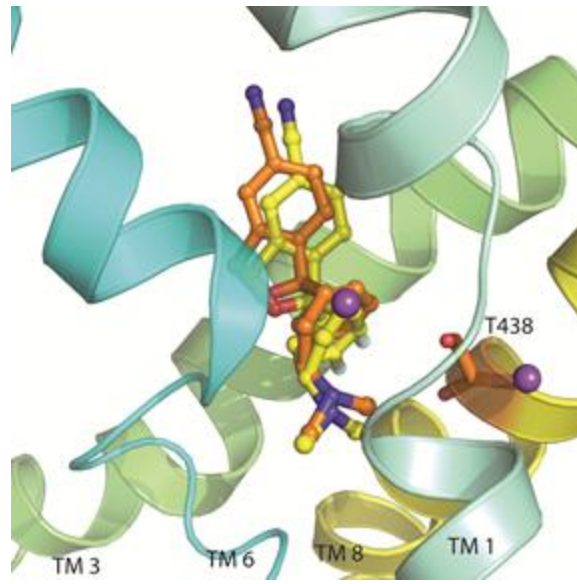


-in

- path
 - database minirosetta_database #this is where your database lives
- file
 - s hSERT1.pdb #starting pdb. Note, you must have HETATM records in your pdb
 - extra_res_fa LG.params #this is the params file you made for your ligand. You must have a params file for each ligand in your pdb
- out
 - mute all #this will mute all output. If you are debugging, take this flag off
 - nstruct 100 #(the number of pdb files you are wanting to create)
- docking
 - uniform_trans 4 #This is the initial placement step. How far from the center of the ligand do you want to sample? Sphere of radius 4 Angstrom
 - randomize2 #Use random conformation from your conformation library as initial placement
- packing # repacking rotamers around the ligand, not around the whole protein!
 - extrachi_cutoff 1
 - ex1
 - ex1aro
 - ex2
- ligand
 - protocol abbrev2 #repack in cycles 1 and 4
 - improve_orientation 1000 #This rotates/slides the ligand around in the pocket 1000 times then chooses the best position...powerful tool to use with rotamers
 - minimize_ligand #minimize ligand rotatable bonds
 - harmonic_torsions 10 #minimizes the ligand with one standard deviation equal to 10 degrees
 - minimize_backbone #minimize backbone around ligand (stretches of residues w/in 6 Angstroms)
 - harmonic_Calphas 0.3
 - soft_rep #uses soft repulsive scoring during initial placement/searching of binding pocket. When minimizing, uses hard repulsive(high resolution scoring function)
 - old_estat #only evaluate the Coulomb term between protein and ligand
 - tether_ligand 0.1 #after initial placement, only allow the ligand to move by .1A

S1: Flags used for RosettaLigand docking. The command line used was: ligand_dock.linuxgccrelease @flags.txt



S2: S-citalopram/S438T-hSERT with Na⁺ present. Wild type hSERT complexed with S-citalopram is shown in yellow. Mutant S438T hSERT is shown in orange. Na⁺ ions are shown in purple. Na⁺ ion coordinates were taken from the LeuT crystal structure 2A65. The resulting S-citalopram/hSERT models with both Na⁺ ions present resulted in a 0.3 Å shift of the dimethyl-amine tail towards the Na⁺ two site. The resulting Rosetta score was -8.8 REU compared to the -8.1 REU for the original model. The increase in score is attributed to better packing of residues against S-citalopram. When the S438T mutation is introduced into the hSERT model including S-citalopram and Na⁺, the resulting energy is -8.0 REU (as compared to -8.8 REU WT with Na⁺ ions). The dimethyl-amine tail [c] is shifted away from residue T438. The shift of S-citalopram's dimethyl-amine tail [c] is the same result as seen without the Na⁺ present in the S-citalopram /hSERT S438T model. The conclusion is that the Na⁺ ions do not result in a significantly different docked position of S-citalopram.

