

A. Top-30 results of the DALI search seeded with BMP-H protein (PDB id: 2a10)

No:	Chain	Z	rmsd	lali	nres	%id	Description
1:	2g13-A	24.1	0.0	95	95	100	MAJOR CARBOXYSOME SHELL PROTEIN 1A;
2:	5d6v-A	18.7	0.7	89	90	57	CARBOXYSOME SHELL PROTEIN;
3:	4axj-B	17.7	0.8	86	89	67	ETHANOLAMINE CARBOXYSOME STRUCTURAL PROTEIN;
4:	4qiv-A	17.7	0.8	86	86	51	BACTERIAL MICROCOMPARTMENTS FAMILY PROTEIN;
5:	5l38-A	17.5	1.4	90	91	50	MSM0272 - RMM MICROCOMPARTMENT SHELL PROTEIN;
6:	4liw-A	16.9	1.2	90	92	48	CARBON DIOXIDE-CONCENTRATING MECHANISM PROTEIN CC
7:	5djb-A	16.7	0.9	87	98	55	MICROCOMPARTMENTS PROTEIN;
8:	2a1b-A	16.2	1.4	91	101	52	CARBON DIOXIDE CONCENTRATING MECHANISM PROTEIN CC
9:	3mpw-A	16.2	1.1	88	99	53	ETHANOLAMINE UTILIZATION PROTEIN EUTM;
10:	3sss-E	15.8	1.2	89	106	49	CARBON DIOXIDE CONCENTRATING MECHANISM PROTEIN;
11:	4ox6-A	15.8	1.2	89	103	35	CARBON DIOXIDE CONCENTRATING MECHANISM PROTEIN CC
12:	4rbv-B	15.6	2.7	91	94	57	PROPANEDIOL UTILIZATION PROTEIN PDUA;
13:	2a10-C	15.2	1.2	89	107	36	CARBON DIOXIDE CONCENTRATING MECHANISM PROTEIN CC
14:	3vcd-A	14.7	1.8	90	184	29	PROPANEDIOL UTILIZATION POLYHEDRAL BODY PROTEIN P
15:	3pac-A	14.7	1.8	90	183	30	SHELL PROTEIN;
16:	3nwg-A	13.3	2.1	83	180	31	MICROCOMPARTMENTS PROTEIN;
17:	5dih-B	11.7	1.5	88	202	23	MICROCOMPARTMENTS PROTEIN;
18:	5hpn-A	10.3	1.6	68	87	57	PERMUTED PDUA;
19:	3i82-A	8.3	1.6	65	216	23	ETHANOLAMINE UTILIZATION PROTEIN EUTL;
20:	1hwu-B	7.8	2.6	75	101	16	PII PROTEIN;
21:	2pfd-A	7.8	2.8	86	540	9	FORMIMIDOYLTRANSFERASE-CYCLODEAMINASE;
22:	3dfe-B	7.7	2.8	77	83	14	PUTATIVE PII-LIKE SIGNALING PROTEIN;
23:	31f0-B	7.7	3.3	79	112	13	NITROGEN REGULATORY PROTEIN P-II;
24:	3u27-D	7.5	1.7	69	218	22	MICROCOMPARTMENTS PROTEIN;
25:	3io0-A	7.5	2.2	73	229	14	ETUB PROTEIN;
26:	4edi-C	7.3	1.7	69	225	29	ETHANOLAMINE UTILIZATION PROTEIN;
27:	4i61-A	7.3	1.6	66	228	23	PROPANEDIOL UTILIZATION PROTEIN PDUB;
28:	2j9e-B	7.3	3.3	77	119	12	HYPOTHETICAL NITROGEN REGULATORY PII-LIKE
29:	3ta1-D	7.2	3.3	77	115	17	NITROGEN REGULATORY PROTEIN P-II (GLNB-3);
30:	2xbp-A	7.2	3.3	77	113	14	NITROGEN REGULATORY PROTEIN P-II;

Hits to BMC-H homologs are shown in Bold; hits to PII-like proteins are in red, whereas the false-positive hit to formimidoyltransferase-cyclodeaminase is shown in plain font. The false-positive hit was evaluated by direct comparison of the protein structures.

