

## Supplementary Information

**Table 1.** Complete scaling statistics for data sets A-Air to I-Air for the scaling models SCALEPACK-kB, SCALEPACK-ano, SCALA-Batch, SCALA-Det, SCALA-Abs, SCALA-Sec, SCALA-Baniso and SCALA-Ref. The numbers in the first row of each cell refer to the full 360° of data, whereas the numbers in italics in the second row refer to the first 180° of data in each case. The values in parenthesis refer to the respective outermost resolution shells.

<b>A-Air (<math>\lambda=0.80</math> Å)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>
Resolution limit [Å]	99 – 1.65 (1.68 – 1.65)	99 – 1.65 (1.68 – 1.65)	99 – 1.65 (1.69 – 1.65)	99 – 1.65 (1.69 – 1.65)	99 – 1.65 (1.69 – 1.65)	99 – 1.65 (1.69 – 1.65)	99 – 1.65 (1.69 – 1.65)
Total no. of observations	665506 <i>332262</i>	665506 <i>332262</i>	657193 <i>328105</i>	657193 <i>328105</i>	657193 <i>328105</i>	657193 <i>328105</i>	657193 <i>328105</i>
Total no. of reflections	386757 <i>192825</i>	386814 <i>192839</i>	362216 <i>180282</i>	362212 <i>180280</i>	362191 <i>180276</i>	362190 <i>180276</i>	362220 <i>180285</i>
Unique reflections	26987 <i>26973</i>	26987 <i>26973</i>	27039 <i>27020</i>	27039 <i>27020</i>	27039 <i>27020</i>	27039 <i>27020</i>	27039 <i>27020</i>
Rejected reflections	110 <i>60</i>	115 <i>37</i>	1 <i>0</i>	2 <i>1</i>	1 <i>1</i>	0 <i>1</i>	0 <i>0</i>
Redundancy	14.33 <i>7.15</i>	14.33 <i>7.15</i>	13.40 <i>6.67</i>	13.40 <i>6.67</i>	13.40 <i>6.67</i>	13.40 <i>6.67</i>	13.40 <i>6.67</i>
Completeness [%]	99.90 (100) <i>99.90 (100)</i>	99.90 (100) <i>99.80 (100)</i>	100 (100) <i>99.90 (99.90)</i>	100 (100) <i>99.90 (99.90)</i>	100 (100) <i>99.90 (99.90)</i>	100 (100) <i>99.90 (99.90)</i>	100 (100) <i>99.90 (99.90)</i>
I/ $\sigma$ (I)	46.53 (30.25) <i>33.24 (20.78)</i>	35.40 (22.21) <i>22.91 (14.33)</i>	45.10 (23.00) <i>32.10 (16.20)</i>	47.40 (24.80) <i>33.70 (17.50)</i>	47.20 (24.30) <i>33.70 (17.20)</i>	47.20 (24.30) <i>33.70 (17.20)</i>	45.90 (23.50) <i>32.60 (16.60)</i>
R <sub>merge</sub> (%)	5.30 (8.90) <i>5.00 (8.50)</i>	5.30 (8.90) <i>5.00 (8.60)</i>	5.20 (8.80) <i>4.90 (8.40)</i>	5.00 (8.40) <i>4.70 (7.90)</i>	5.00 (8.50) <i>4.70 (8.10)</i>	5.00 (8.50) <i>4.70 (8.10)</i>	5.10 (8.60) <i>4.80 (8.20)</i>
R <sub>r.i.m.</sub> (%)	5.50 (9.30) <i>5.40 (9.30)</i>	5.50 (9.30) <i>5.40 (9.40)</i>	5.40 (9.30) <i>5.30 (9.30)</i>	5.20 (8.80) <i>5.10 (8.70)</i>	5.20 (8.90) <i>5.10 (8.90)</i>	5.20 (8.90) <i>5.10 (8.90)</i>	5.30 (9.00) <i>5.20 (9.00)</i>
R <sub>p.i.m.</sub> (%)	1.50 (2.60) <i>2.00 (3.70)</i>	1.50 (2.60) <i>2.00 (3.70)</i>	1.50 (2.70) <i>2.00 (3.80)</i>	1.40 (2.50) <i>2.00 (3.50)</i>	1.40 (2.60) <i>2.00 (3.60)</i>	1.40 (2.60) <i>2.00 (3.60)</i>	1.50 (2.60) <i>2.00 (3.60)</i>
R <sub>anom</sub> (%)	1.60 (2.50) <i>2.20 (4.40)</i>	1.60 (2.50) <i>2.20 (4.10)</i>	1.60 (2.50) <i>2.20 (3.90)</i>	1.60 (2.50) <i>2.20 (3.80)</i>	1.60 (2.50) <i>2.20 (3.90)</i>	1.60 (2.50) <i>2.20 (3.90)</i>	1.60 (2.50) <i>2.20 (3.80)</i>

<b>B-Air (<math>\lambda=1.50 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)
Total no. of observations	479164 <i>239451</i>	479164 <i>239451</i>	472948 <i>236406</i>	472948 <i>236406</i>	472948 <i>236406</i>	472948 <i>236406</i>	472948 <i>236406</i>	472948 <i>236406</i>
Total no. of reflections	278361 <i>138915</i>	278145 <i>138842</i>	255398 <i>127445</i>	255293 <i>127410</i>	255316 <i>127407</i>	255317 <i>127406</i>	255348 <i>127432</i>	255305 <i>127404</i>
Unique reflections	20156 <i>20119</i>	20156 <i>20119</i>	20198 <i>20156</i>	20198 <i>20156</i>	20198 <i>20156</i>	20198 <i>20156</i>	20198 <i>20156</i>	20198 <i>20156</i>
Rejected reflections	405 <i>76</i>	1069 <i>272</i>	22 <i>2</i>	17 <i>7</i>	11 <i>3</i>	11 <i>2</i>	2 <i>1</i>	6 <i>2</i>
Redundancy	13.81 <i>6.90</i>	13.80 <i>6.90</i>	12.64 <i>6.32</i>	12.64 <i>6.32</i>	12.64 <i>6.32</i>	12.64 <i>6.32</i>	12.64 <i>6.32</i>	12.64 <i>6.32</i>
Completeness [%]	99.80 (100) <i>99.60 (100)</i>	99.80 (100) <i>99.50 (100)</i>	99.70 (99.70) <i>99.70 (99.70)</i>	99.70 (99.70) <i>99.70 (99.70)</i>	99.70 (99.70) <i>99.70 (99.70)</i>	99.70 (99.70) <i>99.70 (99.70)</i>	99.70 (99.70) <i>99.70 (99.70)</i>	99.70 (99.70) <i>99.60 (99.60)</i>
$I/\sigma(I)$	39.26 (33.93) <i>27.81 (23.41)</i>	37.42 (28.98) <i>23.85 (18.30)</i>	47.60 (29.80) <i>32.20 (20.20)</i>	54.00 (34.70) <i>38.80 (24.90)</i>	53.60 (33.60) <i>38.80 (24.50)</i>	53.60 (33.60) <i>33.80 (24.50)</i>	51.50 (32.40) <i>35.10 (22.10)</i>	53.60 (33.50) <i>39.00 (24.10)</i>
$R_{\text{merge}}$ (%)	5.80 (8.40) <i>5.70 (8.20)</i>	5.80 (8.30) <i>5.60 (8.10)</i>	5.60 (8.20) <i>5.40 (8.00)</i>	5.00 (7.30) <i>4.80 (6.80)</i>	5.10 (7.50) <i>4.80 (6.90)</i>	5.10 (7.50) <i>4.80 (6.90)</i>	5.30 (7.60) <i>5.00 (7.20)</i>	5.10 (7.40) <i>4.80 (6.90)</i>
$R_{\text{r.i.m.}}$ (%)	6.00 (8.70) <i>6.10 (8.90)</i>	6.00 (8.70) <i>6.10 (8.80)</i>	5.80 (8.60) <i>5.90 (8.70)</i>	5.30 (7.60) <i>5.20 (7.40)</i>	5.30 (7.80) <i>5.20 (7.50)</i>	5.30 (7.80) <i>5.20 (7.50)</i>	5.50 (7.90) <i>5.50 (7.90)</i>	5.40 (7.80) <i>5.20 (7.50)</i>
$R_{\text{p.i.m.}}$ (%)	1.60 (2.30) <i>2.30 (3.40)</i>	1.60 (2.30) <i>2.30 (3.40)</i>	1.60 (2.40) <i>2.30 (3.40)</i>	1.50 (2.10) <i>2.00 (2.90)</i>	1.50 (2.20) <i>2.00 (3.00)</i>	1.50 (2.20) <i>2.00 (3.00)</i>	1.50 (2.20) <i>2.20 (3.10)</i>	1.50 (2.20) <i>2.10 (3.00)</i>
$R_{\text{anom}}$ (%)	2.70 (4.00) <i>3.20 (4.80)</i>	2.70 (4.00) <i>3.20 (4.80)</i>	2.70 (3.90) <i>3.20 (4.60)</i>	2.70 (3.90) <i>3.10 (4.40)</i>	2.70 (3.90) <i>3.10 (4.50)</i>	2.70 (3.90) <i>3.10 (4.50)</i>	2.70 (3.90) <i>3.10 (4.50)</i>	2.70 (3.90) <i>3.10 (4.50)</i>

<b>C-Air (<math>\lambda=1.70</math> Å)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [Å]	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)
Total no. of observations	451994 226095	451994 226095	445208 222653	445208 222653	445208 222653	445208 222653	445208 222653	445208 222653
Total no. of reflections	261883 30892	261440 130703	242487 121748	242383 121667	242426 121680	242426 121679	242451 121716	242430 121683
Unique reflections	19997 19936	19997 19936	20032 19957	20032 19957	20032 19957	20032 19957	20032 19957	20032 19957
Rejected reflections	1349 367	2217 721	93 26	47 22	6 13	7 11	10 2	7 10
Redundancy	13.10 6.57	13.07 6.56	12.10 6.10	12.10 6.10	12.10 6.10	12.10 6.10	12.10 6.10	12.10 6.10
Completeness [%]	99.00 (96.40) 98.70 (92.30)	98.90 (95.30) 98.40 (90.50)	99.10 (99.10) 98.70 (98.70)	99.10 (99.10) 98.70 (98.70)	99.10 (99.10) 98.70 (98.70)	99.10 (99.10) 98.70 (98.70)	99.10 (99.10) 98.70 (98.70)	99.10 (99.10) 98.70 (98.70)
$I/\sigma(I)$	34.50 (20.82) 25.58 (14.88)	33.29 (17.99) 21.93 (12.31)	42.50 (23.90) 28.80 (16.60)	54.30 (31.40) 39.80 (23.50)	52.30 (29.50) 32.90 (22.70)	52.30 (29.50) 39.10 (22.60)	48.90 (27.70) 33.50 (19.40)	52.30 (29.30) 39.20 (22.50)
$R_{\text{merge}}$ (%)	6.30 (9.70) 6.20 (9.40)	6.20 (9.60) 6.10 (9.40)	5.90 (9.40) 5.80 (9.20)	5.00 (7.50) 4.70 (7.00)	5.10 (8.00) 4.80 (7.20)	5.10 (8.00) 4.80 (7.20)	5.30 (8.00) 5.20 (7.60)	5.10 (7.90) 4.80 (7.20)
$R_{\text{r.i.m.}}$ (%)	6.50 (10.20) 6.70 (10.40)	6.50 (10.10) 6.70 (10.60)	6.20 (10.00) 6.40 (10.40)	5.20 (7.90) 5.20 (7.90)	5.30 (8.50) 5.20 (8.10)	5.30 (8.50) 5.20 (8.10)	5.60 (8.60) 5.60 (8.60)	5.40 (8.40) 5.20 (8.10)
$R_{\text{p.i.m.}}$ (%)	1.80 (3.30) 2.60 (4.60)	1.70 (3.20) 2.50 (4.60)	1.70 (3.30) 2.50 (4.70)	1.50 (2.60) 2.00 (3.60)	1.50 (2.80) 2.10 (3.70)	1.50 (2.80) 2.10 (3.70)	1.60 (2.80) 2.20 (3.90)	1.50 (2.80) 2.10 (3.70)
$R_{\text{anom}}$ (%)	3.10 (4.80) 3.70 (5.80)	3.10 (4.80) 3.70 (6.00)	3.10 (4.70) 3.70 (5.90)	3.10 (4.50) 3.40 (5.20)	3.10 (4.50) 3.50 (5.20)	3.10 (4.50) 3.50 (5.20)	3.10 (4.60) 3.50 (5.30)	3.10 (4.50) 3.50 (5.20)

