

Supporting Information

Conservation of allosteric ligand binding sites in G-protein coupled receptors

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Table S1. RMSD between X-ray structures and AF2 models of the 39 structures with bound allosteric ligands

Target	PDB	Uniprot	RMSD, Å
Class A			
A _{2A}	5UIG	P29274	0.715
β ₂	5X7D	P07550	0.396
β ₂	6N48	P07550	1.148
β ₂	6OBA	P07550	0.404
C5a ₁	5O9H	P21730	0.519
C5a ₁	6C1Q	P21730	0.621
C5a ₁	6C1R	P21730	0.593
CCR2	5T1A	P41597	0.593
CCR5	4MBS	P51681	0.685
CCR7	6QZH	P32248	1.492
CCR9	5LWE	P51686	0.871
CB ₁	6KQI	P21554	1.472
CXCR4	3ODU	P61073	0.626
CXCR4	3OE0	P61073	0.809
FFA1	4PHU	O14842	0.672

FFA1	5KW2	O14842	1.249
FFA1	5TZR	O14842	0.644
FFA1	5TZY	O14842	0.96
GPR52	6LI0	Q9Y2T5	0.654
M ₂	4MQT	P08172	1.059
P2Y ₁	4XNV	P47900	0.608
PAR2	5NDD	P55085	0.716
PAR2	5NDZ	P55085	0.702

Class B

CRF ₁	4K5Y	P34998	1.975
GLP-1	5VEW	P43220	1.885
GLP-1	5VEX	P43220	2.193
GLP-1	6KJV	P43220	2.098
GLP-1	6KK7	P43220	2.282
GLP-1	6LN2	P43220	2.02
GCGR	5EE7	P47871	1.505
GCGR	5XEZ	P47871	1.923

Class C

mGlu ₁	4OR2	Q13255	0.681
mGlu ₅	4OO9	P41594	0.653
mGlu ₅	5CGC	P41594	0.741
mGlu ₅	5CGD	P41594	0.729
mGlu ₅	6FFH	P41594	0.711
mGlu ₅	6FFI	P41594	0.745

Class F

SMO	4N4W	Q99835	0.445
SMO	5L7I	Q99835	0.421

Average 1.006

Table S2. Overlapping probe atoms among the allosteric sites of the 21 GPCR structures with ligand and strong hot spot^a

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
1. 3ODU	213	172	16	262	107	97	52	92	5	0	18	0	191	0	0	6	0	116	0	88	0
2. 3OE0	143	279	0	248	93	43	54	101	31	16	66	0	126	0	0	11	16	189	0	95	0
3. 4K5Y	48	24	169	13	0	69	71	65	9	0	1	0	47	12	0	20	0	0	0	35	0
4. 4MBS	83	119	14	339	16	107	140	85	17	47	22	0	130	0	0	16	47	47	0	89	0
5. 4MQT	162	230	2	181	204	25	25	74	34	0	10	22	67	0	19	31	0	178	15	21	24
6. 4N4W	30	197	38	75	56	152	57	31	0	52	212	0	55	6	37	0	51	67	23	16	38
7. 4OO9	78	84	6	63	30	36	102	122	48	40	2	0	57	11	0	50	18	28	0	0	18
8. 4OR2	107	150	28	63	23	44	97	191	58	0	34	0	0	6	0	58	0	0	0	44	0
9. 4PHU	1	19	0	3	0	0	18	20	104	202	0	0	0	0	0	104	204	0	29	0	4
10.5KW2	0	0	0	0	0	0	0	0	0	296	0	0	0	20	0	0	286	0	0	0	4
11.5L7I	6	215	0	26	23	99	20	1	0	45	213	8	34	2	0	0	48	25	29	44	46
12.5LWE	23	68	0	53	21	0	26	16	18	87	10	169	22	0	128	17	85	42	130	23	115
13.5NDD	62	69	0	81	40	40	0	12	0	50	56	0	97	49	0	0	64	26	0	49	0
14.5NDZ	77	54	5	78	33	44	0	6	0	69	53	0	101	70	0	0	69	38	0	54	0
15.5T1A	100	86	16	157	9	44	43	52	20	55	19	186	96	0	194	24	55	24	178	24	168
16.5TZR	6	26	0	5	11	8	26	31	149	135	6	0	7	0	0	149	140	13	27	15	0
17.5TZY	0	46	0	20	18	0	23	25	83	178	6	63	0	0	42	83	178	0	52	0	55
18.5UIG	143	158	0	122	100	97	19	70	44	0	51	100	118	0	16	38	5	170	56	39	15
19.5X7D	88	128	3	187	61	115	57	69	20	0	39	133	88	0	123	20	0	124	129	63	128
20.6LI0	47	21	0	33	41	29	0	0	0	163	41	10	52	50	9	0	160	47	7	157	10
21.6QZH	48	95	10	93	95	14	0	3	0	0	67	170	72	0	143	0	0	79	123	122	180

^a For example, Table S2 shows that the hot spot in 4OO9 (Column 7) overlaps with its own ligand (102 probe atoms) and the ligand in 4OR2 (Column 8, 122 probe atoms).

Table S3. The 10 proteins with the highest level of hot spot overlap with the allosteric ligand bound to 21 GPCRs with strong hot spots at the ligand binding site. Each of the 21 “parent” structures with the bound ligand is listed in bold.

Class	Uniprot	PDB	Overlap	Volume Å³	RMSD, Å	Sequence similarity, %	dpocket
A	aa2ar_human	5UIG	170	344.4			
A	5ht2b_human	6DRZ	260	366.9	2.7	60.6	0.257
A	agtr1_human	4ZUD	252	511.9	6.4	52.0	0.302
A	5ht2b_human	5TUD	241	378.4	3.0	60.6	0.242
A	aa2ar_human	5WF6	235	346.6	1.4	99.6	0.167
A	aa2ar_human	3QAK	231	359.9	1.6	99.3	0.198
A	apj_human	5VBL	231	317.5	6.5	49.3	0.226
A	opr_d_human	4N6H	230	273.1	2.7	59.0	0.256
A	5ht2b_human	6DRY	222	340.5	2.8	59.5	0.284
A	aa2ar_human	3VG9	219	330.5	0.9	98.6	0.168
A	5ht2c_human	6BQG	218	473.8	2.4	61.9	0.245
A	5ht2b_human	6DRX	218	459.6	4.3	59.8	0.278
A	adrb2_human	5X7D	129	69			
A	ccr2_human	5T1A	178	188.1	3.6	56.3	0.251
A	gpr52_human	6L11	147	139.3	1.8	55.0	0.257
A	aa2ar_human	3PWH	143	176.7	1.6	57.7	0.264
A	ccr9_human	5LWE	130	175.8	3.5	52.8	0.233
A	aa2ar_human	5OLV	121	146.5	1.5	58.1	0.253
A	aa2ar_human	3UZA	119	170.2	1.7	57.7	0.254
A	aa2ar_human	5OLG	114	117.1	1.5	58.1	0.247
A	aa2ar_human	5IUB	108	131.7	1.5	58.1	0.251
A	aa1r_human	5N2S	107	95.5	1.8	54.5	0.285
A	adrb2_human	2R4R	106	57.3	0.8	91.7	0.176
A	adrb2_human	3KJ6	105	66.9	0.7	92.3	0.194
A	ccr2_human	5T1A	194	235.6			
A	ccr7_human	6QZH	143	156.8	2.0	69.4	0.159
A	gpr52_human	6L11	137	111.4	2.6	51.8	0.231
A	ccr9_human	5LWE	128	196.6	2.4	66.1	0.262
A	adrb2_human	5X7D	123	57.7	3.6	56.3	0.180
A	aa2ar_human	5OLV	107	115.7	3.7	52.7	0.359
A	ednrb_human	6IGL	103	47.2	4.2	56.2	0.427
A	ntr1_rat	4BUO	102	135.2	2.9	58.3	0.364

A	aa2ar_human	5OM4	99	58.9	3.7	52.3	0.361
A	aa2ar_human	5IUB	96	114.9	3.6	52.7	0.333
F	smo_human	4QIM	94	70.8	7.1	48.8	0.332
A	aa2ar_human	5OLZ	93	103.4	3.8	52.7	0.368
A	ccr5_human	4MBS	339	839.8			
A	ccr5_human	6AKY	384	796.0	0.4	100	0.169
A	ccr5_human	6MEO	346	702.8	0.9	98.6	0.141
A	ccr5_human	6MET	340	694.9	0.9	98.6	0.140
A	ccr5_human	5UIW	339	651.9	0.7	100.0	0.161
A	adrb1_melga	2VT4	333	564.2	1.9	58.2	0.373
A	ccr2_human	6GPX	317	574.0	0.8	92.0	0.279
B	glp1r_human	6LN2	317	586.5	7.4	50.7	0.277
A	ccr5_human	6AKX	313	747.6	0.2	100.0	0.059
A	5ht2b_human	5TUD	299	643.1	3.6	54.1	0.212
A	opr_x_human	4EA3	294	622.3	1.8	63.3	0.229
A	ccr7_human	6QZH	180	300			
A	ccr2_human	5T1A	168	183.9	2.0	69.4	0.212
A	gpr52_human	6LI1	141	130.9	4.9	52.6	0.247
A	adrb2_human	5X7D	128	132.9	4.4	51.9	0.180
A	adrb2_human	6OBA	116	180.5	2.3	53.0	0.235
A	ccr9_human	5LWE	115	153.6	2.4	65.7	0.245
A	ntr1_rat	4BUO	110	181.1	3.7	57.5	0.227
A	ednrb_human	6IGL	107	50.2	3.9	57.8	0.415
A	ntr1_rat	3ZEV	97	199.7	3.0	57.5	0.249
A	adrb1_melga	2YCY	86	76.9	3.6	53.7	0.247
F	smo_human	4QIM	83	63.6	7.6	50.4	0.226
A	adrb2_human	3NY9	83	59.6	4.5	53.4	0.355
A	ccr9_human	5LWE	169	277.5			
A	ccr2_human	5T1A	186	205.9	2.4	66.1	0.292
A	ccr7_human	6QZH	170	265.0	2.4	65.7	0.199
A	gpr52_human	6LI1	139	116.4	3.4	49.8	0.298
A	aa2ar_human	5OM4	137	114.8	4.8	52.0	0.245
A	lpar1_human	4Z36	134	240.6	6.9	51.7	0.171
A	adrb2_human	5X7D	133	105.7	3.5	52.8	0.268
A	ntr1_rat	3ZEV	129	211.7	4.5	57.6	0.300
A	aa2ar_human	5OLV	129	95.1	4.8	51.7	0.249
A	ntr1_rat	4BUO	126	265	6.3	57.6	0.253
A	aa2ar_human	5IUA	122	94.2	4.3	51.3	0.255

A	aa2ar_human	5OLH	122	102.7	4.3	51.7	0.230
A	cxcr4_human	3ODU	213	403.5			
A	pd2r2_human	6D26	329	380.2	1.8	57.4	0.368
A	pd2r2_human	6D27	286	409.4	1.8	56.0	0.409
A	aa2ar_human	3REY	253	362.7	5.7	52.3	0.465
A	ox1r_human	4ZJ8	248	416.8	2.6	58.8	0.159
A	aa2ar_human	3VG9	226	266.5	5.7	49.8	0.406
A	acm2_human	6OIK	222	231.4	6.6	51.3	0.576
A	ox2r_human	5WS3	217	436.8	2.1	57.8	0.232
A	aa1r_human	5UEN	214	345.7	4.6	50.5	0.350
A	cxcr4_human	3OE8	211	353.5	0.6	99.3	0.170
A	ox1r_human	4ZJC	209	472.5	2.5	58.8	0.219
A	drd4_human	5WIU	200	302.1	7.2	51.5	0.272
A	cxcr4_human	3OE0	279	1149.8			
A	ntr1_rat	4XEE	318	634.3	4.0	55.3	0.422
A	apj_human	5VBL	312	876.2	1.3	60.8	0.340
A	ntr1_rat	4XES	299	566.4	4.2	55.7	0.362
A	ntr1_rat	4GRV	299	660.4	3.7	54.9	0.408
A	lpar1_human	4Z34	292	475	6.1	51.3	0.433
A	adrb1_melga	2YCZ	290	687.8	5.3	50.5	0.441
A	adrb1_melga	2Y03	286	596.6	3.3	50.5	0.429
A	lpar1_human	4Z36	280	486.1	6.2	47.6	0.423
A	adrb1_melga	2Y02	279	670.7	4.4	50.9	0.458
A	aa2ar_human	5WF6	276	462.5	5.7	48.7	0.490
A	adrb2_human	2RH1	275	758.9	4.7	53.8	0.416
A	adrb1_melga	2Y00	271	650.7	5.5	50.9	0.564
A	adrb1_melga	3ZPQ	271	610.1	5.6	50.9	0.548
A	par2_human	5NDD	97	119.8			
A	cxcr4_human	3OE8	251	278.7	2.4	60.1	0.401
A	cxcr4_human	3OE9	222	283.8	2.6	58.6	0.356
A	ccr2_human	6GPX	221	206.1	2.2	59.9	0.236
A	cxcr4_human	3OE6	217	200.8	3.9	60.4	0.375
A	pd2r2_human	6D26	217	228.8	2.3	58.0	0.222
A	aa2ar_human	3VG9	210	176.1	5.1	51.2	0.245
A	agtr1_human	4YAY	198	212.0	3.1	59.4	0.201
A	cxcr4_human	3ODU	191	212.3	3.9	58.1	0.280
A	ox1r_human	4ZJ8	190	163.1	4.3	56.6	0.238
A	adrb1_melga	2VT4	189	201.9	5.0	53.2	0.385

