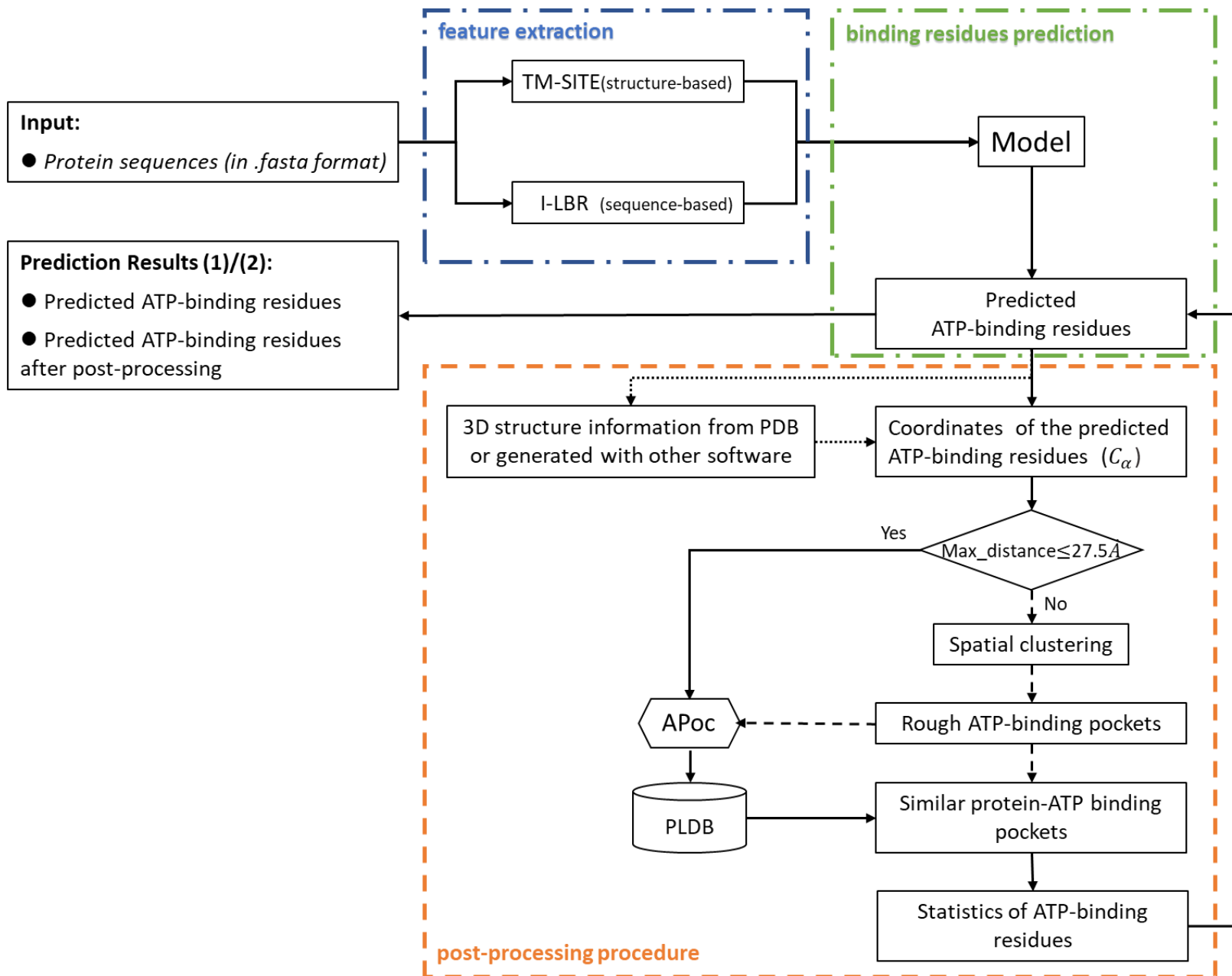


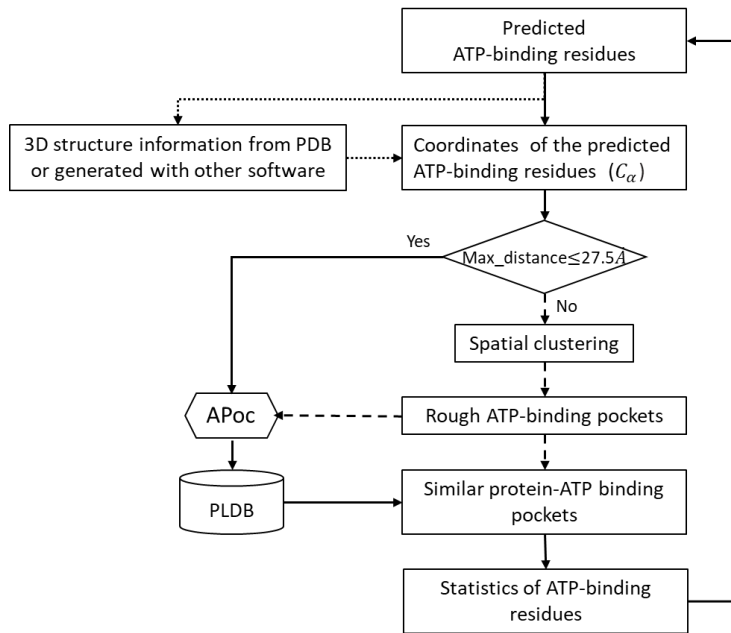
Work Report

贾宁欣

08-29-2021



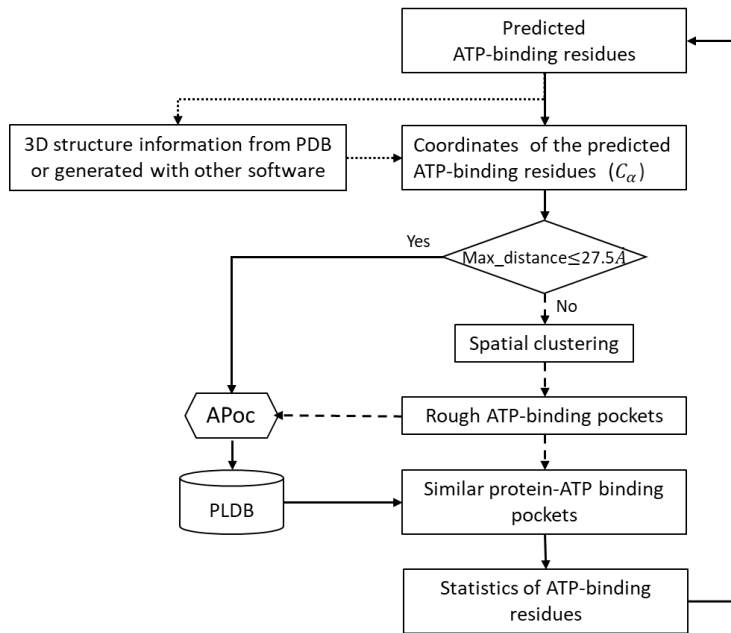
Post-processing procedure



TM-SITE I-LBR label

	TM-SITE	I-LBR	label
1	0.000	0.000002	0.0
2	0.000	0.002964	0.0
3	0.000	0.000001	0.0
4	0.000	0.000000	0.0
5	0.000	0.000000	0.0
6	0.000	0.000000	0.0
7	0.000	0.000000	0.0
8	0.000	0.000000	0.0
9	0.000	0.000000	0.0
10	0.000	0.000001	0.0
11	0.000	0.000000	0.0
12	0.000	0.011167	0.0
13	0.000	0.000000	0.0
14	0.000	0.007261	0.0
15	0.000	0.004631	0.0
16	1.000	0.155886	1.0
17	1.000	0.013850	1.0
18	1.000	0.014945	1.0
19	1.000	0.000000	1.0
20	0.667	0.000002	1.0
21	1.000	0.037511	1.0
22	0.000	0.000000	0.0
23	0.000	0.000000	0.0
24	0.000	0.000000	0.0
25	0.000	0.000001	0.0
26	0.000	0.000000	0.0
27	0.000	0.000006	0.0
28	0.000	0.000005	0.0
29	0.000	0.000000	0.0
30	0.000	0.000000	0.0
31	0.000	0.000001	0.0
32	0.000	0.000001	0.0
33	0.000	0.000000	0.0
34	0.000	0.000009	0.0
35	0.000	0.000005	0.0
36	0.000	0.000008	0.0
37	0.000	0.000000	0.0
38	0.000	0.000000	0.0
39	0.000	0.000011	0.0
40	0.000	0.000000	0.0
41	0.333	0.000001	0.0
42	0.000	0.000000	0.0
43	0.000	0.000000	0.0
44	0.000	0.000002	0.0

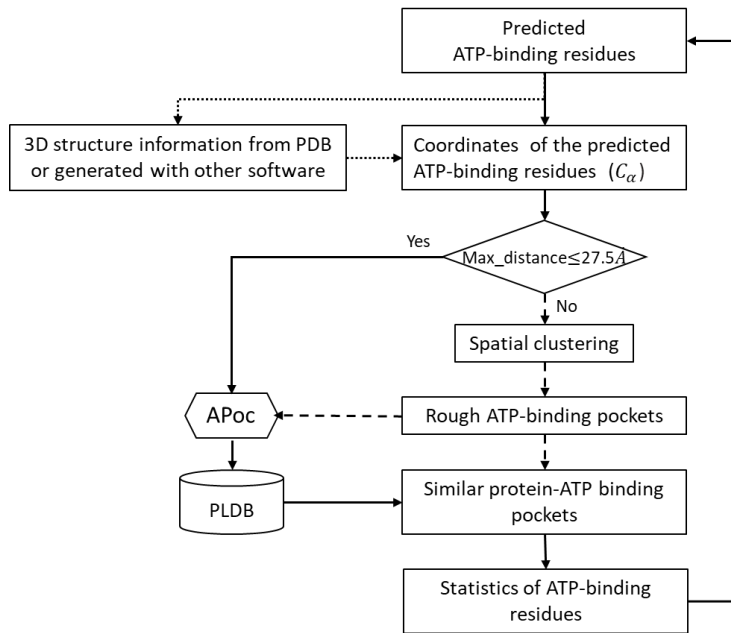
Post-processing procedure



label P-True P-False Result

label	P-True	P-False	Result
1	0.000000	0.002808	0.997192 0
2	0.000000	0.003136	0.996864 0
3	0.000000	0.002796	0.997204 0
4	0.000000	0.002823	0.997177 0
5	0.000000	0.002825	0.997175 0
6	0.000000	0.002806	0.997194 0
7	0.000000	0.002772	0.997228 0
8	0.000000	0.002551	0.997449 0
