



STRUCTURAL BIOLOGY
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Supporting information for article:

Crystal structure of an inorganic pyrophosphatase from *Chlamydia trachomatis* D/UW-3/Cx

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Figure S1 DALI analysis of *CtPPase* (<http://ekhidna2.biocenter.helsinki.fi/dali/>) (Holm, 2020)

Table S1 Results from *PDBeFold P* (<http://www.ebi.ac.uk/msd-srv/ssm/>) analysis of *CtPPase* (Krissinel & Henrick, 2004)

References

Holm, L. (2020). *Protein Sci* **29**, 128-140.

Krissinel, E. & Henrick, K. (2004). *Acta crystallographica. Section D, Biological crystallography* **60**, 2256-2268.

RESULT SUMMARY

##	Q-score	P-score	Z-score	RMSD	Nalgn	Nsse	Ngaps	Seq-%	Nmd	Nres-Q	Nsse-Q	Nres-T	Nsse-T	Query	Target
1	1	41.41	19.31	0.000	206	10	0	1	0	206	10	206	10	PDB 6we5:A	PDB 6we5:A
2	0.9867	29.22	16.16	0.349	206	10	0	1	0	206	10	206	10	PDB 6we5:A	PDB 6we5:B
3	0.9789	25.05	14.94	0.325	205	10	0	1	0	206	10	206	10	PDB 6we5:A	PDB 6we5:C
4	0.6942	13.32	11.12	1.179	169	7	4	0.3669	0	206	10	173	9	PDB 6we5:A	PDB 5ty5:F
5	0.6902	12.96	10.98	1.179	169	7	4	0.3669	0	206	10	174	9	PDB 6we5:A	PDB 5ty5:D
6	0.6801	12.08	10.49	1.192	168	7	6	0.369	0	206	10	174	9	PDB 6we5:A	PDB 3r5v:F
7	0.6795	12.73	10.77	1.196	168	7	6	0.369	0	206	10	174	9	PDB 6we5:A	PDB 3r5v:E
8	0.6777	12.81	10.8	1.207	168	7	6	0.369	0	206	10	174	9	PDB 6we5:A	PDB 3r5v:D
9	0.6771	12.88	10.83	1.211	168	7	6	0.369	0	206	10	174	9	PDB 6we5:A	PDB 5ty5:E
10	0.6768	12.77	10.79	1.188	168	7	6	0.369	0	206	10	175	9	PDB 6we5:A	PDB 3q3l:F
11	0.6768	12.55	10.69	1.188	168	7	6	0.369	0	206	10	175	9	PDB 6we5:A	PDB 3i98:F
12	0.6748	11.93	10.43	1.227	169	7	5	0.3609	0	206	10	176	9	PDB 6we5:A	PDB 3q5v:B
13	0.6747	12.77	10.79	1.174	167	7	6	0.3713	0	206	10	174	9	PDB 6we5:A	PDB 3q3l:E
14	0.6746	12.51	10.68	1.175	167	7	6	0.3713	0	206	10	174	9	PDB 6we5:A	PDB 3i98:E
15	0.6705	12.08	10.49	1.228	168	7	6	0.369	0	206	10	175	9	PDB 6we5:A	PDB 3q3l:D
16	0.6689	11.93	10.43	1.238	168	7	6	0.369	0	206	10	175	9	PDB 6we5:A	PDB 3i98:D
17	0.6596	11.55	10.31	1.247	167	7	6	0.3713	0	206	10	175	10	PDB 6we5:A	PDB 3r6e:C
18	0.6547	12.66	10.74	1.225	165	7	7	0.3697	0	206	10	173	9	PDB 6we5:A	PDB 3r6e:D
19	0.6493	12.11	10.55	1.361	168	7	5	0.3512	0	206	10	175	10	PDB 6we5:A	PDB 3r6e:F
20	0.6178	14.32	11.27	1.315	162	8	8	0.2901	0	206	10	173	9	PDB 6we5:A	PDB 6k27:F
