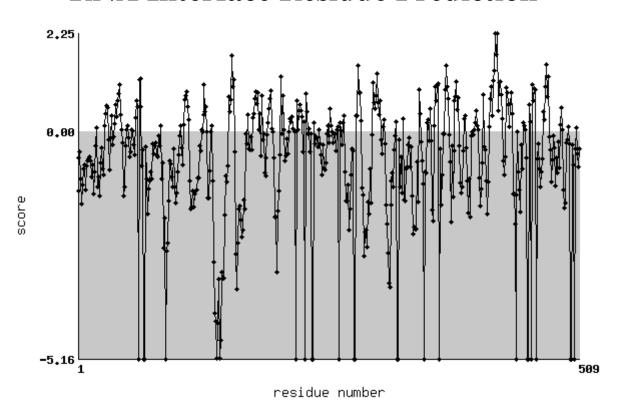
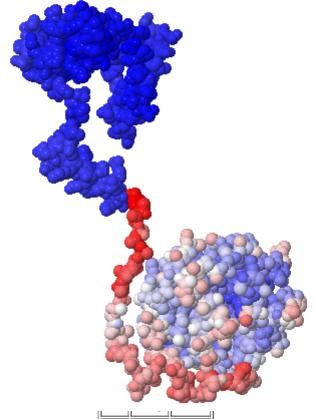
## **RNA Interface Residue Prediction**



RNA interface prediction by averaged ((averaged singlet) + doublet)  $[A^2SD]$ The higher the propensity is, the more likely it is to be an interface.



JSmol

15	THR	-1.03
16	TYR	-0.74
17	GLU	-1.41
18	THR	-0.90
19	MET	-0.31
20	PHE	0.09
21	ALA	-1.25
22	PRO	-1.03
23	GLU	-1.45
24	PHE	-0.70
25	GLY	-0.35
26	PRO	-0.85
27	GLU	-0.97
28	ASN	0.13
29	PRO	0.41
30	PHE	0.60
31	ARG	0.56
32	THR	-0.17
33	GLN	-0.86

34	GLN	-0.13
35	MET	0.36
36	ALA	-0.30
37	ALA	-0.11
38	PRO	0.19
39	ARG	0.62
40	ASN	0.34
41	MET	0.70
42	LEU	0.87
43	SER	1.07
44	GLY	0.40
45	TYR	0.05
46	ALA	-0.25
47	GLU	-1.45
48	PRO	-1.26
49	ALA	-0.31
50	HIS	0.06
51	ILE	0.14
52	ASN	-0.13
53	ASP	-0.56
54	PHE	-0.46
55	MET	0.04
56	PHE	0.03
57	GLU	-0.30
58	GLN	-0.53
59	GLN	0.33
60	ARG	0.70
61	ARG	0.57
62	THR	-5.16
63	PHE	1.19
64	ALA	1.22
65	THR	
	TYR	
67	GLY	-0.41
	TYR	
		-5.16
70	LEU	-0.33
71	ASP	
72		-1.87
73	SER	
74	LEU	
	$\overline{}$	

75	ASP	-0.91
76	ASN	-1.06
77	HIS	-0.28
78	GLN	-0.49
79	VAL	-0.32
80	SER	-0.24
81	ALA	-0.51
82	LYS	-0.56
83	TYR	-0.09
84	ILE	-0.32
85	GLY	0.14
86	SER	-1.07
87	VAL	-0.71
88	GLU	-2.63
89	GLU	-1.96
90	ALA	-5.16
91	GLU	-2.72
92	LYS	-2.53
93	ASN	-1.57
94	GLN	-0.65
95	GLY	-0.73
96	LEU	-1.03
97	THR	-1.26
98	VAL	-0.39
99	PHE	-1.24
	GLU	
	THR	
	GLY	
	GLN	
	LYS	
	LYS	
	THR	
107	GLU	-0.75
108	LYS	0.17
109	ARG	0.73
110	ARG LYS	0.82
111	LYS	0.92
112	LYS PHE	0.58
113	LYS	0.27
114	GLU	-1.11
115	ASN	-1.75