A	pd2r2_human	6D27	184	243.2	2.4	58	0.214
A	par2_human	5NDZ	70	26.1			
A	par1_human	3VW7	95	49.1	1.0	67.7	0.140
A	p2ry1_human	4XNW	81	31	2.1	59.9	0.113
A	pe2r3_human	6AK3	79	87	5.2	56.4	0.225
A	gpr52_human	6LI2	67	32.3	5.6	47.7	0.291
A	opsd_bovin	2I37	65	36.4	4.6	52.2	0.393
A	opsd_bovin	2I36	53	9.0	4.2	52.5	0.288
A	par2_human	5NJ6	51	16.5	0.2	100	0.138
A	pe2r4_human	5YWY	50	13.2	4.5	50.7	0.155
A	gpr52_human	6LI0	50	14.8	5.2	48.4	0.380
A	adrb2_human	3KJ6	49	10.0	4.7	53.6	0.293
A	par2_human	5NDD	49	21.8	0.2	100	0.082
A	ffar1_human	4PHU	104	178.4			
A	ffar1_human	5TZR	149	246.3	0.2	99.6	0.073
A	adrb2_human	3SN6	129	98.3	3.7	45.9	0.337
A	lpar1_human	4Z34	110	190.2	4.2	42.2	0.343
B	glp1r_human	5VEX	110	139.0	7.4	46.9	0.263
A	cxcr4_human	3OE6	100	65.4	4.6	48.8	0.344
B	pth1r_human	6FJ3	95	73.7	5.6	47.4	0.247
A	lpar1_human	4Z35	90	197.0	3.8	42.2	0.369
A	lpar1_human	4Z36	84	152.2	4.1	45.6	0.320
A	ffar1_human	5TZY	83	98.4	1.0	98.1	0.240
A	acm2_human	5ZKC	80	46.6	3.1	50.0	0.380
A	ffar1_human	5KW2	296	407.2			
A	ffar1_human	4PHU	202	236	1.2	96.8	0.208
A	gpr52_human	6LI1	183	246.9	3.7	47.4	0.412
A	ffar1_human	5TZY	178	253.3	1.1	99.6	0.132
A	gpr52_human	6LI0	163	247.5	3.9	51.4	0.388
A	gpr52_human	6LI2	161	252.0	3.4	48.6	0.319
A	p2y12_human	4PXZ	160	212.3	3.6	49.0	0.319
A	hrh1_human	3RZE	156	125.4	3.3	49.4	0.284
A	aa2ar_human	3VGA	144	175.7	3.2	54.7	0.249
A	p2y12_human	4PY0	138	97.1	3.6	49.0	0.324
A	ffar1_human	5TZR	135	80.3	1.2	96.8	0.218
A	ffar1_human	5TZR	149	242.2			
B	glr_human	5XF1	124	61.5	6.4	49.5	0.442

A	adrb2_human	3SN6	119	83.9	5.0	46.2	0.538
B	glp1r_human	5VEX	115	188.1	6.9	46.6	0.322
A	lpar1_human	4Z34	107	154.7	4.1	41.8	0.357
A	ffar1_human	4PHU	104	172.5	0.2	99.6	0.142
A	cxcr4_human	3OE6	99	62.7	4.6	48.5	0.408
A	ptafr_human	5ZKP	93	139.5	3.3	49.8	0.374
A	lpar1_human	4Z35	90	198.8	3.6	41.4	0.442
A	lpar1_human	4Z36	89	169.9	4.3	45.4	0.383
A	ffar1_human	5TZY	83	98.4	1.0	97.1	0.285
B	pth1r_human	6FJ3	78	55.5	6.3	48.2	0.362
A	ffar1_human	5TZY	178	253.3			
A	ffar1_human	5KW2	286	399.1	1.1	99.6	0.144
A	ffar1_human	4PHU	204	249.7	1.0	98.1	0.237
A	gpr52_human	6LI1	176	231.1	4.2	45.3	0.292
A	p2y12_human	4PXZ	166	250.3	4.8	47.4	0.278
A	gpr52_human	6LI2	162	228.9	4.8	44.2	0.319
A	gpr52_human	6LI0	160	242.7	5.7	47.1	0.295
A	p2y12_human	4PY0	144	100	4.8	47.1	0.212
A	ffar1_human	5TZR	140	97.7	1.0	97.1	0.238
A	hrh1_human	3RZE	132	84.4	2.8	48.1	0.302
A	aa2ar_human	3VGA	127	137.4	4.6	50.4	0.207
A	gpr52_human	6LI0	157	473.9			
A	agtr1_human	4YAY	264	304.9	5.3	51.6	0.301
A	agtr1_human	4ZUD	205	194.2	4.1	51.3	0.316
A	q80km9_hcmv	5WB1	164	276.5	4.9	53.4	0.438
A	agtr2_human	5UNG	162	183	5.9	54.1	0.447
A	ccr2_human	6GPX	158	215	2.5	54.2	0.525
A	apj_human	5VBL	155	161.1	6.0	49.1	0.438
A	ccr2_human	6GPS	140	248.6	5.0	51.8	0.419
A	pe2r3_human	6M9T	132	90.5	3.7	45.8	0.447
A	ntr1_rat	5T04	127	147.5	4.7	48.0	0.492
A	ntr1_rat	4XEE	126	84.2	5.2	47.3	0.422
A	agtr2_human	5UNF	125	150.6	5.7	52.0	0.531
B	glr_human	5XEZ	125	210.3	5.0	44.1	0.554
A	acm2_human	4MQT	204	275.3			
A	p2ry1_human	4XNV	217	314.2	4.1	49.8	0.307
A	acm2_human	6OIK	216	298.2	0.8	99.6	0.152
A	ntr1_rat	4XES	204	299.5	3.1	56.7	0.205

A	ntr1_rat	5T04	195	430.4	2.5	55.6	0.168
A	ntr1_rat	4XEE	178	322.6	3.6	55.3	0.195
A	ntr1_rat	4GRV	174	273.8	2.9	53.5	0.228
A	apj_human	5VBL	165	304.9	3.6	54.5	0.295
A	ntr1_rat	4BUO	162	330.5	2.4	56.4	0.234
A	ntr1_rat	3ZEV	161	312.3	2.8	56.7	0.183
F	smo_human	4O9R	160	324.3	5.1	49.5	0.214
A	ntr1_rat	4BV0	157	243.1	4.6	57.5	0.205
A	cxcr4_human	3OE8	155	321	5.9	51.7	0.314
F	smo_human	4QIN	154	204.7	3.9	49.5	0.218

B	crfr1_human	4K5Y	169	325.2			
B	glr_human	5YQZ	147	121.6	3.3	64.4	0.254
B	crfr1_human	4Z9G	113	247.3	0.8	100.0	0.090
A	cxcr4_human	3OE9	103	152.2	6.0	53.4	0.219
B	glp1r_human	5NX2	89	113.7	4.2	63.6	0.233
A	opsd_bovin	6FKA	85	49.5	5.1	50.6	0.239
A	opsd_bovin	6FKC	70	27.3	4.9	50.6	0.240
A	opsd_bovin	6FK6	63	36.6	5.1	50.6	0.300
A	opsd_bovin	6FK8	57	21	5.0	50.6	0.258
A	drd2_human	6CM4	56	111.7	5.4	49.4	0.277
A	opsd_bovin	6FK7	53	20.6	5.1	50.6	0.233

C	grm1_human	4OR2	191	411			
B	pth1r_human	6FJ3	263	368	5.6	46.6	0.237
A	acm2_human	5ZK8	262	381	4.9	43.9	0.205
A	opsd_bovin	5TE5	243	238.9	6.8	50.2	0.292
A	acm3_rat	5ZHP	224	330.5	7.4	47.5	0.154
A	oprdr_human	4N6H	202	185	6.3	48.2	0.276
A	oprdr_human	4RWA	200	246.2	5.7	47.5	0.241
A	acm3_rat	4U14	198	338.2	5.7	47.5	0.206
A	opsd_bovin	6FK6	198	475	6.3	49.8	0.263
A	oprdr_mouse	4EJ4	191	201.4	5.4	47.1	0.200
A	ox1r_human	4ZJC	191	313.8	6.2	52.9	0.214
A	acm2_human	5ZKC	191	266.7	5.2	46.7	0.162

C	grm5_human	4O09	102	250.2			
C	gabr2_human	7C7Q	230	464.7	3.9	58.4	0.187
A	oprdr_mouse	6DDE	228	192.9	7.0	50.6	0.232
A	oprdr_mouse	6DDF	226	259.6	7.7	50.6	0.135
A	oprdr_mouse	4EJ4	224	180.3	6.5	48.2	0.133

A	oprm_mouse	4DKL	218	294	5.8	51	0.184
B	g1sgd4_rabbit	5VAI	217	279.3	9.0	46.5	0.365
B	pth1r_human	6FJ3	216	204.5	5.6	43.3	0.245
A	oprd_human	4N6H	213	164.2	6.8	49.0	0.163
A	lpar1_human	4Z36	206	231.6	10.4	49.8	0.180
A	acm2_human	5ZKC	203	279.2	6.5	47.8	0.175
B	glp1r_human	6B3J	200	186	10.3	46.9	0.310
A	oprd_human	4RWA	194	127.6	5.6	49.8	0.148
C	gabr2_human	6UO8	190	371.9	3.6	57.6	0.360

F	smo_human	4N4W	152	273.5			
A	drd2_human	6CM4	220	393.8	5.1	49.8	0.312
A	agtr1_human	4YAY	203	359.4	7.3	46.9	0.324
F	fzd4_human	6BD4	197	309.4	1.3	58.8	0.263
A	opsd_bovin	5TE5	195	189.5	4.6	45.4	0.487
A	5ht2b_human	5TUD	188	335.8	8.3	53.4	0.244
A	lpar1_human	4Z34	186	345.6	6.3	50.7	0.274
A	lpar1_human	4Z35	181	291.3	6.2	51.2	0.350
A	lpar1_human	4Z36	180	305.2	6.3	52.2	0.298
A	opsd_bovin	6FKA	179	661.9	4.8	53.7	0.347
A	acm3_rat	4DAJ	179	239.8	5.6	48.2	0.218
A	opsd_bovin	6FK6	172	663.2	4.4	48.2	0.376
A	opsd_bovin	6FK7	169	607.4	5.2	48.2	0.455

F	smo_human	5L7I	213	530.1			
F	smo_human	4QIN	243	367.3	0.6	98.8	0.147
F	smo_human	4O9R	234	475.8	0.7	98.8	0.163
F	smo_human	5V56	217	445.8	1.1	99.4	0.144
F	smo_human	4JKV	215	412.2	0.6	98.1	0.117
F	smo_human	4N4W	212	487.7	0.5	98.8	0.080
F	smo_human	5V57	212	435.2	1.1	98.4	0.110
F	smo_human	5L7D	184	374.9	1.9	96.4	0.123
A	aa2ar_human	3QAK	166	257.4	4.6	48.2	0.280
F	smo_human	4QIM	162	339.2	0.7	99.7	0.120
F	fzd4_human	6BD4	160	393.5	1.0	56.2	0.313
A	p2ry1_human	4XNV	149	413.7	5.9	46.2	0.415

Table S4. “Parent” structures without strong hot spots at the allosteric site

PDB ID	Number of “daughter” structures
4XNV	max 53 ^a
5CGC	126 > 84 ^b
5CGD	109 > 84
5EE7	max 40
5O9H	16 > 84
5VEW	max 73
5VEX	max 72
5XEZ	max 70
6C1Q	19 > 84
6C1R	9 > 84
6FFH	91 > 84
6FFI	78 > 84
6KJV	max 77
6KK7	max 73
6KQI	1 > 84
6LN2	95 > 84
6N48	max 80
6OBA	11 > 84

^a Indicates that the strongest hot spot in any structure at the location of the ligand in 4XNV jaf only 53 probes. Similar notation is used for other structures with no corresponding hot spots.