9	0.000000	0.001530	0.998470 0
10	0.000000	0.001534	0.998466 0
11	0.000000	0.001535	0.998465 0
12	0.000000	0.001533	0.998467 0
13	0.000000	0.001532	0.998468 0
14	0.000000	0.006632	0.993368 0
15	0.000000	0.044501	0.955499 0
16	1.000000	0.757359	0.242641 1
17	1.000000	0.688865	0.311135 1
18	1.000000	0.755391	0.244609 1
19	1.000000	0.708924	0.291076 1
20	1.000000	0.318519	0.681481 0
21	1.000000	0.653547	0.346453 1
22	0.000000	0.050510	0.949490 0
23	0.000000	0.038035	0.961965 0
24	0.000000	0.047679	0.952321 0
25	0.000000	0.026292	0.973708 0
26	0.000000	0.016834	0.983166 0
27	0.000000	0.004799	0.995201 0
28	0.000000	0.013747	0.986252 0
29	0.000000	0.014132	0.985868 0
30	0.000000	0.002751	0.997248 0
31	0.000000	0.002751	0.997249 0
32	0.000000	0.002751	0.997249 0
33	0.000000	0.004760	0.995240 0
34	0.000000	0.002838	0.997162 0
35	0.000000	0.009765	0.990235 0
36	0.000000	0.006282	0.993718 0
37	0.000000	0.017794	0.982206 0
38	0.000000	0.011278	0.988722 0
39	0.000000	0.025211	0.974789 0
40	0.000000	0.022582	0.977418 0
41	0.000000	0.178193	0.821807 0
42	0.000000	0.020179	0.979821 0
43	0.000000	0.032543	0.967457 0
44	0.000000	0.001546	0.998454 0

Post-processing procedure

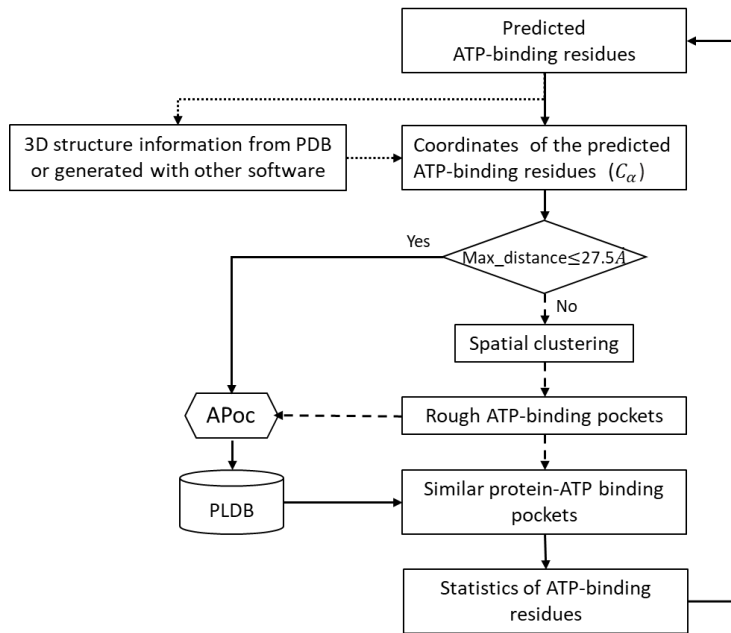


Predicted ATP-binding residues

The screenshot shows a text editor window with the title 'SevGA'. The editor displays a list of predicted ATP-binding residues, numbered 1 through 43. The residues are listed in a column, with some numbers appearing in red text, indicating they are the predicted binding sites. The list is as follows:

Residue Number	Residue Number
1	16
2	17
3	18
4	19
5	21
6	51
7	52
8	65
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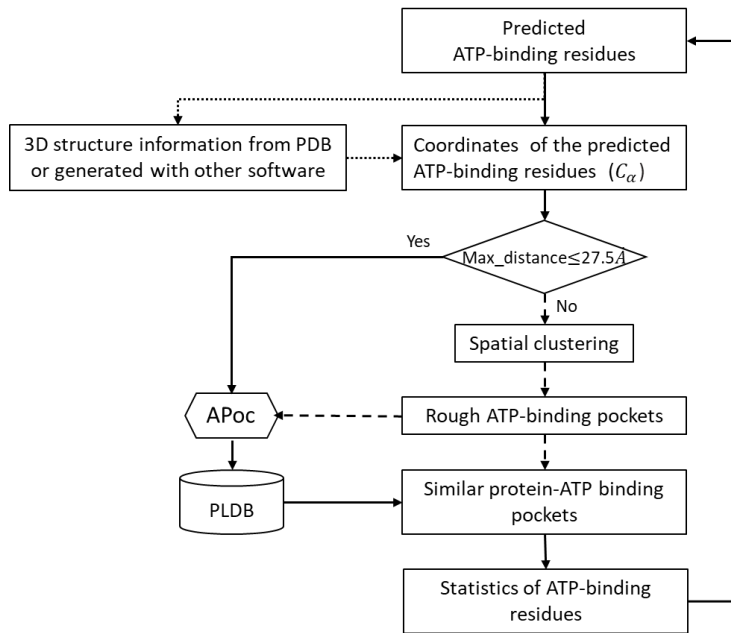
Post-processing procedure



Coordinates of the predicted ATP-binding residues

1	ATOM	105	N	ASP	A	16	19.814	34.584	12.375	1.00	00.00	N
2	ATOM	106	CA	ASP	A	16	19.939	35.801	11.579	1.00	00.00	C
3	ATOM	107	C	ASP	A	16	18.564	36.159	11.023	1.00	00.00	O
4	ATOM	108	O	ASP	A	16	18.007	35.393	10.237	1.00	00.00	O
5	ATOM	109	CB	ASP	A	16	20.951	35.556	10.449	1.00	00.00	C
6	ATOM	110	CG	ASP	A	16	21.365	36.813	9.724	1.00	00.00	C
7	ATOM	111	OD1	ASP	A	16	20.558	37.723	9.618	1.00	00.00	O
8	ATOM	112	OD2	ASP	A	16	22.520	36.880	9.243	1.00	00.00	O
9	ATOM	113	N	MET	A	17	18.026	37.323	11.388	1.00	00.00	N
10	ATOM	114	CA	MET	A	17	16.697	37.674	10.883	1.00	00.00	C
11	ATOM	115	C	MET	A	17	16.746	37.931	9.375	1.00	00.00	C
12	ATOM	116	O	MET	A	17	17.665	38.568	8.871	1.00	00.00	O
13	ATOM	117	CB	MET	A	17	16.140	38.905	11.610	1.00	00.00	C
14	ATOM	118	CG	MET	A	17	16.174	38.798	13.128	1.00	00.00	C
15	ATOM	119	SD	MET	A	17	15.311	37.352	13.741	1.00	00.00	S
16	ATOM	120	CE	MET	A	17	13.631	37.635	13.223	1.00	00.00	C
17	ATOM	121	N	ASP	A	18	15.768	37.403	8.641	1.00	00.00	N
18	ATOM	122	CA	ASP	A	18	15.724	37.654	7.200	1.00	00.00	C
19	ATOM	123	C	ASP	A	18	15.263	39.083	6.936	1.00	00.00	C
20	ATOM	124	O	ASP	A	18	14.326	39.560	7.579	1.00	00.00	O
21	ATOM	125	CB	ASP	A	18	14.782	36.665	6.505	1.00	00.00	C
22	ATOM	126	CG	ASP	A	18	15.216	35.209	6.693	1.00	00.00	C
23	ATOM	127	OD1	ASP	A	18	16.430	34.953	6.715	1.00	00.00	O
24	ATOM	128	OD2	ASP	A	18	14.345	34.327	6.797	1.00	00.00	O
25	ATOM	129	N	CYS	A	19	15.922	39.753	5.978	1.00	00.00	N
26	ATOM	130	CA	CYS	A	19	15.672	41.148	5.593	1.00	00.00	C
27	ATOM	131	C	CYS	A	19	14.979	41.943	6.698	1.00	00.00	C
28	ATOM	132	O	CYS	A	19	13.823	42.357	6.550	1.00	00.00	O
29	ATOM	133	CB	CYS	A	19	14.864	41.207	4.289	1.00	00.00	C
30	ATOM	134	SG	CYS	A	19	13.358	40.193	4.192	1.00	00.00	S
31	ATOM	146	N	PHE	A	21	14.797	44.838	8.596	1.00	00.00	N
32	ATOM	147	CA	PHE	A	21	14.042	46.098	8.615	1.00	00.00	C
33	ATOM	148	C	PHE	A	21	12.797	45.996	7.726	1.00	00.00	C
34	ATOM	149	O	PHE	A	21	11.739	46.579	8.033	1.00	00.00	O
35	ATOM	150	CB	PHE	A	21	14.914	47.277	8.154	1.00	00.00	C
36	ATOM	151	CG	PHE	A	21	15.955	47.747	9.146	1.00	00.00	C
37	ATOM	152	CD1	PHE	A	21	16.357	46.973	10.212	1.00	00.00	C
38	ATOM	153	CD2	PHE	A	21	16.546	49.001	8.976	1.00	00.00	C
39	ATOM	154	CE1	PHE	A	21	17.328	47.426	11.099	1.00	00.00	C
40	ATOM	155	CE2	PHE	A	21	17.504	49.461	9.861	1.00	00.00	C
41	ATOM	156	CZ	PHE	A	21	17.896	48.669	10.924	1.00	00.00	C
42	ATOM	386	N	ILE	A	51	18.656	50.626	2.714	1.00	00.00	N
43	ATOM	387	CA	ILE	A	51	19.310	49.940	3.820	1.00	00.00	C
44	ATOM	388	C	ILE	A	51	18.859	48.474	3.964	1.00	00.00	C
45	ATOM	389	O	ILE	A	51	19.582	47.686	4.593	1.00	00.00	O
46	ATOM	390	CB	ILE	A	51	19.097	50.721	5.142	1.00	00.00	C
47	ATOM	391	CG1	ILE	A	51	19.892	50.134	6.313	1.00	00.00	C
48	ATOM	392	CG2	ILE	A	51	17.620	50.844	5.497	1.00	00.00	C