<b>D-Air (<math>\lambda=1.90 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)	99 – 1.82 (1.87 – 1.82)
Total no. of observations	417767 209243	417767 209243	410764 205791	410764 205791	410764 205791	410764 205791	410764 205791	410764 205791
Total no. of reflections	239199 119549	238469 119493	221977 111947	221738 111768	221846 111806	221844 111807	221898 111891	221844 111807
Unique reflections	19974 19919	19974 19918	19975 19908	19975 19908	19975 19908	19975 19908	19975 19908	19975 19908
Rejected reflections	2529 1047	4103 1268	191 68	118 57	31 27	35 30	21 11	26 23
Redundancy	11.98 6.00	11.94 6.00	11.11 5.62	11.10 5.61	11.11 5.62	11.11 5.62	11.11 5.62	11.11 5.62
Completeness [%]	98.90 (100) 98.60 (100)	98.80 (100) 98.10 (99.30)	98.80 (98.80) 98.50 (98.50)	98.80 (98.80) 98.50 (98.50)	98.80 (98.80) 98.50 (98.50)	98.80 (98.80) 98.50 (98.50)	98.80 (98.80) 98.50 (98.50)	98.80 (98.80) 98.50 (98.50)
$I/\sigma(I)$	27.10 (18.55) 18.96 (12.57)	26.06 (15.62) 16.84 (9.94)	34.10 (20.80) 23.00 (14.00)	47.30 (29.60) 34.70 (21.70)	45.20 (27.60) 33.90 (22.70)	45.30 (27.70) 33.90 (22.70)	41.00 (25.20) 28.00 (17.20)	45.30 (27.70) 33.90 (20.70)
$R_{\text{merge}}$ (%)	7.70 (12.20) 7.50 (11.80)	7.60 (12.00) 7.50 (11.80)	7.20 (11.70) 7.00 (11.50)	5.70 (8.80) 5.30 (8.40)	5.80 (9.50) 5.40 (8.90)	5.80 (9.40) 5.40 (8.80)	6.20 (9.60) 5.90 (9.30)	5.80 (9.50) 5.40 (8.80)
$R_{\text{r.i.m.}}$ (%)	8.00 (12.90) 8.20 (13.10)	8.00 (12.70) 8.20 (13.10)	7.50 (12.40) 7.70 (12.90)	6.00 (9.30) 5.90 (9.40)	6.00 (10.10) 5.90 (10.00)	6.00 (9.90) 5.90 (9.90)	6.40 (10.20) 6.40 (10.50)	6.10 (10.10) 5.90 (9.90)
$R_{\text{p.i.m.}}$ (%)	2.20 (4.00) 3.20 (5.70)	2.20 (4.00) 3.20 (5.70)	2.20 (4.00) 3.20 (5.80)	1.70 (3.00) 2.40 (4.20)	1.80 (3.30) 2.40 (4.50)	1.80 (3.20) 2.40 (4.40)	1.90 (3.30) 2.60 (4.80)	1.80 (3.30) 2.40 (4.50)
$R_{\text{anom}}$ (%)	3.70 (6.20) 4.40 (7.20)	3.70 (5.90) 4.50 (7.50)	3.80 (6.00) 4.40 (7.60)	3.70 (5.50) 4.10 (6.20)	3.70 (5.50) 4.10 (6.50)	3.70 (5.50) 4.10 (6.40)	3.70 (5.50) 4.10 (6.40)	3.70 (5.50) 4.10 (6.50)

<b>E-Air (<math>\lambda=2.10</math> Å)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [Å]	99 – 1.94 (1.97 – 1.94)	99 – 1.94 (1.97 – 1.94)	99 – 1.94 (1.99 – 1.94)	99 – 1.94 (1.99 – 1.94)	99 – 1.94 (1.99 – 1.94)	99 – 1.94 (1.99 – 1.94)	99 – 1.94 (1.99 – 1.94)	99 – 1.94 (1.99 – 1.94)
Total no. of observations	325860 <i>163411</i>	325860 <i>163411</i>	320686 <i>160895</i>	320686 <i>160895</i>	320686 <i>160895</i>	320686 <i>160895</i>	320686 <i>160895</i>	320686 <i>160895</i>
Total no. of reflections	185597 <i>92601</i>	185023 <i>92413</i>	167188 <i>83935</i>	166910 <i>83810</i>	167015 <i>83828</i>	167008 <i>83825</i>	167127 <i>83903</i>	167034 <i>83843</i>
Unique reflections	16520 <i>16466</i>	16519 <i>16465</i>	16539 <i>16463</i>	16539 <i>16463</i>	16539 <i>16463</i>	16539 <i>16463</i>	16539 <i>16463</i>	16539 <i>16463</i>
Rejected reflections	2378 <i>698</i>	3752 <i>1389</i>	192 <i>58</i>	108 <i>56</i>	63 <i>23</i>	64 <i>21</i>	30 <i>7</i>	67 <i>35</i>
Redundancy	11.23 <i>5.62</i>	11.20 <i>5.61</i>	10.11 <i>5.10</i>	10.09 <i>5.09</i>	10.10 <i>5.09</i>	10.10 <i>5.09</i>	10.11 <i>5.10</i>	10.10 <i>5.09</i>
Completeness [%]	98.60 (99.60) <i>98.30 (99.50)</i>	99.40 (99.60) <i>97.20 (97.20)</i>	98.60 (98.60) <i>98.20 (98.20)</i>	98.60 (98.60) <i>98.20 (98.20)</i>	98.60 (98.60) <i>98.20 (98.20)</i>	98.60 (98.60) <i>98.20 (98.20)</i>	98.60 (98.60) <i>98.20 (98.20)</i>	98.60 (98.60) <i>98.20 (98.20)</i>
I/ $\sigma$ (I)	23.67 (15.71) <i>16.43 (10.73)</i>	22.62 (13.07) <i>15.47 (9.42)</i>	29.80 (17.30) <i>20.10 (11.60)</i>	44.00 (26.20) <i>30.70 (18.20)</i>	42.60 (24.90) <i>30.20 (17.60)</i>	42.70 (25.00) <i>30.10 (17.50)</i>	37.20 (22.00) <i>24.60 (14.40)</i>	42.20 (24.80) <i>29.90 (17.50)</i>
R <sub>merge</sub> (%)	8.60 (12.10) <i>8.50 (11.30)</i>	8.50 (12.00) <i>8.40 (10.90)</i>	8.10 (11.70) <i>8.00 (11.10)</i>	6.10 (8.90) <i>5.80 (8.60)</i>	6.00 (9.60) <i>5.80 (9.10)</i>	6.00 (9.40) <i>5.80 (9.00)</i>	6.80 (9.50) <i>6.50 (9.20)</i>	6.20 (9.60) <i>5.90 (9.20)</i>
R <sub>r.i.m.</sub> (%)	9.00 (13.00) <i>9.30 (13.00)</i>	8.90 (12.80) <i>9.20 (12.60)</i>	8.50 (12.50) <i>8.80 (13.00)</i>	6.40 (9.60) <i>6.40 (10.00)</i>	6.30 (10.30) <i>6.40 (10.70)</i>	6.30 (10.00) <i>6.40 (10.60)</i>	7.10 (10.20) <i>7.20 (10.80)</i>	6.50 (10.40) <i>6.50 (10.80)</i>
R <sub>p.i.m.</sub> (%)	2.50 (4.50) <i>3.70 (6.30)</i>	2.50 (4.50) <i>3.70 (6.10)</i>	2.50 (4.60) <i>3.70 (6.60)</i>	1.90 (3.50) <i>2.70 (5.00)</i>	1.90 (3.80) <i>2.70 (5.40)</i>	1.90 (3.70) <i>2.70 (5.30)</i>	2.10 (3.70) <i>3.00 (5.40)</i>	1.90 (3.80) <i>2.70 (5.40)</i>
R <sub>anom</sub> (%)	4.10 (6.10) <i>4.90 (7.50)</i>	4.10 (6.20) <i>4.90 (7.50)</i>	4.20 (6.30) <i>5.10 (7.80)</i>	4.10 (5.70) <i>4.50 (6.10)</i>	4.10 (5.80) <i>4.50 (6.60)</i>	4.10 (5.80) <i>4.50 (6.50)</i>	4.10 (5.70) <i>4.60 (6.60)</i>	4.20 (5.80) <i>4.60 (6.70)</i>

