

Supplementary Table 1

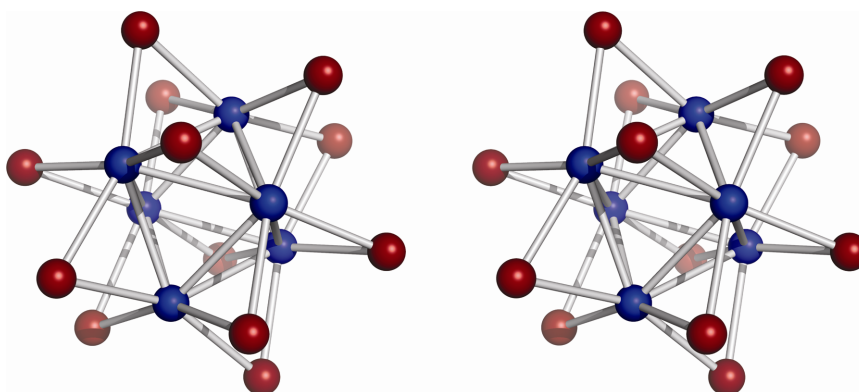
Ta₆Br₁₂²⁺ cluster sites. Positions are given in fractional coordinates. Data are from *SHELXD* (Schneider & Sheldrick, 2002). All sites except those on special positions conform to the twofold crystallographic symmetry. Sites that follow the fivefold non-crystallographic symmetry (5-fold NCS) are indicated. Filled diamonds (◆) show sites that are at probable crystal contact interfaces and stars (*) show sites that are not at probable crystal contact interfaces, but that bind to the protein.

Cluster	x	y	z	Occupancy	Notes
TA01	0.912003	0.687546	0.219412	1.0000	5-fold NCS
TA02	1.077408	0.328148	0.486746	0.9401	*
TA03	1.023376	0.532524	0.508825	0.9033	5-fold NCS
TA04	0.952812	0.692360	0.235182	0.8881	5-fold NCS
TA05	0.946335	0.663536	-0.013130	0.8834	◆
TA06	0.937874	0.939735	0.323057	0.8628	5-fold NCS
TA07	0.790428	0.587830	-0.045240	0.8589	◆
TA08	0.678879	0.584846	-0.093970	0.8390	◆
TA09	0.800270	0.781761	0.219824	0.7934	5-fold NCS
TA10	0.978195	0.945724	0.337774	0.7747	5-fold NCS
TA11	1.101631	0.634140	0.385580	0.7490	5-fold NCS
TA12	0.846466	0.937828	0.406164	0.6924	5-fold NCS
TA13	1.010902	1.136360	0.247015	0.6868	*
TA14	1.168343	0.596947	0.652807	0.6371	5-fold NCS
TA15	0.948898	0.712997	0.257940	0.6356	5-fold NCS
TA16	1.093102	0.845062	0.350660	0.6347	5-fold NCS
TA17	0.936989	0.765862	0.359457	0.6183	5-fold NCS
TA18	0.979828	0.928894	0.370207	0.6170	5-fold NCS
TA19	0.933434	0.683922	0.265760	0.6027	5-fold NCS
TA20	1.008095	0.563377	0.486883	0.5755	5-fold NCS
TA21	0.938736	0.736755	0.396986	0.5573	5-fold NCS
TA22	1.002510	0.813515	0.397962	0.5536	5-fold NCS
TA23	0.950989	0.910439	0.334089	0.5261	5-fold NCS
TA24	1.026978	0.818619	0.465956	0.5257	5-fold NCS
TA25	1.038223	0.861229	0.546278	0.5223	5-fold NCS
TA26	1.018158	0.739983	0.430197	0.5177	5-fold NCS
TA27	1.037910	0.689636	0.511312	0.4780	5-fold NCS
TA28	1.041000	0.660889	0.558645	0.4647	5-fold NCS
TA29	1.051125	0.814964	0.569403	0.4374	5-fold NCS
TA30	0.743645	0.605835	-0.039120	0.4306	◆
TA31	1.005577	0.693207	0.405851	0.3949	5-fold NCS
TA32	0.986244	0.659348	-0.046860	0.3761	◆
TA33	0.729370	0.571899	-0.104960	0.3696	◆
TA34	1.000000	0.501976	0.499998	0.1761	special position

TA35	1.000000	0.873489	0.499998	0.1696	special position
TA36	1.230766	0.372429	0.835790	0.3019	♦
TA37	1.084259	0.304176	0.466802	0.2794	*
TA38	1.051285	0.242027	0.498159	0.2723	*
TA39	1.134453	0.476067	0.839643	0.1836	♦
TA40	0.675537	0.545746	-0.079700	0.1391	♦
TA41	1.000000	0.466873	0.499998	0.0542	special position
TA42	1.014580	1.046440	0.198225	0.1062	*

Supplementary Figure 1

Stereo view of a $\text{Ta}_6\text{Br}_{12}^{2+}$ cluster. Ta atoms are coloured blue and Br atoms are coloured red. The structure of $\text{Ta}_6\text{Br}_{12}^{2+}$ was obtained from PDB entry 2bvl (Reinert *et al.*, 2005).



References

- Reinert, D. J., Jank, T., Aktories, K. & Schulz, G. E. (2005). *J. Mol. Biol.* **351**, 973-981.
 Schneider, T. R. & Sheldrick, G. M. (2002). *Acta Cryst.* **D58**, 1772-1779.