Post-processing procedure

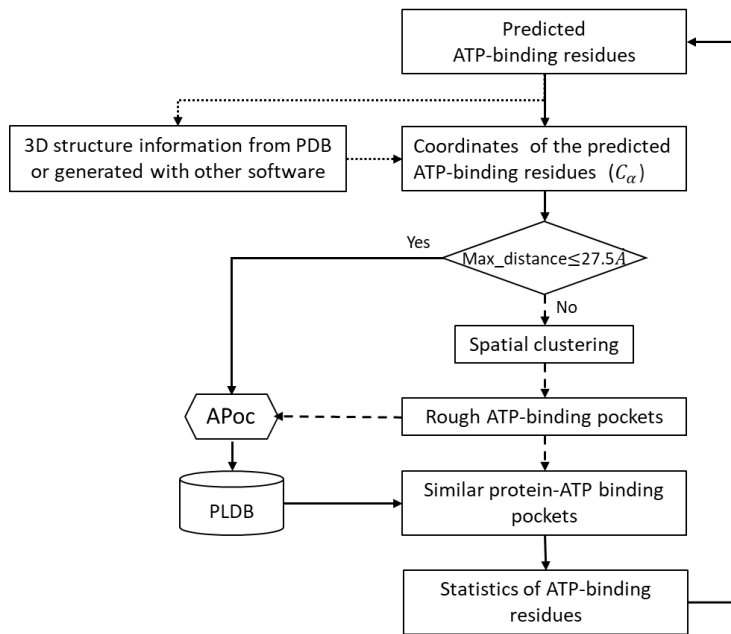


Positions of C_{α} atoms of the predicted binding residues

The screenshot shows a text editor window with the following data:

1	16	19.939	35.801	11.579
2	17	16.697	37.674	10.883
3	18	15.724	37.654	7.200
4	19	15.672	41.148	5.593
5	21	14.042	46.098	8.615
6	51	19.310	49.940	3.820
7	52	17.245	46.693	3.465
8	65	23.614	51.020	-0.460
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Post-processing procedure

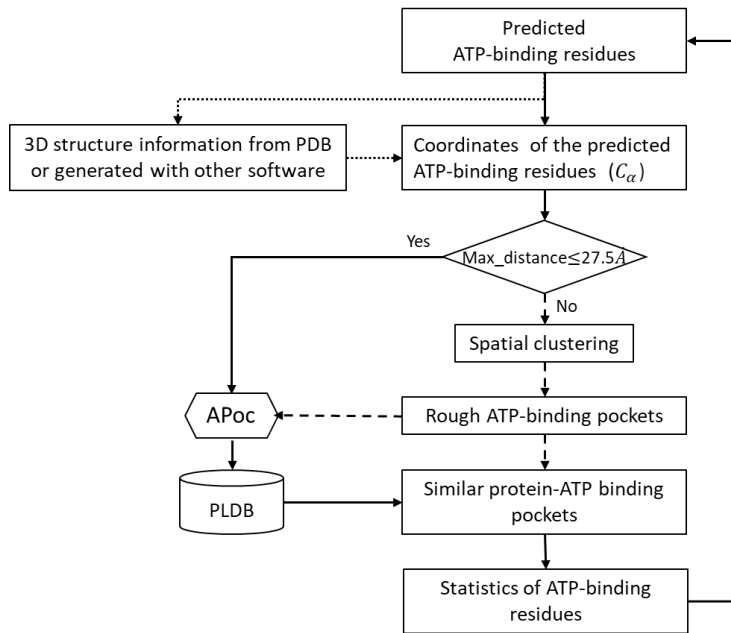


Distance between any two predicted binding residues

The screenshot shows a text file with pairwise distances between predicted binding residues. The data is organized in columns, with each column representing a residue and its coordinates. The rows show the distance between each residue and all other residues. An arrow points to the bottom of the file, indicating the end of the data.

Residue 1	Residue 2	Distance (Å)
18	18	0.0
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
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18	52	3.465
18	65	-0.46
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18	52	3.465
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18	21	8.615
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18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
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18	52	3.465
18	65	-0.46
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18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
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18	52	3.465
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18	52	3.465
18	65	-0.46
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18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
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18	17	10.883
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18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
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18	17	10.883
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18	17	10.883
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18	16	11.579
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18	17	10.883
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18	52	3.465
18	65	-0.46
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18	17	10.883
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18	21	8.615
18	51	3.82
18	52	3.465
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18	16	11.579
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18	21	8.615
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18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
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18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465
18	65	-0.46
18	16	11.579
18	17	10.883
18	19	5.593
18	21	8.615
18	51	3.82
18	52	3.465

Post-processing procedure



Spatial clustering algorithm

Algorithm	$BindingSiteClusters = SpatialClustering(C, T_{Cluster})$
Input	C : the set of predicted ATP-binding residues; $T_{Cluster}$ – threshold for spatial clustering.
Output	$BindingSiteClusters$ – a set of clusters, residues in each cluster constitute a candidate binding site.
1	Calculate $max_distance$: the maximal distance between any two residues in C .
2	IF the $max_distance$ is greater than the pre-defined threshold $T_{Cluster}$
2.1	Clustering the residues in C into two smaller clusters according to their spatial positions: C_First and C_Second
2.2	$BindingSiteClusters_First = SpatialClustering(C_First, T_{Cluster})$
2.3	$BindingSiteClusters_Second = SpatialClustering(C_Second, T_{Cluster})$
2.4	$BindingSiteClusters = BindingSiteClusters_First \cup BindingSiteClusters_Second$
	ELSE
2.5	$BindingSiteClusters = C$
	END
	IF
3	RETURN $BindingSiteClusters$