<b>F-Air (<math>\lambda=2.25 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 2.08 (2.12 – 2.08)	99 – 2.08 (2.12 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)
Total no. of observations	261900 <i>130264</i>	261900 <i>130264</i>	256142 <i>127490</i>	256142 <i>127490</i>	256142 <i>127490</i>	256142 <i>127490</i>	256142 <i>127490</i>	256142 <i>127490</i>
Total no. of reflections	149920 <i>74404</i>	149249 <i>74353</i>	130595 <i>65352</i>	130199 <i>65159</i>	130309 <i>65165</i>	130298 <i>65170</i>	130489 <i>65312</i>	130389 <i>65216</i>
Unique reflections	13640 <i>13530</i>	13640 <i>13530</i>	13617 <i>13464</i>	13617 <i>13464</i>	13617 <i>13464</i>	13617 <i>13464</i>	13617 <i>13464</i>	13617 <i>13464</i>
Rejected reflections	1749 <i>801</i>	3148 <i>767</i>	148 <i>43</i>	156 <i>62</i>	73 <i>37</i>	69 <i>37</i>	33 <i>16</i>	65 <i>31</i>
Redundancy	10.99 <i>5.50</i>	10.94 <i>5.50</i>	9.59 <i>4.85</i>	9.56 <i>4.84</i>	9.57 <i>4.84</i>	9.57 <i>4.84</i>	9.58 <i>4.85</i>	9.58 <i>4.84</i>
Completeness [%]	99.80 (99.80) <i>99.00 (99.80)</i>	99.60 (99.80) <i>97.80 (98.30)</i>	99.50 (99.50) <i>98.50 (98.50)</i>	99.50 (99.50) <i>98.50 (98.50)</i>	99.50 (99.50) <i>98.50 (98.50)</i>	99.50 (99.50) <i>98.50 (98.50)</i>	99.50 (99.50) <i>98.50 (98.50)</i>	99.50 (99.50) <i>98.50 (98.50)</i>
$I/\sigma(I)$	21.39 (14.64) <i>14.62 (9.62)</i>	20.10 (12.33) <i>12.74 (7.53)</i>	26.30 (16.50) <i>18.00 (11.30)</i>	43.00 (27.40) <i>30.10 (19.00)</i>	41.00 (26.00) <i>29.60 (18.70)</i>	41.10 (26.10) <i>29.50 (18.60)</i>	34.10 (21.90) <i>22.60 (14.40)</i>	39.60 (25.50) <i>28.80 (18.50)</i>
$R_{\text{merge}}$ (%)	9.70 (12.40) <i>9.60 (11.30)</i>	9.60 (12.30) <i>9.60 (11.60)</i>	9.20 (11.60) <i>9.10 (10.80)</i>	6.40 (8.50) <i>6.10 (8.20)</i>	6.30 (9.10) <i>6.00 (8.50)</i>	6.20 (8.90) <i>6.00 (8.50)</i>	7.40 (9.70) <i>7.30 (9.20)</i>	6.50 (9.40) <i>6.20 (8.60)</i>
$R_{\text{r.i.m.}}$ (%)	10.10 (13.30) <i>10.50 (13.00)</i>	10.00 (12.10) <i>10.50 (13.30)</i>	9.70 (12.50) <i>10.10 (12.60)</i>	6.70 (9.10) <i>6.70 (9.60)</i>	6.60 (9.80) <i>6.70 (10.00)</i>	6.60 (9.60) <i>6.70 (9.90)</i>	7.80 (10.40) <i>8.10 (10.80)</i>	6.90 (10.10) <i>6.90 (10.00)</i>
$R_{\text{p.i.m.}}$ (%)	2.90 (4.60) <i>4.20 (6.30)</i>	2.90 (4.50) <i>4.20 (6.40)</i>	3.00 (4.60) <i>4.30 (6.50)</i>	2.00 (3.30) <i>2.90 (4.80)</i>	2.00 (3.60) <i>2.90 (5.10)</i>	2.00 (3.50) <i>2.90 (5.10)</i>	2.40 (3.80) <i>3.50 (5.50)</i>	2.10 (3.70) <i>3.00 (5.10)</i>
$R_{\text{anom}}$ (%)	4.40 (5.90) <i>5.30 (7.30)</i>	4.40 (6.00) <i>5.40 (7.80)</i>	4.70 (6.20) <i>5.80 (8.00)</i>	4.40 (5.70) <i>4.90 (6.40)</i>	4.40 (5.70) <i>4.90 (6.50)</i>	4.40 (5.60) <i>4.90 (6.50)</i>	4.50 (6.00) <i>5.10 (6.70)</i>	4.50 (5.70) <i>5.00 (6.70)</i>

<b>G-Air (<math>\lambda=2.40</math> Å)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [Å]	99 – 2.22 (2.26 – 2.22)	99 – 2.22 (2.26 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)
Total no. of observations	213174 <i>106427</i>	213174 <i>106427</i>	209402 <i>104535</i>	209402 <i>104535</i>	209402 <i>104535</i>	209402 <i>104535</i>	209402 <i>104535</i>	209402 <i>104535</i>
Total no. of reflections	121318 <i>60332</i>	121010 <i>60438</i>	105563 <i>52929</i>	105311 <i>52814</i>	105399 <i>52830</i>	105391 <i>52824</i>	105478 <i>52901</i>	105470 <i>52858</i>
Unique reflections	11222 <i>11113</i>	11223 <i>11114</i>	11224 <i>11078</i>	11224 <i>11078</i>	11224 <i>11078</i>	11224 <i>11078</i>	11224 <i>11078</i>	11224 <i>11078</i>
Rejected reflections	1140 <i>171</i>	2022 <i>493</i>	125 <i>32</i>	104 <i>40</i>	67 <i>22</i>	65 <i>22</i>	52 <i>15</i>	46 <i>19</i>
Redundancy	10.81 <i>5.43</i>	10.78 <i>5.44</i>	9.41 <i>4.78</i>	9.38 <i>4.77</i>	9.39 <i>4.77</i>	9.39 <i>4.77</i>	9.40 <i>4.78</i>	9.40 <i>4.77</i>
Completeness [%]	99.20 (99.80) <i>98.20 (99.50)</i>	99.10 (99.10) <i>97.10 (98.10)</i>	99.10 (99.10) <i>97.90 (97.90)</i>	99.10 (99.10) <i>97.90 (97.90)</i>	99.10 (99.10) <i>97.90 (97.90)</i>	99.10 (99.10) <i>97.90 (97.90)</i>	99.10 (99.10) <i>97.90 (97.90)</i>	99.10 (99.10) <i>97.90 (97.90)</i>
$I/\sigma(I)$	19.99 (13.33) <i>13.94 (8.89)</i>	17.92 (10.74) <i>11.52 (6.65)</i>	23.30 (14.40) <i>16.10 (9.70)</i>	38.10 (23.50) <i>26.50 (16.20)</i>	37.10 (23.00) <i>26.20 (16.00)</i>	37.20 (23.10) <i>26.20 (16.00)</i>	30.20 (19.10) <i>20.00 (12.40)</i>	35.70 (22.60) <i>24.90 (15.60)</i>
$R_{\text{merge}}$ (%)	10.30 (14.00) <i>10.20 (12.90)</i>	10.30 (13.70) <i>10.30 (14.20)</i>	10.10 (13.20) <i>9.80 (12.70)</i>	6.70 (9.70) <i>6.40 (9.80)</i>	6.40 (10.00) <i>6.30 (9.90)</i>	6.40 (9.90) <i>6.30 (9.00)</i>	6.20 (6.20) <i>7.70 (10.60)</i>	6.80 (10.50) <i>6.60 (10.20)</i>
$R_{\text{r.i.m.}}$ (%)	10.80 (15.00) <i>11.20 (14.80)</i>	10.70 (14.70) <i>11.30 (16.30)</i>	10.60 (14.20) <i>10.90 (14.90)</i>	7.10 (10.50) <i>7.10 (11.40)</i>	6.80 (10.80) <i>7.00 (11.60)</i>	6.80 (10.70) <i>7.00 (11.60)</i>	8.50 (11.60) <i>8.60 (12.40)</i>	7.20 (11.30) <i>7.40 (12.00)</i>
$R_{\text{p.i.m.}}$ (%)	3.10 (5.20) <i>4.50 (7.20)</i>	3.10 (5.10) <i>4.50 (7.80)</i>	3.20 (5.20) <i>4.60 (7.70)</i>	2.20 (3.80) <i>3.00 (5.80)</i>	2.10 (4.00) <i>3.00 (5.90)</i>	2.10 (3.90) <i>3.00 (5.90)</i>	2.60 (4.30) <i>3.60 (6.40)</i>	2.20 (4.20) <i>3.20 (6.10)</i>
$R_{\text{anom}}$ (%)	4.20 (6.30) <i>5.30 (8.40)</i>	4.20 (6.20) <i>5.40 (9.10)</i>	4.50 (6.50) <i>5.90 (8.70)</i>	4.10 (5.40) <i>4.70 (6.20)</i>	4.10 (5.60) <i>4.70 (6.90)</i>	4.10 (5.50) <i>4.70 (6.70)</i>	4.20 (5.70) <i>5.00 (7.20)</i>	4.20 (5.60) <i>4.90 (7.00)</i>

<b>H-Air (<math>\lambda=2.50 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 2.30 (2.34 – 2.30)	99 – 2.30 (2.34 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)
Total no. of observations	190532 94933	190532 94933	187586 93470	187586 93470	187586 93470	187586 93470	187586 93470	187586 93470
Total no. of reflections	108762 54243	108626 54266	94096 47151	93844 47073	93959 47081	93947 47078	94012 47130	94012 47104
Unique reflections	10073 9989	10073 9989	10091 9991	10091 9991	10091 9991	10091 9991	10091 9991	10091 9991
Rejected reflections	990 80	1385 158	151 46	104 30	64 23	68 22	54 14	56 23
Redundancy	10.80 5.43	10.78 5.43	9.32 4.72	9.30 4.71	9.31 4.71	9.31 4.71	9.32 4.72	9.32 4.71
Completeness [%]	98.80 (85.20) 98.00 (82.00)	98.50 (83.50) 96.90 (79.20)	98.80 (98.80) 98.30 (98.30)	98.80 (98.80) 98.30 (98.30)	98.80 (98.80) 98.30 (98.30)	98.80 (98.80) 98.30 (98.30)	98.80 (98.80) 98.30 (98.30)	98.80 (98.80) 98.30 (98.30)
$I/\sigma(I)$	20.49 (11.97) 13.88 (8.40)	17.11 (9.15) 10.76 (6.22)	22.20 (12.00) 14.70 (8.10)	39.20 (21.40) 26.40 (14.60)	38.40 (20.90) 26.70 (14.90)	38.50 (20.90) 26.60 (14.80)	30.20 (16.90) 18.90 (10.70)	36.80 (20.30) 24.20 (13.60)
$R_{\text{merge}}$ (%)	10.50 (13.90) 10.80 (15.10)	10.40 (13.60) 10.70 (15.40)	10.20 (13.40) 10.20 (12.90)	6.10 (9.00) 6.00 (9.60)	5.70 (10.10) 5.70 (10.10)	5.70 (9.90) 5.70 (10.00)	7.80 (10.30) 7.80 (10.90)	6.10 (10.20) 6.30 (11.00)
$R_{\text{r.i.m.}}$ (%)	10.90 (15.00) 11.80 (17.50)	10.90 (14.70) 11.80 (17.90)	10.80 (14.60) 11.40 (15.50)	6.40 (9.80) 6.70 (11.50)	6.00 (11.00) 6.30 (12.20)	6.30 (10.80) 6.30 (12.00)	8.20 (11.30) 8.70 (13.10)	6.50 (11.20) 7.00 (13.20)
$R_{\text{p.i.m.}}$ (%)	3.10 (5.50) 4.70 (8.60)	3.10 (5.30) 4.70 (8.80)	3.30 (5.60) 4.90 (8.30)	1.90 (3.80) 2.80 (6.10)	1.80 (4.30) 2.70 (6.60)	1.80 (4.20) 2.70 (6.50)	2.50 (4.40) 3.70 (7.10)	2.00 (4.00) 3.00 (7.00)
$R_{\text{anom}}$ (%)	3.50 (5.50) 5.00 (9.10)	3.60 (5.40) 5.10 (10.00)	3.80 (6.50) 5.60 (9.70)	3.30 (5.00) 4.00 (6.60)	3.30 (5.30) 3.90 (7.10)	3.30 (5.30) 3.90 (7.00)	3.50 (5.50) 4.40 (7.70)	3.40 (5.20) 4.20 (7.60)



