

Macromolecular crystallography for mammalian body temperature structures in support of molecular biophysics methods

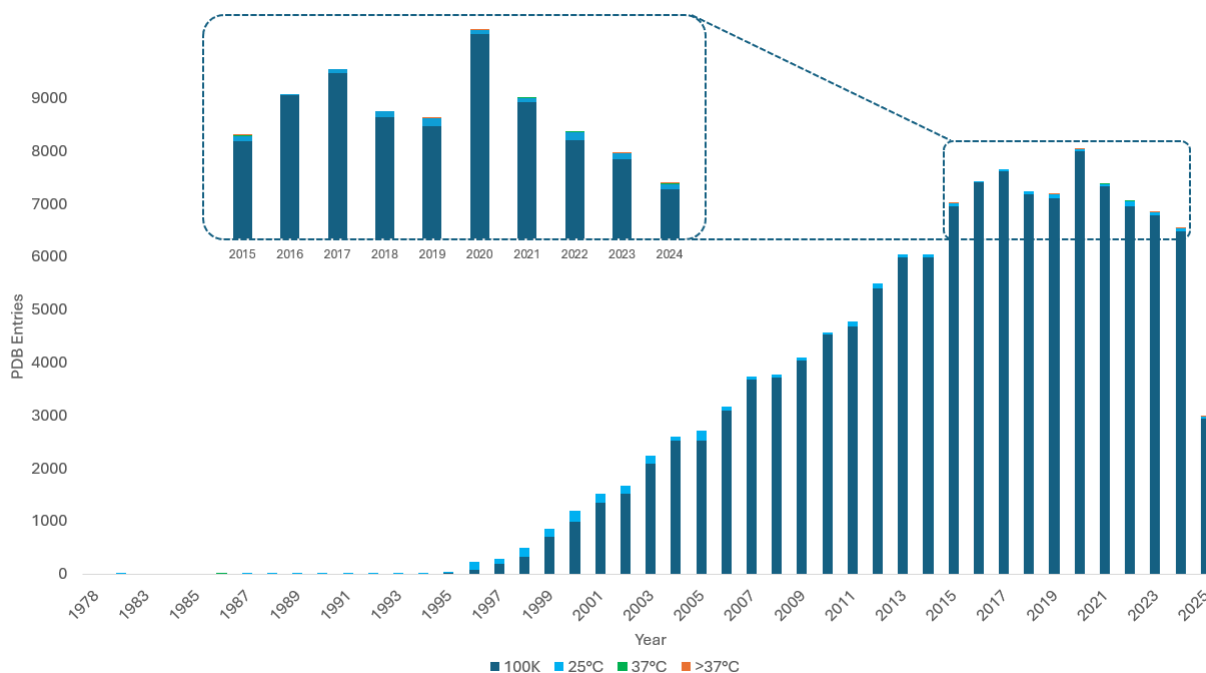
Alice Brink^a, John R Helliwell^b and Francois Jacobs^a

^a Chemistry Department, University of the Free State, Nelson Mandela Drive, Bloemfontein, South Africa.

^a Department of Chemistry, University of Manchester, Oxford Road, Manchester, UK

