SUPPLEMENTAL DIGITAL CONTENT 1

Table 1. Crystallographic Data and Refinement Statistics for Each Protein-Gas Complex

Prot.	Gas pressure (bar)	Reso. (Å)	Cell a (Å)	Cell b (Å)	Cell c (Å)	Cell beta (°)	Complet. (%)	Redund.	Unique reflections	Rsym* (%)	I/σ(I)	Rwork[§] (%)	Rfree[#] (%)	mean B factor (Å^2)	r.m.s. / Length (Å)	ideality Angle (°)
UOX	0	1.77	79.82	96.16	105.44		99.3 (95.6)	5.0 (4.5)	39,546 (1,838)	4.9 (32.5)	33.1 (4.4)	15.84	18.92	22.79	0.010	1.433
	Xe 10	1.70	80.12	96.18	105.46		97.1 (84.4)	4.9 (3.7)	43,762 (3,740)	4.5 (29.6)	31.8 (3.5)	16.47	19.01	21.46	0.010	1.396
	Xe 20	1.60	80.32	96.32	105.58		99.2 (97.5)	4.6 (3.9)	53,446 (7,550)	4.6 (27.6)	19.8 (5.6)	17.60	18.80	22.71	0.009	1.364
	Xe 30	1.85	80.41	96.31	105.59		99.9 (99.9)	4.8 (4.8)	35,288 (5,112)	5.7 (27.7)	15.3 (5.1)	15.57	18.53	26.40	0.012	1.474
	N2O 10	1.75	80.12	96.21	105.46		99.1 (91.7)	4.9 (4.5)	41,022 (3,756)	4.4 (20,0)	34.0 (5.5)	16.01	19.24	21.53	0.010	1.409
	N2O 20	1.75	80.24	86.26	105.54		97.8 (97.1)	4.8 (4.2)	40,615 (3,982)	4.6 (22.2)	35.4 (5.3)	16.29	18.20	23.69	0.011	1.493
	N2O 30	1.65	80.22	96.28	105.57		99.9 (99.6)	4.8 (4.8)	49,352 (,7101)	4.9 (33.2)	15.9 (4.2)	16.39	18.36	25.75	0.010	1.417
LYSO	0	1.55	79.25	79.25	38.17		99.7 (100)	6.8 (7.0)	18,166 (2,603)	6.7 (31.6)	16.6 (6.2)	17.65	18.79	19.22	0.008	1.248
	Xe 10	1.55	79.18	79.18	37.97		96.1 (97.7)	9.7 (8.8)	17,312 (2,520)	4.5 (29.5)	27.7 (7.2)	17.06	19.16	21.50	0.008	1.263
	Xe 20	1.55	79.16	79.16	37.97		96.2 (97.7)	9.8 (9.6)	17,307 (2,525)	4.7 (25.5)	28.5 (9.0)	17.19	19.60	19.74	0.008	1.253
	Xe 30	1.65	79.31	79.31	38.07		99.6 (100)	6.8 (7.0)	15,059 (2,155)	6.4 (32.1)	17.7 (7.3)	17.35	20.82	19.91	0.009	1.310
	N2O 10	1.48	79.18	79.18	37.94		99.6 (98.9)	7.7 (6.6)	20,645 (2,006)	4.1 (35.2)	45.6 (5.1)	17.31	19.76	21.58	0.008	1.263
	N2O 20	1.50	79.18	79.18	37.94		99.7 (100)	7.7 (7.1)	19,887 (1,953)	3.9 (32.9)	47.2 (2.5)	17.23	19.30	21.10	0.008	1.271
	N2O 30	1.58	79.19	79.19	37.94		99.7 (100)	7.3 (5.8)	17,064 (1,656)	4.8 (34.3)	41.3 (4.6)	16.95	19.99	22.88	0.009	1.325
MB	0	1.40	35.03	30.61	63.40	104.45	94.2 (92.0)	4.2 (4.3)	24,493 (3,453)	5.0 (27.6)	13.8 (4.4)	19.30	22.70	20.79	0.009	3.013