Post-processing procedure

Spatial clustering algorithm

4rx6B.pdb	4rx6B.pdb
85	39 [-60.033 -13.827 5.803] 38 [-58.441 -10.795 4.247] 3.761465671782742
86	39 [-60.033 -13.827 5.803] 39 [-60.033 -13.827 5.803] 0.0
87	39 [-60.033 -13.827 5.803] 40 [-63.007 -14.025 8.133] 3.7832234932660236
88	39 [-60.033 -13.827 5.803] 65 [-48.369 1.713 5.788] 19.430407123887033
89	39 [-60.033 -13.827 5.803] 66 [-47.607 5.24 6.962] 22.788138274110946
90	39 [-60.033 -13.827 5.803] 89 [-67.905 -4.735 7.978] 12.221434981212312
91	39 [-60.033 -13.827 5.803] 90 [-64.827 -4.491 5.829] 10.494951548244517
92	39 [-60.033 -13.827 5.803] 91 [-64.329 -0.983 7.164] 13.61162271736915
93	39 [-60.033 -13.827 5.803] 92 [-61.049 -2.353 8.512] 11.833157355498997
94	39 [-60.033 -13.827 5.803] 93 [-58.724 -1.731 11.438] 13.408203533658043
95	39 [-60.033 -13.827 5.803] 95 [-52.605 -0.865 14.008] 17.044373059752008
96	39 [-60.033 -13.827 5.803] 104 [-33.334 7.761 4.167] 34.37375221008029
97	40 [-63.007 -14.025 8.133] 10 [-56.107 -2.772 6.55] 13.294581527825537
98	40 [-63.007 -14.025 8.133] 30 [-45.57 9.618 1.379] 30.14393693597437
99	40 [-63.007 -14.025 8.133] 31 [-47.096 6.256 2.047] 26.486190326281356
100	40 [-63.007 -14.025 8.133] 32 [-46.917 2.621 0.986] 24.229259687411002
101	40 [-63.007 -14.025 8.133] 38 [-58.441 -10.795 4.247] 6.81045167371445
102	40 [-63.007 -14.025 8.133] 39 [-60.033 -13.827 5.803] 3.7832234932660236
103	40 [-63.007 -14.025 8.133] 40 [-63.007 -14.025 8.133] 0.0
104	40 [-63.007 -14.025 8.133] 65 [-48.369 1.713 5.788] 21.6207010293376
105	40 [-63.007 -14.025 8.133] 66 [-47.607 5.24 6.962] 24.69152619827296
106	40 [-63.007 -14.025 8.133] 89 [-67.905 -4.735 7.978] 10.503262778774985
107	40 [-63.007 -14.025 8.133] 90 [-64.827 -4.491 5.829] 9.9758694859145
108	40 [-63.007 -14.025 8.133] 91 [-64.329 -0.983 7.164] 13.144596190069894
109	40 [-63.007 -14.025 8.133] 92 [-61.049 -2.353 8.512] 11.841156573578445
110	40 [-63.007 -14.025 8.133] 93 [-58.724 -1.731 11.438] 13.43166220291278
111	40 [-63.007 -14.025 8.133] 95 [-52.605 -0.865 14.008] 17.773655476575435
112	40 [-63.007 -14.025 8.133] 104 [-33.334 7.761 4.167] 37.02493593512351
113	65 [-48.369 1.713 5.788] 10 [-56.107 -2.772 6.55] 13.97621930436194
114	65 [-48.369 1.713 5.788] 30 [-45.57 9.618 1.379] 9.474318286821486
115	65 [-48.369 1.713 5.788] 31 [-47.096 6.256 2.047] 6.021167577804159
116	65 [-48.369 1.713 5.788] 32 [-46.917 2.621 0.986] 5.098232242650387
117	65 [-48.369 1.713 5.788] 38 [-58.441 -10.795 4.247] 16.132883468245844
118	65 [-48.369 1.713 5.788] 39 [-60.033 -13.827 5.803] 19.430407123887033
119	65 [-48.369 1.713 5.788] 40 [-63.007 -14.025 8.133] 21.6207010293376
120	65 [-48.369 1.713 5.788] 65 [-48.369 1.713 5.788] 0.0
121	65 [-48.369 1.713 5.788] 66 [-47.607 5.24 6.962] 3.794555178146709
122	65 [-48.369 1.713 5.788] 89 [-67.905 -4.735 7.978] 20.6883998681415
123	65 [-48.369 1.713 5.788] 90 [-64.827 -4.491 5.829] 17.5885491442586
124	65 [-48.369 1.713 5.788] 91 [-64.329 -0.983 7.164] 16.24448804979707
125	65 [-48.369 1.713 5.788] 92 [-61.049 -2.353 8.512] 13.591722922425985
126	65 [-48.369 1.713 5.788] 93 [-58.724 -1.731 11.438] 12.28859882167206
127	65 [-48.369 1.713 5.788] 95 [-52.605 -0.865 14.008] 9.599905207865334
128	65 [-48.369 1.713 5.788] 104 [-33.334 7.761 4.167] 16.286717594408024
129	66 [-47.607 5.24 6.962] 10 [-56.107 -2.772 6.55] 11.688108829062125
130	66 [-47.607 5.24 6.962] 30 [-45.57 9.618 1.379] 9.7381472888252046
131	66 [-47.607 5.24 6.962] 31 [-47.096 6.256 2.047] 5.04485896730523
132	66 [-47.607 5.24 6.962] 32 [-46.917 2.621 0.986] 6.561085047459756
133	66 [-47.607 5.24 6.962] 38 [-58.441 -10.795 4.247] 19.54144329367716
134	66 [-47.607 5.24 6.962] 39 [-60.033 -13.827 5.803] 22.788138274110946
135	66 [-47.607 5.24 6.962] 40 [-63.007 -14.025 8.133] 24.69152619827296
136	66 [-47.607 5.24 6.962] 65 [-48.369 1.713 5.788] 3.794555178146709
137	66 [-47.607 5.24 6.962] 66 [-47.607 5.24 6.962] 0.0
138	66 [-47.607 5.24 6.962] 89 [-67.905 -4.735 7.978] 22.6393834942562
139	66 [-47.607 5.24 6.962] 90 [-64.827 -4.491 5.829] 17.5885491442586

4rx6B.pdb	4rx6B.pdb
1	10
2	30
3	31
4	32
5	38
6	39
7	40
8	65
9	66
10	89
11	90
12	91
13	92
14	93
15	95
16	104

4rx6B.pdb	4rx6B.pdb
88	39 [-60.033 -13.827 5.803] 65 [-48.369 1.713 5.788] 19.430407123887033
89	39 [-60.033 -13.827 5.803] 66 [-47.607 5.24 6.962] 22.788138274110946
90	39 [-60.033 -13.827 5.803] 89 [-67.905 -4.735 7.978] 12.221434981212312
91	39 [-60.033 -13.827 5.803] 90 [-64.827 -4.491 5.829] 10.494951548244517
92	39 [-60.033 -13.827 5.803] 91 [-64.329 -0.983 7.164] 13.61162271736915
93	39 [-60.033 -13.827 5.803] 92 [-61.049 -2.353 8.512] 11.833157355498997
94	39 [-60.033 -13.827 5.803] 93 [-58.724 -1.731 11.438] 13.408203533658043
95	39 [-60.033 -13.827 5.803] 95 [-52.605 -0.865 14.008] 17.044373059752008
96	39 [-60.033 -13.827 5.803] 104 [-33.334 7.761 4.167] 34.37375221008029
97	40 [-63.007 -14.025 8.133] 10 [-56.107 -2.772 6.55] 13.294581527825537
98	40 [-63.007 -14.025 8.133] 30 [-45.57 9.618 1.379] 30.14393693597437
99	40 [-63.007 -14.025 8.133] 31 [-47.096 6.256 2.047] 26.486190326281356
100	40 [-63.007 -14.025 8.133] 32 [-46.917 2.621 0.986] 24.229259687411002
101	40 [-63.007 -14.025 8.133] 38 [-58.441 -10.795 4.247] 6.81045167371445
102	40 [-63.007 -14.025 8.133] 39 [-60.033 -13.827 5.803] 3.7832234932660236
103	40 [-63.007 -14.025 8.133] 40 [-63.007 -14.025 8.133] 0.0
104	65 [-48.369 1.713 5.788] 21.6207010293376
105	40 [-63.007 -14.025 8.133] 66 [-47.607 5.24 6.962] 24.69152619827296
106	40 [-63.007 -14.025 8.133] 89 [-67.905 -4.735 7.978] 10.503262778774985
107	40 [-63.007 -14.025 8.133] 90 [-64.827 -4.491 5.829] 9.9758694859145
108	40 [-63.007 -14.025 8.133] 91 [-64.329 -0.983 7.164] 13.144596190069894
109	40 [-63.007 -14.025 8.133] 92 [-61.049 -2.353 8.512] 11.841156573578445
110	40 [-63.007 -14.025 8.133] 93 [-58.724 -1.731 11.438] 13.43166220291278
111	40 [-63.007 -14.025 8.133] 95 [-52.605 -0.865 14.008] 17.773655476575435
112	40 [-63.007 -14.025 8.133] 104 [-33.334 7.761 4.167] 37.02493593512351
113	65 [-48.369 1.713 5.788] 10 [-56.107 -2.772 6.55] 13.97621930436194
114	65 [-48.369 1.713 5.788] 30 [-45.57 9.618 1.379] 9.474318286821486
115	65 [-48.369 1.713 5.788] 31 [-47.096 6.256 2.047] 6.021167577804159
116	65 [-48.369 1.713 5.788] 32 [-46.917 2.621 0.986] 5.098232242650387
117	65 [-48.369 1.713 5.788] 38 [-58.441 -10.795 4.247] 16.132883468245844
118	65 [-48.369 1.713 5.788] 39 [-60.033 -13.827 5.803] 19.430407123887033
119	65 [-48.369 1.713 5.788] 40 [-63.007 -14.025 8.133] 21.6207010293376
120	65 [-48.369 1.713 5.788] 65 [-48.369 1.713 5.788] 0.0
121	65 [-48.369 1.713 5.788] 66 [-47.607 5.24 6.962] 3.794555178146709