S-citalopram/hSERT				Andersen's Model			
mutation	Upper	Ki	-ln(ki)	mutation	REU	Ki	-ln(ki)
A169D	-8.16441	103	-4.63473	A169D	-6.27268	103	-4.63473
A169I	-7.97825	9	-2.19722	A169I	-7.62365	9	-2.19722
A169S	-8.0122	26	-3.2581	A169S	-7.39255	26	-3.2581
A173G	-8.04718	7	-1.94591	A173G	-7.24725	7	-1.94591
A173I	-8.08233	31	-3.43399	A173I	-7.00635	31	-3.43399
A173S	-7.30289	7	-1.94591	A173S	-7.37286	7	-1.94591
A441G	-7.97508	12	-2.48491	A441G	-8.13865	12	-2.48491
C166I	-7.58802	34	-3.52636	C166I	-7.61337	34	-3.52636
F170L	-8.0881	22	-3.09104	F170L	-7.91533	22	-3.09104
F335A	-5.6068	30	-3.4012	F335A	-6.75377	30	-3.4012
F335E	-6.00514	16	-2.77259	F335E	-7.54129	16	-2.77259
F335H	-7.054	22	-3.09104	F335H	-7.58296	22	-3.09104
F335I	-6.12769	198	-5.28827	F335I	-7.06384	198	-5.28827
F335W	-6.57622	116	-4.75359	F335W	-6.9065	116	-4.75359
F335Y	-7.99716	21	-3.04452	F335Y	-7.5074	21	-3.04452
F341A	-8.04596	16	-2.77259	F341A	-6.8588	16	-2.77259
F341I	-8.25073	58	-4.06044	F341I	-6.94841	58	-4.06044
F341L	-8.01354	133	-4.89035	F341L	-7.82786	133	-4.89035
F341Y	-8.0535	1691	-7.43308	F341Y	-6.02449	1691	-7.43308
G100A	-7.15759	66	-4.18965	G100A	-7.61848	66	-4.18965
G442A	-6.66257	6	-1.79176	G442A	-6.69277	6	-1.79176
G445A	-8.13758	17	-2.83321	G445A	-7.67601	17	-2.83321
I165N	-7.46763	57	-4.04305	I165N	-7.07692	57	-4.04305
I165V	-7.99712	21	-3.04452	I165V	-7.7427	21	-3.04452
I172A	-8.08316	8	-2.07944	I172A	-6.71586	8	-2.07944
I172E	-7.67652	578	-6.35957	I172E	-7.23447	578	-6.35957
I172F	-8.64935	1687	-7.43071	I172F	-5.43139	1687	-7.43071
I172Q	-6.68379	77	-4.34381	I172Q	-6.70788	77	-4.34381
I172V	-7.36709	17	-2.83321	I172V	-7.12462	17	-2.83321
L443A	-7.966	30	-3.4012	L443A	-7.12112	30	-3.4012
L443F	-7.45638	30	-3.4012	L443F	-7.63919	30	-3.4012
L443G	-8.3491	8	-2.07944	L443G	-7.96099	8	-2.07944
L443M	-7.95557	8	-2.07944	L443M	-6.11128	8	-2.07944
L443V	-7.86685	8	-2.07944	L443V	-5.29498	8	-2.07944
N177A	-8.5494	158	-5.0626	N177A	-6.91581	158	-5.0626
N177E	-7.95533	15	-2.70805	N177E	-7.46134	15	-2.70805
N177S	-8.05422	332	-5.80513	N177S	-7.85973	332	-5.80513
S174F	-7.96368	23	-3.13549	S174F	-6.79934	23	-3.13549
S438A	-7.89379	89	-4.48864	S438A	-7.31585	89	-4.48864
S438T	-7.1424	7693	-8.94807	S438T	-7.54486	7693	-8.94807
T439A	-8.12008	4	-1.38629	T439A	-7.33229	4	-1.38629

T439S	-8.31658	35	-3.55535	T439S	-7.02994	35	-3.55535
T439V	-7.30897	20	-2.99573	T439V	-8.14342	20	-2.99573
V343N	-7.49659	8	-2.07944	V343N	-7.00492	8	-2.07944
V343S	-8.04836	7	-1.94591	V343S	-7.62298	7	-1.94591
Y175F	-7.80679	6	-1.79176	Y175F	-7.68673	6	-1.79176
Y176F	-7.72629	23	-3.13549	Y176F	-7.32217	23	-3.13549

S3: A comparison of mutations between the presented model and Andersen's models.

