```
>P1;combined_proteinligint
structureX:combined_proteinligint:   1 :A:+535 :I:::-1.00:-1.00
--DERETWSGKVDFLLSVIGFAVDLANVWRFPYLCYKNGGGAFLVPYGIMLAVGGIPLFYMELALGQHNRKGAIT
CWGRLVPLFKGIGYAVVLIAFYVDFYYNVIIAWSLRFFFASFTNSLPWTSCNNIWNTPNCRPFESQ---------
----------------------------------GFQSAASEYFNRYILELNRSEGIHDLGAIKWDMALCLLIVY
LICYFSLWKGISTSGKVVWFTALFPYAALLILLIRGLTLPGSFLGIQYYLTPNFSAIYKAEVWADAATQVFFSLG
PGFGVLLAYASYNKYHNNVYKDALLTSFINSATSFIAGFVIFSVLGYMAHTLGVRIEDVATEGPGLVFVVYPAAI
ATMPASTFWALIFFMMLATLGLDSSFGGSEAIITALSDEFPKIKRNRELFVAGLFSLYFVVGLASCTQGGFYFFH
LLDRYAAGYSILVAVFFEAIAVSWIYGTNRFSEDIRDMIGFPPGRYWQVCWRFVAPIFLLFITVYLLIGYEPLTY
ADYVYPSWANALGWCIAGSSVVMIPAVAIFKLLSTPGSLRQRFTILTTPWRD/iiz*

>P1;DAT
sequence:DAT::::::: 0.00: 0.00
EAQDRETWGKKIDFLLSVIGFAVDLANVWRFPYLCYKNGGGAFLVPYLLFMVIAGMPLFYMELALGQFNREGAAG
VW-KICPILKGVGFTVILISLYVGFFYNVIIAWALHYLFSSFTTELPWIHCNNSWNSPNC---------------
---------------SDAHPGDSSGDSSGLNDTFG-TTPAAEYFERGVLHLHQSHGIDDLGPPRWQLTACLVLVI
VLLYFSLWKGVKTSGKVVWITATMPYVVLTALLLRGVTLPGAIDGIRAYLSVDFYRLCEASVWIDAATQVCFSLG
VGFGVLIAFSSYNKFTNNCYRDAIVTTSINSLTSFSSGFVVFSFLGYMAQKHSVPIGDVAKDGPGLIFIIYPEAI
ATLPLSSAWAVVFFIMLLTLGIDSAMGGMESVITGLIDEFQLLHRHRELFTLFIVLATFLLSLFCVTNGGIYVFT
LLDHFAAGTSILFGVLIEAIGVAWFYGVGQFSDDIQQMTGQRPSLYWRLCWKLVSPCFLLFVVVVSIVTFRPPHY
GAYIFPDWANALGWVIATSSMAMVPIYAAYKFCSLPGSFREKLAYAIAPEKD/iiz*
```

Supplementary Figure 1:

Modeller alignment file (hDAT_dDAT.ali) in the PIR format of the crystal structure of *drosophila melanogaster* dopamine transporter (dDAT, combined_proteinligint, PDB ID: 4M48) and human dopamine transporter (hDAT, DAT). The dDAT pdb file was manually edited before the alignment, to keep only transmembrane regions, as indicated in the alignment file (hDAT_dDAT.ali).

```
from modeller import *
from modeller.automodel import *

env = environ()
log.verbose()
env.io.hetatm = True
# env.io.atom_files_directory = './:../atoms_files'

# Redefine the special_patches routine to include the additional disulfides
# (this routine is empty by default):
class MyModel(automodel):
    def special_patches(self, aln):
# Disulfide bond for residues 180 and 189 of SERT:
        self.patch(residue_type='DISU', residues=(self.residues['125:A'],
                                                  self.residues['134:A']))
    def special_restraints(self,aln):
        rsr = self.restraints
        at = self.atoms

# Build 20 models and assess DOPE and GA2341
a = MyModel(env, alnfile='hDAT_dDAT.ali',
              knowns=('combined_proteinligint'), sequence='DAT',
              assess_methods=(assess.DOPE, assess.GA341))
a.md_level = refine.slow
a.starting_model = 1
a.ending_model = 20
a.make()
```

Supplementary Figure 2:

Modeller script used to model human dopamine transporter (hDAT, DAT) from the crystal structure of Drosophila melanogaster dopamine transporter (dDAT, combined_proteinligint, PDB ID: 4M48). This script calls on the alignment file (hDAT_dDAT.ali).

```
% sequence identity      :    55.888000
Sequence length          :          545
Compactness              :     0.149967
Native energy (pair)     :  -300.420047
Native energy (surface)  :    -9.429987
Native energy (combined) :    -5.898352
Z score (pair)           :    -8.043409
Z score (surface)        :    -5.680203
Z score (combined)       :    -8.836174
GA341 score              :     1.000000


>> Summary of successfully produced models:
Filename                          molpdf     DOPE score    GA341 score
------------------------------------------------------------------------
DAT.B99990001.pdb             2037.88318   -78576.17969        1.00000
DAT.B99990002.pdb             2490.99805   -78602.85938        1.00000
DAT.B99990003.pdb             2268.05835   -78770.38281        1.00000
DAT.B99990004.pdb             2020.34912   -79091.36719        1.00000
DAT.B99990005.pdb             2232.26514   -79429.78906        1.00000
DAT.B99990006.pdb             2025.55774   -79382.17969        1.00000
DAT.B99990007.pdb             2231.56787   -78983.81250        1.00000
DAT.B99990008.pdb             2311.54932   -79134.69531        1.00000
DAT.B99990009.pdb             2267.56567   -78452.00781        1.00000
DAT.B99990010.pdb             2231.79517   -79161.78906        1.00000
DAT.B99990011.pdb             2180.65601   -79195.74219        1.00000
DAT.B99990012.pdb             2536.64331   -78169.07812        1.00000
DAT.B99990013.pdb             2318.51782   -78540.07812        1.00000
DAT.B99990014.pdb             2154.47656   -79418.70312        1.00000
DAT.B99990015.pdb             2339.25464   -78628.23438        1.00000
DAT.B99990016.pdb             3272.49951   -78337.07812        1.00000
DAT.B99990017.pdb             2097.79443   -78957.49219        1.00000
DAT.B99990018.pdb             2192.01074   -78966.17188        1.00000
DAT.B99990019.pdb             2125.33643   -79112.62500        1.00000
DAT.B99990020.pdb             2116.80273   -79124.82812        1.00000


Dynamically allocated memory at          finish [B,KiB,MiB]:     30999958   30273.396    29.564
Starting time                                               : 2013/12/13 16:03:17
Closing time                                                : 2013/12/13 16:40:23
Total CPU time [seconds]                                    :    2223.40
```

Supplementary Figure 3:

Snapshot of the last 41 lines in the Modeller output from running the script shown in Supplementary Figure 2. This highlights the outputs for the different scoring functions (e.g. DOPE), as well as outputs for % sequence identity and Z score.