## B. Top-30 results of the DALI search seeded with BMP-P protein (PDB id: 2rcf)

No:	Chain	Z	rmsd	lali	nres	%id	Description
1:	2rcf-A	20.0	0.0	82	82	100	UNIDENTIFIED CARBOXYSOME POLYPEPTIDE;
2:	2hd3-B	13.1	2.3	82	97	39	ETHANOLAMINE UTILIZATION PROTEIN EUTN;
3:	4i7a-D	12.4	2.4	78	87	32	ETHANOLAMINE UTILIZATION PROTEIN EUTN/CARBOXYSOME
4:	5l37-C	12.3	2.3	81	86	30	MSM0273;
5:	4jvz-C	11.9	2.3	81	97	31	CARBON DIOXIDE CONCENTRATING MECHANISM PROTEIN;
6:	4n8x-1	11.8	2.2	81	99	32	CARBON DIOXIDE CONCENTRATING MECHANISM PROTEIN;
7:	4jw0-B	11.8	2.3	81	97	36	CARBON DIOXIDE CONCENTRATING MECHANISM PROTEIN;
8:	2qw7-H	11.7	2.3	81	98	36	CARBON DIOXIDE CONCENTRATING MECHANISM PROTEIN CC
9:	4q15-A	6.4	2.1	53	68	17	TRANSLATION INITIATION FACTOR IF-1;
10:	2eif-A	6.2	2.7	54	133	15	PROTEIN (EUKARYOTIC TRANSLATION INITIATION FACTOR
11:	2wfw-B	6.1	2.6	57	125	16	ARC;
12:	2dgy-A	6.1	3.2	61	111	15	MGC11102 PROTEIN;
13:	2wg5-A	6.0	2.0	51	87	22	GENERAL CONTROL PROTEIN GCN4, PROTEASOME-ACTIVATI
14:	3i4o-A	6.0	2.1	53	68	17	TRANSLATION INITIATION FACTOR IF-1;
15:	liz6-A	5.9	2.8	55	136	15	INITIATION FACTOR 5A;
16:	1fjg-Q	5.8	2.7	56	104	14	30S RIBOSOMAL PROTEIN S17;
17:	2ot2-A	5.8	1.6	51	90	16	HYDROGENASE ISOENZYMES FORMATION PROTEIN HYPC;
18:	2n8n-A	5.8	2.3	52	72	21	TRANSLATION INITIATION FACTOR IF-1;
19:	5mp9-J	5.8	2.0	52	386	10	PROTEASOME SUBUNIT ALPHA TYPE-1;
20:	1u0l-A	5.7	3.3	57	278	14	PROBABLE GTPASE ENG C;
21:	3m9b-A	5.6	2.6	56	186	18	PROTEASOME-ASSOCIATED ATPASE;
22:	3iz6-P	5.6	3.9	65	85	2	40S RIBOSOMAL PROTEIN RACK1 (RACK1);
23:	3h43-I	5.6	2.1	54	79	17	PROTEASOME-ACTIVATING NUCLEOTIDASE;
24:	5mp9-I	5.6	3.0	55	385	18	PROTEASOME SUBUNIT ALPHA TYPE-1;
25:	5kzf-H	5.5	2.6	55	478	18	PROTEASOME-ASSOCIATED ATPASE;
26:	4bpe-0	5.5	2.4	56	99	23	TRANSLATION INITIATION FACTOR EIF-1A FAMILY PROTE
27:	5mmj-q	5.4	3.1	60	86	13	50S RIBOSOMAL PROTEIN L31;
28:	2z1c-B	5.4	1.8	51	74	22	HYDROGENASE EXPRESSION/FORMATION PROTEIN HYPC;
29:	1bkb-A	5.3	2.7	53	136	11	TRANSLATION INITIATION FACTOR 5A;
30:	2z6b-A	5.3	3.7	62	573	10	TAIL-ASSOCIATED LYSOZYME;

Hits to BMC-P homologs are shown in Bold; hits to OB-fold proteins are in red, whereas the two false-positives are shown in plain font. The false-positives were evaluated by direct comparison of the protein structures. In both cases, the proteins have highly enriched in beta-strands, but do not share the same fold as BMC-P.

