

S2 Table The xenon sites in OprN - β barrel domain

| Site Label / subunit | Refined occupancy (%) / height in initial anomalous map (σ) | Location | Distances (\AA)...residue | |
|----------------------|--|------------------------------------|---|---|
| Xe 506 / A | 35 / 5.7 | β -domain, inter-subunit A/C | 4.30 ...CB Ser 84 A 4.15 ...CA Arg 85 A 4.61 ...CB Ala 86 A 4.27 ...CG1 Ile 323 C | 4.56 ...CB Trp 325 C 4.07 ...O Ile 323 C 3.61 ...OG Ser 84 A |
| Xe 507 / A | 20 / 4.9 | β -domain, intra-subunit A | 4.09 ...CB Leu 299 A 4.07 ...CB Ser 114 A 5.09 ...CG1 Val 82 A | 4.75 ...N Leu 299 A 4.60 ...OG Ser 114 A |
| Xe 501 / B | 45 / 9.8 | β -domain, intra-subunit B | 4.32 ...CG1 Ile 309 B 4.62 ...CD2 Tyr 108 B 4.10 ...CB Leu 110 B 4.03 ...CB Ala 86 B 4.59 ...Xe 502 B | 4.51 ...CG2 Ile 309 B 4.70 ...CB Tyr 108 B 4.69 ...CD1 Leu 110 B 4.34 ...CA Ala 86 B |
| Xe 502 / B | 35 / 8.1 | β -domain, inter-subunit A/B | 4.39 ...CD1 Ile 323 A 4.48 ...C Pro 321 A 4.65 ...CG Pro 321 A 4.19 ...CA Ser 87 B | 4.35 ...CG1 Ile 323 A 4.47 ...CB Pro 321 A 4.33 ...CB Ala 86 B 4.59 ...Xe 501 B |
| Xe 503 / B | 35 / 5.3 | β -domain, inter-subunit A/B | 4.56 ...CB Ala 86 B 4.42 ...C Arg 85 B 4.31 ...N Arg 85 B 4.45 ...CB Ser 84B | 4.50 ...CG2 Ile 323 A 4.52 ...CA Arg 85 B 4.51 ...C Ser 84 B 4.49 ...CB Trp 325 A |
| Xe 501 / C | 22 / 6.4 | β -domain, intra-subunit C | 4.29 ...CG1 Val 293 C 4.48 ...CD1 Leu 295 C 3.99 ...CB Plm 501 A * | 4.49 ...CD2 Leu 118 C 4.38 ...CB Pro 321 C |
| Xe 507 / C | 25 / 5.5 | tunnel ^a | 3.75 ...CG Arg 225 C 4.47 ...CD Gln 159 C 4.18 ...CA Ala 222 C | 4.26 ...CB Arg 225 C 4.42 ...CB Ala 222 C 3.15 ...O HOH 761 C |
| Xe 508/ C | 20 / 3.7 | β -domain, inter-subunit B/C | 4.41 ...CB Trp 325 B 4.53 ...CG2 Ile 323 B 4.52 ...C Arg 85 C 4.41 ...CB Ser 84 C | 4.68 ...CC PLM 504 B 4.60 ...CB Ala 86 C 4.60 ...CA Arg 85 C 3.62 ...OG Ser 84 C |

^a This xenon is located on the inner bank of the tunnel, at the level of the buoy domain.