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**Supplemental Information**

**Interfacial Binding Sites for Cholesterol on G Protein-Coupled  
Receptors**

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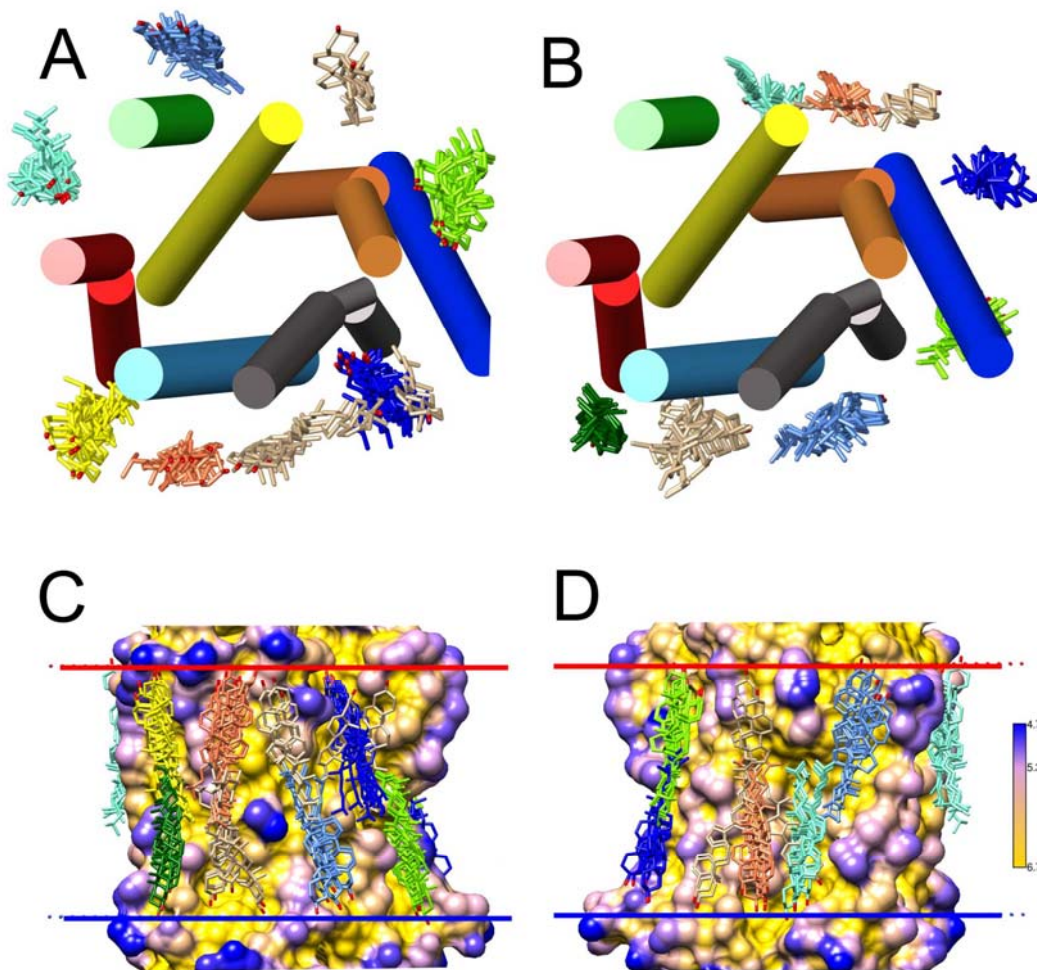


FIGURE S1 Docking to 3D4S with tilted interface planes around the protein. A set of 9 pairs of interface planes were generated by  $5^\circ$  rotations about the Chimera x and z axes. Docking to these structures resulted in the clusters shown in (A) and (B) for the EC and IC monolayers, respectively, coloured as in Fig. 4, and both viewed from the EC side. (C, D) show surface views of 3D4S coloured by distance from a bulk 'solvent' layer calculated using the Depth program (29) with distances ( $\text{\AA}$ ) given by the scale on the right. Clusters are coloured as in Fig. 4.

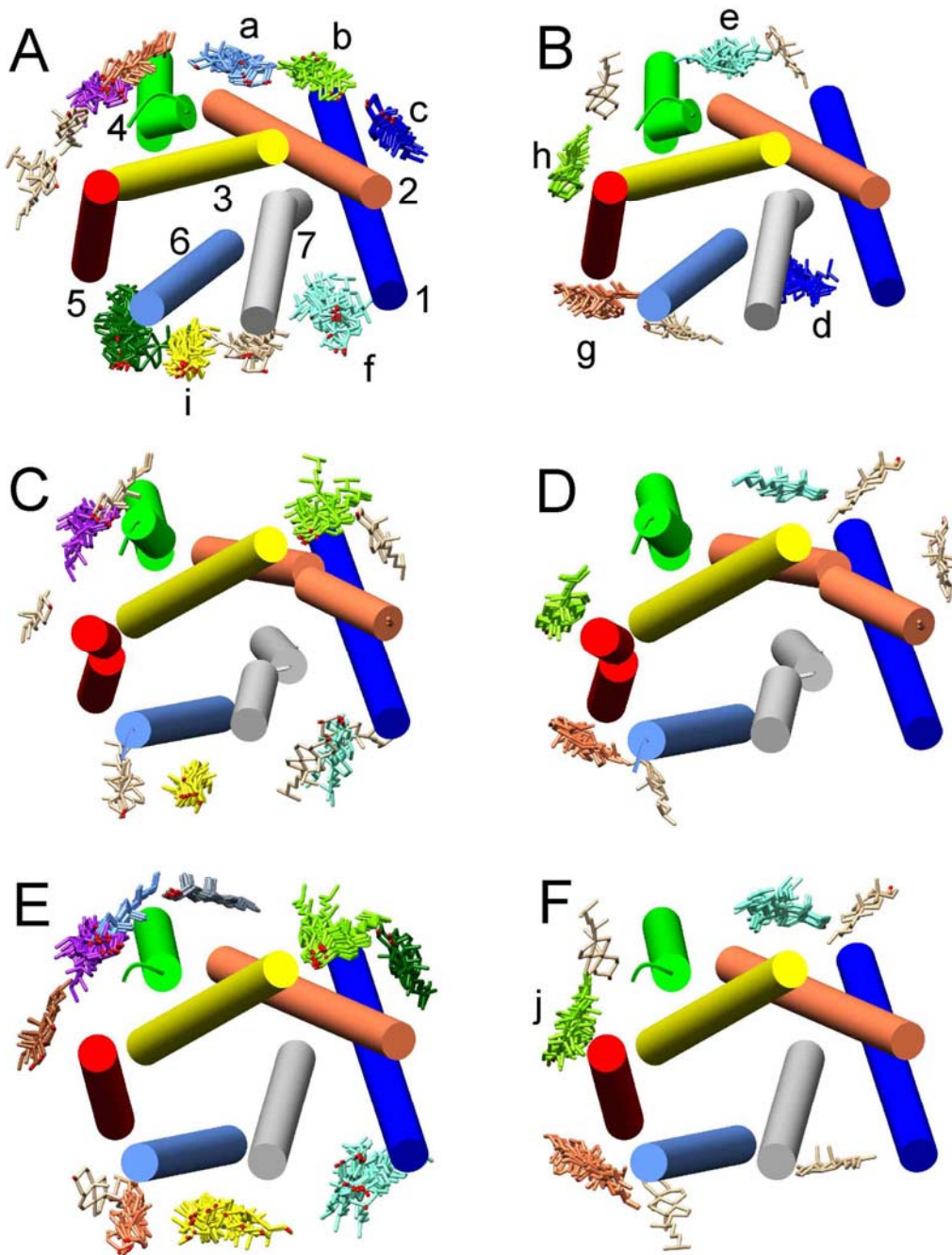


FIGURE S2 Docking to rhodopsin and opsin, all views being from the EC side. Shown are the EC (A, C, E) and IC (B, D, F) monolayers, for the inactive (A, B) and active (C, D) states of rhodopsin and for opsin (E, F). Poses are clustered, with single poses coloured tan. The letters *a-j* relate to clusters identified in Table S6.

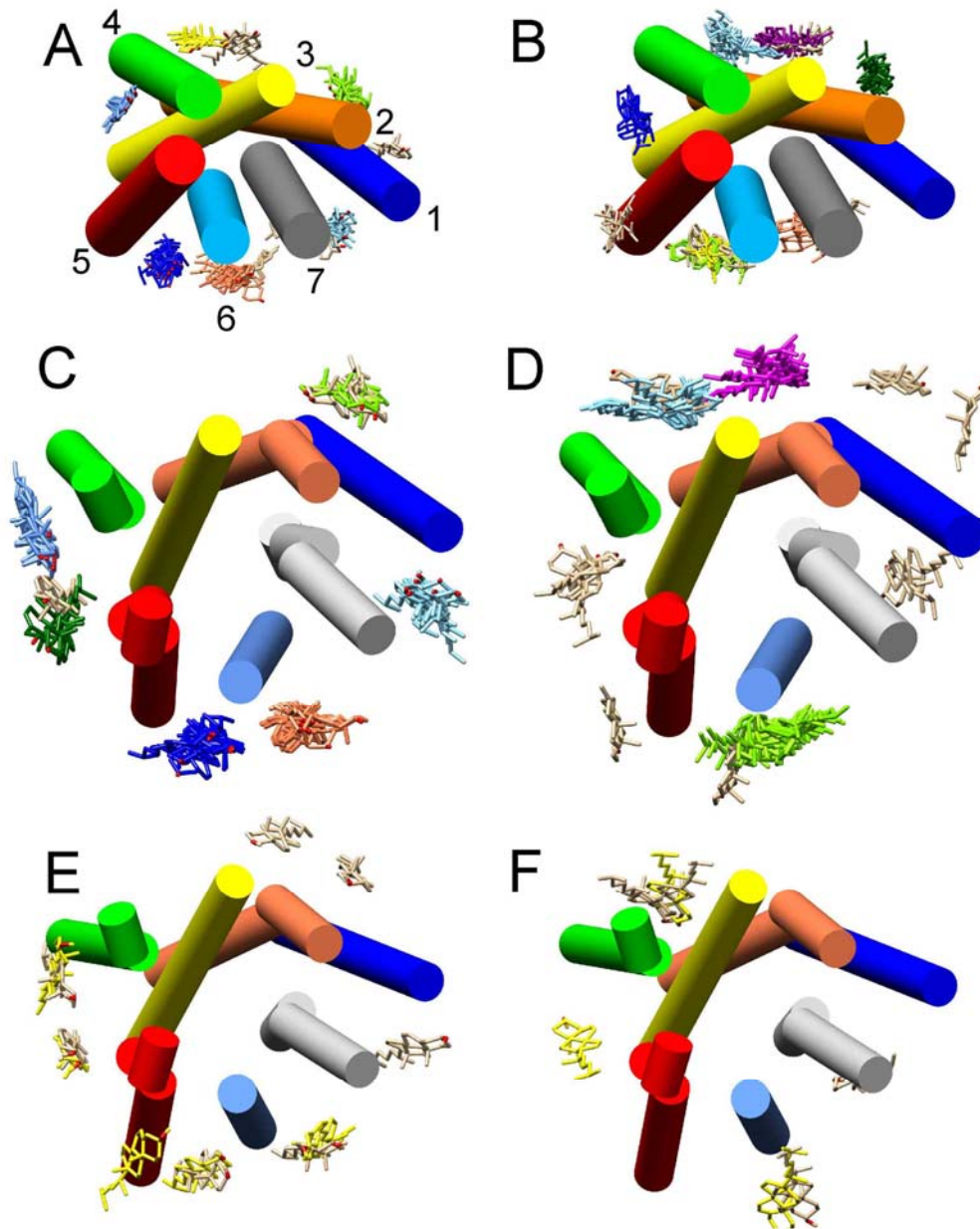


FIGURE S3 Docking to A2A in the inactive, active intermediate, and fully active states, all views being from the EC side. Shown are the EC (A, C, E) and IC (B, D, F) monolayers, for the inactive (A, B), active intermediate (C, D) and active (E, F) states. Only crystallographic structures with no resolved cholesterol molecules are included in this analysis. For the inactive and active intermediate states poses are clustered, with single poses coloured tan. For the active state, poses for the two available structures, 5G53 and 6GDG, are coloured tan and yellow, respectively.

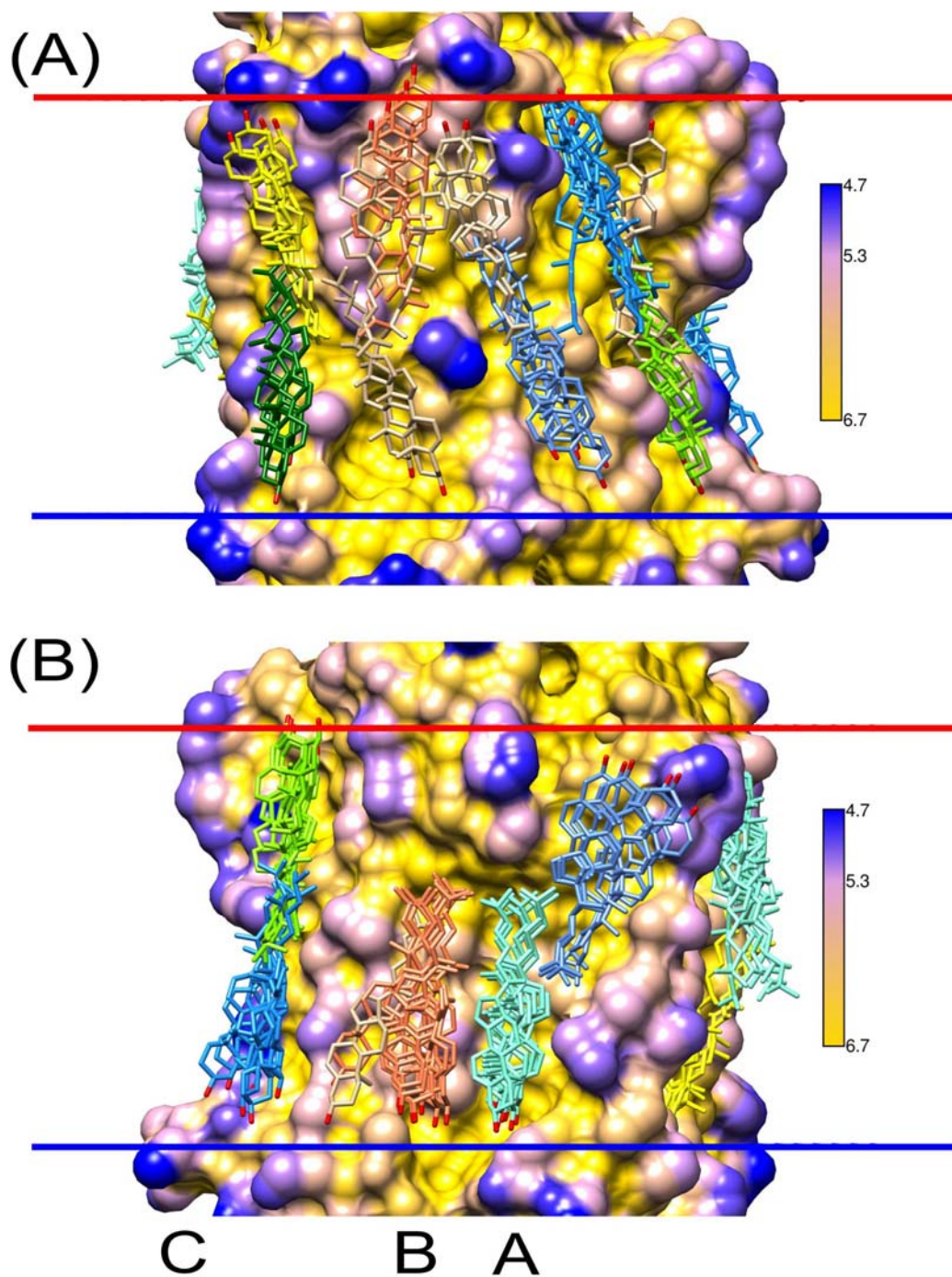


FIGURE S4 Surface view of inactive  $\beta_2$ AR with docking clusters. A and B show two views, related by a 180° rotation, of the surface of 3D4S coloured by distance from a bulk 'solvent' layer calculated using the Depth program (29) with distances (Å) given by the scales on the right. Clusters are shown coloured as in Fig. 4, with the three crystallographic sites A-C marked.

TABLE S1 Cholesterol binding to the A<sub>2A</sub> receptor (EC side)

PDB	Binding site <sup>a</sup>				
	A	B	C	D	Others
5iu4	CLR2402	CLR2403	<i>CLR2404</i>	<i>CLR2405</i>	
4eiy		CLR2403	<i>CLR2404</i>	<i>CLR2405</i>	
5iu7	CLR2402	CLR2403	<i>CLR2404</i>	<i>CLR2405</i>	
5iu8	CLR2406	CLR2403	<i>CLR2404</i>	<i>CLR2405</i>	
5iua	CLR2402	CLR2403	<i>CLR2404</i>	<i>CLR2405</i>	
5iub	OLA2416	CLR2402	<i>CLR2403</i>	CLR2404	
5jtb	OLC1221	CLR1202	CLR1203	<i>CLR1204</i>	
5k2a	OLC1226	CLR1203	<i>CLR1204</i>	<i>CLR1205</i>	
5k2b	OLC1222	<i>CLR1205</i>	<i>CLR1204</i>	<i>CLR1203</i>	
5k2c	OLC1207	CLR1203	<i>CLR1204</i>	<i>CLR1205</i>	
5k2d	OLC1222	CLR1205	<i>CLR1204</i>	<i>CLR1203</i>	
5mzj	OLA2426	CLR2402	<i>CLR2403</i>	<i>CLR2404</i>	
5mzp	CLR2402	CLR2403	<i>CLR2404</i>	<i>CLR2405</i>	
5nlx		CLR506			CLR507/508 <sup>b</sup>
5nm2		CLR1222	<i>CLR1223</i>	<i>CLR1224</i>	
5nm4		CLR508	<i>CLR510</i>		CLR509 <sup>b</sup>
5n2r	OLA2408	CLR2402	<i>CLR2403</i>	<i>CLR2404</i>	
5olg	OLC1228	CLR1202	<i>CLR1203</i>	<i>CLR1204</i>	CLR1205
5olh		CLR1204	<i>CLR1205</i>	<i>CLR1206</i>	
5olo		CLR1202	<i>CLR1203</i>	<i>CLR1204</i>	
5olv	CLR1203	CLR1204	<i>CLR1205</i>	<i>CLR1206</i>	
5olz	CLR1202	CLR1203	<i>CLR1204</i>	<i>CLR1205</i>	
5om1	CLR1204	CLR1205	<i>CLR1206</i>	<i>CLR1207</i>	
5om4	CLR1203	CLR1204	<i>CLR1205</i>	<i>CLR1206</i>	
5uvi		CLR1204	<i>CLR1203</i>	<i>CLR1202</i>	
5vra	OLC2409	CLR2405	<i>CLR2403</i>	<i>CLR2404</i>	
6aqf	OLC1216	CLR1204	<i>CLR1202</i>	<i>CLR1203</i>	

<sup>a</sup> The nomenclature for bound cholesterol (CLR) molecules is that given in the respective PDB file. In some structures, as indicated, binding site A is occupied by a molecule of oleic acid (OLA) or 1-oleoyl-*R*-glycerol (OLC). Entries in italics indicate that a docking pose occupies the site as indicated by an rmsd with the crystallographic CLR molecule of 4 Å or less.

<sup>b</sup> These cholesterol molecules make no contact with protein and so are not included in the analysis.

TABLE S2 Cholesterol binding to other GPCRs

PDB	Binding site <sup>a</sup>	
	EC side	IC side
5-hydroxytryptamine receptor 2B:		
4ib4		<i>CLR2003</i>
4nc3		<i>CLR1203</i>
5tvn		<i>CLR2002</i>
6drx		CLR1202
6dry		CLR2002
6drz		<i>CLR1201</i>
6ds0		<i>CLR1201</i>
Cannabinoid receptor 1:		
5xr8		<i>CLR1203</i>
5xra		<i>CLR608</i>
C-C chemokine receptor type 9:		
5lwe		CLR417
Opioid mu receptor:		
4dkl	<i>CLR614</i>	
Opioid kappa receptor:		
6b73	<i>CLR2002</i>	
P2Y purinoreceptor 12:		
4ntj	CLR1202	<i>CLR1203</i>
4pxz		<i>CLR1202</i>
Metabotropic glutamate receptor (GPCR Class C)		
4or2 (dimer)	CLR1902.A, <i>CLR1903.A</i> , CLR1904.A, <i>CLR1905.A</i> , <i>CLR1905.B</i> , <i>CLR1906.B</i>	
Viral GPCR		
4xt1	<i>CLR401</i> , CLR402	

<sup>a</sup> The nomenclature for bound cholesterol (CLR) molecules is that given in the respective PDB file. Entries in italics indicate that a docking pose occupies the site as indicated by an rmsd with the crystallographic CLR molecule of 4 Å or less.

TABLE S3 Docking of cholesterol on the IC side of the  $\beta_2$ -adrenergic receptor

E <sup>a</sup>	Docking site <sup>b</sup>	Local Residues (within 4 Å of a cholesterol molecule)
3D4S docking sites:		
-14.5	A	Tyr70, Thr73, Ser74, Cys77, Val81, Phe108, Ile112, Leu115, Arg151, Ile154, Leu155, Trp158, Phe166
-13.3	C	Val44, Leu45, Val48, Phe49, Val52, Leu53, Thr56, Leu339
-13.0	d	Ile43, Ala46, Phe49, Leu53, Val317, Pro323, Leu324, Phe336, Gln337, Leu340
-13.0	B	Ile55, Ala59, Thr73, Cys77, Leu80, Val81, Leu84, Ala85
5D5A docking sites:		
-14.6	A	Tyr70, Thr73, Ser74, Ile112, Leu115, Arg151, Ile154, Leu155, Trp158, Phe166
-13.7	C	Val44, Leu45, Val48, Phe49, Val52, Leu53, Leu339, Leu340
-13.1	g	Tyr209, Val213, Val216, Phe217, Ser220, Gln224, Ile291, Ile294
-12.9	h	Cys125, Val126, Val129, Asp130, Leu145, Ile153, Val206, Val210, Pro211, Ile214
-12.7	f	Val216, Tyr219, Phe223, Gly276, Met279, Gly280, Thr283, Leu284, Leu287, Ile291
-12.7	B	Ile55, Ala59, Thr73, Cys77, Leu80, Val81, Ala85, Trp105, Phe108, Ile112
3D4S crystallographic sites:		
	A	Tyr70, Thr73, Ser74, Cys77, Val81, Ile112, Leu115, Arg151, Ile154, Trp158
	B	Ile55, Ala59, Thr73, Cys77, Leu80, Val81, Leu84, Ala85
5D5A crystallographic sites:		
	A	Tyr70, Thr73, Ser74, Cys77, Val81, Ile112, Leu115, Arg151, Ile154, Leu155, Trp158
	B	Ile55, Ala59, Thr73, Cys77, Leu80, Val81, Leu84, Ala85
	C	Val44, Leu45, Val48, Phe49, Val52, Leu53, Thr56, Leu84, Leu339, Leu340

<sup>a</sup> Docking energy, kcal mol<sup>-1</sup>.

<sup>b</sup> Sites of cholesterol binding observed in X-ray crystal structures (Table 1) are given in capitals and additional docking sites are lower case (see Fig. 4).



TABLE S4 Cholesterol docking to A<sub>2A</sub> receptor structures showing no crystallographic cholesterol molecules (EC side)

Inactive			Active Intermediate		
PDB	Pose No. <sup>a</sup>		PDB	Pose No. <sup>a</sup>	
	Site C <sup>b</sup>	Site D <sup>b</sup>		Site C <sup>b</sup>	Site D <sup>b</sup>
3eml	4	3	2ydo	3	2
3pwh	2	1	2ydv	3	2
3rey	5	2	3qak	1	3
3rfm	-	3	4ug2	3	4
3uza	5	3	4uhr	3	2
3uzc	3	1	5wf5	1	5
3vg9	-	5	5wf6	3	5
5uig	-	2	Active		
			5g53	4	8
			6gdg	9	5

<sup>a</sup> Pose number as listed in Table S7.

<sup>b</sup> Sites labelled as in Table S1 and Fig. 7.

TABLE S5 A<sub>2</sub>AR: comparison of MD and docking results for 4EIY

Site <sup>a</sup>	Local Residues <sup>b</sup>
EC side:	
MD IS1	V8, Y9, V12, L272
Dock g	A0, G5, V8, Y9, V12, W268, Y271, L272, V275, T279
MD IS2	V57, L58, P61, F62, T65, F70, F79, I80, F83
Dock f	V57, L58, P61, F62, T65, F70, A72, G76, I80
MD h60	L247, P248, I251, I252, F255, S263, A265, P266,
Dock C	I244, P248, I251, I252, F255, S263, H264, A265, L269
IC side:	
MD IS3	I24, F93, L96, A97, I100, Y103, I104, R107, L115, C128, L131, L192,
Dock c	F93, L96, A97, I100, I104, L115, V116, I124, I135
MD h56i	L194, F201, K233, A236, I237, G240, A243
Dock b	F182, L187, L194, K233, A236, I237, G240, A243, L247

<sup>a</sup> MD refers to sites detected by MD simulations (17, 36) and Dock refers to docking poses, as given in Fig. 6.

<sup>b</sup> Residues close to bound cholesterol as reported in the MD simulation papers (17, 36) or within 4 Å of a docking pose (Table S7).

TABLE S6 Comparison of MD and docking results for rhodopsin in the inactive state, and for opsin

MD Group <sup>a</sup>	Docking Cluster <sup>b</sup>	Residue Numbers <sup>c</sup>	Ref. <sup>d</sup>
Rhodopsin:			
A1	-	53, 56, 57, 60, 320, 321	38
A2	d	252, 255, 256, 259, 260, 305,308,309	38
A3	a	108, <i>111, 112, 115, 172</i>	38
B1	b, c	96, <i>105,108,112,115</i>	39
B2	e	63, 74, <i>154</i>	39
C1	d, f	43, 46, 50, 53, 56, 294, 301, 321, 322, 323	40
C2	g, h	126, 159, 206, 209, 210, 213, 214, 220, 221	40
C3	i	263	40
Opsin:			
D1	-	50, 53, 54, 56, 318, 321, 322, 323	40
D2	j	126, 159, 162, 206, 209, 210, 213, 214, 220	40
D3	-	256, 259, 263	40

<sup>a</sup> Groups of residues showing preferential interaction with cholesterol, numbered as in the original references.

<sup>b</sup> Docking clusters, labelled as in Fig. S2.

<sup>c</sup> Residue numbers for residues showing preferential interaction with cholesterol in MD simulations. Residues also within 4 Å of a docking pose in the given cluster or clusters are indicated in italics.

<sup>d</sup> References for MD simulations.

TABLE S7 Interfacial binding sites for cholesterol on GPCRs

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
GPCR Class A		
5-hydroxytryptamine (Serotonin) receptor		
5-Hydroxytryptamine receptor 5HT1B, inactive, Human 4iaq		
4iaq_EC	-13.3	V175[4.51], S179[4.55], P183[4.59], F186[4.62], H205[5.35], L207[5.37], Y208[5.38], Y211[5.41]
4iaq_IC	-14.0	V74[1.57], Y86[2.41], A89[2.44], S90[2.45], V93[2.48], I170[4.46], A171[4.47], W174[4.50], I178[4.54]
	-13.1	L145[3.48], Y148[3.51], W149[3.52], F219[5.49], L222[5.52], L223[5.53], A226[5.56], L227[5.57]
	-12.9	L145[3.48], W149[3.52], R165[4.41], M169[4.45], L172[4.48], F176[4.52], S179[4.55], Y211[5.41]
	-12.4	F217[5.47], Y218[5.48], T221[5.51], I225[5.55], Y228[5.58], Y232[5.62], I324[6.45], L328[6.49]
5-Hydroxytryptamine receptor 5HT1B, inactive, Human 4iar		
4iar_EC	-14.5	V175[4.51], F176[4.52], S179[4.55], P183[4.59], F186[4.62], H205[5.35], L207[5.37], Y208[5.38], Y211[5.41]
	-12.8	Y40, I44, L52[1.35], L55[1.38], I59[1.42], H347[7.31], A349[7.33], F353[7.37]
4iar_IC	-14.1	Y86[2.41], S90[2.45], V93[2.48], L97[2.52], L101[2.56], P163[4.39], A166[4.42], A167[4.43], I170[4.46], A171[4.47], W174[4.50]
	-13.3	T64[1.47], L65[1.48], A68[1.51], F69[1.52], A72[1.55], R76[1.59], L96[2.51], I100[2.55], L383[8.57]
	-13.3	W138[3.41], L145[3.48], W149[3.52], R165[4.41], M169[4.45], L172[4.48], F176[4.52], Y211[5.41], G215[5.45], F219[5.49]
	-12.8	Y228[5.58], G317[6.38], L320[6.41], G321[6.42], I324[6.45], V325[6.46], L328[6.49], P329[6.50]
	-13.0	I71[1.54], Y75[1.58], A89[2.44], V93[2.48], L96[2.51], L97[2.52], I100[2.55], L101[2.56]
5-Hydroxytryptamine receptor 5HT2B, inactive, with cholesterol, Human 4ib4		
4ib4_EC	-14.5	K53, W56[1.34], L59[1.37], L60[1.38], I115[2.65], M336[6.47], E363[7.36], I364[7.37], W367[7.40], I368[7.41], V371[7.44]
	-14.2	I182[4.52], G185[4.55], I186[4.56], P189[4.59], D216[5.37], F217[5.38], F220[5.41], G221[5.42]
	-12.5	L102[2.52], V126[3.23], P129[3.26], A130[3.27], F133[3.30], L134[3.31], F138[3.35], P191[4.61]
	-12.3	W56[1.34], L59[1.37], L60[1.38], M63[1.41], V64[1.42], M360[7.33], I364[7.37], I368[7.41], V371[7.44]
	-12.2	F331[6.42], L335[6.46], C338[6.49], P339[6.50], I342[6.53], T343[6.54], L358[7.31], L361[7.34], F365[7.38]
	-12.1	F227[5.48], L230[5.51], F331[6.42], I342[6.53], I345[6.56], T346[6.57], L349[6.60], C350[6.61]
	-11.9	L335[6.46], M336[6.47], P339[6.50], I342[6.53], T346[6.57], C353, L358[7.31], L361[7.34], F365[7.38]
	-11.7	I61[1.39], I65[1.43], I66[1.44], I69[1.47], P109[2.59], L113[2.63], M116[2.66], F117[2.67], P122, L123
4ib4_IC	-14.3	I61[1.39], I65[1.43], I66[1.44], I69[1.47], G70[1.48], T73[1.51], L77[1.55], Y394[8.57], I395[8.58], C397, Y399
	-13.2	Y91[2.41], S95[2.45], V98[2.48], F133[3.30], L137[3.34], R169[4.39], F173[4.43], I176[4.46], W180[4.50]
	-12.4	V151[3.48], Y154[3.51], I155[3.52], A231[5.52], I232[5.53], V235[5.56], T236[5.57], L239[5.60]
	-12.4	I76[1.54], S80[1.58], M94[2.44], V98[2.48], L101[2.51], L102[2.52], L134[3.31], F138[3.35]
	-12.3	L59[1.37], L60[1.38], M63[1.41], V64[1.42], P67[1.45], I368[7.41], V371[7.44], V375[7.48], V379[7.52], L382[7.55]
	-12.3	W144[3.41], V151[3.48], I155[3.52], T171[4.41], K175[4.45], V178[4.48], I182[4.52], T228[5.49]
5-Hydroxytryptamine receptor 5HT2B, inactive, with cholesterol, Human 4nc3		
4nc3_EC	-15.6	K53, W56[1.34], L59[1.37], L60[1.38], M63[1.41], V64[1.42], I115[2.65], E363[7.36], I364[7.37], W367[7.40], V371[7.44]
	-14.8	V178[4.48], L181[4.51], I182[4.52], G185[4.55], I186[4.56], P189[4.59], K193[4.63], D216[5.37], F217[5.38], F220[5.41], G221[5.42]
	-13.2	L102[2.52], P129[3.26], A130[3.27], F133[3.30], L134[3.31], F138[3.35], P191[4.61], I192[4.62]
	-12.6	L332[6.43], L335[6.46], C338[6.49], P339[6.50], I342[6.53], T343[6.54], T346[6.57], L358[7.31], L361[7.34], F365[7.38]
	-11.7	F227[5.48], L230[5.51], I234[5.55], F331[6.42], I342[6.53], I345[6.56], T346[6.57], L349[6.60]
	-12.0	L219[5.40], L223[5.44], F227[5.48], A231[5.52], I234[5.55], V235[5.56], I345[6.56], L349[6.60]
4nc3_IC	-14.6	Y91[2.41], M94[2.44], S95[2.45], V98[2.48], F133[3.30], L137[3.34], F138[3.35], F173[4.43], I176[4.46], W180[4.50], I184[4.54]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.9	I61[1.39], I65[1.43], I66[1.44], I69[1.47], G70[1.48], P109[2.59], L112[2.62], Y399
	-12.8	I76[1.54], S80[1.58], M94[2.44], V98[2.48], L102[2.52], F106[2.56], L134[3.31], F138[3.35]
	-12.6	L59[1.37], L60[1.38], M63[1.41], V64[1.42], V371[7.44], V375[7.48], V379[7.52], L382[7.55]
	-12.6	V151[3.48], Y154[3.51], I155[3.52], A231[5.52], I232[5.53], V235[5.56], T236[5.57], L239[5.60]
	-12.7	W144[3.41], V151[3.48], I155[3.52], K175[4.45], V178[4.48], I182[4.52], A224[5.45], T228[5.49], I232[5.53]
5-Hydroxytryptamine receptor 5HT2B, inactive, with cholesterol, Human 5tvn		
5tvn_EC	-15.3	K53, W56[1.34], L60[1.38], I115[2.65], E118, M336[6.47], E363[7.36], I364[7.37], W367[7.40], I368[7.41], V371[7.44]
	-13.7	V178[4.48], L181[4.51], I182[4.52], G185[4.55], I186[4.56], P189[4.59], D216[5.37], F217[5.38], F220[5.41]
	-13.3	L335[6.46], P339[6.50], I342[6.53], T343[6.54], T346[6.57], C353, L358[7.31], F365[7.38]
	-12.4	F226[5.47], F227[5.48], L230[5.51], I234[5.55], F331[6.42], C338[6.49], I342[6.53], I345[6.56], T346[6.57], L349[6.60]
	-12.0	L219[5.40], F220[5.41], L223[5.44], T228[5.49], A231[5.52], I232[5.53], V235[5.56], L349[6.60]
	-11.7	I61[1.39], I65[1.43], I66[1.44], I69[1.47], P109[2.59], L112[2.62], L113[2.63], M116[2.66], F117[2.67], P122, L123
5tvn_IC	-13.6	I61[1.39], I65[1.43], I66[1.44], I69[1.47], G70[1.48], T73[1.51], L77[1.55], Y399
	-13.4	Y91[2.41], M94[2.44], S95[2.45], V98[2.48], L102[2.52], F133[3.30], L134[3.31], L137[3.34], F138[3.35], F173[4.43], I176[4.46], W180[4.50], I184[4.54]
	-12.7	L60[1.38], M63[1.41], V64[1.42], M336[6.47], W367[7.40], I368[7.41], V371[7.44], V375[7.48], V379[7.52], L382[7.55]
	-13.5	I76[1.54], S80[1.58], M94[2.44], V98[2.48], L102[2.52], F106[2.56], L134[3.31], F138[3.35]
	-12.5	W144[3.41], V151[3.48], I155[3.52], Y166, N167, T171[4.41], I174[4.44], K175[4.45], V178[4.48], I182[4.52], T228[5.49], I232[5.53]
	-12.2	V151[3.48], Y154[3.51], I155[3.52], A231[5.52], I232[5.53], V235[5.56], T236[5.57], L239[5.60]
5-Hydroxytryptamine receptor 5HT2B, inactive, with cholesterol, Human 6drx		
6drx_EC	-16.4	W56[1.34], L60[1.38], I115[2.65], M360[7.33], E363[7.36], I364[7.37], W367[7.40], V371[7.44]
	-14.8	V178[4.48], I182[4.52], G185[4.55], I186[4.56], P189[4.59], K193[4.63], D216[5.37], F217[5.38], F220[5.41], G221[5.42]
	-12.6	L335[6.46], P339[6.50], I342[6.53], T343[6.54], T346[6.57], C353, L358[7.31], L361[7.34], F365[7.38]
	-12.4	L102[2.52], V126[3.23], P129[3.26], A130[3.27], F133[3.30], L134[3.31], F138[3.35], P191[4.61]
	-12.0	F227[5.48], L230[5.51], I234[5.55], F331[6.42], L335[6.46], I342[6.53], I345[6.56], L349[6.60], C350[6.61]
	-12.2	L219[5.40], F220[5.41], L223[5.44], F227[5.48], A231[5.52], I234[5.55], V235[5.56], I345[6.56], L349[6.60]
6drx_IC	-12.6	S80[1.58], Y91[2.41], M94[2.44], S95[2.45], L137[3.34], F173[4.43], I176[4.46], W180[4.50], I184[4.54]
	-12.3	W144[3.41], V151[3.48], Y154[3.51], I155[3.52], K158[3.55], T228[5.49], I232[5.53], T236[5.57], L239[5.60]
	-11.7	M63[1.41], P67[1.45], V371[7.44], V375[7.48], L378[7.51], L382[7.55], F391[8.54], I395[8.58]
	-12.6	L332[6.43], M336[6.47], I368[7.41], V371[7.44], V375[7.48], V379[7.52], L382[7.55], F383[7.56]
	-12.0	I76[1.54], L77[1.55], S80[1.58], L81[1.59], M94[2.44], V98[2.48], L101[2.51], L102[2.52], F138[3.35]
5-Hydroxytryptamine receptor 5HT2B, inactive, with cholesterol, Human 6dry		
6dry_EC	-15.3	K53, W56[1.34], L59[1.37], L60[1.38], I115[2.65], M336[6.47], E363[7.36], I364[7.37], W367[7.40], I368[7.41], V371[7.44]
	-13.6	I182[4.52], G185[4.55], I186[4.56], P189[4.59], D216[5.37], F217[5.38], F220[5.41], G221[5.42], A224[5.45]
	-13.1	L102[2.52], P129[3.26], A130[3.27], F133[3.30], L134[3.31], F138[3.35], P191[4.61], I192[4.62]
	-12.8	L335[6.46], P339[6.50], I342[6.53], T343[6.54], T346[6.57], C353, L358[7.31], F365[7.38]
	-12.3	F227[5.48], L230[5.51], I234[5.55], F331[6.42], L335[6.46], I342[6.53], I345[6.56], T346[6.57], L349[6.60]
6dry_IC	-14.5	W144[3.41], A148[3.45], V151[3.48], D152[3.49], I155[3.52], N167, T171[4.41], K175[4.45], V178[4.48], I182[4.52]
	-13.9	Y91[2.41], M94[2.44], S95[2.45], V98[2.48], L137[3.34], F138[3.35], F173[4.43], I176[4.46], W180[4.50], I184[4.54]
	-12.5	M63[1.41], P67[1.45], M336[6.47], V371[7.44], V375[7.48], L378[7.51], L382[7.55], F391[8.54], I395[8.58]
	-12.9	V151[3.48], Y154[3.51], I155[3.52], T228[5.49], A231[5.52], I232[5.53], V235[5.56], T236[5.57]
	-12.5	I76[1.54], L77[1.55], S80[1.58], L81[1.59], M94[2.44], V98[2.48], L101[2.51], L102[2.52], F138[3.35]
5-Hydroxytryptamine receptor 5HT2B, inactive, with cholesterol, Human 6drz		

