.79673100 | -1.89062100 | -3.97858000 |
| H | 4.66992500 | -1.75086900 | -2.92513400 | H | -1.15848500 | -1.17575400 | -0.68856500 |
| H | 3.73885300 | -1.24481600 | -0.81621100 | H | -0.25663900 | 2.59931100 | -0.05475700 |
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| H | 7.03212400 | -4.28539700 | 4.86669700 | H | -5.42124300 | 3.74127300 | -1.91292900 |
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| | | | | | | | |
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| H | 3.88859600 | 3.03872500 | -0.07100500 | H | -9.81675900 | -4.25689300 | 10.63262800 |
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| H | 6.02444100 | 0.20480800 | -8.52462900 | | | | |
| H | -0.24340700 | -2.36303400 | -8.75619000 | C | -8.76184100 | 1.99075500 | 2.70388000 |
| H | -0.11355700 | -3.97112900 | -8.02610600 | C | -8.88391700 | 0.90373400 | 1.66471700 |
| H | -5.23452000 | -0.50610600 | -7.59775900 | O | -9.81835900 | 0.09613000 | 1.67751300 |
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| H | 8.75281800 | -6.08113500 | -2.35728500 | O | -6.92076100 | 1.84704500 | -1.41807100 |
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| H | 4.42742800 | -0.97755400 | 9.09091700 | N | -0.36944500 | -0.58834600 | -4.63528400 |
| H | 4.02608600 | -2.68361400 | 9.38865500 | N | 0.36768600 | -1.70255600 | -6.95284800 |
| | | | | N | 6.81470897 | 3.63876398 | 5.93955265 |

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| N | 6.12615600 | 1.30209600 | -1.58885000 | C | 8.53291008 | 0.76549807 | 2.90666218 |
| N | 4.76174800 | 2.63702600 | -0.47352700 | C | 8.33601936 | 2.28393468 | 2.86428744 |
| N | 6.91535700 | 4.61298300 | -3.58123500 | C | 7.51765365 | 0.08000803 | 1.98304147 |
| N | 3.55948800 | 4.18032600 | -3.36074000 | C | 8.19782900 | 6.38463600 | 2.57674200 |
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| C | 1.02425000 | -0.40731000 | -4.98454300 | C | 4.55699900 | -2.92620400 | -1.24592200 |
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| C | 0.49446800 | -2.20015300 | -8.30304000 | C | 7.91381643 | -2.91530115 | 4.74921493 |
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| C | 2.49126000 | 1.05679000 | 1.65868800 | H | -5.81821700 | 7.97077800 | 4.40094900 |
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| C | -9.87700000 | 3.64030900 | -1.43489000 | H | -8.40173700 | 5.53334200 | 0.92363700 |
| C | 0.89780400 | -3.10031600 | 1.33303500 | H | -4.29992100 | 5.78723200 | -0.31359900 |
| O | -2.61279200 | -1.48800300 | -6.81100900 | H | -7.70197300 | 4.81097400 | -1.13572300 |
| O | -1.14057600 | 1.48191800 | -5.22749900 | H | -6.49368800 | 5.89629700 | 5.46804000 |
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| H | -5.29253491 | 3.98712908 | -1.72502278 | H | 0.05334600 | -2.35020000 | 6.68884400 |
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|---|--------------|-------------|-------------|---|-------------|-------------|------------|
| H | -9.99246600 | -5.19763200 | 9.90640600 | H | 2.32477800 | -3.80818100 | 6.69566100 |
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