^b Indicates that strong hot spot with more than 84 probes at the location of ligand in 5CGC has been found in 126 structures. Similar notation is used to indicate the number of “daughter” structures with more than 84 probes.

Table S5. “Parent” and “daughter” structures for validation by docking

Allosteric “parent”	“Daughter” PDB	Probe overlap	Family
4OR2	1F88	103	Opsins
4OR2	1GZM	127	Opsins
4OR2	1HZX	107	Opsins
4N4W	1L9H	90	Opsins
4OR2	1U19	125	Opsins
4OR2	2G87	124	Opsins
4OR2	2HPY	189	Opsins
4OR2	2I35	178	Opsins
4MBS	2I36	190	Opsins
4OR2	2I37	101	Opsins
4OO9	2J4Y	160	Opsins
4OR2	2PED	149	Opsins
4MBS	2VT4	333	Adrenoceptors
4MBS	2X72	224	Opsins
3OE0	2Y00	271	Adrenoceptors
3OE0	2Y01	254	Adrenoceptors
3OE0	2Y02	279	Adrenoceptors
3OE0	2Y03	286	Adrenoceptors
3OE0	2Y04	264	Adrenoceptors
3OE0	2YCW	230	Adrenoceptors
4MBS	2YCX	283	Adrenoceptors
4MBS	2YCY	257	Adrenoceptors
3OE0	2YCZ	290	Adrenoceptors
4MBS	2Z73	114	Opsins
4MBS	2Z1Y	236	Opsins
4MBS	3AYM	161	Opsins
4MBS	3AYN	137	Opsins
4OR2	3C9L	137	Opsins
4OR2	3C9M	158	Opsins
4MBS	3CAP	108	Opsins

4MBS	3DQB	130	Opsins
4OR2	3OAX	103	Opsins
5NDD	3OE9	222	Chemokine
4MBS	3PBL	225	Dopamine
4MBS	3PQR	187	Opsins
5X7D	3PWH	143	Adenosine
4MBS	3PXO	158	Opsins
5KW2	3RZE	156	Histamine
5UIG	3V2W	109	Lysophospholipid (S1P)
3OE0	3V2Y	113	Lysophospholipid (S1P)
3OE0	3VW7	237	Proteinase-activated
3OE0	3ZEV	164	Neurotensin
3OE0	3ZPQ	271	Adrenoceptors
3OE0	3ZPR	247	Adrenoceptors
4MBS	4A4M	192	Opsins
4MBS	4AMI	243	Adrenoceptors
3OE0	4AMJ	259	Adrenoceptors
4MBS	4BEY	195	Opsins
4MBS	4BEZ	206	Opsins
4MQT	4BUO	162	Neurotensin
3OE0	4BV0	189	Neurotensin
3OE0	4BVN	221	Adrenoceptors
3OE0	4BWB	196	Neurotensin
4MBS	4DAJ	253	Acetylcholine (muscarinic)
4MBS	4DJH	182	Opioid
4OO9	4DKL	218	Opioid
4MBS	4EA3	294	Opioid
4OO9	4EJ4	224	Opioid
5UIG	4GPO	173	Adrenoceptors
3OE0	4GRV	299	Neurotensin
4MBS	4IAQ	198	5-Hydroxytryptamine
3OE0	4IB4	220	5-Hydroxytryptamine
4MBS	4J4Q	201	Opsins

3OEO	4L6R	215	Glucagon
4MBS	4N6H	251	Opioid
4MBS	4NC3	274	5-Hydroxytryptamine
4OR2	4NTJ	107	P2Y
4MBS	4PXF	169	Opsins
5TZY	4PYO	144	P2Y
4MBS	4RWA	211	Opioid
4MBS	4RWD	271	Opioid
4MBS	4S0V	256	Orexin
4MBS	4U14	252	Acetylcholine (muscarinic)
4MBS	4U15	233	Acetylcholine (muscarinic)
4MBS	4U16	196	Acetylcholine (muscarinic)
4MBS	4X1H	195	Opsins
3OEO	4XEE	318	Neurotensin
3OEO	4XES	299	Neurotensin
4MQT	4XNV	217	P2Y
3OEO	4XNW	159	P2Y
4MBS	4XT1	252	Unclassified
4MBS	4XT3	228	Unclassified
6LIO	4YAY	264	Angiotensin
3OEO	4Z34	292	Lysophospholipid (LPA)
3OEO	4Z35	234	Lysophospholipid (LPA)
3OEO	4Z36	280	Lysophospholipid (LPA)
4MBS	4ZJ8	266	Orexin
4MBS	4ZJC	261	Orexin
4MBS	4ZUD	274	Angiotensin
4MBS	4ZWJ	217	Opsins
4MBS	5A8E	184	Adrenoceptors
4MBS	5C1M	219	Opioid
4MBS	5CXV	181	Acetylcholine (muscarinic)
4N4W	5CXV	164	Acetylcholine (muscarinic)
4MBS	5D5A	249	Adrenoceptors
4MBS	5DGY	211	Opsins

4MBS	5DHG	285	Opioid
4MBS	5DHH	281	Opioid
4MBS	5DSG	210	Acetylcholine (muscarinic)
3OE0	5DYS	172	Opsins
4MBS	5EE7	95	Glucagon
4MBS	5EN0	167	Opsins
4MBS	5F8U	250	Adrenoceptors
3ODU	5GLH	199	Endothelin
4OO9	5GLI	159	Endothelin
5UIG	5N2S	156	Adenosine
4OO9	5NX2	173	Glucagon
4MBS	5O9H	162	Complement peptide
3OE0	5T04	270	Neurotensin
4MBS	5TE3	157	Opsins
4OR2	5TE5	243	Opsins
4MBS	5TGZ	119	Cannabinoid
4MBS	5TUD	299	5-Hydroxytryptamine
4MBS	5TVN	221	5-Hydroxytryptamine
3OE0	5U09	112	Cannabinoid
3ODU	5UEN	214	Adenosine
4MBS	5UNF	229	Angiotensin
4MBS	5UNG	263	Angiotensin
4MBS	5UNH	251	Angiotensin
4MBS	5V54	147	5-Hydroxytryptamine
3OE0	5VBL	312	Apelin
4MBS	5VEW	131	Glucagon
4OO9	5VEX	150	Glucagon
3OE0	5W0P	176	Opsins
4MBS	5WB1	284	Unclassified
4MBS	5WB2	233	Unclassified
4MBS	5WIU	210	Dopamine
4MBS	5WIV	193	Dopamine
4MBS	5WKT	162	Opsins

4MBS	5WQC	285	Orexin
4MBS	5WS3	285	Orexin
4MBS	5X33	211	Leukotriene
4MBS	5X93	161	Endothelin
4MBS	5XEZ	256	Glucagon
3OEO	5XF1	244	Glucagon
4MBS	5XJM	282	Angiotensin
4MBS	5XPR	207	Endothelin
3OEO	5XR8	157	Cannabinoid
3OEO	5XRA	194	Cannabinoid
5NDD	5XSZ	135	Lysophospholipid (LPA)
4MBS	5YHL	117	Prostanoid
4K5Y	5YQZ	147	Glucagon
4MBS	5YWY	123	Prostanoid
4MBS	5ZBH	197	Neuropeptide Y
3OEO	5ZBQ	195	Neuropeptide Y
4MBS	5ZHP	241	Acetylcholine (muscarinic)
4MBS	5ZKP	272	Platelet-activating factor
4MBS	5ZKQ	234	Platelet-activating factor
3OEO	5ZTY	232	Cannabinoid
3OEO	6A93	227	5-Hydroxytryptamine
4MBS	6A94	182	5-Hydroxytryptamine
4MBS	6AKX	313	Chemokine
4MBS	6AKY	384	Chemokine
4OO9	6B73	168	Opioid
3OEO	6BD4	204	Frizzled
4MBS	6BQG	283	5-Hydroxytryptamine
3OEO	6BQH	223	5-Hydroxytryptamine
4MBS	6C1Q	248	Complement peptide
4MBS	6C1R	227	Complement peptide
4N4W	6CM4	220	Dopamine
3ODU	6D26	329	Prostanoid
3ODU	6D27	286	Prostanoid

5L7I	6D32	221	Frizzled
5L7I	6D35	177	Frizzled
4MBS	6DO1	252	Angiotensin
4MBS	6DRX	264	5-Hydroxytryptamine
4MBS	6DRY	237	5-Hydroxytryptamine
4MBS	6DRZ	263	5-Hydroxytryptamine
4MBS	6DS0	200	5-Hydroxytryptamine
4MBS	6E59	275	Tachykinin
4MBS	6E67	214	Adrenoceptors
4OR2	6FJ3	263	Parathyroid hormone
4OR2	6FK6	198	Opsins
4N4W	6FK7	169	Opsins
4OO9	6FK8	183	Opsins
4OR2	6FK9	185	Opsins
4OO9	6FKA	185	Opsins
4N4W	6FKB	145	Opsins
4OR2	6FKC	190	Opsins
4OO9	6FKD	165	Opsins
4MBS	6FUF	198	Opsins
4MBS	6GPS	218	Chemokine
4MBS	6GPX	317	Chemokine
4MBS	6GT3	205	Adenosine
4MBS	6H7J	170	Adrenoceptors
4MBS	6H7L	191	Adrenoceptors
4MBS	6H7M	223	Adrenoceptors
4MBS	6H7N	192	Adrenoceptors
4MBS	6H7O	186	Adrenoceptors
4MBS	6HLL	287	Tachykinin
3OE0	6HLO	293	Tachykinin
4MBS	6HLP	332	Tachykinin
5LWE	6I9K	174	Opsins
5KW2	6IBB	99	Succinate
4MBS	6IBL	158	Adrenoceptors

3ODU	6IGK	178	Endothelin
4MBS	6IGL	212	Endothelin
6LIO	6IIV	98	Prostanoid
3ODU	6IQL	219	Dopamine
4MBS	6J20	248	Tachykinin
4MBS	6J21	266	Tachykinin
4MBS	6JOD	311	Angiotensin
3OEO	6JZH	174	Adenosine
4MBS	6K1Q	188	Endothelin
4MBS	6KJV	178	Glucagon
4OR2	6KK1	149	Glucagon
3OEO	6KK7	152	Glucagon
3OEO	6KNM	290	Apelin
3OEO	6KO5	340	Ghrelin
4MBS	6KP6	213	Acetylcholine (muscarinic)
3OEO	6KQI	169	Cannabinoid
3OEO	6KUW	245	Adrenoceptors
3OEO	6KUX	321	Adrenoceptors
4MBS	6KUY	268	Adrenoceptors
4MBS	6LN2	317	Glucagon
4MBS	6LRY	175	Endothelin
4MBS	6LUQ	177	Dopamine
4MBS	6LW5	243	Formylpeptide
6LIO	6M9T	132	Prostanoid
4MBS	6ME2	122	Melatonin
5TZY	6ME3	108	Melatonin
4MBS	6ME4	123	Melatonin
4MBS	6ME5	137	Melatonin
3OEO	6ME6	156	Melatonin
5KW2	6ME7	96	Melatonin
3OEO	6ME8	153	Melatonin
3OEO	6ME9	226	Melatonin
3OEO	6MH8	237	Adenosine

