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Supporting information for article:

Coarse snapshots of oxygen-dissociation intermediates of a giant hemoglobin elucidated by determining the oxygen saturation in individual subunits in the crystalline state

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Table S1 Refined *B*-factors and occupancies of the atoms of oxygen-surrounding residues.

Cryst 1 (69% oxy)				Cryst 2 (58% oxy)			
A1				A1			
Residue	atom	<i>B</i> -factor	Occ.	Residue	atom	<i>B</i> -factor	Occ.
Heme	FE	51.23	1	Heme	FE	63.33	1
	NA	49.24		NA	67.63		
	NB	48.40		NB	67.26		
	NC	52.48		NC	67.97		
	ND	53.55		ND	66.10		
His94 (F8)	NE2	52.06		His94 (F8)	NE2	66.16	
His62 (E7)	NE2	48.31		His62 (E7)	NE2	65.15	
Phe46 (CD1)	CE1	50.66		Phe46 (CD1)	CE1	63.85	
Val66 (E11)	CG2	47.49		Val66 (E11)	CG2	59.86	
Phe32 (B10)	CZ	47.49		Phe32 (B10)	CZ	65.88	
	<i>Average</i>	50.09			<i>Average</i>	65.32	
	<i>S.D.</i>	2.20			<i>S.D.</i>	2.44	
O ₂	O1	50.95	0.75	O ₂	O1	66.48	0.40
	O2	48.38		O ₂	O2	66.01	
A2				A2			
Residue	atom	<i>B</i> -factor	Occ.	Residue	atom	<i>B</i> -factor	Occ.
Heme	FE	43.04	1	Heme	FE	53.25	1
	NA	46.78		NA	53.76		
	NB	43.69		NB	52.23		
	NC	47.01		NC	55.71		
	ND	43.61		ND	55.49		
His94 (F8)	NE2	48.11		His94 (F8)	NE2	61.13	
His62 (E7)	NE2	45.09		His62 (E7)	NE2	57.46	
Phe46 (CD1)	CE1	46.50		Phe46 (CD1)	CE1	56.91	
Val66 (E11)	CG2	41.54		Val66 (E11)	CG2	53.91	
Trp32 (B10)	CH2	48.11		Trp32 (B10)	CH2	57.47	
	<i>Average</i>	45.35			<i>Average</i>	55.72	
	<i>S.D.</i>	2.29			<i>S.D.</i>	2.64	
O ₂	O1	46.13	0.65	O ₂	O1	56.18	0.60
	O2	44.28		O ₂	O2	56.16	
B1				B1			
Residue	atom	<i>B</i> -factor	Occ.	Residue	atom	<i>B</i> -factor	Occ.
Heme	FE	47.20	1	Heme	FE	67.66	1
	NA	47.23		NA	66.28		
	NB	46.40		NB	63.17		
	NC	49.14		NC	68.13		
	ND	45.62		ND	67.12		
His96(F8)	NE2	52.37		His96(F8)	NE2	66.66	
Gln64 (E7)	NE2	55.19		Gln64 (E7)	NE2	66.41	
Phe51 (CD1)	CE2	53.97		Phe51 (CD1)	CE2	64.17	
Val68 (E11)	CG2	48.70		Val68 (E11)	CG2	61.46	
Phe36 (B10)	CZ	51.44		Phe36 (B10)	CZ	66.57	

	<i>Average</i>	49.73			<i>Average</i>	65.76	
	<i>S.D.</i>	3.33			<i>S.D.</i>	2.13	
O ₂	O1	49.62	0.60	O ₂	O1	65.45	0.32
	O2	49.74			O2	66.78	
B2				B2			
Residue	atom	<i>B-factor</i>	Occ.	Residue	atom	<i>B-factor</i>	Occ.
Heme	FE	48.85	1	Heme	FE	67.41	1
	NA	50.72			NA	71.23	
	NB	51.71			NB	72.04	
	NC	50.63			NC	72.60	
	ND	53.00			ND	74.11	
His98 (F8)	NE2	45.55		His98 (F8)	NE2	66.70	
His66 (E7)	NE2	52.02		His66 (E7)	NE2	64.49	
Phe50 (CD1)	CE2	51.47		Phe50 (CD1)	CE2	69.37	
Val70 (E11)	CG2	49.04		Val70 (E11)	CG2	66.30	
Phe36 (B10)	CZ	50.90		Phe36 (B10)	CZ	61.95	
	<i>Average</i>	50.39			<i>Average</i>	68.62	
	<i>S.D.</i>	2.12			<i>S.D.</i>	3.90	
O ₂	O1	49.30	0.70	O ₂	O1	71.55	0.70
	O2	48.94			O2	71.84	

