

COMPND W:\zeph\SINDHU\ .DLG FILES\mutant5drug4\complex54.pdbqt

GENERATED BY OPEN BABEL 2.3.1

REMARK 4 XXXX COMPLIES WITH FORMAT V. 2.0

[illegible]

ATOM	7109	O	ALA	744	8.513	58.181	15.698	1.00	0.00	O
ATOM	7110	N	VAL	745	7.646	58.645	17.725	1.00	0.00	N
ATOM	7111	HN	VAL	745	7.311	59.353	18.378	1.00	0.00	H
ATOM	7112	CA	VAL	745	7.759	57.280	18.130	1.00	0.00	C
ATOM	7113	CB	VAL	745	7.510	57.077	19.595	1.00	0.00	C
ATOM	7115	CG2	VAL	745	8.579	57.860	20.378	1.00	0.00	C
ATOM	7141	CD	GLN	748	11.560	54.523	15.311	1.00	0.00	C
ATOM	7143	NE2	GLN	748	12.469	55.466	14.949	1.00	0.00	N
ATOM	7144	1HE2	GLN	748	13.433	55.311	15.244	1.00	0.00	H
ATOM	7145	2HE2	GLN	748	12.212	56.291	14.407	1.00	0.00	H
ATOM	8571	CA	GLN	900	14.632	58.917	13.586	1.00	0.00	C
ATOM	8572	CB	GLN	900	13.491	57.948	13.941	1.00	0.00	C
ATOM	8573	CG	GLN	900	12.718	57.423	12.731	1.00	0.00	C
ATOM	8576	NE2	GLN	900	11.752	59.672	12.859	1.00	0.00	N
ATOM	8577	1HE2	GLN	900	11.250	60.447	12.426	1.00	0.00	H
ATOM	8578	2HE2	GLN	900	12.068	59.737	13.827	1.00	0.00	H
ATOM	8579	C	GLN	900	15.303	59.225	14.900	1.00	0.00	C
ATOM	8580	O	GLN	900	15.197	60.338	15.419	1.00	0.00	O
ATOM	8581	N	VAL	901	16.035	58.253	15.474	1.00	0.00	N
ATOM	8583	CA	VAL	901	16.604	58.476	16.780	1.00	0.00	C
ATOM	8584	CB	VAL	901	17.379	57.298	17.277	1.00	0.00	C
ATOM	8585	CG1	VAL	901	18.218	57.767	18.466	1.00	0.00	C
ATOM	8587	C	VAL	901	17.547	59.615	16.692	1.00	0.00	C
ATOM	8588	O	VAL	901	17.591	60.490	17.560	1.00	0.00	O
ATOM	8595	C	SER	902	18.739	61.880	14.917	1.00	0.00	C
ATOM	8597	N	SER	903	17.395	62.020	14.848	1.00	0.00	N
ATOM	8598	HN	SER	903	16.766	61.286	15.173	1.00	0.00	H
ATOM	8599	CA	SER	903	16.891	63.256	14.293	1.00	0.00	C
ATOM	8603	C	SER	903	15.726	63.792	15.081	1.00	0.00	C
ATOM	8604	O	SER	903	15.338	63.229	16.104	1.00	0.00	O
ATOM	8605	N	PHE	904	15.191	64.961	14.632	1.00	0.00	N
ATOM	8607	CA	PHE	904	14.042	65.597	15.236	1.00	0.00	C
ATOM	8608	CB	PHE	904	12.840	64.672	15.541	1.00	0.00	C
ATOM	8615	C	PHE	904	14.402	66.327	16.497	1.00	0.00	C
ATOM	8616	O	PHE	904	15.541	66.733	16.721	1.00	0.00	O
ATOM	8617	N	ALA	905	13.373	66.477	17.357	1.00	0.00	N
ATOM	8618	HN	ALA	905	12.501	66.027	17.080	1.00	0.00	H
ATOM	8619	CA	ALA	905	13.334	67.183	18.611	1.00	0.00	C
ATOM	8620	CB	ALA	905	12.027	66.841	19.361	1.00	0.00	C
ATOM	8621	C	ALA	905	14.518	66.766	19.429	1.00	0.00	C
ATOM	8622	O	ALA	905	15.176	65.780	19.093	1.00	0.00	O
ATOM	8623	N	PRO	906	14.844	67.550	20.450	1.00	0.00	N
ATOM	8624	CA	PRO	906	15.959	67.248	21.305	1.00	0.00	C
ATOM	8628	C	PRO	906	15.718	65.841	21.747	1.00	0.00	C
ATOM	8629	O	PRO	906	14.549	65.487	21.861	1.00	0.00	O
ATOM	8630	N	ASP	907	16.773	65.050	22.082	1.00	0.00	N
ATOM	8631	HN	ASP	907	17.685	65.506	22.084	1.00	0.00	H
ATOM	8632	CA	ASP	907	16.772	63.637	22.438	1.00	0.00	C
ATOM	8633	CB	ASP	907	18.177	63.093	22.737	1.00	0.00	C
ATOM	8634	CG	ASP	907	18.111	61.573	22.636	1.00	0.00	C
ATOM	8635	OD1	ASP	907	17.000	61.042	22.367	1.00	0.00	O
ATOM	8636	OD2	ASP	907	19.173	60.921	22.822	1.00	0.00	O
ATOM	8637	C	ASP	907	15.918	63.456	23.679	1.00	0.00	C
ATOM	8638	O	ASP	907	15.942	62.436	24.359	1.00	0.00	O
ATOM	8639	N	TYR	908	15.329	64.554	24.143	1.00	0.00	N
ATOM	8640	HN	TYR	908	15.499	65.408	23.612	1.00	0.00	H
ATOM	8641	CA	TYR	908	14.496	64.690	25.279	1.00	0.00	C
ATOM	8642	CB	TYR	908	14.111	63.444	26.115	1.00	0.00	C
ATOM	8643	CG	TYR	908	12.827	62.863	25.628	1.00	0.00	C
ATOM	8644	CD1	TYR	908	11.674	63.591	25.808	1.00	0.00	C
ATOM	8645	CD2	TYR	908	12.739	61.614	25.054	1.00	0.00	C
ATOM	8646	CE1	TYR	908	10.459	63.104	25.394	1.00	0.00	C
ATOM	8647	CE2	TYR	908	11.523	61.120	24.637	1.00	0.00	C
ATOM	8648	CZ	TYR	908	10.381	61.866	24.803	1.00	0.00	C
TER	11280		ALA	1185						
HETATM11281	O	LIG		1	15.050	59.439	20.745	1.00	0.00	O
HETATM11282	O	LIG		1	12.410	63.150	19.250	1.00	0.00	O
HETATM11283	O	LIG		1	16.948	63.036	18.637	1.00	0.00	O
HETATM11284	N	LIG		1	15.962	61.233	19.657	1.00	0.00	N
HETATM11285	N	LIG		1	14.670	63.045	18.924	1.00	0.00	N
HETATM11286	C	LIG		1	13.501	61.071	19.849	1.00	0.00	C
HETATM11287	C	LIG		1	14.891	60.502	20.142	1.00	0.00	C
HETATM11288	C	LIG		1	13.461	62.512	19.331	1.00	0.00	C
HETATM11289	C	LIG		1	15.928	62.473	19.039	1.00	0.00	C