Corresponding authors: brinka@ufs.ac.za and john.helliwell@manchester.ac.uk

Supporting Information

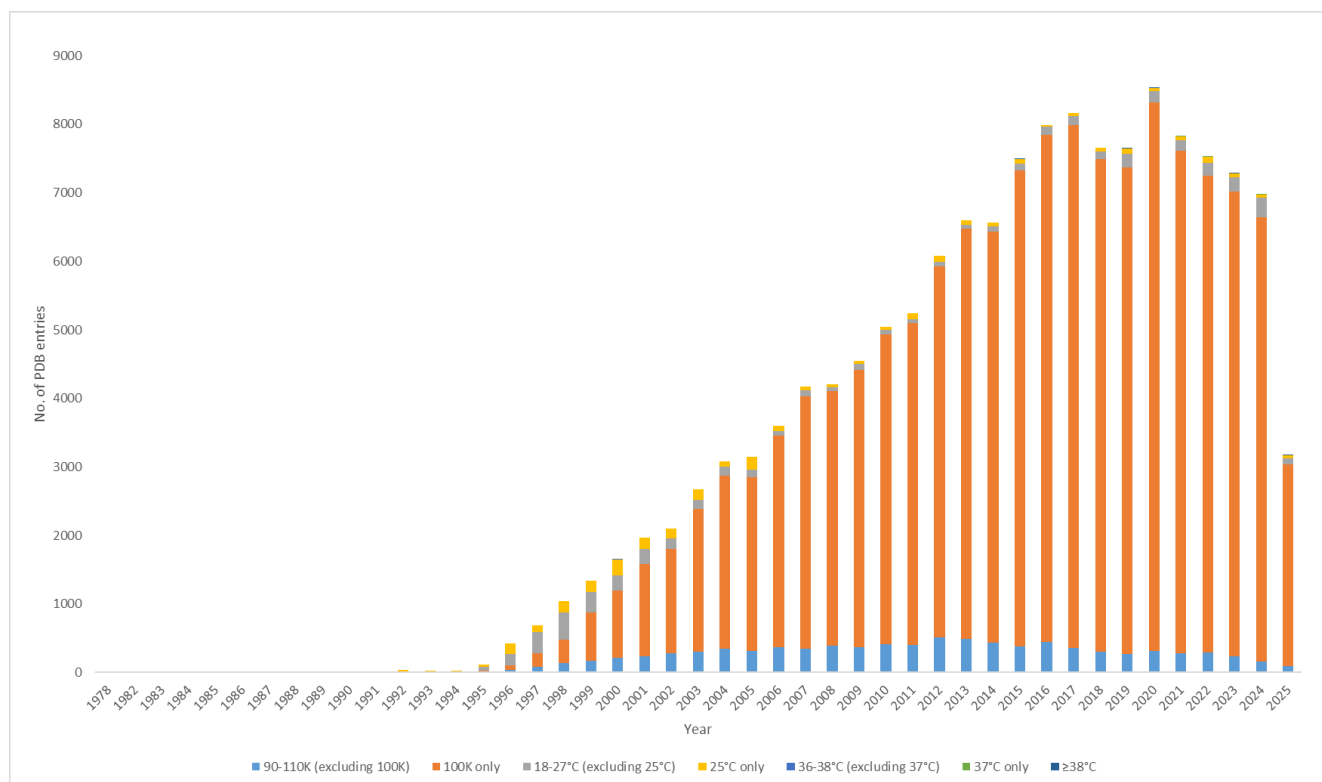


SI Fig.1. X-ray crystallographic structures available from the PDB obtained at low (100 K) and high (25°C, 37°C and >37°C) sample analysis temperatures plotted per year. The inset shows an enlarged section for the years 2015-2024 to clearly highlight the notable disparity between the high ($\geq 37^\circ\text{C}$) and low temperature ($100\text{K} \leq 25^\circ\text{C}$) crystal data sets.

SI Table.1. The X-ray crystallographic structures at low (100 K) and high (25°C, 37°C and >37°C) temperatures tabulated per year as found on the PDB.

