

## Recognition of ATP binding sites by searching the ASTRAL dataset.

The Table presents a list of proteins (top 400) whose binding sites were recognized to be similar to the ATP binding site of the “hypothetical” protein MJ0577 (1mjh). The proteins are listed in order of decreasing similarity to the query binding site.

Rank	PDB code	Match Score	t-score	p-value	SCOP Family	SCOP Remarks
1	1mjhA	100	273	0.02	52436	complexed with atp
2	1o97C	44	90	1.30	52432	complexed with amp, fad
3	1efvB	42	84	1.35	52432	complexed with amp, fad
4	1iw7D	40	77	1.39	64490	None
5	1jqnA	40	77	1.39	51632	complexed with asp, dco, mn
6	1n7vA	39	74	1.42	89429	complexed with act, ca
7	1ihuA	39	74	1.42	52652	None
8	1i0zA	39	74	1.42	51848	None
9	3grs	39	74	1.42	51943	None
10	1lldA	39	74	1.42	51848	None
11	1ldm	38	71	1.44	51848	complexed with nad, oxm
12	1ufhA	38	71	1.44	55730	None
13	1nvmB	38	71	1.44	51800	None
14	1n6bA	38	71	1.44	48265	complexed with dmz, hem, so4
15	1d0cA	38	71	1.44	56513	None
16	1qkrA	38	71	1.44	47221	None
17	1rgs	38	71	1.44	51210	None
18	1hjzA	38	71	1.44	89724	None
19	1e3hA	38	71	1.44	46916	complexed with so4
20	1ng7A	38	71	1.44	89044	None
21	1jmvA	38	71	1.44	52436	None
22	1hyuA	38	71	1.44	51943	None
23	1ja1A	38	71	1.44	50438	None
24	1cipA	38	71	1.44	47896	complexed with gnp, mg
25	1bjbA	38	71	1.44	49159	a single-chain construct with epsilon chain domain, includes part of the linker
26	1lnzA	38	71	1.44	82052	None
27	1ek6A	38	71	1.44	51751	None
28	1trb	38	71	1.44	51943	None
29	1hyeA	37	68	1.46	51848	complexed with nap
30	1af7	37	68	1.46	47758	complexed with sah
31	1onfA	37	68	1.46	51943	None
32	1o0sA	37	68	1.46	51883	None
33	1lh0A	37	68	1.46	53272	None
34	1mdbA	37	68	1.46	56802	complexed with amp, dbh, so4
35	2pia	37	68	1.46	63381	complexed with fes, fmn
36	1jyeA	37	68	1.46	53823	complexed with gol; mutant
37	1cgmE	37	68	1.46	47196	None
38	1ni3A	37	68	1.46	52592	complexed with mse, so4

39	lgehA	37	68	1.46	51650	None
40	locyA	37	68	1.46	88875	complexed with cit, so4, zn
41	le9xA	37	68	1.46	48265	complexed with hem, pim; mutant
42	lfurA	37	68	1.46	48558	None
43	lnp7A	37	68	1.46	48174	None
44	ll7vA	37	68	1.46	75648	None
45	1k4zA	37	68	1.46	69341	None
46	lj7lA	37	68	1.46	64411	None
47	lby5A	37	68	1.46	56948	complexed with c8e, fe, orn
48	1k32A	37	68	1.46	68933	None
49	lrypD	37	68	1.46	56251	None
50	ldabA	37	68	1.46	51153	None
51	lnkr	37	68	1.46	49159	None
52	lazsC	37	68	1.46	47896	complexed with fkp, gsp, mg; mutant
53	lfo4A	37	68	1.46	47742	None
54	linp	37	68	1.46	56656	complexed with mg
55	lkekA	37	68	1.46	88746	None
56	ldgtB	36	64	1.49	47786	complexed with amp, zn
57	lmswD	36	64	1.49	56691	elongation complex; shows dramatic conformational changes in the transition from initiation to elongation transcription
58	lcliA	36	64	1.49	55327	None
59	lqorA	36	64	1.49	50136	None
60	lkk8A	36	64	1.49	50085	complexed with adp, bef, ca, gol, mg; mutant
61	3pmgA	36	64	1.49	53739	None
62	lezvA	36	64	1.49	63412	None
63	ldzlA	36	64	1.49	88649	mutant
64	ldl6A	36	64	1.49	57784	complexed with zn
65	lldnA	36	64	1.49	51848	None
66	llfpA	36	64	1.49	75626	structural genomics
67	lb35A	36	64	1.49	88634	None
68	la8o	36	64	1.49	47354	mutant
69	lky9B	36	64	1.49	74933	None
70	lp3hA	36	64	1.49	50130	None
71	lhy0A	36	64	1.49	48558	None
72	lm6nA	36	64	1.49	81768	complexed with so4
73	2pii	36	64	1.49	54914	None
74	2mysA	36	64	1.49	50085	complexed with mg, mly, so4
75	lkzqA	36	64	1.49	74878	None
76	lfmk	36	64	1.49	50045	None
77	ljfbA	36	64	1.49	48265	complexed with gol, hem
78	ljhdA	36	64	1.49	63801	complexed with br, so4
79	ln12A	36	64	1.49	49405	None
80	li12A	36	64	1.49	55730	None
81	lhwxA	36	64	1.49	51883	None
82	lfftC	36	64	1.49	81451	None