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
6drz_EC	-14.3	W56[1.34], L60[1.38], M63[1.41], M336[6.47], I364[7.37], W367[7.40], I368[7.41], V371[7.44]
	-14.0	W144[3.41], I182[4.52], I186[4.56], P189[4.59], K193[4.63], D216[5.37], F217[5.38], F220[5.41], G221[5.42], A224[5.45], T228[5.49]
	-12.9	L332[6.43], L335[6.46], M336[6.47], C338[6.49], P339[6.50], I342[6.53], T343[6.54], L358[7.31], L361[7.34], F365[7.38]
	-12.7	V126[3.23], P129[3.26], A130[3.27], F133[3.30], L134[3.31], L137[3.34], I188[4.58], P191[4.61]
	-12.1	F227[5.48], L230[5.51], I234[5.55], F331[6.42], C338[6.49], I342[6.53], I345[6.56], T346[6.57], L349[6.60]
6drz_IC	-15.6	I61[1.39], I65[1.43], I66[1.44], I69[1.47], G70[1.48], Y394[8.57], I395[8.58], C397, Y399
	-14.3	W144[3.41], A148[3.45], V151[3.48], D152[3.49], I155[3.52], K175[4.45], V178[4.48], I182[4.52]
	-13.5	Y91[2.41], M94[2.44], S95[2.45], V98[2.48], L102[2.52], L134[3.31], F173[4.43], I176[4.46]
	-12.9	V151[3.48], Y154[3.51], I155[3.52], T228[5.49], A231[5.52], I232[5.53], V235[5.56], T236[5.57], L239[5.60]
	-12.2	M63[1.41], P67[1.45], L74[1.52], M336[6.47], V371[7.44], V375[7.48], L378[7.51], L382[7.55], F391[8.54], I395[8.58]

## 5-Hydroxytryptamine receptor 5HT2B, inactive, with cholesterol, Human 6ds0

6ds0_EC	-14.2	K53, W56[1.34], L59[1.37], L60[1.38], M63[1.41], I115[2.65], M360[7.33], E363[7.36], I364[7.37], W367[7.40], V371[7.44]
	-13.0	W144[3.41], I182[4.52], G185[4.55], I186[4.56], P189[4.59], K193[4.63], F217[5.38], F220[5.41], A224[5.45], T228[5.49], I232[5.53]
	-12.6	L102[2.52], V126[3.23], P129[3.26], A130[3.27], F133[3.30], L134[3.31], F138[3.35], P191[4.61]
	-12.2	L335[6.46], M336[6.47], P339[6.50], I342[6.53], T343[6.54], T346[6.57], C353, F365[7.38]
6ds0_IC	-14.1	I61[1.39], I65[1.43], I66[1.44], I69[1.47], G70[1.48], T73[1.51], P109[2.59], Y394[8.57], I395[8.58], C397, Y399
	-13.3	Y91[2.41], M94[2.44], S95[2.45], V98[2.48], F133[3.30], L137[3.34], F173[4.43], I176[4.46], W180[4.50], I184[4.54]
	-12.4	T73[1.51], I76[1.54], L77[1.55], S80[1.58], L81[1.59], L101[2.51], L105[2.55], F106[2.56]
	-12.3	I76[1.54], S80[1.58], M94[2.44], V98[2.48], L101[2.51], L102[2.52], L134[3.31], F138[3.35]
	-12.3	M63[1.41], P67[1.45], I368[7.41], V371[7.44], V375[7.48], L378[7.51], V379[7.52], L382[7.55]

## Adenosine A1 receptor

## Adenosine A1 receptor, inactive, Human 5n2s

5n2s_EC	-13.1	F185[5.43], F186[5.44], L190[5.48], L193[5.51], L248[6.49], I252[6.53], C255[6.56], I256[6.57], F259[6.60]
	-11.9	I13[1.36], V17[1.40], V24[1.47], A60[2.55], P64[2.59], I67[2.62], L68[2.63], I71[2.66]
	-12.2	L57[2.52], L61[2.56], L65[2.60], M82[3.27], V83[3.28], P86[3.31], L90[3.35], W132[4.50], F136[4.54]
5n2s_IC	-13.5	F185[5.43], L190[5.48], L193[5.51], V197[5.55], Y200[5.58], L201[5.59], F204[5.62], A237[6.38], F241[6.42], A244[6.45], L238[6.39], I252[6.53]
	-13.1	V53[2.48], L57[2.52], L61[2.56], P86[3.31], A125[4.43], I128[4.46], A129[4.47], W132[4.50], F136[4.54]

## Adenosine A1 receptor, inactive, residues renumbered, Human 5uen

5uen_EC	-13.4	L134[4.52], V137[4.55], T141[4.59], F144[4.62], G145[4.63], W146, F183[5.41], W188[5.46]
	-12.9	F185[5.43], F186[5.44], L190[5.48], L193[5.51], L194[5.52], V197[5.55], L248[6.49], I252[6.53], C255[6.56], I256[6.57], F259[6.60], C260[6.61]
	-12.2	V17[1.40], A20[1.43], L21[1.44], V24[1.47], G59[2.54], A60[2.55], P64[2.59], I67[2.62], L68[2.63], I71[2.66]
5uen_IC	-13.5	F185[5.43], L190[5.48], V197[5.55], F204[5.62], A237[6.38], L240[6.41], F241[6.42], A244[6.45], L248[6.49]
	-13.4	I15[1.38], I19[1.42], L238[6.39], L242[6.43], F275[7.40], M283[7.48], I286[7.51], V287[7.52], F290[7.55], R291[7.56]
	-12.8	G14[1.37], V17[1.40], L18[1.41], L21[1.44], W303[8.58], F307[8.62], R308[8.63], C309[8.64]
	-12.5	S50[2.45], V53[2.48], L61[2.56], A125[4.43], I128[4.46], A129[4.47], W132[4.50], F136[4.54]

## Adenosine A2A receptor

## A2A active state no cholesterol

## A2A adenosine receptor, active state, with agonist and G protein, Human 5g53

5g53_EC	-13.6	S6[1.32], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], L276[7.41], T279[7.44]
	-12.6	I10[1.36], L14[1.40], V18[1.44], P61[2.59], I64[2.62], T65[2.63], T68[2.66], F70

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.4	A243[6.45], L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], P266[7.31], L269[7.34]
	-12.4	I127[4.48], V130[4.51], L131[4.52], A134[4.55], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.3	L131[4.52], W143, Y179[5.40], F180[5.41], F183[5.44], A184[5.45], V188[5.49], L192[5.53]
	-12.1	V57[2.55], L58[2.56], F62[2.60], T65[2.63], F70, A72, G76[3.24], I80[3.28]
	-12.0	F182[5.43], L190[5.51], L191[5.52], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
5g53_IC	-13.5	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.5	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L58[2.56], F83[3.31], K122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-12.7	V229[6.31], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50]
	-12.7	V12[1.38], L241[6.43], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V282[7.47], V283[7.48], F286[7.51], I287[7.52]
A2A adenosine receptor, active state, with agonist and G protein, Human 6gdg		
6gdg_EC	-13.3	F182[5.43], L187[5.48], L191[5.52], L194[5.55], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
	-13.1	I127[4.48], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], G142[4.63], F180[5.41]
	-12.1	L131[4.52], W143, Y179[5.40], F180[5.41], F183[5.44], A184[5.45], V188[5.49], L192[5.53]
	-12.8	V178[5.39], Y179[5.40], F182[5.43], F183[5.44], L187[5.48], L191[5.52], C254[6.56], F257[6.59], F258[6.60]
	-12.1	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, L269[7.34], L272[7.37]
6gdg_IC	-13.4	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], K122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.1	V229[6.31], A232[6.34], K233[6.35], A236[6.38], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50]
	-12.7	L96[3.44], I100[3.48], I104[3.52], L115, V116, I124[4.45], F183[5.44], A184[5.45], V188[5.49]
A2A active intermediate state no cholesterol		
A2A adenosine receptor, active intermediate state, with agonist, Human 2ydo		
2ydo_EC	-14.4	V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], L276[7.41], T279[7.44]
	-12.7	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.5	A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], P266[7.31], W268[7.33], L269[7.34]
	-12.7	L14[1.40], V18[1.44], I21[1.47], P61[2.59], F62[2.60], I64[2.62], A65[2.63], F70
	-12.0	I127[4.48], V130[4.51], L131[4.52], A134[4.55], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.7	F93[3.41], L131[4.52], I135[4.56], Y179[5.40], F180[5.41], F183[5.44], A184[5.45], V188[5.49], P189[5.50]
2ydo_IC	-13.7	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], F133[4.54]
	-13.5	L194[5.55], Y197[5.58], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-12.9	F182[5.43], L187[5.48], L190[5.51], L194[5.55], Y197[5.58], A236[6.38], V239[6.41], G240[6.42], A243[6.45], L247[6.49]
A2A adenosine receptor, active intermediate state, with agonist, Human 2ydv		
2ydv_EC	-13.9	S6[1.32], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-12.5	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.5	A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, P266[7.31], L269[7.34]
	-12.2	I127[4.48], V130[4.51], L131[4.52], A134[4.55], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.9	L131[4.52], W143, Y179[5.40], F180[5.41], F183[5.44], A184[5.45], V188[5.49], L192[5.53]
2ydv_IC	-13.7	L194[5.55], Y197[5.58], A236[6.38], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.3	V25[1.51], C28[1.54], W29[1.55], W32[1.58], A50[2.48], I53[2.51], L54[2.52], V57[2.55], L58[2.56]
	-13.3	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], F133[4.54]
	-13.0	F182[5.43], L187[5.48], L190[5.51], L194[5.55], Y197[5.58], V239[6.41], A243[6.45], L247[6.49]
	-12.7	V18[1.44], I21[1.47], L22[1.48], V25[1.51], W29[1.55], V57[2.55], I302[8.57], H306[8.61]
A2A adenosine receptor, active intermediate state, with agonist, Human 3qak		
3qak_EC	-13.7	A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], H264, A265, L269[7.34]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
3qak_IC	-12.9	V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-12.5	F183[5.44], L187[5.48], L191[5.52], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-13.2	C28[1.54], V31[1.57], W32[1.58], V46[2.44], A50[2.48], I53[2.51], V57[2.55], L58[2.56]
	-12.8	Y43[2.41], S47[2.45], A50[2.48], L58[2.56], F83[3.31], L87[3.35], K122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-12.7	L194[5.55], Y197[5.58], A236[6.38], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-12.6	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], I124[4.45], I127[4.48], L131[4.52], I135[4.56], F180[5.41], A184[5.45]
A2A adenosine receptor, active intermediate state, with agonist, Human 4ug2		
4ug2_EC	-13.8	S6[1.32], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-12.8	L131[4.52], W143, Y179[5.40], F180[5.41], F183[5.44], A184[5.45], V188[5.49], L192[5.53]
	-12.7	G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], L269[7.34]
	-12.3	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
	-12.1	I127[4.48], V130[4.51], L131[4.52], A134[4.55], T138[4.59], L141[4.62], W143, F180[5.41]
4ug2_IC	-13.2	V25[1.51], C28[1.54], W29[1.55], W32[1.58], I53[2.51], L54[2.52], V57[2.55], L58[2.56]
	-13.1	Y197[5.58], F201[5.62], A236[6.38], V239[6.41], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-12.7	Y43[2.41], L54[2.52], L58[2.56], F83[3.31], L87[3.35], K122[4.43], W129[4.50], F133[4.54]
	-12.5	F183[5.44], L187[5.48], V188[5.49], L191[5.52], L192[5.53], G195[5.56], L198[5.59], R199[5.60]
	-12.4	L96[3.44], I100[3.48], R120[4.41], I124[4.45], F183[5.44], A184[5.45], V188[5.49], L192[5.53]
	-12.2	V12[1.38], A15[1.41], I16[1.42], L19[1.45], V282[7.47], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
	-12.8	L194[5.55], Y197[5.58], L198[5.59], F201[5.62], L202[5.63], R205[5.66], L247[6.49], I251[6.53]
A2A adenosine receptor, active intermediate state, with agonist, Human 4uhr		
4uhr_EC	-13.5	S6[1.32], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-13.1	F182[5.43], L187[5.48], L190[5.51], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.8	G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, L269[7.34]
	-12.6	L14[1.40], V18[1.44], I21[1.47], V57[2.55], P61[2.59], F62[2.60], A65[2.63], I80[3.28]
	-12.7	L96[3.44], L131[4.52], W143, F180[5.41], F183[5.44], A184[5.45], V188[5.49], L192[5.53]
	-11.8	I127[4.48], V130[4.51], L131[4.52], A134[4.55], T138[4.59], L141[4.62], W143, F180[5.41]
4uhr_IC	-13.7	T11[1.37], L14[1.40], A15[1.41], V18[1.44], L22[1.48], H306[8.61], V307[8.62], Q310[8.65]
	-13.4	Y197[5.58], A236[6.38], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.4	V25[1.51], C28[1.54], W29[1.55], W32[1.58], A50[2.48], I53[2.51], L54[2.52], V57[2.55], L58[2.56]
	-13.1	Y43[2.41], V46[2.44], A50[2.48], L54[2.52], F83[3.31], I125[4.46], W129[4.50], F133[4.54]
A2A adenosine receptor, active intermediate state, with agonist, Human 5wf5		
5wf5_EC	-13.9	A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], S263, H264, A265, L269[7.34]
	-13.5	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-12.3	L14[1.40], A17[1.43], V18[1.44], I21[1.47], L22[1.48], V57[2.55], P61[2.59], I64[2.62]
	-12.3	I127[4.48], V130[4.51], L131[4.52], A134[4.55], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.3	F182[5.43], L187[5.48], L190[5.51], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
5wf5_IC	-13.3	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I124[4.45], L131[4.52], I135[4.56], F180[5.41]
	-13.0	L194[5.55], Y197[5.58], A236[6.38], V239[6.41], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.0	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], K122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-12.7	V25[1.51], C28[1.54], W29[1.55], W32[1.58], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F83[3.31]
	-12.4	V12[1.38], I16[1.42], L19[1.45], L272[7.37], V275[7.40], T279[7.44], V282[7.47], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
A2A adenosine receptor, active intermediate state, with agonist, Human 5wf6		



PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Swf6_EC	-13.5	G5[1.31], S6[1.32], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-12.6	L14[1.40], A17[1.43], V18[1.44], I21[1.47], L22[1.48], G56[2.54], V57[2.55], I60[2.58], P61[2.59], I64[2.62], T65[2.63]
	-12.5	G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, P266[7.31], L269[7.34]
	-12.1	I127[4.48], V130[4.51], L131[4.52], A134[4.55], T138[4.59], L141[4.62], W143, F180[5.41]
	-11.9	F182[5.43], L187[5.48], L190[5.51], L191[5.52], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
Swf6_IC	-14.0	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.7	L194[5.55], Y197[5.58], A236[6.38], V239[6.41], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.7	C28[1.54], W29[1.55], W32[1.58], V46[2.44], A50[2.48], I53[2.51], A54[2.52], L58[2.56], L87[3.35], F133[4.54]
	-13.6	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L58[2.56], F83[3.31], L87[3.35], K122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.0	F182[5.43], L190[5.51], L194[5.55], Y197[5.58], A236[6.38], V239[6.41], G240[6.42], A243[6.45], L247[6.49], I251[6.53]

## A2A inactive state no cholesterol

## A2A adenosine receptor, inactive state, Human 3eml

3eml_EC	-14.2	L14[1.40], A17[1.43], I21[1.47], L22[1.48], I60[2.58], P61[2.59], I64[2.62], T65[2.63]
	-14.2	G5[1.31], S6[1.32], V8[1.34], Y9[1.35], V12[1.38], Y271[7.36], L272[7.37], V275[7.40]
	-12.8	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], L194[5.55], A243[6.45], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
	-12.9	G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], L269[7.34]
3eml_IC	-12.1	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
	-13.9	F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], L244[6.46], L247[6.49], I251[6.53]
	-13.4	Y43[2.41], V46[2.44], K122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.3	I237[6.39], L241[6.43], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55], R291[7.56]
-13.2	V46[2.44], S47[2.45], A50[2.48], A54[2.52], L58[2.56], F83[3.31], K122[4.43], I125[4.46], W129[4.50], F133[4.54]	

## A2A adenosine receptor, inactive state, Human 3pwh

3pwh_EC	-13.1	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-13.0	L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, L269[7.34]
	-12.3	H75[3.23], F79[3.27], A126[4.47], W129[4.50], V130[4.51], F133[4.54], L137[4.58], M140[4.61]
	-12.2	S7[1.33], I10[1.36], T11[1.37], L14[1.40], A15[1.41], V18[1.44], L19[1.45], L22[1.48]
3pwh_IC	-14.5	L194[5.55], Y197[5.58], L198[5.59], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50]
	-13.0	Y43[2.41], V46[2.44], A122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-12.6	L187[5.48], L194[5.55], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
	-13.6	C28[1.54], W32[1.58], V46[2.44], A50[2.48], I53[2.51], L54[2.52], V57[2.55], L58[2.56]
	-13.1	I21[1.47], L22[1.48], V25[1.51], L26[1.52], W29[1.55], V57[2.55], I302[8.57], I303[8.58], S305[8.60]
-12.5	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], V116, I124[4.45], A184[5.45], C185[5.46], V188[5.49]	
-12.4	Y103[3.51], V188[5.49], L191[5.52], L192[5.53], G195[5.56], V196[5.57], L198[5.59], R199[5.60]	

## A2A adenosine receptor, inactive state, Human 3rey

3rey_EC	-15.0	L14[1.40], A17[1.43], V18[1.44], L22[1.48], P61[2.59], F62[2.60], I64[2.62], T65[2.63]
	-13.2	F182[5.43], F183[5.44], L187[5.48], L194[5.55], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.8	H75[3.23], F79[3.27], A126[4.47], W129[4.50], V130[4.51], F133[4.54], L137[4.58], M140[4.61]
	-12.3	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
3rey_IC	-12.2	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, L269[7.34], L272[7.37], L276[7.41]
	-13.4	I21[1.47], L22[1.48], V25[1.51], L26[1.52], W29[1.55], V57[2.55], I302[8.57], I303[8.58]
	-13.4	V31[1.57], Y43[2.41], V46[2.44], A122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.0	L187[5.48], L194[5.55], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
	-12.9	I237[6.39], L241[6.43], V275[7.40], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55], R291[7.56]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.3	F93[3.41], L96[3.44], I100[3.48], I104[3.52], I124[4.45], I135[4.56], A184[5.45], C185[5.46]
A2A adenosine receptor, inactive state, Human 3rfm		
3rfm_EC	-14.6	L14[1.40], A17[1.43], I21[1.47], L22[1.48], G56[2.54], P61[2.59], I64[2.62], T65[2.63]
	-14.2	H75[3.23], A126[4.47], W129[4.50], V130[4.51], F133[4.54], L137[4.58], M140[4.61], L141[4.62]
	-13.2	F182[5.43], F183[5.44], L187[5.48], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
3rfm_EC	-14.6	I21[1.47], L22[1.48], V25[1.51], L26[1.52], W29[1.55], V57[2.55], I302[8.57], I303[8.58], R304[8.59], S305[8.60]
	-14.0	L194[5.55], Y197[5.58], L198[5.59], F201[5.62], A236[6.38], G240[6.42], L244[6.46], L247[6.49]
	-13.0	Y43[2.41], V46[2.44], S47[2.45], A122[4.43], I125[4.46], A126[4.47], W129[4.50], F133[4.54]
	-14.0	C28[1.54], V31[1.57], W32[1.58], V46[2.44], A50[2.48], L54[2.52], L58[2.56], F83[3.31], F133[4.54]
A2A adenosine receptor, inactive state, Human 3uza		
3uza_EC	-14.4	L14[1.40], A17[1.43], V18[1.44], I21[1.47], L22[1.48], P61[2.59], I64[2.62], T65[2.63]
	-14.2	Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V283[7.48]
	-13.3	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], L194[5.55], A243[6.45], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
	-13.2	H75[3.23], A126[4.47], W129[4.50], V130[4.51], F133[4.54], L137[4.58], M140[4.61], L141[4.62]
	-12.2	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], L269[7.34], L272[7.37], L276[7.41]
	-12.0	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
3uza_IC	-14.0	I21[1.47], L22[1.48], V25[1.51], L26[1.52], W29[1.55], V57[2.55], I302[8.57], I303[8.58], S305[8.60]
	-13.3	L194[5.55], Y197[5.58], L198[5.59], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50]
	-13.2	V31[1.57], Y43[2.41], V46[2.44], A122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.1	V25[1.51], C28[1.54], W29[1.55], W32[1.58], L33[1.59], I53[2.51], L54[2.52], V57[2.55], L58[2.56]
A2A adenosine receptor, inactive state, Human 3uzc		
3uzc_EC	-12.6	F183[5.44], L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-14.3	L14[1.40], A17[1.43], V18[1.44], I21[1.47], L22[1.48], P61[2.59], I64[2.62], T65[2.63]
	-12.3	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], S263, A265, P266[7.31], L269[7.34]
	-12.2	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.1	S47[2.45], A50[2.48], L54[2.52], L58[2.56], F79[3.27], F83[3.31], W129[4.50], F133[4.54]
3uzc_IC	-14.3	L241[6.43], L272[7.37], L276[7.41], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55], R291[7.56]
	-13.6	F183[5.44], A184[5.45], V188[5.49], L191[5.52], L192[5.53], G195[5.56], L198[5.59], R199[5.60]
	-13.5	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], L194[5.55], A236[6.38], G240[6.42], A243[6.45], L247[6.49]
	-13.5	I21[1.47], L22[1.48], V25[1.51], L26[1.52], W29[1.55], I302[8.57], I303[8.58], S305[8.60]
	-13.5	V31[1.57], Y43[2.41], V46[2.44], A122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-12.6	C28[1.54], W29[1.55], V31[1.57], W32[1.58], V46[2.44], A50[2.48], L54[2.52], V57[2.55], L58[2.56]
A2A adenosine receptor, inactive state, Human 3vg9		
3vg9_EC	-14.3	S6[1.32], V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-12.7	L14[1.40], A17[1.43], I21[1.47], V57[2.55], I60[2.58], P61[2.59], I64[2.62], T65[2.63]
	-12.3	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
	-12.1	A50[2.48], I53[2.51], A54[2.52], V57[2.55], L58[2.56], F79[3.27], F83[3.31], F133[4.54], M140[4.61]
3vg9_IC	-13.9	Y43[2.41], V46[2.44], A50[2.48], L58[2.56], F83[3.31], K122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.7	V25[1.51], C28[1.54], W29[1.55], W32[1.58], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F83[3.31], F133[4.54]
	-13.2	F93[3.41], L96[3.44], I100[3.48], R120[4.41], I124[4.45], I127[4.48], C128[4.49], L131[4.52], I135[4.56], F180[5.41], C185[5.46]
	-13.2	L190[5.51], L194[5.55], F201[5.62], A236[6.38], V239[6.41], G240[6.42], A243[6.45], L247[6.49], I251[6.53]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
A2A adenosine receptor, inactive state, Human 3vga		
3vga_EC	-12.7	I10[1.36], L14[1.40], I21[1.47], V25[1.51], G56[2.54], V57[2.55], P61[2.59], I64[2.62]
	-12.4	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L194[5.55], A243[6.45], L247[6.49], I251[6.53], C254[6.56], F258[6.60]
	-12.4	G240[6.42], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], L269[7.34]
	-12.1	L241[6.43], L244[6.46], C245[6.47], W268[7.33], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V283[7.48]
	-12.2	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
3vga_IC	-15.4	F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], L241[6.43], A243[6.45], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-14.0	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], A54[2.52], L58[2.56], F83[3.31], K122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.1	I237[6.39], L241[6.43], L244[6.46], V275[7.40], L276[7.41], T279[7.44], V283[7.48], I287[7.52], Y290[7.55]
	-13.1	V12[1.38], I16[1.42], V275[7.40], T279[7.44], V282[7.47], V283[7.48], F286[7.51], Y290[7.55]
	-12.9	C28[1.54], V31[1.57], W32[1.58], V46[2.44], A50[2.48], I53[2.51], V57[2.55], L58[2.56]
A2A adenosine receptor, inactive state, Human 5uig		
5uig_EC	-13.5	G5[1.31], S6[1.32], V8[1.34], Y9[1.35], V12[1.38], Y271[7.36], L272[7.37], V275[7.40]
	-12.7	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
5uig_IC	-14.8	N42[2.40], Y43[2.41], F44[2.42], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], F133[4.54]
	-14.4	L241[6.43], L244[6.46], L272[7.37], L276[7.41], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
	-13.4	V25[1.51], C28[1.54], W29[1.55], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
	-12.5	F93[3.41], L96[3.44], I100[3.48], I104[3.52], I124[4.45], I127[4.48], L131[4.52], I135[4.56], F180[5.41], C185[5.46]
A2A inactive state with cholesterol		
A2A adenosine receptor, inactive state, with cholesterol, Human 4eiy		
4eiy_EC	-14.3	A0, G5[1.31], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.4	F182[5.43], F183[5.44], L187[5.48], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.4	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], S263, H264, A265, L269[7.34]
	-12.3	I10[1.36], L14[1.40], V18[1.44], I21[1.47], P61[2.59], I64[2.62], T65[2.63], T68[2.66]
	-12.0	V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, A72, G76[3.24], I80[3.28]
4eiy_IC	-14.1	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], F133[4.54]
	-13.5	K233[6.35], A236[6.38], I237[6.39], G240[6.42], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.2	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], I135[4.56]
	-13.0	F182[5.43], L187[5.48], L194[5.55], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
	-12.7	V12[1.38], L241[6.43], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V283[7.48], F286[7.51], I287[7.52]
	-13.3	C28[1.54], V46[2.44], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
	-12.5	L96[3.44], I100[3.48], Y103[3.51], I104[3.52], A184[5.45], V188[5.49], P189[5.50], L192[5.53]
A2A adenosine receptor, inactive state, with cholesterol, Human 5iu4		
5iu4_EC	-14.4	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-14.3	I251[6.53], I252[6.54], F255[6.57], S263, H264, A265, P266[7.31], L269[7.34]
	-13.2	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.9	V57[2.55], L58[2.56], F62[2.60], T65[2.63], F70, A72, G76[3.24], C77[3.25], F79[3.27], I80[3.28]
5iu4_IC	-14.6	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, T117[4.38], R120[4.41], I124[4.45], P189[5.50]
	-13.9	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], F83[3.31], A122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.3	L187[5.48], L191[5.52], L194[5.55], F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
A2A adenosine receptor, inactive state, with cholesterol, Human 5iu7		
5iu7_EC	-14.1	A0, G5[1.31], V8[1.34], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-13.6	I251[6.53], I252[6.54], F255[6.57], C262, S263, H264, A265, L269[7.34]
	-12.9	F182[5.43], F183[5.44], L187[5.48], L191[5.52], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.0	I21[1.47], V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, I80[3.28]
	-12.7	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.5	V57[2.55], L58[2.56], F62[2.60], H75[3.23], G76[3.24], F79[3.27], I80[3.28], M140[4.61]
	-12.2	F93[3.41], L96[3.44], F180[5.41], A184[5.45], C185[5.46], V188[5.49], P189[5.50], L192[5.53]
Siu7_IC	-14.8	C28[1.54], V31[1.57], W32[1.58], V46[2.44], A50[2.48], I125[4.46], W129[4.50], V130[4.51], F133[4.54]
	-13.4	F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.2	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, T117[4.38], I124[4.45], I135[4.56]
	-12.7	L14[1.40], A17[1.43], V18[1.44], I21[1.47], L22[1.48], G56[2.54], H306[8.61], V307[8.62]
	-12.7	L96[3.44], I100[3.48], Y103[3.51], I104[3.52], I108[3.56], L115, V188[5.49], L192[5.53]
	-12.6	I237[6.39], L241[6.43], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V283[7.48], I287[7.52], R291[7.56]
A2A adenosine receptor, inactive state, with cholesterol, Human Siu8		
Siu8_EC	-14.8	L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], C262, S263, A265, L269[7.34]
	-14.7	A0, P2[1.28], G5[1.31], V8[1.34], Y9[1.35], V12[1.38], I16[1.42], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-13.4	F182[5.43], L187[5.48], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
Siu8_IC	-14.8	C28[1.54], V31[1.57], W32[1.58], V46[2.44], A50[2.48], I125[4.46], W129[4.50], V130[4.51], F133[4.54]
	-13.6	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], I135[4.56], C185[5.46]
	-13.2	F182[5.43], L187[5.48], L191[5.52], L194[5.55], F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
	-13.0	V25[1.51], C28[1.54], W29[1.55], W32[1.58], A50[2.48], I53[2.51], L54[2.52], L58[2.56], F83[3.31]
A2A adenosine receptor, inactive state, with cholesterol, Human Siua		
Siua_EC	-14.4	A0, G5[1.31], V8[1.34], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-14.2	I251[6.53], I252[6.54], F255[6.57], C262, S263, H264, A265, L269[7.34]
	-13.1	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.7	V57[2.55], L58[2.56], F62[2.60], F70, A72, G76[3.24], C77[3.25], F79[3.27], I80[3.28]
	-12.1	L14[1.40], I21[1.47], V57[2.55], P61[2.59], I64[2.62], T65[2.63], T68[2.66], F70
	-12.1	F79[3.27], A126[4.47], W129[4.50], V130[4.51], F133[4.54], L137[4.58], M140[4.61], L141[4.62]
Siua_IC	-13.9	F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.6	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], L58[2.56], F83[3.31], A122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.4	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], I135[4.56], C185[5.46]
	-13.3	C28[1.54], W29[1.55], W32[1.58], V46[2.44], A50[2.48], L54[2.52], L58[2.56], F83[3.31], F133[4.54]
	-12.3	I237[6.39], L241[6.43], L244[6.46], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V283[7.48], I287[7.52], R291[7.56]
A2A adenosine receptor, inactive state, with cholesterol, Human Siub		
Siub_EC	-14.8	I251[6.53], I252[6.54], F255[6.57], T256[6.58], S263, H264, A265, L269[7.34]
	-14.7	A0, G5[1.31], V8[1.34], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.2	F182[5.43], F183[5.44], L187[5.48], L191[5.52], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.4	I21[1.47], V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, I80[3.28]
	-12.7	L14[1.40], V18[1.44], I21[1.47], P61[2.59], I64[2.62], T65[2.63], T68[2.66], F70
Siub_IC	-14.9	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45]
	-14.0	C28[1.54], W29[1.55], V31[1.57], W32[1.58], V46[2.44], I125[4.46], W129[4.50], V130[4.51], F133[4.54]
	-13.9	F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.4	V25[1.51], C28[1.54], W29[1.55], W32[1.58], I53[2.51], L54[2.52], V57[2.55], L58[2.56]
	-12.7	I237[6.39], L241[6.43], L244[6.46], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V283[7.48], I287[7.52], R291[7.56]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.7	L96[3.44], I100[3.48], Y103[3.51], I104[3.52], I108[3.56], L115, V188[5.49], L192[5.53], V196[5.57]
A2A adenosine receptor, inactive state, with cholesterol, Human 5jtb		
5jtb_EC	-14.3	A0, G5[1.31], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.5	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-13.3	V57[2.55], L58[2.56], F62[2.60], T65[2.63], F70, A72, A73[3.21], G76[3.24], C77[3.25], I80[3.28]
	-12.5	L14[1.40], A17[1.43], V18[1.44], I21[1.47], V57[2.55], P61[2.59], I64[2.62], T65[2.63], T68[2.66], F70
5jtb_IC	-13.3	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L58[2.56], F79[3.27], F83[3.31], I125[4.46], W129[4.50], F133[4.54]
	-13.0	F182[5.43], L187[5.48], L190[5.51], L194[5.55], Y197[5.58], F201[5.62], K233[6.35], A236[6.38], V239[6.41], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-12.6	V25[1.51], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
	-12.4	F93[3.41], L96[3.44], I100[3.48], I104[3.52], I124[4.45], L131[4.52], I135[4.56], A184[5.45], C185[5.46]
	-12.3	V12[1.38], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V283[7.48], F286[7.51], Y290[7.55]
A2A adenosine receptor, inactive state, with cholesterol, Human 5k2a		
5k2a_EC	-15.1	A0, P2[1.28], G5[1.31], V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-13.4	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L194[5.55], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.9	L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], A265, P266[7.31], L269[7.34]
	-12.7	I10[1.36], L14[1.40], A17[1.43], V57[2.55], P61[2.59], I64[2.62], T65[2.63], T68[2.66], F70
	-12.6	V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, A72, A73[3.21], G76[3.24], C77[3.25], I80[3.28]
	-12.5	A73[3.21], H75[3.23], G76[3.24], F79[3.27], V130[4.51], F133[4.54], L137[4.58], M140[4.61]
	-12.4	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
5k2a_IC	-14.4	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], F133[4.54]
	-13.6	F93[3.41], L96[3.44], A97[3.45], I100[3.48], L115, V116, R120[4.41], I124[4.45], C185[5.46], P189[5.50]
	-13.0	V25[1.51], C28[1.54], W29[1.55], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
	-12.8	F182[5.43], L187[5.48], L191[5.52], L194[5.55], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
	-12.5	V12[1.38], L241[6.43], L272[7.37], V275[7.40], T279[7.44], V282[7.47], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
	-12.5	L241[6.43], L244[6.46], C245[6.47], L272[7.37], L276[7.41], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
A2A adenosine receptor, inactive state, with cholesterol, Human 5k2b		
5k2b_EC	-15.0	A0, P1[1.27], P2[1.28], G5[1.31], V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-13.9	V57[2.55], L58[2.56], F62[2.60], T65[2.63], F70, A72, A73[3.21], G76[3.24], C77[3.25], I80[3.28]
	-13.8	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], A243[6.45], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-13.0	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], C262, S263, A265, L269[7.34]
	-12.3	H75[3.23], F79[3.27], W129[4.50], V130[4.51], F133[4.54], L137[4.58], M140[4.61], L141[4.62]
5k2b_IC	-14.3	Y43[2.41], F44[2.42], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], F133[4.54]
	-14.0	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], P189[5.50]
	-13.2	V25[1.51], C28[1.54], W29[1.55], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
	-13.1	L187[5.48], L191[5.52], L194[5.55], F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
A2A adenosine receptor, inactive state, with cholesterol, Human 5k2c		
5k2c_EC	-14.2	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.5	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-13.2	F62[2.60], T65[2.63], F70, A72, G76[3.24], C77[3.25], F79[3.27], I80[3.28]
	-12.5	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, P266[7.31], L269[7.34]
	-13.6	L14[1.40], A17[1.43], V18[1.44], I21[1.47], P61[2.59], I64[2.62], T65[2.63], F70