HETATM C	1	C1	LG1	A	1	0.868	-1.527	-1.046	1.00	0.00
HETATM N	2	N1	LG1	A	1	-0.462	-6.712	-1.597	1.00	0.00
HETATM O	3	O1	LG1	A	1	2.722	-0.490	-0.074	1.00	0.00
HETATM C	4	C2	LG1	A	1	-0.361	-1.854	-1.602	1.00	0.00
HETATM N	5	N2	LG1	A	1	2.115	3.375	2.025	1.00	0.00
HETATM C	6	C3	LG1	A	1	-0.696	-3.205	-1.747	1.00	0.00
HETATM C	7	C4	LG1	A	1	0.194	-4.213	-1.332	1.00	0.00
HETATM C	8	C5	LG1	A	1	-0.170	-5.595	-1.478	1.00	0.00
HETATM C	9	C6	LG1	A	1	1.428	-3.869	-0.770	1.00	0.00
HETATM C	10	C7	LG1	A	1	1.741	-2.523	-0.633	1.00	0.00
HETATM C	11	C8	LG1	A	1	2.961	-1.916	-0.056	1.00	0.00
HETATM C	12	C9	LG1	A	1	0.603	0.589	0.297	1.00	0.00
HETATM C	13	C10	LG1	A	1	1.322	1.043	1.582	1.00	0.00
HETATM C	14	C11	LG1	A	1	2.444	2.052	1.363	1.00	0.00
HETATM C	15	C12	LG1	A	1	1.465	-0.175	-0.749	1.00	0.00
HETATM C	16	C13	LG1	A	1	2.284	2.082	-4.375	1.00	0.00
HETATM C	17	C14	LG1	A	1	0.993	1.649	-4.115	1.00	0.00
HETATM C	18	C15	LG1	A	1	0.729	0.930	-2.946	1.00	0.00
HETATM C	19	C16	LG1	A	1	1.756	0.623	-2.029	1.00	0.00

HETATM C	20	C17	LG1	A	1	3.053	1.095	-2.318	1.00	0.00
HETATM C	21	C18	LG1	A	1	3.316	1.815	-3.487	1.00	0.00
HETATM C	22	C19	LG1	A	1	1.782	4.423	0.995	1.00	0.00
HETATM C	23	C20	LG1	A	1	3.190	3.864	2.959	1.00	0.00
HETATM F	24	F1	LG1	A	1	2.537	2.771	-5.495	1.00	0.00
HETATM H	25	H1	LG1	A	1	-1.062	-1.089	-1.920	1.00	0.00
HETATM H	26	H2	LG1	A	1	-1.659	-3.466	-2.181	1.00	0.00
HETATM H	27	H3	LG1	A	1	2.127	-4.633	-0.441	1.00	0.00
HETATM H	28	H4	LG1	A	1	3.847	-2.129	-0.660	1.00	0.00
HETATM H	29	H5	LG1	A	1	3.124	-2.224	0.981	1.00	0.00
HETATM H	30	H6	LG1	A	1	0.086	1.444	-0.153	1.00	0.00
HETATM H	31	H7	LG1	A	1	-0.199	-0.081	0.641	1.00	0.00
HETATM H	32	H8	LG1	A	1	1.709	0.157	2.098	1.00	0.00
HETATM H	33	H9	LG1	A	1	0.567	1.476	2.249	1.00	0.00
HETATM H	34	H10	LG1	A	1	1.263	3.240	2.587	1.00	0.00
HETATM H	35	H11	LG1	A	1	2.556	2.258	0.293	1.00	0.00
HETATM H	36	H12	LG1	A	1	3.398	1.719	1.780	1.00	0.00
HETATM H	37	H13	LG1	A	1	0.196	1.874	-4.818	1.00	0.00
HETATM H	38	H14	LG1	A	1	-0.293	0.606	-2.762	1.00	0.00
HETATM H	39	H15	LG1	A	1	3.881	0.918	-1.636	1.00	0.00
HETATM H	40	H16	LG1	A	1	4.318	2.173	-3.705	1.00	0.00
HETATM H	41	H17	LG1	A	1	0.940	4.061	0.400	1.00	0.00
HETATM H	42	H18	LG1	A	1	2.663	4.589	0.369	1.00	0.00
HETATM H	43	H19	LG1	A	1	1.495	5.339	1.520	1.00	0.00
HETATM H	44	H20	LG1	A	1	4.126	3.952	2.399	1.00	0.00
HETATM H	45	H21	LG1	A	1	3.286	3.154	3.783	1.00	0.00

