

```

HEADER      ModPipe Model of GI 115833068                2018-01-2
TITLE      Model of Sequence 2 from patent US 7105656
SOURCE
EXPDTA     THEORETICAL MODEL, MODELLER SVN 2018/01/27 03:13:33
AUTHOR      URSULA PIEPER, BENJAMIN WEBB, EASHWAR NARAYANAN, ANDREJ SALI
REMARK 220 Original ID: MDR1_HUMAN_MUT
REMARK 220 EXPERIMENTAL DETAILS
REMARK 220 EXPERIMENT TYPE: THEORETICAL MODEL
REMARK 220 METHOD: HOMOLOGY MODELING
REMARK 220 PROGRAM: MODPIPE
REMARK 220 SEQUENCE IDENTITY:                89.00
REMARK 220 GA341 SCORE:                      1.00
REMARK 220 EVALUE:                          0
REMARK 220 MPQS:                            1.9388
REMARK 220 zDOPE SCORE:                     -0.33
REMARK 220 TSVMOD METHOD:                    NA
REMARK 220 TSVMOD RMSD:
REMARK 220 TSVMOD NO35:
REMARK 220 TEMPLATE PDB:                    5ko2
REMARK 220 TEMPLATE CHAIN:                  A
REMARK 220 TARGET LENGTH:                   1280
REMARK 220 TARGET BEGIN:                    29
REMARK 220 TARGET END:                     1276
REMARK 220 TEMPLATE BEGIN:                  28
REMARK 220 TEMPLATE END:                   1272
REMARK 220 MODPIPE RUN:                     MW-hPGPmutantG185V
REMARK 220 MODPIPE MODEL ID:                444f339089431267be00029d242df5ac
REMARK 220 MODPIPE ALIGN ID:                fdb3ed07482b784b780105ef8458cc3e
REMARK 220 MODPIPE SEQUENCE ID:             60d39a16bd58385778d9588e6f45244eMDLETKRQ
REMARK      6 MODELLER OBJECTIVE FUNCTION:    7692.9263
REMARK      6 MODELLER BEST TEMPLATE % SEQ ID: 88.861
REMARK      6 GENERATED BY MODPIPE VERSION SVN.r1610
HELIX 121 121 VAL      36  TYR      42  1              7
HELIX 122 122 TRP      45  LEU      85  1             41
HELIX 123 123 ILE      98  ARG     157  1             60
HELIX 124 124 ILE     160  VAL     165  1              6
HELIX 125 125 VAL     168  ILE     186  1             19
HELIX 126 126 ASP     188  PHE     267  1             80
HELIX 127 127 LYS     272  LYS     279  1              8
HELIX 128 128 GLU     282  LEU     322  1             41
HELIX 129 129 ILE     328  ASP     370  1             43
HELIX 130 130 SER     434  MET     440  1              7
HELIX 131 131 ILE     458  THR     460  1              3
HELIX 132 132 VAL     463  ILE     469  1              7
HELIX 133 133 ILE     484  ARG     489  1              6
HELIX 134 134 MET     497  ALA     507  1             11
HELIX 135 135 TYR     510  LYS     515  1              6
HELIX 136 136 GLY     533  ARG     547  1             15
HELIX 137 137 THR     563  ARG     577  1             15
HELIX 138 138 LEU     589  ASN     594  1              6
HELIX 139 139 HIS     612  GLU     618  1              7
HELIX 140 140 ILE     621  THR     630  1             10
HELIX 141 141 PHE     697  ASN     704  1              8
HELIX 142 142 TRP     708  ARG     741  1             34
HELIX 143 143 PRO     745  ARG     798  1             54
HELIX 144 144 VAL     801  ASP     805  1              5
HELIX 145 145 THR     811  TYR     853  1             43
HELIX 146 146 TRP     855  GLU     902  1             48
HELIX 147 147 PHE     904  LEU     910  1              7
HELIX 148 148 GLU     913  ALA     965  1             53
HELIX 149 149 PHE     971  PHE     994  1             24
HELIX 150 150 TYR     998  GLU    1013  1             16
HELIX 151 151 LYS    1076  GLU    1084  1              9
HELIX 152 152 VAL    1106  HIS    1112  1              7
HELIX 153 153 ILE    1127  GLY    1134  1              8
HELIX 154 154 GLN    1142  ALA    1152  1             11
HELIX 155 155 HIS    1155  SER    1160  1              6
HELIX 156 156 GLY    1178  ARG    1192  1             15
HELIX 157 157 THR    1208  ARG    1222  1             15
HELIX 158 158 LEU    1234  ASN    1239  1              6
HELIX 159 159 HIS    1257  GLN    1263  1              7
HELIX 160 160 ILE    1266  ALA    1275  1             10
SHEET   55  55  1 LEU     392  ARG     395  0
SHEET   56  56  1 LEU     415  VAL     417  0