<b>I-Air (<math>\lambda=2.65 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 2.44 (2.48 – 2.44)	99 – 2.44 (2.48 – 2.44)	99 – 2.44 (2.50 2.44)	99 – 2.44 (2.50 2.44)	99 – 2.44 (2.50 2.44)	99 – 2.44 (2.50 2.44)	99 – 2.44 (2.50 2.44)	99 – 2.44 (2.50 2.44)
Total no. of observations	163207 <i>81712</i>	163207 <i>81712</i>	161214 <i>80734</i>	161214 <i>80734</i>	161214 <i>80734</i>	161214 <i>80734</i>	161214 <i>80734</i>	161214 <i>80734</i>
Total no. of reflections	93466 <i>46751</i>	93509 <i>46795</i>	78706 <i>39073</i>	78612 <i>39051</i>	78672 <i>39040</i>	78662 <i>39039</i>	78674 <i>39074</i>	78730 <i>39058</i>
Unique reflections	8525 <i>8512</i>	8525 <i>8512</i>	8554 <i>8506</i>	8554 <i>8506</i>	8554 <i>8506</i>	8554 <i>8506</i>	8554 <i>8506</i>	8554 <i>8506</i>
Rejected reflections	648 <i>33</i>	569 <i>28</i>	101 <i>21</i>	51 <i>19</i>	31 <i>18</i>	33 <i>21</i>	29 <i>11</i>	33 <i>16</i>
Redundancy	10.96 <i>5.49</i>	10.97 <i>5.50</i>	9.20 <i>4.59</i>	9.19 <i>4.59</i>	9.20 <i>4.59</i>	9.20 <i>4.59</i>	9.20 <i>4.59</i>	9.20 <i>4.59</i>
Completeness [%]	98.30 (87.30) <i>99.10 (85.10)</i>	99.20 (86.00) <i>98.70 (82.80)</i>	99.40 (99.40) <i>98.90 (98.90)</i>	99.40 (99.40) <i>98.90 (98.90)</i>	99.40 (99.40) <i>98.90 (98.90)</i>	99.40 (99.40) <i>98.90 (98.90)</i>	99.40 (99.40) <i>98.90 (98.90)</i>	99.40 (99.40) <i>98.90 (98.90)</i>
$I/\sigma(I)$	21.09 (11.40) <i>13.69 (7.59)</i>	16.02 (8.23) <i>10.03 (5.25)</i>	20.90 (7.60) <i>13.90 (5.10)</i>	36.00 (13.50) <i>23.90 (9.00)</i>	35.20 (13.00) <i>24.40 (9.10)</i>	35.40 (13.00) <i>24.50 (9.20)</i>	28.20 (10.80) <i>18.20 (7.00)</i>	32.60 (10.50) <i>22.40 (7.40)</i>
$R_{\text{merge}}$ (%)	11.40 (17.90) <i>11.60 (18.70)</i>	11.40 (17.60) <i>11.50 (19.10)</i>	11.00 (17.50) <i>11.00 (17.90)</i>	5.90 (13.70) <i>5.80 (14.70)</i>	5.60 (14.40) <i>5.50 (14.40)</i>	5.60 (14.00) <i>5.60 (14.20)</i>	8.00 (14.10) <i>8.30 (14.30)</i>	6.50 (15.20) <i>6.40 (15.30)</i>
$R_{\text{r.i.m.}}$ (%)	11.90 (19.20) <i>12.60 (21.80)</i>	11.90 (20.00) <i>12.60 (22.30)</i>	11.50 (19.10) <i>12.30 (21.40)</i>	6.20 (14.90) <i>6.50 (17.40)</i>	5.90 (15.70) <i>6.20 (17.10)</i>	5.90 (15.30) <i>6.20 (16.90)</i>	8.40 (15.40) <i>9.20 (17.00)</i>	6.90 (16.60) <i>7.20 (18.20)</i>
$R_{\text{p.i.m.}}$ (%)	3.40 (6.90) <i>5.10 (10.90)</i>	3.40 (7.20) <i>5.10 (11.20)</i>	3.50 (7.30) <i>5.30 (11.50)</i>	1.90 (5.70) <i>2.80 (9.10)</i>	1.80 (6.00) <i>2.70 (9.10)</i>	1.80 (5.90) <i>2.70 (8.90)</i>	2.60 (6.00) <i>3.90 (8.90)</i>	2.20 (6.40) <i>3.20 (9.60)</i>
$R_{\text{anom}}$ (%)	2.70 (5.90) <i>4.40 (9.70)</i>	2.80 (6.50) <i>4.70 (10.70)</i>	3.40 (7.10) <i>5.60 (12.50)</i>	2.50 (5.30) <i>3.40 (8.50)</i>	2.40 (5.60) <i>3.30 (8.90)</i>	2.40 (5.50) <i>3.30 (8.70)</i>	2.70 (5.80) <i>4.10 (9.40)</i>	2.70 (6.40) <i>4.00 (10.60)</i>

**Table 2.** Complete scaling statistics for data sets B-He to I-He for the scaling models SCALEPACK-kB, SCALEPACK-ano, SCALA-Batch, SCALA-Det, SCALA-Abs, SCALA-Sec, SCALA-Baniso and SCALA-Ref. The numbers in the first row of each cell refer to the full 360° of data, whereas the numbers in italics in the second row refer to the first 180° of data in each case. The values in parenthesis refer to the respective outermost resolution shells.

<b>B-He (<math>\lambda=1.50</math> Å)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [Å]	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)
Total no. of observations	499329 <i>249492</i>	499329 <i>249492</i>	483221 <i>241354</i>	483221 <i>241354</i>	483221 <i>241354</i>	483221 <i>241354</i>	483221 <i>241354</i>	483221 <i>241354</i>
Total no. of reflections	272014 <i>136146</i>	271642 <i>135971</i>	256885 <i>128300</i>	256885 <i>128070</i>	256670 <i>128111</i>	256671 <i>128115</i>	256802 <i>128254</i>	256020 <i>127786</i>
Unique reflections	19897 <i>19852</i>	19897 <i>19852</i>	19939 <i>19892</i>	19939 <i>19892</i>	19939 <i>19892</i>	19939 <i>19892</i>	19939 <i>19892</i>	19884 <i>19892</i>
Rejected reflections	2686 <i>855</i>	3375 <i>1160</i>	285 <i>76</i>	244 <i>97</i>	176 <i>74</i>	177 <i>77</i>	142 <i>42</i>	169 <i>69</i>
Redundancy	13.67 <i>6.86</i>	13.65 <i>6.85</i>	12.88 <i>6.45</i>	12.87 <i>6.44</i>	12.87 <i>6.44</i>	12.87 <i>6.44</i>	12.88 <i>6.45</i>	12.88 <i>6.44</i>
Completeness [%]	98.10 (100) <i>97.80 (100)</i>	97.80 (100) <i>97.50 (100)</i>	98.20 (98.20) <i>98.00 (98.00)</i>	98.20 (98.20) <i>98.00 (98.00)</i>	98.20 (98.20) <i>98.00 (98.00)</i>	98.20 (98.20) <i>98.00 (98.00)</i>	98.20 (98.20) <i>98.00 (98.00)</i>	98.20 (98.20) <i>98.00 (98.00)</i>
I/ $\sigma$ (I)	54.55 (31.33) <i>38.37 (21.33)</i>	53.77 (23.52) <i>36.80 (15.21)</i>	67.60 (32.70) <i>42.20 (20.30)</i>	87.80 (43.40) <i>64.60 (32.10)</i>	83.90 (40.70) <i>62.10 (30.20)</i>	83.90 (40.70) <i>62.10 (30.20)</i>	74.50 (36.10) <i>47.60 (23.10)</i>	83.80 (41.10) <i>61.80 (30.30)</i>
R <sub>merge</sub> (%)	3.70 (8.00) <i>3.80 (8.40)</i>	3.70 (8.00) <i>3.80 (8.40)</i>	3.50 (8.00) <i>3.60 (8.40)</i>	2.90 (6.40) <i>2.80 (6.10)</i>	3.00 (6.90) <i>2.90 (6.50)</i>	3.00 (6.90) <i>2.90 (6.50)</i>	3.30 (7.40) <i>3.30 (7.60)</i>	3.10 (6.80) <i>3.00 (6.40)</i>
R <sub>r.i.m.</sub> (%)	3.80 (8.30) <i>4.10 (9.10)</i>	3.80 (8.30) <i>4.10 (9.10)</i>	3.70 (8.30) <i>3.90 (9.20)</i>	3.10 (6.70) <i>3.10 (6.70)</i>	3.10 (7.20) <i>3.10 (7.10)</i>	3.10 (7.20) <i>3.10 (7.10)</i>	3.40 (7.70) <i>3.60 (8.60)</i>	3.30 (7.10) <i>3.30 (7.00)</i>
R <sub>p.i.m.</sub> (%)	1.00 (2.30) <i>1.60 (3.50)</i>	1.00 (2.30) <i>1.60 (3.50)</i>	1.00 (2.40) <i>1.50 (3.70)</i>	0.80 (1.90) <i>1.20 (2.70)</i>	0.90 (2.10) <i>1.20 (2.80)</i>	0.90 (2.10) <i>1.20 (2.80)</i>	0.90 (2.20) <i>1.40 (3.40)</i>	0.90 (2.00) <i>1.30 (2.80)</i>
R <sub>anom</sub> (%)	2.10 (3.10) <i>2.30 (3.90)</i>	2.10 (3.20) <i>2.20 (2.50)</i>	2.10 (3.40) <i>2.30 (4.30)</i>	2.10 (3.20) <i>2.20 (3.70)</i>	2.10 (3.20) <i>2.20 (3.80)</i>	2.10 (3.20) <i>2.20 (3.80)</i>	2.10 (3.20) <i>2.20 (4.00)</i>	2.10 (3.20) <i>2.20 (3.80)</i>

<b>C-He (<math>\lambda=1.70 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)
Total no. of observations	439618 217098	439618 217098	430259 212225	430259 212225	430259 212225	430259 212225	430259 212225	430259 212225
Total no. of reflections	243229 120274	242744 120037	227071 112937	226796 112661	226908 112722	226909 112724	226999 112891	226807 112682
Unique reflections	19498 19093	19498 19093	19509 19055	19509 19055	19509 19055	19509 19055	19509 19055	19459 19023
Rejected reflections	1875 282	2867 697	119 13	75 62	30 24	31 23	15 6	34 24
Redundancy	12.47 6.30	12.44 6.29	11.64 5.93	11.63 5.91	11.63 5.92	11.63 5.92	11.64 5.92	11.66 5.92
Completeness [%]	96.00 (99.80) 94.10 (97.90)	95.90 (99.60) 93.50 (96.30)	96.10 (96.10) 93.90 (93.90)	96.10 (96.10) 93.90 (93.90)	96.10 (96.10) 93.90 (93.90)	96.10 (96.10) 93.90 (93.90)	96.10 (96.10) 93.90 (93.90)	96.20 (96.20) 94.10 (94.10)
$I/\sigma(I)$	38.61 (25.87) 28.11 (17.94)	38.74 (19.84) 27.73 (13.50)	49.60 (24.00) 33.00 (17.10)	69.80 (34.90) 57.70 (31.00)	66.30 (32.20) 54.60 (28.60)	66.30 (32.20) 54.60 (28.50)	57.40 (28.00) 39.20 (20.40)	66.20 (33.10) 54.20 (28.80)
$R_{\text{merge}}$ (%)	5.00 (8.90) 5.00 (9.20)	4.90 (8.90) 5.00 (9.20)	4.60 (8.30) 4.60 (8.30)	3.60 (6.40) 3.40 (5.80)	3.70 (7.00) 3.50 (6.30)	3.70 (7.00) 3.50 (6.30)	4.10 (7.50) 4.00 (7.10)	3.90 (7.00) 3.60 (6.30)
$R_{\text{r.i.m.}}$ (%)	5.20 (9.50) 5.40 (10.20)	5.20 (9.50) 5.40 (10.20)	4.80 (8.90) 5.10 (9.30)	3.80 (6.80) 3.70 (6.60)	3.90 (7.50) 3.80 (7.00)	3.90 (7.50) 3.80 (7.10)	4.30 (8.00) 4.40 (8.10)	4.00 (7.50) 3.90 (7.10)
$R_{\text{p.i.m.}}$ (%)	1.40 (3.00) 2.10 (4.50)	1.40 (3.00) 2.10 (4.50)	1.40 (3.00) 2.00 (4.20)	1.10 (2.20) 1.50 (3.00)	1.10 (2.50) 1.50 (3.20)	1.10 (2.50) 1.50 (3.20)	1.20 (2.70) 1.70 (3.70)	1.10 (2.50) 1.60 (3.20)
$R_{\text{anom}}$ (%)	2.70 (4.00) 3.00 (4.60)	2.70 (4.10) 3.00 (4.70)	2.60 (4.00) 3.00 (4.70)	2.60 (3.60) 2.80 (4.00)	2.60 (3.70) 2.80 (4.10)	2.60 (3.70) 2.80 (4.10)	2.60 (3.70) 2.80 (4.30)	2.60 (3.60) 2.80 (4.10)

