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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  41  41  VAL    36  TYR    42  1              7
HELIX  42  42  TRP    45  LEU    85  1             41
HELIX  43  43  ILE    98  ARG   157  1             60
HELIX  44  44  ILE   160  VAL   165  1              6
HELIX  45  45  VAL   168  ILE   186  1             19
HELIX  46  46  ASP   188  PHE   267  1             80
HELIX  47  47  LYS   272  LYS   279  1              8
HELIX  48  48  GLU   282  LEU   322  1             41
HELIX  49  49  ILE   328  ASP   370  1             43
HELIX  50  50  SER   434  MET   440  1              7
HELIX  51  51  ILE   458  THR   460  1              3
HELIX  52  52  VAL   463  ILE   469  1              7
HELIX  53  53  ILE   484  ARG   489  1              6
HELIX  54  54  MET   497  ALA   507  1             11
HELIX  55  55  TYR   510  LYS   515  1              6
HELIX  56  56  GLY   533  ARG   547  1             15
HELIX  57  57  THR   563  ARG   577  1             15
HELIX  58  58  LEU   589  ASN   594  1              6
HELIX  59  59  HIS   612  GLU   618  1              7
HELIX  60  60  ILE   621  THR   630  1             10
HELIX  61  61  PHE   697  ASN   704  1              8
HELIX  62  62  TRP   708  ARG   741  1             34
HELIX  63  63  PRO   745  ARG   798  1             54
HELIX  64  64  VAL   801  ASP   805  1              5
HELIX  65  65  THR   811  TYR   853  1             43
HELIX  66  66  TRP   855  GLU   902  1             48
HELIX  67  67  PHE   904  LEU   910  1              7
HELIX  68  68  GLU   913  ALA   965  1             53
HELIX  69  69  PHE   971  PHE   994  1             24
HELIX  70  70  TYR   998  GLU  1013  1             16
HELIX  71  71  LYS  1076  GLU  1084  1              9
HELIX  72  72  VAL  1106  HIS  1112  1              7
HELIX  73  73  ILE  1127  GLY  1134  1              8
HELIX  74  74  GLN  1142  ALA  1152  1             11
HELIX  75  75  HIS  1155  SER  1160  1              6
HELIX  76  76  GLY  1178  ARG  1192  1             15
HELIX  77  77  THR  1208  ARG  1222  1             15
HELIX  78  78  LEU  1234  ASN  1239  1              6
HELIX  79  79  HIS  1257  GLN  1263  1              7
HELIX  80  80  ILE  1266  ALA  1275  1             10
SHEET  19  19  1  LEU   392  ARG   395  0
SHEET  20  20  1  LEU   415  VAL   417  0

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SHEET	21	21	1	THR	422	GLY	427	0											
SHEET	22	22	1	MET	450	VAL	453	0											
SHEET	23	23	1	ILE	470	VAL	473	0											
SHEET	24	24	1	ILE	551	ASP	555	0											
SHEET	25	25	1	THR	581	ILE	585	0											
SHEET	26	26	1	VAL	597	ASP	602	0											
SHEET	27	27	1	VAL	605	GLY	610	0											
SHEET	28	28	1	VAL	1035	GLY	1038	0											
SHEET	29	29	1	LEU	1058	VAL	1060	0											
SHEET	30	30	1	THR	1065	GLY	1070	0											
SHEET	31	31	1	LYS	1093	LEU	1096	0											
SHEET	32	32	1	LEU	1113	VAL	1116	0											
SHEET	33	33	1	ILE	1196	ASP	1200	0											
SHEET	34	34	1	THR	1226	ILE	1230	0											