116	ASP	-1.71
117	ALA	-1.35
118	SER	-1.70
119	ASN	-1.42
120	ILE	-1.35
121	ASP	-1.31
122	GLY	-1.05
123	PHE	-1.04
124	LEU	-0.31
125	GLY	-0.43
126	PRO	0.04
127	TRP	0.01
128	ALA	0.39
129	LYS	1.08
130	TYR	0.46
131	VAL	0.58
132	ASP	-0.00
133	GLU	-1.50
134	LYS	-1.51
135	ASP	-0.88
136	VAL	0.00
137	ALA	0.15
138	LYS	-1.11
139	PRO	-2.96
140	SER	-4.13
141	GLU	-4.31
142	GLU	-5.14
143	GLU	-4.35
144	GLN	-3.34
145	LYS	-5.14
146	GLU	-4.74
147	LEU	-3.18
148	ASP	-3.33
149	GLU	-3.32
150	ILE	-1.89
151	THR	-0.99
152	ALA	-1.13
153	LYS	-0.77
154	ARG	0.80
155	GLN	0.46

150	Lvc	1 0 74
	LYS	
157	LYS	1.74
	GLY	
	LYS	
	GLN	
161	GLU	-2.77
	GLU	
	GLU	
	LYS	
	PRO	
	GLY	
	GLU	
	GLU	
	LYS	
170	THR	-1.74
171	ILE	-0.04
172	LEU	-0.28
173	HIS	0.39
174	VAL	-0.39
175	LYS	-0.40
	GLU	
177	MET	-0.40
178	TYR	0.32
179	ASP	0.42
180	TYR	0.76
181	GLN	0.92
182	GLY	0.64
183	ARG	0.90
184	SER	0.06
185	TYR	0.42
186	LEU	-0.54
187	HIS	0.82
188	ILE	-0.18
189	PRO	-0.04
190	GLN	-0.92
191	ASP	-0.99
192	VAL	-0.59
193		-0.06
194	VAL	0.20
	ASN	0.52
	LEU	0.76
_		

197	ARG	0.95
198	SER	0.07
199	THR	0.01
200	MET	-0.58
201	PRO	-1.93
202	PRO	-1.94
203	GLU	-3.18
204	LYS	-1.79
205	CYS	-1.34
206	TYR	-0.52
207	LEU	1.26
208	PRO	-0.04
209	LYS	0.83
210	LYS	0.04
211	GLN	-0.66
212	ILE	-0.55
213	HIS	-0.15
214	VAL	-0.49
215	TRP	-0.00
216	SER	0.31
217	GLY	0.23
218	HIS	0.34
219	THR	0.07
220	LYS	0.06
221	GLY	0.01
222	VAL	-5.16
223	SER	0.70
224	ALA	0.04
225	VAL	0.48
226	ARG	0.62
227	LEU	0.49
228	PHE	0.35
		-0.45
		0.24
		-5.16
232		0.86
233		0.46
234	LEU	-0.03
	$\overline{}$	0.08
	LEU	
	SER	
	-	•

238	CYS	-5.16
239	SER	-5.16
240	MET	0.22
241	ASP	-0.27
242	CYS	-0.12
243	LYS	-0.13
244	ILE	-0.34
245	LYS	0.06
246	LEU	-0.28
247	TRP	-0.51
248	GLU	-0.98
249	VAL	-0.29
250	TYR	-0.81
251	GLY	-0.86
252	GLU	-0.71
253	ARG	-0.03
254	ARG	0.13
255	CYS	-0.24
256	LEU	-0.09
257	ARG	0.54
258	THR	0.15
259	PHE	0.01
260	ILE	-0.25
261	GLY	-0.03
262	HIS	-0.04
263	SER	-0.42
264	LYS	0.05
265	ALA	0.11
266	VAL	-5.16
267	ARG	0.20
268	ASP	0.02
269	ILE	-0.30
270	CYS	0.20
271	PHE	0.37
272	ASN	-0.91
273	THR	-1.58
274	ALA	-1.56
275	GLY	-1.20
276	THR	-2.22
277	GLN	-1.74