HETATM11290	H	LIG	1	16.883	60.826	19.798	1.00	0.00	H
HETATM11291	H	LIG	1	14.638	63.978	18.522	1.00	0.00	H
HETATM11292	C	LIG	1	12.815	60.181	18.851	1.00	0.00	C
HETATM11293	C	LIG	1	13.072	60.344	17.496	1.00	0.00	C
HETATM11294	C	LIG	1	12.435	59.518	16.570	1.00	0.00	C
HETATM11295	C	LIG	1	11.546	58.534	17.007	1.00	0.00	C
HETATM11296	C	LIG	1	11.295	58.379	18.369	1.00	0.00	C
HETATM11297	C	LIG	1	11.931	59.206	19.296	1.00	0.00	C
HETATM11298	C	LIG	1	12.710	61.039	21.164	1.00	0.00	C
HETATM11299	C	LIG	1	13.070	62.215	22.046	1.00	0.00	C

CONECT1128611298112871128811292

CONECT11287112811128411286

CONECT11288112821128511286

CONECT11289112831128411285

CONECT11292112971128611293

CONECT112931129211294

CONECT112941129511293

CONECT112951129611294

CONECT112961129511297

CONECT112971129611292

CONECT112981129911286

CONECT1129911298

CONECT1129011284

CONECT1129111285

CONECT11284112871128911290

CONECT11285112881128911291

CONECT1128111287

CONECT1128211288

CONECT1128311289

END