Post-processing procedure

Spatial clustering algorithm

4rx6B.pdb	4rx6B.pdb
85	39 [-60.033 -13.827 5.803] 38 [-58.441 -10.795 4.247] 3.761465671782742
86	39 [-60.033 -13.827 5.803] 39 [-60.033 -13.827 5.803] 0.0
87	39 [-60.033 -13.827 5.803] 40 [-63.007 -14.025 8.133] 3.7832234932660236
88	39 [-60.033 -13.827 5.803] 65 [-48.369 1.713 5.788] 19.430407123887033
89	39 [-60.033 -13.827 5.803] 66 [-47.607 5.24 6.962] 22.788138274110946
90	39 [-60.033 -13.827 5.803] 89 [-67.905 -4.735 7.978] 12.221434981212312
91	39 [-60.033 -13.827 5.803] 90 [-64.827 -4.491 5.829] 10.494951548244517
92	39 [-60.033 -13.827 5.803] 91 [-64.329 -0.983 7.164] 13.61162271736915
93	39 [-60.033 -13.827 5.803] 92 [-61.049 -2.353 8.512] 11.833157355498997
94	39 [-60.033 -13.827 5.803] 93 [-58.724 -1.731 11.438] 13.408203533658043
95	39 [-60.033 -13.827 5.803] 95 [-52.605 -0.865 14.008] 17.044373059752008
96	39 [-60.033 -13.827 5.803] 104 [-33.334 7.761 4.167] 34.37375221008029
97	40 [-63.007 -14.025 8.133] 10 [-56.107 -2.772 6.55] 13.294581527825537
98	40 [-63.007 -14.025 8.133] 30 [-45.57 9.618 1.379] 30.14393693597437
99	40 [-63.007 -14.025 8.133] 31 [-47.096 6.256 2.047] 26.486190326281356
100	40 [-63.007 -14.025 8.133] 32 [-46.917 2.621 0.986] 24.229259687411002
101	40 [-63.007 -14.025 8.133] 38 [-58.441 -10.795 4.247] 6.81045167371445
102	40 [-63.007 -14.025 8.133] 39 [-60.033 -13.827 5.803] 3.7832234932660236
103	40 [-63.007 -14.025 8.133] 40 [-63.007 -14.025 8.133] 0.0
104	40 [-63.007 -14.025 8.133] 65 [-48.369 1.713 5.788] 21.6207010293376
105	40 [-63.007 -14.025 8.133] 66 [-47.607 5.24 6.962] 24.69152619827296
106	40 [-63.007 -14.025 8.133] 89 [-67.905 -4.735 7.978] 10.503262778774985
107	40 [-63.007 -14.025 8.133] 90 [-64.827 -4.491 5.829] 9.9758694859145
108	40 [-63.007 -14.025 8.133] 91 [-64.329 -0.983 7.164] 13.144596190069894
109	40 [-63.007 -14.025 8.133] 92 [-61.049 -2.353 8.512] 11.841156573578445
110	40 [-63.007 -14.025 8.133] 93 [-58.724 -1.731 11.438] 13.431662220291278
111	40 [-63.007 -14.025 8.133] 95 [-52.605 -0.865 14.008] 17.773655476575435
112	40 [-63.007 -14.025 8.133] 104 [-33.334 7.761 4.167] 37.02493593512351
113	65 [-48.369 1.713 5.788] 10 [-56.107 -2.772 6.55] 8.97621930436194
114	65 [-48.369 1.713 5.788] 30 [-45.57 9.618 1.379] 9.474318286821486
115	65 [-48.369 1.713 5.788] 31 [-47.096 6.256 2.047] 6.021167577804159
116	65 [-48.369 1.713 5.788] 32 [-46.917 2.621 0.986] 5.098232242650387
117	65 [-48.369 1.713 5.788] 38 [-58.441 -10.795 4.247] 16.132883468245844
118	65 [-48.369 1.713 5.788] 39 [-60.033 -13.827 5.803] 19.430407123887033
119	65 [-48.369 1.713 5.788] 40 [-63.007 -14.025 8.133] 21.6207010293376
120	65 [-48.369 1.713 5.788] 65 [-48.369 1.713 5.788] 0.0
121	65 [-48.369 1.713 5.788] 66 [-47.607 5.24 6.962] 3.794555178146709
122	65 [-48.369 1.713 5.788] 89 [-67.905 -4.735 7.978] 20.68883998681415
123	65 [-48.369 1.713 5.788] 90 [-64.827 -4.491 5.829] 17.5885491442586
124	65 [-48.369 1.713 5.788] 91 [-64.329 -0.983 7.164] 16.24448804979707
125	65 [-48.369 1.713 5.788] 92 [-61.049 -2.353 8.512] 13.591722922425985
126	65 [-48.369 1.713 5.788] 93 [-58.724 -1.731 11.438] 12.28859882167206
127	65 [-48.369 1.713 5.788] 95 [-52.605 -0.865 14.008] 9.599905207865334
128	65 [-48.369 1.713 5.788] 104 [-33.334 7.761 4.167] 16.286717594408024
129	66 [-47.607 5.24 6.962] 10 [-56.107 -2.772 6.55] 11.688108829062125
130	66 [-47.607 5.24 6.962] 30 [-45.57 9.618 1.379] 7.381472888252046
131	66 [-47.607 5.24 6.962] 31 [-47.096 6.256 2.047] 5.04485896730523
132	66 [-47.607 5.24 6.962] 32 [-46.917 2.621 0.986] 6.561085047459756
133	66 [-47.607 5.24 6.962] 38 [-58.441 -10.795 4.247] 19.54144329367716
134	66 [-47.607 5.24 6.962] 39 [-60.033 -13.827 5.803] 22.788138274110946
135	66 [-47.607 5.24 6.962] 40 [-63.007 -14.025 8.133] 24.69152619827296
136	66 [-47.607 5.24 6.962] 65 [-48.369 1.713 5.788] 3.794555178146709
137	66 [-47.607 5.24 6.962] 66 [-47.607 5.24 6.962] 0.0
138	66 [-47.607 5.24 6.962] 89 [-67.905 -4.735 7.978] 22.6393834942562