ATOM H	488	3HG2	VAL X	30	12.091	-7.837	21.848	1.00	0.00
ATOM N	489	N	VAL X	31	11.273	-6.682	26.762	1.00	0.00
ATOM C	490	CA	VAL X	31	10.676	-6.826	28.084	1.00	0.00
ATOM C	491	C	VAL X	31	9.256	-6.279	28.113	1.00	0.00
ATOM O	492	O	VAL X	31	8.915	-5.365	27.359	1.00	0.00
ATOM C	493	CB	VAL X	31	11.511	-6.111	29.163	1.00	0.00
ATOM C	494	CG1	VAL X	31	12.888	-6.746	29.277	1.00	0.00
ATOM C	495	CG2	VAL X	31	11.632	-4.628	28.847	1.00	0.00
ATOM H	496	H	VAL X	31	11.567	-5.767	26.452	1.00	0.00
ATOM H	497	HA	VAL X	31	10.575	-7.876	28.361	1.00	0.00
ATOM H	498	HB	VAL X	31	10.994	-6.188	30.120	1.00	0.00
ATOM H	499	1HG1	VAL X	31	13.464	-6.229	30.045	1.00	0.00
ATOM H	500	2HG1	VAL X	31	12.784	-7.796	29.550	1.00	0.00
ATOM H	501	3HG1	VAL X	31	13.406	-6.667	28.321	1.00	0.00
ATOM H	502	1HG2	VAL X	31	12.225	-4.138	29.620	1.00	0.00
ATOM H	503	2HG2	VAL X	31	12.121	-4.503	27.881	1.00	0.00
ATOM H	504	3HG2	VAL X	31	10.639	-4.179	28.812	1.00	0.00
ATOM N	505	N	PRO X	32	8.428	-6.845	28.984	1.00	0.00
ATOM C	506	CA	PRO X	32	8.852	-7.940	29.846	1.00	0.00
ATOM C	507	C	PRO X	32	8.807	-9.271	29.105	1.00	0.00
ATOM O	508	O	PRO X	32	7.983	-9.468	28.212	1.00	0.00
ATOM C	509	CB	PRO X	32	7.862	-7.898	31.022	1.00	0.00
ATOM C	510	CG	PRO X	32	6.590	-7.344	30.440	1.00	0.00
ATOM C	511	CD	PRO X	32	7.215	-6.182	29.484	1.00	0.00
ATOM H	512	HA	PRO X	32	9.784	-7.787	30.161	1.00	0.00
ATOM H	513	1HB	PRO X	32	7.721	-8.792	31.157	1.00	0.00

ATOM H	774	2HG	PRO	X	51	-1.034	-1.605	28.987	1.00	0.00
ATOM H	775	1HD	PRO	X	51	-1.317	-3.836	27.958	1.00	0.00
ATOM H	776	2HD	PRO	X	51	0.046	-2.973	27.720	1.00	0.00
ATOM N	777	N	SER	X	52	0.593	-4.773	32.640	1.00	0.00
ATOM C	778	CA	SER	X	52	0.000	-5.382	33.823	1.00	0.00
ATOM C	779	C	SER	X	52	0.458	-4.677	35.095	1.00	0.00
ATOM O	780	O	SER	X	52	1.648	-4.655	35.413	1.00	0.00
ATOM C	781	CB	SER	X	52	0.349	-6.856	33.882	1.00	0.00
ATOM O	782	OG	SER	X	52	-0.168	-7.474	35.027	1.00	0.00
ATOM H	783	H	SER	X	52	1.511	-4.357	32.708	1.00	0.00
ATOM H	784	HA	SER	X	52	-1.089	-5.418	33.791	1.00	0.00
ATOM H	785	1HB	SER	X	52	-0.059	-7.346	32.999	1.00	0.00
ATOM H	786	2HB	SER	X	52	1.434	-6.959	33.885	1.00	0.00
ATOM H	787	HG	SER	X	52	0.190	-7.051	35.811	1.00	0.00
ATOM N	788	N	PRO	X	53	-0.493	-4.099	35.818	1.00	0.00
ATOM C	789	CA	PRO	X	53	-1.896	-4.152	35.422	1.00	0.00
ATOM C	790	C	PRO	X	53	-2.167	-3.245	34.230	1.00	0.00
ATOM O	791	O	PRO	X	53	-1.564	-2.182	34.093	1.00	0.00
ATOM C	792	CB	PRO	X	53	-2.659	-3.699	36.678	1.00	0.00
ATOM C	793	CG	PRO	X	53	-1.699	-2.805	37.414	1.00	0.00
ATOM C	794	CD	PRO	X	53	-0.321	-3.576	37.179	1.00	0.00
ATOM H	795	HA	PRO	X	53	-2.146	-5.083	35.172	1.00	0.00
ATOM H	796	1HB	PRO	X	53	-3.291	-3.154	36.306	1.00	0.00
ATOM H	797	2HB	PRO	X	53	-2.714	-4.442	37.118	1.00	0.00
ATOM H	798	1HG	PRO	X	53	-1.664	-2.060	37.014	1.00	0.00
ATOM H	799	2HG	PRO	X	53	-1.747	-3.028	38.324	1.00	0.00

