Report for 5C1M : Crystal Structure Of Active Mu-Opioid Receptor Bound To The Agonist Bu72 Chain A

List of all contacts can be downloaded here (../../structures_database/5C1M/5C1M_txt.zip)

Thu Aug 10 2017

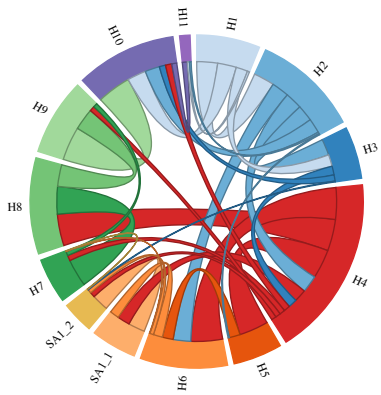

Figure 1: Chord plot showing secondary structure elements

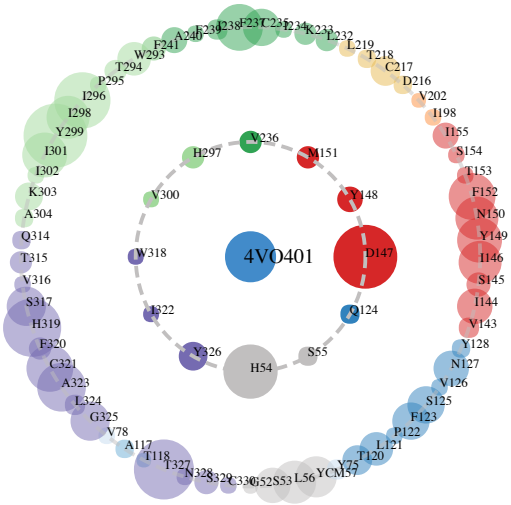

Figure 2: Asteroid Plot for selected residue 4VO401

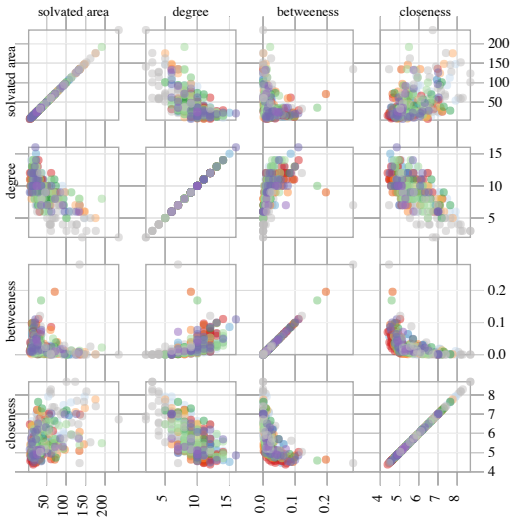

Figure 3: Network statistics

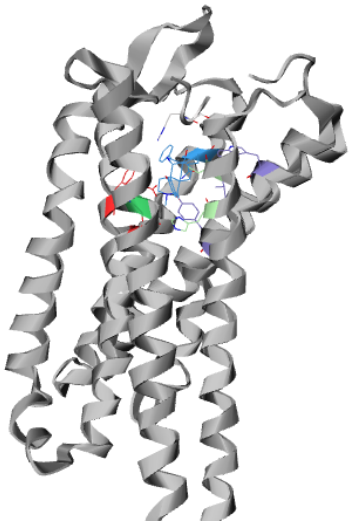

Figure 4: The 3D structure view of 5C1M A

Name	Solvated Area	Degree	Betweenness	Closeness
F347	234.87	2	0	6.726
R277	191.55	8	0.022	5.49
L265	176.07	3	0	7.414
Y210	175.27	5	0.001	7.764
OLC403	162.29	5	0.025	5.538
Q212	152.09	3	0	8.183
R211	148.08	6	0.008	7.317
M65	147.51	5	0	7.914
H223	146	5	0.001	7.643
R182	145.9	6	0.001	5.431

Table 1: Top ten residues with highest solvated area

Name	Solvated Area	Degree	Betweenness	Closeness
G325	6.97	9	0.01	5.16
C140	7.22	12	0.01	6.469
A184	7.38	11	0.014	4.893
G199	8.16	10	0.014	5.41
S162	8.21	11	0.038	4.571
A111	8.44	11	0.017	4.907
A337	9.12	10	0.036	4.767
A102	9.46	9	0.018	4.836
S195	9.67	12	0.032	4.876
A175	9.73	10	0.005	5.01