21	0.6168	14.39	11.39	1.321	162	8	8	0.2901	0	206	10	173	10	PDB 6we5:A	PDB 6k27:G
22	0.6166	12.01	10.46	1.322	162	7	8	0.2901	0	206	10	173	8	PDB 6we5:A	PDB 6k27:C
23	0.6152	14.2	11.22	1.331	162	8	8	0.2901	0	206	10	173	9	PDB 6we5:A	PDB 6k27:D
24	0.6151	14.36	11.29	1.332	162	8	8	0.2901	0	206	10	173	9	PDB 6we5:A	PDB 6k27:H
25	0.6141	16.35	12.06	1.232	159	8	7	0.3082	0	206	10	171	9	PDB 6we5:A	PDB 6n1c:D
26	0.6127	14.53	11.35	1.298	161	8	7	0.2919	0	206	10	173	9	PDB 6we5:A	PDB 6k27:B
27	0.6098	14.24	11.24	1.367	162	8	8	0.2901	0	206	10	173	9	PDB 6we5:A	PDB 6k27:E
28	0.6087	14.07	11.17	1.374	162	8	8	0.2901	0	206	10	173	9	PDB 6we5:A	PDB 6k27:A
29	0.6064	13.9	11.56	1.440	164	8	5	0.311	0	206	10	175	11	PDB 6we5:A	PDB 5h4f:A
30	0.6055	11.48	10.23	1.395	162	7	8	0.2901	0	206	10	173	8	PDB 6we5:A	PDB 6ki8:B
31	0.6053	13.75	11.04	1.396	162	8	8	0.284	0	206	10	173	9	PDB 6we5:A	PDB 6ki7:B
32	0.6052	13.95	11.12	1.397	162	8	8	0.284	0	206	10	173	9	PDB 6we5:A	PDB 6ki7:C
33	0.6016	13.43	10.91	1.467	163	8	7	0.2883	0	206	10	173	9	PDB 6we5:A	PDB 6k21:A
34	0.5991	15.98	11.92	1.230	157	8	8	0.3121	0	206	10	171	9	PDB 6we5:A	PDB 6n1c:B
35	0.598	13.77	11.5	1.463	161	8	7	0.354	0	206	10	170	11	PDB 6we5:A	PDB 2bqy:A
36	0.5972	13.66	11.15	1.235	155	7	7	0.3097	0	206	10	167	8	PDB 6we5:A	PDB 6n1c:C
37	0.5948	12.39	10.74	1.364	159	7	8	0.3145	0	206	10	171	8	PDB 6we5:A	PDB 6n1c:F
38	0.5942	12.11	10.5	1.321	159	7	8	0.2956	0	206	10	173	8	PDB 6we5:A	PDB 6ki8:C
39	0.5938	12.86	11.14	1.492	162	8	6	0.2901	0	206	10	172	11	PDB 6we5:A	PDB 3sw5:B
40	0.5937	12.94	11.17	1.492	162	8	6	0.2901	0	206	10	172	11	PDB 6we5:A	PDB 3sw5:E
41	0.593	12.53	10.73	1.475	162	8	6	0.284	0	206	10	173	9	PDB 6we5:A	PDB 6ki7:F
42	0.593	14.25	11.69	1.402	160	8	6	0.3125	0	206	10	172	11	PDB 6we5:A	PDB 5h4f:B
43	0.5925	11.69	10.49	1.498	161	8	6	0.3168	0	206	10	170	10	PDB 6we5:A	PDB 3tr4:F
44	0.5912	14.52	11.44	1.391	160	8	8	0.2875	0	206	10	173	10	PDB 6we5:A	PDB 6ki7:A
45	0.5902	11.89	10.25	1.446	161	8	9	0.2857	0	206	10	173	10	PDB 6we5:A	PDB 5tea:E
46	0.59	11.14	10.08	1.447	161	7	8	0.2857	0	206	10	173	8	PDB 6we5:A	PDB 6ki8:A
47	0.5898	13.21	10.91	1.401	160	8	8	0.2875	0	206	10	173	10	PDB 6we5:A	PDB 6ki7:E
48	0.5883	12.94	11.17	1.380	158	8	9	0.3101	0	206	10	170	11	PDB 6we5:A	PDB 3i4q:A
49	0.5875	13.89	11.19	1.415	160	8	7	0.2875	0	206	10	173	10	PDB 6we5:A	PDB 6ki7:G
50	0.5874	12.3	10.64	1.417	160	8	8	0.2875	0	206	10	173	9	PDB 6we5:A	PDB 6ki7:H