ATOM H	1970	1HD1	ILE X 130	8.395	0.656	15.775	1.00	0.00
ATOM H	1971	2HD1	ILE X 130	10.047	0.035	15.530	1.00	0.00
ATOM H	1972	3HD1	ILE X 130	9.794	1.722	16.039	1.00	0.00
ATOM N	1973	N	PRO X 131	13.059	1.823	11.516	1.00	0.00
ATOM C	1974	CA	PRO X 131	14.308	2.434	11.044	1.00	0.00
ATOM C	1975	C	PRO X 131	14.297	2.854	9.574	1.00	0.00
ATOM O	1976	O	PRO X 131	14.848	3.898	9.221	1.00	0.00
ATOM C	1977	CB	PRO X 131	15.372	1.350	11.287	1.00	0.00
ATOM C	1978	CG	PRO X 131	14.835	0.527	12.425	1.00	0.00
ATOM C	1979	CD	PRO X 131	13.259	0.436	11.947	1.00	0.00
ATOM H	1980	HA	PRO X 131	14.509	3.254	11.572	1.00	0.00
ATOM H	1981	1HB	PRO X 131	15.277	0.846	10.529	1.00	0.00
ATOM H	1982	2HB	PRO X 131	16.026	1.825	11.595	1.00	0.00
ATOM H	1983	1HG	PRO X 131	14.215	0.030	12.128	1.00	0.00
ATOM H	1984	2HG	PRO X 131	15.544	0.361	13.014	1.00	0.00
ATOM H	1985	1HD	PRO X 131	12.533	-0.031	11.544	1.00	0.00
ATOM H	1986	2HD	PRO X 131	13.265	0.510	12.896	1.00	0.00
ATOM N	1987	N	LEU X 132	13.660	2.065	8.713	1.00	0.00
ATOM C	1988	CA	LEU X 132	13.604	2.428	7.301	1.00	0.00
ATOM C	1989	C	LEU X 132	12.846	3.729	7.076	1.00	0.00
ATOM O	1990	O	LEU X 132	13.243	4.539	6.247	1.00	0.00
ATOM C	1991	CB	LEU X 132	12.958	1.300	6.489	1.00	0.00
ATOM C	1992	CG	LEU X 132	13.836	0.060	6.282	1.00	0.00
ATOM C	1993	CD1	LEU X 132	13.021	-1.056	5.643	1.00	0.00
ATOM C	1994	CD2	LEU X 132	15.030	0.422	5.410	1.00	0.00
ATOM H	1995	H	LEU X 132	13.215	1.218	9.036	1.00	0.00