4OO9	6NWE	191	Opsins
4N4W	6O3C	289	Frizzled
4MBS	6OL9	236	Acetylcholine (muscarinic)
6LIO	6OS0	223	Angiotensin
4MBS	6OS1	229	Angiotensin
4MBS	6OS2	256	Angiotensin
4OO9	6PEL	155	Opsins
4MBS	6PGS	142	Opsins
4MBS	6PH7	125	Opsins
3OE0	6PRZ	223	Adrenoceptors
4MBS	6PS0	234	Adrenoceptors
4MBS	6PS1	139	Adrenoceptors
3OE0	6PS2	208	Adrenoceptors
4MBS	6PS3	206	Adrenoceptors
3OE0	6PS4	252	Adrenoceptors
4MBS	6PS5	179	Adrenoceptors
4MBS	6PS6	175	Adrenoceptors
3OE0	6PS7	181	Adenosine
4MBS	6PS8	144	Melatonin
4OO9	6PT2	244	Opioid
4OO9	6PT3	230	Opioid
3ODU	6RNK	181	Succinate
3OE0	6RZ4	324	Leukotriene
3OE0	6RZ5	242	Leukotriene
3OE0	6RZ6	218	Leukotriene
3OE0	6RZ7	279	Leukotriene
3OE0	6RZ8	244	Leukotriene
3OE0	6RZ9	253	Leukotriene
3ODU	6S0Q	128	Adenosine
3ODU	6TO7	197	Orexin
4MBS	6TOD	270	Orexin
4MBS	6TOS	237	Orexin
4MBS	6TOT	232	Orexin

4MBS	6TP3	221	Orexin
4MBS	6TP4	195	Orexin
4MBS	6TP6	237	Orexin
4MBS	6TPG	246	Orexin
4MBS	6TPJ	223	Orexin
3OEO	6TPK	187	Vasopressin and oxytocin
3ODU	6TPN	211	Orexin
4MBS	6TQ4	203	Orexin
4MBS	6TQ6	191	Orexin
3ODU	6TQ7	160	Orexin
4MBS	6TQ9	152	Orexin
4MBS	6V9S	216	Orexin
4MBS	6VI4	189	Opioid
4MBS	6W25	262	Melanocortin
3OEO	6WJC	214	Acetylcholine (muscarinic)
3OEO	7C61	250	5-Hydroxytryptamine
3OEO	7C6A	283	Angiotensin

Table S6. Docking results

Target_Parent_Ligand ^a	Distance to FTMap results			Distance to ligand in parent structure		
	Pose ^b	Hot spot ^c	Distance to hot spot ^d	Pose ^e	Ligand in parent ^f	Distance to ligand in parent ^g
1F88_4OR2_ASD02820003	6	4.008	2.64	6	FM9	1.92
1GZM_4OR2_ASD02820003	6	5.005	1.28	9	FM9	2.32
1HZX_4N4W_ASD02820003	2	7.003	1.74	7	SNT	3.93
1HZX_4OR2_ASD02820003	8	7.003	1.12	4	FM9	1.65
1L9H_4N4W_ASD02820003	9	8.005	1.85	9	SNT	3.83
1U19_4N4W_ASD02820003	7	8.005	1.67	4	SNT	4.21
1U19_4OR2_ASD02820003	7	8.005	1.79	7	FM9	1.55
2G87_4N4W_ASD02820003	2	0.013	2.34	4	SNT	3.88
2G87_4OR2_ASD02820003	7	0.013	1.61	4	FM9	2.55
2HPY_4N4W_ASD02820003	6	3.008	1.01	9	SNT	3.43
2HPY_4OR2_ASD02820003	8	3.008	0.99	8	FM9	2.59
2I35_4N4W_ASD02820003	5	2.012	2.06	5	SNT	3.99
2I35_4OR2_ASD02820003	7	2.012	1.88	6	FM9	2.69
2I36_4MBS_ASD02820003	6	0.013	1.45	4	MRV	3.17
2I36_4N4W_ASD02820003	7	3.011	1.40	2	SNT	3.96
2I37_4N4W_ASD02820003	4	3.011	1.63	7	SNT	3.54
2I37_4OR2_ASD02820003	4	1.016	3.26	1	FM9	1.90
2J4Y_4N4W_ASD02820003	8	4.01	1.83	8	SNT	3.30
2J4Y_4OO9_ASD02820003	4	2.012	2.13	2	2U8	3.39
2PED_4N4W_ASD02820003	5	5.005	1.01	5	SNT	3.88
2PED_4OR2_ASD02820003	6	5.005	1.48	2	FM9	2.59
2X72_4MBS_ASD02820003	7	4.008	1.02	7	MRV	2.13
3C9L_4N4W_ASD02820003	6	5.008	0.91	8	SNT	3.66
3C9L_4OR2_ASD02820003	5	5.008	0.88	6	FM9	2.36
3C9M_4N4W_ASD02820003	5	5.007	2.17	2	SNT	3.78
3C9M_4OR2_ASD02820003	7	5.007	1.32	3	FM9	3.29
3CAP_4MBS_ASD02820003	3	6.006	1.65	3	MRV	2.56
3DQB_4MBS_ASD02820003	7	1.012	1.04	5	MRV	3.11
3OAX_4N4W_ASD02820003	6	12.003	1.84	7	SNT	3.59

3OAX_4OR2_ASD02820003	7	12.003	1.26	8	FM9	1.30
3OE9_3ODU_ASD04570023	1	5.007	2.90	5	ITD	1.97
3OE9_4K5Y_ASD04570023	1	9.003	6.31	1	1Q5	19.26
3OE9_5NDD_ASD04570023	2	3.009	2.95	2	8TZ	2.78
3PBL_4MBS_ASD04640014	8	1.014	1.44	3	MRV	1.98
3PBL_4N4W_ASD04640014	5	1.014	1.39	6	SNT	3.71
3PBL_5KW2_ASD04640014	3	2.011	1.86	3	6XQ	2.56
3PBL_5NDD_ASD04640014	4	1.014	1.36	2	8TZ	0.97
3PQR_4MBS_ASD02820003	3	3.009	2.02	3	MRV	3.12
3PQR_4N4W_ASD02820003	7	3.009	1.86	6	SNT	3.87
3PWH_3ODU_ASD03130013	6	7.005	2.59	6	ITD	2.26
3PWH_5TZY_ASD03130013	2	1.015	3.31	7	7OS	4.11
3PWH_5X7D_ASD03130013	1	0.024	2.92	4	8VS	3.33
3PXO_4MBS_ASD02820003	9	2.013	1.70	9	MRV	3.30
3PXO_4N4W_ASD02820003	9	2.013	1.69	8	SNT	4.20
3PXO_4N4W_ASD05688001	1	11.001	12.04	1	SNT	16.60
3VW7_3OE0_ASD05503050	1	3.01	1.90	6	PRD- chain I	5.23
3VW7_3OE0_ASD05503052	3	0.018	1.79	2	PRD- chain I	2.17
3VW7_5NDZ_ASD05503050	3	5.005	1.34	1	8UN	1.96
3VW7_5NDZ_ASD05503052	1	5.005	2.19	3	8UN	2.34
4A4M_4MBS_ASD02820003	1	0.014	1.61	9	MRV	3.94
4A4M_4MBS_ASD05688001	6	4.009	1.69	10	MRV	3.63
4A4M_4N4W_ASD02820003	5	0.014	1.29	2	SNT	3.37
4A4M_4N4W_ASD05688001	1	0.014	1.82	1	SNT	3.50
4BEY_4MBS_ASD02820003	2	0.019	1.97	5	MRV	2.41
4BEY_4MBS_ASD05688001	3	1.016	2.71	2	MRV	3.33
4BEY_4N4W_ASD02820003	2	2.010	1.72	1	SNT	3.01
4BEY_4N4W_ASD05688001	9	12.002	13.76	1	SNT	17.15
4BEZ_4MBS_ASD02820003	4	2.011	1.06	10	MRV	2.33
4BEZ_4MBS_ASD05688001	1	1.013	2.13	1	MRV	3.16
4BEZ_4N4W_ASD02820003	5	1.013	1.47	7	SNT	3.01
4BEZ_4N4W_ASD05688001	1	8.004	12.68	1	SNT	17.09
4DJH_4MBS_ASD00170299	10	4.007	1.87	8	MRV	1.43
4DJH_4MBS_ASD03170003	1	1.023	2.49	2	MRV	2.34

4DJH_5NDD_ASD00170299	5	4.007	1.86	2	8TZ	2.16
4DJH_5NDD_ASD03170003	2	4.007	2.42	5	8TZ	1.94
4DJH_6LI0_ASD00170299	10	0.027	1.45	8	D7W	4.46
4DJH_6LI0_ASD03170003	1	10.001	1.88	2	D7W	4.75
4EJ4_4N4W_ASD03180043	7	7.005	3.22	1	SNT	3.69
4EJ4_4N4W_ASD16020002	2	7.005	2.52	1	SNT	3.85
4EJ4_4OO9_ASD03180043	3	7.005	2.61	4	2U8	4.57
4EJ4_4OO9_ASD16020002	3	0.022	2.14	3	2U8	3.57
4EJ4_5KW2_ASD03180043	2	6.006	3.15	1	6XQ	3.71
4EJ4_5KW2_ASD16020002	2	6.006	3.31	2	6XQ	4.16
4J4Q_4MBS_ASD02820003	8	0.017	1.25	3	MRV	2.43
4J4Q_4MBS_ASD05688001	7	0.017	1.66	5	MRV	2.94
4J4Q_4N4W_ASD02820003	5	2.015	0.71	3	SNT	3.67
4J4Q_4N4W_ASD05688001	5	2.015	1.70	4	SNT	3.47
4L6R_3OE0_ASD04910208	1	1.017	0.80	7	PRD- chain I	7.84
4L6R_5NDD_ASD04910208	5	5.007	0.69	3	8TZ	1.66
4N6H_4MBS_ASD03180043	1	4.011	3.47	2	MRV	0.39
4N6H_4MBS_ASD16020002	2	4.011	3.03	9	MRV	0.59
4N6H_4N4W_ASD03180043	7	4.011	3.59	1	SNT	4.48
4N6H_4N4W_ASD16020002	2	3.011	2.97	8	SNT	3.52
4NTJ_4OR2_ASD13170001	3	6.005	2.48	2	FM9	1.73
4NTJ_4OR2_ASD13170002	3	6.005	1.57	1	FM9	1.61
4NTJ_5KW2_ASD13170001	1	0.017	2.25	2	6XQ	3.74
4NTJ_5KW2_ASD13170002	1	0.017	2.16	1	6XQ	3.68
4PXF_4MBS_ASD02820003	9	2.011	1.15	9	MRV	2.92
4PXF_4MBS_ASD05688001	3	6.006	2.36	9	MRV	3.49
4PXZ_5TZY_ASD13170001	4	0.015	2.62	1	7OS	2.53
4PXZ_5TZY_ASD13170002	1	0.015	2.94	1	7OS	2.54
4PY0_3OE0_ASD13170001	5	5.006	2.10	3	PRD- chain I	8.88
4PY0_3OE0_ASD13170002	3	5.006	2.00	6	PRD- chain I	8.15
4PY0_5TZY_ASD13170001	3	0.014	2.43	3	7OS	3.73
4PY0_5TZY_ASD13170002	1	0.014	2.95	1	7OS	4.37
4RWA_4MBS_ASD03180043	3	7.003	2.95	10	MRV	0.94
4RWA_4MBS_ASD16020002	5	3.012	2.71	4	MRV	0.92