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
5k2c_IC	-13.9	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.5	F201[5.62], K233[6.35], A236[6.38], I237[6.39], G240[6.42], L244[6.46], L247[6.49], P248[6.50], I251[6.53]
	-13.3	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], I135[4.56]
	-13.0	C28[1.54], W32[1.58], V46[2.44], A50[2.48], I53[2.51], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
A2A adenosine receptor, inactive state, with cholesterol, Human 5k2d		
5k2d_EC	-14.5	A0, G5[1.31], V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.4	F182[5.43], F183[5.44], L187[5.48], L194[5.55], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
	-12.6	V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, A72, G76[3.24], I80[3.28]
	-12.6	L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, L269[7.34]
	-12.5	L14[1.40], A17[1.43], V18[1.44], I21[1.47], P61[2.59], I64[2.62], T65[2.63], T68[2.66], F70
	-12.3	H75[3.23], W129[4.50], V130[4.51], F133[4.54], A134[4.55], L137[4.58], M140[4.61], L141[4.62]
	-12.2	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
5k2d_IC	-14.1	F93[3.41], L96[3.44], A97[3.45], I100[3.48], L115, V116, T117[4.38], R120[4.41], I124[4.45], P189[5.50]
	-14.0	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.4	L241[6.43], L272[7.37], V275[7.40], L276[7.41], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
	-12.8	L187[5.48], L191[5.52], L194[5.55], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
	-13.4	C28[1.54], W32[1.58], V46[2.44], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
A2A adenosine receptor, inactive state, with cholesterol, Human 5mzj		
5mzj_EC	-14.2	I251[6.53], I252[6.54], F255[6.57], S263, H264, A265, P266[7.31], L269[7.34]
	-14.0	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.0	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.8	F79[3.27], A126[4.47], W129[4.50], V130[4.51], F133[4.54], L137[4.58], M140[4.61], L141[4.62]
	-12.6	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.3	F93[3.41], L96[3.44], F180[5.41], A184[5.45], C185[5.46], V188[5.49], P189[5.50], L192[5.53]
	-12.1	I21[1.47], V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, I80[3.28]
5mzj_IC	-14.0	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-13.9	C28[1.54], W29[1.55], W32[1.58], V46[2.44], A50[2.48], L54[2.52], L58[2.56], F83[3.31], F133[4.54]
	-13.7	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], F83[3.31], A122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-12.8	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], V116, I124[4.45], I135[4.56]
	-12.5	L241[6.43], L244[6.46], C245[6.47], L272[7.37], L276[7.41], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
-12.2	V12[1.38], L272[7.37], V275[7.40], T279[7.44], V282[7.47], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]	
A2A adenosine receptor, inactive state, with cholesterol, Human 5mzp		
5mzp_EC	-14.1	A0, G5[1.31], V8[1.34], Y9[1.35], V12[1.38], I16[1.42], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.0	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.7	I251[6.53], I252[6.54], F255[6.57], C262, S263, H264, A265, L269[7.34]
	-12.5	F93[3.41], L96[3.44], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], F180[5.41]
	-12.4	V18[1.44], I21[1.47], V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, I80[3.28]
5mzp_IC	-13.7	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-13.6	C28[1.54], W29[1.55], V31[1.57], W32[1.58], V46[2.44], A50[2.48], W129[4.50], F133[4.54]
	-13.3	C28[1.54], W29[1.55], W32[1.58], V46[2.44], A50[2.48], L54[2.52], L58[2.56], F83[3.31], F133[4.54]
	-13.1	Q89[3.37], F93[3.41], L96[3.44], A97[3.45], I100[3.48], L115, V116, R120[4.41], I124[4.45], A184[5.45], C185[5.46], P189[5.50]
-12.3	V12[1.38], L272[7.37], V275[7.40], T279[7.44], V282[7.47], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]	

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
A2A adenosine receptor, inactive state, with cholesterol, Human 5n2r		
5n2r_EC	-14.0	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-13.1	F182[5.43], F183[5.44], L187[5.48], L191[5.52], A243[6.45], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.4	L14[1.40], A17[1.43], V18[1.44], I21[1.47], L22[1.48], V57[2.55], P61[2.59], I64[2.62]
	-12.3	L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, P266[7.31], L269[7.34]
	-12.9	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.6	F93[3.41], L96[3.44], F180[5.41], A184[5.45], C185[5.46], V188[5.49], P189[5.50], L192[5.53]
5n2r_IC	-13.9	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49]
	-13.8	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], L58[2.56], F83[3.31], A122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.9	C28[1.54], V31[1.57], W32[1.58], V46[2.44], A50[2.48], L54[2.52], V57[2.55], L58[2.56]
	-12.8	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, I124[4.45], L131[4.52], I135[4.56], A184[5.45], C185[5.46]
	-12.6	V25[1.51], C28[1.54], W29[1.55], W32[1.58], L33[1.59], I53[2.51], L54[2.52], V57[2.55], L58[2.56]
A2A adenosine receptor, inactive state, with cholesterol, Human 5nlx		
5nlx_EC	-13.6	G14[1.40], V17[1.43], Y18[1.44], V21[1.47], W373, Y376, L377, V380
	-13.5	F191[5.52], L196[5.57], L200[5.61], L352, I356, C359, F360, F363, C364
	-13.4	L349, P353, I357, F360, C367, S368, A370, L374
	-12.9	F102[3.50], L140[4.61], A143, I144, T147, L150, W152, F189[5.50]
	-12.5	L23[1.49], V27[1.53], I30[1.56], L31[1.57], V66[2.64], P70, I73[3.21], T74[3.22]
5nlx_IC	-13.9	Y52[2.50], V55[2.53], S56[2.54], A59[2.57], L63[2.61], L67[2.65], F92[3.40], G127[4.48], A131[4.52], I134[4.55], W138[4.59], F142[4.63]
	-13.6	F191[5.52], F192[5.53], L196[5.57], L199[5.60], L203[5.64], A341, G345, A348, L352
	-13.6	C37, V40[2.38], W41[2.39], V55[2.53], A59[2.57], L63[2.61], V66[2.64], L67[2.65]
A2A adenosine receptor, inactive state, with cholesterol, Human 5nm2		
5nm2_EC	-14.3	A0, G5[1.31], V8[1.34], Y9[1.35], V12[1.38], I16[1.42], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-14.1	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], C262, S263, A265, L269[7.34]
	-13.0	F182[5.43], L187[5.48], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61], C262
	-12.6	F93[3.41], L96[3.44], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], F180[5.41]
	-12.3	I21[1.47], V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, I80[3.28]
5nm2_IC	-13.8	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-13.4	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], L58[2.56], F83[3.31], A122[4.43], I125[4.46], W129[4.50]
	-13.2	F93[3.41], L96[3.44], A97[3.45], I100[3.48], L115, V116, I124[4.45], C185[5.46]
	-13.5	C28[1.54], W32[1.58], V46[2.44], A50[2.48], I53[2.51], L54[2.52], V57[2.55], L58[2.56]
A2A adenosine receptor, inactive state, with cholesterol, Human 5nm4		
5nm4_EC	-14.2	P353, I356, I357, F360, C367, S368, H369, A370, L374
	-13.7	G14[1.40], V17[1.43], Y18[1.44], V21[1.47], I25[1.51], W373, Y376, L377, V380, T384
	-13.0	F192[5.53], L196[5.57], L200[5.61], L352, I356, C359, F360, F363, C364
	-12.5	F102[3.50], L105[3.53], L140[4.61], A143, I144, T147, L150, F189[5.50]
5nm4_IC	-13.9	F191[5.52], F192[5.53], L196[5.57], L199[5.60], L203[5.64], K338, A341, G345, A348, L352
	-13.8	Y52[2.50], V55[2.53], S56[2.54], A59[2.57], L63[2.61], L67[2.65], F92[3.40], A131[4.52], I134[4.55], W138[4.59], F142[4.63]
	-13.6	C37, W41[2.39], V55[2.53], A59[2.57], I62[2.60], L63[2.61], V66[2.64], L67[2.65]
A2A adenosine receptor, inactive state, with cholesterol, Human Solg		
Solg_EC	-14.4	A0, G5[1.31], V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-13.9	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], C262, S263, A265, P266[7.31], L269[7.34]
	-12.9	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.6	F93[3.41], L96[3.44], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], F180[5.41]
Solg_IC	-14.3	C28[1.54], W29[1.55], V31[1.57], W32[1.58], V46[2.44], A50[2.48], I125[4.46], W129[4.50], V130[4.51], F133[4.54]
	-13.8	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-13.5	F44[2.42], F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], C128[4.49], L131[4.52], I135[4.56]
A2A adenosine receptor, inactive state, with cholesterol, Human 50lh		
Solh_EC	-13.8	I251[6.53], I252[6.54], F255[6.57], C262, S263, H264, A265, P266[7.31]
	-13.7	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], I16[1.42], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.2	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.2	F93[3.41], L96[3.44], L131[4.52], I135[4.56], T138[4.59], L141[4.62], F180[5.41], P189[5.50]
Solh_IC	-13.6	Y43[2.41], V46[2.44], S47[2.45], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.4	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
A2A adenosine receptor, inactive state, with cholesterol, Human Solo		
Solo_EC	-13.0	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-13.0	F79[3.27], A126[4.47], W129[4.50], V130[4.51], F133[4.54], L137[4.58], M140[4.61], L141[4.62]
	-12.8	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], A243[6.45], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.4	L14[1.40], A17[1.43], V18[1.44], I21[1.47], L22[1.48], G56[2.54], V57[2.55], P61[2.59], I64[2.62]
	-12.2	A50[2.48], L54[2.52], L58[2.56], F62[2.60], F79[3.27], F83[3.31], W129[4.50], F133[4.54]
	-12.3	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, P266[7.31], L269[7.34]
Solo_IC	-14.0	Y43[2.41], V46[2.44], S47[2.45], A122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-13.9	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-12.9	C28[1.54], V31[1.57], W32[1.58], V46[2.44], A50[2.48], L54[2.52], V57[2.55], L58[2.56]
	-12.5	V12[1.38], I16[1.42], I237[6.39], L241[6.43], V275[7.40], T279[7.44], V283[7.48], F286[7.51], I287[7.52], R291[7.56]
A2A adenosine receptor, inactive state, with cholesterol, Human Solv		
Solv_EC	-14.7	I251[6.53], I252[6.54], F255[6.57], C262, S263, H264, A265, L269[7.34]
	-13.9	L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-13.6	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], I16[1.42], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
Solv_IC	-13.7	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], L58[2.56], F83[3.31], A122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.7	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L194[5.55], A236[6.38], G240[6.42], A243[6.45], L247[6.49]
	-13.5	V25[1.51], C28[1.54], W29[1.55], W32[1.58], V46[2.44], A50[2.48], L54[2.52], L58[2.56], F83[3.31], F133[4.54]
	-12.8	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], I124[4.45], L131[4.52], I135[4.56], A184[5.45], C185[5.46]
A2A adenosine receptor, inactive state, with cholesterol, Human Solz		
Solz_EC	-13.9	G5[1.31], V8[1.34], Y9[1.35], V12[1.38], I16[1.42], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.8	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.5	L244[6.46], P248[6.50], I252[6.54], F255[6.57], C262, A265, L269[7.34], L276[7.41]
	-12.5	F93[3.41], L96[3.44], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], F180[5.41]
	-12.4	I21[1.47], V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, I80[3.28]
	-12.1	L244[6.46], L247[6.49], P248[6.50], I251[6.53], I252[6.54], F255[6.57], A265, P266[7.31], L269[7.34]
Solz_IC	-13.5	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], L58[2.56], F83[3.31], I125[4.46], W129[4.50], F133[4.54]



PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-13.5	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49]
	-13.5	F44[2.42], F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], I135[4.56]
	-13.4	C28[1.54], W29[1.55], W32[1.58], V46[2.44], A50[2.48], L54[2.52], L58[2.56], F83[3.31], F133[4.54]
	-12.8	L241[6.43], L244[6.46], C245[6.47], P248[6.50], L272[7.37], L276[7.41], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
A2A adenosine receptor, inactive state, with cholesterol, Human 5om1		
5om1_EC	-14.5	I251[6.53], I252[6.54], F255[6.57], T256[6.58], C262, S263, H264, A265, L269[7.34]
	-13.9	A0, G5[1.31], V8[1.34], Y9[1.35], V12[1.38], I16[1.42], W268[7.33], Y271[7.36], L272[7.37], V275[7.40]
	-13.6	L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.6	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
	-12.2	V18[1.44], I21[1.47], V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, I80[3.28]
5om1_IC	-14.0	L187[5.48], L191[5.52], L194[5.55], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
	-13.5	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], F83[3.31], I125[4.46], W129[4.50], F133[4.54]
	-13.2	C28[1.54], V31[1.57], W32[1.58], V46[2.44], A50[2.48], L54[2.52], V57[2.55], L58[2.56]
A2A adenosine receptor, inactive state, with cholesterol, Human 5om4		
5om4_EC	-14.7	I251[6.53], I252[6.54], F255[6.57], C262, S263, H264, A265, L269[7.34]
	-14.0	A0, G5[1.31], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.2	F182[5.43], F183[5.44], L187[5.48], L191[5.52], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
5om4_IC	-14.1	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-13.7	Y43[2.41], V46[2.44], S47[2.45], A50[2.48], L54[2.52], L58[2.56], F83[3.31], A122[4.43], I125[4.46], W129[4.50], F133[4.54]
	-13.3	V25[1.51], C28[1.54], W29[1.55], W32[1.58], V46[2.44], A50[2.48], L54[2.52], L58[2.56], F133[4.54]
	-13.0	Q89[3.37], F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], I135[4.56], A184[5.45], C185[5.46], P189[5.50]
	-12.5	L241[6.43], L244[6.46], C245[6.47], L272[7.37], L276[7.41], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
A2A adenosine receptor, inactive state, with cholesterol, Human 5uvi		
5uvi_EC	-14.3	P2[1.28], G5[1.31], V8[1.34], Y9[1.35], V12[1.38], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.4	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], A243[6.45], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60]
	-12.5	L244[6.46], P248[6.50], I251[6.53], I252[6.54], F255[6.57], S263, A265, L269[7.34]
5uvi_IC	-14.2	Y43[2.41], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50], F133[4.54]
	-13.3	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], F201[5.62], K233[6.35], A236[6.38], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-13.2	F93[3.41], L96[3.44], A97[3.45], I100[3.48], I104[3.52], L115, V116, I124[4.45], I135[4.56], A184[5.45], C185[5.46], P189[5.50]
	-13.8	C28[1.54], W32[1.58], V46[2.44], A50[2.48], I53[2.51], A54[2.52], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
	-12.4	V12[1.38], L272[7.37], V275[7.40], T279[7.44], V282[7.47], V283[7.48], F286[7.51], I287[7.52]
A2A adenosine receptor, inactive state, with cholesterol, Human 5vra		
5vra_EC	-14.6	A0, P2[1.28], G5[1.31], V8[1.34], Y9[1.35], V12[1.38], I16[1.42], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-13.5	I251[6.53], I252[6.54], F255[6.57], S263, H264, A265, P266[7.31], L269[7.34]
	-13.3	F182[5.43], F183[5.44], L187[5.48], L190[5.51], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.9	I10[1.36], L14[1.40], V18[1.44], P61[2.59], I64[2.62], T65[2.63], T68[2.66], F70
	-13.3	V57[2.55], L58[2.56], P61[2.59], F62[2.60], T65[2.63], F70, A72, I80[3.28]
	-12.6	F93[3.41], L131[4.52], A134[4.55], I135[4.56], T138[4.59], L141[4.62], W143, F180[5.41]
5vra_IC	-14.8	Y43[2.41], F44[2.42], V46[2.44], S47[2.45], K122[4.43], I125[4.46], A126[4.47], W129[4.50]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-13.5	F182[5.43], L187[5.48], L190[5.51], L191[5.52], L194[5.55], Y197[5.58], F201[5.62], A236[6.38], V239[6.41], G240[6.42], A243[6.45], L247[6.49], I251[6.53]
	-13.3	F93[3.41], L96[3.44], A97[3.45], I100[3.48], L115, V116, I124[4.45], I135[4.56], A184[5.45], C185[5.46], P189[5.50]
	-12.8	V25[1.51], C28[1.54], A50[2.48], I53[2.51], A54[2.52], V57[2.55], L58[2.56], F79[3.27], F83[3.31], F133[4.54]
	-12.2	V8[1.34], V12[1.38], I16[1.42], L272[7.37], V275[7.40], T279[7.44], V282[7.47], F286[7.51], Y290[7.55]
	-12.8	L241[6.43], L244[6.46], C245[6.47], P248[6.50], L276[7.41], V283[7.48], F286[7.51], I287[7.52]
A2A adenosine receptor, inactive state, with cholesterol, Human 6aqf		
6aqf_EC	-14.5	A0, P2[1.28], G5[1.31], V8[1.34], Y9[1.35], V12[1.38], L267[7.32], W268[7.33], Y271[7.36], L272[7.37], V275[7.40], T279[7.44]
	-14.0	I251[6.53], I252[6.54], F255[6.57], C262, S263, H264, A265, P266[7.31], L269[7.34]
	-13.1	F182[5.43], F183[5.44], L187[5.48], L191[5.52], L247[6.49], I251[6.53], C254[6.56], F255[6.57], F258[6.60], C259[6.61]
	-12.2	F93[3.41], L96[3.44], L131[4.52], I135[4.56], T138[4.59], L141[4.62], F180[5.41], P189[5.50], L192[5.53]
6aqf_IC	-14.7	C28[1.54], V31[1.57], W32[1.58], V46[2.44], K122[4.43], I125[4.46], A126[4.47], W129[4.50], V130[4.51], F133[4.54]
	-12.7	L187[5.48], L191[5.52], L194[5.55], K233[6.35], A236[6.38], I237[6.39], G240[6.42], A243[6.45], L247[6.49]
	-12.3	V12[1.38], L272[7.37], V275[7.40], T279[7.44], V283[7.48], F286[7.51], I287[7.52], Y290[7.55]
Adrenergic Beta-1 receptor		
Beta-1 adrenergic, inactive, Turkey 2vt4		
2vt4_EC	-16.1	V172[4.56], P176[4.60], W181, W182, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-14.0	S45[1.36], M48[1.39], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63]
	-13.6	L47[1.38], M48[1.39], L50[1.41], V51[1.42], L54[1.45], V102[2.65], W323[7.33], V326[7.36], A327[7.37], W330[7.40]
	-12.3	Y217[5.48], L221[5.52], L304[6.49], L308[6.53], I311[6.56], V312[6.57], F315[6.60], N316[6.61], L319
2vt4_IC	-13.7	L78[2.41], T81[2.44], S82[2.45], C85[2.48], K159[4.43], I162[4.46], C163[4.47], W166[4.50]
	-12.8	I224[5.55], A227[5.58], L228[5.59], G293[6.38], G297[6.42], T300[6.45], L301[6.46], L304[6.49], P305[6.50], L308[6.53]
	-12.5	A49[1.40], V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L356[8.57], L357[8.58]
	-12.0	V60[1.51], I63[1.54], A64[1.55], G67[1.58], L88[2.51], V89[2.52], L92[2.55], L93[2.56]
	-12.5	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I161[4.45], I168[4.52], V172[4.56], I214[5.45], P219[5.50]
Beta-1 adrenergic, inactive, partial agonist, Turkey 2y00		
2y00_EC	-15.1	V172[4.56], P176[4.60], W181, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-14.6	W40[1.31], M48[1.39], V51[1.42], L54[1.45], V102[2.65], A327[7.37], W330[7.40], L331[7.41], A334[7.44], A337[7.47], M338[7.48], I341[7.51]
	-14.3	S45[1.36], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66]
	-12.6	Y217[5.48], L220[5.51], L221[5.52], L304[6.49], L308[6.53], I311[6.56], V312[6.57], F315[6.60], L319
	-12.4	L301[6.46], P305[6.50], L319, V320, P321[7.31], L324[7.34], F328[7.38], L331[7.41]
2y00_IC	-13.6	L78[2.41], T81[2.44], S82[2.45], C85[2.48], K159[4.43], I162[4.46], C163[4.47], W166[4.50], A170[4.54], F174[4.58]
	-13.0	I224[5.55], A227[5.58], L228[5.59], Y231[5.62], G297[6.42], T300[6.45], L301[6.46], L304[6.49], L308[6.53]
	-12.7	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], A64[1.55], L356[8.57], L357[8.58]
	-12.5	L50[1.41], L53[1.44], L54[1.45], A57[1.48], L61[1.52], I341[7.51], C344[7.54], R350[8.51], F353[8.54], L357[8.58]
	-12.4	L54[1.45], I294[6.39], V298[6.43], A334[7.44], M338[7.48], I341[7.51], I342[7.52], R345[7.55]
Beta-1 adrenergic, inactive, partial agonist, Turkey 2y01		
2y01_EC	-14.5	W40[1.31], V51[1.42], L54[1.45], V102[2.65], A327[7.37], W330[7.40], L331[7.41], A334[7.44], A337[7.47], M338[7.48], I341[7.51]
	-14.2	S45[1.36], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
2y01_IC	-13.8	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L92[2.55], L356[8.57], L357[8.58]
	-12.9	M223[5.54], I224[5.55], A227[5.58], L228[5.59], G293[6.38], I294[6.39], M296[6.41], G297[6.42], T300[6.45], L301[6.46], L304[6.49], L308[6.53]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.8	L78[2.41], T81[2.44], S82[2.45], C85[2.48], V89[2.52], L93[2.56], L116[3.27], L120[3.31], K159[4.43], I162[4.46], C163[4.47], W166[4.50], F174[4.58]
	-12.4	I294[6.39], V298[6.43], L301[6.46], F328[7.38], L331[7.41], M338[7.48], I341[7.51], I342[7.52], R345[7.55]
	-12.5	L46[1.37], L50[1.41], L53[1.44], L54[1.45], A57[1.48], G58[1.49], L61[1.52], C344[7.54], F353[8.54], L357[8.58]
	-12.2	Y217[5.48], L221[5.52], I224[5.55], F225[5.56], L228[5.59], R229[5.60], L308[6.53], I311[6.56]
	-11.9	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I161[4.45], V165[4.49], I168[4.52], I214[5.45], I218[5.49], I222[5.53]
Beta-1 adrenergic, inactive, agonist, Turkey 2y02		
2y02_EC	-14.3	P176[4.60], W181, W182, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-14.2	S45[1.36], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66]
	-14.2	W40[1.31], M44[1.35], M48[1.39], V51[1.42], L54[1.45], V102[2.65], A327[7.37], W330[7.40], L331[7.41], A334[7.44], A337[7.47], M338[7.48], I341[7.51]
	-12.6	Y217[5.48], L220[5.51], L221[5.52], L304[6.49], L308[6.53], I311[6.56], V312[6.57], F315[6.60], N316[6.61], L319
	-12.6	L301[6.46], L304[6.49], P305[6.50], L308[6.53], L319, V320, P321[7.31], L324[7.34], F328[7.38]
2y02_IC	-13.6	V52[1.43], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L92[2.55], L356[8.57], L357[8.58]
	-12.9	L78[2.41], T81[2.44], S82[2.45], C85[2.48], V89[2.52], L93[2.56], L116[3.27], L120[3.31], K159[4.43], I162[4.46], C163[4.47], F174[4.58]
	-12.8	I224[5.55], G293[6.38], I294[6.39], G297[6.42], T300[6.45], L301[6.46], L304[6.49], L308[6.53]
	-12.8	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I168[4.52], V172[4.56], I214[5.45], P219[5.50]
Beta-1 adrenergic, inactive, agonist, Turkey 2y03		
2y03_EC	-15.7	P176[4.60], W181, W182, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-14.4	W40[1.31], M44[1.35], M48[1.39], V51[1.42], L54[1.45], V102[2.65], A327[7.37], W330[7.40], L331[7.41], A334[7.44], A337[7.47], M338[7.48], I341[7.51]
	-14.1	S45[1.36], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
	-12.4	Y217[5.48], L221[5.52], L308[6.53], I311[6.56], V312[6.57], F315[6.60], N316[6.61], L319
	-12.3	A206[5.37], I209[5.40], A210[5.41], I213[5.44], I214[5.45], I218[5.49], V314[6.59], F315[6.60]
	-12.0	L301[6.46], L304[6.49], L308[6.53], L319, V320, P321[7.31], L324[7.34], F328[7.38]
2y03_IC	-13.9	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L356[8.57], L357[8.58]
	-13.6	L78[2.41], T81[2.44], S82[2.45], C85[2.48], V89[2.52], L116[3.27], L120[3.31], K159[4.43], I162[4.46], C163[4.47], W166[4.50], F174[4.58]
	-12.9	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I168[4.52], V172[4.56], I214[5.45], P219[5.50]
	-12.3	I224[5.55], L228[5.59], G297[6.42], T300[6.45], L301[6.46], L304[6.49], P305[6.50], L308[6.53]
	-12.0	A49[1.40], L50[1.41], L53[1.44], L54[1.45], A57[1.48], L61[1.52], F353[8.54], K354[8.55], L357[8.58]
Beta-1 adrenergic, inactive, partial agonist, Turkey 2y04		
2y04_EC	-14.4	W40[1.31], M48[1.39], V51[1.42], L54[1.45], V102[2.65], A327[7.37], W330[7.40], L331[7.41], A334[7.44], A337[7.47], M338[7.48], I341[7.51]
	-14.3	S45[1.36], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
	-13.1	I168[4.52], L171[4.55], V172[4.56], W181, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-12.5	Y217[5.48], L220[5.51], L221[5.52], L304[6.49], L308[6.53], I311[6.56], V312[6.57], F315[6.60]
2y04_IC	-13.6	V52[1.43], V56[1.47], A57[1.48], V60[1.51], L92[2.55], L356[8.57], L357[8.58], A358[8.59]
	-13.4	M223[5.54], I224[5.55], A227[5.58], L228[5.59], G293[6.38], M296[6.41], G297[6.42], T300[6.45], L301[6.46], L304[6.49], L308[6.53]
	-13.1	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I161[4.45], I168[4.52], V172[4.56], I214[5.45], P219[5.50]
	-12.9	T81[2.44], S82[2.45], C85[2.48], L123[3.34], I162[4.46], C163[4.47], W166[4.50], A170[4.54], F174[4.58]
	-12.4	L46[1.37], A49[1.40], L50[1.41], L53[1.44], L54[1.45], A57[1.48], G58[1.49], L61[1.52], F353[8.54], L357[8.58]
	-12.1	I294[6.39], V298[6.43], L301[6.46], L331[7.41], M338[7.48], I341[7.51], I342[7.52], R345[7.55]
Beta-1 adrenergic, inactive, antagonist, Turkey 2ycw		
2ycw_EC	-14.2	M44[1.35], L47[1.38], M48[1.39], V51[1.42], L54[1.45], V102[2.65], W323[7.33], V326[7.36], A327[7.37], W330[7.40], A334[7.44], M338[7.48]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-14.1	E41[1.32], S45[1.36], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
	-12.6	L301[6.46], P305[6.50], V309[6.54], L319, V320, P321[7.31], L324[7.34], F328[7.38]
2ycw_IC	-13.3	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L123[3.34], I162[4.46], C163[4.47], W166[4.50], A170[4.54], F174[4.58]
	-12.7	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L356[8.57], L357[8.58]
	-12.2	V51[1.42], I294[6.39], V298[6.43], A334[7.44], M338[7.48], I341[7.51], I342[7.52], R345[7.55]
	-12.8	I224[5.55], G293[6.38], I294[6.39], G297[6.42], T300[6.45], L301[6.46], L304[6.49], L308[6.53]
	-12.3	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I161[4.45], V165[4.49], I168[4.52], V172[4.56], I214[5.45], P219[5.50]
Beta-1 adrenergic, inactive, antagonist, Turkey 2ycx		
2ycx_EC	-13.7	T300[6.45], L301[6.46], L304[6.49], P305[6.50], L308[6.53], V309[6.54], L319, V320, P321[7.31], L324[7.34], F328[7.38]
	-13.3	W40[1.31], M44[1.35], M48[1.39], V51[1.42], A334[7.44], A337[7.47], M338[7.48], I341[7.51]
	-12.9	S45[1.36], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
	-12.7	V172[4.56], P176[4.60], W181, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-12.7	Y217[5.48], L221[5.52], L304[6.49], L308[6.53], I311[6.56], V312[6.57], F315[6.60], L319
2ycx_IC	-13.8	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L123[3.34], K159[4.43], I162[4.46], C163[4.47], W166[4.50], A170[4.54], F174[4.58]
	-13.7	I224[5.55], G293[6.38], M296[6.41], G297[6.42], T300[6.45], L301[6.46], L304[6.49], L308[6.53]
	-12.8	I63[1.54], A64[1.55], G67[1.58], L88[2.51], V89[2.52], L92[2.55], L93[2.56], L120[3.31]
	-12.6	V160[4.44], C163[4.47], T164[4.48], A167[4.51], A170[4.54], L171[4.55], F174[4.58], L175[4.59]
	-11.9	I294[6.39], V298[6.43], L301[6.46], F328[7.38], L331[7.41], M338[7.48], I342[7.52], R345[7.55]
Beta-1 adrenergic, inactive, antagonist, Turkey 2ycy		
2ycy_EC	-12.3	M44[1.35], V298[6.43], L301[6.46], W323[7.33], A327[7.37], F328[7.38], L331[7.41], M338[7.48]
	-14.9	P176[4.60], W181, W182, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
2ycy_IC	-14.3	I224[5.55], A227[5.58], L228[5.59], Y231[5.62], G297[6.42], T300[6.45], L301[6.46], L304[6.49]
	-13.6	M44[1.35], L47[1.38], I294[6.39], V298[6.43], L331[7.41], M338[7.48], I341[7.51], I342[7.52], R345[7.55]
	-13.4	V52[1.43], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L92[2.55], L356[8.57], L357[8.58]
	-13.3	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L116[3.27], L120[3.31], L123[3.34], I162[4.46], C163[4.47], W166[4.50], F174[4.58]
Beta-1 adrenergic, inactive, antagonist, Turkey 2ycz		
2ycz_EC	-15.6	P176[4.60], W181, W182, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-14.7	V51[1.42], L54[1.45], W323[7.33], V326[7.36], A327[7.37], W330[7.40], A334[7.44], A337[7.47], M338[7.48], I341[7.51]
	-14.1	E41[1.32], S45[1.36], M48[1.39], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66]
	-12.1	L301[6.46], P305[6.50], L308[6.53], V309[6.54], V312[6.57], L319, V320, L324[7.34], F328[7.38]
2ycz_IC	-14.5	M223[5.54], I224[5.55], A227[5.58], L228[5.59], Y231[5.62], G293[6.38], M296[6.41], G297[6.42], T300[6.45], L301[6.46], L304[6.49]
	-13.9	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L120[3.31], L123[3.34], I162[4.46], C163[4.47], W166[4.50], F174[4.58]
	-13.0	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L92[2.55], L356[8.57], L357[8.58]
	-12.5	V51[1.42], I294[6.39], V298[6.43], A334[7.44], M338[7.48], I341[7.51], I342[7.52], R345[7.55]
Beta-1 adrenergic, inactive, agonist, Turkey 3zpq		
3zpq_EC	-14.0	I168[4.52], L171[4.55], V172[4.56], P176[4.60], W181, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-13.8	M44[1.35], L47[1.38], M48[1.39], V51[1.42], L54[1.45], V102[2.65], V326[7.36], A327[7.37], W330[7.40], A334[7.44], A337[7.47], M338[7.48]
	-13.3	S45[1.36], A49[1.40], V52[1.43], L53[1.44], V56[1.47], P96[2.59], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
	-12.8	Y217[5.48], L220[5.51], L221[5.52], L308[6.53], I311[6.56], V312[6.57], F315[6.60], L319
3zpq_IC	-13.9	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L92[2.55], P96[2.59], L356[8.57], L357[8.58], A358[8.59]
	-13.2	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L123[3.34], I162[4.46], C163[4.47], W166[4.50], A170[4.54], F174[4.58]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.3	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I161[4.45], V165[4.49], I168[4.52], V172[4.56], I214[5.45]
Beta-1 adrenergic, inactive, agonist, Turkey 3zpr		
3zpr_EC	-16.0	V172[4.56], P176[4.60], W181, W182, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-13.7	W40[1.31], M44[1.35], L47[1.38], M48[1.39], V51[1.42], L54[1.45], V102[2.65], V326[7.36], A327[7.37], W330[7.40], L331[7.41], A334[7.44], A337[7.47], M338[7.48]
	-13.3	S45[1.36], M48[1.39], A49[1.40], V52[1.43], L53[1.44], V56[1.47], P96[2.59], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
	-12.7	Y217[5.48], L220[5.51], L221[5.52], L304[6.49], L308[6.53], I311[6.56], V312[6.57], F315[6.60], N316[6.61], L319
3zpr_IC	-14.0	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L92[2.55], P96[2.59], L356[8.57], L357[8.58]
	-13.3	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L123[3.34], K159[4.43], I162[4.46], C163[4.47], W166[4.50], A170[4.54], F174[4.58]
	-12.4	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I161[4.45], V165[4.49], I168[4.52], V172[4.56], I214[5.45]
Beta-1 adrenergic, inactive, agonist, Turkey 4ami		
4ami_EC	-17.2	P176[4.60], W181, W182, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-13.6	E41[1.32], S45[1.36], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66]
	-13.6	W40[1.31], M44[1.35], L47[1.38], M48[1.39], V51[1.42], L54[1.45], V102[2.65], A327[7.37], W330[7.40], A334[7.44], A337[7.47], M338[7.48], I341[7.51]
	-13.2	L301[6.46], P305[6.50], L308[6.53], V309[6.54], V312[6.57], L319, V320, P321[7.31], L324[7.34], F328[7.38]
4ami_IC	-13.6	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], L356[8.57], L357[8.58]
	-13.1	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L123[3.34], I162[4.46], C163[4.47], W166[4.50], A170[4.54], F174[4.58]
	-12.9	I224[5.55], A227[5.58], L228[5.59], G293[6.38], I294[6.39], M296[6.41], G297[6.42], T300[6.45], L304[6.49], L308[6.53]
	-12.4	L46[1.37], A49[1.40], L50[1.41], L53[1.44], L54[1.45], A57[1.48], G58[1.49], L61[1.52], F353[8.54], L357[8.58]
	-12.1	V134[3.45], I137[3.48], I161[4.45], T164[4.48], V165[4.49], I168[4.52], I214[5.45], I218[5.49]
Beta-1 adrenergic, inactive, agonist, Turkey 4amj		
4amj_EC	-17.0	V172[4.56], P176[4.60], W181, W182, N204[5.35], A206[5.37], Y207[5.38], A210[5.41], I214[5.45]
	-14.0	W40[1.31], M44[1.35], L47[1.38], M48[1.39], V51[1.42], V102[2.65], W330[7.40], A334[7.44], A337[7.47], M338[7.48]
	-13.2	S45[1.36], A49[1.40], V52[1.43], V56[1.47], L92[2.55], P96[2.59], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
	-12.6	Y217[5.48], L220[5.51], L221[5.52], L304[6.49], L308[6.53], I311[6.56], V312[6.57], F315[6.60], N316[6.61], L319
4amj_IC	-13.7	V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L92[2.55], L356[8.57], L357[8.58], A358[8.59]
	-13.1	I224[5.55], A227[5.58], G293[6.38], M296[6.41], G297[6.42], T300[6.45], L301[6.46], L304[6.49], L308[6.53]
	-13.0	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L116[3.27], L120[3.31], K159[4.43], I162[4.46], W166[4.50], F174[4.58]
	-12.9	L46[1.37], A49[1.40], L50[1.41], L53[1.44], L54[1.45], A57[1.48], G58[1.49], L61[1.52], C344[7.54], F353[8.54], L357[8.58]
	-12.8	E130[3.41], C133[3.44], V134[3.45], I137[3.48], I161[4.45], I168[4.52], V172[4.56], I214[5.45]
	-12.4	I294[6.39], V298[6.43], L301[6.46], F328[7.38], L331[7.41], M338[7.48], I341[7.51], I342[7.52], R345[7.55]
Beta-1 adrenergic, inactive, Turkey 4gpo		
4gpo_EC	-14.4	L47[1.38], L50[1.41], V51[1.42], L54[1.45], W323[7.33], V326[7.36], A327[7.37], W330[7.40]
	-13.1	S45[1.36], A49[1.40], V52[1.43], L53[1.44], V56[1.47], P96[2.59], A99[2.62], T100[2.63], V103[2.66]
	-12.9	L301[6.46], P305[6.50], L308[6.53], V309[6.54], V312[6.57], L319, V320, L324[7.34], F328[7.38]
	-12.4	V89[2.52], L116[3.27], L120[3.31], L123[3.34], W166[4.50], A170[4.54], F174[4.58], M178[4.62]
	-12.0	Y217[5.48], L221[5.52], I224[5.55], L308[6.53], I311[6.56], V312[6.57], F315[6.60], N316[6.61]
4gpo_IC	-13.1	L78[2.41], T81[2.44], S82[2.45], C85[2.48], L93[2.56], L120[3.31], K159[4.43], I162[4.46], C163[4.47], W166[4.50]
	-12.9	L220[5.51], I224[5.55], A227[5.58], L228[5.59], Y231[5.62], G293[6.38], M296[6.41], G297[6.42], T300[6.45], L304[6.49], L308[6.53]
	-12.7	C133[3.44], V134[3.45], I137[3.48], M153, I161[4.45], I213[5.44], I214[5.45], I218[5.49]
	-12.3	L47[1.38], L50[1.41], V51[1.42], L54[1.45], I294[6.39], A334[7.44], M338[7.48], I341[7.51], I342[7.52]
	-12.0	A49[1.40], V52[1.43], L53[1.44], V56[1.47], A57[1.48], V60[1.51], L61[1.52], A64[1.55], L356[8.57]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
<b>Beta-1 adrenergic, inactive, inverse agonist, Turkey 5a8e</b>		
5a8e_EC	-15.9	S45[1.36], M48[1.39], A49[1.40], V52[1.43], L53[1.44], V56[1.47], A99[2.62], T100[2.63], V103[2.66], R104[2.67]
	-14.1	W40[1.31], M44[1.35], L47[1.38], M48[1.39], V51[1.42], V102[2.65], W323[7.33], V326[7.36], A327[7.37], W330[7.40], A334[7.44]
	-14.0	Q38[1.29], E41[1.32], A42[1.33], S45[1.36], L46[1.37], A49[1.40], L53[1.44], R104[2.67]
	-13.7	I168[4.52], V172[4.56], P176[4.60], W181, N204[5.35], A206[5.37], Y207[5.38], I214[5.45]
	-12.3	Y217[5.48], L220[5.51], L221[5.52], L304[6.49], L308[6.53], I311[6.56], V312[6.57], F315[6.60]
	-12.0	L304[6.49], P305[6.50], L308[6.53], V309[6.54], V312[6.57], L319, L324[7.34], F328[7.38]
5a8e_IC	-15.2	L78[2.41], F79[2.42], T81[2.44], S82[2.45], C85[2.48], K159[4.43], I162[4.46], C163[4.47], W166[4.50]
	-12.7	L47[1.38], V51[1.42], L54[1.45], W330[7.40], A334[7.44], M338[7.48], I341[7.51], R345[7.55]
<b>Adrenergic beta-2 receptor</b>		
<b>Beta-2 adrenergic receptor, active state, Human 3p0g</b>		
3p0g_EC	-14.9	M156[4.48], V160[4.52], L163[4.55], P168[4.60], W173, Y174, N196[5.35], Y199[5.38], A202[5.41], V206[5.45]
	-13.8	G280[6.42], T283[6.45], L284[6.46], L287[6.49], P288[6.50], I291[6.53], V292[6.54], V295[6.57], L302, I303, V307[7.34], L311[7.38]
	-13.4	S41[1.40], V44[1.43], L45[1.44], V48[1.47], L84[2.55], P88[2.59], A91[2.62], A92[2.63], L95[2.66], M96[2.67]
	-13.1	W32[1.31], M36[1.35], V39[1.38], M40[1.39], I43[1.42], I94[2.65], I309[7.36], L310[7.37], W313[7.40], V317[7.44], F321[7.48]
	-13.0	I201[5.40], I205[5.44], Y209[5.48], L212[5.51], V213[5.52], V216[5.55], I294[6.56], V297[6.59], I298[6.60]
	-12.9	L155[4.47], W158[4.50], I159[4.51], G162[4.54], F166[4.58], L167[4.59], Q170[4.62], M171[4.63]
	-12.2	E30[1.29], V33[1.32], V34[1.33], G37[1.36], I38[1.37], S41[1.40], L45[1.44], L95[2.66]
3p0g_IC	-14.6	V216[5.55], Y219[5.58], S220[5.59], F223[5.62], M279[6.41], T283[6.45], L287[6.49], I291[6.53]
	-14.1	Y70[2.41], C77[2.48], V81[2.52], A85[2.56], F108[3.27], I112[3.31], L115[3.34], I154[4.46], W158[4.50], F166[4.58]
	-14.0	V52[1.51], I55[1.54], T56[1.55], A59[1.58], L80[2.51], V81[2.52], L84[2.55], A85[2.56], W105[3.24]
	-13.7	Y70[2.41], L115[3.34], R151[4.43], I154[4.46], L155[4.47], W158[4.50], G162[4.54], F166[4.58]
	-13.4	C125[3.44], V126[3.45], V129[3.48], D130[3.49], L145, I153[4.45], M156[4.48], V160[4.52], V206[5.45], V210[5.49], I214[5.53]
<b>Beta-2 adrenergic receptor, active state, Human 3sn6</b>		
3sn6_EC	-22.8	M156[4.48], V160[4.52], L163[4.55], T164[4.56], P168[4.60], W173, Y174, N196[5.35], A198[5.37], Y199[5.38], A202[5.41], V206[5.45]
	-21.6	T283[6.45], L284[6.46], L287[6.49], P288[6.50], I291[6.53], V292[6.54], V295[6.57], L302, I303
	-21.5	Y209[5.48], L212[5.51], V213[5.52], V216[5.55], I291[6.53], I294[6.56], V295[6.57], I298[6.60], Q299[6.61], L302
	-21.0	L284[6.46], P288[6.50], V292[6.54], L302, I303, R304[7.31], V307[7.34], L311[7.38], I314[7.41]
	-20.6	V44[1.43], L45[1.44], V48[1.47], P88[2.59], A92[2.63], L95[2.66], T96[2.67], F101
	-21.7	Q197[5.36], I201[5.40], I205[5.44], Y209[5.48], V213[5.52], I294[6.56], V297[6.59], I298[6.60]
3sn6_IC	-23.0	V216[5.55], Y219[5.58], S220[5.59], F223[5.62], L275[6.37], M279[6.41], T283[6.45], L287[6.49]
	-22.3	Y70[2.41], T73[2.44], S74[2.45], C77[2.48], L115[3.34], R151[4.43], I154[4.46], L155[4.47], W158[4.50], F166[4.58]
	-21.8	Y209[5.48], L212[5.51], V216[5.55], L272[6.34], L275[6.37], G276[6.38], M279[6.41], G280[6.42], T283[6.45], L287[6.49], I291[6.53]
	-21.6	F71[2.42], E122[3.41], C125[3.44], V126[3.45], V129[3.48], I153[4.45], I205[5.44], V206[5.45], V210[5.49], I214[5.53]
	-22.1	V129[3.48], Y132[3.51], F133[3.52], I205[5.44], V210[5.49], V213[5.52], I214[5.53], F217[5.56], V218[5.57]
	-21.1	I55[1.54], T73[2.44], C77[2.48], L80[2.51], V81[2.52], L84[2.55], A85[2.56], F108[3.27], I112[3.31]
<b>Beta-2 adrenergic receptor, active state, Human, residues renumbered 6mxt</b>		
6mxt_EC	-16.4	L163[4.55], P168[4.60], W173, Y174, N196[5.35], A198[5.37], Y199[5.38], A202[5.41]
	-14.3	T283[6.45], L284[6.46], L287[6.49], P288[6.50], I291[6.53], V292[6.54], L302, I303, R304[7.31], V307[7.34], L311[7.38]
	-13.9	Y209[5.48], L212[5.51], V213[5.52], I291[6.53], I294[6.56], V295[6.57], I298[6.60], Q299[6.61], L302
	-12.9	L155[4.47], W158[4.50], I159[4.51], G162[4.54], F166[4.58], L167[4.59], Q170[4.62], M171[4.63]
	-12.8	S41[1.40], V44[1.43], L45[1.44], V48[1.47], L84[2.55], P88[2.59], A92[2.63], L95[2.66], T96[2.67]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
6mxt_IC	-14.0	Y70[2.41], R151[4.43], I154[4.46], L155[4.47], W158[4.50], I159[4.51], G162[4.54], F166[4.58]
	-13.5	V39[1.38], L42[1.41], I43[1.42], A46[1.45], L310[7.37], W313[7.40], I314[7.41], V317[7.44], G320[7.47], F321[7.48], L324[7.51]
	-13.1	E122[3.41], C125[3.44], V126[3.45], V129[3.48], I153[4.45], I205[5.44], V206[5.45], V210[5.49], P211[5.50], I214[5.53]
	-13.1	V52[1.51], I55[1.54], T56[1.55], L80[2.51], V81[2.52], L84[2.55], A85[2.56], F108[3.27], I112[3.31]
	-15.7	Y70[2.41], T73[2.44], S74[2.45], C77[2.48], V81[2.52], F108[3.27], I154[4.46], W158[4.50]
	-12.5	G276[6.38], I277[6.39], M279[6.41], G280[6.42], T283[6.45], L284[6.46], L287[6.49], I291[6.53]
	-12.4	V44[1.43], L45[1.44], V48[1.47], F49[1.48], V52[1.51], L53[1.52], T56[1.55], L84[2.55], P88[2.59], L339[8.57]
Beta-2 adrenergic receptor, inactive state, with cholesterol, Human 2rh1		
2rh1_EC	-13.1	L155[4.47], W158[4.50], I159[4.51], G162[4.54], L163[4.55], F166[4.58], L167[4.59], Q170[4.62], M171[4.63]
	-13.0	S41[1.40], V44[1.43], V48[1.47], L84[2.55], P88[2.59], A91[2.62], A92[2.63], L95[2.66], M96[2.67]
	-12.8	W32[1.31], M36[1.35], M40[1.39], I43[1.42], I94[2.65], I309[7.36], L310[7.37], W313[7.40], V317[7.44]
2rh1_IC	-14.5	Y70[2.41], C77[2.48], V81[2.52], F108[3.27], I112[3.31], L115[3.34], R151[4.43], I154[4.46], W158[4.50], F166[4.58]
	-14.3	V44[1.43], L45[1.44], V48[1.47], F49[1.48], V52[1.51], L53[1.52], L84[2.55], L339[8.57], L340[8.58], C341[8.59]
	-13.4	I43[1.42], A46[1.45], F49[1.48], G50[1.49], L53[1.52], V317[7.44], G320[7.47], P323[7.50], L324[7.51], F336[8.54], L340[8.58]
	-13.4	I55[1.54], A59[1.58], T73[2.44], C77[2.48], L80[2.51], V81[2.52], L84[2.55], A85[2.56]
	-12.4	I277[6.39], T281[6.43], L284[6.46], C285[6.47], P288[6.50], I314[7.41], F321[7.48], L324[7.51], I325[7.52], C327[7.54], R328[7.55]
Beta-2 adrenergic receptor, inactive state, with cholesterol, Human 3d4s		
3d4s_EC	-17.1	T164[4.56], P168[4.60], W173, Y174, N196[5.35], A198[5.37], Y199[5.38], A202[5.41], V206[5.45]
	-13.8	Y209[5.48], L212[5.51], V213[5.52], L287[6.49], I291[6.53], I294[6.56], V295[6.57], I298[6.60], Q299[6.61]
	-12.8	M36[1.35], V39[1.38], M40[1.39], I43[1.42], I94[2.65], E306[7.33], I309[7.36], L310[7.37], W313[7.40], V317[7.44]
	-12.7	S41[1.40], V44[1.43], L45[1.44], V48[1.47], L84[2.55], P88[2.59], A91[2.62], A92[2.63], L95[2.66]
	-12.5	W32[1.31], M36[1.35], V39[1.38], I43[1.42], V317[7.44], G320[7.47], F321[7.48], L324[7.51]
	-12.3	L284[6.46], L287[6.49], P288[6.50], I291[6.53], V292[6.54], V295[6.57], L302, I303
	-12.7	T281[6.43], L284[6.46], C285[6.47], P288[6.50], R304[7.31], V307[7.34], L310[7.37], L311[7.38], I314[7.41]
3d4s_IC	-14.5	Y70[2.41], T73[2.44], S74[2.45], C77[2.48], V81[2.52], F108[3.27], I112[3.31], L115[3.34], R151[4.43], I154[4.46], L155[4.47], W158[4.50], F166[4.58]
	-13.3	V44[1.43], L45[1.44], V48[1.47], F49[1.48], V52[1.51], L53[1.52], T56[1.55], L339[8.57]
	-13.0	I43[1.42], A46[1.45], F49[1.48], G50[1.49], L53[1.52], V317[7.44], G320[7.47], P323[7.50], L324[7.51], F336[8.54], Q337[8.55], L340[8.58], L342
	-13.0	I55[1.54], A59[1.58], T73[2.44], C77[2.48], L80[2.51], V81[2.52], L84[2.55], A85[2.56]
Beta-2 adrenergic receptor, inactive state, with cholesterol, Human 3ny8		
3ny8_EC	-13.8	T281[6.43], L284[6.46], C285[6.47], P288[6.50], R304[7.31], V307[7.34], L310[7.37], L311[7.38], I314[7.41]
	-13.7	T164[4.56], P168[4.60], W173, N196[5.35], A198[5.37], Y199[5.38], A202[5.41], V206[5.45]
	-13.7	T283[6.45], L284[6.46], L287[6.49], P288[6.50], V292[6.54], R304[7.31], V307[7.34], L311[7.38]
	-13.4	F108[3.27], W158[4.50], I159[4.51], G162[4.54], L163[4.55], F166[4.58], L167[4.59], Q170[4.62]
	-13.2	M36[1.35], M40[1.39], I94[2.65], I309[7.36], L310[7.37], W313[7.40], I314[7.41], V317[7.44], F321[7.48]
	-13.0	S41[1.40], V44[1.43], L45[1.44], V48[1.47], P88[2.59], A91[2.62], A92[2.63], L95[2.66]
	-12.4	Y209[5.48], L212[5.51], V213[5.52], L287[6.49], I291[6.53], I294[6.56], V295[6.57], I298[6.60]
3ny8_IC	-14.6	Y70[2.41], T73[2.44], S74[2.45], C77[2.48], V81[2.52], F108[3.27], I112[3.31], L115[3.34], A150[4.42], R151[4.43], I154[4.46], L155[4.47], W158[4.50], F166[4.58]
	-14.5	L45[1.44], V48[1.47], F49[1.48], V52[1.51], L53[1.52], T56[1.55], L84[2.55], L339[8.57], L340[8.58], C341[8.59]
	-13.3	I43[1.42], A46[1.45], F49[1.48], G50[1.49], L53[1.52], V317[7.44], G320[7.47], P323[7.50], L324[7.51], F336[8.54], L340[8.58], L342
	-13.1	I55[1.54], A59[1.58], T73[2.44], C77[2.48], L80[2.51], V81[2.52], L84[2.55], A85[2.56]
	-12.8	F223[5.62], K273[6.35], G276[6.38], I277[6.39], G280[6.42], T283[6.45], L284[6.46], L287[6.49], I291[6.53]
	-12.8	I277[6.39], T281[6.43], L284[6.46], I314[7.41], F321[7.48], L324[7.51], I325[7.52], R328[7.55]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.6	Y209[5.48], V213[5.52], V216[5.55], F217[5.56], S220[5.59], Q224[5.63], L287[6.49], I291[6.53]
Beta-2 adrenergic receptor, inactive state, with cholesterol, Human 3ny9		
3ny9_EC	-15.4	T164[4.56], P168[4.60], W173, Y174, N196[5.35], A198[5.37], Y199[5.38], A202[5.41], V206[5.45]
	-13.9	M36[1.35], V39[1.38], M40[1.39], I43[1.42], I94[2.65], E306[7.33], I309[7.36], L310[7.37], W313[7.40], V317[7.44], F321[7.48]
	-13.6	L284[6.46], L287[6.49], P288[6.50], I291[6.53], V292[6.54], L302, I303, R304[7.31], V307[7.34], L311[7.38]
	-13.4	S41[1.40], V44[1.43], L45[1.44], V48[1.47], L84[2.55], P88[2.59], A91[2.62], A92[2.63], L95[2.66], M96[2.67]
	-13.1	F108[3.27], W158[4.50], I159[4.51], G162[4.54], L163[4.55], F166[4.58], L167[4.59], Q170[4.62]
3ny9_IC	-14.1	Y209[5.48], V213[5.52], V216[5.55], F217[5.56], S220[5.59], L287[6.49], I291[6.53], I294[6.56]
	-13.6	Y70[2.41], T73[2.44], S74[2.45], C77[2.48], V81[2.52], F108[3.27], I112[3.31], L115[3.34], I154[4.46], L155[4.47], W158[4.50], F166[4.58]
	-12.9	L45[1.44], V48[1.47], F49[1.48], V52[1.51], L53[1.52], L84[2.55], L339[8.57], L340[8.58]
	-12.6	I55[1.54], A59[1.58], C77[2.48], L80[2.51], V81[2.52], A85[2.56], W105[3.24], I112[3.31]
	-12.5	I277[6.39], T281[6.43], L284[6.46], C285[6.47], I314[7.41], F321[7.48], L324[7.51], I325[7.52]
Beta-2 adrenergic receptor, inactive state, with cholesterol, Human 3nya		
3nya_EC	-17.2	T164[4.56], P168[4.60], W173, Y174, N196[5.35], A198[5.37], Y199[5.38], A202[5.41], V206[5.45]
	-14.1	M36[1.35], V39[1.38], M40[1.39], I43[1.42], I94[2.65], E306[7.33], I309[7.36], L310[7.37], W313[7.40], V317[7.44]
	-13.4	L284[6.46], L287[6.49], P288[6.50], I291[6.53], V292[6.54], V295[6.57], L302, I303, V307[7.34]
	-13.3	F104[3.23], F108[3.27], W158[4.50], I159[4.51], G162[4.54], F166[4.58], Q170[4.62], M171[4.63]
	-13.1	Y209[5.48], L212[5.51], L287[6.49], I291[6.53], I294[6.56], V295[6.57], I298[6.60], Q299[6.61]
	-12.9	S41[1.40], V44[1.43], L45[1.44], V48[1.47], L84[2.55], P88[2.59], A91[2.62], A92[2.63], L95[2.66]
3nya_IC	-13.4	V39[1.38], I43[1.42], A46[1.45], F49[1.48], L53[1.52], V317[7.44], G320[7.47], F321[7.48], P323[7.50], L324[7.51], C327[7.54], F336[8.54], L340[8.58]
	-13.4	T73[2.44], S74[2.45], C77[2.48], F108[3.27], L115[3.34], R151[4.43], I154[4.46], L155[4.47], W158[4.50], F166[4.58]
	-12.9	I277[6.39], T281[6.43], L284[6.46], C285[6.47], P288[6.50], L311[7.38], I314[7.41], F321[7.48], I325[7.52], R328[7.55]
	-12.9	I55[1.54], A59[1.58], C77[2.48], L80[2.51], V81[2.52], A85[2.56], W105[3.24], F108[3.27], I112[3.31]
	-12.7	V44[1.43], L45[1.44], V48[1.47], F49[1.48], V52[1.51], L53[1.52], T56[1.55], L339[8.57]
Beta-2 adrenergic receptor, inactive state, with cholesterol, Human 3pds		
3pds_EC	-12.8	L163[4.55], T164[4.56], P168[4.60], W173, N196[5.35], Y199[5.38], A202[5.41], V206[5.45]
	-12.5	V44[1.43], L45[1.44], V48[1.47], F49[1.48], P88[2.59], A92[2.63], M96[2.67], F101
3pds_IC	-14.1	Y70[2.41], T73[2.44], S74[2.45], C77[2.48], V81[2.52], I112[3.31], L115[3.34], R151[4.43], I154[4.46], L155[4.47], W158[4.50], F166[4.58]
	-13.0	C125[3.44], V126[3.45], V129[3.48], D130[3.49], L145, I153[4.45], I205[5.44], V206[5.45], V210[5.49], I214[5.53]
	-12.8	I55[1.54], A59[1.58], T73[2.44], C77[2.48], L80[2.51], V81[2.52], L84[2.55], A85[2.56]
	-12.5	I277[6.39], T281[6.43], L284[6.46], C285[6.47], P288[6.50], I314[7.41], F321[7.48], I325[7.52], R328[7.55]
Beta-2 adrenergic receptor, inactive state, with cholesterol, Human 5d5a		
5d5a_EC	-16.0	V160[4.52], L163[4.55], T164[4.56], P168[4.60], W173, Y174, N196[5.35], A198[5.37], Y199[5.38], A202[5.41], S203[5.42], V206[5.45]
	-13.0	S41[1.40], V44[1.43], L45[1.44], V48[1.47], L84[2.55], P88[2.59], A91[2.62], A92[2.63], L95[2.66], M96[2.67]
	-12.6	W32[1.31], M36[1.35], V39[1.38], I43[1.42], E306[7.33], L310[7.37], W313[7.40], V317[7.44]
	-12.6	L212[5.51], L287[6.49], I291[6.53], I294[6.56], V295[6.57], I298[6.60], Q299[6.61], L302
	-12.3	L115[3.34], W158[4.50], I159[4.51], G162[4.54], F166[4.58], L167[4.59], Q170[4.62], M171[4.63]
5d5a_IC	-14.6	Y70[2.41], T73[2.44], S74[2.45], I112[3.31], L115[3.34], R151[4.43], I154[4.46], L155[4.47], W158[4.50], F166[4.58]
	-13.7	V44[1.43], L45[1.44], V48[1.47], F49[1.48], V52[1.51], L53[1.52], L339[8.57], L340[8.58]
	-12.9	C125[3.44], V126[3.45], V129[3.48], D130[3.49], L145, I153[4.45], V206[5.45], V210[5.49], P211[5.50], I214[5.53]
	-12.7	V216[5.55], Y219[5.58], F223[5.62], G276[6.38], M279[6.41], G280[6.42], T283[6.45], L284[6.46], L287[6.49], I291[6.53]
	-12.7	I55[1.54], A59[1.58], T73[2.44], C77[2.48], L80[2.51], V81[2.52], A85[2.56], W105[3.24], F108[3.27], I112[3.31]
	-13.1	Y209[5.48], V213[5.52], V216[5.55], F217[5.56], S220[5.59], Q224[5.63], I291[6.53], I294[6.56]
Beta-2 adrenergic receptor, inactive state, with cholesterol, Human 5x7d		
5x7d_EC	-14.2	M36[1.35], V39[1.38], M40[1.39], I43[1.42], I94[2.65], K305[7.32], E306[7.33], I309[7.36], L310[7.37], W313[7.40]



PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-14.1	V160[4.52], T164[4.56], P168[4.60], W173, Y199[5.38], A202[5.41], S203[5.42], V206[5.45]
	-13.1	L284[6.46], L287[6.49], P288[6.50], I291[6.53], V292[6.54], L302, I303, R304[7.31], V307[7.34], L311[7.38]
	-12.3	L155[4.47], W158[4.50], I159[4.51], G162[4.54], L163[4.55], F166[4.58], L167[4.59], Q170[4.62], M171[4.63]
5x7d_IC	-14.4	Y70[2.41], T73[2.44], S74[2.45], C77[2.48], V81[2.52], F108[3.27], I112[3.31], L115[3.34], R151[4.43], I154[4.46], L155[4.47], W158[4.50], F166[4.58]
	-13.7	Y209[5.48], V213[5.52], V216[5.55], F217[5.56], S220[5.59], L287[6.49], I291[6.53], I294[6.56]
	-13.1	E122[3.41], C125[3.44], V126[3.45], V129[3.48], D130[3.49], I153[4.45], V160[4.52], T164[4.56], V206[5.45], P211[5.50]
	-13.1	V39[1.38], L42[1.41], I43[1.42], A46[1.45], F49[1.48], L310[7.37], V317[7.44], G320[7.47], F321[7.48], L324[7.51]
	-12.6	V52[1.51], I55[1.54], T56[1.55], A59[1.58], L80[2.51], V81[2.52], L84[2.55], A85[2.56], W105[3.24], F108[3.27], I112[3.31]
Angiotensin II receptor Type 1 (AT1)		
Angiotensin receptor Type II AT1, inactive, Human 4yay		
4yay_EC	-14.7	L155[4.52], L158[4.55], A159[4.56], L161[4.58], P162[4.59], I165[4.62], H166[4.63], E185, L195[5.38]
	-12.6	Y26[1.30], P255[6.50], R275[7.26], I279[7.30], T282[7.33], A283[7.34], I286[7.37], I290[7.41]
4yay_IC	-14.3	V40[1.44], F44[1.48], G45[1.49], L48[1.52], P299[7.50], Y302[7.53], G303[7.54], L305[7.56], G306[8.47]
	-13.2	K240[6.35], A244[6.39], L247[6.42], F248[6.43], F251[6.46], I290[7.41], F301[7.52], F304[7.55]
	-12.2	N200[5.43], F204[5.47], L205[5.48], F208[5.51], L209[5.52], L212[5.55], T213[5.56], T216[5.59], I254[6.49], Q257[6.52]
Angiotensin receptor Type II AT1, inactive, Human 4zud		
4zud_EC	-14.7	F117[3.41], L155[4.52], A159[4.56], P162[4.59], H166[4.63], F182, L195[5.38], T198[5.41], K199[5.42], L202[5.45]
	-11.9	H24, Y26[1.30], P255[6.50], F259[6.54], D278[7.29], I279[7.30], T282[7.33], A283[7.34], I286[7.37]
	-11.7	Y99[3.23], K102[3.26], I103[3.27], I150[4.47], W153[4.50], L154[4.51], G157[4.54], I164[4.61]
4zud_IC	-15.3	V62[2.38], F66[2.42], C121[3.45], I124[3.48], D125[3.49], T141[4.38], V144[4.41], A145[4.42], T148[4.45], L155[4.52]
	-13.6	F208[5.51], I211[5.54], L212[5.55], Y215[5.58], T216[5.59], W219[5.62], M243[6.38], L247[6.42], F250[6.45], F251[6.46], I254[6.49]
	-13.4	K240[6.35], M243[6.38], A244[6.39], L247[6.42], F248[6.43], F251[6.46], I290[7.41], F301[7.52]
	-13.2	F248[6.43], I290[7.41], F293[7.44], L297[7.48], L300[7.51], F301[7.52], G303[7.54], F304[7.55]
Angiotensin II receptor Type 2 (AT2)		
Angiotensin receptor Type II AT2, active-like state, Human 5unf		
5unf_EC	-13.1	Y52[1.40], F55[1.43], F59[1.47], L91[2.51], L92[2.52], A95[2.55], P98[2.58], L99[2.59], T102[2.62], Y106[2.66], F112
	-13.0	Q206[5.33], W207[5.34], G210[5.37], I211[5.38], M214[5.41], I217[5.44], L218[5.45], I222[5.49]
	-12.6	M170[4.52], L173[4.55], L176[4.58], P177[4.59], Y180[4.62], F181[4.63], W207[5.34], M214[5.41], L218[5.45], I222[5.49]
5unf_IC	-13.5	I81[2.41], F84[2.44], N85[2.45], V88[2.48], L92[2.52], F123[3.31], A160[4.42], S161[4.43], V164[4.46], P165[4.47]
	-13.1	A260[6.39], I267[6.46], L305[7.40], L306[7.41], T309[7.44], V313[7.48], F316[7.51], L317[7.52], V321[7.56]
	-12.5	Y82[2.42], C137[3.45], V140[3.48], I163[4.45], L166[4.48], M170[4.52], L218[5.45], I222[5.49], F226[5.53]
	-12.5	L224[5.51], Y231[5.58], F232[5.59], A259[6.38], V262[6.41], L263[6.42], I266[6.45], L270[6.49], V274[6.53]
	-12.2	I53[1.41], V56[1.44], I57[1.45], L60[1.48], V61[1.49], V64[1.52], F316[7.51], F320[7.55]
Angiotensin receptor Type II AT2, active-like state, Human 5ung		
5ung_EC	-13.6	Y52[1.40], F55[1.43], F59[1.47], I63[1.51], L91[2.51], L92[2.52], A95[2.55], P98[2.58], L99[2.59], T102[2.62], F112
	-13.0	Q206[5.33], A209[5.36], G210[5.37], L213[5.40], M214[5.41], I217[5.44], L218[5.45], I222[5.49], M284[6.63]
	-12.9	M170[4.52], L173[4.55], S174[4.56], L176[4.58], P177[4.59], Y180[4.62], M214[5.41], L218[5.45]
	-12.2	I266[6.45], I267[6.46], L270[6.49], P271[6.50], V274[6.53], L275[6.54], L278[6.57], V292[7.27], V295[7.30], I296[7.31]
5ung_IC	-13.3	L92[2.52], F123[3.31], L126[3.34], N127[3.35], S161[4.43], V164[4.46], P165[4.47], W168[4.50]
	-13.0	I54[1.42], A260[6.39], L263[6.42], A264[6.43], I267[6.46], C268[6.47], L305[7.40], L306[7.41], T309[7.44], V313[7.48], L317[7.52]
	-12.9	L224[5.51], Y231[5.58], F232[5.59], A259[6.38], V262[6.41], L263[6.42], I266[6.45], L270[6.49], V274[6.53]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.5	T136[3.44], C137[3.45], V140[3.48], I163[4.45], M170[4.52], L218[5.45], I222[5.49], F226[5.53]
Angiotensin receptor Type II AT2, active-like state, Human Sunh		
Sunh_IC	-13.8	I81[2.41], N85[2.45], F123[3.31], L126[3.34], S161[4.43], V164[4.46], P165[4.47], W168[4.50]
	-13.5	Y82[2.42], T136[3.44], C137[3.45], V140[3.48], I163[4.45], M170[4.52], L218[5.45], I222[5.49], F226[5.53]
	-13.1	F220[5.47], I221[5.48], L224[5.51], I225[5.52], A228[5.55], T229[5.56], F232[5.59], L270[6.49], V274[6.53]
	-12.7	I54[1.42], K256[6.35], A260[6.39], L263[6.42], A264[6.43], I267[6.46], C268[6.47], L305[7.40], L306[7.41], T309[7.44], V313[7.48]
	-11.8	Y231[5.58], F232[5.59], R235[5.62], V262[6.41], L263[6.42], I266[6.45], L270[6.49], V274[6.53]
Cannabinoid CB1 receptor		
Cannabinoid CB1, inactive, Human 5tgz		
5tgz_EC	-13.3	I353[6.45], I354[6.46], P358[6.50], A361[6.53], Y365[6.57], N372[7.28], L374[7.30], I375[7.31], V378[7.34]
	-13.0	A120[1.36], V121[1.37], L124[1.40], T125[1.41], F174[2.61], H178[2.65], V179[2.66], H181
	-12.1	L287[5.51], V291[5.55], I353[6.45], G357[6.49], L360[6.52], A361[6.53], V364[6.56], Y365[6.57]
5tgz_IC	-15.4	L142[1.58], R148, H154[2.41], V161[2.48], L165[2.52], R230[4.39], V234[4.43], C238[4.47]
	-13.4	F208[3.44], L209[3.45], I212[3.48], I227, K232[4.41], A236[4.45], L239[4.48], I243[4.52], L286[5.50]
Cannabinoid CB1, inactive, Human 5u09		
5u09_EC	-12.9	T274[5.38], M277[5.41], F278[5.42], G281[5.45], V282[5.46], V285[5.49], F289[5.53], F368[6.60]
	-12.7	I354[6.46], P358[6.50], A361[6.53], I362[6.54], Y365[6.57], K370, N372[7.28], I375[7.31], V378[7.34]
	-12.7	L138[1.54], V161[2.48], L164[2.51], L165[2.52], V168[2.55], I169[2.56], Y172[2.59], R182, V188[3.24], F191[3.27], K192[3.28]
	-12.6	L124[1.40], T125[1.41], T128[1.44], F129[1.45], L132[1.48], I175[2.62], V179[2.66], F180
	-12.6	L287[5.51], L288[5.52], V291[5.55], I353[6.45], A361[6.53], V364[6.56], Y365[6.57], F368[6.60], G369[6.61]
5u09_IC	-15.7	I141[1.57], L142[1.58], L147, R148, Y153[2.40], H154[2.41], I156[2.43], G157[2.44], S158[2.45], V161[2.48]
	-12.7	F208[3.44], L209[3.45], K232[4.41], A236[4.45], L239[4.48], I243[4.52], I247[4.56], V282[5.46]
Cannabinoid CB1, active intermediate, with cholesterol, Human 5xr8		
5xr8_EC	-13.7	L135[1.51], L164[2.51], L165[2.52], V168[2.55], I169[2.56], Y172[2.59], R182, K192[3.28]
	-12.9	L124[1.40], T128[1.44], L132[1.48], V171[2.58], Y172[2.59], I175[2.62], D176[2.63], F180
	-12.9	L117[1.33], A120[1.36], V121[1.37], L124[1.40], T125[1.41], T128[1.44], F129[1.45], L132[1.48], V179[2.66]
5xr8_IC	-15.2	I141[1.57], Y153[2.40], H154[2.41], G157[2.44], S158[2.45], V161[2.48], L165[2.52], W241[4.50], I245[4.54]
	-13.1	K343[6.35], L347[6.39], V351[6.43], I354[6.46], V392[7.48], I395[7.51], I396[7.52], L399[7.55], R400[7.56]
	-12.4	F208[3.44], L209[3.45], I212[3.48], K232[4.41], A236[4.45], I243[4.52], F278[5.42], V282[5.46]
	-12.8	F208[3.44], I212[3.48], I216[3.52], I227, G281[5.45], V282[5.46], V285[5.49], F289[5.53]
Cannabinoid CB1, active intermediate, with cholesterol, Human 5xra		
5xra_EC	-13.7	L124[1.40], T128[1.44], L132[1.48], V171[2.58], Y172[2.59], I175[2.62], D176[2.63], F180
5xra_IC	-15.8	H154[2.41], G157[2.44], S158[2.45], V161[2.48], L165[2.52], F237[4.46], C238[4.47], W241[4.50], I245[4.54]
	-12.9	F208[3.44], L209[3.45], K232[4.41], A233[4.42], V235[4.44], A236[4.45], L239[4.48], I243[4.52], F278[5.42], V282[5.46]
	-12.4	F208[3.44], I212[3.48], I216[3.52], I227, G281[5.45], V282[5.46], V285[5.49], L286[5.50]
	-14.2	I212[3.48], Y215[3.51], I216[3.52], R220[3.56], V285[5.49], L288[5.52], F289[5.53], Y292[5.56]
Chemokine CC receptor		
Chemokine CC receptor, Type 2, inactive, Human 5t1a		

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
5t1a_EC	-13.1	L90[2.52], K114[3.26], L115[3.27], G118[3.30], L119[3.31], I122[3.34], W165[4.50], V169[4.54], I176[4.61]
	-13.1	V167[4.52], F170[4.55], V173[4.58], P174[4.59], I177[4.62], F178[4.63], W198[5.35], F201[5.38]
	-12.9	F253[6.45], L254[6.46], T257[6.49], P258[6.50], I261[6.53], V262[6.54], L265[6.57], L283[7.30], A286[7.33]
	-12.8	S50[1.40], F53[1.43], I54[1.44], F57[1.47], V58[1.48], P96[2.58], A99[2.61], H100[2.62], A103[2.65]
	-12.2	I40[1.30], L44[1.34], L48[1.38], V289[7.36], T292[7.39], L293[7.40], T296[7.43], C299[7.46], I300[7.47]
	-13.7	F53[1.43], F57[1.47], M61[1.51], I93[2.55], P96[2.58], L97[2.59], H100[2.62], F108
5t1a_IC	-13.5	L73, I79[2.41], L82[2.44], N83[2.45], I86[2.48], L90[2.52], L119[3.31], I122[3.34], V158[4.43], V162[4.47], W165[4.50], V169[4.54]
	-12.9	T247[6.39], V251[6.43], L254[6.46], F255[6.47], T296[7.43], I300[7.47], I304[7.51], F307[7.54], V308[7.55]
	-12.4	I132[3.44], L133[3.45], I136[3.48], F156[4.41], V167[4.52], M205[5.42], L209[5.46], L213[5.50]

## Chemokine CC receptor, Type 5, inactive, Human 4mbs

4mbs_EC	-14.1	Q102[3.26], L103[3.27], G106[3.30], I110[3.34], V150[4.47], W153[4.50], V154[4.51], V157[4.54], I164[4.61]
	-12.4	V155[4.52], F158[4.55], A159[4.56], L161[4.58], P162[4.59], W190[5.35], F193[5.38], K197[5.42], L201[5.46]
	-12.2	F245[6.45], L246[6.46], A249[6.49], P250[6.50], I253[6.53], V254[6.54], L257[6.57], R274[7.29]
	-12.2	L32[1.34], L36[1.38], F247[6.47], V281[7.36], T284[7.39], L285[7.40], T288[7.43], I292[7.47], I295[7.50]
4mbs_IC	-12.8	I124[3.48], Y127[3.51], I200[5.45], V204[5.49], L205[5.50], L208[5.53], V209[5.54], I212[5.57], C213[5.58]
	-12.4	L61, I67[2.41], N71[2.45], F78[2.52], V146[4.43], V150[4.47], W153[4.50], V157[4.54]
	-12.4	R235[6.35], T239[6.39], V243[6.43], F247[6.47], I292[7.47], I295[7.50], I296[7.51], F299[7.54], V300[7.55]
	-13.5	M64[2.38], I120[3.44], L121[3.45], I124[3.48], L128[3.52], F144[4.41], T148[4.45], L201[5.46], L205[5.50]
-12.6	F45[1.47], V46[1.48], M49[1.51], L50[1.52], L53[1.55], I54[1.56], Y307[8.53], F311[8.57]	

## Chemokine CC receptor, Type 9, inactive, with cholesterol, Human 5lwe

5lwe_EC	-13.6	R44[1.28], F46[1.30], A47[1.31], F50[1.34], L51[1.35], I297[7.32], Q300[7.35], V301[7.36], A304[7.39], I305[7.40]
	-12.6	L175[4.52], A178[4.55], L179[4.56], I181[4.58], P182[4.59], L185[4.62], Y186[4.63], V214[5.39], L217[5.42], K218[5.43], L221[5.46]
	-12.4	F117[3.23], K120[3.26], V121[3.27], S124[3.30], M125[3.31], W173[4.50], V174[4.51], I184[4.61]
5lwe_IC	-13.6	W74[1.58], M85[2.41], L88[2.44], N89[2.45], I92[2.48], L96[2.52], K166[4.43], F170[4.47], W173[4.50]
	-12.9	K254[6.35], T258[6.39], T261[6.42], V262[6.43], L265[6.46], I305[7.40], F308[7.43], L312[7.47], L316[7.51]
	-12.4	F50[1.34], L54[1.38], L57[1.41], F308[7.43], L312[7.47], V315[7.50], L316[7.51], F319[7.54]

## Chemokine CXC receptor

## Chemokine CXC Receptor Type 4, inactive, Human 3odu

3odu_EC	-12.6	L167[4.56], L194[5.34], V197[5.37], V198[5.38], F201[5.41], Q202[5.42], M205[5.45], V206[5.46]
	-12.6	P163[4.52], L166[4.55], L167[4.56], I169[4.58], P170[4.59], I173[4.62], F174[4.63], W195[5.35]
	-12.1	L208[5.48], F249[6.45], L253[6.49], Y256[6.52], I257[6.53], S260[6.56], I261[6.57], F264[6.60], I270
	-12.1	K38[1.32], I39[1.33], P42[1.36], T43[1.37], S46[1.40], I47[1.41], L50[1.44], V99[2.65]
	-12.9	V197[5.37], Q200[5.40], F201[5.41], I204[5.44], I209[5.49], S263[6.59], L266[6.62], L267[6.63]
3odu_IC	-14.2	H79[2.45], V82[2.48], L86[2.52], A111[3.27], V114[3.30], I115[3.31], Y157[4.46], W161[4.50], L165[4.54]
	-13.3	I60[1.54], Y65[1.59], V82[2.48], L85[2.51], L86[2.52], I89[2.55], T90[2.56], F93[2.59], I115[3.31]
	-13.0	I47[1.41], T51[1.45], G55[1.49], L58[1.52], F293[7.43], C296[7.46], P299[7.49], I300[7.50], A303[7.53], F304[7.54]
	-12.7	W125[3.41], F129[3.45], L132[3.48], L151[4.40], V155[4.44], G159[4.48], P163[4.52], L167[4.56], Q202[5.42], V206[5.46], L210[5.50]
	-12.6	A247[6.43], A250[6.46], C251[6.47], P254[6.50], L290[7.40], L297[7.47], I300[7.50], L301[7.51], F304[7.54]
	-12.3	I215[5.55], L216[5.56], Y219[5.59], V242[6.38], I245[6.41], L246[6.42], F249[6.45], L253[6.49], Y256[6.52]