Year	Number of PDB entries			
	100K	25°C	37°C	>37°C
1978	0	0	0	0
1982	0	1	0	0
1983	0	0	0	0
1984	0	0	0	0
1985	0	0	0	0
1986	0	0	1	0
1987	0	3	0	0
1988	0	1	0	0
1989	1	4	0	0
1990	1	5	0	0
1991	0	11	0	0
1992	3	18	0	0
1993	1	2	0	0
1994	4	10	0	0
1995	18	33	0	0
1996	75	153	0	0
1997	194	97	0	0
1998	336	169	0	0
1999	702	157	0	0
2000	984	222	0	0
2001	1343	171	0	0
2002	1524	147	0	0
2003	2083	158	0	0
2004	2519	75	0	0
2005	2534	184	0	0
2006	3089	81	0	0
2007	3688	59	0	0
2008	3724	47	0	0
2009	4049	48	0	0
2010	4525	40	0	0
2011	4692	93	0	0
2012	5413	81	0	0
2013	5984	72	0	0
2014	5998	48	0	0
2015	6952	57	1	1
2016	7407	14	0	0
2017	7625	41	0	0
2018	7190	59	0	0

2019	7104	80	0	1
2020	8003	38	0	2
2021	7334	47	1	0
2022	6961	83	2	0
2023	6783	55	2	8
2024	6489	44	7	1
2025	2942	43	1	3
Total	128274	2751	15	16



SI Fig.2. Extended data bin range of X-ray crystallographic structures available from the PDB indicating sample analysis temperature versus year published. The data is indicated within bin ranges of 90-110 K (bottom light blue, excluding 100 K); 100 K only (middle orange); 18-27 °C (top grey, excluding 25°C); 36-38°C (top blue, excluding 37°C); 37°C only (top green) and >38°C (top navy-blue). Data collections sampled at low temperature 90-110K (bottom light blue) + 100K (middle orange) clearly indicate the marked number of low temperature data versus the barely visible, high temperature ranges (18-38°C) indicated at the top of the histograms.

SI Table.2. Extended data bin range of X-ray crystallographic structures available from the PDB indicating sample analysis temperature versus year published (data visually indicated in Fig SI 2).

Year	Number of PDB entries						
	90-110K (excluding 100K)	100K only	18-27°C (excluding 25°C)	25°C only	36-38°C (excluding 37°C)	37°C only	≥38°C
1978	0	0	0	0	0	0	0
1982	0	0	1	1	0	0	0
1983	0	0	0	0	0	0	0
1984	0	0	0	0	0	0	0
1985	0	0	0	0	0	0	0
1986	0	0	0	0	0	1	0
1987	0	0	3	3	0	0	0
1988	0	0	1	1	0	0	0
1989	0	1	4	4	0	0	0
1990	0	1	2	5	0	0	0
1991	1	0	2	11	0	0	0
1992	0	3	12	18	0	0	0
1993	1	1	9	2	0	0	0
1994	2	4	13	10	0	0	0
1995	7	18	54	33	0	0	0
1996	32	75	166	153	0	0	0
1997	85	194	308	97	0	0	0
1998	138	336	398	169	0	0	0
1999	172	702	302	157	0	0	0
2000	213	984	223	222	1	0	0
2001	235	1343	218	171	0	0	0
2002	275	1524	154	147	0	0	0
2003	302	2083	131	158	0	0	0
2004	348	2519	136	75	0	0	0
2005	317	2534	111	184	0	0	0
2006	364	3089	69	81	0	0	0
2007	345	3688	79	59	0	0	0
2008	386	3724	46	47	0	0	0
2009	369	4049	82	48	0	0	0
2010	412	4525	65	40	0	0	0
2011	405	4692	52	93	0	0	0
2012	509	5413	73	81	0	0	0
2013	488	5984	58	72	0	0	0
2014	438	5998	77	48	0	0	0
2015	376	6952	102	57	1	1	1

2016	440	7407	123	14	0	0	0
2017	361	7625	139	41	0	0	0
2018	306	7190	102	59	0	0	0
2019	269	7104	191	80	0	0	1
2020	314	8003	173	38	0	0	2
2021	278	7334	160	47	0	1	0
2022	290	6961	190	83	0	2	0
2023	236	6783	211	55	0	2	8
2024	157	6489	279	44	0	7	0
2025	94	2942	91	43	0	1	3
Total	8965	128274	4610	2751	2	15	15