<b>D-He (<math>\lambda=1.90 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.85 – 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)	99 – 1.82 (1.87– 1.82)
Total no. of observations	470684 233565	470684 233565	406641 201552	406641 201552	406641 201552	406641 201552	406641 201552	406641 201552
Total no. of reflections	228184 <i>113402</i>	227643 <i>113217</i>	214601 <i>105742</i>	214186 <i>105532</i>	214347 <i>105582</i>	214344 <i>105582</i>	214490 <i>105700</i>	213618 <i>105235</i>
Unique reflections	19141 <i>18831</i>	19141 <i>18831</i>	19168 <i>18837</i>	19168 <i>18837</i>	19168 <i>18837</i>	19168 <i>18837</i>	19168 <i>18837</i>	19168 <i>18762</i>
Rejected reflections	3201 <i>568</i>	4345 <i>906</i>	225 <i>41</i>	89 <i>36</i>	38 <i>16</i>	37 <i>17</i>	19 <i>4</i>	40 <i>19</i>
Redundancy	11.92 <i>6.02</i>	11.89 <i>6.01</i>	11.20 <i>5.61</i>	11.17 <i>5.60</i>	11.18 <i>5.61</i>	11.18 <i>5.61</i>	11.19 <i>5.61</i>	11.19 <i>5.61</i>
Completeness [%]	94.20 (100) <i>92.70 (100)</i>	93.90 (100) <i>92.20 (100)</i>	94.40 (94.40) <i>92.80 (92.80)</i>	94.40 (94.40) <i>92.80 (92.80)</i>	94.40 (94.40) <i>92.80 (92.80)</i>	94.40 (94.40) <i>92.80 (92.80)</i>	94.40 (94.40) <i>92.80 (92.80)</i>	94.40 (94.40) <i>92.80 (92.80)</i>
$I/\sigma(I)$	33.49 (25.28) <i>24.54 (16.89)</i>	34.38 (19.55) <i>23.72 (12.43)</i>	42.40 (22.20) <i>27.20 (14.50)</i>	65.40 (35.10) <i>48.10 (26.40)</i>	61.50 (32.30) <i>45.60 (24.50)</i>	61.60 (32.40) <i>45.60 (24.50)</i>	50.40 (26.60) <i>33.20 (17.80)</i>	61.50 (32.60) <i>45.20 (24.60)</i>
$R_{\text{merge}}$ (%)	5.90 (9.90) <i>5.90 (10.30)</i>	5.80 (9.90) <i>5.80 (10.40)</i>	5.50 (9.90) <i>5.50 (10.20)</i>	4.10 (7.40) <i>3.90 (7.10)</i>	4.20 (8.00) <i>4.00 (7.50)</i>	4.20 (8.00) <i>4.00 (7.50)</i>	4.70 (8.70) <i>4.50 (8.60)</i>	4.30 (8.10) <i>4.10 (7.60)</i>
$R_{\text{r.i.m.}}$ (%)	6.10 (10.40) <i>6.40 (11.50)</i>	6.10 (10.40) <i>6.30 (11.50)</i>	5.80 (10.40) <i>6.10 (11.40)</i>	4.30 (7.80) <i>4.30 (7.90)</i>	4.40 (8.50) <i>4.40 (8.40)</i>	4.40 (8.40) <i>4.40 (8.40)</i>	4.90 (9.20) <i>5.00 (9.70)</i>	4.50 (8.50) <i>4.50 (8.50)</i>
$R_{\text{p.i.m.}}$ (%)	1.70 (3.20) <i>2.50 (5.00)</i>	1.70 (3.20) <i>2.50 (5.00)</i>	1.70 (3.30) <i>2.40 (5.10)</i>	1.20 (2.40) <i>1.70 (3.50)</i>	1.20 (2.70) <i>1.80 (3.70)</i>	1.20 (2.70) <i>1.80 (3.70)</i>	1.40 (2.90) <i>2.00 (4.30)</i>	1.30 (2.70) <i>1.80 (3.80)</i>
$R_{\text{anom}}$ (%)	3.10 (4.40) <i>3.50 (5.50)</i>	3.20 (4.70) <i>3.50 (5.60)</i>	3.20 (4.70) <i>3.50 (5.90)</i>	3.10 (4.10) <i>3.20 (4.70)</i>	3.10 (4.20) <i>3.30 (4.90)</i>	3.10 (4.20) <i>3.30 (4.80)</i>	3.10 (4.20) <i>3.30 (5.00)</i>	3.10 (4.20) <i>3.30 (4.80)</i>

<b>E-He (<math>\lambda=2.10 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 1.94 (1.97 – 1.94)	99 – 1.94 (1.97 – 1.94)	99 – 1.94 (1.99– 1.94)	99 – 1.94 (1.99– 1.94)	99 – 1.94 (1.99– 1.94)	99 – 1.94 (1.99 – 1.94)	99 – 1.94 (1.99 – 1.94)	99 – 1.94 (1.99 – 1.94)
Total no. of observations	363682 <i>180586</i>	363682 <i>180586</i>	347129 <i>172357</i>	347129 <i>172357</i>	347129 <i>172357</i>	347129 <i>172357</i>	347129 <i>172357</i>	347129 <i>172357</i>
Total no. of reflections	194852 <i>96997</i>	194262 <i>96780</i>	180127 <i>89954</i>	179513 <i>89669</i>	179728 <i>89725</i>	179724 <i>89718</i>	180043 <i>89902</i>	173993 <i>89514</i>
Unique reflections	16491 <i>16189</i>	16491 <i>16189</i>	16519 <i>16207</i>	16519 <i>16207</i>	16519 <i>16207</i>	16519 <i>16207</i>	16519 <i>16207</i>	16472 <i>16160</i>
Rejected reflections	2955 <i>536</i>	4124 <i>938</i>	229 <i>38</i>	162 <i>58</i>	82 <i>41</i>	75 <i>37</i>	31 <i>7</i>	79 <i>39</i>
Redundancy	11.82 <i>5.99</i>	11.78 <i>5.98</i>	10.90 <i>5.50</i>	10.87 <i>5.53</i>	10.88 <i>5.54</i>	10.88 <i>5.54</i>	10.90 <i>5.55</i>	10.89 <i>5.54</i>
Completeness [%]	97.90 (100) <i>96.10 (100)</i>	97.50 (100) <i>95.80 (100)</i>	98.00 (98.00) <i>96.20 (96.20)</i>	98.00 (98.00) <i>96.20 (96.20)</i>	98.00 (98.00) <i>96.20 (96.20)</i>	98.00 (98.00) <i>96.20 (96.20)</i>	98.00 (98.00) <i>96.20 (96.20)</i>	98.00 (98.00) <i>96.20 (96.20)</i>
I/ $\sigma$ (I)	29.97 (20.13) <i>20.88 (13.18)</i>	29.99 (15.28) <i>19.83 (9.38)</i>	37.50 (19.00) <i>23.60 (12.40)</i>	65.70 (34.10) <i>46.60 (25.20)</i>	61.40 (31.40) <i>44.10 (23.30)</i>	61.60 (31.30) <i>44.10 (23.30)</i>	47.00 (24.00) <i>29.40 (15.60)</i>	60.70 (30.60) <i>43.90 (23.10)</i>
R <sub>merge</sub> (%)	6.70 (12.60) <i>6.90 (12.80)</i>	6.70 (12.60) <i>6.80 (12.40)</i>	6.50 (12.20) <i>6.60 (11.80)</i>	4.40 (8.50) <i>4.30 (8.40)</i>	4.30 (9.90) <i>4.30 (9.10)</i>	4.30 (9.80) <i>4.30 (8.90)</i>	5.30 (10.50) <i>5.20 (10.20)</i>	4.60 (10.10) <i>4.50 (9.20)</i>
R <sub>r.i.m.</sub> (%)	7.00 (13.30) <i>7.50 (13.80)</i>	7.00 (13.30) <i>7.40 (13.90)</i>	6.80 (13.00) <i>7.20 (13.40)</i>	4.60 (9.00) <i>4.70 (9.40)</i>	4.50 (10.50) <i>4.70 (10.20)</i>	4.50 (10.40) <i>4.70 (10.10)</i>	5.60 (11.10) <i>5.80 (11.60)</i>	4.80 (10.70) <i>4.90 (10.30)</i>
R <sub>p.i.m.</sub> (%)	2.00 (4.20) <i>2.90 (6.00)</i>	1.90 (4.20) <i>2.90 (6.10)</i>	2.00 (4.30) <i>2.90 (6.10)</i>	1.30 (2.90) <i>1.90 (4.20)</i>	1.30 (3.40) <i>1.90 (4.60)</i>	1.30 (3.40) <i>1.90 (4.60)</i>	1.60 (3.70) <i>2.30 (5.30)</i>	1.40 (3.50) <i>2.00 (4.70)</i>
R <sub>anom</sub> (%)	3.40 (4.80) <i>3.90 (5.80)</i>	3.40 (5.10) <i>3.90 (5.80)</i>	3.50 (5.30) <i>4.00 (6.30)</i>	3.30 (4.30) <i>3.50 (4.90)</i>	3.30 (4.50) <i>3.60 (5.10)</i>	3.30 (4.50) <i>3.60 (5.10)</i>	3.40 (4.60) <i>3.60 (5.50)</i>	3.40 (4.60) <i>3.60 (5.10)</i>