278	PHE	-0.97
279	LEU	-0.38
280	SER	-0.44
281	ALA	-5.16
282	ALA	-5.16
283	TYR	0.36
284	ASP	0.37
285	ARG	1.50
286	TYR	0.90
287	LEU	0.90
288	LYS	0.25
289	LEU	-1.28
290	TRP	-1.44
291	ASP	-2.83
292	THR	-2.27
293	GLU	-2.23
294	THR	-2.61
295	GLY	-1.60
296	GLN	-1.87
297	CYS	-0.85
298	ILE	-1.62
299	SER	-0.06
300	ARG	1.13
301	PHE	0.67
302	THR	0.54
	ASN	
	ARG	
305	LYS	0.67
306	VAL	0.39
307	PRO	0.70
308	TYR	-0.17
309	CYS	-0.50
310	VAL	0.12
311	LYS	0.28
312	PHE	-0.27
313	ASN	-1.67
314	PRO	-2.10
315	ASP	-2.75
316	GLU	-3.43
317	ASP	-3.53
318	LYS	-1.66

319	GLN	-1.12
320	ASN	-0.92
321	LEU	-1.26
322	PHE	-0.41
323	VAL	-0.08
324	ALA	0.23
325	GLY	-5.16
326	MET	-5.16
327	SER	-0.18
328	ASP	-1.26
329	LYS	-0.57
330	LYS	-1.39
331	ILE	0.29
	VAL	
333	GLN	-1.56
334	TRP	-0.85
335	ASP	-0.80
336	ILE	-0.29
337	ARG	-0.13
338	SER	-0.79
339	GLY	-0.34
340	GLU	-1.45
341	ILE	-2.31
	VAL	
343	GLN	-2.20
344	GLU	-2.21
345	TYR ASP	-0.68
346	ASP	-1.59
347	ARG	0.97
348	HIS	0.42
349	LEU	-0.23
	GLY	
351	ALA	-1.19
352	VAL	-5.16
353	ASN	-0.91
353 354	ASN THR	-0.91 -0.92
353 354	ASN THR	-0.91 -0.92
353 354 355 356	ASN THR ILE VAL	-0.91 -0.92 0.20 0.28
353 354 355 356	ASN THR ILE VAL	-0.91 -0.92 0.20 0.28
353 354 355 356 357 358	ASN THR	-0.91 -0.92 0.20 0.28 -0.21 0.54

,		
360	GLU	-1.77
361	ASN	-2.02
362	ARG	0.15
363	ARG	1.04
364	PHE	0.71
365	VAL	1.05
366	SER	1.10
367	THR	-5.16
368	SER	-0.38
369	ASP	-1.67
370	ASP	-0.98
371	LYS	-0.03
372	SER	-0.03
373	LEU	0.97
374	ARG	1.52
375	VAL	1.04
376	TRP	0.76
377	GLU	-0.07
378	TRP	-0.68
379	ASP	-2.04
380	ILE	-0.31
381	PRO	-1.47
382	VAL	-0.44
383	ASP	0.70
384	PHE	0.81
385	LYS	1.15
386	TYR	0.51
387	ILE	0.78
388	ALA	-0.31
389	GLU	-1.15
390	PRO	-1.39
391	SER	-1.26
392	MET	-0.44
393	HIS	0.31
394	SER	0.37
395	MET	-0.36
396	PRO	-1.12
397	ALA	-1.85
398	VAL	-1.07
399	THR	-1.94