```

[illegible]

HETATM	9714	C	LIG	0	14.181	77.375	28.849	0.00	0.00	C
HETATM	9715	O	LIG	0	14.414	76.202	28.631	0.00	0.00	O
HETATM	9716	N	LIG	0	13.376	78.016	27.996	0.00	0.00	N
HETATM	9717	C	LIG	0	13.058	79.319	28.154	0.00	0.00	C
HETATM	9718	O	LIG	0	12.326	79.888	27.372	0.00	0.00	O
HETATM	9719	C	LIG	0	14.446	81.216	28.831	0.00	0.00	C
HETATM	9720	C	LIG	0	15.554	81.000	28.032	0.00	0.00	C
HETATM	9721	C	LIG	0	16.285	82.073	27.559	0.00	0.00	C
HETATM	9722	C	LIG	0	15.907	83.363	27.883	0.00	0.00	C
HETATM	9723	C	LIG	0	14.798	83.579	28.680	0.00	0.00	C
HETATM	9724	C	LIG	0	14.065	82.506	29.150	0.00	0.00	C
HETATM	9725	H	LIG	0	10.892	79.818	31.400	0.00	0.00	H
HETATM	9726	H	LIG	0	11.314	78.804	30.001	0.00	0.00	H
HETATM	9727	H	LIG	0	12.375	78.834	31.429	0.00	0.00	H
HETATM	9728	H	LIG	0	11.836	81.187	29.561	0.00	0.00	H
HETATM	9729	H	LIG	0	12.898	81.217	30.989	0.00	0.00	H
HETATM	9730	H	LIG	0	15.320	77.385	30.490	0.00	0.00	H
HETATM	9731	H	LIG	0	13.008	77.531	27.240	0.00	0.00	H
HETATM	9732	H	LIG	0	15.850	79.992	27.779	0.00	0.00	H
HETATM	9733	H	LIG	0	17.151	81.905	26.936	0.00	0.00	H
HETATM	9734	H	LIG	0	16.477	84.202	27.514	0.00	0.00	H
HETATM	9735	H	LIG	0	14.504	84.586	28.934	0.00	0.00	H
HETATM	9736	H	LIG	0	13.200	82.674	29.773	0.00	0.00	H
CONNECT	9708	9726	9727	9709	9725					
CONNECT	9709	9710	9729	9728	9708					
CONNECT	9710	9711	9717	9719	9709					
CONNECT	9711	9710	9712	9713						
CONNECT	9714	9713	9715	9716						
CONNECT	9717	9710	9718	9716						
CONNECT	9719	9710	9720	9724						
CONNECT	9720	9719	9721	9732						
CONNECT	9721	9720	9733	9722						
CONNECT	9722	9721	9734	9723						
CONNECT	9723	9735	9722	9724						
CONNECT	9724	9719	9736	9723						
CONNECT	9725	9708								
CONNECT	9726	9708								
CONNECT	9727	9708								
CONNECT	9728	9709								
CONNECT	9729	9709								
CONNECT	9730	9713								
CONNECT	9731	9716								
CONNECT	9732	9720								
CONNECT	9733	9721								
CONNECT	9734	9722								
CONNECT	9735	9723								
CONNECT	9736	9724								
CONNECT	9713	9711	9714	9730						
CONNECT	9716	9714	9717	9731						
CONNECT	9712	9711								
CONNECT	9715	9714								
CONNECT	9718	9717								