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Supporting Material

The Structure of Neuroglobin at High Xe and Kr Pressure Reveals Partial Conservation of Globin Internal Cavities

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Supplementary Table 1: Data collection and refinement statistics*

	metNgb•Xe	metNgb•Kr	NgbCO•Xe
Data collection			
Space group	R 32 [†]	R 32 [†]	R 32 [†]
a, b, c (Å)	88.83, 88.83, 110.93	88.80, 88.80, 113.50	88.68, 88.68, 109.83
α, β, γ (°)	90, 90, 120	90, 90, 120	90, 90, 120
Resolution Range (Å)	44.99-1.80(1.90-1.80)	19.5-1.86 (2.1-1.86)	31.47-2.25 (2.37-2.25)
Completeness (%)	100 (100)	99.7 (100)	97.5 (84.7)
Redundancy (%)	10.8(10.8)	6.17 (6.22)	9.3 (7.6)
R _{meas}	0.06 (0.38)	0.05 (0.38)	0.059 (0.22)
$\langle I / \sigma I \rangle$	31.3 (5.6)	22.84 (5.03)	29.6 (8.7)
Refinement			
Resolution (Å)	1.80	1.86	2.26
No. of reflections	15036	13599	7509
R _{cryst} / R _{free} (%)	18.6/ 21.0	17.2/20.8	19.2/25.4
No. of protein atoms	1297	1285	1257
No. of ligand atoms (Xe or Kr)	6	2	5
No. of ion atoms	5	5	5
No. of water oxygens	83	75	47
B-factors (Å²)			
Protein	21.6	28.3	35.8
Ligand	16.8	42.1	37.2
Ion	22.7	35.3	28.8
Water	32.3	41.0	44.1
overall	22.3	29.0	36.0
R.m.s deviations			
Bond lengths (Å)	0.014	0.016	0.013
Bond angles (°)	1.332	1.452	1.814

*Highest resolution shell is shown in parenthesis.

[†] Based on the Laue classes; in this case, it was the hexagonal setting H 3 2

Tab.1: Data collection and refinement statistics

Data collection and refinement statistics for metNgb-Xe, metNgb-Kr and NgbCO-Xe.

PDB codes are, respectively: 3GK9, 3GKT, 3GLN.