4RWA_4N4W_ASD03180043	2	7.003	2.98	2	SNT	3.63
4RWA_4N4W_ASD16020002	8	7.003	2.77	2	SNT	3.91
4RWD_4MBS_ASD03180043	3	2.013	3.12	4	MRV	0.91
4RWD_4MBS_ASD16020002	4	6.007	2.74	7	MRV	1.29
4RWD_4N4W_ASD03180043	6	2.013	3.00	2	SNT	4.80
4RWD_4N4W_ASD16020002	7	3.01	3.38	3	SNT	4.87
4RWD_5NDD_ASD03180043	5	6.007	2.75	5	8TZ	4.12
4RWD_5NDD_ASD16020002	4	6.007	2.94	3	8TZ	4.24
4X1H_4MBS_ASD02820003	3	1.017	1.38	3	MRV	2.17
4X1H_4MBS_ASD05688001	3	1.017	1.29	7	MRV	2.77
4X1H_4N4W_ASD02820003	4	1.017	0.86	1	SNT	3.56
4X1H_4N4W_ASD05688001	2	1.017	1.41	1	SNT	3.26
4XNV_4MQT_ASD03570002	2	3.011	2.93	2	2CU	4.54
4XNV_4MQT_ASD03570029	4	3.011	1.98	5	2CU	2.60
4XNV_5L7I_ASD03570002	1	3.011	2.91	4	VIS	2.46
4XNV_5L7I_ASD03570029	9	3.011	2.02	3	VIS	2.07
4XNV_6LI0_ASD03570002						
4XNV_6LI0_ASD03570029						
4XNW_3OE0_ASD03570002	8	6.005	2.41	1	PRD- chain I	5.67
4XNW_3OE0_ASD03570029	4	6.005	1.95	8	PRD- chain I	5.46
4XT1_4MBS_ASD01350033	10	2.01	1.40	10	MRV	3.37
4XT1_4MBS_ASD01350061	8	2.01	1.70	8	MRV	3.58
4XT1_5NDD_ASD01350033	1	4.008	1.99	8	8TZ	1.67
4XT1_5NDD_ASD01350061	4	4.008	1.73	2	8TZ	0.73
4XT1_6LI0_ASD01350033	1	10.003	1.57	1	D7W	5.66
4XT1_6LI0_ASD01350061	1	10.003	1.69	1	D7W	5.95
4XT3_4MBS_ASD01350033	8	1.012	2.01	6	MRV	3.36
4XT3_4MBS_ASD01350061	2	0.019	1.73	7	MRV	4.03
4XT3_5NDD_ASD01350033	5	0.019	2.12	6	8TZ	1.44
4XT3_5NDD_ASD01350061	6	1.012	1.31	4	8TZ	0.68
4XT3_6LI0_ASD01350033	6	5.009	1.64	9	D7W	7.06
4XT3_6LI0_ASD01350061	1	7.005	2.31	6	D7W	6.94
4Z34_3OE0_ASD14870001	7	7.003	1.84	4	PRD- chain I	9.31
4Z34_3OE0_ASD14870005	6	7.003	2.11	5	PRD- chain I	8.98

4Z34_4N4W_ASD14870001	1	7.003	2.08	10	SNT	2.74
4Z34_4N4W_ASD14870005	3	7.003	2.05	1	SNT	3.81
4Z34_4PHU_ASD14870001	1	1.014	1.80	1	2YB	13.17
4Z34_4PHU_ASD14870005	1	5.006	2.13	1	2YB	4.26
4Z34_5LWE_ASD14870001	3	7.003	1.59	6	79K	3.72
4Z34_5LWE_ASD14870005	1	7.003	2.02	1	79K	3.74
4Z35_3OE0_ASD14870001	2	3.008	3.68	5	PRD- chain I	9.20
4Z35_3OE0_ASD14870005	7	4.006	2.68	2	PRD- chain I	8.54
4Z35_4N4W_ASD14870001	4	3.008	3.43	9	SNT	2.80
4Z35_4N4W_ASD14870005	7	10.004	2.30	4	SNT	3.50
4Z35_4PHU_ASD14870001	1	4.006	2.23	1	2YB	12.86
4Z35_4PHU_ASD14870005	3	1.016	2.19	2	2YB	3.14
4Z35_5LWE_ASD14870001	2	3.008	3.86	3	79K	2.40
4Z35_5LWE_ASD14870005	8	10.004	3.40	1	79K	3.58
4Z36_3OE0_ASD14870001	5	4.008	2.64	7	PRD- chain I	8.97
4Z36_3OE0_ASD14870005	1	5.007	2.45	1	PRD- chain I	8.69
4Z36_4N4W_ASD14870001	6	4.008	2.65	8	SNT	3.24
4Z36_4N4W_ASD14870005	3	4.008	2.19	9	SNT	3.56
4Z36_5LWE_ASD14870001	8	4.008	2.49	3	79K	2.75
4Z36_5LWE_ASD14870005	3	4.008	2.73	4	79K	2.45
4Z36_5TZR_ASD14870001	4	5.007	1.81	4	MK6	13.30
4Z36_5TZR_ASD14870005	1	9.004	2.18	1	MK6	4.94
5CXV_4MBS_ASD01810699	1	0.026	0.34	6	MRV	4.80
5CXV_4MBS_ASD01811561	5	0.026	1.04	5	MRV	4.97
5CXV_4N4W_ASD01810699	1	0.026	0.17	2	SNT	4.33
5CXV_4N4W_ASD01811561	7	1.018	1.10	4	SNT	5.59
5D5A_4MBS_ASD01580008	10	0.018	1.08	6	MRV	3.75
5D5A_4MBS_ASD03130023	3	11.002	1.47	4	MRV	1.25
5DSG_4MBS_ASD01840213	10	2.015	2.12	3	MRV	4.71
5DSG_4MBS_ASD01914813	4	2.015	1.32	3	MRV	4.29
5DSG_4N4W_ASD01840213	1	3.011	2.42	6	SNT	5.55
5DSG_4N4W_ASD01914813	9	6.004	1.03	2	SNT	4.65
5DYS_3OE0_ASD02820003	3	1.013	1.71	7	PRD- chain I	12.70
5DYS_3OE0_ASD05688001	3	1.013	2.74	6	PRD- chain I	12.99

5DYS_4N4W_ASD02820003	7	3.011	2.00	7	SNT	3.59
5DYS_4N4W_ASD05688001	4	0.014	1.79	4	SNT	3.39
5EE7_4MBS_ASD04910208	6	0.014	1.43	10	MRV	5.30
5EE7_6LI0_ASD04910208	2	3.01	0.24	2	D7W	0.89
5EN0_4MBS_ASD02820003	8	3.01	1.92	8	MRV	2.59
5EN0_4MBS_ASD05688001	3	3.01	2.82	3	MRV	3.39
5EN0_4N4W_ASD02820003	2	1.014	1.64	5	SNT	4.86
5EN0_4N4W_ASD05688001	4	1.014	1.56	9	SNT	1.24
5N2S_5NDD_ASD00170496	7	7.007	1.72	7	8TZ	1.46
5N2S_5NDD_ASD00170902						
5N2S_5UIG_ASD00170496	1	7.007	1.53	7	8D1	1.87
5N2S_5UIG_ASD00170902						
5N2S_6LI0_ASD00170496	3	7.007	2.93	2	D7W	4.58
5N2S_6LI0_ASD00170902						
5NX2_4K5Y_ASD01180443	2	3.009	0.59	10	1Q5	4.19
5NX2_4N4W_ASD01180443	1	2.013	0.40	1	SNT	4.24
5NX2_4OO9_ASD01180443	1	2.013	0.38	9	2U8	3.41
5O9H_3ODU_ASD03160012	1	11.001	2.81	3	ITD	2.51
5O9H_3ODU_ASD11780002	5	11.001	2.12	6	ITD	1.94
5O9H_4MBS_ASD03160012	4	11.001	3.13	4	MRV	3.11
5O9H_4MBS_ASD11780002	8	11.001	0.77	2	MRV	2.82
5O9H_5NDD_ASD03160012	2	2.013	2.79	2	8TZ	2.63
5O9H_5NDD_ASD11780002	1	2.013	3.19	3	8TZ	2.95
5O9H_6LI0_ASD03160012						
5O9H_6LI0_ASD11780002						
5TE3_4MBS_ASD02820003	1	9.005	1.49	8	MRV	3.00
5TE3_4MBS_ASD05688001	8	9.005	1.40	8	MRV	2.98
5TE3_4N4W_ASD02820003	6	2.01	1.53	5	SNT	3.89
5TE3_4N4W_ASD05688001	1	1.011	1.66	2	SNT	4.07
5TE5_4N4W_ASD02820003	9	3.013	2.25	9	SNT	4.33
5TE5_4N4W_ASD05688001	2	2.014	3.08	7	SNT	4.44
5TE5_4OR2_ASD02820003	5	3.013	1.58	4	FM9	2.30
5TE5_4OR2_ASD05688001	3	3.013	2.23	10	FM9	2.49
5TGZ_4MBS_ASD03331126	6	0.019	2.18	4	MRV	0.97

5TGZ_4MBS_ASD03331623	7	0.019	1.82	2	MRV	1.40
5U09_3OE0_ASD03331126	1	1.019	2.27	5	PRD- chain I	10.57
5U09_3OE0_ASD03331623	9	1.019	3.57	7	PRD- chain I	11.92
5U09_4N4W_ASD03331126	3	1.019	2.49	6	SNT	4.65
5U09_4N4W_ASD03331623	3	1.019	3.74	5	SNT	4.03
5UEN_3ODU_ASD00170496	4	8.002	0.83	9	ITD	1.23
5UEN_3ODU_ASD00170902						
5UEN_5L7I_ASD00170496	3	8.002	0.78	10	VIS	4.88
5UEN_5L7I_ASD00170902						
5UEN_5NDD_ASD00170496	9	8.002	1.03	2	8TZ	0.58
5UEN_5NDD_ASD00170902						
5VEW_4MBS_ASD01180443	10	0.027	0.92	4	MRV	6.57
5VEW_4N4W_ASD01180443	8	0.027	0.52	5	SNT	5.97
5VEX_4OO9_ASD01180443	1	9.002	0.60	10	2U8	1.72
5VEX_5TZR_ASD01180443	9	1.014	0.59	1	MK6	3.49
5WIU_4MBS_ASD00170350	9	1.013	1.25	8	MRV	0.75
5WIU_5NDD_ASD00170350	1	0.015	1.28	6	8TZ	2.22
5WIV_4MBS_ASD00170350	2	1.014	1.15	9	MRV	1.52
5WIV_5NDD_ASD00170350	10	1.014	0.91	1	8TZ	1.65
5WKT_4MBS_ASD02820003	5	4.01	0.62	10	MRV	2.71
5WKT_4MBS_ASD05688001	9	4.01	0.72	3	MRV	2.72
5WKT_4N4W_ASD02820003	9	3.011	1.58	10	SNT	3.49
5WKT_4N4W_ASD05688001	1	0.023	1.97	1	SNT	3.66
5XEZ_4MBS_ASD04910208	5	1.018	0.24	6	MRV	3.80
5XEZ_5NDD_ASD04910208	5	0.027	0.14	8	8TZ	1.51
5XEZ_6LI0_ASD04910208	7	2.016	1.38	5	D7W	3.02
5XF1_3OE0_ASD04910208	6	4.007	0.28	9	PRD- chain I	8.26
5XF1_4N4W_ASD04910208	3	1.018	1.56	5	SNT	5.45
5XF1_5NDD_ASD04910208	4	2.016	0.65	3	8TZ	1.69
5XF1_5TZR_ASD04910208	10	1.018	0.39	10	MK6	11.88
5XF1_6LI0_ASD04910208	5	0.018	0.32	1	D7W	3.41
5XR8_3OE0_ASD03331126	8	1.015	2.85	1	PRD- chain I	11.08
5XR8_3OE0_ASD03331623	4	1.015	3.03	10	PRD- chain I	10.89
5XR8_3OE0_ASD03331727	3	2.013	2.83	8	PRD- chain I	12.16