<b>F-He (<math>\lambda=2.25 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 2.08 (2.12 – 2.08)	99 – 2.08 (2.12 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)	99 – 2.08 (2.13 – 2.08)
Total no. of observations	291398 <i>143854</i>	291398 <i>143854</i>	278204 <i>137272</i>	278204 <i>137272</i>	278204 <i>137272</i>	278204 <i>137272</i>	278204 <i>137272</i>	278204 <i>137272</i>
Total no. of reflections	156318 <i>77443</i>	155802 <i>77248</i>	141919 <i>70082</i>	141246 <i>69744</i>	141509 <i>69808</i>	141506 <i>69089</i>	141825 <i>70053</i>	141065 <i>69631</i>
Unique reflections	13398 <i>13068</i>	13398 <i>13068</i>	13421 <i>13067</i>	13421 <i>13067</i>	13421 <i>13067</i>	13421 <i>13067</i>	13421 <i>13067</i>	13364 <i>13010</i>
Rejected reflections	2306 <i>387</i>	3357 <i>746</i>	192 <i>25</i>	158 <i>63</i>	90 <i>45</i>	94 <i>44</i>	37 <i>8</i>	85 <i>39</i>
Redundancy	11.67 <i>5.93</i>	11.63 <i>5.91</i>	10.57 <i>5.36</i>	10.52 <i>5.34</i>	10.54 <i>5.34</i>	10.54 <i>5.34</i>	10.57 <i>5.36</i>	10.56 <i>5.35</i>
Completeness [%]	97.50 (100) <i>95.10 (100)</i>	97.20 (100) <i>94.60 (99.90)</i>	97.60 (97.60) <i>95.10 (95.10)</i>	97.60 (97.60) <i>95.10 (95.10)</i>	97.60 (97.60) <i>95.10 (95.10)</i>	97.60 (97.60) <i>95.10 (95.10)</i>	97.60 (97.60) <i>95.10 (95.10)</i>	97.60 (97.60) <i>95.10 (95.10)</i>
$I/\sigma(I)$	25.10 (19.71) <i>17.57 (12.47)</i>	24.49 (15.52) <i>16.75 (9.27)</i>	33.10 (19.90) <i>21.60 (13.20)</i>	61.10 (37.10) <i>44.40 (27.60)</i>	56.00 (33.80) <i>41.80 (25.70)</i>	56.10 (33.90) <i>41.80 (25.70)</i>	41.60 (25.30) <i>27.40 (16.90)</i>	55.20 (33.40) <i>39.80 (24.70)</i>
$R_{\text{merge}}$ (%)	7.90 (11.80) <i>7.80 (11.80)</i>	7.80 (11.80) <i>7.80 (11.90)</i>	7.60 (11.50) <i>7.50 (11.40)</i>	4.90 (7.60) <i>4.70 (7.50)</i>	4.80 (9.20) <i>4.70 (8.30)</i>	4.80 (9.10) <i>4.70 (8.20)</i>	6.10 (9.70) <i>5.90 (9.70)</i>	5.10 (9.30) <i>4.90 (8.40)</i>
$R_{\text{r.i.m.}}$ (%)	8.20 (12.40) <i>8.50 (13.20)</i>	8.20 (12.50) <i>8.50 (13.30)</i>	8.00 (12.20) <i>8.20 (13.00)</i>	5.10 (8.10) <i>5.10 (8.40)</i>	5.00 (9.80) <i>5.20 (9.50)</i>	5.00 (9.60) <i>5.20 (9.40)</i>	6.40 (10.30) <i>6.50 (11.10)</i>	5.30 (9.90) <i>5.40 (9.40)</i>
$R_{\text{p.i.m.}}$ (%)	2.30 (4.00) <i>3.30 (5.80)</i>	2.30 (4.00) <i>3.30 (5.80)</i>	2.30 (4.10) <i>3.40 (6.10)</i>	1.50 (2.60) <i>2.10 (3.80)</i>	1.50 (3.20) <i>2.10 (4.40)</i>	1.50 (3.20) <i>2.10 (4.30)</i>	1.90 (3.40) <i>2.70 (5.20)</i>	1.60 (3.30) <i>2.20 (4.30)</i>
$R_{\text{anom}}$ (%)	3.70 (4.60) <i>4.30 (5.70)</i>	3.70 (4.90) <i>4.40 (5.80)</i>	3.90 (5.30) <i>4.60 (6.90)</i>	3.60 (4.40) <i>3.80 (5.00)</i>	3.60 (4.70) <i>3.90 (5.20)</i>	3.60 (4.60) <i>3.90 (5.20)</i>	3.70 (4.70) <i>4.00 (5.70)</i>	3.70 (4.60) <i>4.00 (5.10)</i>

<b>G-He (<math>\lambda=2.40 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 2.22 (2.26 – 2.22)	99 – 2.22 (2.26 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)	99 – 2.22 (2.28 – 2.22)
Total no. of observations	213174 <i>106427</i>	213174 <i>106427</i>	227210 <i>112940</i>	227210 <i>112940</i>	227210 <i>112940</i>	227210 <i>112940</i>	227210 <i>112940</i>	227210 <i>112940</i>
Total no. of reflections	121318 <i>60332</i>	121010 <i>60438</i>	113178 <i>56439</i>	112742 <i>56211</i>	112894 <i>56261</i>	112883 <i>56257</i>	113092 <i>56408</i>	112442 <i>56071</i>
Unique reflections	11222 <i>11113</i>	11223 <i>11114</i>	11037 <i>10906</i>	11037 <i>10906</i>	11037 <i>10906</i>	11037 <i>10906</i>	11037 <i>10906</i>	10975 <i>10844</i>
Rejected reflections	1140 <i>171</i>	2022 <i>493</i>	152 <i>23</i>	129 <i>59</i>	71 <i>31</i>	70 <i>29</i>	19 <i>5</i>	54 <i>26</i>
Redundancy	10.81 <i>5.43</i>	10.78 <i>5.44</i>	10.25 <i>5.18</i>	10.21 <i>5.15</i>	10.23 <i>5.16</i>	10.23 <i>5.16</i>	10.25 <i>5.17</i>	10.25 <i>5.17</i>
Completeness [%]	99.20 (99.80) <i>98.20 (99.50)</i>	98.90 (99.70) <i>97.10 (98.10)</i>	97.00 (97.00) <i>96.00 (96.00)</i>	97.00 (97.00) <i>96.00 (96.00)</i>	97.00 (97.00) <i>96.00 (96.00)</i>	97.00 (97.00) <i>96.00 (96.00)</i>	97.00 (97.00) <i>96.00 (96.00)</i>	97.00 (97.00) <i>95.90 (95.90)</i>
I/ $\sigma$ (I)	19.99 (13.33) <i>13.94 (8.89)</i>	17.92 (10.74) <i>11.52 (6.65)</i>	28.10 (18.50) <i>19.20 (12.90)</i>	52.30 (34.70) <i>39.80 (26.80)</i>	50.20 (33.20) <i>38.00 (25.60)</i>	50.20 (33.20) <i>37.90 (25.60)</i>	36.60 (24.60) <i>24.80 (16.80)</i>	47.30 (32.40) <i>34.20 (23.70)</i>
R <sub>merge</sub> (%)	10.30 (14.00) <i>10.20 (12.90)</i>	10.30 (13.70) <i>10.30 (14.20)</i>	8.70 (12.70) <i>8.40 (12.20)</i>	5.30 (8.00) <i>4.90 (8.20)</i>	4.90 (9.80) <i>4.70 (8.50)</i>	4.90 (9.60) <i>4.70 (8.50)</i>	6.70 (10.30) <i>6.40 (10.30)</i>	5.30 (10.60) <i>5.10 (9.30)</i>
R <sub>r.i.m.</sub> (%)	10.80 (15.00) <i>11.20 (14.80)</i>	10.70 (14.70) <i>11.30 (16.30)</i>	9.10 (13.50) <i>9.30 (13.90)</i>	5.50 (8.50) <i>5.50 (9.20)</i>	5.10 (10.40) <i>5.30 (9.70)</i>	5.10 (10.20) <i>5.30 (9.60)</i>	7.10 (11.00) <i>7.10 (11.80)</i>	5.60 (11.20) <i>5.60 (10.50)</i>
R <sub>p.i.m.</sub> (%)	3.10 (5.20) <i>4.50 (7.20)</i>	3.10 (5.10) <i>4.50 (7.80)</i>	2.70 (4.50) <i>3.90 (6.60)</i>	1.60 (2.80) <i>2.30 (4.20)</i>	1.50 (3.40) <i>2.20 (4.50)</i>	1.50 (3.40) <i>2.20 (4.50)</i>	2.10 (3.70) <i>3.00 (5.60)</i>	1.70 (3.70) <i>2.40 (4.80)</i>
R <sub>anom</sub> (%)	4.20 (6.30) <i>5.40 (8.40)</i>	4.20 (6.20) <i>5.40 (9.10)</i>	3.90 (5.30) <i>4.90 (7.70)</i>	3.60 (4.30) <i>3.80 (5.20)</i>	3.50 (4.40) <i>3.80 (5.60)</i>	3.50 (4.40) <i>3.80 (5.50)</i>	3.70 (4.70) <i>4.10 (6.30)</i>	3.50 (4.30) <i>3.90 (5.60)</i>

<b>H-He (<math>\lambda=2.50 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 2.30 (2.34 – 2.30)	99 – 2.30 (2.34 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)	99 – 2.30 (2.36 – 2.30)
Total no. of observations	217832 <i>107562</i>	217832 <i>107562</i>	210429 <i>103841</i>	210429 <i>103841</i>	210429 <i>103841</i>	210429 <i>103841</i>	210429 <i>103841</i>	210429 <i>103841</i>
Total no. of reflections	120555 <i>59671</i>	118074 <i>58397</i>	102294 <i>50714</i>	101930 <i>50602</i>	102169 <i>50613</i>	102160 <i>50616</i>	102196 <i>50705</i>	101663 <i>50345</i>
Unique reflections	10146 <i>9992</i>	10146 <i>9993</i>	10178 <i>9999</i>	10178 <i>9999</i>	10178 <i>9999</i>	10178 <i>9999</i>	10178 <i>9999</i>	10111 <i>9932</i>
Rejected reflections	1816 <i>377</i>	1609 <i>262</i>	141 <i>15</i>	116 <i>25</i>	32 <i>20</i>	41 <i>18</i>	29 <i>4</i>	33 <i>18</i>
Redundancy	11.64 <i>5.85</i>	11.64 <i>5.84</i>	10.05 <i>5.07</i>	10.01 <i>5.06</i>	10.04 <i>5.06</i>	10.04 <i>5.06</i>	10.04 <i>5.07</i>	10.05 <i>5.07</i>
Completeness [%]	98.90 (100) <i>97.30 (99.80)</i>	98.80 (100) <i>97.30 (99.80)</i>	99.00 (99.00) <i>97.40 (97.40)</i>	99.00 (99.00) <i>97.40 (97.40)</i>	99.00 (99.00) <i>97.40 (97.40)</i>	99.00 (99.00) <i>97.40 (97.40)</i>	99.00 (99.00) <i>97.40 (97.40)</i>	99.00 (99.00) <i>97.40 (97.40)</i>
$I/\sigma(I)$	24.84 (28.76) <i>17.49 (20.67)</i>	20.67 (12.43) <i>17.49 (20.67)</i>	27.30 (14.30) <i>18.30 (9.90)</i>	53.70 (28.90) <i>36.70 (20.10)</i>	47.50 (25.00) <i>36.50 (19.80)</i>	47.60 (25.10) <i>36.40 (19.80)</i>	36.70 (19.80) <i>23.40 (12.80)</i>	45.40 (21.40) <i>32.80 (16.10)</i>
$R_{\text{merge}}$ (%)	9.10 (14.70) <i>8.60 (14.90)</i>	9.10 (15.10) <i>8.70 (15.50)</i>	8.90 (14.90) <i>8.50 (14.90)</i>	4.70 (9.90) <i>4.50 (10.10)</i>	4.40 (11.80) <i>4.30 (10.30)</i>	4.40 (11.70) <i>4.30 (10.30)</i>	6.80 (12.60) <i>6.40 (12.50)</i>	5.10 (12.60) <i>4.80 (11.40)</i>
$R_{\text{r.i.m.}}$ (%)	9.40 (15.50) <i>9.40 (16.80)</i>	9.50 (16.00) <i>9.50 (17.40)</i>	9.30 (15.90) <i>9.40 (17.20)</i>	4.90 (10.50) <i>5.00 (11.50)</i>	4.70 (12.60) <i>4.80 (11.80)</i>	4.70 (12.50) <i>4.80 (11.80)</i>	7.10 (13.40) <i>7.10 (14.40)</i>	5.30 (13.40) <i>5.40 (13.10)</i>
$R_{\text{p.i.m.}}$ (%)	2.60 (5.10) <i>3.70 (7.50)</i>	2.60 (5.20) <i>3.70 (7.80)</i>	2.80 (5.50) <i>4.00 (8.40)</i>	1.40 (3.50) <i>2.10 (5.40)</i>	1.40 (4.30) <i>2.00 (5.70)</i>	1.40 (4.30) <i>2.00 (5.70)</i>	2.10 (4.60) <i>3.00 (6.90)</i>	1.60 (4.60) <i>2.30 (6.20)</i>
$R_{\text{anom}}$ (%)	2.90 (4.20) <i>3.80 (6.10)</i>	2.90 (4.70) <i>3.90 (6.80)</i>	3.30 (5.30) <i>4.50 (8.40)</i>	2.80 (3.90) <i>3.10 (5.10)</i>	2.80 (4.30) <i>3.10 (5.50)</i>	2.80 (4.30) <i>3.10 (5.50)</i>	3.00 (4.50) <i>3.50 (6.30)</i>	2.90 (4.60) <i>3.30 (5.80)</i>