SHEET	35	35	1	LEU	1242	GLN	1247	0											
SHEET	36	36	1	ARG	1250	GLY	1255	0											
ATOM	2124	CG1	ILE	299			17.640	75.413	19.933	1.00	148.39								C
ATOM	2126	CD1	ILE	299			19.165	75.329	19.892	1.00	148.39								C
ATOM	2146	CG	PHE	303			16.989	72.791	16.510	1.00	150.69								C
ATOM	2147	CD1	PHE	303			17.366	71.476	16.359	1.00	150.69								C
ATOM	2148	CD2	PHE	303			17.422	73.492	17.611	1.00	150.69								C
ATOM	2149	CE1	PHE	303			18.173	70.862	17.284	1.00	150.69								C
ATOM	2150	CE2	PHE	303			18.231	72.880	18.540	1.00	150.69								C
ATOM	2151	CZ	PHE	303			18.607	71.568	18.380	1.00	150.69								C
ATOM	2184	CE1	TYR	307			14.897	69.405	13.551	1.00	63.89								C
ATOM	2186	CZ	TYR	307			14.462	68.112	13.719	1.00	63.89								C
ATOM	2187	OH	TYR	307			14.560	67.488	14.981	1.00	63.89								O
ATOM	5400	CA	ASN	721			9.343	68.559	20.656	1.00	148.14								C
ATOM	5401	CB	ASN	721			10.116	69.877	20.901	1.00	148.14								C
ATOM	5402	CG	ASN	721			10.269	70.263	22.355	1.00	148.14								C
ATOM	5405	C	ASN	721			10.062	67.347	21.154	1.00	148.14								C
ATOM	5406	O	ASN	721			11.044	66.920	20.551	1.00	148.14								O
ATOM	5407	N	GLY	722			9.608	66.777	22.287	1.00	49.22								N
ATOM	5408	CA	GLY	722			10.158	65.549	22.783	1.00	49.22								C
ATOM	5416	CA	LEU	724			10.059	65.055	17.209	1.00	84.37								C
ATOM	5417	CB	LEU	724			10.536	66.503	17.027	1.00	84.37								C
ATOM	5418	CG	LEU	724			9.374	67.508	17.047	1.00	84.37								C
ATOM	5419	CD1	LEU	724			9.872	68.951	16.860	1.00	84.37								C
ATOM	5423	N	GLN	725			12.009	63.918	18.133	1.00	162.48								N
ATOM	5426	CG	GLN	725			14.755	64.232	19.738	1.00	162.48								C
ATOM	5427	CD	GLN	725			15.952	64.328	18.803	1.00	162.48								C
ATOM	5428	OE1	GLN	725			16.630	65.352	18.742	1.00	162.48								O
ATOM	5752	OG	SER	766			12.975	72.141	16.106	1.00	55.67								O
ATOM	5787	CE1	PHE	770			14.193	73.911	21.347	1.00	80.80								C
ATOM	5789	CZ	PHE	770			14.242	72.841	20.486	1.00	80.80								C
ATOM	6320	CD	GLN	838			12.480	69.602	25.548	1.00	108.23								C
ATOM	6321	OE1	GLN	838			12.820	70.663	26.068	1.00	108.23								O
ATOM	6322	NE2	GLN	838			13.110	69.088	24.457	1.00	108.23								N
ATOM	7482	C	MET	986			20.987	63.283	23.282	1.00	62.73								C
ATOM	7483	O	MET	986			21.468	64.232	23.901	1.00	62.73								O
ATOM	7484	N	ALA	987			19.701	63.256	22.898	1.00	64.86								N
ATOM	7485	CA	ALA	987			18.828	64.390	23.018	1.00	64.86								C
ATOM	7486	CB	ALA	987			17.424	64.111	22.453	1.00	64.86								C
ATOM	7487	C	ALA	987			18.641	64.858	24.438	1.00	64.86								C
ATOM	7488	O	ALA	987			18.627	66.062	24.697	1.00	64.86								O
ATOM	7489	N	VAL	988			18.485	63.938	25.406	1.00	63.48								N
ATOM	7502	CB	GLN	990			21.110	68.342	23.723	1.00	52.91								C
ATOM	7503	CG	GLN	990			21.254	69.725	23.084	1.00	52.91								C
ATOM	7504	CD	GLN	990			20.976	69.589	21.595	1.00	52.91								C
ATOM	7505	OE1	GLN	990			21.488	68.685	20.935	1.00	52.91								O
ATOM	7506	NE2	GLN	990			20.138	70.509	21.047	1.00	52.91								N