5XR8_4N4W_ASD03331126	1	1.015	2.11	3	SNT	3.75
5XR8_4N4W_ASD03331623	10	1.015	2.14	6	SNT	4.05
5XR8_4N4W_ASD03331727	10	1.015	2.07	7	SNT	3.77
5XR8_5NDD_ASD03331126	6	1.015	2.20	2	8TZ	1.68
5XR8_5NDD_ASD03331623	5	1.015	1.74	5	8TZ	1.56
5XR8_5NDD_ASD03331727	6	1.015	2.82	6	8TZ	1.92
5XR8_6LI0_ASD03331126	7	2.013	2.05	7	D7W	5.01
5XR8_6LI0_ASD03331623	3	2.013	2.08	5	D7W	5.44
5XR8_6LI0_ASD03331727	5	2.013	2.20	5	D7W	4.91
5XRA_3OE0_ASD03331126	3	3.011	2.98	9	PRD- chain I	11.74
5XRA_3OE0_ASD03331623	8	1.016	2.74	3	PRD- chain I	10.80
5XRA_3OE0_ASD03331727	7	3.011	1.89	10	PRD- chain I	10.80
5XRA_4N4W_ASD03331126	9	3.011	2.79	7	SNT	3.64
5XRA_4N4W_ASD03331623	10	1.016	2.01	3	SNT	4.26
5XRA_4N4W_ASD03331727	4	1.016	3.75	6	SNT	4.16
5XRA_5NDD_ASD03331126	2	1.016	2.31	5	8TZ	1.75
5XRA_5NDD_ASD03331623	1	1.016	2.22	8	8TZ	2.12
5XRA_5NDD_ASD03331727	9	1.016	1.90	5	8TZ	2.26
5XRA_6LI0_ASD03331126	3	2.012	2.43	2	D7W	4.98
5XRA_6LI0_ASD03331623	2	2.012	1.95	2	D7W	4.88
5XRA_6LI0_ASD03331727	2	2.012	2.40	3	D7W	4.23
5YQZ_4K5Y_ASD04910208	1	2.018	0.69	2	1Q5	1.96
5YQZ_4O09_ASD04910208	8	3.016	0.39	9	2U8	4.31
5YQZ_4OR2_ASD04910208	4	0.018	0.61	9	FM9	3.46
5YQZ_5NDD_ASD04910208	6	1.018	0.38	7	8TZ	1.27
5ZTY_3OE0_ASD01150307	4	7.005	90.72	4	PRD	121.08
5ZTY_3OE0_ASD03331798	4	7.005	91.16	4	PRD	121.65
5ZTY_3OE0_ASD11730002	3	7.005	88.93	3	PRD	119.38
5ZTY_5NDD_ASD01150307	8	7.005	90.54	8	8TZ	110.23
5ZTY_5NDD_ASD03331798	4	7.005	91.61	4	8TZ	111.45
5ZTY_5NDD_ASD11730002	9	7.005	89.30	9	8TZ	108.60
6AKX_4MBS_ASD00601006	2	8.002	1.94	7	MRV	1.98
6AKX_4MBS_ASD00601007	3	1.018	1.97	8	MRV	2.68
6AKX_4MBS_ASD03570003	1	8.002	1.80	5	MRV	0.77

6AKX_4N4W_ASD00601006	5	1.018	1.51	4	SNT	5.98
6AKX_4N4W_ASD00601007	6	1.018	1.82	10	SNT	5.44
6AKX_4N4W_ASD03570003	4	1.018	2.99	5	SNT	3.68
6AKX_5NDD_ASD00601006	8	8.002	1.68	10	8TZ	1.07
6AKX_5NDD_ASD00601007	7	8.002	2.21	10	8TZ	0.68
6AKX_5NDD_ASD03570003	3	8.002	2.73	2	8TZ	1.15
6AKX_6LI0_ASD00601006	1	1.018	1.97	7	D7W	4.92
6AKX_6LI0_ASD00601007	5	1.018	2.48	8	D7W	5.20
6AKX_6LI0_ASD03570003	3	1.018	3.19	2	D7W	5.96
6AKY_4MBS_ASD00601006	2	4.012	1.58	8	MRV	2.43
6AKY_4MBS_ASD00601007	4	4.012	1.97	6	MRV	2.21
6AKY_4MBS_ASD03570003	1	4.012	1.79	4	MRV	1.32
6AKY_4N4W_ASD00601006	2	3.014	2.05	9	SNT	3.79
6AKY_4N4W_ASD00601007	4	3.014	1.86	7	SNT	3.68
6AKY_4N4W_ASD03570003	6	8.001	2.70	1	SNT	2.82
6AKY_5NDD_ASD00601006	1	0.019	2.56	8	8TZ	0.91
6AKY_5NDD_ASD00601007	8	4.012	2.19	2	8TZ	1.09
6AKY_5NDD_ASD03570003	10	4.012	3.40	1	8TZ	1.86
6AKY_6LI0_ASD00601006	1	3.014	2.20	5	D7W	5.15
6AKY_6LI0_ASD00601007	4	3.014	2.32	3	D7W	5.28
6AKY_6LI0_ASD03570003	2	3.014	3.26	5	D7W	5.96
6B73_4N4W_ASD00170299	5	6.007	1.76	3	SNT	1.85
6B73_4N4W_ASD03170003	2	6.007	2.14	2	SNT	2.54
6B73_4N4W_ASD03170006	5	6.007	1.59	2	SNT	2.37
6B73_4O09_ASD00170299	5	6.007	1.87	1	2U8	2.01
6B73_4O09_ASD03170003	3	6.007	1.65	2	2U8	2.74
6B73_4O09_ASD03170006	2	6.007	1.50	1	2U8	2.13
6BQG_4MBS_ASD00110052	9	0.016	2.24	9	MRV	1.34
6BQG_4MBS_ASD00111114	1	2.012	2.09	8	MRV	1.83
6BQG_4MBS_ASD00111115	9	4.01	1.90	5	MRV	1.98
6BQG_4N4W_ASD00110052	9	0.016	2.36	3	SNT	4.79
6BQG_4N4W_ASD00111114	7	0.016	2.40	2	SNT	4.28
6BQG_4N4W_ASD00111115	4	0.016	1.79	9	SNT	3.89
6BQG_5NDD_ASD00110052	3	0.016	2.16	6	8TZ	2.46

6BQG_5NDD_ASD00111114	10	0.016	2.38	3	8TZ	1.21
6BQG_5NDD_ASD00111115	7	0.016	1.54	4	8TZ	2.56
6BQG_6LI0_ASD00110052	9	0.016	2.36	2	D7W	4.38
6BQG_6LI0_ASD00111114	5	0.016	2.47	10	D7W	3.01
6BQG_6LI0_ASD00111115	3	0.016	2.24	1	D7W	4.10
6BQH_3OE0_ASD00110052	7	0.018	2.16	7	PRD- chain I	10.01
6BQH_3OE0_ASD00111114	9	3.012	1.75	10	PRD- chain I	8.62
6BQH_3OE0_ASD00111115	9	3.012	2.14	1	PRD- chain I	9.08
6BQH_4N4W_ASD00110052	7	4.01	1.33	7	SNT	4.25
6BQH_4N4W_ASD00111114	7	4.01	1.12	10	SNT	4.10
6BQH_4N4W_ASD00111115	2	7.004	1.97	3	SNT	5.43
6BQH_5NDD_ASD00110052	10	0.018	1.83	2	8TZ	2.75
6BQH_5NDD_ASD00111114	5	3.012	1.60	8	8TZ	1.98
6BQH_5NDD_ASD00111115	8	3.012	1.75	2	8TZ	2.06
6C1Q_4MBS_ASD03160012	8	3.014	3.58	10	MRV	3.15
6C1Q_4MBS_ASD11780002	5	2.017	3.94	2	MRV	3.57
6C1Q_5NDD_ASD03160012	6	2.017	3.95	2	8TZ	3.12
6C1Q_5NDD_ASD11780002	5	0.017	4.02	7	8TZ	3.26
6C1Q_6LI0_ASD03160012	1	2.017	3.06	1	D7W	7.30
6C1Q_6LI0_ASD11780002	1	2.017	1.81	1	D7W	8.48
6C1R_4MBS_ASD03160012	5	12.002	1.68	8	MRV	1.99
6C1R_4MBS_ASD11780002	6	12.002	0.55	2	MRV	3.06
6C1R_5NDD_ASD03160012	2	12.002	0.62	4	8TZ	2.63
6C1R_5NDD_ASD11780002	1	12.002	0.46	9	8TZ	2.44
6CM4_4N4W_ASD00990001	4	1.016	0.59	9	SNT	3.93
6CM4_4N4W_ASD00990027	10	4.01	1.16	1	SNT	2.66
6CM4_4N4W_ASD00990028	8	4.01	1.17	9	SNT	2.80
6CM4_5NDD_ASD00990001	8	2.014	0.65	7	8TZ	3.14
6CM4_5NDD_ASD00990027	5	4.01	1.10	3	8TZ	2.32
6CM4_5NDD_ASD00990028	7	7.005	0.96	4	8TZ	1.69
6CM4_5UIG_ASD00990001	5	4.01	0.74	5	8D1	5.09
6CM4_5UIG_ASD00990027	7	7.005	1.29	4	8D1	1.41
6CM4_5UIG_ASD00990028	8	4.01	1.08	7	8D1	2.52
6CM4_6LI0_ASD00990001	5	1.016	0.59	8	D7W	1.37

6CM4_6LI0_ASD00990027	9	4.01	1.11	7	D7W	1.84
6CM4_6LI0_ASD00990028	10	1.016	0.60	6	D7W	2.29
6E59_4MBS_ASD06720001	8	8.003	1.87	9	MRV	2.37
6E59_4N4W_ASD06720001	4	8.003	1.89	5	SNT	4.62
6E67_4MBS_ASD01580008	2	0.023	0.62	6	MRV	4.79
6E67_4MBS_ASD03130018	2	8.002	2.08	5	MRV	1.44
6E67_4MBS_ASD03130023	3	8.002	1.86	4	MRV	1.82
6E67_5NDD_ASD01580008	3	8.002	0.26	10	8TZ	0.35
6E67_5NDD_ASD03130018	1	8.002	1.93	3	8TZ	2.35
6E67_5NDD_ASD03130023	3	8.002	2.24	3	8TZ	2.85
6FK6_4N4W_ASD02820003	2	8.003	1.33	9	SNT	2.61
6FK6_4N4W_ASD05688001	10	8.003	2.05	5	SNT	3.18
6FK6_4OR2_ASD02820003	3	0.019	1.97	9	FM9	1.50
6FK6_4OR2_ASD05688001	2	0.019	2.14	8	FM9	1.78
6FK7_4N4W_ASD02820003	2	5.009	1.63	6	SNT	2.76
6FK7_4N4W_ASD05688001	7	7.005	1.86	8	SNT	3.75
6FK7_4OO9_ASD02820003	9	6.006	1.93	4	2U8	3.18
6FK7_4OO9_ASD05688001	6	7.005	1.78	5	2U8	4.27
6FK8_4N4W_ASD02820003	6	2.011	2.51	2	SNT	2.91
6FK8_4N4W_ASD05688001	1	1.015	2.42	2	SNT	2.60
6FK8_4OO9_ASD02820003	1	1.015	1.69	3	2U8	3.48
6FK8_4OO9_ASD05688001	7	1.015	2.22	9	2U8	3.79
6FK9_4N4W_ASD02820003	9	2.011	1.80	3	SNT	2.39
6FK9_4N4W_ASD05688001	5	2.011	2.32	6	SNT	3.46
6FK9_4OR2_ASD02820003	5	2.011	2.12	5	FM9	2.12
6FK9_4OR2_ASD05688001	3	0.022	2.49	9	FM9	1.73
6FKA_4K5Y_ASD02820003	3	2.012	1.60	2	1Q5	6.60
6FKA_4K5Y_ASD05688001	1	2.012	1.55	1	1Q5	8.06
6FKA_4N4W_ASD02820003	2	10.004	1.12	9	SNT	3.06
6FKA_4N4W_ASD05688001	4	5.006	2.21	8	SNT	3.45
6FKA_4OO9_ASD02820003	2	1.013	1.73	6	2U8	2.62
6FKA_4OO9_ASD05688001	7	11.003	0.86	5	2U8	3.74
6FKB_4MBS_ASD02820003	1	4.008	1.53	8	MRV	4.08
6FKB_4MBS_ASD05688001	7	7.005	2.56	9	MRV	3.77