4rx6B.pdb

4rx6B.pdb

new 1

1	40	[-63.007	-14.025	8.133]	40	[-63.007	-14.025	8.133]	0.0
2	40	[-63.007	-14.025	8.133]	39	[-60.033	-13.827	5.803]	3.7832234932660236
3	40	[-63.007	-14.025	8.133]	38	[-58.441	-10.795	4.247]	6.81045167371445
4	40	[-63.007	-14.025	8.133]	90	[-64.827	-4.491	5.829]	9.9758694859145
5	40	[-63.007	-14.025	8.133]	89	[-67.905	-4.735	7.978]	10.503262778774985
6	40	[-63.007	-14.025	8.133]	92	[-61.049	-2.353	8.512]	11.841156573578445
7	40	[-63.007	-14.025	8.133]	91	[-64.329	-0.983	7.164]	13.144596190069894
8	40	[-63.007	-14.025	8.133]	10	[-56.107	-2.772	6.55]	13.294581527825537
9	40	[-63.007	-14.025	8.133]	93	[-58.724	-1.731	11.438]	13.431662220291278
10	40	[-63.007	-14.025	8.133]	95	[-52.605	-0.865	14.008]	17.773655476575435
11	40	[-63.007	-14.025	8.133]	65	[-48.369	1.713	5.788]	21.6207010293376
12	40	[-63.007	-14.025	8.133]	32	[-46.917	2.621	0.986]	24.229259687411002
13	40	[-63.007	-14.025	8.133]	66	[-47.607	5.24	6.962]	24.69152619827296
14	40	[-63.007	-14.025	8.133]	31	[-47.096	6.256	2.047]	26.486190326281356
15	40	[-63.007	-14.025	8.133]	30	[-45.57	9.618	1.379]	30.14393693597437
16	40	[-63.007	-14.025	8.133]	104	[-33.334	7.761	4.167]	37.02493593512351

Post-processing procedure

Spatial clustering algorithm

4rx6B.pdb	4rx6B.pdb
85	39 [-60.033 -13.827 5.803] 38 [-58.441 -10.795 4.247] 3.761465671782742
86	39 [-60.033 -13.827 5.803] 39 [-60.033 -13.827 5.803] 0.0
87	39 [-60.033 -13.827 5.803] 40 [-63.007 -14.025 8.133] 3.7832234932660236
88	39 [-60.033 -13.827 5.803] 65 [-48.369 1.713 5.788] 19.430407123887033
89	39 [-60.033 -13.827 5.803] 66 [-47.607 5.24 6.962] 22.788138274110946
90	39 [-60.033 -13.827 5.803] 89 [-67.905 -4.735 7.978] 12.221434981212312
91	39 [-60.033 -13.827 5.803] 90 [-64.827 -4.491 5.829] 10.494951548244517
92	39 [-60.033 -13.827 5.803] 91 [-64.329 -0.983 7.164] 13.61162271736915
93	39 [-60.033 -13.827 5.803] 92 [-61.049 -2.353 8.512] 11.833157355498997
94	39 [-60.033 -13.827 5.803] 93 [-58.724 -1.731 11.438] 13.408203533658043
95	39 [-60.033 -13.827 5.803] 95 [-52.605 -0.865 14.008] 17.044373059752008
96	39 [-60.033 -13.827 5.803] 104 [-33.334 7.761 4.167] 34.37375221008029
97	40 [-63.007 -14.025 8.133] 10 [-56.107 -2.772 6.55] 13.294581527825537
98	40 [-63.007 -14.025 8.133] 30 [-45.57 9.618 1.379] 30.14393693597437
99	40 [-63.007 -14.025 8.133] 31 [-47.096 6.256 2.047] 26.486190326281356
100	40 [-63.007 -14.025 8.133] 32 [-46.917 2.621 0.986] 24.229259687411002
101	40 [-63.007 -14.025 8.133] 38 [-58.441 -10.795 4.247] 6.81045167371445
102	40 [-63.007 -14.025 8.133] 39 [-60.033 -13.827 5.803] 3.7832234932660236
103	40 [-63.007 -14.025 8.133] 40 [-63.007 -14.025 8.133] 0.0
104	40 [-63.007 -14.025 8.133] 65 [-48.369 1.713 5.788] 21.6207010293376
105	40 [-63.007 -14.025 8.133] 66 [-47.607 5.24 6.962] 24.69152619827296
106	40 [-63.007 -14.025 8.133] 89 [-67.905 -4.735 7.978] 10.503262778774985
107	40 [-63.007 -14.025 8.133] 90 [-64.827 -4.491 5.829] 9.9758694859145
108	40 [-63.007 -14.025 8.133] 91 [-64.329 -0.983 7.164] 13.144596190069894
109	40 [-63.007 -14.025 8.133] 92 [-61.049 -2.353 8.512] 11.841156573578445
110	40 [-63.007 -14.025 8.133] 93 [-58.724 -1.731 11.438] 13.431662220291278
111	40 [-63.007 -14.025 8.133] 95 [-52.605 -0.865 14.008] 17.773655476575435
112	40 [-63.007 -14.025 8.133] 104 [-33.334 7.761 4.167] 37.02493593512351
113	65 [-48.369 1.713 5.788] 10 [-56.107 -2.772 6.55] 13.294581527825537
114	65 [-48.369 1.713 5.788] 30 [-45.57 9.618 1.379] 30.14393693597437
115	65 [-48.369 1.713 5.788] 31 [-47.096 6.256 2.047] 26.486190326281356
116	65 [-48.369 1.713 5.788] 32 [-46.917 2.621 0.986] 24.229259687411002
117	65 [-48.369 1.713 5.788] 38 [-58.441 -10.795 4.247] 6.81045167371445
118	65 [-48.369 1.713 5.788] 39 [-60.033 -13.827 5.803] 3.7832234932660236
119	65 [-48.369 1.713 5.788] 40 [-63.007 -14.025 8.133] 0.0
120	65 [-48.369 1.713 5.788] 65 [-48.369 1.713 5.788] 0.0
121	65 [-48.369 1.713 5.788] 66 [-47.607 5.24 6.962] 24.69152619827296
122	65 [-48.369 1.713 5.788] 89 [-67.905 -4.735 7.978] 10.503262778774985
123	65 [-48.369 1.713 5.788] 90 [-64.827 -4.491 5.829] 9.9758694859145
124	65 [-48.369 1.713 5.788] 91 [-64.329 -0.983 7.164] 13.144596190069894
125	65 [-48.369 1.713 5.788] 92 [-61.049 -2.353 8.512] 11.841156573578445
126	65 [-48.369 1.713 5.788] 93 [-58.724 -1.731 11.438] 13.431662220291278
127	65 [-48.369 1.713 5.788] 95 [-52.605 -0.865 14.008] 17.773655476575435
128	65 [-48.369 1.713 5.788] 104 [-33.334 7.761 4.167] 37.02493593512351
129	66 [-47.607 5.24 6.962] 10 [-56.107 -2.772 6.55] 13.294581527825537
130	66 [-47.607 5.24 6.962] 30 [-45.57 9.618 1.379] 30.14393693597437
131	66 [-47.607 5.24 6.962] 31 [-47.096 6.256 2.047] 26.486190326281356
132	66 [-47.607 5.24 6.962] 32 [-46.917 2.621 0.986] 24.229259687411002
133	66 [-47.607 5.24 6.962] 38 [-58.441 -10.795 4.247] 6.81045167371445
134	66 [-47.607 5.24 6.962] 39 [-60.033 -13.827 5.803] 3.7832234932660236
135	66 [-47.607 5.24 6.962] 40 [-63.007 -14.025 8.133] 0.0
136	66 [-47.607 5.24 6.962] 65 [-48.369 1.713 5.788] 21.6207010293376
137	66 [-47.607 5.24 6.962] 66 [-47.607 5.24 6.962] 0.0
138	66 [-47.607 5.24 6.962] 89 [-67.905 -4.735 7.978] 10.503262778774985