<b>I-He (<math>\lambda=2.65 \text{ \AA}</math>)</b>	<b>SCALEPACK-kB</b>	<b>SCALEPACK-ano</b>	<b>SCALA-Batch</b>	<b>SCALA-Det</b>	<b>SCALA-Abs</b>	<b>SCALA-Sec</b>	<b>SCALA-Baniso</b>	<b>SCALA-Ref</b>
Resolution limit [ $\text{\AA}$ ]	99 – 2.44 (2.48 – 2.44)	99 – 2.44 (2.48 – 2.44)	99 – 2.44 (2.50 – 2.44)	99 – 2.44 (2.50 – 2.44)	99 – 2.44 (2.50 – 2.44)	99 – 2.44 (2.50 – 2.44)	99 – 2.44 (2.50 – 2.44)	99 – 2.44 (2.50 – 2.44)
Total no. of observations	186255 92938	186255 92938	179509 85519	179509 85519	179509 85519	179509 85519	179509 85519	179509 85519
Total no. of reflections	100798 50376	100815 50396	86834 43504	86562 43466	86779 43472	86774 43470	86733 43499	86457 43283
Unique reflections	8600 8557	8600 8557	8627 8581	8627 8581	8627 8581	8627 8581	8627 8581	8579 8533
Rejected reflections	1191 151	1155 101	200 22	116 17	77 13	78 12	78 8	70 11
Redundancy	11.72 5.89	11.72 5.89	10.07 5.07	10.03 5.07	10.06 5.07	10.06 5.07	10.05 5.07	10.08 5.07
Completeness [%]	99.60 (100) 99.10 (100)	99.60 (100) 99.10 (100)	99.70 (99.70) 99.20 (99.20)	99.70 (99.70) 99.20 (99.20)	99.70 (99.70) 99.20 (99.20)	99.70 (99.70) 99.20 (99.20)	99.70 (99.70) 99.20 (99.20)	99.70 (99.70) 99.20 (99.20)
$I/\sigma(I)$	24.30 (15.10) 16.86 (10.39)	19.12 (10.78) 12.71 (7.17)	26.20 (12.30) 17.30 (8.30)	53.10 (25.60) 35.00 (17.10)	50.80 (23.90) 35.70 (17.30)	50.80 (23.90) 35.70 (17.20)	35.50 (17.20) 23.30 (11.50)	46.20 (17.50) 31.60 (12.50)
$R_{\text{merge}}$ (%)	9.60 (16.30) 9.50 (16.20)	9.60 (16.50) 9.50 (17.30)	9.40 (16.10) 9.40 (15.60)	4.30 (10.50) 4.20 (11.50)	3.80 (12.30) 3.70 (11.10)	3.80 (12.20) 3.80 (10.90)	6.80 (12.80) 6.60 (12.70)	4.60 (13.70) 4.50 (12.10)
$R_{\text{r.i.m.}}$ (%)	10.00 (17.30) 10.30 (18.20)	10.00 (17.50) 10.40 (19.40)	9.80 (17.20) 10.40 (18.00)	4.50 (11.20) 4.60 (13.10)	4.00 (13.20) 4.10 (12.80)	4.00 (13.00) 4.10 (12.50)	7.10 (13.70) 7.30 (14.60)	4.90 (14.70) 5.00 (13.80)
$R_{\text{p.i.m.}}$ (%)	2.80 (5.70) 4.00 (8.10)	2.80 (5.80) 4.00 (8.70)	2.90 (6.00) 4.30 (8.70)	1.30 (3.80) 1.90 (6.30)	1.20 (4.60) 1.70 (6.10)	1.20 (4.50) 1.70 (6.00)	2.10 (4.80) 3.00 (7.10)	1.50 (5.10) 2.10 (6.70)
$R_{\text{anom}}$ (%)	2.00 (4.70) 3.30 (6.70)	2.10 (5.30) 3.40 (7.80)	2.70 (5.40) 4.10 (9.00)	1.90 (3.40) 2.30 (4.90)	1.80 (4.30) 2.20 (6.00)	1.80 (4.30) 2.20 (5.90)	2.20 (4.50) 2.90 (6.70)	2.00 (4.60) 2.60 (7.00)

**Table 3. Anomalous difference Patterson syntheses for data sets A-Air to I-He.** The resolution range was 30.0 to 2.44 Å in all cases. The two columns of numbers refer to the full 360° of data and to the first 180° (in italics).

Data Set		A-Air ( $\lambda=0.80$ Å)	B-Air ( $\lambda=1.50$ Å)	C-Air ( $\lambda=1.70$ Å)	D-Air ( $\lambda=1.90$ Å)	E-Air ( $\lambda=2.10$ Å)	F-Air ( $\lambda=2.25$ Å)	G-Air ( $\lambda=2.40$ Å)	H-Air ( $\lambda=2.50$ Å)	I-Air ( $\lambda=2.65$ Å)
SCALEPACK- kB	No. of reflections	7156 <i>7121</i>	7108 <i>7059</i>	6993 <i>6960</i>	6933 <i>6825</i>	6915 <i>6856</i>	7120 <i>6910</i>	7037 <i>6856</i>	7106 <i>6934</i>	7109 <i>7032</i>
	$P_{\max}$	9.6 <i>17.5</i>	28.8 <i>37.9</i>	35.8 <i>46.1</i>	48.7 <i>63.9</i>	57.3 <i>72.1</i>	62.1 <i>77.9</i>	42.1 <i>57.4</i>	27.4 <i>45.3</i>	11.8 <i>29.7</i>
	$P_{\min}$	-1.4 <i>-3.9</i>	-3.0 <i>-5.8</i>	-3.9 <i>-7.3</i>	-4.7 <i>-8.4</i>	-5.1 <i>-9.4</i>	-6.2 <i>-8.9</i>	-4.8 <i>-6.8</i>	-3.6 <i>-6.6</i>	-2.4 <i>-6.4</i>
	Standard deviation [ $\sigma$ ]	0.11 <i>0.21</i>	0.27 <i>0.39</i>	0.32 <i>0.48</i>	0.48 <i>0.70</i>	0.53 <i>0.71</i>	0.56 <i>0.74</i>	0.40 <i>0.59</i>	0.27 <i>0.49</i>	0.11 <i>0.34</i>
SCALEPACK- ano	No. of reflections	7156 <i>7121</i>	7106 <i>7048</i>	6976 <i>6927</i>	6903 <i>6791</i>	6886 <i>6803</i>	7085 <i>6890</i>	7023 <i>6833</i>	7100 <i>6931</i>	7109 <i>7032</i>
	$P_{\max}$	9.7 <i>16.0</i>	28.1 <i>37.5</i>	35.5 <i>45.2</i>	48.2 <i>63.6</i>	55.8 <i>69.7</i>	61.8 <i>79.4</i>	44.1 <i>60.0</i>	28.3 <i>46.7</i>	12.7 <i>31.3</i>
	$P_{\min}$	-1.4 <i>-3.6</i>	-3.0 <i>-5.8</i>	-3.9 <i>-7.0</i>	-4.9 <i>-8.9</i>	-5.1 <i>-9.6</i>	-6.8 <i>-9.5</i>	-5.4 <i>-7.5</i>	-4.0 <i>-7.1</i>	-2.8 <i>-6.8</i>
	Standard deviation [ $\sigma$ ]	0.11 <i>0.19</i>	0.26 <i>0.38</i>	0.32 <i>0.47</i>	0.48 <i>0.71</i>	0.52 <i>0.70</i>	0.56 <i>0.77</i>	0.41 <i>0.61</i>	0.28 <i>0.49</i>	0.12 <i>0.34</i>
SCALA-Batch	No. of reflections	7154 <i>7110</i>	7110 <i>7007</i>	6996 <i>6912</i>	6920 <i>6799</i>	6913 <i>6780</i>	7086 <i>6739</i>	7032 <i>6656</i>	7090 <i>6721</i>	7093 <i>6686</i>
	$P_{\max}$	6.3 <i>11.5</i>	18.5 <i>23.8</i>	23.5 <i>29.1</i>	33.6 <i>43.6</i>	40.6 <i>54.0</i>	49.3 <i>70.1</i>	40.1 <i>62.1</i>	27.4 <i>53.0</i>	17.6 <i>46.5</i>
	$P_{\min}$	-0.9 <i>-2.3</i>	-1.7 <i>-3.0</i>	-2.5 <i>-4.1</i>	-3.5 <i>-5.7</i>	-3.9 <i>-7.9</i>	-6.1 <i>-9.3</i>	-4.9 <i>-9.6</i>	-4.1 <i>-9.2</i>	-4.6 <i>-10.9</i>
	Standard deviation [ $\sigma$ ]	0.07 <i>0.15</i>	0.17 <i>0.23</i>	0.22 <i>0.29</i>	0.32 <i>0.46</i>	0.38 <i>0.53</i>	0.56 <i>0.70</i>	0.40 <i>0.67</i>	0.31 <i>0.68</i>	0.22 <i>0.63</i>
SCALA-Baniso	No. of reflections	7154 <i>7110</i>	7110 <i>7007</i>	6996 <i>6908</i>	6916 <i>6793</i>	6911 <i>6772</i>	7080 <i>6724</i>	7032 <i>6654</i>	7090 <i>6720</i>	7093 <i>6685</i>
	$P_{\max}$	6.2 <i>11.4</i>	18.0 <i>22.8</i>	22.5 <i>27.0</i>	31.1 <i>38.1</i>	36.4 <i>44.0</i>	41.4 <i>52.6</i>	30.8 <i>41.2</i>	19.1 <i>30.0</i>	8.6 <i>20.1</i>
	$P_{\min}$	-0.9 <i>-2.3</i>	-1.6 <i>-2.8</i>	-2.3 <i>-3.7</i>	-3.1 <i>-4.5</i>	-3.0 <i>-5.4</i>	-4.0 <i>-5.8</i>	-2.7 <i>-5.0</i>	-1.8 <i>-3.9</i>	-1.1 <i>-3.7</i>
	Standard deviation [ $\sigma$ ]	0.07 <i>0.15</i>	0.17 <i>0.23</i>	0.21 <i>0.27</i>	0.30 <i>0.40</i>	0.34 <i>0.43</i>	0.40 <i>0.53</i>	0.30 <i>0.43</i>	0.21 <i>0.34</i>	0.10 <i>0.27</i>
SCALA-Det	No. of reflections	7154 <i>7110</i>	7109 <i>7005</i>	6994 <i>6896</i>	6914 <i>6769</i>	6899 <i>6743</i>	7060 <i>6672</i>	7025 <i>6634</i>	7088 <i>6714</i>	7093 <i>6684</i>
	$P_{\max}$	6.2 <i>11.2</i>	18.0 <i>22.5</i>	22.7 <i>26.4</i>	32.1 <i>38.0</i>	37.2 <i>42.9</i>	42.5 <i>49.9</i>	32.7 <i>39.4</i>	20.4 <i>26.9</i>	8.7 <i>16.0</i>
	$P_{\min}$	-0.9 <i>-2.2</i>	-1.6 <i>-2.6</i>	-2.2 <i>-3.2</i>	-3.0 <i>-3.8</i>	-3.0 <i>-4.6</i>	-3.7 <i>-4.8</i>	-3.2 <i>-4.1</i>	-1.8 <i>-2.9</i>	-1.0 <i>-2.0</i>
	Standard deviation [ $\sigma$ ]	0.07 <i>0.15</i>	0.17 <i>0.22</i>	0.21 <i>0.26</i>	0.30 <i>0.41</i>	0.34 <i>0.41</i>	0.39 <i>0.49</i>	0.31 <i>0.41</i>	0.20 <i>0.29</i>	0.09 <i>0.19</i>
SCALA-Abs	No. of reflections	7154 <i>7109</i>	7110 <i>7006</i>	6994 <i>6900</i>	6916 <i>6776</i>	6899 <i>6750</i>	7061 <i>6675</i>	7025 <i>6637</i>	7087 <i>6714</i>	7093 <i>6684</i>
	$P_{\max}$	6.3 <i>11.5</i>	18.5 <i>23.1</i>	23.4 <i>27.5</i>	33.2 <i>39.7</i>	39.0 <i>45.1</i>	44.8 <i>52.6</i>	34.7 <i>42.3</i>	21.7 <i>28.1</i>	9.5 <i>17.9</i>
	$P_{\min}$	-0.9 <i>-2.3</i>	-1.7 <i>-2.7</i>	-2.3 <i>-3.5</i>	-3.1 <i>-4.3</i>	-3.1 <i>-4.8</i>	-3.9 <i>-4.9</i>	-3.1 <i>-4.4</i>	-1.9 <i>-2.8</i>	-1.2 <i>-2.4</i>
	Standard deviation [ $\sigma$ ]	0.07 <i>0.15</i>	0.17 <i>0.23</i>	0.21 <i>0.27</i>	0.32 <i>0.43</i>	0.36 <i>0.43</i>	0.41 <i>0.52</i>	0.32 <i>0.42</i>	0.22 <i>0.29</i>	0.10 <i>0.21</i>
SCALA-Sec	No. of reflections	7154 <i>7110</i>	7110 <i>7006</i>	6994 <i>6900</i>	6916 <i>6776</i>	6899 <i>6750</i>	7061 <i>6677</i>	7026 <i>6636</i>	7087 <i>6714</i>	7092 <i>6684</i>
	$P_{\max}$	6.3 <i>11.5</i>	18.5 <i>23.1</i>	23.4 <i>27.5</i>	33.2 <i>39.7</i>	39.0 <i>45.2</i>	44.9 <i>53.0</i>	34.8 <i>42.5</i>	21.8 <i>28.2</i>	9.4 <i>17.6</i>
	$P_{\min}$	-0.9 <i>-2.3</i>	-1.7 <i>-2.7</i>	-2.3 <i>-3.5</i>	-3.1 <i>-4.3</i>	-3.1 <i>-4.8</i>	-3.9 <i>-5.0</i>	-3.1 <i>-4.5</i>	-1.9 <i>-2.9</i>	-1.2 <i>-2.3</i>
	Standard deviation [ $\sigma$ ]	0.07 <i>0.15</i>	0.17 <i>0.23</i>	0.21 <i>0.27</i>	0.32 <i>0.43</i>	0.36 <i>0.43</i>	0.41 <i>0.52</i>	0.32 <i>0.42</i>	0.22 <i>0.29</i>	0.10 <i>0.21</i>
SCALA-Ref	No. of reflections	-	7127 <i>7022</i>	7012 <i>6917</i>	6934 <i>6794</i>	6918 <i>6764</i>	7080 <i>6703</i>	7032 <i>6648</i>	7084 <i>6713</i>	7092 <i>6684</i>
	$P_{\max}$	-	19.5 <i>24.2</i>	25.2 <i>29.6</i>	36.1 <i>42.6</i>	47.2 <i>52.3</i>	60.4 <i>66.9</i>	53.9 <i>61.6</i>	36.3 <i>47.4</i>	22.0 <i>44.8</i>
	$P_{\min}$	-	-1.9 <i>-2.9</i>	-2.6 <i>-3.9</i>	-3.5 <i>-4.6</i>	-4.1 <i>-5.7</i>	-6.1 <i>-6.5</i>	-5.9 <i>-6.4</i>	-4.4 <i>-6.0</i>	-4.8 <i>-10.5</i>
	Standard deviation [ $\sigma$ ]	-	0.18 <i>0.24</i>	0.23 <i>0.29</i>	0.34 <i>0.44</i>	0.43 <i>0.49</i>	0.53 <i>0.63</i>	0.48 <i>0.59</i>	0.39 <i>0.50</i>	0.24 <i>0.60</i>