ATOM H	1996	HA	LEU X 132	14.613	2.599	6.928	1.00	0.00
ATOM H	1997	1HB	LEU X 132	12.125	1.061	7.147	1.00	0.00
ATOM H	1998	2HB	LEU X 132	12.575	1.658	5.534	1.00	0.00
ATOM H	1999	HG	LEU X 132	14.215	-0.236	7.260	1.00	0.00
ATOM H	2000	1HD1	LEU X 132	13.653	-1.933	5.499	1.00	0.00
ATOM H	2001	2HD1	LEU X 132	12.185	-1.315	6.293	1.00	0.00
ATOM H	2002	3HD1	LEU X 132	12.641	-0.723	4.678	1.00	0.00
ATOM H	2003	1HD2	LEU X 132	15.653	-0.460	5.264	1.00	0.00
ATOM H	2004	2HD2	LEU X 132	14.679	0.783	4.443	1.00	0.00
ATOM H	2005	3HD2	LEU X 132	15.615	1.200	5.899	1.00	0.00
ATOM N	2006	N	PHE X 133	11.747	3.935	7.799	1.00	0.00
ATOM C	2007	CA	PHE X 133	10.994	5.178	7.644	1.00	0.00
ATOM C	2008	C	PHE X 133	11.902	6.350	8.025	1.00	0.00
ATOM O	2009	O	PHE X 133	11.938	7.368	7.336	1.00	0.00
ATOM C	2010	CB	PHE X 133	9.730	5.168	8.504	1.00	0.00
ATOM C	2011	CG	PHE X 133	8.865	6.383	8.327	1.00	0.00
ATOM C	2012	CD1	PHE X 133	9.298	7.455	7.559	1.00	0.00
ATOM C	2013	CD2	PHE X 133	7.617	6.457	8.927	1.00	0.00
ATOM C	2014	CE1	PHE X 133	8.504	8.573	7.395	1.00	0.00
ATOM C	2015	CE2	PHE X 133	6.821	7.574	8.764	1.00	0.00
ATOM C	2016	CZ	PHE X 133	7.265	8.633	7.997	1.00	0.00
ATOM H	2017	H	PHE X 133	11.434	3.233	8.455	1.00	0.00
ATOM H	2018	HA	PHE X 133	10.704	5.307	6.600	1.00	0.00
ATOM H	2019	1HB	PHE X 133	9.113	4.307	8.254	1.00	0.00
ATOM H	2020	2HB	PHE X 133	9.997	5.127	9.561	1.00	0.00
ATOM H	2021	HD1	PHE X 133	10.278	7.407	7.082	1.00	0.00

ATOM C	1993	CD1	LEU	X	132	12.822	-1.037	6.417	1.00	0.00
ATOM C	1994	CD2	LEU	X	132	14.729	0.583	6.313	1.00	0.00
ATOM H	1995	H	LEU	X	132	12.557	1.380	9.725	1.00	0.00
ATOM H	1996	HA	LEU	X	132	14.008	2.790	7.656	1.00	0.00
ATOM H	1997	1HB	LEU	X	132	11.640	1.057	7.762	1.00	0.00
ATOM H	1998	2HB	LEU	X	132	12.177	1.621	6.163	1.00	0.00
ATOM H	1999	HG	LEU	X	132	13.793	-0.076	8.105	1.00	0.00
ATOM H	2000	1HD1	LEU	X	132	13.528	-1.866	6.367	1.00	0.00
ATOM H	2001	2HD1	LEU	X	132	11.950	-1.339	6.998	1.00	0.00
ATOM H	2002	3HD1	LEU	X	132	12.510	-0.765	5.410	1.00	0.00
ATOM H	2003	1HD2	LEU	X	132	15.427	-0.253	6.259	1.00	0.00
ATOM H	2004	2HD2	LEU	X	132	14.446	0.886	5.305	1.00	0.00
ATOM H	2005	3HD2	LEU	X	132	15.206	1.421	6.823	1.00	0.00
ATOM N	2006	N	PHE	X	133	11.005	3.921	8.329	1.00	0.00
ATOM C	2007	CA	PHE	X	133	10.163	5.089	8.077	1.00	0.00
ATOM C	2008	C	PHE	X	133	10.975	6.346	8.385	1.00	0.00
ATOM O	2009	O	PHE	X	133	11.082	7.246	7.549	1.00	0.00
ATOM C	2010	CB	PHE	X	133	8.890	5.021	8.922	1.00	0.00
ATOM C	2011	CG	PHE	X	133	8.015	6.235	8.799	1.00	0.00
ATOM C	2012	CD1	PHE	X	133	8.401	7.309	8.009	1.00	0.00
ATOM C	2013	CD2	PHE	X	133	6.804	6.308	9.470	1.00	0.00
ATOM C	2014	CE1	PHE	X	133	7.598	8.427	7.894	1.00	0.00
ATOM C	2015	CE2	PHE	X	133	5.997	7.424	9.355	1.00	0.00
ATOM C	2016	CZ	PHE	X	133	6.396	8.485	8.567	1.00	0.00
ATOM H	2017	H	PHE	X	133	10.727	3.235	9.016	1.00	0.00
ATOM H	2018	HA	PHE	X	133	9.882	5.122	7.023	1.00	0.00