	Xe 10	1.45	35.25	30.72	63.50	104.50	93.2 (86.4)	3.8 (2.5)	22,115 (1,020)	5.6 (20.5)	38.3 (5.3)	20.51	23.18	21.25	0.010	3.074
	Xe 20	1.55	35.29	30.64	63.57	104.45	91.4 (82.1)	3.8 (2.6)	17,741 (779)	5.8 (17.3)	5.9 (37.4)	20.00	23.69	24.34	0.011	3.137
	Xe 30	1.60	35.33	30.66	63.57	104.44	94.9 (86.2)	3.7 (2.4)	16,770 (742)	6.0 (20.4)	5.1 (33.5)	19.06	24.18	23.78	0.011	3.170
	N2O 10	1.40	35.26	30.67	63.57	104.59	94.2 (92.3)	4.2 (4.2)	24,287 (3,528)	5.6 (29.6)	13.1 (3.9)	19.45	21.63	22.54	0.010	3.033
	N2O 20	1.45	35.36	30.62	63.57	104.59	94.8 (93.0)	4.2 (4.2)	22,577 (3,216)	4.9 (27.3)	14.6 (4.2)	19.22	20.95	24.10	0.010	3.061
	N2O 30	1.55	35.45	30.55	63.63	104.57	95.3 (93.9)	4.1 (4.2)	18,602 (2,643)	4.3 (25.8)	16.8 (4.5)	18.79	22.36	26.40	0.011	3.058
NGB	0	1.70	89.01	89.01	115.33		98.7 (98.9)	7.4 (7.3)	19,208 (2,788)	6.0 (32.0)	18.4 (5.9)	17.12	19.58	26.19	0.011	3.002
	Xe 10	1.70	89.03	89.03	115.10		99.7 (97.1)	7.2 (5.3)	19,471 (1,856)	4.4 (31.5)	42.9 (3.6)	17.31	20.29	28.87	0.011	3.015
	Xe 20	2.00	89.10	89.10	115.06		99.5 (99.9)	3.8 (3.6)	22,926 (1,146)	6.3 (27.1)	40.6 (10.2)	16.37	22.28	28.98	0.015	3.136
	Xe 30	1.90	89.10	89.10	114.82		98.1 (98.0)	6.9 (4.0)	13,763 (673)	6.6 (38.9)	35.3 (4.0)	17.01	21.26	30.53	0.014	3.105
	N2O 10	1.75	89.05	89.05	114.93		99.9 (100)	7.3 (7.3)	17,892 (2,596)	4.4 (34.1)	24.6 (5.9)	16.89	18.81	30.32	0.012	3.122
	N2O 20	1.70	89.17	89.17	114.86		99.8 (99.8)	7.3 (7.6)	19,538 (2,816)	4.0 (27.7)	26.9 (7.0)	17.22	19.61	27.93	0.012	3.162
	N2O 30	1.70	89.28	89.28	114.76		99.9 (99.9)	7.3 (7.3)	19,567 (2,835)	4.1 (29.8)	26.1 (6.4)	17.17	18.74	28.59	0.011	3.074

Each crystallographic data collection is named by its gas pressure given in bars. Data between parentheses correspond to the highest resolution shell.
*Rsym = $\sum_{h,k,l}\sum_i |I_i(h,k,l) - \langle I_i(h,k,l)\rangle| / \sum_{h,k,l}\sum_i I_i(h,k,l)$, where $I_i(h,k,l)$ is the intensity of observed reflections and $\langle I_i(h,k,l)\rangle$ the weighted mean of all observations after rejection of outliers.
[§]Rwork = $\sum|Fo|-|Fc| / \sum|Fo|$; indicates accuracy of the model. [#]Rfree is a cross validation residual using 5% of the native data which were randomly chosen and excluded from the refinement.