Data Set	Scaling Protocol	-	B-He	C-He	D-He	E-He	F-He	G-He	H-He	I-He
			( $\lambda=1.50 \text{ \AA}$ )	( $\lambda=1.70 \text{ \AA}$ )	( $\lambda=1.90 \text{ \AA}$ )	( $\lambda=2.10 \text{ \AA}$ )	( $\lambda=2.25 \text{ \AA}$ )	( $\lambda=2.40 \text{ \AA}$ )	( $\lambda=2.50 \text{ \AA}$ )	( $\lambda=2.65 \text{ \AA}$ )
SCALEPACK-kB	No. of reflections	-	6771 6720	6518 6382	6265 6144	6803 6564	6846 6547	6892 6795	7097 6939	7178 7135
	$P_{\max}$	-	15.1 16.5	17.5 19.3	28.6 30.6	33.3 33.0	34.0 36.0	25.0 32.2	13.1 20.0	4.9 11.2
	$P_{\min}$	-	-1.3 -1.6	-1.4 -1.8	-3.2 -3.0	-2.6 -3.0	-3.3 -3.4	-2.7 -4.0	-1.2 -3.4	-0.7 -2.8
	Standard deviation [ $\sigma$ ]	-	0.14 0.16	0.18 0.20	0.45 0.32	0.36 0.34	0.34 0.37	0.28 0.34	0.14 0.24	0.05 0.15
SCALEPACK-ano	No. of reflections	-	6819 6758	6570 6410	6239 6103	6769 6515	6814 6499	6885 6774	7098 6929	7177 7135
	$P_{\max}$	-	14.7 16.2	18.0 19.6	27.9 29.4	32.4 32.3	33.4 35.8	25.7 33.6	13.5 20.5	5.3 12.3
	$P_{\min}$	-	-1.2 -1.5	-1.4 -1.9	-3.3 -2.9	-2.7 -3.2	-3.2 -3.5	-2.9 -4.3	-1.4 -3.6	-1.0 -3.2
	Standard deviation [ $\sigma$ ]	-	0.14 0.15	0.19 0.21	0.46 0.30	0.35 0.33	0.33 0.37	0.30 0.36	0.15 0.25	0.06 0.16
SCALA-Batch	No. of reflections	-	6767 6718	6505 6345	6255 6133	6806 6561	6845 6525	6851 6695	7094 6841	7167 7032
	$P_{\max}$	-	8.5 9.4	9.1 9.4	15.2 17.8	21.1 19.4	24.8 27.5	26.3 35.6	14.8 25.2	8.8 19.2
	$P_{\min}$	-	-0.6 -0.8	-0.7 -0.8	-1.4 -1.8	-2.0 -1.9	-2.4 -3.2	-3.6 -6.1	-2.2 -5.2	-1.7 -4.6
	Standard deviation [ $\sigma$ ]	-	0.08 0.09	0.09 0.09	0.15 0.18	0.21 0.19	0.25 0.28	0.39 0.41	0.16 0.33	0.14 0.26
SCALA-Baniso	No. of reflections	-	6763 6712	6499 6340	6252 6124	6792 6547	6839 6518	6848 6690	7094 6841	7166 7032
	$P_{\max}$	-	8.3 8.9	8.7 8.7	14.3 15.8	18.8 16.0	22.0 21.0	21.7 24.3	11.2 14.4	4.9 8.3
	$P_{\min}$	-	-0.6 -0.7	-0.7 -0.8	-1.3 -1.6	-1.4 -1.5	-1.7 -1.9	-2.4 -3.0	-1.0 -2.1	-0.6 -1.3
	Standard deviation [ $\sigma$ ]	-	0.08 0.08	0.08 0.09	0.14 0.16	0.19 0.16	0.22 0.22	0.28 0.26	0.13 0.17	0.07 0.12
SCALA-Det	No. of reflections	-	6749 6684	6490 6294	6224 6081	6752 6481	6790 6422	6823 6629	7087 6824	7167 7032
	$P_{\max}$	-	8.2 8.7	8.8 8.4	14.4 15.4	18.7 15.2	21.1 19.1	20.3 21.7	10.6 12.3	4.1 5.7
	$P_{\min}$	-	-0.6 -0.7	-0.7 -0.8	-1.2 -1.6	-1.5 -1.3	-1.6 -1.7	-2.0 -2.4	-0.9 -1.3	-0.5 -0.7
	Standard deviation [ $\sigma$ ]	-	0.08 0.08	0.08 0.08	0.14 0.15	0.18 0.15	0.21 0.19	0.22 0.22	0.11 0.14	0.08 0.07
SCALA-Abs	No. of reflections	-	6756 6691	6495 6311	6231 6092	6756 6487	6790 6436	6819 6636	7090 6824	7165 7032
	$P_{\max}$	-	8.3 8.9	8.9 8.5	14.7 16.1	19.2 15.9	21.9 20.4	20.7 22.7	11.2 12.9	4.1 6.1
	$P_{\min}$	-	-0.6 -0.7	-0.7 -0.8	-1.3 -1.5	-1.5 -1.4	-1.8 -1.9	-1.8 -2.2	-0.8 -1.2	-0.4 -0.6
	Standard deviation [ $\sigma$ ]	-	0.08 0.08	0.09 0.08	0.15 0.16	0.18 0.15	0.21 0.20	0.21 0.23	0.12 0.14	0.04 0.07
SCALA-Sec	No. of reflections	-	6756 6691	6495 6311	6232 6092	6756 6487	6790 6437	6820 6636	7090 6824	7165 7032
	$P_{\max}$	-	8.3 8.9	8.9 8.6	14.7 16.1	19.2 15.9	22.0 20.5	20.7 22.8	11.3 13.0	4.1 6.1
	$P_{\min}$	-	-0.6 -0.7	-0.7 -0.8	-1.3 -1.5	-1.5 -1.4	-1.8 -1.9	-1.8 -2.2	-0.9 -1.2	-0.4 -0.6
	Standard deviation [ $\sigma$ ]	-	0.08 0.08	0.09 0.08	0.15 0.16	0.18 0.15	0.21 0.20	0.21 0.23	0.12 0.14	0.04 0.07
SCALA-Ref	No. of reflections	-	6734 6672	6470 6286	6203 6066	6735 6464	6766 6424	6788 6619	7044 6786	7122 6987
	$P_{\max}$	-	10.2 11.0	11.5 10.9	28.7 21.0	28.4 23.0	36.2 31.0	37.3 40.1	25.4 27.9	13.5 22.4
	$P_{\min}$	-	-0.80 -1.08	-1.0 -1.1	-2.6 -1.9	-2.7 -2.3	-3.4 -3.6	-3.8 -5.0	-2.5 -3.4	-1.9 -4.5
	Standard deviation [ $\sigma$ ]	-	0.09 0.10	0.11 0.10	0.27 0.20	0.25 0.21	0.32 0.28	0.34 0.37	0.23 0.26	0.36 0.26