

S1 Table The xenon sites in OprN - α domain (at 20 bar)

Site Label / subunit	Refined occupancy (%) / height in initial anomalous map (σ)	Location	Distances (\AA)...residue	
Xe 503 / A	100 / 31.0	site M1 on axis (iris)	3.94 ...CD1 Leu 405 A 3.96 ...CD2 Leu 405 B 3.88 ...CD1 Leu 405 C 3.63 ...OD1 Asp 409 A 3.81 ...OD1 Asp 409 B	3.66 ...OD1 Asp 409 C 3.78 ...NH1 Arg 412 A 4.07 ...NH1 Arg 412 B 4.09 ...NH1 Arg 412 C
Xe 504 / A	30 / 7.0	Site S1 intra-subunit A	3.84 ...CA Ala 201 A 3.92 ...CB Gln 177 A 4.11 ...CG Arg 204 A 4.76 ...CD1 Leu 408 A	3.79 ...O Ala 201 A 3.85 ...O Gln 177 A 4.50 ...N Arg 181 A 4.23 ...CZ Phe 404 A
Xe 506 / B	30 / 6.3	Site S1 intra-subunit B	3.78 ...CB Ala 201 B 3.78 ...CB Gln 177 B 3.99 ...CG Arg 204 B 3.90 ...CB Ser 180 B 3.18 ...OE1 Glu 411 B	3.58 ...O Ala 201 B 4.05 ...CG Gln 177 B 4.46 ...N Arg 181 B 4.47 ...CZ Phe 404 B 4.57 ...OE2 Glu 411 B
Xe 505 / C	30 / 4.9	Site S1 intra-subunit C	3.79 ...CB Ala 201 C 3.74 ...CB Gln 177 C 4.16 ...CG Arg 204 C 4.23 ...CB Ser 180 C 3.31 ...OE1 Glu 411 C 3.47 ...O Gln 177 C	3.64 ...O Ala 201 C 3.95 ...CG Gln 177 C 4.49 ...N Arg 181 C 4.19 ...CZ Phe 404 C 4.45 ...CD Glu 411 C
Xe 505 / A	45 / 12.5	Site S2 inter-subunit A/C	3.66 ...CA Gln 214 A 4.06 ...C Pro 213 A 3.82 ...CB Lys 371 C 4.10 ...CD Arg 375 C 4.19 ...CB Ala 217 A	3.49 ...OE1 Gln 214 A 3.92 ...O Pro 213 A 3.67 ...CG Arg 372 C 4.37 ...CB Arg 375 C 3.32 ...O HOH 683 C
Xe 508 / A	35 / 9.5	Site S2 inter-subunit A/B	3.59 ...CA Gln 214 B 4.22 ...C Pro 213 B 4.22 ...CB Lys 371 A 3.99 ...CD Arg 375 A 4.25 ...CB Ala 217 B	3.49 ...OE1 Gln 214 A 3.92 ...O Pro 213 A 3.67 ...CG Arg 372 C 4.45 ...CB Arg 375 A 3.38 ...O HOH 654 A
Xe 509 / B	40 / 9.0	Site S2 inter-subunit B/C	3.65 ...CA Gln 214 C 4.03 ...CB Gln 214 C 4.25 ...C Pro 213 C 4.10 ...CB Lys 371 B 4.00 ...CD Arg 375 B 4.29 ...CB Ala 217 C 4.01 ...C Lys 371 B	4.00 ...CG Gln 214 C 4.30 ...OE1 Gln 214 C 4.13 ...O Pro 213 C 3.69 ...CG Arg 372 B 4.35 ...CB Arg 375 B 3.38 ...O HOH 689 B 3.72 ...N Arg 372 B
Xe 507 / B	25 / 7.5	Site S3 intra-subunit B	3.17 ...CG Leu 149 B 3.82 ...CD2 Leu 51 B 4.31 ...CD2 Leu 57 B 2.95 ...CD1 Leu 149 B 4.37 ...N Ile 150 B	4.10 ...CB Ser 50 B 3.41 ...OG Ser 50 B 4.08 ...O Ser 50 B 4.73 ...CG1 Ile 150 B 2.94 ...CB Leu 149 B
Xe 506 / C	23 / 7.6	Site S3 intra-subunit C	3.67 ...CG Leu 149 C 4.12 ...CD2 Leu 51 C 4.12 ...CD1 Leu 57 C 3.78 ...CD1 Leu 149 C 4.30 ...N Ile 150 C 4.23 ...O Ser 50 C 4.53 ...CG Asn 54 C	4.08 ...CB Ser 50 C 3.23 ...OG Ser 50 C 4.20 ...CG Leu 57 C 4.73 ...CG1 Ile 150 C 3.09 ...CB Leu 149 C 4.24 ...CB Asn 54 C 4.33 ...C Ser 50 C