6FKB_4N4W_ASD02820003	1	4.008	1.53	2	SNT	3.51
6FKB_4N4W_ASD05688001	8	7.005	2.52	6	SNT	2.07
6FKC_4N4W_ASD02820003	3	6.008	2.67	5	SNT	2.80
6FKC_4N4W_ASD05688001	2	7.006	2.26	4	SNT	3.31
6FKC_4OR2_ASD02820003	8	7.006	2.76	8	FM9	3.35
6FKC_4OR2_ASD05688001	4	7.006	2.11	4	FM9	2.31
6FKD_4N4W_ASD02820003	1	6.008	1.71	5	SNT	2.72
6FKD_4N4W_ASD05688001	5	4.01	2.14	9	SNT	3.09
6FKD_4OO9_ASD02820003	1	6.008	1.35	3	2U8	3.39
6FKD_4OO9_ASD05688001	1	6.008	1.72	2	2U8	4.57
6FUF_4MBS_ASD02820003	8	2.017	1.69	8	MRV	3.51
6FUF_4MBS_ASD05688001	4	2.017	1.65	6	MRV	3.38
6FUF_4N4W_ASD02820003	6	4.006	1.15	10	SNT	3.18
6FUF_4N4W_ASD05688001	3	1.017	1.70	3	SNT	3.21
6GPS_4MBS_ASD10910002	3	2.013	2.54	6	MRV	5.01
6GPS_5NDD_ASD10910002	9	2.013	2.13	1	8TZ	1.40
6GPS_6LI0_ASD10910002	1	5.007	1.29	3	D7W	7.73
6GPX_4MBS_ASD10910002	1	1.015	2.07	6	MRV	3.45
6GPX_5NDD_ASD10910002	1	1.015	2.08	1	8TZ	1.73
6GPX_6LI0_ASD10910002	1	10.003	1.13	5	D7W	7.84
6GT3_4MBS_ASD00180010	7	1.015	1.93	6	MRV	2.27
6GT3_4MBS_ASD00180044	5	8.004	2.12	5	MRV	1.25
6GT3_4MBS_ASD03130013	2	8.004	2.23	5	MRV	1.63
6GT3_4N4W_ASD00180010	3	1.015	2.15	5	SNT	2.49
6GT3_4N4W_ASD00180044	4	8.004	2.10	7	SNT	2.95
6GT3_4N4W_ASD03130013	1	8.004	2.43	2	SNT	4.21
6GT3_5LWE_ASD00180010	7	0.018	2.15	1	79K	2.88
6GT3_5LWE_ASD00180044	1	0.018	1.36	2	79K	2.87
6GT3_5LWE_ASD03130013	2	0.018	3.10	2	79K	3.33
6GT3_5NDD_ASD00180010	3	1.015	2.21	8	8TZ	0.83
6GT3_5NDD_ASD00180044	7	8.004	2.47	3	8TZ	0.86
6GT3_5NDD_ASD03130013	5	2.011	2.86	3	8TZ	1.13
6HLL_4MBS_ASD06720001	1	3.013	74.34	1	MRV	105.06
6HLL_4N4W_ASD06720001	2	3.013	73.02	2	SNT	100.41

6HLL_5NDD_ASD06720001	5	3.013	77.01	5	8TZ	108.15
6HLO_3OE0_ASD06720001	8	6.006	3.55	10	PRD	7.50
6HLO_4N4W_ASD06720001	2	0.017	2.47	2	SNT	5.17
6HLO_5NDD_ASD06720001	5	0.017	2.06	4	8TZ	4.33
6HLP_4MBS_ASD06720001	2	2.017	2.68	2	MRV	1.44
6HLP_4N4W_ASD06720001	2	2.017	2.65	2	SNT	4.73
6HLP_4PHU_ASD06720001	6	1.022	3.06	3	2YB	11.77
6HLP_5NDD_ASD06720001	1	2.017	2.46	6	8TZ	5.15
6J20_4MBS_ASD06720001	9	6.008	280.19	9	MRV	299.82
6J20_4N4W_ASD06720001	2	6.008	276.74	2	SNT	292.65
6J20_5NDD_ASD06720001	1	6.008	277.88	1	8TZ	297.81
6J21_4MBS_ASD06720001	4	3.015	193.28	4	MRV	197.63
6J21_4N4W_ASD06720001	7	3.015	195.65	7	SNT	196.88
6JZH_3OE0_ASD00180010	3	14.001	1.25	6	PRD	11.17
6JZH_3OE0_ASD00180044	4	14.001	1.16	10	PRD	9.96
6JZH_3OE0_ASD03130013	4	0.017	1.51	6	PRD	8.91
6KJV_4MBS_ASD01180443	5	5.009	0.68	7	MRV	5.90
6KJV_4N4W_ASD01180443	5	2.013	0.47	9	SNT	1.78
6KJV_5NDD_ASD01180443	7	2.013	0.48	8	8TZ	4.16
6KK1_4N4W_ASD01180443	6	0.014	0.32	6	SNT	2.72
6KK1_4OR2_ASD01180443	2	1.013	0.91	3	FM9	3.04
6KK7_3OE0_ASD01180443	4	10.002	75.42	4	PRD	117.05
6KK7_4N4W_ASD01180443	1	10.002	71.86	1	SNT	102.05
6KP6_4MBS_ASD01840213	10	5.005	89.83	10	MRV	118.88
6KP6_4MBS_ASD01841006	7	5.005	86.55	7	MRV	115.66
6KP6_4MBS_ASD01914813	7	5.005	85.87	7	MRV	115.43
6KP6_4N4W_ASD01840213	5	5.005	85.44	5	SNT	112.26
6KP6_4N4W_ASD01841006	7	5.005	81.65	7	SNT	108.18
6KP6_4N4W_ASD01914813	4	5.005	79.95	4	SNT	106.33
6KP6_5NDD_ASD01840213	5	5.005	90.08	5	8TZ	120.35
6KP6_5NDD_ASD01841006	3	5.005	91.52	3	8TZ	121.87
6KP6_5NDD_ASD01914813	9	5.005	90.66	9	8TZ	121.10
6KPC_3OE0_ASD01150307	5	4.009	65.98	5	PRD	99.15
6KPC_3OE0_ASD03331798	2	4.009	67.28	2	PRD	99.63

6KPC_3OE0_ASD11730002	7	4.009	65.14	7	PRD	98.44
6KPC_5NDD_ASD01150307	9	4.009	65.32	9	8TZ	87.51
6KPC_5NDD_ASD03331798	4	4.009	64.49	4	8TZ	86.50
6KPC_5NDD_ASD11730002	1	4.009	64.97	1	8TZ	86.76
6KQI_3OE0_ASD03331126	3	0.019	1.91	3	PRD	10.07
6KQI_3OE0_ASD03331623	7	1.012	3.27	9	PRD	10.21
6KQI_3OE0_ASD03331727	9	0.019	2.65	3	PRD	10.08
6KQI_4N4W_ASD03331126	2	0.019	2.32	9	SNT	4.28
6KQI_4N4W_ASD03331623	10	0.019	3.63	7	SNT	4.38
6KQI_4N4W_ASD03331727	1	0.019	3.54	9	SNT	4.37
6KUX_3OE0_ASD00170351	6	0.02	31.75	6	PRD	26.68
6KUX_3OE0_ASD03050002	5	0.02	31.51	5	PRD	26.23
6KUX_3OE0_ASD03070001						
6KUX_4N4W_ASD00170351	1	4.009	36.91	1	SNT	47.14
6KUX_4N4W_ASD03050002	4	0.02	37.81	4	SNT	48.26
6KUX_4N4W_ASD03070001						
6KUX_5NDD_ASD00170351	6	4.009	34.41	6	8TZ	38.19
6KUX_5NDD_ASD03050002	7	4.009	32.84	7	8TZ	36.67
6KUX_5NDD_ASD03070001						
6KUY_4MBS_ASD00170351	10	2.016	1.72	7	MRV	1.35
6KUY_4MBS_ASD03050002	5	2.016	2.18	4	MRV	1.43
6KUY_4MBS_ASD03070001						
6KUY_4N4W_ASD00170351	10	0.019	2.07	10	SNT	4.29
6KUY_4N4W_ASD03050002	3	0.019	2.83	1	SNT	4.50
6KUY_4N4W_ASD03070001						
6KUY_4PHU_ASD00170351	4	2.016	2.00	3	2YB	11.50
6KUY_4PHU_ASD03050002	2	2.016	1.88	2	2YB	11.57
6KUY_4PHU_ASD03070001						
6LN2_4MBS_ASD01180443	8	3.011	0.46	7	MRV	4.67
6LN2_4N4W_ASD01180443	5	3.011	0.50	9	SNT	3.15
6LUQ_4MBS_ASD00990001	2	1.017	0.39	6	MRV	4.78
6LUQ_4MBS_ASD00990027	8	1.017	0.65	4	MRV	2.74
6LUQ_4MBS_ASD00990028	4	1.017	0.74	5	MRV	1.83
6LUQ_4N4W_ASD00990001	2	1.017	0.37	6	SNT	3.86

6LUQ_4N4W_ASD00990027	6	1.017	1.69	3	SNT	3.01
6LUQ_4N4W_ASD00990028	5	1.017	0.66	6	SNT	3.42
6LUQ_5NDD_ASD00990001	5	0.017	1.82	6	8TZ	4.60
6LUQ_5NDD_ASD00990027	2	0.017	1.64	2	8TZ	4.41
6LUQ_5NDD_ASD00990028	5	1.017	1.80	3	8TZ	4.98
6LUQ_5TZY_ASD00990001	8	2.014	0.71	6	7OS	1.75
6LUQ_5TZY_ASD00990027	8	6.007	1.65	1	7OS	1.81
6LUQ_5TZY_ASD00990028	9	2.014	1.39	4	7OS	1.60
6MH8_3OE0_ASD00180010	8	0.017	0.83	4	PRD	8.05
6MH8_3OE0_ASD00180044	2	0.017	1.14	9	PRD	8.16
6MH8_3OE0_ASD03130013	5	2.014	2.70	2	PRD	7.08
6MH8_4N4W_ASD00180010	7	0.017	1.42	10	SNT	3.47
6MH8_4N4W_ASD00180044	3	0.017	1.15	6	SNT	3.83
6MH8_4N4W_ASD03130013	6	0.017	2.41	3	SNT	4.88
6MH8_5NDD_ASD00180010	3	3.011	2.08	2	8TZ	1.02
6MH8_5NDD_ASD00180044	7	0.017	2.50	2	8TZ	1.62
6MH8_5NDD_ASD03130013	2	3.011	2.91	4	8TZ	1.60
6NWE_4N4W_ASD02820003	8	9.001	2.18	9	SNT	3.36
6NWE_4N4W_ASD05688001	4	6.008	2.20	4	SNT	3.71
6NWE_4OO9_ASD02820003	4	0.017	1.08	7	2U8	0.33
6NWE_4OO9_ASD05688001	2	0.017	2.10	2	2U8	0.74
6OL9_4MBS_ASD01850003	9	9.002	61.17	9	MRV	68.37
6OL9_4N4W_ASD01850003	1	9.002	64.21	1	SNT	74.75
6PEL_4N4W_ASD02820003	5	0.018	1.26	2	SNT	3.70
6PEL_4N4W_ASD05688001	3	0.018	1.15	2	SNT	4.07
6PEL_4OO9_ASD02820003	1	0.018	1.41	7	2U8	1.02
6PEL_4OO9_ASD05688001	3	0.018	1.15	2	2U8	1.53
6PGS_4MBS_ASD02820003	10	0.015	1.32	10	MRV	3.78
6PGS_4MBS_ASD05688001	6	0.015	1.97	5	MRV	3.07
6PGS_4N4W_ASD02820003	1	0.015	1.38	5	SNT	1.90
6PGS_4N4W_ASD05688001	3	0.015	1.00	4	SNT	2.42
6PH7_4MBS_ASD02820003	9	9.004	2.00	9	MRV	3.73
6PH7_4MBS_ASD05688001	5	9.004	1.42	4	MRV	2.87
6PRZ_3OE0_ASD01580008	10	6.005	0.65	9	PRD	6.57