4rx6B.pdb	4rx6B.pdb	new 1
1	40 [-63.007 -14.025 8.133]	40 [-63.007 -14.025 8.133] 0.0
2	40 [-63.007 -14.025 8.133]	39 [-60.033 -13.827 5.803] 3.7832234932660236
3	40 [-63.007 -14.025 8.133]	38 [-58.441 -10.795 4.247] 6.81045167371445
4	40 [-63.007 -14.025 8.133]	90 [-64.827 -4.491 5.829] 9.9758694859145
5	40 [-63.007 -14.025 8.133]	89 [-67.905 -4.735 7.978] 10.503262778774985
6	40 [-63.007 -14.025 8.133]	92 [-61.049 -2.353 8.512] 11.841156573578445
7	40 [-63.007 -14.025 8.133]	91 [-64.329 -0.983 7.164] 13.144596190069894
8	40 [-63.007 -14.025 8.133]	10 [-56.107 -2.772 6.55] 13.294581527825537
9	40 [-63.007 -14.025 8.133]	93 [-58.724 -1.731 11.438] 13.43166220291278
10	40 [-63.007 -14.025 8.133]	95 [-52.605 -0.865 14.008] 17.773655476575435
11	40 [-63.007 -14.025 8.133]	65 [-48.369 1.713 5.788] 21.6207010293376
12	40 [-63.007 -14.025 8.133]	32 [-46.917 2.621 0.986] 24.229259687411002
13	40 [-63.007 -14.025 8.133]	66 [-47.607 5.24 6.962] 24.69152619827296
14	40 [-63.007 -14.025 8.133]	31 [-47.096 6.256 2.047] 26.486190326281356
15	40 [-63.007 -14.025 8.133]	30 [-45.57 9.618 1.379] 30.14393693597437
16	40 [-63.007 -14.025 8.133]	104 [-33.334 7.761 4.167] 37.02493593512351

README

4rx6B_ATP_BS01.apoc.pdb

4rx6B_ATP_BS02.apoc.pdb

4rx6B.txt

1

PKT1

2

3

10、38、61、89、90、91、92、93

4

5

10 [-56.107 -2.772 6.55]13.294581527825537

6

38 [-58.441 -10.795 4.247]6.81045167371445

7

61

8

89 [-67.905 -4.735 7.978]10.503262778774985

9

90 [-64.827 -4.491 5.829]9.9758694859145

10

91 [-64.329 -0.983 7.164]13.144596190069894

11

92 [-61.049 -2.353 8.512]11.841156573578445

12

93 [-58.724 -1.731 11.438]13.431662220291278

13

14

PKT2

15

16

31、32、65、66、67、106

17

18

31 [-47.096 6.256 2.047]26.486190326281356

19

32 [-46.917 2.621 0.986]24.229259687411002

20

65 [-48.369 1.713 5.788]21.6207010293376

21

66 [-47.607 5.24 6.962]24.69152619827296

22

67

23

106

24

25

26

Post-processing procedure



名称	修改日期	类型	大小
1qngA_ATP_BS01.apoc.pdb	2018/11/6 18:09	Program Debug ...	405 KB
1r0zC_ATP_BS01.apoc.pdb	2018/11/6 18:07	Program Debug ...	182 KB
1r4nB_ATP_BS01.apoc.pdb	2018/11/6 18:09	Program Debug ...	261 KB
1rdqE_ATP_BS02.apoc.pdb	2018/11/6 18:09	Program Debug ...	230 KB
1s9iA_ATP_BS01.apoc.pdb	2018/11/6 17:35	Program Debug ...	199 KB
1s9iB_ATP_BS01.apoc.pdb	2018/11/6 18:04	Program Debug ...	192 KB
1su2A_ATP_BS01.apoc.pdb	2018/11/6 17:41	Program Debug ...	104 KB
1su2A_ATP_BS02.apoc.pdb	2018/11/6 18:04	Program Debug ...	102 KB
1svmC_ATP_BS01.apoc.pdb	2018/11/6 18:11	Program Debug ...	243 KB
1sx3E_ATP_BS01.apoc.pdb	2018/11/6 17:40	Program Debug ...	314 KB
1tc0B_ATP_BS01.apoc.pdb	2018/11/6 18:03	Program Debug ...	123 KB

```
Scoring parameters: normalization length = 25, d0 = 1.280
Alignment search mode: non-sequential
Best alignment search: initial = 32
Sequence similarity (BLOSUM62): sum = -6, sum_pos = 9
Running time: 0.02370 seconds
```

Post-processing procedure

[illegible]

XXX

Work on my paper.

localizing protein-ATP binding residues is critical to understanding the interactions between protein and ATP, which is of significant importance for both protein function analysis and drug discovery. ↵

V1.5↵

Adenosine 5'-triphosphate (ATP) is an important small molecule in cells, which is the energy source for organisms to maintain membrane transport, cellular motility, muscle contraction, signaling, replication and transcription of DNA, and various metabolic processes. For protein, ATP as a ligand interacts with it through ATP-binding residues. ATP is hydrolyzed to remove a terminal phosphate group and converted into ADP, and a large amount of energy is released

at the same time. The released energy and phosphate group work together to change the protein structure at the ATP-binding residues, thereby further causing changes in protein activity. Previous studies have shown that protein-ligand binding residues tend to form spatial clusters, forming protein-ligand binding sites (pockets), which are valuable drug targets for antibacterial and anti-cancer chemotherapy. Hence, accurately localizing protein-ATP binding residues is critical to understanding the interactions between protein and ATP, which is of significant importance for both protein function analysis and drug discovery. ↵

↵

ATP 是什么↵

对于 protein, ATP 作为其 ligand 通过 ATP-binding residues 与其相互作用↵

ATP 对蛋白质起作用的方式: hydrolyze↵

绑定残基空间聚类形成 binding sites (pockets)↵

定位 protein-ligand binding residues 很重要↵

↵

D2.D3.D4 研究方法概述: ↵

实验方法↵

计算方法: ↵

基于序列的↵

基于结构的↵

基于序列和结构的 (本文 TM-SITE [结构] 和 I-LBR [序列]) ↵

↵

D2↵

V1.1↵

Experimental methods are the most accurate techniques to identify the protein-ATP binding residues, but it relies too much on manpower and equipment resources, and is expensive and time-consuming. As the alternate techniques, computational methods have been used successfully for predicting the protein-ligand binding residues during the past decade. For the prediction of the protein-ATP binding residues, the highest Matthews correlation coefficient (MCC) value reached 0.685. According to the different types of information on

Post-processing procedure