Table 2: Bottom ten residues with lowest solvated area

Name	Solvated Area	Degree	Betweenness	Closeness
Y326	21.24	16	0.11	4.855
Y106	22.83	15	0.086	4.517
I107	16.36	14	0.052	4.607
F289	18.81	14	0.058	4.712
W318	23.11	14	0.049	5.693
H297	15.26	14	0.067	4.888
Y299	14.96	14	0.028	5.576
M255	21.29	14	0.038	4.986
Y148	29.21	14	0.111	5.033
I93	10.27	14	0.037	5.102

Table 3: Top ten residues with highest degree values

Name	Solvated Area	Degree	Betweenness	Closeness
F347	234.87	2	0	6.726
T307	141.1	2	0	6.895
P63	101.17	3	0	8.686
PO4405	61.19	3	0	8.29
L265	176.07	3	0	7.414
S62	123.39	3	0	8.686
Q212	152.09	3	0	8.183
T60	127.77	4	0.001	7.695
G61	61.14	4	0.008	8.067
C346	60.13	4	0.003	6.114

Table 4: Bottom ten residues with lowest degree values

Name	Solvated Area	Degree	Betweenness	Closeness
P6G406	134.51	7	0.281	4.455
D177	70.89	9	0.196	4.636
M243	35.8	10	0.169	4.588
4VO401	33.2	12	0.121	5.036
Y148	29.21	14	0.111	5.033
Y326	21.24	16	0.11	4.855
N328	19.45	13	0.1	4.619
L176	14.04	13	0.099	4.843
F241	13.49	13	0.098	4.743
A168	12.1	11	0.097	4.76

Table 5: Top ten residues with highest betwenness values

Name	Solvated Area	Degree	Betweenness	Closeness
F347	234.87	2	0	6.726
G213	58.44	4	0	8.181
PO4405	61.19	3	0	8.29
T311	61.98	6	0	7.031
Q212	152.09	3	0	8.183
S266	64.82	5	0	7.369
M65	147.51	5	0	7.914
P309	91.62	4	0	7.086
S62	123.39	3	0	8.686
T307	141.1	2	0	6.895

Table 6: Bottom ten residues with lowest betwenness values

Name	Solvated Area	Degree	Betweenness	Closeness
S62	123.39	3	0	8.686
P63	101.17	3	0	8.686
PO4405	61.19	3	0	8.29
Q212	152.09	3	0	8.183
G213	58.44	4	0	8.181
G61	61.14	4	0.008	8.067
S64	54.04	6	0.011	7.919
M65	147.51	5	0	7.914
Y210	175.27	5	0.001	7.764
T60	127.77	4	0.001	7.695

Table 7: Top ten residues with highest closeness values

Name	Solvated Area	Degree	Betweenness	Closeness
T160	15.66	12	0.07	4.381
P6G406	134.51	7	0.281	4.455
L158	15.74	11	0.073	4.455
M161	23.05	11	0.038	4.471
L110	13.59	12	0.057	4.471
N332	17.5	12	0.086	4.514
F178	23.35	11	0.093	4.514
Y106	22.83	15	0.086	4.517
T157	15.44	11	0.026	4.533
Y336	36.23	10	0.077	4.552

Table 8: Bottom ten residues with lowest closeness values

Ligand	Residue/Ligand	Number of contacts
YCM57	P58	19
4VO401	D147	16
YCM57	L56	13
4VO401	H54	13
YCM57	W318	11
YCM57	Q59	10
PO4405	T225	9
P6G406	F178	8
OLC403	OLC402	7
OLC402	OLC403	7

Table 9: Top ten residues with highest number of atomic contacts with a ligand

Ligand	Residue/Ligand	Number of contacts
P6G406	D177	1
YCM57	S53	1
P6G407	F87	1
4VO401	V300	1
P6G407	L83	1
P6G407	V80	1
4VO401	W318	1
P6G406	L194	1
4VO401	I322	1
CLR404	C321	1

Table 10: Bottom ten residues with lowest number of atomic contacts with a ligand