ATOM	7509	N	VAL	991			19.275	68.647	26.266	1.00	81.26								N
ATOM	7510	CA	VAL	991			18.261	69.427	26.922	1.00	81.26								C
ATOM	7511	CB	VAL	991			16.952	68.696	27.030	1.00	81.26								C
ATOM	7512	CG1	VAL	991			15.981	69.545	27.868	1.00	81.26								C
ATOM	7513	CG2	VAL	991			16.439	68.394	25.612	1.00	81.26								C
ATOM	7514	C	VAL	991			18.655	69.849	28.324	1.00	81.26								C
ATOM	7530	CB	PHE	994			19.692	73.681	26.961	1.00	70.83								C
ATOM	7531	CG	PHE	994			19.199	75.064	26.708	1.00	70.83								C
ATOM	7533	CD2	PHE	994			17.945	75.439	27.132	1.00	70.83								C
TER	9707		GLY	1276															
HETATM	9708	C	LIG	0			13.901	68.293	18.746	0.00	0.00								C
HETATM	9709	C	LIG	0			13.906	67.973	20.091	0.00	0.00								C
HETATM	9710	C	LIG	0			15.075	68.074	20.822	0.00	0.00								C

HETATM	9711	C	LIG	0	16.239	68.495	20.208	0.00	0.00
HETATM	9712	C	LIG	0	16.235	68.814	18.863	0.00	0.00
HETATM	9713	C	LIG	0	15.066	68.714	18.133	0.00	0.00
HETATM	9714	C	LIG	0	17.514	68.606	21.005	0.00	0.00
HETATM	9715	C	LIG	0	17.775	67.327	21.774	0.00	0.00
HETATM	9716	O	LIG	0	17.075	66.833	22.633	0.00	0.00
HETATM	9717	N	LIG	0	18.946	66.852	21.307	0.00	0.00
HETATM	9718	C	LIG	0	19.457	67.646	20.357	0.00	0.00
HETATM	9719	O	LIG	0	20.506	67.426	19.786	0.00	0.00
HETATM	9720	N	LIG	0	18.678	68.714	20.108	0.00	0.00
HETATM	9721	C	LIG	0	17.451	69.785	21.941	0.00	0.00
HETATM	9722	C	LIG	0	16.686	69.714	23.090	0.00	0.00
HETATM	9723	C	LIG	0	16.628	70.796	23.950	0.00	0.00
HETATM	9724	C	LIG	0	17.334	71.947	23.660	0.00	0.00
HETATM	9725	C	LIG	0	18.101	72.018	22.511	0.00	0.00
HETATM	9726	C	LIG	0	18.162	70.935	21.654	0.00	0.00
HETATM	9727	H	LIG	0	12.989	68.210	18.175	0.00	0.00
HETATM	9728	H	LIG	0	12.996	67.645	20.572	0.00	0.00
HETATM	9729	H	LIG	0	15.078	67.824	21.873	0.00	0.00
HETATM	9730	H	LIG	0	17.145	69.143	18.383	0.00	0.00
HETATM	9731	H	LIG	0	15.062	68.963	17.082	0.00	0.00
HETATM	9732	H	LIG	0	19.368	66.036	21.619	0.00	0.00
HETATM	9733	H	LIG	0	18.850	69.418	19.464	0.00	0.00
HETATM	9734	H	LIG	0	16.133	68.814	23.317	0.00	0.00
HETATM	9735	H	LIG	0	16.029	70.741	24.847	0.00	0.00
HETATM	9736	H	LIG	0	17.289	72.793	24.330	0.00	0.00
HETATM	9737	H	LIG	0	18.652	72.918	22.283	0.00	0.00
HETATM	9738	H	LIG	0	18.760	70.990	20.756	0.00	0.00
CONNECT	9708	9709	9713	9727					
CONNECT	9709	9710	9708	9728					
CONNECT	9710	9709	9711	9729					
CONNECT	9711	9710	9712	9714					
CONNECT	9712	9711	9713	9730					
CONNECT	9713	9708	9712	9731					
CONNECT	9714	9711	9715	9720	9721				
CONNECT	9715	9714	9716	9717					
CONNECT	9718	9717	9719	9720					
CONNECT	9721	9714	9722	9726					
CONNECT	9722	9721	9723	9734					
CONNECT	9723	9722	9724	9735					
CONNECT	9724	9723	9725	9736					
CONNECT	9725	9724	9726	9737					
CONNECT	9726	9721	9725	9738					
CONNECT	9727	9708							
CONNECT	9728	9709							
CONNECT	9729	9710							
CONNECT	9730	9712							
CONNECT	9731	9713							
CONNECT	9732	9717							
CONNECT	9733	9720							
CONNECT	9734	9722							
CONNECT	9735	9723							
CONNECT	9736	9724							
CONNECT	9737	9725							