

COMPND W:\zeph\SINDHU\ .DLG FILES\mutant2drug2\comples22.pdbqt

GENERATED BY OPEN BABEL 2.3.1

REMARK 4 XXXX COMPLIES WITH FORMAT V. 2.0

HELIX	205	205	SER	2	PHE	7	1				6
HELIX	206	206	TRP	12	LEU	52	1				41
HELIX	207	207	SER	63	ASP	131	1				69
HELIX	208	208	GLY	136	THR	176	1				41
HELIX	209	209	THR	182	VAL	220	1				39
HELIX	210	210	ILE	228	PHE	234	1				7
HELIX	211	211	LYS	239	ILE	256	1				18
HELIX	212	212	ILE	260	SER	290	1				31
HELIX	213	213	VAL	298	ASP	337	1				40
HELIX	214	214	LYS	400	GLN	408	1				9
HELIX	215	215	ILE	425	THR	427	1				3
HELIX	216	216	VAL	430	ILE	436	1				7
HELIX	217	217	ILE	451	GLY	458	1				8
HELIX	218	218	MET	464	GLU	473	1				10
HELIX	219	219	TYR	477	LYS	482	1				6
HELIX	220	220	LYS	486	ASP	488	1				3
HELIX	221	221	GLY	500	ARG	514	1				15
HELIX	222	222	THR	530	ARG	544	1				15
HELIX	223	223	LEU	556	VAL	559	1				4
HELIX	224	224	HIS	579	GLU	585	1				7
HELIX	225	225	ILE	588	THR	594	1				7
HELIX	226	226	ARG	609	THR	616	1				8
HELIX	227	227	VAL	622	THR	650	1				29
HELIX	228	228	THR	657	ARG	708	1				52
HELIX	229	229	VAL	711	ASP	715	1				5
HELIX	230	230	THR	721	ILE	762	1				42
HELIX	231	231	THR	768	GLU	812	1				45
HELIX	232	232	PHE	814	THR	816	1				3
HELIX	233	233	GLU	823	ALA	871	1				49
HELIX	234	234	GLU	882	VAL	901	1				20
HELIX	235	235	ALA	909	GLU	923	1				15
HELIX	236	236	ARG	957	ASP	959	1				3
HELIX	237	237	LYS	986	GLU	994	1				9
HELIX	238	238	VAL	1016	ALA	1021	1				6
HELIX	239	239	ILE	1037	ILE	1041	1				5
HELIX	240	240	GLN	1052	ALA	1062	1				11
HELIX	241	241	HIS	1065	GLU	1069	1				5
HELIX	242	242	LYS	1074	SER	1076	1				3
HELIX	243	243	ASP	1081	GLY	1083	1				3
HELIX	244	244	GLY	1088	ARG	1102	1				15
HELIX	245	245	THR	1118	ALA	1131	1				14
HELIX	246	246	THR	1146	GLN	1148	1				3
HELIX	247	247	HIS	1167	ALA	1172	1				6
HELIX	248	248	ILE	1176	GLN	1184	1				9
SHEET	92	92	1 LEU	359	ARG	362	0				
SHEET	93	93	1 VAL	364	PHE	366	0				
SHEET	94	94	1 LEU	377	LEU	380	0				
SHEET	95	95	1 LEU	382	VAL	384	0				
SHEET	96	96	1 THR	389	VAL	393	0				
SHEET	97	97	1 MET	417	SER	419	0				
SHEET	98	98	1 ILE	437	SER	441	0				
SHEET	99	99	1 I								