## Chemokine CXC Receptor Type 4, inactive, Human 3oe0

3oe0_EC	-13.0	K38[1.32], I39[1.33], P42[1.36], T43[1.37], S46[1.40], I47[1.41], L50[1.44], V99[2.65]
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PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.4	L208[5.48], L253[6.49], I257[6.53], S260[6.56], I261[6.57], F264[6.60], I270, F276[7.26]
	-12.8	P42[1.36], S46[1.40], F49[1.43], L50[1.44], I53[1.47], P92[2.58], A95[2.61], V96[2.62], V99[2.65]
	-12.3	P163[4.52], L166[4.55], L167[4.56], I169[4.58], P170[4.59], I173[4.62], W195[5.35], F199[5.39], Q202[5.42]
3oe0_IC	-13.1	G64[1.58], L78[2.44], H79[2.45], V82[2.48], L86[2.52], V114[3.30], V118[3.34], Y157[4.46], W161[4.50], L165[4.54]
	-13.0	W125[3.41], F129[3.45], L132[3.48], L151[4.40], V155[4.44], G159[4.48], P163[4.52], L167[4.56], Q202[5.42], V206[5.46], L210[5.50]
Chemokine CXC Receptor Type 4, inactive, Human 3oe6		
3oe6_EC	-15.6	P254[6.50], I257[6.53], G258[6.54], I261[6.57], F276[7.26], T279[7.29], V280[7.30], W283[7.33], T287[7.37]
	-13.0	P163[4.52], L166[4.55], L167[4.56], I169[4.58], P170[4.59], I173[4.62], F174[4.63], W195[5.35], F199[5.39], Q202[5.42], V206[5.46]
	-12.5	F49[1.43], I53[1.47], I89[2.55], P92[2.58], F93[2.59], V96[2.62], Y103, F104
	-12.0	K38[1.32], I39[1.33], P42[1.36], T43[1.37], S46[1.40], I47[1.41], L50[1.44], V99[2.65]
3oe6_IC	-13.7	L216[5.56], Y219[5.59], I223[5.63], V242[6.38], I245[6.41], L246[6.42], F249[6.45], L253[6.49], Y256[6.52]
	-12.9	W125[3.41], F129[3.45], L132[3.48], L151[4.40], V155[4.44], V158[4.47], G159[4.48], P163[4.52], L167[4.56], V206[5.46]
	-12.8	R70, L78[2.44], H79[2.45], V82[2.48], L86[2.52], V114[3.30], I115[3.31], V118[3.34], Y157[4.46], W161[4.50], L165[4.54]
	-12.4	I243[6.39], A247[6.43], P254[6.50], L290[7.40], F293[7.43], L297[7.47], I300[7.50], L301[7.51]
	-12.7	L132[3.48], Y135[3.51], M205[5.45], L210[5.50], I213[5.53], V214[5.54], S217[5.57], I221[5.61]
	-12.3	I44[1.38], I47[1.41], I48[1.42], T51[1.45], L290[7.40], F293[7.43], I300[7.50], F304[7.54]
Chemokine CXC Receptor Type 4, inactive, Human 3oe8		
3oe8_EC	-13.2	L208[5.48], I209[5.49], G212[5.52], I213[5.53], F249[6.45], Y256[6.52], I257[6.53], S260[6.56], I261[6.57]
3oe8_IC	-13.7	H79[2.45], V82[2.48], L86[2.52], A111[3.27], V114[3.30], I115[3.31], Y157[4.46], W161[4.50], L165[4.54]
	-13.4	T51[1.45], V54[1.48], G55[1.49], L58[1.52], V59[1.53], V62[1.56], K67, P299[7.49], I300[7.50], Y302[7.52], A303[7.53]
	-12.4	F129[3.45], V155[4.44], V158[4.47], G159[4.48], P163[4.52], L166[4.55], L167[4.56], I169[4.58], P170[4.59], Q202[5.42]
	-12.1	W125[3.41], V155[4.44], G159[4.48], P163[4.52], F201[5.41], Q202[5.42], V206[5.46], L210[5.50]
Chemokine CXC Receptor Type 4, inactive, Human 3oe9		
3oe9_EC	-12.4	V196[5.36], V197[5.37], Q200[5.40], F201[5.41], I204[5.44], I209[5.49], I259[6.55], S263[6.59], L266[6.62]
	-12.2	L253[6.49], P254[6.50], I257[6.53], G258[6.54], I261[6.57], V280[7.30], W283[7.33], T287[7.37]
	-11.7	L208[5.48], F249[6.45], L253[6.49], I257[6.53], S260[6.56], I261[6.57], F264[6.60], I270
	-11.6	F40[1.34], A247[6.43], A250[6.46], P254[6.50], K282[7.32], W283[7.33], I286[7.36], L290[7.40]
	-11.6	F49[1.43], I53[1.47], L85[2.51], I89[2.55], P92[2.58], F93[2.59], V96[2.62], F104
3oe9_IC	-12.9	V82[2.48], L86[2.52], F107[3.23], A111[3.27], V114[3.30], Y157[4.46], W161[4.50], L165[4.54], F172[4.61]
	-12.9	V155[4.44], V158[4.47], G159[4.48], P163[4.52], L167[4.56], P170[4.59], F199[5.39], Q202[5.42], V206[5.46]
	-12.8	I243[6.39], A247[6.43], A250[6.46], C251[6.47], L297[7.47], I300[7.50], L301[7.51], A303[7.53]
	-12.3	I47[1.41], L50[1.44], T51[1.45], V54[1.48], G55[1.49], L58[1.52], P299[7.49], Y302[7.52]
Chemokine CXC Receptor Type 4, inactive, Human 4rws		
4rws_EC	-13.2	P163[4.52], L166[4.55], L167[4.56], I169[4.58], P170[4.59], I173[4.62], W195[5.35], F199[5.39], Q202[5.42], V206[5.46], L210[5.50]
4rws_IC	-13.2	I204[5.44], L208[5.48], I209[5.49], G212[5.52], I215[5.55], L216[5.56], Y219[5.59], V242[6.38], I245[6.41], L246[6.42], F249[6.45]
	-13.0	I47[1.41], L50[1.44], T51[1.45], V54[1.48], G55[1.49], L58[1.52], P299[7.49], I300[7.50], Y302[7.52], A303[7.53]
	-12.9	A247[6.43], A250[6.46], C251[6.47], P254[6.50], L290[7.40], F293[7.43], L297[7.47], I300[7.50], L301[7.51], A303[7.53]
	-12.5	W125[3.41], F129[3.45], L132[3.48], L151[4.40], V155[4.44], G159[4.48], P163[4.52], L166[4.55], L167[4.56], V206[5.46]
	-13.9	I44[1.38], I47[1.41], I48[1.42], T51[1.45], L290[7.40], F293[7.43], I300[7.50], A303[7.53]
	-13.9	G64[1.58], Y65[1.59], L78[2.44], V82[2.48], L86[2.52], V118[3.34], Y157[4.46], L165[4.54]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Complement C5a receptor		
Complement C5a receptor, inactive, Human 5o9h		
5o9h_EC	-13.1	I253[6.46], L256[6.49], P257[6.50], V260[6.53], M264[6.57], T274[7.27], L278[7.31], F288[7.41]
	-13.0	F48[1.43], V52[1.47], F83[2.51], L87[2.55], P90[2.58], A91[2.59], F104, A108[3.24], L112[3.28]
	-12.7	V80[2.48], L84[2.52], S110[3.26], I111[3.27], L115[3.31], L118[3.34], L165[4.54], A172[4.61], L173[4.62]
	-12.4	L207[5.43], F211[5.47], L212[5.48], L215[5.51], L256[6.49], V260[6.53], I263[6.56], M264[6.57], F267[6.60]
	-12.9	V80[2.48], F83[2.51], L84[2.52], L87[2.55], A107[3.23], A108[3.24], I111[3.27], L112[3.28]
	-11.7	L33, I38[1.33], L41[1.36], V42[1.37], A45[1.40], V46[1.41], L49[1.44], F93[2.61], V97[2.65]
	-11.8	F48[1.43], L49[1.44], L53[1.48], P90[2.58], F93[2.61], T94[2.62], V97[2.65], Q98[2.66]
5o9h_IC	-13.1	I253[6.46], L256[6.49], P257[6.50], V260[6.53], M264[6.57], T274[7.27], L278[7.31], F288[7.41]
	-13.0	F48[1.43], V52[1.47], F83[2.51], L87[2.55], P90[2.58], A91[2.59], F104, A108[3.24], L112[3.28]
	-12.7	V80[2.48], L84[2.52], S110[3.26], I111[3.27], L115[3.31], L118[3.34], L165[4.54], A172[4.61], L173[4.62]
	-12.4	L207[5.43], F211[5.47], L212[5.48], L215[5.51], L256[6.49], V260[6.53], I263[6.56], M264[6.57], F267[6.60]
	-12.9	V80[2.48], F83[2.51], L84[2.52], L87[2.55], A107[3.23], A108[3.24], I111[3.27], L112[3.28]
	-11.7	L33, I38[1.33], L41[1.36], V42[1.37], A45[1.40], V46[1.41], L49[1.44], F93[2.61], V97[2.65]
	-11.8	F48[1.43], L49[1.44], L53[1.48], P90[2.58], F93[2.61], T94[2.62], V97[2.65], Q98[2.66]
Complement C5a receptor, inactive, residues renumbered, Human 6c1q		
6c1q_EC	-13.9	L163[4.52], L167[4.56], P170[4.59], Y174[4.63], R198[5.34], V202[5.38], V205[5.41], L209[5.45]
	-13.6	F48[1.43], V52[1.47], F83[2.51], L87[2.55], I91[2.59], F190, A108[3.24], L112[3.28]
	-12.0	I253[6.46], L256[6.49], P257[6.50], V260[6.53], T261[6.54], M264[6.57], T274[7.27], L277[7.30], L278[7.31], L281[7.34]
	-12.0	F48[1.43], L49[1.44], L53[1.48], P90[2.58], I91[2.59], T94[2.62], Q98[2.66], P189, F190
	-11.9	F83[2.51], L84[2.52], L87[2.55], F190, A107[3.23], A108[3.24], I111[3.27], L112[3.28]
	-11.8	L207[5.43], F211[5.47], L212[5.48], L215[5.51], L256[6.49], V260[6.53], I263[6.56], M264[6.57], F267[6.60]
	-11.6	V35[1.30], P36[1.31], L39[1.34], I253[6.46], L256[6.49], P257[6.50], L277[7.30], L281[7.34], L284[7.37], F288[7.41]
6c1q_IC	-13.9	L163[4.52], L167[4.56], P170[4.59], Y174[4.63], R198[5.34], V202[5.38], V205[5.41], L209[5.45]
	-13.6	F48[1.43], V52[1.47], F83[2.51], L87[2.55], I91[2.59], F190, A108[3.24], L112[3.28]
	-12.0	I253[6.46], L256[6.49], P257[6.50], V260[6.53], T261[6.54], M264[6.57], T274[7.27], L277[7.30], L278[7.31], L281[7.34]
	-12.0	F48[1.43], L49[1.44], L53[1.48], P90[2.58], I91[2.59], T94[2.62], Q98[2.66], P189, F190
	-11.9	F83[2.51], L84[2.52], L87[2.55], F190, A107[3.23], A108[3.24], I111[3.27], L112[3.28]
	-11.8	L207[5.43], F211[5.47], L212[5.48], L215[5.51], L256[6.49], V260[6.53], I263[6.56], M264[6.57], F267[6.60]
	-11.6	V35[1.30], P36[1.31], L39[1.34], I253[6.46], L256[6.49], P257[6.50], L277[7.30], L281[7.34], L284[7.37], F288[7.41]
Complement C5a receptor, inactive, residues renumbered, Human 6c1r		
6c1r_EC	-13.1	F48[1.43], V52[1.47], F83[2.51], L87[2.55], P90[2.58], I91[2.59], F190, G105[3.21], A108[3.24], L112[3.28]
	-12.7	R197[5.33], R200[5.36], A201[5.37], I204[5.40], V205[5.41], V208[5.44], L209[5.45], W213[5.49]
	-12.4	L207[5.43], F211[5.47], L212[5.48], L215[5.51], L256[6.49], V260[6.53], I263[6.56], M264[6.57], F267[6.60]
	-12.4	V80[2.48], F83[2.51], L84[2.52], L87[2.55], A107[3.23], A108[3.24], I111[3.27], L112[3.28], L115[3.31]
	-12.3	I253[6.46], L256[6.49], P257[6.50], V260[6.53], T261[6.54], M264[6.57], T274[7.27], L277[7.30], L278[7.31], L281[7.34]
	-12.2	V35[1.30], P36[1.31], L39[1.34], I253[6.46], F254[6.47], L277[7.30], L281[7.34], L284[7.37], F288[7.41]
	-12.1	F48[1.43], L49[1.44], P90[2.58], I91[2.59], T94[2.62], Q98[2.66], P189, F190
6c1r_IC	-13.1	F48[1.43], V52[1.47], F83[2.51], L87[2.55], P90[2.58], I91[2.59], F190, G105[3.21], A108[3.24], L112[3.28]
	-12.7	R197[5.33], R200[5.36], A201[5.37], I204[5.40], V205[5.41], V208[5.44], L209[5.45], W213[5.49]
	-12.4	L207[5.43], F211[5.47], L212[5.48], L215[5.51], L256[6.49], V260[6.53], I263[6.56], M264[6.57], F267[6.60]
	-12.4	V80[2.48], F83[2.51], L84[2.52], L87[2.55], A107[3.23], A108[3.24], I111[3.27], L112[3.28], L115[3.31]
	-12.3	I253[6.46], L256[6.49], P257[6.50], V260[6.53], T261[6.54], M264[6.57], T274[7.27], L277[7.30], L278[7.31], L281[7.34]
	-12.2	V35[1.30], P36[1.31], L39[1.34], I253[6.46], F254[6.47], L277[7.30], L281[7.34], L284[7.37], F288[7.41]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.1	F48[1.43], L49[1.44], P90[2.58], I91[2.59], T94[2.62], Q98[2.66], P189, F190
Dopamine receptor		
Dopamine receptor D2, inactive, Human 6c38		
6c38_EC	-13.7	L162[4.52], I166[4.56], P169[4.59], L174, N175, N176, Y192[5.41], V196[5.45]
	-12.6	V190[5.39], V191[5.40], I195[5.44], Y199[5.48], I203[5.52], L206[5.55], I415[7.42], I418[7.45]
	-12.5	T42[1.40], I45[1.43], V49[1.47], T85[2.55], P89[2.59], V92[2.62], Y93[2.63], V96[2.66], V97[2.67]
	-13.0	F202[5.51], L206[5.55], I404[7.31], L408[7.35], I412[7.39], I415[7.42], L416[7.43], H419[7.46]
6c38_IC	-14.6	Y209[5.58], I210[5.59], I212[5.61], Y213[5.62], A397[6.59], G401, I404[7.31], I405[7.32], L408[7.35], P409[7.36], I412[7.39]
	-14.4	L82[2.52], L86[2.56], L113[3.31], M116[3.34], M117[3.35], T153[4.43], I156[4.46], S157[4.47], W160[4.50]
	-12.5	C126[3.44], I130[3.48], R151[4.41], M155[4.45], I158[4.48], L162[4.52], V196[5.45], V200[5.49]
	-12.4	L40[1.38], V47[1.45], F50[1.48], L54[1.52], I445, T448, F458, L462
	-12.4	T42[1.40], I45[1.43], A46[1.44], V49[1.47], F50[1.48], L54[1.52], M57[1.55], I461, L462
Dopamine receptor D3, inactive, Human 3pbl		
3pbl_EC	-14.7	I339[6.45], V340[6.46], L343[6.49], P344[6.50], L347[6.53], T348[6.54], H359, L364[7.34]
	-13.4	I190[5.40], V194[5.44], Y198[5.48], F201[5.51], G202[5.52], V205[5.55], V350[6.56], H354[6.60]
	-12.6	I40[1.43], L41[1.44], V44[1.47], T80[2.55], P84[2.59], V87[2.62], Y88[2.63], V91[2.66]
3pbl_IC	-15.0	Y208[5.58], I211[5.61], Y212[5.62], A332[6.38], L335[6.41], G336[6.42], I339[6.45], V340[6.46], L343[6.49], P344[6.50]
	-13.5	S35[1.38], A38[1.41], L39[1.42], A42[1.45], F45[1.48], G46[1.49], L49[1.52], W370[7.40], A377[7.47], V381[7.51], T384[7.54], F394[8.54], L398[8.58]
	-13.2	Y66[2.41], V69[2.44], S70[2.45], A151[4.43], I154[4.46], T155[4.47], W158[4.50], V159[4.51], F162[4.54]
	-12.5	W119[3.41], R149[4.41], L152[4.44], M153[4.45], A156[4.48], L160[4.52], V195[5.45], L199[5.49]
	-12.4	I40[1.43], L41[1.44], V44[1.47], F45[1.48], L49[1.52], M52[1.55], I397[8.57], L398[8.58]
	-12.4	V44[1.47], G48[1.51], C51[1.54], M52[1.55], L55[1.58], L76[2.51], T80[2.55], L81[2.56]
Dopamine receptor D4, inactive, Human 5wiu		
5wiu_EC	-14.0	G40[1.38], L43[1.41], R428[7.33], L429[7.34], S431[7.36], A432[7.37], W435[7.40], V439[7.44]
	-13.1	V42[1.40], I45[1.43], G46[1.44], L49[1.47], A50[1.48], P89[2.59], L90[2.60], V92[2.62], Y93[2.63]
	-12.3	F202[5.48], P206[5.52], L209[5.55], L210[5.56], V412[6.53], I415[6.56], T416[6.57], L419[6.60]
	-12.5	F124[3.41], C127[3.44], A128[3.45], T159[4.49], L162[4.52], V166[4.56], Y195[5.41], C199[5.45], L203[5.49]
	-12.4	V194[5.40], V198[5.44], F202[5.48], L203[5.49], P206[5.52], L210[5.56], I415[6.56], L419[6.60]
5wiu_IC	-14.0	S71[2.41], V74[2.44], S75[2.45], A78[2.48], L82[2.52], L86[2.56], M114[3.31], M117[3.34], L153[4.43], I156[4.46], W160[4.50]
	-13.5	R394[6.35], P397[6.38], V398[6.39], G401[6.42], L404[6.45], L405[6.46], T408[6.49], F451[7.56]
	-13.2	L209[5.55], Y212[5.58], F216[5.62], P397[6.38], V400[6.41], G401[6.42], L404[6.45], L405[6.46], T408[6.49]
	-12.9	C56[1.54], V57[1.55], V59[1.57], A60[1.58], V74[2.44], A78[2.48], L82[2.52], L85[2.55], L86[2.56]
Dopamine receptor D4, inactive, Human 5wiv		
5wiv_EC	-13.8	Q33[1.31], A36[1.34], A37[1.35], G40[1.38], R428[7.33], W435[7.40], V439[7.44], L443[7.48]
	-13.4	V42[1.40], I45[1.43], G46[1.44], L49[1.47], A50[1.48], P89[2.59], L90[2.60], V92[2.62], Y93[2.63]
	-11.7	F202[5.48], L209[5.55], L404[6.45], T408[6.49], V412[6.53], I415[6.56], T416[6.57], L419[6.60]
5wiv_IC	-13.9	S71[2.41], V74[2.44], S75[2.45], A78[2.48], L82[2.52], L86[2.56], L153[4.43], I156[4.46]
	-13.1	L209[5.55], Y212[5.58], W213[5.59], F216[5.62], P397[6.38], G401[6.42], L404[6.45], L405[6.46], T408[6.49], P409[6.50]
	-13.2	C56[1.54], V59[1.57], A60[1.58], V74[2.44], L81[2.51], L82[2.52], L85[2.55], L86[2.56]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Endothelin ETB receptor		
Endothelin ETB receptor, inactive, Human 5glh		
5glh_EC	-13.0	V228[4.52], V231[4.55], L232[4.56], V234[4.58], P235[4.59], I238[4.62], T263[5.28], F265[5.30], M266[5.31]
	-12.1	E172[3.23], K175[3.26], F179[3.30], V227[4.51], V230[4.54], V231[4.55], V234[4.58], A237[4.61]
5glh_IC	-15.3	L286[5.51], A290[5.55], Y293[5.58], K323[6.35], T324[6.36], F326[6.38], C327[6.39], L330[6.42]
	-13.8	L190[3.41], A194[3.45], I197[3.48], R201[3.52], E221[4.45], L224[4.48], V228[4.52], L232[4.56]
	-13.5	L110[1.41], V113[1.44], L114[1.45], I117[1.48], F397[8.54], K398[8.55], A400[8.57], L401[8.58]
	-13.1	F112[1.43], V113[1.44], I116[1.47], I117[1.48], S120[1.51], T121[1.52], Y124[1.55], K128[1.59]
	-12.8	I138[2.41], L145[2.48], A219[4.43], I222[4.46], V223[4.47], W226[4.50], V227[4.51], V230[4.54]
Endothelin ETB receptor, inactive, Human 5gli		
5gli_EC	-12.8	N104[1.35], D147[2.50], H150[2.53], I155[2.58], N158[2.61], K161[2.64], L162[2.65], Q181[3.32], V185[3.36], T188[3.39], W336[6.48], I372[7.39], A375[7.42], S376[7.43], N378[7.45], S379[7.46]
	-12.1	I116[1.47], V152[2.55], I153[2.56], P156[2.59], I157[2.60], Y160[2.63], F169, M173[3.24]
5gli_IC	-14.0	I116[1.47], S120[1.51], T121[1.52], Y124[1.55], L148[2.51], V152[2.55], A400[8.57], L401[8.58], C403[8.60]
	-13.4	A194[3.45], I197[3.48], D198[3.49], R201[3.52], E221[4.45], L224[4.48], V228[4.52], L232[4.56]
	-13.1	Y127[1.58], L145[2.48], F179[3.30], V214[4.38], A219[4.43], I222[4.46], V223[4.47], W226[4.50], V230[4.54]
	-12.3	F278[5.43], F282[5.47], L286[5.51], A290[5.55], Y293[5.58], T294[5.59], F326[6.38], A333[6.45], L337[6.49]
Endothelin ETB receptor, inactive, agonist bound, Human 5x93		
5x93_EC	-12.9	K175[3.26], F179[3.30], V223[4.47], V227[4.51], V230[4.54], V234[4.58], A237[4.61], I238[4.62]
	-12.5	F112[1.43], I116[1.47], V152[2.55], P156[2.59], I157[2.60], Y160[2.63], F169, M173[3.24]
5x93_IC	-14.4	I116[1.47], I117[1.48], S120[1.51], T121[1.52], Y124[1.55], V152[2.55], A400[8.57], L401[8.58], W404
	-14.4	L190[3.41], C193[3.44], A194[3.45], I197[3.48], D198[3.49], R201[3.52], E221[4.45], W276[5.41], F280[5.45], L284[5.49], I288[5.53]
	-13.7	L123[1.54], Y124[1.55], Y127[1.58], L145[2.48], L148[2.51], L149[2.52], V152[2.55], I153[2.56]
	-12.8	F278[5.43], F282[5.47], L286[5.51], A290[5.55], Y293[5.58], T294[5.59], F326[6.38], L337[6.49]
	-12.8	I138[2.41], L145[2.48], L149[2.52], V214[4.38], T218[4.42], A219[4.43], I222[4.46], V223[4.47], W226[4.50]
	-12.9	C327[6.39], V331[6.43], L334[6.46], P338[6.50], M374[7.41], I384[7.51], A385[7.52], L388[7.55], V389[7.56]
Free Fatty Acid receptor FFAR1		
Free fatty acid receptor FFAR1, residues renumbered, inactive, Human 4phu		
4phu_EC	-13.3	L231[4.55], L234[4.58], L235[4.59], P239[4.63], A242, S243, A246, S247, L253, W257
	-13.2	Q6, L7, F9, G10, V13, A14, A17, L18
	-12.8	W131, A132, L135[2.38], C136[2.39], G139[2.42], F142[2.45], G143[2.46], G149[2.52], W150[2.53], L158[2.61]
	-12.7	L133, H137[2.40], V141[2.44], S178[3.29], P181[3.32], A182[3.33], S185[3.36], L189[3.40]
	-12.5	F192[3.43], L195[3.46], A199[3.50], L230[4.54], L234[4.58], A242, S243, A246, L253, W257
4phu_IC	-12.4	F20, V24, I27, R28, L53, L54, V57, V81, A85
	-12.3	A102[1.33], Y105[1.36], L106[1.37], L193[3.44], A196[3.47], I197[3.48], F200[3.51], C201[3.52]
	-13.9	Y44, A99[1.30], A102[1.33], A103[1.34], V126[1.57], I130, L189[3.40], L193[3.44], I197[3.48]
Histamine H1 receptor		
Histamine H1 receptor, inactive, Human 3rze		
3rze_EC	-14.1	L154[4.52], L157[4.55], I160[4.58], P161[4.59], G164[4.62], W165, N166, H167, F190[5.38]
	-12.8	S35[1.40], C38[1.43], V42[1.47], L46[1.51], L74[2.51], A78[2.55], P82[2.59], I85[2.62], L86[2.63], L89[2.66]
3rze_IC	-13.9	L207[5.55], Y210[5.58], G418[6.38], A422[6.42], I425[6.45], L426[6.46], I429[6.49], I433[6.53]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
-13.8		L39[1.44], V42[1.47], G43[1.48], L46[1.51], I482[8.57], L483[8.58], H484[8.59], I485
-13.1		L49[1.54], Y50[1.55], R53[1.58], V71[2.48], L74[2.51], I75[2.52], V79[2.56], F102[3.27], M106[3.31]
-13.3		L64[2.41], V67[2.44], S68[2.45], V71[2.48], F102[3.27], I148[4.46], W152[4.50], F156[4.54]
Leukotriene BLT1 receptor		
Leukotriene BLT1 receptor, inactive, Human 5x33		
5x33_EC	-14.5	S28[1.42], M31[1.45], V32[1.46], L35[1.49], P36[1.50], P74[2.60], L77[2.63], H78[2.64], T81, W82
	-13.8	R93[3.28], Y97[3.32], V141[4.49], G145[4.53], F148[4.56], L149[4.57], T152[4.60], L155[4.63]
	-13.4	I19[1.33], A234[6.48], F235[6.49], P238[6.52], Q261[7.29], A265[7.33], V268[7.36], C269[7.37], L272[7.40]
	-13.3	A234[6.48], L237[6.51], P238[6.52], V241[6.55], V242[6.56], V245[6.59], L262[7.30], A265[7.33]
	-13.0	L71[2.57], T72[2.58], F75[2.61], F87[3.22], A90[3.25], G91[3.26], L94[3.29], C95[3.30]
	-12.9	L64[2.50], A90[3.25], R93[3.28], L94[3.29], Y97[3.32], I98[3.33], F148[4.56], L155[4.63]
5x33_IC	-15.1	N61[2.47], L64[2.50], I98[3.33], V101[3.36], R137[4.45], L140[4.48], V141[4.49], W144[4.52], F148[4.56]
	-12.6	L108[3.43], T111[3.46], A112[3.47], L115[3.50], D116[3.51], L139[4.47], A146[4.54], L150[4.58], F186[5.43]
	-12.4	F196[5.53], V200[5.57], Y203[5.60], A204[5.61], S207[5.64], I229[6.43], L230[6.44], L237[6.51]
Lysophosphatidic acid receptor 1		
Lysophosphatidic acid receptor 1, inactive, Human 4z34		
4z34_EC	-16.0	F97[2.52], L122[3.26], L123[3.27], G126[3.30], L127[3.31], T130[3.34], I176[4.54], G179[4.57], S183[4.61]
	-14.8	I268[6.45], T272[6.49], P273[6.50], V276[6.53], L280[6.57], D288[7.30], Y292[7.34], F296[7.38]
	-12.8	L215[5.48], F218[5.51], V219[5.52], V222[5.55], T272[6.49], V276[6.53], L279[6.56], L280[6.57], C283[6.60]
	-12.0	W45, M53[1.36], G54[1.37], I57[1.40], T58[1.41], I61[1.44], L65[1.48], F107[2.62]
	-11.6	M64[1.47], L65[1.48], L68[1.51], F96[2.51], L100[2.55], F103[2.58], Y104[2.59], F107[2.62]
4z34_IC	-13.0	M71[1.54], Y75[1.58], Y86[2.41], A93[2.48], F97[2.52], I168[4.46], W172[4.50], I176[4.54]
	-13.2	M64[1.47], L65[1.48], L68[1.51], L69[1.52], F96[2.51], L100[2.55], I325[8.57], L326[8.58]
Lysophosphatidic acid receptor 1, inactive, Human 4z35		
4z35_EC	-14.7	F97[2.52], L123[3.27], L127[3.31], T130[3.34], W172[4.50], I176[4.54], G179[4.57], A180[4.58], S183[4.61]
	-13.0	I212[5.45], L215[5.48], V219[5.52], V276[6.53], L279[6.56], L280[6.57], C283[6.60], C284[6.61]
	-12.4	I268[6.45], I269[6.46], T272[6.49], P273[6.50], V276[6.53], L280[6.57], C284[6.61], C287, D288[7.30]
	-11.7	L140[3.44], M174[4.52], V177[4.55], M178[4.56], I181[4.59], W186, F209[5.42], F213[5.46]
4z35_IC	-14.9	M71[1.54], I74[1.57], Y75[1.58], Y86[2.41], A89[2.44], A93[2.48], I168[4.46], W172[4.50], I176[4.54]
Lysophosphatidic acid receptor 1, inactive, Human 4z36		
4z36_EC	-14.8	F97[2.52], L122[3.26], L123[3.27], G126[3.30], L127[3.31], T130[3.34], W172[4.50], I176[4.54], G179[4.57], A180[4.58], S183[4.61]
	-12.5	I268[6.45], I269[6.46], T272[6.49], P273[6.50], V276[6.53], L280[6.57], D288[7.30], Y292[7.34]
	-12.2	I212[5.45], L215[5.48], F218[5.51], V219[5.52], V222[5.55], I268[6.45], T272[6.49], V276[6.53], L279[6.56], C283[6.60]
4z36_IC	-14.1	M71[1.54], I74[1.57], Y75[1.58], Y86[2.41], A89[2.44], N90[2.45], I168[4.46], W172[4.50], I176[4.54]
	-12.6	L140[3.44], I144[3.48], H147[3.51], I148[3.52], M174[4.52], M178[4.56], F213[5.46], L224[5.57]
	-12.5	L140[3.44], A141[3.45], I144[3.48], E145[3.49], I148[3.52], V167[4.45], V170[4.48], M178[4.56]
	-13.0	L68[1.51], M71[1.54], V72[1.55], Y75[1.58], V76[1.59], F96[2.51], F97[2.52], L100[2.55]
	-12.4	V222[5.55], F229[5.62], V261[6.38], G265[6.42], I268[6.45], I269[6.46], T272[6.49], V276[6.53]
	-12.3	I262[6.39], A266[6.43], I269[6.46], F296[7.38], L299[7.41], M306[7.48], Y313[7.55], R314[7.56]



PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Muscarinic AChR		
Muscarinic M1 receptor, inactive, Human 5cxv		
5cxv_EC	-14.2	K20, Q24[1.31], F27[1.34], I28[1.35], T31[1.38], L86[2.65], T398[7.33], E401[7.36], L402[7.37], W405[7.40]
	-13.3	L376[6.46], T379[6.49], P380[6.50], I383[6.53], M384[6.54], V387[6.57], C394, V395, P396[7.31], L399[7.34]
	-12.6	V25[1.32], G29[1.36], G33[1.40], S36[1.43], L37[1.44], V40[1.47], T76[2.55], N80[2.59], T84[2.63], L87[2.66], M88[2.67]
	-12.6	Q110[3.37], M114[3.41], L156[4.56], W164[4.64], F182, I188[5.38], T192[5.42], A195[5.45], A196[5.46]
5cxv_IC	-14.9	Y62[2.41], L65[2.44], S66[2.45], C69[2.48], A143[4.43], I146[4.46], G147[4.47], W150[4.50], F154[4.54]
	-12.8	I73[2.52], L104[3.31], V107[3.34], A143[4.43], L144[4.44], G147[4.47], L148[4.48], W150[4.50], L151[4.51], F154[4.54]
	-12.7	A369[6.39], L376[6.46], L406[7.41], V409[7.44], I413[7.48], M416[7.51], C417[7.52], L420[7.55]
	-12.7	S36[1.43], L37[1.44], V40[1.47], T41[1.48], L44[1.51], L45[1.52], I48[1.55], L432[8.57], L433[8.58], C435
	-12.1	L34[1.41], L37[1.44], A38[1.45], T41[1.48], G42[1.49], L45[1.52], M416[7.51], L420[7.55], F429[8.54], L433[8.58]
Muscarinic M2 receptor, inactive, Human 3uon		
3uon_EC	-14.9	I26[1.35], V29[1.38], A30[1.39], L33[1.42], T81[2.62], T84[2.65], V85[2.66], T423[7.36], W427[7.40], I431[7.44]
	-13.4	N108[3.37], V111[3.40], M112[3.41], L154[4.56], W162[4.64], F180, F181, V186[5.38], T190[5.42], A193[5.45], A194[5.46]
	-12.7	V27[1.36], G31[1.40], S34[1.43], I38[1.47], N78[2.59], T81[2.62], L82[2.63], V85[2.66]
	-12.3	I398[6.46], A401[6.49], P402[6.50], V405[6.53], M406[6.54], C416, I417, P418[7.31], V421[7.34]
3uon_IC	-15.0	L98[3.27], A101[3.30], L102[3.31], G141[4.43], I144[4.46], A145[4.47], W148[4.50], V149[4.51], F152[4.54]
	-13.9	V29[1.38], L33[1.42], V36[1.45], I431[7.44], T434[7.47], I435[7.48], A438[7.51], A441[7.54], L442[7.55], K448[8.51]
	-13.2	L35[1.44], I38[1.47], I39[1.48], I42[1.51], L43[1.52], V46[1.55], L454[8.57], L455[8.58]
	-12.8	A391[6.39], L394[6.42], A395[6.43], I398[6.46], L428[7.41], I431[7.44], I435[7.48], C439[7.52], C443[7.56]
	-12.5	M112[3.41], L115[3.44], F119[3.48], F123[3.52], M143[4.45], L150[4.52], L154[4.56], T190[5.42], A193[5.45], A194[5.46]
	-12.2	F195[5.47], Y196[5.48], V199[5.51], T203[5.55], Y206[5.58], W207[5.59], S210[5.62], I397[6.45], A401[6.49], N404[6.52], V405[6.53]
	-12.2	S32[1.41], L35[1.44], V36[1.45], I39[1.48], L43[1.52], K448[8.51], F451[8.54], L455[8.58]
Muscarinic M2 receptor, active state, agonist bound, Human 4mq5		
4mq5_EC	-14.4	E22[1.31], V23[1.32], F25[1.34], I26[1.35], V29[1.38], L33[1.42], I424[7.37], I431[7.44]
	-12.5	L394[6.42], I398[6.46], P402[6.50], V405[6.53], M406[6.54], I409[6.57], I417, V421[7.34]
4mq5_IC	-14.6	T203[5.55], Y206[5.58], W207[5.59], S210[5.62], I389[6.37], L390[6.38], L393[6.41], L394[6.42], I397[6.45]
	-13.6	F63[2.44], S64[2.45], I71[2.52], L102[3.31], I144[4.46], A145[4.47], W148[4.50], F152[4.54], A156[4.58]
	-13.4	L35[1.44], I38[1.47], I39[1.48], I42[1.51], L43[1.52], V74[2.55], L454[8.57], L455[8.58]
	-13.0	A391[6.39], A395[6.43], I398[6.46], L428[7.41], I431[7.44], I435[7.48], A438[7.51], C439[7.52], C443[7.56]
	-12.4	V29[1.38], L33[1.42], V36[1.45], L43[1.52], I431[7.44], T434[7.47], I435[7.48], L442[7.55], F451[8.54]
	-13.4	L28[1.37], S32[1.41], L35[1.44], V36[1.45], I39[1.48], L43[1.52], F451[8.54], L455[8.58]
Muscarinic M3 receptor, inactive, Rat 4daj		
4daj_EC	-13.5	N152[3.37], V155[3.40], M156[3.41], L198[4.56], A202[4.60], W206[4.64], F224, T234[5.42], A237[5.45], A238[5.46], M241[5.49], P242[5.50]
	-13.3	V197[4.55], L198[4.56], P201[4.59], A202[4.60], F205[4.63], W206[4.64], Y208[4.66], F209[4.67]
	-13.3	I70[1.35], A71[1.36], L73[1.38], T74[1.39], L77[1.42], I128[2.65], L527[7.37], W530[7.40], L531[7.41], I534[7.44]
4daj_IC	-14.0	Y104[2.41], L107[2.44], S108[2.45], C111[2.48], I115[2.52], I146[3.31], G189[4.47], W192[4.50], F196[4.54]
	-13.1	M156[3.41], L159[3.44], V160[3.45], F163[3.48], F167[3.52], M187[4.45], I194[4.52], L198[4.56], A237[5.45], A238[5.46], M241[5.49]
	-12.5	A494[6.39], L497[6.42], A498[6.43], I501[6.46], T502[6.47], L531[7.41], I534[7.44], V538[7.48], C542[7.52], L545[7.55], C546[7.56]
Muscarinic M4 receptor, inactive, Human 5dsg		
5dsg_EC	-14.6	E31[1.31], F34[1.34], I35[1.35], V38[1.38], I93[2.65], T433[7.33], I437[7.37], W440[7.40], L441[7.41], V444[7.44]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-13.9	H24, T29[1.29], M32[1.32], V33[1.33], A36[1.36], G40[1.40], L44[1.44], N87[2.59], I94[2.66]
	-13.4	L411[6.46], T414[6.49], P415[6.50], V418[6.53], M419[6.54], V422[6.57], C429, I430, P431[7.31], V434[7.34]
	-13.0	V103[3.23], D106[3.26], L107[3.27], F161[4.54], L169[4.62], F170[4.63], Q172[4.65], R178
	-12.2	N117[3.37], M121[3.41], L163[4.56], F189, V195[5.38], T199[5.42], A202[5.45], A203[5.46]
5dsg_IC	-14.2	Y69[2.41], F72[2.44], S73[2.45], I80[2.52], L111[3.31], G150[4.43], I153[4.46], A154[4.47], W157[4.50], F161[4.54]
	-14.0	R400[6.35], F403[6.38], A404[6.39], L407[6.42], L411[6.46], L441[7.41], I448[7.48], C452[7.52], C456[7.56]
	-13.4	N117[3.37], M121[3.41], L124[3.44], I125[3.45], F128[3.48], F132[3.52], Y140, M152[4.45], L163[4.56], A202[5.45], A203[5.46]
	-13.2	L42[1.42], V45[1.45], G49[1.49], L52[1.52], V444[7.44], T447[7.47], I448[7.48], P450[7.50], A451[7.51], A454[7.54], F464[8.54], L468[8.58]
	-12.1	M54[1.54], K58[1.58], F72[2.44], C76[2.48], L79[2.51], I80[2.52], F84[2.56], L111[3.31]
	-12.0	I51[1.51], M54[1.54], L55[1.55], K58[1.58], F72[2.44], L79[2.51], A83[2.55], F84[2.56]
Neuropeptide Y1 receptor		
Neuropeptide Y1 receptor, inactive, Human 5zbh		
5zbh_EC	-12.9	W129[3.41], L165[4.52], A168[4.55], S169[4.56], P172[4.59], Y211[5.38], L214[5.41], Q219[5.46]
	-12.5	F84[2.48], I91[2.55], M92[2.56], F96[2.60], F108, G109[3.21], A111[3.23], M112[3.24]
	-12.2	V274[6.46], L277[6.49], P278[6.50], I281[6.53], F282[6.54], V285[6.57], L301[7.34], C305[7.38]
5zbh_IC	-14.5	W129[3.41], V132[3.44], L133[3.45], V136[3.48], W148, H154[4.41], G158[4.45], V161[4.48], L165[4.52]
	-13.2	L66[1.58], I77[2.41], V80[2.44], N81[2.45], F84[2.48], Y156[4.43], I159[4.46], W163[4.50]
Neuropeptide Y1 receptor, inactive, Human 5zbq		
5zbq_EC	-13.5	L165[4.52], A168[4.55], S169[4.56], P172[4.59], I175[4.62], Y176[4.63], L214[5.41], L218[5.45]
	-12.2	M39[1.31], T42[1.34], L43[1.35], A46[1.38], L300[7.33], L304[7.37], L307[7.40], I311[7.44]
	-12.0	I51[1.43], V55[1.47], L59[1.51], I91[2.55], P95[2.59], F96[2.60], V99[2.63], F108
	-12.8	I40[1.32], A44[1.36], G48[1.40], I51[1.43], I52[1.44], F98[2.62], V99[2.63], L102[2.66]
5zbq_IC	-13.4	L66[1.58], I77[2.41], V80[2.44], F84[2.48], Y156[4.43], I159[4.46], W163[4.50], V167[4.54]
	-12.6	S267[6.39], V274[6.46], T308[7.41], V315[7.48], I318[7.51], F319[7.52], F322[7.55], Q328[8.51]
Neurotensin NTS1 receptor		
Neurotensin receptor NTS1, active intermediate, agonist bound, Rat 3zev		
3zev_EC	-13.6	D60, Y62[1.30], S63[1.31], L66[1.34], V67[1.35], I70[1.38], Y349[7.33], M352[7.36], L353[7.37], L357[7.41], V360[7.44]
	-12.6	L199[4.55], L200[4.56], I202[4.58], P203[4.59], F206[4.62], T207[4.63], V229, T233[5.34], V237[5.38]
	-12.4	L247[5.48], L251[5.52], L322[6.49], V326[6.53], L329[6.56], M330[6.57], Y333[6.60], I334[6.61]
	-12.7	V319[6.46], L322[6.49], P323[6.50], V326[6.53], M330[6.57], I334[6.61], L343[7.27], F346[7.30], F350[7.34]
	-12.1	A140[3.23], R143[3.26], G144[3.27], F147[3.30], W194[4.50], L195[4.51], A198[4.54], L205[4.61]
	-12.6	L115[2.52], L119[2.56], V123[2.60], A136, F137, G138[3.21], G141[3.24], L148[3.31]
3zev_IC	-14.9	F75[1.43], T79[1.47], V80[1.48], S83[1.51], V84[1.52], F87[1.55], L118[2.55], T383[8.57], L384[8.58], C386
	-14.2	L247[5.48], L251[5.52], S254[5.55], T258[5.59], R311[6.38], V314[6.41], I315[6.42], V318[6.45], L322[6.49]
	-12.9	Y104[2.41], L111[2.48], F147[3.30], I190[4.46], S191[4.47], W194[4.50], L195[4.51], A198[4.54]
	-13.3	A69[1.37], I70[1.38], A73[1.41], V77[1.45], I367[7.51], N370[7.54], F380[8.54], L381[8.55]
	-12.5	A312[6.39], I315[6.42], A316[6.43], V319[6.46], C320[6.47], L353[7.37], L357[7.41], V360[7.44], L368[7.52]
	-12.8	I70[1.38], L74[1.42], A356[7.40], L357[7.41], V360[7.44], I364[7.48], I367[7.51], L371[7.55]
Neurotensin receptor NTS1, active intermediate, agonist bound, Rat 4buo		
4buo_EC	-14.3	D60, Y62[1.30], S63[1.31], L66[1.34], V67[1.35], I70[1.38], Y349[7.33], M352[7.36], L353[7.37], A356[7.40], L357[7.41], V360[7.44]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
4buo_IC	-13.6	F75[1.43], T79[1.47], V80[1.48], S83[1.51], V84[1.52], F87[1.55], L118[2.55], P122[2.59], T383[8.57], L384[8.58]
Neurotensin receptor NTS1, active intermediate, agonist bound, Rat 4bv0		
4bv0_EC	-14.5	D60, S63[1.31], L66[1.34], V67[1.35], I70[1.38], Y349[7.33], L353[7.37], A356[7.40], L357[7.41], V360[7.44]
	-12.7	L111[2.48], L115[2.52], F119[2.56], F137, G138[3.21], A140[3.23], G141[3.24], L148[3.31]
4bv0_IC	-14.6	T79[1.47], V80[1.48], G83[1.51], V84[1.52], F87[1.55], L118[2.55], F119[2.56], T383[8.57], L384[8.58], C386, L387
	-14.0	S254[5.55], N257[5.58], T258[5.59], A261[5.62], R311[6.38], V314[6.41], I315[6.42], V318[6.45], L322[6.49]
	-13.5	Y104[2.41], G107[2.44], S108[2.45], L111[2.48], F147[3.30], I190[4.46], S191[4.47], W194[4.50], A198[4.54]
	-13.5	G83[1.51], L86[1.54], F87[1.55], A90[1.58], L111[2.48], L114[2.51], L115[2.52], F119[2.56]
Neurotensin receptor NTS1, active state, Rat 4grv		
4grv_EC	-14.0	D60, S63[1.31], L66[1.34], V67[1.35], I70[1.38], Y349[7.33], M352[7.36], L353[7.37], A356[7.40], L357[7.41], A360[7.44]
	-12.8	K235[5.36], V236[5.37], Q239[5.40], V240[5.41], F243[5.44], M244[5.45], F248[5.49], Y333[6.60]
	-12.8	L199[4.55], L200[4.56], I202[4.58], P203[4.59], F206[4.62], T207[4.63], V229, V237[5.38]
	-13.0	F75[1.43], T79[1.47], L118[2.55], P122[2.59], L125[2.62], Y126[2.63], W130[2.67], V131[2.68]
4grv_IC	-13.5	Y104[2.41], S108[2.45], L111[2.48], F147[3.30], L148[3.31], K187[4.43], I190[4.46], S191[4.47], W194[4.50]
	-13.3	M250[5.51], S254[5.55], T258[5.59], R311[6.38], V314[6.41], I315[6.42], V318[6.45], L322[6.49]
	-12.6	I70[1.38], L74[1.42], L308[6.35], A312[6.39], I315[6.42], A316[6.43], V319[6.46], C320[6.47], A356[7.40], L357[7.41], A360[7.44], I364[7.48]
	-12.2	F75[1.43], T79[1.47], V80[1.48], S83[1.51], V84[1.52], F87[1.55], L118[2.55], P122[2.59]
Neurotensin receptor NTS1, active state, Rat 4xee		
4ee_EC	-14.5	D60, S63[1.31], L66[1.34], I70[1.38], Y349[7.33], M352[7.36], L353[7.37], A356[7.40], L357[7.41], A360[7.44]
	-13.3	L247[5.48], L251[5.52], L322[6.49], V326[6.53], L329[6.56], M330[6.57], Y333[6.60], I334[6.61]
	-12.9	A196[4.52], L199[4.55], L200[4.56], I202[4.58], P203[4.59], F206[4.62], T207[4.63], T233[5.34], V237[5.38]
	-12.7	L72[1.40], F75[1.43], V76[1.44], T79[1.47], L125[2.62], Y126[2.63], W130[2.67], V131[2.68]
	-12.5	A140[3.23], R143[3.26], G144[3.27], F147[3.30], L195[4.51], A198[4.54], I202[4.58], L205[4.61]
	-12.6	I61[1.29], V65[1.33], T68[1.36], A69[1.37], L72[1.40], A73[1.41], V76[1.44], W130[2.67]
	-12.5	F75[1.43], T79[1.47], L118[2.55], P122[2.59], V123[2.60], Y126[2.63], A136, F137
4xee_IC	-14.2	S83[1.51], V84[1.52], L86[1.54], F87[1.55], L111[2.48], L114[2.51], L115[2.52], L118[2.55], L119[2.56]
	-13.3	Y104[2.41], S108[2.45], L111[2.48], F147[3.30], L148[3.31], K187[4.43], I190[4.46], S191[4.47], W194[4.50]
	-13.3	F75[1.43], T79[1.47], V80[1.48], S83[1.51], V84[1.52], L118[2.55], T383[8.57], L384[8.58]
	-13.2	M250[5.51], S254[5.55], T258[5.59], R311[6.38], V314[6.41], I315[6.42], V318[6.45], L322[6.49]
	-13.0	I70[1.38], L74[1.42], A312[6.39], A316[6.43], A356[7.40], L357[7.41], A360[7.44], I364[7.48], L368[7.52]
	-12.8	L158[3.41], K188[4.44], F189[4.45], A192[4.48], I193[4.49], A196[4.52], L200[4.56], V240[5.41], M244[5.45]
Neurotensin receptor NTS1, active state, Rat 4xes		
4xes_EC	-13.3	D60, S63[1.31], L66[1.34], V67[1.35], I70[1.38], L74[1.42], Y349[7.33], M352[7.36], L353[7.37], A356[7.40], A360[7.44]
	-12.9	F246[5.47], L247[5.48], M250[5.51], L251[5.52], L322[6.49], V326[6.53], L329[6.56], M330[6.57], I334[6.61]
	-12.7	L118[2.55], L119[2.56], V123[2.60], F137, G138[3.21], A140[3.23], G141[3.24], C142[3.25]
4xes_IC	-14.2	A69[1.37], A73[1.41], V76[1.44], V77[1.45], V80[1.48], F380[8.54], L381[8.55], T383[8.57]
	-13.6	L111[2.48], L115[2.52], L119[2.56], L148[3.31], K187[4.43], I190[4.46], S191[4.47], W194[4.50]
	-13.4	F246[5.47], M250[5.51], S254[5.55], T258[5.59], R311[6.38], V314[6.41], V318[6.45], L322[6.49]
	-13.1	I70[1.38], L74[1.42], V77[1.45], A356[7.40], L357[7.41], A360[7.44], I364[7.48], I367[7.51], F380[8.54]
	-13.0	S83[1.51], L86[1.54], F87[1.55], L111[2.48], L114[2.51], L115[2.52], L118[2.55], L119[2.56]
	-12.7	I70[1.38], L74[1.42], A312[6.39], A316[6.43], A356[7.40], L357[7.41], A360[7.44], I364[7.48], L368[7.52]
	-13.0	F75[1.43], T79[1.47], V80[1.48], S83[1.51], V84[1.52], F87[1.55], L118[2.55], P122[2.59]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Neurotensin receptor NTS1, active state, Rat 5t04		
5t04_EC	-13.1	D60, S63[1.31], L66[1.34], V67[1.35], I70[1.38], L74[1.42], Y349[7.33], M352[7.36], L353[7.37], L357[7.41], A360[7.44]
	-12.7	D139[3.22], A140[3.23], R143[3.26], G144[3.27], F147[3.30], L148[3.31], L195[4.51], A198[4.54], L205[4.61]
	-13.3	L111[2.48], L115[2.52], L119[2.56], F137, A140[3.23], G141[3.24], G144[3.27], L148[3.31]
	-12.9	L247[5.48], M250[5.51], L251[5.52], L322[6.49], V326[6.53], L329[6.56], M330[6.57], Y333[6.60], I334[6.61]
	-12.5	T68[1.36], L72[1.40], F75[1.43], T79[1.47], P122[2.59], L125[2.62], Y126[2.63], W130[2.67], V131[2.68]
	-12.2	V319[6.46], L322[6.49], P323[6.50], V326[6.53], M330[6.57], I334[6.61], F346[7.30], F350[7.34]
5t04_IC	-14.0	M250[5.51], S254[5.55], T258[5.59], R311[6.38], V314[6.41], I315[6.42], V318[6.45], L322[6.49]
	-13.5	Y104[2.41], L111[2.48], L115[2.52], L119[2.56], L148[3.31], K187[4.43], I190[4.46], S191[4.47], W194[4.50]
	-13.0	L86[1.54], F87[1.55], A90[1.58], L111[2.48], L114[2.51], L115[2.52], L118[2.55], L119[2.56]
	-12.3	I70[1.38], L308[6.35], A312[6.39], I315[6.42], A316[6.43], V319[6.46], C320[6.47], L353[7.37], A356[7.40], L357[7.41], A360[7.44], I364[7.48], L368[7.52]
Opioid receptor		
Opioid delta receptor, inactive, Mouse 4ej4		
4ej4_EC	-12.7	V271[6.45], V272[6.46], A275[6.49], P276[6.50], I279[6.53], F280[6.54], V283[6.57], I289, V296[7.31]
	-12.7	L175[4.52], G178[4.55], V179[4.56], P182[4.59], M186[4.63], F202, W209[5.34], V212[5.37], T213[5.38], F220[5.45]
	-12.6	T53[1.36], S57[1.40], A61[1.44], L65[1.48], P103[2.58], S106[2.61], A107[2.62], L110[2.65], M111[2.66], F116
	-12.6	F218[5.43], F222[5.47], V223[5.48], I226[5.51], L227[5.52], I279[6.53], I282[6.56], V283[6.57], L286[6.60], V287[6.61]
4ej4_IC	-14.6	F89[2.44], N90[2.45], L93[2.48], L97[2.52], Y130[3.34], K166[4.43], N169[4.46], I170[4.47], W173[4.50]
	-12.6	V144[3.48], Y147[3.51], I148[3.52], V224[5.49], L227[5.52], I228[5.53], V231[5.56], C232[5.57]
	-12.3	R261[6.35], V265[6.39], A269[6.43], V272[6.46], L302[7.37], L306[7.41], L313[7.48], L317[7.52]
	-12.8	F137[3.41], M141[3.45], V144[3.48], F159, K164[4.41], L167[4.44], I168[4.45], L175[4.52], F220[5.45], V224[5.49], P225[5.50]
	-13.7	F222[5.47], R261[6.35], L264[6.38], V265[6.39], G268[6.42], V271[6.45], V272[6.46], A275[6.49], I279[6.53]
Opioid delta receptor, inactive, Human 4n6h		
4n6h_EC	-15.1	F133[3.37], F137[3.41], L175[4.52], G178[4.55], V179[4.56], F202, W209[5.34], V212[5.37], T213[5.38], C216[5.41], F220[5.45]
	-13.7	V272[6.46], A275[6.49], P276[6.50], I279[6.53], F280[6.54], V283[6.57], I289, V296[7.31], A299[7.34], C303[7.38]
	-12.7	S44[1.27], A47[1.30], L48[1.31], A51[1.34], L55[1.38], P294[7.29], A298[7.33], L302[7.37]
	-12.4	F218[5.43], F222[5.47], I226[5.51], A275[6.49], I279[6.53], I282[6.56], V283[6.57], V287[6.61]
	-12.0	T53[1.36], S57[1.40], A61[1.44], L65[1.48], P103[2.58], S106[2.61], A107[2.62], L110[2.65]
	-11.9	L64[1.47], M71[1.54], L93[2.48], A96[2.51], L97[2.52], S100[2.55], L119[3.23], L120[3.24], A123[3.27]
	-12.3	L93[2.48], L119[3.23], K122[3.26], A123[3.27], S126[3.30], Y130[3.34], W173[4.50], M184[4.61]
4n6h_IC	-13.6	I74[1.57], V75[1.58], K81, I86[2.41], F89[2.44], K166[4.43], N169[4.46], I170[4.47], W173[4.50]
	-13.6	L64[1.47], L65[1.48], V68[1.51], L69[1.52], F72[1.55], L332[8.57], C333[8.58], K335[8.60], P336
Opioid delta receptor, inactive, Human 4rwa		
4rwa_EC	-13.4	S44[1.27], A47[1.30], L48[1.31], A51[1.34], L55[1.38], P294[7.29], L295[7.30], A298[7.33], L302[7.37]
	-13.2	V272[6.46], A275[6.49], P276[6.50], I279[6.53], F280[6.54], V283[6.57], I289, V296[7.31], A299[7.34]
	-12.7	F137[3.41], L175[4.52], V179[4.56], Y208[5.33], W209[5.34], V212[5.37], T213[5.38], C216[5.41], F220[5.45]
	-12.6	V174[4.51], L175[4.52], G178[4.55], V181[4.58], P182[4.59], V185[4.62], M186[4.63], W209[5.34]
4rwa_IC	-14.3	A58[1.41], A61[1.44], V62[1.45], L65[1.48], L69[1.52], F329[8.54], R330[8.55], L332[8.57], C333[8.58]
	-13.1	V75[1.58], K81, I86[2.41], F89[2.44], L93[2.48], Y130[3.34], K166[4.43], I170[4.47], W173[4.50]
	-12.4	F222[5.47], I226[5.51], T230[5.55], Y233[5.58], L237[5.62], L264[6.38], V271[6.45], A275[6.49], I279[6.53]
	-12.9	L55[1.38], A58[1.41], V62[1.45], V316[7.51], A319[7.54], F320[7.55], F329[8.54], R330[8.55]
	-12.4	V68[1.51], M71[1.54], F72[1.55], V75[1.58], R76[1.59], L93[2.48], L97[2.52], S100[2.55]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.3	F137[3.41], T140[3.44], M141[3.45], V144[3.48], Y147[3.51], I148[3.52], H152[3.56], L175[4.52], F220[5.45], V224[5.49], I228[5.53]
	-12.4	L55[1.38], L306[7.41], A309[7.44], L313[7.48], V316[7.51], L317[7.52], F320[7.55], L321[7.56]
Opioid delta receptor, inactive, Human 4rwd		
4rwd_EC	-14.5	L175[4.52], G178[4.55], V179[4.56], P182[4.59], M186[4.63], F202, W209[5.34], D210[5.35], V212[5.37], T213[5.38], C216[5.41], F220[5.45]
	-13.4	V272[6.46], A275[6.49], P276[6.50], I279[6.53], F280[6.54], V283[6.57], I289, V296[7.31], A299[7.34], C303[7.38]
	-12.6	F218[5.43], F222[5.47], V223[5.48], I226[5.51], I279[6.53], I282[6.56], V283[6.57], V287[6.61]
	-12.0	S57[1.40], C60[1.43], A61[1.44], P103[2.58], S106[2.61], A107[2.62], L110[2.65], M111[2.66]
4rwd_IC	-16.1	I74[1.57], V75[1.58], K81, I86[2.41], F89[2.44], N90[2.45], L93[2.48], Y130[3.34], K166[4.43], N169[4.46], I170[4.47], W173[4.50], S177[4.54]
	-12.8	F137[3.41], T140[3.44], V144[3.48], Y147[3.51], K155, F159, L175[4.52], F220[5.45], V224[5.49], P225[5.50], I228[5.53]
	-12.5	F222[5.47], V223[5.48], I226[5.51], T230[5.55], Y233[5.58], L237[5.62], L264[6.38], V271[6.45]
Opioid kappa receptor, inactive, Human 4djh		
4djh_EC	-14.0	Y66[1.39], S67[1.40], F70[1.43], V71[1.44], P113[2.58], S116[2.61], T117[2.62], L120[2.65]
	-13.5	F143[3.37], F147[3.41], L185[4.52], S188[4.55], V189[4.56], S192[4.59], L196[4.63], W222[5.34], F225[5.37], M226[5.38], C229[5.41], F233[5.45]
4djh_IC	-13.6	F99[2.44], L103[2.48], L107[2.52], I137[3.31], Y140[3.34], K176[4.43], I180[4.47], W183[4.50]
	-12.4	A64[1.37], S67[1.40], V68[1.41], V71[1.44], V72[1.45], V75[1.48], L79[1.52], F341[8.54], C345[8.58]
	-11.9	Y246[5.58], I250[5.62], L277[6.38], A281[6.42], V284[6.45], V285[6.46], T288[6.49], P289[6.50]
	-11.8	R274[6.35], V278[6.39], V282[6.43], V285[6.46], L318[7.41], T321[7.44], L325[7.48], L329[7.52], L333[7.56]
Opioid kappa receptor, active, with cholesterol, Human 6b73		
6b73_EC	-12.9	F147[3.41], L185[4.52], S188[4.55], V189[4.56], S192[4.59], L196[4.63], W222[5.34], F225[5.37], M226[5.38], F233[5.45], I237[5.49]
	-12.6	V284[6.45], V285[6.46], T288[6.49], P289[6.50], I292[6.53], F293[6.54], V296[6.57], T302
	-12.0	L107[2.52], K132[3.26], I133[3.27], S136[3.30], I137[3.31], Y140[3.34], N141[3.35], I194[4.61]
	-12.0	F231[5.43], F235[5.47], V239[5.51], L240[5.52], I292[6.53], L295[6.56], V296[6.57], L299[6.60]
	-12.0	F70[1.43], V71[1.44], V75[1.48], P113[2.58], S116[2.61], T117[2.62], L120[2.65], M121[2.66]
6b73_IC	-13.4	M90, I96[2.41], F99[2.44], N100[2.45], L103[2.48], Y140[3.34], K176[4.43], N179[4.46], W183[4.50]
	-13.2	V154[3.48], Y157[3.51], I158[3.52], V236[5.48], I237[5.49], L240[5.52], I241[5.53], V244[5.56], C245[5.57]
Opioid mu receptor, inactive, with cholesterol, Mouse 4dkl		
4dkl_EC	-14.2	L194[4.52], A197[4.55], I198[4.56], F221, W228[5.34], L231[5.37], L232[5.38], C235[5.41]
	-14.0	I290[6.45], V291[6.46], T294[6.49], P295[6.50], I298[6.53], Y299[6.54], I302[6.57], I308, P309, F313[7.30], S317[7.34]
	-12.7	F237[5.43], F241[5.47], I242[5.48], V245[5.51], I298[6.53], I301[6.56], I302[6.57], L305[6.60], I306[6.61]
4dkl_IC	-13.7	F108[2.44], L112[2.48], L116[2.52], I146[3.31], Y149[3.34], K185[4.43], V189[4.47], W192[4.50]
	-13.2	V245[5.51], Y252[5.58], L283[6.38], V284[6.39], V286[6.41], A287[6.42], I290[6.45], T294[6.49], I298[6.53]
	-12.3	Y106[2.42], C159[3.44], T160[3.45], V163[3.48], D164[3.49], V187[4.45], L194[4.52], F239[5.45], I247[5.53]
Opioid mu receptor, active, with cholesterol, Mouse 5c1m		
5c1m_EC	-15.4	L194[4.52], A197[4.55], I198[4.56], P201[4.59], M205[4.63], F221, S222, W228[5.34], L231[5.37], C235[5.41], F239[5.45]
	-14.4	I290[6.45], T294[6.49], P295[6.50], I298[6.53], Y299[6.54], I302[6.57], I308, F313[7.30], Q314[7.31], S317[7.34]
	-13.6	V291[6.46], P295[6.50], Y299[6.54], I302[6.57], I308, F313[7.30], Q314[7.31], S317[7.34], F320[7.37], C321[7.38], L324[7.41]
5c1m_IC	-13.6	Y166[3.51], I238[5.44], F239[5.45], M243[5.49], L246[5.52], I247[5.53], V250[5.56], C251[5.57], L254[5.60]
	-13.1	M99, I105[2.41], F108[2.44], N109[2.45], L112[2.48], I146[3.31], Y149[3.34], K185[4.43], N188[4.46], W192[4.50]
	-12.6	T249[5.55], Y252[5.58], G253[5.59], I256[5.62], V282[6.37], L283[6.38], V286[6.41], I290[6.45]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.6	F237[5.43], F241[5.47], I242[5.48], V245[5.51], L246[5.52], T249[5.55], G253[5.59], I256[5.62], L283[6.38], V286[6.41], I290[6.45]
	-12.5	F87[1.51], M90[1.54], Y91[1.55], V94[1.58], R95[1.59], L112[2.48], L116[2.52], I146[3.31]
	-12.5	L74[1.38], I77[1.41], V81[1.45], F84[1.48], L88[1.52], T327[7.44], C330[7.47], L331[7.48], V334[7.51], F338[7.55]
Opioid NOP receptor, inactive, Human 4ea3		
4ea3_EC	-13.5	L95[2.48], L99[2.52], K124[3.26], T125[3.27], A128[3.30], Y132[3.34], W175[4.50], V183[4.58], A186[4.61], I187[4.62]
	-13.3	F135[3.37], F139[3.41], L177[4.52], V180[4.55], V181[4.56], P184[4.59], F215[5.38], C218[5.41], I219[5.42], F222[5.45], V226[5.49]
	-11.9	L50[1.31], A299[7.33], I300[7.34], F303[7.37], C304[7.38], L307[7.41], V310[7.44], L314[7.48]
4ea3_IC	-14.7	L77[1.58], F91[2.44], L95[2.48], Y132[3.34], Q168[4.43], N171[4.46], V172[4.47], W175[4.50], S179[4.54], V183[4.58]
	-13.0	I231[5.54], S232[5.55], Y235[5.58], S236[5.59], I239[5.62], L266[6.38], A270[6.42], V273[6.45], G274[6.46], T277[6.49]
	-12.7	L57[1.38], A60[1.41], G64[1.45], G68[1.49], L71[1.52], C313[7.47], P316[7.50], I317[7.51], A320[7.54], F330[8.54]
	-12.7	F139[3.41], T142[3.44], A143[3.45], V146[3.48], V170[4.45], L177[4.52], F222[5.45], V230[5.53]
	-13.3	V146[3.48], Y149[3.51], F222[5.45], V226[5.49], L229[5.52], V230[5.53], V233[5.56], C234[5.57]
	-12.8	R263[6.35], L266[6.38], V267[6.39], A270[6.42], V271[6.43], G274[6.46], P278[6.50], L307[7.41]
	-12.7	L57[1.38], V267[6.39], V271[6.43], L307[7.41], V310[7.44], L314[7.48], L318[7.52], L322[7.56]
Opioid NOP receptor, inactive, Human 5dhg		
5dhg_EC	-13.7	L95[2.48], L99[2.52], K124[3.26], T125[3.27], A128[3.30], Y132[3.34], W175[4.50], V183[4.58], A186[4.61], I187[4.62]
	-12.9	F139[3.41], L177[4.52], V180[4.55], V181[4.56], P184[4.59], M188[4.63], P205, W211[5.34], F215[5.38], I219[5.42], F222[5.45]
	-11.8	L50[1.31], T296[7.30], A299[7.33], I300[7.34], F303[7.37], L307[7.41], V310[7.44], L314[7.48]
5dhg_IC	-14.1	L77[1.58], F91[2.44], L95[2.48], Y132[3.34], Q168[4.43], V172[4.47], W175[4.50], S179[4.54]
Opioid NOP receptor, inactive, Human 5dhh		
5dhh_EC	-12.9	F135[3.37], F139[3.41], L177[4.52], V181[4.56], P184[4.59], M188[4.63], P205, W211[5.34], F215[5.38], F222[5.45]
	-12.5	L99[2.52], A121[3.23], K124[3.26], T125[3.27], A128[3.30], I129[3.31], Y132[3.34], A186[4.61]
5dhh_IC	-14.5	I88[2.41], F91[2.44], L95[2.48], Y132[3.34], Q168[4.43], N171[4.46], V172[4.47], W175[4.50], V183[4.58]
	-13.2	F139[3.41], T142[3.44], A143[3.45], V146[3.48], V170[4.45], L177[4.52], F222[5.45], V230[5.53]
	-13.2	C70[1.51], Y74[1.55], L77[1.58], R78[1.59], T98[2.51], L99[2.52], L102[2.55], I129[3.31]
	-12.8	V146[3.48], Y149[3.51], F222[5.45], V226[5.49], L229[5.52], V230[5.53], V233[5.56], C234[5.57], L237[5.60]
Opsin		
Opsin, Bovine 3cap		
3cap_EC	-14.2	V81[2.48], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.3	W35[1.30], Q36[1.31], M39[1.34], Y43[1.38], L46[1.41], L50[1.45], I286[7.33], F293[7.40]
	-12.9	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-12.7	L216[5.51], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], T277[6.60], H278[6.61]
	-12.5	I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], Y96[2.63], F105
	-12.3	A158[4.47], W161[4.50], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-12.0	L262[6.45], I263[6.46], L266[6.49], P267[6.50], I286[7.33], F287[7.34], I290[7.37], F294[7.41]
3cap_IC	-14.3	F208[5.43], F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60], L266[6.49]
	-13.0	W126[3.41], I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
	-12.9	I133[3.48], E134[3.49], V137[3.52], F148, M155[4.44], G156[4.45], F159[4.48], V162[4.51]
	-12.5	T62[1.57], Y74[2.41], L77[2.44], N78[2.45], V81[2.48], F85[2.52], F116[3.31], W161[4.50]
Opsin, Bovine 3dqb		

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
3dq <sub>b</sub> _EC	-14.2	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.1	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F283, F287[7.34]
	-13.1	F159[4.48], V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-12.6	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], L46[1.41], I286[7.33], F293[7.40]
	-13.7	L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], H278[6.61]
	-13.0	I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], Y96[2.63], F105
	-13.0	W175, S202[5.37], F203[5.38], I205[5.40], Y206[5.41], V209[5.44], V210[5.45], I214[5.49]
3dq <sub>b</sub> _IC	-14.0	F208[5.43], F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60]
	-13.5	L59[1.54], T62[1.57], V63[1.58], R69, L77[2.44], V81[2.48], F85[2.52], F116[3.31], W161[4.50]
	-13.2	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
Opsin, Bovine 4j4q		
4j4q_EC	-15.2	F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28]
	-13.5	V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175, Y206[5.41]
	-12.8	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F283, F287[7.34]
4j4q_IC	-13.2	F208[5.43], F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], Q225[5.60]
	-12.7	Y43[1.38], L46[1.41], R252[6.35], I256[6.39], F293[7.40], Y301[7.48], V304[7.51], M309[7.56]
	-12.4	F220[5.55], G224[5.59], V227[5.62], V254[6.37], I255[6.38], V258[6.41], I259[6.42], L262[6.45]
Opsin, Bovine 4pxf		
4pxf_EC	-14.5	F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], C110[3.25], L112[3.27], E113[3.28]
	-13.4	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], F293[7.40]
	-13.0	L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], T277[6.60], H278[6.61]
	-13.0	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F283, F287[7.34]
	-12.2	F159[4.48], V162[4.51], M163[4.52], A166[4.55], P170[4.59], V173[4.62], W175, Y206[5.41]
	-12.4	W175, S202[5.37], F203[5.38], I205[5.40], Y206[5.41], V209[5.44], V210[5.45], I214[5.49]
4pxf_IC	-12.9	F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60], L266[6.49]
	-12.8	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
Opsin, Bovine 4x1h		
4x1h_EC	-14.6	F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28]
	-13.2	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F283, F287[7.34]
	-12.8	Q36[1.31], F37[1.32], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], F293[7.40]
	-12.3	W175, E201[5.36], S202[5.37], I205[5.40], Y206[5.41], V209[5.44], V210[5.45], I214[5.49]
	-12.4	F159[4.48], V162[4.51], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175, Y206[5.41]
	-14.7	L59[1.54], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
4x1h_IC	-13.2	F208[5.43], F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], Q225[5.60]
	-12.7	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], V210[5.45], I214[5.49], V218[5.53], F221[5.56]
Opsin, Bovine 5te3		
5te3_EC	-14.5	F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28]
	-14.1	F159[4.48], V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175
	-13.6	Q36[1.31], F37[1.32], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], F293[7.40]
	-12.8	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-13.5	L216[5.51], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], T277[6.60], H278[6.61]
	-12.4	I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], Y96[2.63], F105
5te3_IC	-12.9	F208[5.43], F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], L266[6.49]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.4	W126[3.41], I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56]
	-12.3	Y74[2.41], L77[2.44], N78[2.45], V81[2.48], F85[2.52], F116[3.31], V157[4.46], W161[4.50]
	-12.2	F56[1.51], L59[1.54], Y60[1.55], V63[1.58], Q64[1.59], L84[2.51], F85[2.52], F88[2.55]
Opsin, Bovine 5wkt		
5wkt_EC	-14.2	F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.2	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F283, F287[7.34]
	-13.0	Q36[1.31], F37[1.32], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], F293[7.40]
	-12.5	F159[4.48], V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
5wkt_IC	-13.7	F208[5.43], F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], Q225[5.60]
	-12.3	W126[3.41], I133[3.48], Y136[3.51], V137[3.52], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
Opsin, Bovine 6fk6		
6fk6_EC	-14.6	F85[2.52], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-12.9	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], A42[1.37], Y43[1.38], L46[1.41], M183, I286[7.33], F293[7.40]
	-12.8	F208[5.43], L216[5.51], L262[6.45], W265[6.48], L266[6.49], A269[6.52], A272[6.55], F273[6.56], F276[6.59]
	-12.6	F159[4.48], M163[4.52], A166[4.55], P170[4.59], V173[4.62], W175, Y206[5.41], V210[5.45]
	-12.2	A158[4.47], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-12.1	F85[2.52], F115[3.30], F116[3.31], L119[3.34], W161[4.50], L165[4.54], A169[4.58], L172[4.61], V173[4.62]
6fk6_IC	-13.7	I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60], W265[6.48]
	-13.7	L59[1.54], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
	-12.9	I133[3.48], Y136[3.51], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56]
Opsin, Bovine 6fk7		
6fk7_EC	-14.3	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.6	I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], I286[7.33], F287[7.34], I290[7.37]
	-13.6	W35[1.30], Q36[1.31], M39[1.34], Y43[1.38], L46[1.41], L50[1.45], F293[7.40], F294[7.41], T297[7.44]
	-12.9	F159[4.48], V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175
	-12.3	F85[2.52], F115[3.30], F116[3.31], L119[3.34], W161[4.50], L165[4.54], A169[4.58], L172[4.61], V173[4.62]
6fk7_IC	-14.0	L59[1.54], Y60[1.55], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
Opsin, Bovine 6fk8		
6fk8_EC	-14.5	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.3	I263[6.46], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34], I290[7.37], P291[7.38]
	-13.0	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], L46[1.41], M183, I286[7.33], F293[7.40]
	-12.9	F159[4.48], V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175
	-12.3	V81[2.48], F85[2.52], F115[3.30], F116[3.31], L119[3.34], W161[4.50], L165[4.54], A169[4.58], L172[4.61], V173[4.62]
6fk8_IC	-14.0	L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60], W265[6.48], L266[6.49]
	-13.8	L59[1.54], T62[1.57], V63[1.58], R69, L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
	-12.7	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
Opsin, Bovine 6fk9		
6fk9_EC	-14.4	F88[2.55], G89[2.56], T92[2.59], T93[2.60], F103, F105, G109[3.24], C110[3.25], L112[3.27], E113[3.28]
	-13.7	W35[1.30], Q36[1.31], M39[1.34], Y43[1.38], L46[1.41], L50[1.45], F293[7.40], F294[7.41], T297[7.44]
	-13.6	V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175
	-12.4	F159[4.48], M163[4.52], W175, S202[5.37], I205[5.40], Y206[5.41], V209[5.44], V210[5.45]
	-12.2	L262[6.45], I263[6.46], L266[6.49], P267[6.50], V271[6.54], I286[7.33], F287[7.34], I290[7.37]



PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
6fk9_IC	-12.2	F85[2.52], F115[3.30], F116[3.31], L119[3.34], W161[4.50], L165[4.54], A169[4.58], L172[4.61], V173[4.62]
	-13.7	L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60], W265[6.48], L266[6.49]
	-13.7	L59[1.54], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
	-12.9	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
Opsin, Bovine 6fka		
6fka_EC	-14.5	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.3	W35[1.30], Q36[1.31], M39[1.34], Y43[1.38], L46[1.41], L50[1.45], F293[7.40], F294[7.41], T297[7.44]
	-12.6	A158[4.47], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-12.5	F159[4.48], V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
6fka_IC	-12.5	V81[2.48], F85[2.52], F115[3.30], F116[3.31], L119[3.34], W161[4.50], L165[4.54], A169[4.58], L172[4.61], V173[4.62]
	-14.2	L59[1.54], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
	-13.9	L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60], W265[6.48], L266[6.49]
Opsin, Bovine 6fkb		
6fkb_EC	-14.5	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.6	W35[1.30], Q36[1.31], M39[1.34], Y43[1.38], L46[1.41], L50[1.45], F293[7.40], F294[7.41], T297[7.44]
	-12.8	F159[4.48], V162[4.51], M163[4.52], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175
	-12.3	A158[4.47], W161[4.50], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-12.6	F85[2.52], F115[3.30], L119[3.34], W161[4.50], L165[4.54], A169[4.58], L172[4.61], V173[4.62]
6fkb_IC	-13.1	I133[3.48], Y136[3.51], P142, M163[4.52], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
Opsin, Bovine 6fkc		
6fkc_EC	-15.1	I263[6.46], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F283, F287[7.34], M288[7.35], I290[7.37], P291[7.38]
	-14.3	F88[2.55], G89[2.56], T92[2.59], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28]
	-13.8	W35[1.30], Q36[1.31], M39[1.34], Y43[1.38], L46[1.41], F293[7.40], F294[7.41], T297[7.44]
	-12.7	A158[4.47], W161[4.50], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
6fkc_IC	-14.0	L59[1.54], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
Opsin, Bovine 6fkd		
6fkd_EC	-14.6	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.0	Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], L46[1.41], M183, I286[7.33], F293[7.40]
	-13.0	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], I286[7.33], F287[7.34], I290[7.37]
	-13.0	V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175
6fkd_IC	-14.1	F208[5.43], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], Q225[5.60], W265[6.48]
	-13.3	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
	-13.7	L59[1.54], T62[1.57], V63[1.58], R69, L77[2.44], V81[2.48], F85[2.52], W161[4.50]
Orexin receptor		
Orexin receptor Type 1, inactive, Human 4zjc		
4zjc_EC	-17.0	K43, V48[1.34], L49[1.35], A52[1.38], A338[7.33], T341[7.36], F342[7.37], W345[7.40]
	-13.1	I175[4.56], P178[4.59], W206, Y211[5.34], I214[5.37], Y215[5.38], C218[5.41], V222[5.45]
	-12.7	F220[5.43], Y224[5.47], L225[5.48], L228[5.51], A308[6.45], L312[6.49], V316[6.53], I319[6.56], L320[6.57], F324[6.61]
	-12.4	A117[3.23], K120[3.26], V121[3.27], Y124[3.30], A170[4.51], L173[4.54], A174[4.55], V177[4.58], A180[4.61]
	-12.1	L309[6.46], L312[6.49], P313[6.50], V316[6.53], L317[6.54], C339[7.34], F342[7.37], L346[7.41]
4zjc_IC	-14.0	A51[1.37], V54[1.40], A55[1.41], V58[1.44], V59[1.45], I356[7.51], N359[7.54], F360[7.55]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.8	N87[2.45], L90[2.48], L94[2.52], L125[3.31], R162[4.43], I165[4.46], L166[4.47], W169[4.50]
	-12.6	K298[6.35], V302[6.39], V306[6.43], L309[6.46], F342[7.37], L346[7.41], I356[7.51], I357[7.52], F360[7.55], L361[7.56]
	-13.1	F57[1.43], L61[1.47], V62[1.48], T65[1.51], L66[1.52], L69[1.55], A97[2.55], A372[8.57], F373[8.58]
Orexin receptor Type 2, inactive, Human 4s0v		
4s0v_EC	-14.0	Y53[1.31], V56[1.34], L57[1.35], G60[1.38], I63[1.41], A344[7.33], F348[7.37], W351[7.40]
	-13.3	S125[3.23], K128[3.26], V129[3.27], Y132[3.30], I178[4.51], C181[4.54], I182[4.55], I185[4.58], A188[4.61]
	-12.8	V179[4.52], I183[4.56], P186[4.59], W214, Y219[5.34], Y223[5.38], C226[5.41], V230[5.45]
	-12.4	I315[6.46], L318[6.49], P319[6.50], I322[6.53], L323[6.54], L326[6.57], F333, W345[7.34]
4s0v_IC	-13.7	L98[2.48], Y132[3.30], L133[3.31], R170[4.43], I173[4.46], V174[4.47], W177[4.50], C181[4.54]
	-13.1	F228[5.43], M233[5.48], L236[5.51], V240[5.55], M307[6.38], L310[6.41], L311[6.42], A314[6.45], I322[6.53]
Orexin receptor Type 2, inactive, Human 5wqc		
5wqc_EC	-13.9	Y53[1.31], V56[1.34], L57[1.35], G60[1.38], I63[1.41], A344[7.33], F348[7.37], W351[7.40]
	-13.4	S125[3.23], K128[3.26], V129[3.27], Y132[3.30], I178[4.51], C181[4.54], I182[4.55], I185[4.58]
	-13.3	V179[4.52], I183[4.56], P186[4.59], W214, Y219[5.34], P220[5.35], M222[5.37], Y223[5.38], C226[5.41]
	-12.6	Y53[1.31], V56[1.34], L57[1.35], Y343[7.32], A344[7.33], W345[7.34], T347[7.36], F348[7.37], W351[7.40]
5wqc_IC	-13.7	I62[1.40], I63[1.41], V66[1.44], V67[1.45], I362[7.51], N365[7.54], F375[8.54], F379[8.58]
	-12.9	L143[3.41], C147[3.45], L150[3.48], S172[4.45], I175[4.48], V179[4.52], I183[4.56], V230[5.45]
	-12.9	M233[5.48], L236[5.51], V240[5.55], Y243[5.58], M307[6.38], L310[6.41], L311[6.42], A314[6.45], I322[6.53]
	-12.9	F65[1.43], L69[1.47], I70[1.48], V73[1.51], L74[1.52], A378[8.57], F379[8.58], C382
	-13.5	L98[2.48], Y132[3.30], L133[3.31], R170[4.43], I173[4.46], V174[4.47], W177[4.50], C181[4.54]
	-12.8	G60[1.38], I63[1.41], V64[1.42], V312[6.43], W351[7.40], A359[7.48], I362[7.51], I363[7.52], F366[7.55], L367[7.56]
Orexin receptor Type 2, inactive, Human 5ws3		
5ws3_EC	-13.7	Y53[1.31], V56[1.34], L57[1.35], G60[1.38], I63[1.41], A344[7.33], F348[7.37], W351[7.40]
	-13.5	Q124[3.22], S125[3.23], K128[3.26], V129[3.27], Y132[3.30], I178[4.51], C181[4.54], I182[4.55], I185[4.58], A188[4.61]
	-12.6	L143[3.41], V179[4.52], I183[4.56], P186[4.59], W214, Y219[5.34], Y223[5.38], C226[5.41], V230[5.45]
5ws3_IC	-14.8	Y132[3.30], R170[4.43], V174[4.47], W177[4.50], I178[4.51], C181[4.54], I182[4.55], I185[4.58]
	-14.4	L236[5.51], M239[5.54], V240[5.55], Y243[5.58], L244[5.59], L310[6.41], L311[6.42], A314[6.45], I315[6.46], L318[6.49]
	-13.6	L69[1.47], I70[1.48], V73[1.51], L74[1.52], A378[8.57], F379[8.58], C381, C382
	-15.0	I62[1.40], V66[1.44], V67[1.45], I70[1.48], I362[7.51], N365[7.54], F375[8.54], F379[8.58]
	-12.7	L143[3.41], C147[3.45], L150[3.48], I175[4.48], V179[4.52], I183[4.56], C226[5.41], V230[5.45]
	-12.5	G60[1.38], I63[1.41], V64[1.42], V308[6.39], V312[6.43], W351[7.40], A359[7.48], I362[7.51], I363[7.52], F366[7.55], L367[7.56]
	-13.3	N95[2.45], L98[2.48], L102[2.52], T106[2.56], V129[3.27], L133[3.31], I173[4.46], W177[4.50]
P2Y receptor		
P2Y1 receptor, inactive, with cholesterol, Human 4xnv		
4xnv_EC	-12.9	I178[4.52], V181[4.55], A182[4.56], P185[4.59], Y189[4.63], Y217[5.38], C220[5.41], A224[5.45]
	-12.7	I59[1.40], F62[1.43], I63[1.44], L67[1.48], P105[2.58], I108[2.61], F109[2.62], F112[2.65]
	-12.2	F215[5.36], M219[5.40], F226[5.47], C227[5.48], L230[5.51], L234[5.55], I274[6.49], V278[6.53], T281[6.56], R285[6.60]
	-12.5	G48, F49[1.30], Y52[1.33], Y53[1.34], A56[1.37], V57[1.38], L60[1.41], L315[7.44], V319[7.48]
	-12.1	A270[6.45], I274[6.49], P275[6.50], V278[6.53], M279[6.54], M282[6.57], V302[7.31], T305[7.34]
4xnv_IC	-13.5	W83, V88[2.41], F91[2.44], N92[2.45], L95[2.48], I169[4.43], S172[4.46], V173[4.47], W176[4.50], V180[4.54]
	-13.0	Y89[2.42], L140[3.41], C144[3.45], A147[3.48], H148[3.49], I171[4.45], V175[4.49], I178[4.52], A224[5.45], M225[5.46], L232[5.53]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
P2Y1 receptor, inactive, Human 4xnw		
4xnw_EC	-14.4	I178[4.52], V181[4.55], A182[4.56], P185[4.59], Y189[4.63], S213[5.34], I216[5.37], Y217[5.38], C220[5.41]
	-13.6	F215[5.36], M219[5.40], T222[5.43], F226[5.47], C227[5.48], L230[5.51], L234[5.55], I274[6.49], V278[6.53], T281[6.56], R285[6.60]
	-13.1	F215[5.36], M219[5.40], V223[5.44], C227[5.48], V228[5.49], V231[5.52], T281[6.56], R285[6.60]
	-12.2	F49[1.30], Y53[1.34], V57[1.38], V271[6.46], V308[7.37], L312[7.41], L315[7.44], V319[7.48]
	-11.8	I59[1.40], F62[1.43], I63[1.44], L67[1.48], P105[2.58], I108[2.61], F109[2.62], F119
	-12.2	T267[6.42], A270[6.45], V271[6.46], P275[6.50], A304[7.33], T305[7.34], V308[7.37], T309[7.38], L312[7.41]
4xnw_IC	-13.7	W83, V88[2.41], F91[2.44], N92[2.45], L95[2.48], F129[3.30], K165[4.39], I169[4.43], V173[4.47], W176[4.50], V180[4.54]
	-13.0	V61[1.42], Y260[6.35], I264[6.39], L315[7.44], C318[7.47], V319[7.48], I322[7.51], L326[7.55]
	-12.9	Y89[2.42], L140[3.41], C144[3.45], A147[3.48], R162, I171[4.45], I178[4.52], A182[4.56], A224[5.45], M225[5.46]
P2Y12 receptor, inactive, with cholesterol, Human 4ntj		
4ntj_EC	-14.6	Y192[5.41], Q195[5.44], V196[5.45], W199[5.48], L203[5.52], R256[6.55], T260[6.59], L261[6.60]
	-14.5	F36[1.43], L40[1.47], L75[2.55], P78[2.58], F79[2.59], L82[2.62], R93[3.21], V96[3.24]
	-13.8	F246[6.45], I247[6.46], V250[6.49], P251[6.50], F254[6.53], A255[6.54], P258[6.57], Y259[6.58], V279[7.34]
	-13.0	I247[6.46], T275[7.30], Y278[7.33], V279[7.34], S282[7.37], T283[7.38], W285[7.40], L286[7.41], L289[7.44]
	-12.8	Q25[1.32], V26[1.33], P29[1.36], L30[1.37], T33[1.40], F37[1.44], I81[2.61], A85[2.65], L87
4ntj_IC	-14.4	N235[6.34], V236[6.35], F239[6.38], I242[6.41], A243[6.42], F246[6.45], I247[6.46], V250[6.49], P251[6.50]
	-13.8	I61[2.41], N65[2.45], I68[2.48], L72[2.52], F106[3.34], K142[4.43], V146[4.47], W149[4.50], F153[4.54], M160[4.61]
	-12.9	I120[3.48], Y123[3.51], Q124[3.52], I200[5.49], L203[5.52], I204[5.53], V207[5.56], C208[5.57]
	-13.0	L117[3.45], I120[3.48], Q124[3.52], L144[4.45], F151[4.52], I193[5.42], V196[5.45], I197[5.46], I200[5.49]
P2Y12 receptor, inactive, with cholesterol, Human 4pxz		
4pxz_EC	-12.5	I23[1.30], I247[6.46], P251[6.50], Y278[7.33], V279[7.34], S282[7.37], T283[7.38], L286[7.41]
	-12.4	F95[3.23], Q98[3.26], V99[3.27], I103[3.31], L157[4.58], M160[4.61], I161[4.62], N164
	-12.3	F246[6.45], V250[6.49], P251[6.50], F254[6.53], A255[6.54], P258[6.57], T275[7.30], L276[7.31], V279[7.34]
4pxz_IC	-13.9	I61[2.41], N65[2.45], I68[2.48], L72[2.52], I103[3.31], F106[3.34], K142[4.43], V146[4.47], W149[4.50], F153[4.54], M160[4.61]
	-12.1	L31[1.38], V34[1.41], I240[6.39], W285[7.40], L289[7.44], L293[7.48], F296[7.51], F300[7.55]
	-11.9	L117[3.45], I120[3.48], L144[4.45], Y192[5.41], I193[5.42], V196[5.45], I197[5.46], I200[5.49], I204[5.53]
P2Y12 receptor, inactive, Human 4py0		
4py0_EC	-12.2	V250[6.49], P251[6.50], F254[6.53], A255[6.54], P258[6.57], F268, T275[7.30], L276[7.31], V279[7.34]
	-12.0	F246[6.45], I247[6.46], P251[6.50], T275[7.30], Y278[7.33], V279[7.34], S282[7.37], L286[7.41]
4py0_IC	-13.5	I68[2.48], L72[2.52], I103[3.31], F106[3.34], K142[4.43], V146[4.47], W149[4.50], F153[4.54], M160[4.61]
	-12.5	W199[5.48], F202[5.51], I206[5.55], Y209[5.58], T210[5.59], I242[6.41], F246[6.45], F254[6.53]
	-12.4	L117[3.45], I120[3.48], L144[4.45], V147[4.48], F151[4.52], Y192[5.41], I193[5.42], V196[5.45], I197[5.46], I200[5.49], I204[5.53]
	-11.9	L31[1.38], I240[6.39], I247[6.46], W285[7.40], L289[7.44], L293[7.48], F296[7.51], F300[7.55]
Rhodospin active state		
Rhodopsin activate state, Bovine 2x72		
2x72_EC	-14.5	F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], Q113[3.28]
	-13.4	Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], L46[1.41], M183, I286[7.33], T289[7.36], F293[7.40]
	-12.8	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-13.0	F159[4.48], V162[4.51], M163[4.52], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
2x72_IC	-14.2	L59[1.54], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], L119[3.34], W161[4.50]
	-13.3	I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60], L266[6.49]
	-12.7	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
	-13.0	F56[1.51], L59[1.54], Y60[1.55], V63[1.58], Q64[1.59], L84[2.51], F85[2.52], F88[2.55]
Rhodopsin activate state, MII, Bovine 3pqr		
3pqr_EC	-14.4	V81[2.48], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.0	Q36[1.31], F37[1.32], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], F293[7.40]
	-12.4	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], V271[6.54], F283, F287[7.34]
	-12.4	A158[4.47], W161[4.50], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-12.3	F159[4.48], M163[4.52], A166[4.55], P170[4.59], V173[4.62], W175, Y206[5.41], V210[5.45]
3pqr_IC	-13.2	L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], H278[6.61]
	-12.9	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56]
	-12.8	L59[1.54], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
-12.6	F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], L266[6.49]	
Rhodopsin activate state, MII, Bovine 3pxo		
3pxo_EC	-14.4	F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.6	Q36[1.31], F37[1.32], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], F293[7.40]
	-13.1	F159[4.48], V162[4.51], M163[4.52], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-12.9	L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], H278[6.61]
	-12.7	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], V271[6.54], F283, F287[7.34]
3pxo_IC	-13.4	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
Rhodopsin activate state, MII, Bovine 4a4m		
4a4m_EC	-14.6	V81[2.48], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28], F116[3.31]
	-13.3	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], T289[7.36], F293[7.40]
	-13.2	W175, S202[5.37], F203[5.38], I205[5.40], Y206[5.41], V209[5.44], V210[5.45], I214[5.49]
	-13.0	I48[1.43], M49[1.44], F52[1.47], F88[2.55], T92[2.59], T93[2.60], Y96[2.63], F105
	-12.9	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F283, F287[7.34]
	-12.9	F159[4.48], M163[4.52], A166[4.55], P170[4.59], V173[4.62], W175, Y206[5.41], V210[5.45]
4a4m_IC	-13.5	F208[5.43], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60]
	-13.3	L59[1.54], T62[1.57], V63[1.58], L77[2.44], V81[2.48], F85[2.52], F116[3.31], L119[3.34], W161[4.50]
	-12.2	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56]
Rhodopsin activate state, Bovine4zww		
4zww_EC	-14.2	L88[2.55], G89[2.56], S93[2.60], F103, F105, G109[3.24], C110[3.25], L112[3.27], Q113[3.28], F116[3.31]
	-13.8	F159[4.48], V162[4.51], M163[4.52], L165[4.54], A166[4.55], A169[4.58], P170[4.59], A173[4.62], W175
	-13.8	Q36[1.31], M39[1.34], L183, I286[7.33], T289[7.36], I290[7.37], F293[7.40], F294[7.41]
4zww_IC	-14.0	F208[5.43], F212[5.47], T213[5.48], M216[5.51], I217[5.52], F220[5.55], F221[5.56], Q225[5.60]
	-12.7	F45[1.40], I48[1.43], V49[1.44], F52[1.47], P53[1.48], F56[1.51], L57[1.52], Y60[1.55], T320[8.57]
Rhodopsin activate state, with arrestin, Human 5dys		
5dys_EC	-14.4	F88[2.55], G89[2.56], T93[2.60], F103, F105, G109[3.24], L112[3.27], E113[3.28]
	-12.8	I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F283, F287[7.34]
5dys_IC		

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Rhodopsin activate state, with arrestin, Human 5w0p		
5w0p_EC	-12.8	I259[6.42], L262[6.45], I263[6.46], V266[6.49], P267[6.50], S270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-12.7	A158[4.47], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], A173[4.62], W175
	-12.5	L88[2.55], G89[2.56], S93[2.60], F105, G109[3.24], L112[3.27], Q113[3.28], F116[3.31]
5w0p_IC	-13.9	F220[5.55], Y223[5.58], G224[5.59], V227[5.62], V254[6.37], I255[6.38], V258[6.41], L262[6.45]
	-13.1	F45[1.40], I48[1.43], V49[1.44], F52[1.47], P53[1.48], F56[1.51], L57[1.52], Y60[1.55], T320[8.57]
	-15.3	F208[5.43], T213[5.48], M216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60]
Rhodopsin inactive state		
Rhodopsin inactive state, Bovine 1f88		
1f88_EC	-15.5	Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], T289[7.36], I290[7.37], F293[7.40], F294[7.41], T297[7.44]
	-13.4	L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], T277[6.60], H278[6.61]
	-12.9	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-12.7	A158[4.47], W161[4.50], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62]
	-13.5	W175, E201[5.36], S202[5.37], F203[5.38], I205[5.40], Y206[5.41], V209[5.44], V210[5.45]
1f88_IC	-13.7	T62[1.57], V63[1.58], K66, R69, Y74[2.41], L77[2.44], V157[4.46], W161[4.50], L165[4.54]
	-13.0	Y43[1.38], I256[6.39], A260[6.43], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M309[7.56]
	-12.8	F220[5.55], Y223[5.58], E232[5.67], I259[6.42], L262[6.45], I263[6.46], L266[6.49], P267[6.50]
	-13.0	F212[5.47], I213[5.48], I217[5.52], F220[5.55], F221[5.56], G224[5.59], V227[5.62], L266[6.49]
	-13.0	W126[3.41], V129[3.44], I133[3.48], Y136[3.51], F159[4.48], M163[4.52], V210[5.45], I214[5.49], V218[5.53], C222[5.57]
Rhodopsin inactive state, Bovine 1gzm		
1gzm_EC	-13.9	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], I290[7.37], F294[7.41], T297[7.44]
	-12.5	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-13.6	F212[5.47], L216[5.51], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], H278[6.61]
	-12.9	I263[6.46], P267[6.50], V271[6.54], I286[7.33], F287[7.34], I290[7.37], P291[7.38], F294[7.41]
	-13.2	F85[2.52], T108[3.23], N111[3.26], L112[3.27], F115[3.30], F116[3.31], W161[4.50], L165[4.54]
	-12.5	W126[3.41], F159[4.48], M163[4.52], A166[4.55], W175, Y206[5.41], V210[5.45], I214[5.49]
	-12.2	A158[4.47], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-11.9	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T108[3.23], L112[3.27], F116[3.31]
	-13.2	W175, S202[5.37], I205[5.40], Y206[5.41], V209[5.44], V210[5.45], I214[5.49], I217[5.52]
1gzm_IC	-14.2	R69, Y74[2.41], L77[2.44], N78[2.45], V81[2.48], F85[2.52], I154[4.43], V157[4.46], W161[4.50], L165[4.54]
	-12.8	I133[3.48], V137[3.52], F146, F148, H152[4.41], M155[4.44], G156[4.45], F159[4.48], V162[4.51]
	-13.0	W126[3.41], V129[3.44], I133[3.48], Y136[3.51], F159[4.48], M163[4.52], V210[5.45], I214[5.49], V218[5.53], F221[5.56]
	-12.2	Y43[1.38], L47[1.42], I256[6.39], A260[6.43], T297[7.44], Y301[7.48], I305[7.52], M309[7.56]
Rhodopsin inactive state, Bovine 1hzx		
1hzx_EC	-15.6	Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], T289[7.36], I290[7.37], F293[7.40], F294[7.41], T297[7.44]
	-15.1	F159[4.48], V162[4.51], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175, Y206[5.41]
	-13.8	F212[5.47], L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], T277[6.60], H278[6.61]
	-13.6	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-12.8	F45[1.40], I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], L95[2.62], Y96[2.63], F105
	-12.6	F85[2.52], T108[3.23], N111[3.26], L112[3.27], F115[3.30], F116[3.31], W161[4.50], L165[4.54], L172[4.61]
1hzx_IC	-13.4	Y74[2.41], L77[2.44], V81[2.48], F85[2.52], F116[3.31], I154[4.43], V157[4.46], W161[4.50]
	-13.1	Y43[1.38], I256[6.39], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M308[7.55], M309[7.56]
	-13.1	F212[5.47], I213[5.48], I217[5.52], F220[5.55], F221[5.56], Y223[5.58], G224[5.59], V227[5.62]
	-12.6	I133[3.48], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Rhodospin inactive state, Bovine 1l9h		
1l9h_EC	-14.5	W35[1.30], Q36[1.31], M39[1.34], Y43[1.38], M183, I290[7.37], F294[7.41], T297[7.44]
	-12.6	F85[2.52], T108[3.23], N111[3.26], L112[3.27], F115[3.30], F116[3.31], W161[4.50], L165[4.54], L172[4.61]
	-13.0	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T92[2.59], F105, L112[3.27]
	-12.6	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-14.4	F212[5.47], L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], H278[6.61]
	-13.9	I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], L95[2.62], Y96[2.63], F105
1l9h_IC	-13.4	Y74[2.41], L77[2.44], V81[2.48], F85[2.52], F116[3.31], I154[4.43], V157[4.46], W161[4.50]
	-13.0	Y43[1.38], I256[6.39], I263[6.46], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M308[7.55], M309[7.56]
	-12.6	W126[3.41], I133[3.48], F159[4.48], M163[4.52], Y206[5.41], V210[5.45], I214[5.49], V218[5.53], F221[5.56], C222[5.57]
Rhodospin inactive state, Bovine 1u19		
1u19_EC	-14.5	A32, Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], T289[7.36], I290[7.37], F293[7.40], F294[7.41], T297[7.44]
	-12.9	F45[1.40], I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], L95[2.62], Y96[2.63], F105
	-12.8	A158[4.47], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62], W175
	-13.0	F56[1.51], F85[2.52], F88[2.55], G89[2.56], T92[2.59], T93[2.60], F105, L112[3.27]
	-12.6	F85[2.52], L112[3.27], F115[3.30], F116[3.31], L119[3.34], W161[4.50], L165[4.54], L172[4.61]
	-12.4	F212[5.47], L216[5.51], F220[5.55], L262[6.45], L266[6.49], F273[6.56], Y274[6.57], H278[6.61]
	-13.1	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
1u19_IC	-13.5	Y74[2.41], L77[2.44], V81[2.48], I154[4.43], V157[4.46], A158[4.47], W161[4.50], L165[4.54]
	-13.0	Y43[1.38], I256[6.39], A260[6.43], I263[6.46], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M309[7.56]
	-13.1	F212[5.47], I213[5.48], I217[5.52], F220[5.55], F221[5.56], Y223[5.58], G224[5.59], L266[6.49]
Rhodospin inactive state, bathorhodopsin, Bovine 2g87		
2g87_EC	-14.3	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], T289[7.36], I290[7.37], F293[7.40], F294[7.41], T297[7.44]
	-13.1	F212[5.47], L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], T277[6.60], H278[6.61]
	-12.7	A158[4.47], W161[4.50], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62]
	-12.6	V81[2.48], F85[2.52], T108[3.23], N111[3.26], L112[3.27], F115[3.30], F116[3.31], W161[4.50], L165[4.54], L172[4.61]
	-12.5	F45[1.40], I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], L95[2.62], Y96[2.63], F105
	-12.4	M163[4.52], A166[4.55], P170[4.59], V173[4.62], W175, Y206[5.41], V210[5.45], H211[5.46]
	-13.5	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-12.8	F56[1.51], L59[1.54], V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], L112[3.27]
2g87_IC	-12.9	Y74[2.41], L77[2.44], V81[2.48], F115[3.30], I154[4.43], V157[4.46], W161[4.50], L165[4.54]
	-12.6	Y43[1.38], I256[6.39], A260[6.43], I263[6.46], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M309[7.56]
Rhodospin inactive state, lumirhodopsin, Bovine 2hpy		
2hpy_EC	-14.1	Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], T289[7.36], I290[7.37], F293[7.40], F294[7.41]
	-13.5	F159[4.48], V162[4.51], M163[4.52], A166[4.55], P170[4.59], V173[4.62], G174, W175
	-13.0	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-12.6	I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], L95[2.62], Y96[2.63], F105
	-12.6	V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], T93[2.60], F105, L112[3.27]
	-12.3	V81[2.48], F85[2.52], F115[3.30], F116[3.31], W161[4.50], L165[4.54], A169[4.58], L172[4.61], V173[4.62]
2hpy_IC	-13.5	Y74[2.41], L77[2.44], N78[2.45], V81[2.48], F85[2.52], I154[4.43], V157[4.46], W161[4.50]
	-12.7	Y43[1.38], I256[6.39], A260[6.43], I263[6.46], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M308[7.55], M309[7.56]
	-12.6	F212[5.47], I213[5.48], L216[5.51], I217[5.52], F220[5.55], F221[5.56], G224[5.59], L266[6.49]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Rhodospin inactive state, Bovine 2ped		
2ped_EC	-14.9	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], T289[7.36], I290[7.37], F293[7.40], F294[7.41], T297[7.44]
	-14.0	F212[5.47], L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], T277[6.60], H278[6.61]
	-13.1	I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], L95[2.62], Y96[2.63], F105
	-14.1	F159[4.48], V162[4.51], A166[4.55], A169[4.58], P170[4.59], V173[4.62], G174, W175
	-13.6	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-13.2	I263[6.46], P267[6.50], V271[6.54], I286[7.33], F287[7.34], I290[7.37], P291[7.38], F294[7.41]
	-12.5	F85[2.52], T108[3.23], N111[3.26], L112[3.27], F115[3.30], F116[3.31], W161[4.50], L165[4.54], L172[4.61]
2ped_IC	-13.8	F220[5.55], Y223[5.58], E232[5.67], R252[6.35], I255[6.38], I259[6.42], L262[6.45], L266[6.49]
	-13.2	Y74[2.41], L77[2.44], V81[2.48], F85[2.52], I154[4.43], V157[4.46], A158[4.47], W161[4.50], L165[4.54]
	-12.9	F212[5.47], I213[5.48], I217[5.52], F220[5.55], F221[5.56], G224[5.59], Q225[5.60], L266[6.49]
	-12.6	Y43[1.38], I256[6.39], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M308[7.55], M309[7.56]
Rhodospin inactive state, Bovine 3c9l		
3c9l_EC	-14.2	W35[1.30], Q36[1.31], M39[1.34], Y43[1.38], M183, I286[7.33], I290[7.37], T297[7.44]
	-13.0	F85[2.52], T108[3.23], N111[3.26], L112[3.27], F115[3.30], F116[3.31], W161[4.50], L165[4.54]
	-12.7	L262[6.45], I263[6.46], L266[6.49], P267[6.50], G270[6.53], V271[6.54], Y274[6.57], F287[7.34]
	-12.7	F212[5.47], L216[5.51], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], H278[6.61]
	-12.5	A158[4.47], W161[4.50], V162[4.51], L165[4.54], A166[4.55], A169[4.58], P170[4.59], V173[4.62]
3c9l_IC	-13.8	Y74[2.41], L77[2.44], N78[2.45], V81[2.48], F85[2.52], I154[4.43], V157[4.46], W161[4.50], L165[4.54]
	-12.8	Y43[1.38], I256[6.39], A260[6.43], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M308[7.55], M309[7.56]
	-12.9	L59[1.54], V63[1.58], R69, L77[2.44], V81[2.48], L84[2.51], F85[2.52], F88[2.55]
Rhodospin inactive state, Bovine 3c9m		
3c9m_EC	-14.4	Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], M183, I286[7.33], I290[7.37], F294[7.41]
	-12.9	L262[6.45], I263[6.46], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], T277[6.60], H278[6.61]
3c9m_IC	-12.9	Y43[1.38], I256[6.39], A260[6.43], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M308[7.55], M309[7.56]
	-12.8	Y74[2.41], L77[2.44], V81[2.48], F85[2.52], I154[4.43], V157[4.46], A158[4.47], W161[4.50], L165[4.54]
	-12.6	I133[3.48], Y136[3.51], F159[4.48], M163[4.52], V210[5.45], I214[5.49], V218[5.53], F221[5.56]
Rhodospin inactive state, Bovine 3oax		
3oax_EC	-13.7	W35[1.30], Q36[1.31], M39[1.34], L40[1.35], Y43[1.38], L46[1.41], M183, I286[7.33], I290[7.37]
	-13.1	F159[4.48], V162[4.51], M163[4.52], A166[4.55], P170[4.59], V173[4.62], G174, W175, Y206[5.41]
	-13.0	F45[1.40], I48[1.43], M49[1.44], F52[1.47], P53[1.48], F88[2.55], T92[2.59], L95[2.62], Y96[2.63], F105
	-12.7	I263[6.46], L266[6.49], P267[6.50], V271[6.54], I286[7.33], F287[7.34], I290[7.37], P291[7.38]
	-12.5	F212[5.47], L216[5.51], F220[5.55], L262[6.45], L266[6.49], G270[6.53], F273[6.56], Y274[6.57], H278[6.61]
	-12.5	F85[2.52], T108[3.23], N111[3.26], L112[3.27], F115[3.30], F116[3.31], W161[4.50], L165[4.54], L172[4.61]
	-12.9	L59[1.54], V81[2.48], L84[2.51], F85[2.52], F88[2.55], G89[2.56], L112[3.27], F116[3.31]
3oax_IC	-13.4	V63[1.58], Y74[2.41], L77[2.44], I154[4.43], V157[4.46], A158[4.47], W161[4.50], L165[4.54]
	-12.7	Y43[1.38], I256[6.39], A260[6.43], I263[6.46], F294[7.41], T297[7.44], Y301[7.48], V304[7.51], I305[7.52], M308[7.55], M309[7.56]
Rhodospin inactive state, Squid 2z73		
2z73_EC	-14.3	L272[6.46], P276[6.50], V280[6.54], W291, T293[7.31], Y295[7.33], A296[7.34], P300[7.38], F303[7.41]
	-13.4	F78[2.48], F81[2.51], T82[2.52], L85[2.55], V86[2.56], L91[2.61], F103, G104[3.21], A107[3.24], V110[3.27]
	-13.2	F210[5.48], I213[5.51], V279[6.53], L282[6.56], L283[6.57], F286[6.60], G287[6.61], P288

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.2	F78[2.48], A106[3.23], K109[3.26], V110[3.27], F113[3.30], I114[3.31], W160[4.50], I171[4.61]
2z73_IC	-13.3	I213[5.51], I216[5.54], F217[5.55], Y220[5.58], F221[5.59], V224[5.62], I264[6.38], L271[6.45], S275[6.49], V279[6.53]
	-13.0	G53[1.51], I56[1.54], Y57[1.55], T60[1.58], K61[1.59], F78[2.48], F81[2.51], L85[2.55]
	-13.5	C49[1.47], G50[1.48], G53[1.51], I54[1.52], Y57[1.55], F81[2.51], L85[2.55], F89[2.59], P90[2.60], F330[8.58]
	-12.7	I131[3.48], N135[3.52], I206[5.44], L207[5.45], G211[5.49], L214[5.52], I215[5.53], F218[5.56], C219[5.57]
	-12.5	T60[1.58], M71[2.41], I74[2.44], F153[4.43], I156[4.46], I157[4.47], W160[4.50], L161[4.51], V164[4.54]
Rhodospin inactive state, Squid 3ayn		
3ayn_EC	-14.1	L272[6.46], P276[6.50], V279[6.53], V280[6.54], L283[6.57], W291, T293[7.31], A296[7.34], P300[7.38]
	-14.0	F210[5.48], I213[5.51], L271[6.45], V279[6.53], L282[6.56], L283[6.57], F286[6.60], G287[6.61], P288
	-13.3	L272[6.46], P276[6.50], T293[7.31], Y295[7.33], A296[7.34], L299[7.37], P300[7.38], F303[7.41]
	-12.6	F78[2.48], F81[2.51], T82[2.52], L85[2.55], V86[2.56], P90[2.60], L91[2.61], F103, A107[3.24], V110[3.27]
3ayn_IC	-14.7	I39[1.37], F40[1.38], I43[1.41], I47[1.45], W332, V333, L334, T335, C336
	-14.0	I39[1.37], I43[1.41], I46[1.44], I47[1.45], W332, V333, L334, T335, C336
	-13.4	G45[1.43], I46[1.44], C49[1.47], G50[1.48], G53[1.51], Y57[1.55], F81[2.51], L85[2.55], F89[2.59], F330[8.58]
	-13.3	I213[5.51], I216[5.54], F217[5.55], Y220[5.58], F221[5.59], V224[5.62], L271[6.45], S275[6.49], V279[6.53]
	-12.8	I131[3.48], Y134[3.51], I206[5.44], L207[5.45], L214[5.52], I215[5.53], F218[5.56], C219[5.57]
Sphingosine 1-phosphate receptor (S1P1) receptor		
Sphingosine 1-phosphate receptor (S1P1), inactive, Human 3v2y		
3v2y_EC	-13.0	K41, S44[1.31], T48[1.35], V51[1.38], F52[1.39], I55[1.42], R292[7.34], Y295[7.37]
	-11.8	F133[3.41], I170[4.52], I173[4.55], L174[4.56], L177[4.59], W182, F205[5.42], L213[5.50]
3v2y_IC	-13.9	L61[1.48], I64[1.51], F65[1.52], L68[1.55], I325[8.57], M326[8.58], G327[8.59], R328, L330
	-13.0	L67[1.54], I70[1.57], W71[1.58], Y82[2.41], L89[2.48], F161[4.43], I164[4.46], S165[4.47], W168[4.50], V169[4.51], L172[4.54]
	-12.4	I64[1.51], L67[1.54], I70[1.57], W71[1.58], Y82[2.41], L89[2.48], L92[2.51], L93[2.52], V96[2.55]
Thrombin receptor 1 (PAR1)		
Thrombin receptor 1 (PAR1), inactive, Human 3vw7		
3vw7_EC	-13.1	F319[6.41], I323[6.45], I324[6.46], P328[6.50], F351[7.33], A352[7.34], L355[7.37], C356[7.38]
	-13.1	T110[1.40], F113[1.43], V114[1.44], P118[1.48], P156[2.58], I159[2.61], S160[2.62], F170
	-13.0	A228[4.51], L229[4.52], A232[4.55], P236[4.59], K240[4.63], L263, Y267[5.35], Y270[5.38]
	-12.7	V149[2.51], L150[2.52], S153[2.55], V154[2.56], F157[2.59], E173[3.23], L174[3.24], F177[3.27]
	-12.7	F280[5.48], L283[5.51], F319[6.41], I323[6.45], P328[6.50], V331[6.53], L332[6.54], A352[7.34]
3vw7_IC	-13.5	G111[1.41], V112[1.42], V115[1.45], L119[1.49], C365[7.47], P368[7.50], L369[7.51], Y372[7.54]
	-13.1	V139[2.41], H143[2.45], L216[4.39], S220[4.43], C223[4.46], L224[4.47], W227[4.50], I231[4.54]
	-13.0	Y140[2.42], L191[3.41], T194[3.44], V195[3.45], I198[3.48], T222[4.45], L229[4.52], F274[5.42], V277[5.45], F278[5.46], P282[5.50], I285[5.53]
Viral GPCR Receptor (US28)		
Viral GPCR Receptor (US28), inactive, with cholesterol, 4xt1		
4xt1_EC	-14.4	A77[2.48], L80[2.51], L81[2.52], C84[2.55], L88[2.59], S101[3.22], V102[3.23], P103[3.24]
	-13.3	I238[6.45], I239[6.46], L242[6.49], P243[6.50], L246[6.53], T247[6.54], S268[7.30], L269[7.31], R271[7.33], A272[7.34]
	-12.6	T105[3.26], L106[3.27], A109[3.30], V113[3.34], W152[4.50], V156[4.54], F163[4.61], M164[4.62]
	-12.5	L37[1.36], F38[1.37], G41[1.40], V42[1.41], L45[1.44], F46[1.45], M90[2.61], L94[2.65]



PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Run1.3	-14.0	I64, V70[2.41], I73[2.44], N74[2.45], A77[2.48], L81[2.52], C110[3.31], V113[3.34], C145[4.43], S148[4.46], I149[4.47], W152[4.50]
Run1.11	-13.1	T123[3.44], L127[3.48], Y131[3.52], W151[4.49], F154[4.52], I158[4.56], I199[5.49], V203[5.53]
Run1.14	-12.8	M193[5.43], F197[5.47], V198[5.48], L201[5.51], S202[5.52], S205[5.55], Y206[5.56], Y209[5.59], L246[6.53], F249[6.56]