6PRZ_3OE0_ASD03130018	9	2.01	0.98	5	PRD	3.39
6PRZ_3OE0_ASD03130023	1	2.01	1.60	2	PRD	2.28
6PS0_4MBS_ASD01580008	10	1.014	0.56	2	MRV	5.09
6PS0_4MBS_ASD03130018	8	12.002	2.11	6	MRV	1.48
6PS0_4MBS_ASD03130023	7	12.002	1.42	1	MRV	2.03
6PS0_5NDD_ASD01580008	1	0.014	1.28	1	8TZ	0.75
6PS0_5NDD_ASD03130018	1	12.002	1.83	3	8TZ	1.55
6PS0_5NDD_ASD03130023	2	12.002	2.07	1	8TZ	3.32
6PS1_4MBS_ASD01580008	3	7.005	0.85	2	MRV	3.98
6PS1_4MBS_ASD03130018	10	6.006	1.13	5	MRV	0.83
6PS1_4MBS_ASD03130023	1	6.006	2.96	1	MRV	1.41
6PS2_3OE0_ASD01580008	1	5.005	0.83	9	PRD	6.95
6PS2_3OE0_ASD03130018	2	1.013	1.17	5	PRD	4.06
6PS2_3OE0_ASD03130023	7	12.001	1.10	6	PRD	4.30
6PS3_4MBS_ASD01580008	6	2.01	1.12	3	MRV	3.76
6PS3_4MBS_ASD03130018	6	4.008	1.66	5	MRV	0.89
6PS3_4MBS_ASD03130023	8	6.005	2.92	8	MRV	0.87
6PS3_4N4W_ASD01580008	3	1.01	0.60	3	SNT	4.00
6PS3_4N4W_ASD03130018	4	6.005	2.80	4	SNT	4.43
6PS3_4N4W_ASD03130023	2	10.003	3.23	4	SNT	5.35
6PS3_5NDD_ASD01580008	3	0.017	1.20	3	8TZ	0.64
6PS3_5NDD_ASD03130018	2	0.017	2.12	2	8TZ	1.95
6PS3_5NDD_ASD03130023	4	10.003	2.79	4	8TZ	3.02
6PS4_3OE0_ASD01580008	5	0.02	0.60	4	PRD	11.19
6PS4_3OE0_ASD03130018	10	4.008	1.12	10	PRD	4.13
6PS4_3OE0_ASD03130023	1	0.02	3.89	2	PRD	8.99
6PS4_5NDD_ASD01580008	8	0.02	0.81	9	8TZ	0.84
6PS4_5NDD_ASD03130018	2	0.02	1.71	2	8TZ	1.73
6PS4_5NDD_ASD03130023	3	0.02	2.80	3	8TZ	2.42
6PS4_6LI0_ASD01580008	1	3.011	0.76	1	D7W	4.66
6PS4_6LI0_ASD03130018						
6PS4_6LI0_ASD03130023	1	3.011	0.45	1	D7W	4.41
6PS5_4MBS_ASD01580008	8	0.014	0.94	5	MRV	3.52
6PS5_4MBS_ASD03130018	7	8.005	2.10	1	MRV	0.96

6PS5_4MBS_ASD03130023	5	8.005	2.53	3	MRV	1.47
6PS5_4N4W_ASD01580008	8	0.014	1.00	2	SNT	4.83
6PS5_4N4W_ASD03130018	1	8.005	2.17	2	SNT	4.16
6PS5_4N4W_ASD03130023	2	8.005	2.16	1	SNT	4.06
6PS5_5NDD_ASD01580008	3	0.014	0.96	1	8TZ	1.21
6PS5_5NDD_ASD03130018	1	0.014	2.63	1	8TZ	1.54
6PS5_5NDD_ASD03130023	1	0.014	3.20	1	8TZ	2.35
6PS6_4MBS_ASD01580008	10	0.018	0.73	4	MRV	3.88
6PS6_4MBS_ASD03130018	5	1.014	1.93	3	MRV	0.50
6PS6_4MBS_ASD03130023	5	1.014	4.05	5	MRV	1.38
6PS6_5NDD_ASD01580008	2	0.018	0.99	2	8TZ	0.85
6PS6_5NDD_ASD03130018	1	0.018	2.18	1	8TZ	1.87
6PS6_5NDD_ASD03130023	1	0.018	3.10	1	8TZ	2.91
6PS7_3OE0_ASD00180010	6	3.01	2.38	3	PRD	7.88
6PS7_3OE0_ASD00180044	8	7.005	2.11	5	PRD	8.79
6PS7_3OE0_ASD03130013	3	6.005	2.02	3	PRD	8.02
6PS7_5KW2_ASD00180010	1	0.018	1.09	5	6XQ	5.59
6PS7_5KW2_ASD00180044	1	0.018	1.67	9	6XQ	4.14
6PS7_5KW2_ASD03130013	4	5.006	3.10	4	6XQ	3.05
6PS7_5NDD_ASD00180010	7	3.01	2.30	2	8TZ	1.09
6PS7_5NDD_ASD00180044	10	7.005	2.08	6	8TZ	0.12
6PS7_5NDD_ASD03130013	3	3.01	2.59	5	8TZ	1.44
6PT2_4N4W_ASD03180043	5	8.002	51.95	5	SNT	65.99
6PT2_4N4W_ASD16020002	10	8.002	52.29	10	SNT	66.02
6PT2_4OO9_ASD03180043	5	8.002	56.57	5	2U8	69.75
6PT2_4OO9_ASD16020002	4	8.002	54.41	4	2U8	67.61
6PT3_4N4W_ASD03180043	8	2.01	64.58	8	SNT	86.54
6PT3_4N4W_ASD16020002	9	2.01	63.94	9	SNT	85.90
6PT3_4OO9_ASD03180043	1	2.01	63.67	1	2U8	85.80
6PT3_4OO9_ASD16020002	4	2.01	63.29	4	2U8	85.73
6RZ4_3OE0_ASD01883993	1	0.015	2.20	8	PRD	7.39
6RZ4_3OE0_ASD01885005	1	0.015	2.20	10	PRD	7.13
6RZ4_3OE0_ASD01885006	6	10.004	2.58	6	PRD	7.79
6RZ4_4N4W_ASD01883993	7	5.006	1.55	6	SNT	4.57

6RZ4_4N4W_ASD01885005	8	5.006	1.47	4	SNT	4.55
6RZ4_4N4W_ASD01885006	5	5.006	1.31	10	SNT	5.23
6RZ5_3OE0_ASD01883993	2	8.002	16.75	2	PRD	47.23
6RZ5_3OE0_ASD01885005	1	8.002	16.33	1	PRD	46.93
6RZ5_3OE0_ASD01885006	8	8.002	17.05	4	PRD	46.47
6RZ5_4N4W_ASD01883993	1	8.002	17.48	3	SNT	35.02
6RZ5_4N4W_ASD01885005	2	8.002	17.40	4	SNT	34.99
6RZ5_4N4W_ASD01885006	3	8.002	17.34	7	SNT	34.85
6RZ5_5TZY_ASD01883993	2	8.002	2.44	1	7OS	1.79
6RZ5_5TZY_ASD01885005	8	3.011	1.91	1	7OS	2.01
6RZ5_5TZY_ASD01885006	2	3.011	1.71	4	7OS	1.78
6S0Q_3ODU_ASD00180010	5	8.004	87.83	5	ITD	96.52
6S0Q_3ODU_ASD00180044	4	8.004	87.98	4	ITD	97.54
6S0Q_3ODU_ASD03130013	9	8.004	88.60	9	ITD	97.31
6S0Q_5LWE_ASD00180010	1	8.004	82.44	1	79K	97.36
6S0Q_5LWE_ASD00180044	7	8.004	83.44	7	79K	98.80
6S0Q_5LWE_ASD03130013	4	8.004	83.29	4	79K	98.43
6S0Q_5TZY_ASD00180010	1	8.004	97.49	1	7OS	97.78
6S0Q_5TZY_ASD00180044	10	8.004	97.59	10	7OS	97.91
6S0Q_5TZY_ASD03130013	1	8.004	97.28	1	7OS	97.59
6VI4_4MBS_ASD00170299	6	3.009	11.95	2	MRV	19.22
6VI4_4MBS_ASD03170003	10	3.009	12.02	6	MRV	19.43
6VI4_4MBS_ASD03170006	9	3.009	12.58	1	MRV	19.42
6VI4_5NDD_ASD00170299	10	3.009	22.44	10	8TZ	34.86
6VI4_5NDD_ASD03170003	9	3.009	24.96	9	8TZ	37.23
6VI4_5NDD_ASD03170006	9	3.009	24.15	9	8TZ	36.63
6W25_4MBS_ASD05140009	9	1.011	14.44	9	MRV	21.14
6W25_4MBS_ASD05143009	3	1.011	14.24	3	MRV	20.49
6W25_4MBS_ASD05143011	2	1.011	14.21	2	MRV	20.09
6W25_4N4W_ASD05140009	10	1.011	93.90	10	SNT	99.88
6W25_4N4W_ASD05143009	10	1.011	93.91	10	SNT	99.82
6W25_4N4W_ASD05143011	9	1.011	92.31	9	SNT	98.19
6W25_5NDD_ASD05140009	5	1.011	15.51	5	8TZ	17.55
6W25_5NDD_ASD05143009	1	1.011	14.30	1	8TZ	16.09

6W25_5NDD_ASD05143011	2	1.011	14.27	2	8TZ	15.93
6W25_5TZR_ASD05140009	1	1.011	93.24	1	MK6	90.04
6W25_5TZR_ASD05143009	8	1.011	92.87	4	MK6	89.99
6W25_5TZR_ASD05143011	1	1.011	92.31	1	MK6	88.93
6WJC_3OE0_ASD01810375	7	3.012	1.90	8	PRD	8.53
6WJC_3OE0_ASD01810699	6	1.017	0.43	6	PRD	13.23
6WJC_3OE0_ASD01811561	6	1.017	0.84	10	PRD	9.51
6WJC_4MQT_ASD01810375	1	3.012	1.90	3	2CU	4.69
6WJC_4MQT_ASD01810699	7	6.005	0.63	10	2CU	4.94
6WJC_4MQT_ASD01811561	6	6.005	1.07	6	2CU	5.00
6WJC_4N4W_ASD01810375	3	5.008	1.39	1	SNT	7.20
6WJC_4N4W_ASD01810699	2	0.021	0.81	5	SNT	3.19
6WJC_4N4W_ASD01811561	6	1.017	0.96	7	SNT	3.13

^a "Daughter"_"Parent"_Ligand: "Daughter" and "Parent" structures given as PDB IDs, Ligand as ASD ID

^b Pose ID of the docked ligand that was closest to the hot spot

^c Hot spot ID and the number of probe clusters. E.g. 0.021 means the top hot spot (numbered as 0) with 21 probe clusters, see the FTMap paper.

^d Shortest distance between the center of mass of the docked ligand and the hot spot

^e Pose ID of the docked ligand that had the shortest distance to the allosteric modulator copied from the "parent" protein

^f 3-letter PDB code of the ligand in the "parent" structure

^g Distance between the center of mass of the docked ligand and the center of mass of the ligand from the "parent" structure.

Table S7. Number of structures with conserved sites, grouped by conformational state, for 'parent' structures listed in Table 1.

Parent ^a				Daughter			
PDB	Target	Class	State	Active	Intermediate	Inactive	Other
5UIG	A _{2A}	A	Inactive	73	16	192	1
5X7D	β ₂	A	Inactive			33	
5T1A	CCR2	A	Inactive			19	
4MBS	CCR5	A	Inactive	81	18	219	1
6QZH	CCR7	A	Inactive	1		9	
5LWE	CCR9	A	Inactive	2		44	
3ODU	CXCR4	A	Inactive	40	12	179	1
3OE0	CXCR4	A	Inactive	81	20	218	1
4PHU	FFA1	A	Intermediate	1	2	9	
5KW2	FFA1	A	Intermediate	18	7	21	
5TZR	FFA1	A	Intermediate	1	2	9	1
5TZY	FFA1	A	Intermediate	17	8	23	
6LI0	GPR52	A	Inactive	26	8	59	1
4MQT	M ₂	A	Active	28	15	83	
5NDD	PAR2	A	Intermediate	36	12	140	1
5NDZ	PAR2	A	Intermediate		1		
4K5Y	CRF ₁	B	Inactive	1	1	3	
4OR2	mGlu ₁	C	Inactive	35	12	143	
4OO9	mGlu ₅	C	Inactive	39	5	100	1
4N4W	SMO	F	Inactive	56	12	126	1
5L7I	SMO	F	Inactive	9	7	32	
All structures				88	34	271	1

^a Parent structures with weakly detected, or protein-membrane interfacial sites were left out of this analysis (one active-state, one intermediate and 16 inactive-state structures).