ATOM	5663	C	MET	595	18.001	92.505	49.190	1.00	0.00	C
ATOM	5664	O	MET	595	18.060	91.869	48.140	1.00	0.00	O
ATOM	5665	N	GLN	596	18.619	92.080	50.301	1.00	0.00	N
ATOM	5677	N	THR	597	19.398	89.124	49.082	1.00	0.00	N
ATOM	5678	HN	THR	597	18.396	89.068	49.264	1.00	0.00	H
ATOM	5681	OG1	THR	597	19.543	86.361	49.883	1.00	0.00	O
ATOM	5682	HG1	THR	597	19.840	85.681	50.475	1.00	0.00	H
ATOM	5684	C	THR	597	19.499	87.261	47.107	1.00	0.00	C
ATOM	5685	O	THR	597	18.492	87.929	46.849	1.00	0.00	O
ATOM	5686	N	LEU	598	20.014	86.024	46.335	1.00	0.00	N
ATOM	5687	HN	LEU	598	19.479	85.352	45.785	1.00	0.00	H
ATOM	5689	CA	LEU	598	19.512	84.947	45.212	1.00	0.00	C
ATOM	5690	CB	LEU	598	18.743	85.666	44.073	1.00	0.00	C
ATOM	5691	CG	LEU	598	18.132	84.783	42.949	1.00	0.00	C
ATOM	5693	CD2	LEU	598	17.358	83.595	43.545	1.00	0.00	C
ATOM	6834	CG	PHE	714	7.622	87.329	44.021	1.00	0.00	C
ATOM	6835	CD1	PHE	714	8.841	87.082	43.436	1.00	0.00	C
ATOM	6837	CE1	PHE	714	8.913	86.644	42.136	1.00	0.00	C
ATOM	6862	CD	PRO	717	10.914	86.502	49.250	1.00	0.00	C
ATOM	6863	CB	PRO	717	11.410	85.555	47.079	1.00	0.00	C
ATOM	6864	CG	PRO	717	11.589	86.836	47.906	1.00	0.00	C
ATOM	6865	C	PRO	717	12.803	83.833	48.096	1.00	0.00	C
ATOM	6866	O	PRO	717	13.569	83.900	49.058	1.00	0.00	O
ATOM	6867	N	LYS	718	13.064	83.216	46.923	1.00	0.00	N
ATOM	6868	HN	LYS	718	12.287	83.109	46.271	1.00	0.00	H
ATOM	6869	CA	LYS	718	14.328	82.702	46.515	1.00	0.00	C
ATOM	6870	CB	LYS	718	14.690	81.362	47.182	1.00	0.00	C
ATOM	6878	C	LYS	718	14.239	82.506	45.029	1.00	0.00	C
ATOM	6880	N	ASN	719	13.472	83.370	44.328	1.00	0.00	N
ATOM	6881	HN	ASN	719	12.984	84.132	44.798	1.00	0.00	H
ATOM	6889	C	ASN	719	13.339	84.550	42.293	1.00	0.00	C
ATOM	6890	O	ASN	719	12.272	85.119	42.073	1.00	0.00	O
ATOM	6891	N	THR	720	14.514	85.071	41.909	1.00	0.00	N
ATOM	6893	CA	THR	720	14.551	86.411	41.412	1.00	0.00	C
ATOM	6894	CB	THR	720	15.909	87.032	41.319	1.00	0.00	C
ATOM	6897	CG2	THR	720	16.472	87.198	42.733	1.00	0.00	C
ATOM	6898	C	THR	720	13.967	86.480	40.056	1.00	0.00	C
ATOM	6900	N	THR	721	13.883	87.730	39.574	1.00	0.00	N
ATOM	6901	HN	THR	721	14.242	88.501	40.136	1.00	0.00	H
ATOM	6904	OG1	THR	721	12.662	90.237	38.922	1.00	0.00	O
ATOM	6905	HG1	THR	721	12.689	91.159	38.696	1.00	0.00	H
TER	11274		ALA	1185						
HETATM	11275	O	LIG	1	16.952	89.848	45.312	1.00	0.00	O
HETATM	11276	O	LIG	1	14					

CONECT112921129111293  
CONECT112931129211294  
CONECT112941129311295  
CONECT112951129011294  
CONECT1128211277  
CONECT1128311278  
CONECT11277112791128111282  
CONECT11278112801128111283  
CONECT1127511280  
CONECT1127611281  
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