83	1fy7A	36	64	1.49	55730	complexed with coa, na
84	1esc	36	64	1.49	52267	None
85	1ftt	36	64	1.49	46690	None
86	1kmoA	36	64	1.49	56948	complexed with hto, lda
87	1m4uA	36	64	1.49	82904	complexed with nag
88	1p5hA	36	64	1.49	89797	None
89	1e19A	36	64	1.49	53634	None
90	1mt5A	36	64	1.49	75305	None
91	1f8nA	36	64	1.49	48485	complexed with fe2
92	1e8cA	36	64	1.49	63419	None
93	1jchA	36	64	1.49	63841	None
94	1bx4A	36	64	1.49	53614	complexed with adn, cl, mo4, mo6
95	1fmb	36	64	1.49	50631	complexed with hyb; mutant
96	1qhxA	36	64	1.49	52569	complexed with atp, mg
97	1cydA	36	64	1.49	51751	None
98	1n7dA	36	64	1.49	63826	complexed with ca, keg, man, nag; mutant
99	1gteA	36	64	1.49	46553	None
100	1kqpA	36	64	1.49	52403	None
101	1cjwA	36	64	1.49	55730	complexed with cot
102	1k0mA	36	64	1.49	47617	None
103	1epwA	36	64	1.49	49956	complexed with so4, zn
104	1h29A	36	64	1.49	48696	None
105	1dmuA	36	64	1.49	52990	None
106	1ejdA	36	64	1.49	55209	None
107	1ns5A	36	64	1.49	82371	None
108	1m32A	36	64	1.49	53402	None
109	1h30A	36	64	1.49	49944	None
110	1i5zA	36	64	1.49	46796	None
111	1qczA	36	64	1.49	52256	None
112	1mxiA	36	64	1.49	75218	complexed with iod, sah
113	1pf4A	36	64	1.49	52686	None
114	2trcP	36	64	1.49	52888	complexed with gd
115	1n97A	36	64	1.49	48265	None
116	1f2A	36	64	1.49	51943	None
117	1ih7A	36	64	1.49	53118	complexed with gmp, k
118	451c	36	64	1.49	46627	complexed with hem
119	1he7A	36	64	1.49	49159	swapped N-terminal strand dimer; only one subunit is in the PDB entry
120	1jilA	36	64	1.49	52375	complexed with 485
121	1h6kA	36	64	1.49	48385	None
122	3btaA	36	64	1.49	49956	complexed with zn
123	1rkd	36	64	1.49	53614	complexed with adp, po4, rib
124	1hzfA	36	64	1.49	48251	complexed with mse
125	1cvuA	36	64	1.49	48132	None
126	1gz5A	36	64	1.49	82540	None
127	1fxoA	36	64	1.49	53464	None
128	1qm9A	36	64	1.49	54929	None