400       LEU       -0.08         401       SER       0.00         402       PRO       -0.06         403       ASN       0.04         404       GLY       0.20         405       LYS       0.49         406       TRP       0.15         407       LEU       0.06         408       ALA       -1.04         409       CYS       -1.69         410       GLN       -1.30         411       SER       -0.71         412       MET       0.84         413       ASP       -0.34
402       PRO       -0.06         403       ASN       0.04         404       GLY       0.20         405       LYS       0.49         406       TRP       0.15         407       LEU       0.06         408       ALA       -1.04         409       CYS       -1.69         410       GLN       -1.30         411       SER       -0.71         412       MET       0.84
403 ASN 0.04 404 GLY 0.20 405 LYS 0.49 406 TRP 0.15 407 LEU 0.06 408 ALA -1.04 409 CYS -1.69 410 GLN -1.30 411 SER -0.71 412 MET 0.84
404       GLY       0.20         405       LYS       0.49         406       TRP       0.15         407       LEU       0.06         408       ALA       -1.04         409       CYS       -1.69         410       GLN       -1.30         411       SER       -0.71         412       MET       0.84
405 LYS 0.49 406 TRP 0.15 407 LEU 0.06 408 ALA -1.04 409 CYS -1.69 410 GLN -1.30 411 SER -0.71 412 MET 0.84
406 TRP 0.15 407 LEU 0.06 408 ALA -1.04 409 CYS -1.69 410 GLN -1.30 411 SER -0.71 412 MET 0.84
407       LEU       0.06         408       ALA       -1.04         409       CYS       -1.69         410       GLN       -1.30         411       SER       -0.71         412       MET       0.84
408 ALA -1.04 409 CYS -1.69 410 GLN -1.30 411 SER -0.71 412 MET 0.84
409       CYS       -1.69         410       GLN       -1.30         411       SER       -0.71         412       MET       0.84
410 GLN -1.30 411 SER -0.71 412 MET 0.84
411 SER -0.71 412 MET 0.84
412 MET 0.84
413 ASP -0.34
414 ASN -0.40
415 GLN -1.12
416 ILE -1.86
417 LEU -1.13
418 ILE 0.12
419 PHE 0.75
420 GLY 1.03
421 ALA 0.38
422 GLN 1.17
423 ASN 1.39
424 ARG 2.23
425 PHE 1.77
426 ARG 2.25
427 LEU 0.49
428 ASN 1.12
429 LYS 1.15
430 LYS 0.84
430 LYS 0.84
430 LYS 0.84 431 LYS 0.31
430 LYS 0.84 431 LYS 0.31 432 ILE -0.65
430 LYS 0.84 431 LYS 0.31 432 ILE -0.65 433 PHE -0.97
430       LYS       0.84         431       LYS       0.31         432       ILE       -0.65         433       PHE       -0.97         434       LYS       -0.57
430       LYS       0.84         431       LYS       0.31         432       ILE       -0.65         433       PHE       -0.97         434       LYS       -0.57         435       GLY       1.00
430       LYS       0.84         431       LYS       0.31         432       ILE       -0.65         433       PHE       -0.97         434       LYS       -0.57         435       GLY       1.00         436       HIS       0.90         437       MET       0.63
430       LYS       0.84         431       LYS       0.31         432       ILE       -0.65         433       PHE       -0.97         434       LYS       -0.57         435       GLY       1.00         436       HIS       0.90         437       MET       0.63

441	TYR	0.41
442	ALA	-1.40
443	CYS	-1.41
444	GLN	-2.09
445	VAL	-5.16
446	ASP	-1.43
447	PHE	0.00
448	SER	-0.90
449	PRO	-1.32
450	ASP	-1.81
451	MET	-0.29
452	SER	-0.84
453	TYR	0.21
454	VAL	0.15
455	ILE	0.06
456	SER	-0.58
457	GLY	-5.16
458	ASP	-5.16
459	GLY	0.63
460	ASN	0.24
461	GLY	-5.16
462	LYS	1.08
463	LEU	0.70
464	ASN	0.99
465	ILE	0.97
466	TRP	-5.16
	ASP	
468	TRP	-0.27
	LYS	
	THR	
	THR	b .
	LYS	
	LEU	
474	TYR	0.27
475	SER	1.02
476	ARG	1.53
	PHE	
	LYS	
	ALA	
	HIS	
481	ASP	-1.13

482	LYS	-0.63
483	VAL	-0.09
484	CYS	-0.35
485	ILE	-1.23
486	GLY	-0.59
487	ALA	-0.92
488	VAL	-0.23
489	TRP	-0.82
490	HIS	0.16
491	PRO	0.55
492	HIS	0.04
493	GLU	-1.31
494	THR	-1.72
495	SER	-1.61
496	LYS	-0.25
497	VAL	-0.18
498	ILE	0.12
499	THR	-0.27
500	CYS	-5.16
501	GLY	-5.16
502	TRP	-0.29
503	ASP	-0.74
504	GLY	-5.16
505	LEU	-0.38
506	ILE	0.09
507	LYS	-0.50
508	LEU	-0.79
509	TRP	-0.39

## How to visualize the prediction result at hand

- 1. Download the prediction result file (PDB format) from the following link; Prediction Result
- 2. Launch Rasmol by the following way;
  - % rasmol -script (downloaded file)
- 3. The protein is colour coded residue-wise as shown bellow;
  - red: highly likely to be an interface
  - light blue: unlikely to be an interface
  - o deep blue: buried residue (not considered as an interface residue)
- 4. The scores of the prediction are the numbers between columns 61 and 66 (temperature factor column) of ATOM rows in the file.

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