The mechanism of Iron Uptake by transferrins: the X-ray structures of the 18 kDa N-II domain fragment of duck ovotransferrin and its nitrilotriacetate complex.

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Supplementary table. Iron-binding sites; bond angles (°)

18 kDa fragment		NTA complex		pST: N-lobe*	
O2-Fe-O3	65	O2-Fe-O3	65	O2-Fe-O3	64
O2-Fe-OH1 (Y95)	97	O2-Fe-OH1 (Y95)	-	O2-Fe-OD1 (D63)	86
O2-Fe-OH1 (Y188)	104	O2-Fe-OH1 (Y188)	95	O2-Fe-OH1 (Y95)	93
O2-Fe-O (G260)	85	O2-Fe-O4 (NTA)	80	O2-Fe-OH1 (Y188)	96
O2-Fe-N (G260)	156	O2-Fe-O8 (NTA)	87	O2-Fe-NE2 (H249)	167
O3-Fe-OH1 (Y95)	160	O2-Fe-O12 (NTA)	140	O3-Fe-OD1 (D63)	87
O3-Fe-OH1 (Y188)	93	O2-Fe-N (NTA)	148	O3-Fe-OH1 (Y95)	156
O3-Fe-O (G260)	84	O3-Fe-OH1 (Y95)	-	O3-Fe-OH1 (Y188)	90
O3-Fe-N (G260)	96	O3-Fe-OH1 (Y188)	102	O3-Fe-OH1 (H249)	105
O (G260)-Fe-N (G260)	79	O3-Fe-O4 (NTA)	145	OD1 (D63)-Fe-OH1 (Y95)	87
O (G260)-Fe-OH1 (Y95)	88	O3-Fe-O8 (NTA)	83	OD1 (D63)-Fe-OH1 (Y188)	176
O (G260)-Fe-OH1 (Y188)	169	O3-Fe-O12 (NTA)	75	OD1 (D63)-Fe-NE2 (H249)	87
N (G260)-Fe-OH1 (Y95)	100	O3-Fe-N (NTA)	129	OH1 (Y95)-Fe-OH1 (Y188)	97
N (G260)-Fe-OH1 (Y188)	90	O4 (NTA)-Fe-OH1 (Y95)	-	OH1 (Y95)-Fe-NE2(H249)	98
OH1 (Y95)-Fe-OH1 (Y188)	98	O4 (NTA)-Fe-OH1 (Y188)	82	OH1 (Y188)-Fe-NE2 (H249)	91
		O4 (NTA)-Fe-O8 (NTA)	95		
		O4 (NTA)-Fe-O12 (NTA)	140		
		O4 (NTA)-Fe-N (NTA)	81		
		O8 (NTA)-Fe-OH1 (Y188)	176		
		O8 (NTA)-Fe-O12 (NTA)	86		
		O8 (NTA)-Fe-N (NTA)	69		
		O12 (NTA)-Fe- OH1 (Y188)	94		
		O12 (NTA)-Fe-N (NTA)	62		
		N (NTA)-Fe- OH1 (Y188)	108		
		OH1 (Y95)-Fe-OH1 (Y188)			