Cryst 3 (21% oxy)

A1			
Residue	atom	<i>B-factor</i>	Occ.
Heme	FE	36.14	1
	NA	38.85	
	NB	39.91	
	NC	40.96	
	ND	40.60	
His94 (F8)	NE2	42.98	
His62 (E7)	NE2	32.97	
Phe46 (CD1)	CE1	36.43	
Val66 (E11)	CG2	29.32	
Phe32 (B10)	CZ	37.06	
	<i>Average</i>	37.52	
	<i>S.D.</i>	4.08	
O ₂	O1	38.11	0.25
	O2	40.01	

Cryst 4 (13% oxy)

A1			
Residue	atom	<i>B-factor</i>	Occ.
Heme	FE	35.49	1
	NA	36.97	
	NB	38.46	
	NC	38.62	
	ND	38.55	
His94 (F8)	NE2	37.43	
His62 (E7)	NE2	38.44	
Phe46 (CD1)	CE1	40.18	
Val66 (E11)	CG2	27.36	
Phe32 (B10)	CZ	34.88	
	<i>Average</i>	36.64	
	<i>S.D.</i>	3.62	
O ₂	O1	35.74	0.04
	O2	35.41	

A2			
Residue	atom	<i>B-factor</i>	Occ.
Heme	FE	38.10	1
	NA	34.86	
	NB	35.38	
	NC	39.13	
	ND	35.70	
His94 (F8)	NE2	39.17	
His62 (E7)	NE2	38.36	

A2			
Residue	atom	<i>B-factor</i>	Occ.
Heme	FE	32.69	1
	NA	33.57	
	NB	32.37	
	NC	34.24	
	ND	35.46	
His94 (F8)	NE2	34.54	
His62 (E7)	NE2	28.69	

Phe46 (CD1)	CE1	39.52		Phe46 (CD1)	CE1	28.23	
Val66 (E11)	CG2	31.97		Val66 (E11)	CG2	28.70	
Trp32 (B10)	CH2	37.03		Trp32 (B10)	CH2	31.71	
	<i>Average</i>	36.92			<i>Average</i>	32.02	
	<i>S.D.</i>	2.42			<i>S.D.</i>	2.64	
O ₂	O1	37.02	0.05	O ₂	O1	31.74	0.06
	O2	37.25			O2	31.21	
B1				B1			
Residue	atom	<i>B-factor</i>	Occ.	Residue	atom	<i>B-factor</i>	Occ.
Heme	FE	38.88	1	Heme	FE	36.72	1
	NA	40.92			NA	38.48	
	NB	39.03			NB	34.65	
	NC	40.51			NC	38.28	
	ND	44.89			ND	36.60	
His96(F8)	NE2	40.36		His96(F8)	NE2	39.45	
Gln64 (E7)	NE2	45.34		Gln64 (E7)	NE2	40.71	
Phe51 (CD1)	CE2	45.22		Phe51 (CD1)	CE2	45.01	
Val68 (E11)	CG2	36.58		Val68 (E11)	CG2	38.56	
Phe36 (B10)	CZ	40.18		Phe36 (B10)	CZ	39.46	
	<i>Average</i>	41.19			<i>Average</i>	38.79	
	<i>S.D.</i>	2.99			<i>S.D.</i>	2.79	
O ₂	O1	41.94	0.15	O ₂	O1	38.42	0.05
	O2	42.75			O2	38.40	
B2				B2			
Residue	atom	<i>B-factor</i>	Occ.	Residue	atom	<i>B-factor</i>	Occ.
Heme	FE	47.30	1	Heme	FE	38.17	1
	NA	50.65			NA	42.05	
	NB	53.39			NB	43.15	
	NC	40.34			NC	41.89	
	ND	53.63			ND	41.18	
His98 (F8)	NE2	40.34		His98 (F8)	NE2	34.94	
His66 (E7)	NE2	44.06		His66 (E7)	NE2	34.71	
Phe50 (CD1)	CE2	54.18		Phe50 (CD1)	CE2	41.95	
Val70 (E11)	CG2	37.87		Val70 (E11)	CG2	34.53	
Phe36 (B10)	CZ	36.71		Phe36 (B10)	CZ	32.42	
	<i>Average</i>	47.06			<i>Average</i>	38.50	
	<i>S.D.</i>	6.85			<i>S.D.</i>	4.01	
O ₂	O1	50.92	0.30	O ₂	O1	39.43	0.15
	O2	51.49			O2	39.29	