## Viral GPCR Receptor (US28), inactive, with cholesterol, 4xt3

4xt3_EC	-12.8	I238[6.45], I239[6.46], L242[6.49], P243[6.50], L246[6.53], T247[6.54], V250[6.57], F265[7.27], L269[7.31], A272[7.34]
	-12.5	F154[4.52], I157[4.55], I158[4.56], I160[4.58], P161[4.59], V165, L180, Y184[5.34]
	-12.7	I239[6.46], F240[6.47], S268[7.30], R271[7.33], A272[7.34], L275[7.37], T276[7.38], L279[7.41]
	-11.9	L37[1.36], F38[1.37], G41[1.40], V42[1.41], L45[1.44], F46[1.45], M90[2.61], L94[2.65]
	-12.5	V35[1.34], F38[1.37], L39[1.38], V42[1.41], F46[1.45], R271[7.33], L275[7.37], L279[7.41], C282[7.44], L286[7.48]
Run1.2	-14.0	I64, V70[2.41], I73[2.44], N74[2.45], A77[2.48], L81[2.52], C110[3.31], C145[4.43], S148[4.46], I149[4.47], W152[4.50]
Run1.11	-13.3	L127[3.48], Y131[3.52], F154[4.52], I158[4.56], E191[5.41], L194[5.44], I199[5.49], V203[5.53]
Run1.14	-13.2	L127[3.48], Y130[3.51], Y131[3.52], L194[5.44], V198[5.48], I199[5.49], S202[5.52], V203[5.53]
Run2.8	-13.6	E124[3.45], L127[3.48], R139, F147[4.45], F150[4.48], W151[4.49], F154[4.52], I157[4.55]
Run2.17	-12.8	L201[5.51], S205[5.55], Y208[5.58], Y209[5.59], S212[5.62], I231[6.38], V234[6.41], L235[6.42], I238[6.45]

## GPCR Class B

## Calcitonin receptor-like receptor

## Calcitonin receptor-like receptor, inactive, Human 6e3y

6e3y_EC	-13.5	I123.E, I127.E[1.25], L131.E[1.29], H289, Y292[5.37], C299[5.44], A300[5.45], L303[5.48], V304[5.49], R355
	-12.8	I146[1.44], I153[1.51], A154[1.52], L157[1.55], I192[2.65], I193[2.66], T196[2.69], A197[2.70]
	-12.7	F182[2.55], C186[2.59], V190[2.63], I193[2.66], S211[3.28], C212[3.29], V214[3.31], S215[3.32], I218[3.35], L222[3.39]
	-12.7	N140[1.38], Y143[1.41], L144[1.42], I147[1.45], L151[1.49], I371[7.44], F375[7.48], L378[7.51]
	-12.3	V210[3.27], K213[3.30], V214[3.31], F217[3.34], L264[4.54], C268[4.58], A271[4.61], W283
6e3y_IC	-13.7	R336[6.40], I340[6.44], I371[7.44], F375[7.48], L378[7.51], L379[7.52], T382[7.55], I383[7.56]
	-13.6	F164[1.62], N179[2.52], F182[2.55], F217[3.34], I218[3.35], Y221[3.38], Y256[4.46], W260[4.50], L264[4.54]
	-12.6	L131.E[1.29], A135.E[1.33], V138.E[1.36], K142.E[1.40], L303[5.48], V304[5.49], F307[5.52], F308[5.53]
	-12.8	L157[1.55], L160[1.58], G161[1.59], I162[1.60], F164[1.62], Y165[1.63], F182[2.55], V185[2.58]

## Corticotropin CRF1R

## Corticotropin CRF1R, inactive, Human 4k5y

4k5y_EC	-13.2	G186[3.27], R189[3.30], L190[3.31], A193[3.34], A194[3.35], Y197[3.38], F198[3.39], W236[4.50], F240[4.54], I243[4.57], A247[4.61], L251[4.65], W259
	-12.9	F204[3.45], F207[3.48], I234[4.48], V238[4.52], I242[4.56], A245[4.59], I271[5.38], P275[5.42], L278[5.45], V279[5.46]
4k5y_IC	-13.9	N157[2.52], L164[2.59], A194[3.35], Y197[3.38], F198[3.39], I232[4.46], W236[4.50], F240[4.54]
	-13.5	F207[3.48], C211[3.52], T215[3.56], M230[4.44], F231[4.45], I234[4.48], L278[5.45], I282[5.49], F286[5.53]
	-12.3	H214[3.55], V218[3.59], L278[5.45], L281[5.48], I282[5.49], I285[5.52], F286[5.53], N289[5.56]
	-12.0	L135[1.55], F138[1.58], V139[1.59], L142[1.62], L164[2.59], A167[2.62], T168[2.63], V171[2.66]

## Corticotropin CRF1R, inactive, Human 4z9g

4z9g_EC	-13.5	P321[6.47], I325[6.51], L329[6.55], E336, S340[7.34], V343[7.37], F344[7.38], F347[7.41]
	-13.2	F204[3.45], V238[4.52], I242[4.56], A245[4.59], Y253[4.67], I271[5.38], P275[5.42], L278[5.45]
4z9g_IC	-13.8	F204[3.45], F207[3.48], C211[3.52], T215[3.56], R225, L226[4.40], I234[4.48], V238[4.52], I242[4.56], P275[5.42], L278[5.45], I282[5.49]
	-13.5	L142[1.62], I147, I153[2.48], N157[2.52], L164[2.59], Y197[3.38], I232[4.46], W236[4.50]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Glucagon receptor		
Glucagon receptor, inactive, Human 4l6r		
4l6r_EC	-13.8	I315[5.47], N318[5.50], F319[5.51], F322[5.54], I355[6.46], P356[6.47], V360[6.51], V363[6.54], F367[6.58], V368
	-12.7	F322[5.54], P356[6.47], L357[6.48], V360[6.51], H361[6.52], V364[6.55], K381[7.38], F384[7.41]
	-12.7	M301[5.33], W304[5.36], W305[5.37], F309[5.41], F312[5.44], L313[5.45], L316[5.48], I317[5.49]
	-12.3	Q142[1.40], V143[1.41], T146[1.44], S150[1.48], L153[1.51], L157[1.55], L192[2.65], D195[2.68], G196[2.69]
	-12.2	Q142[1.40], V143[1.41], T146[1.44], S150[1.48], L153[1.51], G154[1.52], L157[1.55], L192[2.65], D195[2.68]
	-12.1	A222[3.27], R225[3.30], V226[3.31], V229[3.34], Y233[3.38], M276[4.54], V280[4.58], V284[4.62], L288[4.66]
4l6r_IC	-12.6	V147[1.45], L151[1.49], F391[7.48], L394[7.51], V398[7.55], F402[7.59], L403[7.60], Q408[8.51]
	-12.5	K349[6.40], T353[6.44], L357[6.48], F387[7.44], L388[7.45], L395[7.52], L399[7.56], L403[7.60]
	-12.8	F345[6.36], K349[6.40], L352[6.43], T353[6.44], P356[6.47], L357[6.48], V360[6.51], H361[6.52]
Glucagon receptor, inactive, Human 5ee7		
5ee7_EC	-14.1	Q142[1.40], T146[1.44], S150[1.48], L153[1.51], A154[1.52], L157[1.55], L192[2.65], D195[2.68], G196[2.69], T200[2.73]
	-13.5	A222[3.27], R225[3.30], V226[3.31], V229[3.34], F230[3.35], Y233[3.38], A283[4.61], C287[4.65], W295
	-12.7	I315[5.47], N318[5.50], F319[5.51], F322[5.54], I355[6.46], P356[6.47], V360[6.51], V363[6.54], V364[6.55], F367[6.58]
5ee7_IC	-14.2	L247[3.52], H250[3.55], L313[5.45], L316[5.48], I317[5.49], F320[5.52], I321[5.53], R324[5.56]
	-13.1	L157[1.55], L160[1.58], A161[1.59], G164[1.62], G165[1.63], L182[2.55], V185[2.58], S189[2.62]
Glucagon receptor, inactive, Human 5xez		
5xez_EC	-15.2	T146[1.44], S150[1.48], L153[1.51], G154[1.52], L192[2.65], D195[2.68], G196[2.69], R199[2.72]
	-13.4	R225[3.30], V226[3.31], V229[3.34], F230[3.35], M276[4.54], V280[4.58], A283[4.61], C287[4.65], N291, W295
	-13.1	W304[5.36], F312[5.44], L316[5.48], F320[5.52], V363[6.54], A366[6.57], F367[6.58], T369, D370
	-13.0	T353[6.44], L357[6.48], V360[6.51], H361[6.52], V364[6.55], K381[7.38], F384[7.41], D385[7.42]
	-12.8	V185[2.58], L186[2.59], V193[2.66], G219, A222[3.27], G223[3.28], V226[3.31], F230[3.35]
5xez_IC	-14.4	S265[4.43], L266[4.44], G269[4.47], G273[4.51], M276[4.54], L277[4.55], V280[4.58], P281[4.59], V284[4.62]
	-12.8	N179[2.52], L186[2.59], V229[3.34], F230[3.35], Y233[3.38], L268[4.46], W272[4.50], M276[4.54], V280[4.58]
	-12.7	L160[1.58], G164[1.62], A178[2.51], A182[2.55], V185[2.58], L186[2.59], S189[2.62], F230[3.35]
Glucagon receptor, inactive, Human 5xf1		
5xf1_EC	-14.2	T146[1.44], S150[1.48], L153[1.51], G154[1.52], L158[1.56], L192[2.65], G196[2.69], R199[2.72]
	-13.7	L153[1.51], L157[1.55], L160[1.58], V185[2.58], S189[2.62], L192[2.65], V193[2.66], G196[2.69], L197[2.70], R199[2.72]
	-13.5	V185[2.58], L186[2.59], S189[2.62], V193[2.66], L197[2.70], G219, G223[3.28], V226[3.31]
	-13.1	T353[6.44], P356[6.47], L357[6.48], V360[6.51], H361[6.52], V364[6.55], K381[7.38], F384[7.41], D385[7.42]
	-12.7	R225[3.30], V226[3.31], V229[3.34], F230[3.35], M276[4.54], V280[4.58], A283[4.61], C287[4.65], W295
5xf1_IC	-13.7	S265[4.43], L268[4.46], G269[4.47], G273[4.51], M276[4.54], L277[4.55], V280[4.58], P281[4.59]
	-12.8	L157[1.55], L160[1.58], G164[1.62], A178[2.51], A182[2.55], V185[2.58], L186[2.59], S189[2.62], F230[3.35]
	-13.2	N179[2.52], L186[2.59], V229[3.34], F230[3.35], Y233[3.38], L268[4.46], W272[4.50], M276[4.54]
	-13.0	K349[6.40], S350[6.41], T353[6.44], L357[6.48], L399[7.56], L403[7.60], N404[8.47], K405[8.48]
Glucagon-like peptide receptor (GLP-1R)		
Glucagon-like peptide receptor (GLP-1R), inactive, Human 5vew		
5vew_EC	-14.9	Y145[1.40], T149[1.44], V150[1.45], A153[1.48], L154[1.49], S157[1.52], I161[1.56], F195[2.65], D198[2.68]
	-12.8	P358[6.47], L359[6.48], T362[6.51], H363[6.52], I366[6.55], F367[6.56], R380[7.35], K383[7.38], L384[7.39]
	-12.8	Q140[1.35], F143[1.38], L144[1.39], I147[1.42], I382[7.37], T386[7.41], S389[7.44], F393[7.48], L396[7.51], M397[7.52]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.7	L224[3.27], L228[3.31], L231[3.34], Y235[3.38], L278[4.54], V282[4.58], I286[4.62], Y289[4.65]
5vew_IC	-13.5	Y242[3.45], L245[3.48], I272[4.48], V276[4.52], L279[4.55], F280[4.56], I308[5.38], P312[5.42], F315[5.45]
	-13.1	L167[1.62], Y178[2.48], L181[2.51], N182[2.52], A185[2.55], L189[2.59], L192[2.62], F266[4.42], W274[4.50]
	-13.1	N182[2.52], L232[3.35], Y235[3.38], F266[4.42], V270[4.46], W274[4.50], L278[4.54], V282[4.58]
Glucagon-like peptide receptor (GLP-1R), inactive, Human 5vex		
5vex_EC	-14.0	A153[1.48], F156[1.51], S157[1.52], V160[1.55], I161[1.56], F195[2.65], D198[2.68], A199[2.69]
	-13.1	F143[1.38], L144[1.39], I147[1.42], T386[7.41], S389[7.44], F390[7.45], F393[7.48], L396[7.51], M397[7.52], I400[7.55]
	-12.6	L279[4.55], F280[4.56], P283[4.59], V287[4.63], Y291[4.67], Y305[5.35], I308[5.38], P312[5.42]
5vex_IC	-13.6	Y242[3.45], L245[3.48], I272[4.48], V276[4.52], F280[4.56], I308[5.38], P312[5.42], F315[5.45]
	-13.6	L231[3.34], L232[3.35], Y235[3.38], R267[4.43], V270[4.46], A271[4.47], W274[4.50], G275[4.51], L278[4.54]
	-12.6	F324[5.54], I328[5.58], K351[6.40], L354[6.43], T355[6.44], P358[6.47], L359[6.48], T362[6.51], I366[6.55]
Glucagon-like peptide receptor (GLP-1R), active, Human 6b3j		
6b3j_EC	-14.7	Y145[1.40], T149[1.44], A153[1.48], F156[1.51], S157[1.52], V160[1.55], F195[2.65], D198[2.68]
	-13.7	F367[6.56], M371, T378[7.33], L379[7.34], I382[7.37], K383[7.38], T386[7.41], F390[7.45]
6b3j_IC	-16.4	L232[3.35], Y235[3.38], R267[4.43], V270[4.46], S271[4.47], W274[4.50], G275[4.51], L278[4.54]
	-13.2	K351[6.40], L354[6.43], T355[6.44], P358[6.47], T386[7.41], S389[7.44], F390[7.45], M397[7.52], L401[7.56]
	-12.6	K346[6.35], L349[6.38], A350[6.39], T353[6.42], L354[6.43], I366[6.55], F367[6.56], M371, T386[7.41]
	-12.3	L154[1.49], S157[1.52], A158[1.53], I161[1.56], L396[7.51], I400[7.55], C403[7.58], F404[7.59]
GPCR Class C		
Metabotropic glutamate receptor (mGlu)		
Metabotropic glutamate receptor mGlu1, inactive, dimer with cholesterol, Human 4or2		
4or2_EC	-13.5	L608.A[1.55], F639.A[2.47], W588.B, S589.B, I594.B[1.41], I597.B[1.44], A598.B[1.45], C601.B[1.48], L605.B[1.52]
	-13.3	W588.A, S589.A, I594.A[1.41], I597.A[1.44], A598.A[1.45], C601.A[1.48], L605.A[1.52], L608.B[1.55], F639.B[2.47]
	-13.3	L605.A[1.52], L608.B[1.55], F639.B[2.47], V643.B[2.51], F646.B[2.54], T647.B[2.55], T653.B, T655.B[3.27], S656.B[3.28], L659.B[3.31]
	-13.1	T793.B[6.45], I796.B[6.48], I797.B[6.49], A800.B[6.52], I804.B[6.56], Y810.B[7.27], I813.B[7.30], T814.B[7.31], F817.B[7.34], L821.B[7.38]
	-13.0	W588.A, I597.A[1.44], C601.A[1.48], L605.A[1.52], F646.A[2.54], I604.B[1.51], L608.B[1.55], F639.B[2.47], F646.B[2.54]
	-13.0	T793.A[6.45], I796.A[6.48], I797.A[6.49], A800.A[6.52], I804.A[6.56], Y810.A[7.27], I813.A[7.30], T814.A[7.31], F817.A[7.34], L821.A[7.38]
	-13.9	W588.A, F639.A[2.47], L640.A[2.48], V643.A[2.51], F646.A[2.54], T647.A[2.55], A650.A, L659.A[3.31], L663.A[3.35]
	-12.4	L713.A[4.39], V716.A[4.42], L720.A[4.46], L751.A[5.38], V754.A[5.41], A755.A[5.42], G758.A[5.45], Y759.A[5.46], L762.A[5.49]
4or2_IC	-14.6	V676.B[3.48], N680.B[3.52], R684.B[3.56], I709.B[4.35], L713.B[4.39], V716.B[4.42], Y759.B[5.46], L762.B[5.49], L763.B[5.50], S766.B[5.53], Y770.B[5.57]
	-13.1	F599.A[1.46], F789.A[6.41], F817.A[7.34], L821.A[7.38], T824.A[7.41], V825.A[7.42], G828.A[7.45], C829.A[7.46], T832.A[7.49]
	-12.7	Y786.B[6.38], T793.B[6.45], L821.B[7.38], V825.B[7.42], G828.B[7.45], C829.B[7.46], T832.B[7.49], P833.B[7.50]
	-12.3	E629.A[2.37], Y632.A[2.40], I633.A[2.41], A636.A[2.44], L640.A[2.48], L662.A[3.34], L663.A[3.35], L666.A[3.38], M670.A[3.42], W704.A[4.30], V707.A[4.33]
	-13.1	T611.A[1.58], V615.A[1.62], Y632.A[2.40], A636.A[2.44], F639.A[2.47], L640.A[2.48], V643.A[2.51], L663.A[3.35]
	-12.7	V676.A[3.48], N680.A[3.52], R684.A[3.56], I709.A[4.35], L713.A[4.39], V716.A[4.42], Y759.A[5.46], L762.A[5.49]
	-12.7	F599.B[1.46], L602.B[1.49], V606.B[1.53], F609.B[1.56], T824.B[7.41], L827.B[7.44], G828.B[7.45], T832.B[7.49], M835.B[7.52], Y836.B[7.53], I839.B[7.56]
	-13.4	L608.A[1.55], T611.A[1.58], L612.A[1.59], V615.A[1.62], F639.A[2.47], V643.A[2.51], L605.B[1.52], F609.B[1.56]
	-12.3	W704.B[4.30], V707.B[4.33], I708.B[4.34], S711.B[4.37], I712.B[4.38], S715.B[4.41], L718.B[4.44], T719.B[4.45], V722.B[4.48]
Metabotropic glutamate receptor mGlu1, inactive, Human 4oo9		

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
4oo9_EC	-12.3	L573, P578[1.38], I581[1.41], A582[1.42], V585[1.45], F586[1.46], L589[1.49], T811[7.41]
	-12.1	T780[6.45], I783[6.48], I784[6.49], I791[6.56], Y797[7.27], T801[7.31], F804[7.34], L808[7.38]
	-12.0	I699[4.38], C702[4.41], I703[4.42], G706[4.45], V709[4.48], A710[4.49], I713[4.52], M714[4.53]
	-11.7	I703[4.42], I707[4.46], L711[4.50], M714[4.53], L738[5.38], A742[5.42], Y746[5.46], L749[5.49]
4oo9_IC	-13.0	V663[3.48], T664[3.49], Y667[3.52], I696[4.35], L700[4.39], Y746[5.46], L749[5.49], L750[5.50]
	-12.5	F586[1.46], L589[1.49], A593[1.53], F596[1.56], V819[7.49], V822[7.52], Y823[7.53], L826[7.56]
	-12.5	E616[2.37], Y619[2.40], I620[2.41], A623[2.44], L627[2.48], L653[3.38], M657[3.42], L694[4.33]
	-13.1	F586[1.46], Y773[6.38], L808[7.38], T811[7.41], V812[7.42], G815[7.45], C816[7.46], V819[7.49], P820[7.50]
GPCR Class F		
Class F Frizzled FZD4		
Class F Frizzled FZD4, inactive, Human 6bd4		
6bd4_EC	-12.8	I318[3.41], I354[4.52], K358[4.56], V361[4.59], M365[4.63], G389[5.45], F390[5.46], P394[5.50], Y398[5.54], I401[5.57]
	-12.6	F218[1.31], W222[1.35], M474[7.35], A475[7.36], M478[7.39], L479[7.40], F482[7.43], M483[7.44]
6bd4_IC	-13.7	I318[3.41], V321[3.44], I322[3.45], L325[3.48], H343[4.41], Y346[4.44], F347[4.45], A350[4.48], I354[4.52], P394[5.50], T397[5.53], Y398[5.54], I401[5.57]
	-13.1	L443[6.39], V446[6.42], I450[6.46], M483[7.44], L486[7.47], M493[7.54], W494[7.55], W496[7.57]
	-12.9	F241[1.54], F257[2.46], M260[2.49], F311[3.34], F312[3.35], H348[4.46], W352[4.50], A356[4.54]
Class F Smoothened SMO		
Class F Smoothened SMO, inactive, dimer, Human 4jkv		
4jkv_EC	-14.0	D229.B[1.31], S232.B[1.34], Y233.B[1.35], A236.B[1.38], F237.B[1.39], V240.B[1.42], K519.B[7.39], I530.B[7.50]
	-13.2	L246[1.48], F275[2.52], I279[2.56], A283[2.60], M286, E292, S313[3.24], I316[3.27], I320[3.31]
	-12.8	A377[4.62], L405.B[5.48], A406.B[5.49], G409.B[5.52], I413.B[5.56], F467.B[6.48], F471.B[6.52], F474.B[6.55]
	-12.8	I413[5.56], G416[5.59], Y417[5.60], I420[5.63], F460[6.41], L464[6.45], F467[6.48], S468[6.49], F471[6.52]
	-12.5	A406[5.49], G409[5.52], L410[5.53], I413[5.56], V414[5.57], F467[6.48], F471[6.52], F474[6.55], F369.B[4.54]
	-12.4	P306.B, L312.B[3.23], V315.B[3.26], I316.B[3.27], V319.B[3.30], W365.B[4.50], F369.B[4.54], L376.B[4.61]
	-12.3	Y233[1.35], A236[1.38], F237[1.39], V240[1.42], F523[7.43], I530[7.50], T534[7.54], W537[7.57]
4jkv_IC	-14.9	R451.B[6.32], I454.B[6.35], F455.B[6.36], L458.B[6.39], F462.B[6.43], F523.B[7.43], T534.B[7.54], W537.B[7.57]
	-13.9	L410[5.53], I413[5.56], W256.B, N260.B, Y269.B[2.46], T357.B[4.42], S358.B[4.43], Y359.B[4.44], H361.B[4.46], L362.B[4.47], F369.B[4.54]
	-13.9	V253[1.55], W256, F268[2.45], Y269[2.46], A272[2.49], V276[2.53], V319[3.30], I320[3.31], Y323[3.34]
	-13.9	Y323[3.34], Y359[4.44], H361[4.46], L362[4.47], W365[4.50], F369[4.54], Y337.B[3.48], H340.B[3.51], Y417.B[5.60], F418.B[5.61], R421.B[5.64]
	-13.5	F237[1.39], E447[6.28], R451[6.32], I454[6.35], F455[6.36], L458[6.39], F523[7.43], I530[7.50], A531[7.51], T534[7.54], W537[7.57]
	-12.9	A239.B[1.41], V240.B[1.42], L243.B[1.45], C244.B[1.46], F247.B[1.49], W537.B[7.57], T538.B[8.47], L542.B[8.51]
-12.7	W339[3.50], L426[5.69], L450[6.31], I454[6.35], F457[6.38], L458[6.39], G461[6.42], L464[6.45], I465[6.46]	
Class F Smoothened SMO, inactive, Human 4n4w		
4n4w_EC	-13.5	I413[5.56], G416[5.59], I420[5.63], F460[6.41], L464[6.45], F467[6.48], S468[6.49], F471[6.52], F475[6.56]
	-13.3	L246[1.48], F275[2.52], I279[2.56], L282[2.59], A283[2.60], F285[2.62], M286, D287
	-13.0	L246[1.48], F275[2.52], I279[2.56], M286, E292, S313[3.24], I316[3.27], I317[3.28], I320[3.31]
	-12.6	L367[4.52], L371[4.56], R398[5.41], Y399[5.42], G402[5.45], F403[5.46], A406[5.49], L410[5.53]
4n4w_IC	-14.1	V319[3.30], Y323[3.34], S358[4.43], H361[4.46], L362[4.47], W365[4.50], S366[4.51], F369[4.54]
	-13.4	V330[3.41], V333[3.44], V334[3.45], Y337[3.48], F360[4.45], L363[4.48], L367[4.52], L371[4.56], P407[5.50], L410[5.53], V414[5.57], F418[5.61]
	-12.8	W256, F268[2.45], Y269[2.46], V276[2.53], V319[3.30], I320[3.31], Y323[3.34], H361[4.46], W365[4.50]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Class F Smoothened SMO, inactive, Human 4o9r		
4o9r_EC	-13.5	L246[1.48], F275[2.52], I279[2.56], L282[2.59], A283[2.60], F285[2.62], M286, D287
	-12.9	F275[2.52], V276[2.53], I279[2.56], E292, S313[3.24], I316[3.27], I317[3.28], I320[3.31]
	-12.8	L412[5.55], I413[5.56], F460[6.41], L464[6.45], F467[6.48], S468[6.49], F471[6.52], Y472[6.53], F475[6.56], N476[6.57]
	-12.7	F460[6.41], G461[6.42], L464[6.45], I465[6.46], S468[6.49], Y472[6.53], V517[7.37], I520[7.40]
4o9r_IC	-14.2	F237[1.39], R451[6.32], I454[6.35], F455[6.36], L458[6.39], F523[7.43], I530[7.50], A531[7.51], T534[7.54], W537[7.57]
Class F Smoothened SMO, inactive, Human 4qim		
4qim_EC	-12.7	I413[5.56], Y417[5.60], I420[5.63], F460[6.41], L464[6.45], F467[6.48], S468[6.49], F471[6.52]
4qim_IC	-14.3	V240[1.42], L243[1.45], F247[1.49], V536[7.56], W537[7.57], T538[8.47], K539[8.48], T541[8.50], L542[8.51]
	-13.1	L450[6.31], R451[6.32], I454[6.35], F455[6.36], L458[6.39], F523[7.43], G527[7.47], I530[7.50], A531[7.51], T534[7.54], W537[7.57]
	-13.1	V319[3.30], Y323[3.34], H361[4.46], L362[4.47], W365[4.50], S366[4.51], F369[4.54], T372[4.57]
	-12.8	W256, F268[2.45], Y269[2.46], A272[2.49], V276[2.53], I279[2.56], I320[3.31], W365[4.50]
Class F Smoothened SMO, inactive, Human 4qin		
4qin_EC	-14.1	F237[1.39], R451[6.32], I454[6.35], F455[6.36], L458[6.39], F523[7.43], I530[7.50], A531[7.51], T534[7.54], W537[7.57]
	-13.4	V319[3.30], Y323[3.34], S358[4.43], H361[4.46], L362[4.47], W365[4.50], F369[4.54], T372[4.57], V373[4.58]
	-12.9	L412[5.55], I413[5.56], G416[5.59], Y417[5.60], I420[5.63], R421[5.64], M424[5.67], L464[6.45], F467[6.48]
	-12.7	V333[3.44], Y337[3.48], F360[4.45], L363[4.48], L367[4.52], A406[5.49], L410[5.53], V414[5.57], F418[5.61]
4qin_IC	-13.0	P306, L312[3.23], V315[3.26], I316[3.27], V319[3.30], Y323[3.34], W365[4.50], F369[4.54], T372[4.57], V373[4.58], L376[4.61]
	-12.8	L246[1.48], F275[2.52], I279[2.56], A283[2.60], M286, L312[3.23], S313[3.24], I316[3.27], I317[3.28]
	-12.7	S366[4.51], L367[4.52], V370[4.55], L371[4.56], A374[4.59], V378[4.63], Y399[5.42], G402[5.45], F403[5.46]
	-12.5	L412[5.55], I413[5.56], G416[5.59], F460[6.41], L464[6.45], F467[6.48], S468[6.49], F471[6.52]
	-12.1	A401[5.44], L405[5.48], A406[5.49], G409[5.52], L412[5.55], I413[5.56], F467[6.48], F471[6.52], F474[6.55], F475[6.56]
	13.2	A239[1.41], L243[1.45], L246[1.48], F247[1.49], L282[2.59], F285[2.62], M286, D287
Class F Smoothened SMO, inactive, Human 5I7d		
5I7d_EC	-14.1	F275[2.52], I279[2.56], T311, L312[3.23], S313[3.24], I316[3.27], I317[3.28], I320[3.31]
	-12.5	L367[4.52], L371[4.56], R398[5.41], Y399[5.42], A401[5.44], G402[5.45], F403[5.46], A406[5.49]
	-12.5	D229[1.31], S232[1.34], Y233[1.35], A236[1.38], F237[1.39], V240[1.42], K519[7.39], I530[7.50], W537[7.57]
	-12.5	L412[5.55], I413[5.56], L464[6.45], F467[6.48], S468[6.49], F471[6.52], Y472[6.53], N476[6.57]
Class F Smoothened SMO, inactive, Human 5I7i		
5I7i_EC	-13.5	F275[2.52], I279[2.56], M286, E292, S313[3.24], I316[3.27], I317[3.28], I320[3.31]
5I7i_IC	-15.3	V240[1.42], L243[1.45], F247[1.49], V536[7.56], W537[7.57], T538[8.47], K539[8.48], T541[8.50], L542[8.51]
	-14.4	F237[1.39], R451[6.32], F455[6.36], L458[6.39], F462[6.43], F523[7.43], G527[7.47], I530[7.50], A531[7.51], T534[7.54], W537[7.57]
	-13.8	V319[3.30], Y323[3.34], S358[4.43], H361[4.46], L362[4.47], W365[4.50], S366[4.51], F369[4.54]
	-13.1	V253[1.55], W256, F268[2.45], Y269[2.46], V276[2.53], V319[3.30], I320[3.31], Y323[3.34]
	-12.6	V330[3.41], V333[3.44], Y337[3.48], F360[4.45], L363[4.48], L367[4.52], L410[5.53], V414[5.57], F418[5.61]
Class F Smoothened SMO, Active, Xenopus 6d32		
6d32_EC	-13.8	I215[1.44], F219[1.48], F248[2.52], I252[2.56], L255[2.59], A256[2.60], F258, M259
	-12.8	L385[5.55], I386[5.56], L437[6.45], F440[6.48], G441[6.49], F444[6.52], Y445[6.53], F448[6.56]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
	-12.4	I340[4.52], L344[4.56], H371[5.41], Y372[5.42], G375[5.45], F376[5.46], A379[5.49], L383[5.53]
	-12.3	I205[1.34], I209[1.38], S212[1.41], V213[1.42], F216[1.45], C217[1.46], F220[1.49], W510[7.57]
	-12.4	F248[2.52], A249[2.53], I252[2.56], A256[2.60], M259, A262, E265, I266, I289[3.27], I290[3.28], I293[3.31]
	-12.3	Y206[1.35], I209[1.38], F210[1.39], V213[1.42], K492[7.39], F496[7.43], I503[7.50], T507[7.54]
6d32_IC	-12.7	L385[5.55], I386[5.56], G389[5.59], Y390[5.60], I393[5.63], F433[6.41], V436[6.44], L437[6.45], F440[6.48]
	-12.6	I292[3.30], Y296[3.34], H334[4.46], L335[4.47], W338[4.50], F342[4.54], T345[4.57], V346[4.58]
	-12.5	R424[6.32], I427[6.35], L431[6.39], F435[6.43], F496[7.43], S504[7.51], T507[7.54], W508[7.55], W510[7.57], T511[8.47]
	-12.5	I303[3.41], V306[3.44], M307[3.45], I336[4.48], I340[4.52], L344[4.56], G375[5.45], F376[5.46], P380[5.50], L383[5.53]
	-13.0	W229, F241[2.45], Y242[2.46], A245[2.49], A249[2.53], I252[2.56], I293[3.31], H334[4.46]

## Class F Smoothened SMO, Active, Xenopus 6d35

6d35_EC	-13.1	F248[2.52], I252[2.56], A256[2.60], M259, E265, S286[3.24], I289[3.27], I290[3.28], I293[3.31]
	-12.9	L385[5.55], I386[5.56], L437[6.45], F440[6.48], G441[6.49], F444[6.52], Y445[6.53], F448[6.56]
	-12.7	I340[4.52], L344[4.56], H371[5.41], Y372[5.42], G375[5.45], F376[5.46], A379[5.49], L383[5.53]
	-12.5	E202[1.31], Y206[1.35], I209[1.38], F210[1.39], V213[1.42], K492[7.39], F496[7.43], I503[7.50], T507[7.54]
	-12.6	I205[1.34], A208[1.37], I209[1.38], S212[1.41], V213[1.42], F216[1.45], F258, W510[7.57]
6d35_IC	-13.2	R424[6.32], I427[6.35], L431[6.39], F496[7.43], S504[7.51], T507[7.54], W508[7.55], T511[8.47]
	-12.9	L423[6.31], G426[6.34], I427[6.35], F430[6.38], L431[6.39], F435[6.43], I438[6.46], F496[7.43]
	-12.4	N233, F241[2.45], Y242[2.46], A245[2.49], A249[2.53], I252[2.56], I293[3.31], H334[4.46]
	-13.2	A249[2.53], I292[3.30], I293[3.31], Y296[3.34], S331[4.43], H334[4.46], L335[4.47], W338[4.50]
	-12.6	I303[3.41], V306[3.44], M307[3.45], F333[4.45], I336[4.48], I340[4.52], L344[4.56], G375[5.45], L383[5.53]
	-12.5	L385[5.55], I386[5.56], G389[5.59], Y390[5.60], I393[5.63], F433[6.41], V436[6.44], L437[6.45], F440[6.48]

## Adiponectin Receptors

## GPCR Adiponectin Receptor

## Adiponectin Receptor, inactive, Human 3wxv

3wxv_EC	-13.7	L276[5], V279[5], T282[5], T286[5], F291, A294, T295, M300[6], G301[6], F304[6]
	-12.9	F145[1], L149[1], I153[1], M156[1], G174[2], L178[2], V181[2], L182[2], S185[2]
	-12.8	W302[6], I339[7], V342[7], L343[7], A346[7], F349[7], V350[7], Y353[7]
3wxv_IC	-14.9	Q265[5], T266[5], G269[5], V270[5], G273[5], L276[5], S277[5], V279[5], V280[5]
	-13.4	Q265[5], L272[5], L276[5], V279[5], I311[6], G315[6], A318[6], A319[6]
	-12.5	F304[6], A307[6], V308[6], I311[6], T312[6], L316[6], I321, F325
	-12.5	R122, F125, K126, I128, F129, F145[1], V146[1], L149[1]

PDB <sup>a</sup>	E <sup>b</sup>	Local Residues <sup>c</sup>
Adiponectin Receptor, inactive, Human 5lwy		
5lwy_EC	-13.2	Q179[2], V183[2], L186[2], L225[3], M228, V232[4], L250[4], I258, I261
	-13.1	L316[6], L320, L350[7], I353[7], F354[7], A357[7], F360, V361, H364
	-11.5	Q244[4], P245[4], I248[4], Y249[4], V252[4], L256[4], I291, H295
5lwy_IC	-13.1	G276[5], V277[5], G280[5], V281[5], G284[5], S288, I290, I291
	-12.8	R213[3], L214[3], K217[3], L218[3], S221[3], L225[3], I261, Q265[5]
Adiponectin Receptor, inactive, Human 5lx9		
5lx9_EC	-13.1	L160, M167, L178[2], K181[2], V182[2], G185[2], F188[2], L189[2], I192[2], S196
	-12.2	V183[2], L186[2], L225[3], M228, V232[4], L250[4], C254[4], I258, I261
	-12.5	L316[6], L320, L350[7], I353[7], F354[7], A357[7], F360, V361, H364
5lx9_IC	-13.5	I139[1], F140[1], R141[1], I142[1], T146[1], W150[1], L154[1], W344[7]
	-13.1	L256[4], G276[5], V277[5], G280[5], V281[5], G284[5], S288, I291
	-13.1	G276[5], A279[5], G280[5], L283[5], G284[5], L287[5], I290, A329
	-12.2	L214[3], K217[3], L218[3], S221[3], L225[3], M228, I261, Q265[5]
	-12.0	V252[4], V255[4], L256[4], A259, V263[5], W266[5], V277[5], V281[5]
Adiponectin Receptor, inactive, Human 5lxa		
5lxa_EC	-12.9	L316[6], L320, L350[7], I353[7], F354[7], A357[7], F360, V361, H364
	-12.7	Q179[2], V182[2], V183[2], Y236[4], F247[4], L250[4], I251[4], C254[4], V255[4], I258
5lxa_IC	-12.9	L189[2], L193[2], L214[3], K217[3], L218[3], S221[3], L225[3], I261, Q265[5]
	-12.0	V252[4], L256[4], V277[5], G280[5], V281[5], G284[5], S288, I291
Adiponectin Receptor, inactive, Human 5lxg		
5lxg_EC	-14.4	Q168, V171[2], V172[2], M175[2], V221[3], Y225[3], L239[4], S240[4], C243[4], V244[4], I247[4]
	-13.6	V279[5], T282[5], M283[5], T286[5], G290, F291, A294, T295, M300[6], G301[6], F304[6], A307[6], I311[6]
	-12.7	W302[6], I339[7], V342[7], L343[7], A346[7], F349[7], V350[7], Y353[7]
5lxg_IC	-12.8	Y209[3], I212[3], I216[3], F220[3], F271[5], L274[5], G275[5], G278[5], F303[6], A307[6], Y310[6], I311[6], A314[6], Y317[6], F340[7]
	-12.7	M175[2], L178[2], L214[3], M217[3], G218[3], V221[3], I247[4], I250[4], I251[4], Q254[4], D256[4], R257
	-12.2	F271[5], L272[5], G275[5], L276[5], G278[5], V279[5], T282[5], A307[6], I311[6]
	-12.3	F145[1], L149[1], I153[1], L178[2], V181[2], L182[2], S185[2], F186[2], L189[2], F204[3]

a. EC and IC refer to the extracellular and intracellular sides of the membrane respectively.

b. Docking energies in kcal mol<sup>-1</sup>.

c. Square brackets give systematic residue numbers from the GPCR database (<http://gpcrdb.org>), or, where these are not available, the TM helix number.