129	1lbvA	36	64	1.49	56656	None
130	1qlaA	36	64	1.49	46978	None
131	2cy3	36	64	1.49	48696	complexed with hem
132	1h41A	36	64	1.49	82253	None
133	1i7nA	36	64	1.49	52463	None
134	1nxiA	36	64	1.49	89947	structural genomics
135	1kyqA	36	64	1.49	75110	None
136	1jvbA	36	64	1.49	50136	complexed with mse, zn
137	1fecA	36	64	1.49	51943	None
138	1ojt	36	64	1.49	51943	None
139	1k4nA	36	64	1.49	75396	structural genomics
140	1ky9A	36	64	1.49	74933	None
141	1o22A	36	64	1.49	90065	structural genomics
142	1jvr	36	64	1.49	47842	None
143	1mqsa	36	64	1.49	56816	complexed with an N-terminal peptide of sed5p, chain B
144	1i7pA	36	64	1.49	63381	complexed with fad
145	1chmA	36	64	1.49	53093	None
146	1d7yA	36	64	1.49	51943	None
147	1pswA	36	64	1.49	89784	structural genomics
148	1d4aA	36	64	1.49	52235	None
149	1jlnA	36	64	1.49	53851	None
150	1ivyA	36	64	1.49	53499	None
151	1jc4A	36	64	1.49	64257	None
152	1e79A	36	64	1.49	47918	None
153	2tpsA	36	64	1.49	51392	None
154	1iknD	36	64	1.49	48404	None
155	1fepA	36	64	1.49	56948	None
156	1gz0A	36	64	1.49	75218	None
157	1qbkB	36	64	1.49	48372	complexed with gnp, mg
158	1hriA	36	64	1.49	48648	complexed with cholesterol
159	1gw5B	36	64	1.49	74771	complexed with ihp
160	1kv3A	36	64	1.49	81289	None
161	1c8dA	36	64	1.49	88646	complexed with ca
162	19hcA	36	64	1.49	48696	None
163	1d0nA	36	64	1.49	55754	None
164	1l11A	36	64	1.49	75131	None
165	1kbiA	36	64	1.49	51396	complexed with fmm, hem, mpd, po4, pyr
166	3cyr	36	64	1.49	48696	complexed with hem
167	1n9pA	35	61	1.51	81966	complexed with mse
168	1f8fA	35	61	1.51	50136	complexed with eoh, nah, so4, zn
169	1i58A	35	61	1.51	55884	None
170	1qamA	35	61	1.51	88784	complexed with act
171	1e5kA	35	61	1.51	53470	complexed with cit, li
172	1j6zA	35	61	1.51	53068	None
173	1m6iA	35	61	1.51	51943	None
174	1j4nA	35	61	1.51	56895	complexed with bng

175	1i50A	35	61	1.51	64485	complexed with mn, zn
176	1k3rA	35	61	1.51	74955	None
177	1hynP	35	61	1.51	64362	None
178	1byi	35	61	1.51	52652	None
179	1k92A	35	61	1.51	52403	complexed with cry, so4; mutant
180	1iqvA	35	61	1.51	47974	None
181	1fftB	35	61	1.51	49541	None
182	1j0mA	35	61	1.51	48234	complexed with ca
183	1ebdA	35	61	1.51	51943	None
184	1gkuB	35	61	1.51	69496	None
185	1n62C	35	61	1.51	55448	None
186	1m7sA	35	61	1.51	56635	None
187	1hm9A	35	61	1.51	51171	None
188	1m1cA	35	61	1.51	82857	None
189	1gg3A	35	61	1.51	47032	None
190	1k3kA	35	61	1.51	56855	mutant
191	1kliH	35	61	1.51	50514	complexed with ben, ca, gol, so4
192	1qb7A	35	61	1.51	53272	complexed with ade, cit, mg
193	1gk8A	35	61	1.51	51650	None
194	1io7A	35	61	1.51	48265	None
195	1c8bA	35	61	1.51	64095	None
196	1fc6A	35	61	1.51	68933	mutant
197	1nuyA	35	61	1.51	56656	complexed with f6p, mg, pi
198	1k28A	35	61	1.51	69256	complexed with k, po4
199	1hdoA	35	61	1.51	51751	complexed with nap
200	1fgjA	35	61	1.51	48711	None
201	1qo8A	35	61	1.51	48711	None
202	1qi9A	35	61	1.51	48321	None
203	1qj5A	35	61	1.51	53417	None
204	2rspA	35	61	1.51	50631	None
205	1mdc	35	61	1.51	50847	complexed with plm, so4
206	1eyqA	35	61	1.51	54627	None
207	1ni5A	35	61	1.51	82359	complexed with mse
208	1hh5A	35	61	1.51	48696	complexed with hec
209	1oxwA	35	61	1.51	89729	None
210	1jgtA	35	61	1.51	52403	None
211	1k9oI	35	61	1.51	56575	Michaelis serpin-trypsin complex
212	1ksiA	35	61	1.51	49999	None
213	1dxrC	35	61	1.51	48707	complexed with bcb, bpb, fe2, hec, lda, mq9, mst, ns5, so4; mutant
214	1gosA	35	61	1.51	51913	None
215	1dceA	35	61	1.51	48440	None
216	1bhgA	35	61	1.51	49304	None
217	1i52A	35	61	1.51	68901	complexed with ca, ctp, mg
218	1kssA	35	61	1.51	48711	complexed with fad, fum, hem, na; mutant
219	1f8mA	35	61	1.51	88704	None
220	1i6lA	35	61	1.51	52375	complexed with gol, nh4, so4, tym