Occ.; Occupancy

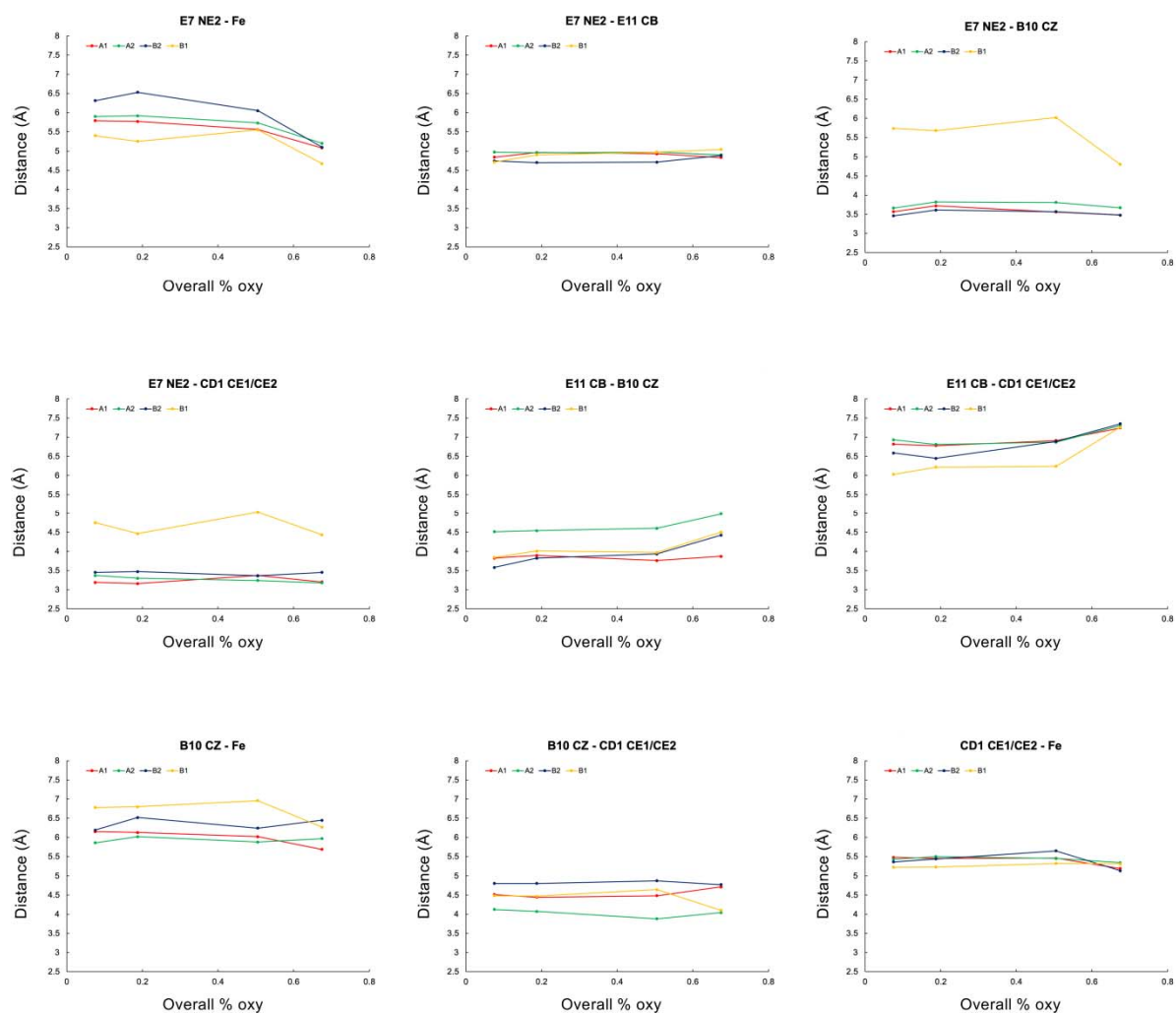


Figure S1 Changes of the distance between the atoms of oxygen-surrounding residues for each subunit (A1, A2, B1, and B2 are drawn as red, green, blue, and yellow line, respectively). The combination of atoms whose distance was measured is shown in the upper part of each graph.