ATOM H	2019	1HB	PHE	X	133	8.284	4.167	8.620	1.00	0.00
ATOM H	2020	2HB	PHE	X	133	9.145	4.929	9.977	1.00	0.00
ATOM H	2021	HD1	PHE	X	133	9.352	7.263	7.476	1.00	0.00
ATOM H	2022	HD2	PHE	X	133	6.490	5.470	10.093	1.00	0.00
ATOM H	2023	HE1	PHE	X	133	7.914	9.263	7.271	1.00	0.00
ATOM H	2024	HE2	PHE	X	133	5.049	7.468	9.888	1.00	0.00
ATOM H	2025	HZ	PHE	X	133	5.762	9.367	8.477	1.00	0.00
ATOM N	2026	N	TYR	X	134	11.555	6.415	9.583	1.00	0.00
ATOM C	2027	CA	TYR	X	134	12.355	7.583	9.935	1.00	0.00
ATOM C	2028	C	TYR	X	134	13.491	7.803	8.951	1.00	0.00
ATOM O	2029	O	TYR	X	134	13.787	8.935	8.574	1.00	0.00
ATOM C	2030	CB	TYR	X	134	12.918	7.439	11.351	1.00	0.00
ATOM C	2031	CG	TYR	X	134	13.809	8.584	11.777	1.00	0.00
ATOM C	2032	CD1	TYR	X	134	13.283	9.846	12.013	1.00	0.00
ATOM C	2033	CD2	TYR	X	134	15.173	8.400	11.943	1.00	0.00
ATOM C	2034	CE1	TYR	X	134	14.092	10.896	12.401	1.00	0.00
ATOM C	2035	CE2	TYR	X	134	15.990	9.443	12.332	1.00	0.00
ATOM C	2036	CZ	TYR	X	134	15.447	10.690	12.559	1.00	0.00
ATOM O	2037	OH	TYR	X	134	16.257	11.732	12.948	1.00	0.00
ATOM H	2038	H	TYR	X	134	11.442	5.661	10.246	1.00	0.00
ATOM H	2039	HA	TYR	X	134	11.737	8.481	9.895	1.00	0.00
ATOM H	2040	1HB	TYR	X	134	12.067	7.367	12.031	1.00	0.00
ATOM H	2041	2HB	TYR	X	134	13.484	6.508	11.381	1.00	0.00
ATOM H	2042	HD1	TYR	X	134	12.211	10.002	11.885	1.00	0.00
ATOM H	2043	HD2	TYR	X	134	15.596	7.413	11.761	1.00	0.00
ATOM H	2044	HE1	TYR	X	134	13.664	11.882	12.582	1.00	0.00

ATOM	9949	OXT	VAL	X	630	10.261	17.982	-26.734	1.00	0.00
O										
ATOM	9950	H	VAL	X	630	8.764	14.130	-28.101	1.00	0.00
H										
ATOM	9951	HA	VAL	X	630	9.902	15.683	-26.077	1.00	0.00
H										
ATOM	9952	HB	VAL	X	630	11.114	13.917	-27.405	1.00	0.00
H										
ATOM	9953	1HG1	VAL	X	630	12.223	14.614	-29.502	1.00	0.00
H										
ATOM	9954	2HG1	VAL	X	630	10.452	14.678	-29.661	1.00	0.00
H										
ATOM	9955	3HG1	VAL	X	630	11.379	16.179	-29.426	1.00	0.00
H										
ATOM	9956	1HG2	VAL	X	630	13.294	15.018	-27.317	1.00	0.00
H										
ATOM	9957	2HG2	VAL	X	630	12.489	16.597	-27.164	1.00	0.00
H										
ATOM	9958	3HG2	VAL	X	630	12.307	15.377	-25.881	1.00	0.00
H										

S5: *R*-citalopram docked into hSERT model.