221	1h6vA	35	61	1.51	51943	None
222	1g9mG	35	61	1.51	56503	complexed with fuc, ioh, nag; mutant
223	1luxy	35	61	1.51	56184	complexed with epu, fad; mutant
224	1hr6A	35	61	1.51	63412	None
225	1iwgA	35	61	1.51	82694	None
226	1pfo	35	61	1.51	56979	None
227	1klfB	35	61	1.51	49405	None
228	1gdnA	35	61	1.51	50514	complexed with gol, so4
229	1o2dA	35	61	1.51	69892	None
230	1hh2P	35	61	1.51	50282	None
231	1adn	35	61	1.51	57885	complexed with zn
232	1edoA	35	61	1.51	51751	complexed with nap
233	2shpA	35	61	1.51	52805	None
234	1ffyA	35	61	1.51	47324	protein/RNA complex; complexed with k, mo2, mo4, mo5, mo6, mrc, zn
235	1bif	35	61	1.51	52589	complexed with atg, gol, mg, po4; mutant
236	1dekA	35	61	1.51	52541	None
237	1lfkA	35	61	1.51	48265	complexed with hem
238	1azsA	35	61	1.51	55074	complexed with fkp, gsp, mg; mutant
239	1ko7A	35	61	1.51	75139	None
240	1zakA	35	61	1.51	52541	None
241	1k3pA	35	61	1.51	48257	None
242	1d4bA	35	61	1.51	54278	None
243	1mbyA	35	61	1.51	82616	None
244	1iz0A	35	61	1.51	50136	complexed with mse, so4
245	1b04A	35	61	1.51	56096	None
246	1o8aA	35	61	1.51	55505	complexed with act, cl, nag, ndg, nxa, zn
247	1ni4B	35	61	1.51	88741	None
248	1fgyA	35	61	1.51	50730	complexed with 4ip
249	1nqeA	35	61	1.51	56948	complexed with c8e, mg
250	7odcA	35	61	1.51	88683	complexed with plp; mutant
251	1hrkA	35	61	1.51	53801	None
252	1tubB	35	61	1.51	52491	complexed with gdp, gtp, txl
253	1bhtA	35	61	1.51	57415	None
254	1odmA	35	61	1.51	51198	complexed with asv, fe2, so4
255	1bdb	35	61	1.51	51751	complexed with nad
256	1ca1	35	61	1.51	48538	complexed with cd, zn
257	1ksfX	35	61	1.51	81924	complexed with adp, ioh, met, mg, pge; mutant
258	1gkrA	35	61	1.51	75044	None
259	4fiv	35	61	1.51	50631	complexed with 1ni
260	1itwA	35	61	1.51	82526	None
261	1n7hA	35	61	1.51	51751	None
262	1gp1A	35	61	1.51	52901	None
263	1hskA	35	61	1.51	56184	complexed with fad
264	1lshA	35	61	1.51	48432	complexed with pca, pld, upl

