

| Plane group | Phase. Residual (degree) ^a | Number. of comparison | Target residual (degree) ^b |
|---------------------------------|--|--------------------------|--|
| p1 | 24.8 ^c | 178 | |
| p2 | 41.0! | 89 | 36.2 |
| p12_b | 79.5 | 64 | 25.9 |
| p12_a | 31.6` | 67 | 26.3 |
| p12 ₁ _b | 19.0* | 64 | 25.9 |
| p12 ₁ _a | 77.2 | 67 | 26.3 |
| c12_b | 79.5 | 64 | 25.9 |
| c12_a | 31.6` | 67 | 26.3 |
| p222 | 65.2 | 220 | 29.4 |
| p222 ₁ b | 64.9 | 220 | 29.4 |
| p222 ₁ a | 32.1! | 220 | 29.4 |
| p22 ₁ 2 ₁ | 62.5 | 220 | 29.4 |
| c222 | 65.2 | 220 | 29.4 |
| p4 | 72.3 | 185 | 30.3 |
| p422 | 68.1 | 402 | 27.3 |
| p42 ₁ 2 | 65.6 | 402 | 27.3 |
| p3 | 65.7 | 84 | 24.8 |
| p3 ₁ 2 | 69.9 | 213 | 25.3 |
| p32 ₁ | 68.7 | 224 | 25.8 |
| p6 | 71.2 | 257 | 28.8 |
| p622 | 72.7 | 526 | 26.7 |

Table S2