### C. Top-30 results of the HHpred search seeded with BMP-P protein sequence (WP\_012823797)

Query WP\_012823797.1 carboxysome peptide A [Halothiobacillus neapolitanus]  
 Match\_columns 83  
 Searched\_HMMs 94372  
 Date Wed Nov 1 08:13:30 2017

No Hit	Prob	E-value	P-value	Score	SS	Cols	Query HMM	Template HMM
1 2RCF_A Crystal Structure of Or	100.0	4E-35	4.3E-40	190.9	12.7	83	1-83	1-83 (91)
2 2RCF_D Crystal Structure of Or	100.0	4E-35	4.3E-40	190.9	12.7	83	1-83	1-83 (91)
3 d2rcfe_b.40.15.1 (E:) Carboxy	100.0	6E-35	6.3E-40	186.0	12.5	80	1-80	1-80 (80)
4 d4jvzb_b.40.15.1 (B:) Carbon	100.0	1E-34	1.1E-39	189.7	12.4	83	1-83	1-88 (94)
5 d2qw7c_b.40.15.1 (C:) Carbon	100.0	1.1E-34	1.2E-39	189.9	12.3	83	1-83	1-88 (95)
6 4I7A_E Ethanolamine utilizatio	100.0	1.1E-34	1.2E-39	190.0	12.3	83	1-83	1-88 (95)
7 5L37_C MSM0273; bacterial micr	100.0	1.5E-34	1.6E-39	189.5	12.6	83	1-83	1-83 (95)
8 5L37_B MSM0273; bacterial micr	100.0	1.5E-34	1.6E-39	189.5	12.6	83	1-83	1-83 (95)
9 d2hd3a1_b.40.15.1 (A:1-95) Eth	100.0	1.9E-34	2E-39	188.7	12.3	83	1-83	1-88 (95)
10 5V74_P1 Ethanolamine utilizati	100.0	1.7E-34	1.8E-39	189.4	12.0	83	1-83	1-88 (96)
11 d4jw0a_b.40.15.1 (A:) automat	100.0	2E-34	2.1E-39	188.6	12.2	83	1-83	1-88 (95)
12 4JVZ_C Carbon dioxide concentr	100.0	2.5E-34	2.6E-39	189.4	12.5	83	1-83	1-88 (99)
13 4JW0_E Carbon dioxide concentr	100.0	4.1E-34	4.3E-39	191.1	12.2	83	1-83	1-88 (108)
14 2HD3_B Ethanolamine utilizatio	100.0	4.3E-34	4.5E-39	189.6	12.1	83	1-83	1-88 (103)
15 2HD3_C Ethanolamine utilizatio	100.0	4.3E-34	4.5E-39	189.6	12.1	83	1-83	1-88 (103)
16 4N8F_B Carbon dioxide concentr	100.0	5.3E-34	5.6E-39	191.6	12.5	83	1-83	1-88 (112)
17 2QW7_F Carbon dioxide concentr	100.0	4.8E-34	5.1E-39	191.6	12.3	83	1-83	1-88 (111)
18 2QW7_H Carbon dioxide concentr	100.0	4.8E-34	5.1E-39	191.6	12.3	83	1-83	1-88 (111)
19 d4n8x2_b.40.15.1 (2:) Carbon	100.0	7.8E-34	8.2E-39	186.1	12.1	83	1-83	1-89 (96)
20 4N8X_B Carbon dioxide concentr	100.0	1.9E-33	2E-38	188.1	12.1	83	1-83	1-89 (109)
21 4N8X_4 Carbon dioxide concentr	100.0	1.9E-33	2E-38	188.1	12.1	83	1-83	1-89 (109)
22 PF03319.12 ; EutN_CcmL ; Ethan	100.0	6.3E-33	6.7E-38	179.7	11.9	78	1-78	1-89 (89)
23 d3vyta_b.40.14.1 (A:) Hydroge	76.7	9.6	0.0001	22.8	2.9	25	31-55	20-45 (52)
24 d1b70b3_b.40.4.4 (B:39-151) Do	76.6	40	0.00042	22.9	7.1	48	6-56	8-56 (113)
25 2XVS_A TETRATRICOPEPTIDE REPEA	74.4	39	0.00041	24.9	5.9	46	6-54	79-130 (166)
26 PF16669.4 ; TTC5_OB ; Tetratri	74.2	50	0.00053	22.8	6.2	44	6-52	20-69 (114)
27 2Z1C_B Hydrogenase expression/	72.2	10	0.00011	24.5	2.4	21	37-57	28-49 (75)
28 d2z1ca1_b.40.14.1 (A:2-72) Hyd	69.0	18	0.00019	23.1	2.9	19	37-55	27-46 (71)
29 PF01455.17 ; HupF_HypC ; HupF/	68.8	48	0.00051	20.9	4.6	40	15-55	8-48 (66)
30 3PCO_B Phenylalanyl-tRNA synth	66.8	77	0.00081	28.4	6.9	51	6-56	46-97 (795)

Hits to BMC-P homologs are shown in Bold; hits to OB-fold proteins are in red.