265	1kk6A	35	61	1.51	51168	None
266	1du2A	35	61	1.51	46576	None
267	1fs0G	35	61	1.51	52944	complexed to the epsilon subunit; the coiled-coil part is disordered
268	1mi1A	35	61	1.51	81838	None
269	1n5uA	35	61	1.51	48553	None
270	1vdc	35	61	1.51	51943	None
271	1e5pA	35	61	1.51	50815	None
272	1rdr	35	61	1.51	56694	complexed with ca
273	1aop	35	61	1.51	55125	None
274	1hxhA	35	61	1.51	51751	None
275	1ecrA	35	61	1.51	56597	protein/DNA complex
276	2tbvA	35	61	1.51	88643	None
277	1gwiA	35	61	1.51	48265	None
278	1cby	35	61	1.51	55677	None
279	1pda	35	61	1.51	53851	complexed with acy, dpm
280	1dmtA	35	61	1.51	55502	complexed with gol, nag, rdf, zn
281	1f1sA	35	61	1.51	48234	None
282	1h4vB	35	61	1.51	52955	complexed with so4
283	1b8oA	35	61	1.51	53168	complexed with imh, mg, po4
284	1ja9A	35	61	1.51	51751	complexed with ndp, pyq
285	1gz2A	35	61	1.51	56437	complexed with sep
286	1uayA	35	61	1.51	51751	None
287	1gy8A	35	61	1.51	51751	None
288	1l1qA	35	61	1.51	53272	complexed with 9da, so4
289	1n62A	35	61	1.51	47742	None
290	1umuA	35	61	1.51	51307	None
291	1eovA	35	61	1.51	50250	None
292	1hdcA	35	61	1.51	51751	None
293	1g0dA	35	61	1.51	81289	complexed with so4
294	1e6uA	35	61	1.51	51751	complexed with nap, so4, trs, uvw
295	1f5nA	35	61	1.51	48341	complexed with gnp, mg; mutant
296	1i16	35	61	1.51	50172	None
297	1a49A	35	61	1.51	50801	None
298	1egaA	35	61	1.51	52592	None
299	1jymA	35	61	1.51	56421	None
300	1aozA	35	61	1.51	49550	None
301	1ciy	35	61	1.51	49796	None
302	1j5sA	35	61	1.51	75082	None
303	1ihmA	35	61	1.51	88637	None
304	1chuA	35	61	1.51	46978	None
305	1psdA	35	61	1.51	51830	None
306	1pymA	35	61	1.51	88704	None
307	1i50B	35	61	1.51	64490	complexed with mn, zn
308	1tgoA	35	61	1.51	53118	None
309	1j6uA	35	61	1.51	51985	structural genomics
310	1cfr	35	61	1.51	52999	None
311	1dosA	35	61	1.51	51591	None