51	0.583	11.34	10.5	1.458	157	7	6	0.3631	0	206	10	166	10	PDB 6we5:A	PDB 2bqx:A
52	0.5827	11.04	10.15	1.438	157	7	6	0.293	0	206	10	167	8	PDB 6we5:A	PDB 3d53:E
53	0.5826	15.93	11.9	1.303	158	8	9	0.3101	0	206	10	175	9	PDB 6we5:A	PDB 6n1c:E
54	0.5818	11.4	10.36	1.516	159	8	6	0.3208	0	206	10	168	10	PDB 6we5:A	PDB 3tr4:D
55	0.5815	11.62	10.46	1.499	160	8	6	0.3187	0	206	10	171	10	PDB 6we5:A	PDB 3tr4:E
56	0.5812	12.43	10.75	1.196	149	7	5	0.3154	0	206	10	160	8	PDB 6we5:A	PDB 4z70:C
57	0.5805	13.28	11.15	1.379	156	8	8	0.2885	0	206	10	168	10	PDB 6we5:A	PDB 3emj:C
58	0.5763	13.66	11.15	1.272	157	7	9	0.3057	0	206	10	176	8	PDB 6we5:A	PDB 6n1c:A
59	0.5734	11.05	9.871	1.555	161	7	6	0.2857	0	206	10	173	7	PDB 6we5:A	PDB 6ki7:D
60	0.5729	11.56	10.38	1.313	150	7	4	0.3133	0	206	10	160	8	PDB 6we5:A	PDB 4z71:C
61	0.5705	11.4	10.36	1.443	155	8	7	0.2903	0	206	10	166	10	PDB 6we5:A	PDB 3emj:B
62	0.5702	11.81	10.49	1.277	149	7	5	0.3154	0	206	10	160	8	PDB 6we5:A	PDB 4z74:C
63	0.5702	12.92	11.01	1.446	155	8	7	0.2903	0	206	10	166	10	PDB 6we5:A	PDB 3emj:G
64	0.5598	11.35	10.29	1.352	149	7	5	0.3154	0	206	10	160	8	PDB 6we5:A	PDB 4z73:C
65	0.5596	11.7	10.44	1.304	149	7	5	0.3154	0	206	10	162	8	PDB 6we5:A	PDB 4z70:B
66	0.5583	11.42	10.14	1.390	155	8	8	0.3613	0	206	10	172	10	PDB 6we5:A	PDB 1ygz:F
67	0.5577	12.71	10.7	1.393	155	8	8	0.3613	0	206	10	172	10	PDB 6we5:A	PDB 1ygz:E
68	0.5577	11.39	10.13	1.394	155	8	8	0.3613	0	206	10	172	10	PDB 6we5:A	PDB 1ygz:D
69	0.5553	11.99	10.57	1.331	148	7	5	0.3041	0	206	10	160	8	PDB 6we5:A	PDB 4z73:J
70	0.5497	9.858	9.489	1.371	148	7	5	0.3108	0	206	10	160	7	PDB 6we5:A	PDB 4z73:H
71	0.546	6.457	8.183	1.916	166	8	5	0.2711	0	206	10	174	11	PDB 6we5:A	PDB 3fq3:I
72	0.5427	10.41	9.871	1.422	148	7	5	0.3108	0	206	10	160	8	PDB 6we5:A	PDB 4z74:H
73	0.5038	6.726	8.163	1.936	159	7	9	0.2704	0	206	10	172	10	PDB 6we5:A	PDB 4xe1:A