

Table 4. Selected active site and metal ligand distances

		Distance, Å		
		Subunit A	Subunit B	Average*
Fe ^{III}	Mn ^{II}	3.24	3.29	3.26
Fe ^{III}	Asp 163 Oδ2	2.24	2.23	2.23
	Asp 134 Oδ2	2.36	2.34	2.35
	Tyr 166 O ⁻	1.85	1.90	1.88
	His 324 Nε2	2.69	2.69	2.69
	PO ₄ O3	2.18	2.81	–
	PO ₄ O1	2.59	1.85	–
	Mn ^{II}	Asp 163 Oδ2	2.21	2.32
Asn 200 Oδ1		2.11	2.07	2.09
His 285 Nε2		2.16	2.10	2.13
His 322 Nδ1		2.15	2.05	2.10
PO ₄ O2		2.69	2.03	–
PO ₄ O3		2.51	3.22	–
PO ₄ (O1)		His 201 Nε2	2.81	2.98
	Glu 365 Oε2	2.83	3.53	–
PO ₄ (O ₂)	Asn 200 Nδ2	2.67	2.71	2.69
PO ₄ (O ₃)	His 322 O	2.56	2.37	2.47
	His 295 Nε2	3.96	3.19	–
PO ₄ (O ₄)	Glu 365 Oε2	3.31	2.97	3.17
	His 295 Nε2	2.77	3.74	–

*No average was calculated if the difference in distances was >0.5 Å.