312	2cmd	35	61	1.51	51848	complexed with cit
313	1bgxT	35	61	1.51	47808	None
314	1lla	35	61	1.51	48051	complexed with cl, cu, na
315	1mpp	35	61	1.51	50646	complexed with so4
316	1mpp	35	61	1.51	50646	complexed with so4
317	2prgA	35	61	1.51	48509	None
318	1kzkA	35	61	1.51	50631	None
319	1tubA	35	61	1.51	52491	complexed with gdp, gtp, txl
320	1lw7A	35	61	1.51	52397	complexed with mse, nad, so4
321	1khvA	35	61	1.51	56694	None
322	1jg1A	35	61	1.51	53354	complexed with sah
323	1h65A	35	61	1.51	52592	None
324	1ngvA	35	61	1.51	89763	None
325	1jmsA	35	61	1.51	47803	complexed with mg, na
326	1f0xA	35	61	1.51	55109	None
327	1ezvB	35	61	1.51	63412	None
328	1dnv	35	61	1.51	88647	None
329	1gkmA	35	61	1.51	48572	complexed with cys, gol, oxo, so4; mutant
330	1mkiA	35	61	1.51	90084	None
331	2hhmA	35	61	1.51	56656	None
332	1ofdA	35	61	1.51	69337	None
333	1jogA	35	61	1.51	81740	None
334	1jboB	35	61	1.51	46532	complexed with cyc, men
335	1hetA	35	61	1.51	50136	None
336	1g2nA	35	61	1.51	48509	complexed with eph
337	1mslA	35	61	1.51	81329	None
338	1gweA	35	61	1.51	56635	complexed with hem, so4
339	1njfA	35	61	1.51	81269	None
340	1kbvA	35	61	1.51	49550	None
341	1guzA	35	61	1.51	51848	None
342	1j18A	35	61	1.51	49453	complexed with acy, ca, glc, so4
343	1jj21	35	61	1.51	48663	complexed with cd, cl, k, mg, na
344	1l8qA	35	61	1.51	81695	complexed with adp, mg, mse
345	1et9A	35	61	1.51	50219	None
346	2ae2A	35	61	1.51	51751	None
347	1kwgA	35	61	1.51	51012	complexed with act, cl, mpd, zn
348	1hyrC	35	61	1.51	48942	None
349	1dz4A	35	61	1.51	48265	None
350	1io1A	35	61	1.51	64519	mutant
351	1jscA	35	61	1.51	52475	None
352	1jwiB	35	61	1.51	56437	None
353	1i6aA	35	61	1.51	53851	mutant
354	1qkiA	35	61	1.51	51800	None
355	1bvsA	34	58	1.53	46930	None
356	1tml	34	58	1.53	51990	complexed with so4
357	2pspA	34	58	1.53	57493	None
358	1cjyA	34	58	1.53	49563	None



359	livhA	34	58	1.53	47204	None
360	liqpA	34	58	1.53	48020	None
361	lfn4A	34	58	1.53	55962	complexed with dho
362	lmpxA	34	58	1.53	69222	None
363	lj33A	34	58	1.53	52734	mutant
364	lk0rA	34	58	1.53	50282	None
365	lga8A	34	58	1.53	53458	complexed with del, mn, upf; mutant
366	lshcA	34	58	1.53	50755	None
367	lliiA	34	58	1.53	53614	complexed with acp, adn, cl, mg
368	lnbaA	34	58	1.53	52500	None
369	lex4A	34	58	1.53	50123	None
370	lgz8A	34	58	1.53	88854	complexed with csw, mbp
371	lji0A	34	58	1.53	52686	complexed with atp, mse
372	liml	34	58	1.53	57736	None
373	lbouA	34	58	1.53	48077	None
374	la3wA	34	58	1.53	50801	None
375	lko9A	34	58	1.53	48157	complexed with so4
376	lceqA	34	58	1.53	51848	None
377	lk75A	34	58	1.53	69602	None
378	lfuiA	34	58	1.53	50444	None
379	lng2A	34	58	1.53	50045	None
380	lkb0A	34	58	1.53	68952	complexed with ca, gol, hec, pqq, tfb
381	loacA	34	58	1.53	49999	None
382	loedC	34	58	1.53	90113	None
383	lmxtA	34	58	1.53	51913	atomic resolution structure
384	ljevB	34	58	1.53	64505	None
385	li7oA	34	58	1.53	56530	None
386	li7oA	34	58	1.53	56530	None
387	lkyA	34	58	1.53	49800	None
388	lhtyA	34	58	1.53	88693	complexed with mpd, nag, trs, zn
389	ll5jA	34	58	1.53	74779	None
390	lkagA	34	58	1.53	52566	None
391	lqe3A	34	58	1.53	53475	complexed with so4, zn
392	le3mA	34	58	1.53	48335	None
393	lgcoA	34	58	1.53	51751	None
394	lezvC	34	58	1.53	81647	complexed with fes, hem, sma, uq6
395	lg10A	34	58	1.53	56030	None
396	lan4A	34	58	1.53	47460	None
397	li1iP	34	58	1.53	55505	complexed with zn
398	le58A	34	58	1.53	53255	complexed with cl, phs, so4; mutant
399	lczaN	34	58	1.53	53083	None
400	lfnhA	34	58	1.53	49266	None