Table 5 Observed and calculated structure factors for 1



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 0 | 1 | 0 | 408 | 409 | 9 |
| -1 | 2 | 0 | 1265 | 1234 | 77 |
| 0 | 2 | 0 | 1483 | 1426 | 18 |
| -1 | 3 | 0 | 665 | 646 | 17 |
| 0 | 3 | 0 | 630 | 575 | 13 |
| -2 | 4 | 0 | 3326 | 3206 | 144 |
| -1 | 4 | 0 | 1211 | 1112 | 17 |
| 0 | 4 | 0 | 1672 | 1520 | 24 |
| -2 | 5 | 0 | 1226 | 1169 | 25 |
| -1 | 5 | 0 | 3222 | 3040 | 69 |
| 0 | 5 | 0 | 1087 | 1057 | 9 |
| -3 | 6 | 0 | 1328 | 1283 | 72 |
| -2 | 6 | 0 | 133 | 91 | 18 |
| -1 | 6 | 0 | 420 | 403 | 14 |
| 0 | 6 | 0 | 1384 | 1326 | 17 |
| -3 | 7 | 0 | 149 | 147 | 24 |
| -2 | 7 | 0 | 2065 | 2012 | 54 |
| -1 | 7 | 0 | 1147 | 1140 | 19 |
| 0 | 7 | 0 | 2124 | 2119 | 33 |
| -4 | 8 | 0 | 521 | 501 | 22 |
| -3 | 8 | 0 | 14 | 125 | -14 |
| -2 | 8 | 0 | 628 | 627 | 21 |
| -1 | 8 | 0 | 784 | 785 | 12 |
| 0 | 8 | 0 | 1891 | 1887 | 27 |
| -4 | 9 | 0 | 451 | 445 | 14 |
| -3 | 9 | 0 | 2373 | 2322 | 62 |
| -2 | 9 | 0 | 862 | 871 | 18 |
| -1 | 9 | 0 | 192 | 194 | 17 |
| 0 | 9 | 0 | 562 | 558 | 12 |
| -5 | 10 | 0 | 934 | 943 | 46 |
| -4 | 10 | 0 | 709 | 705 | 13 |
| -3 | 10 | 0 | 149 | 161 | 22 |
| -2 | 10 | 0 | 1284 | 1279 | 28 |
| -1 | 10 | 0 | 769 | 791 | 19 |
| 0 | 10 | 0 | 316 | 316 | 15 |
| -5 | 11 | 0 | 835 | 823 | 30 |
| -4 | 11 | 0 | 761 | 755 | 17 |
| -3 | 11 | 0 | 348 | 336 | 13 |
| -1 | 2 | 1 | 189 | 191 | 21 |
| -2 | 3 | 1 | 1434 | 1405 | 33 |
| -1 | 3 | 1 | 1075 | 1045 | 30 |
| -3 | 4 | 1 | 144 | 172 | 13 |
| -2 | 4 | 1 | 101 | 127 | 17 |
| -1 | 4 | 1 | 163 | 181 | 15 |
| -4 | 5 | 1 | 2918 | 2809 | 55 |
| -3 | 5 | 1 | 651 | 607 | 21 |
| -2 | 5 | 1 | 614 | 582 | 11 |
| -1 | 5 | 1 | 2824 | 2719 | 55 |
| -5 | 6 | 1 | 344 | 341 | 7 |
| -4 | 6 | 1 | 585 | 588 | 18 |
| -3 | 6 | 1 | 466 | 448 | 18 |
| -2 | 6 | 1 | 743 | 736 | 14 |
| -1 | 6 | 1 | 274 | 259 | 9 |
| -6 | 7 | 1 | 213 | 209 | 14 |
| -5 | 7 | 1 | 946 | 928 | 24 |
| -4 | 7 | 1 | 398 | 385 | 13 |
| -3 | 7 | 1 | 405 | 403 | 12 |
| -2 | 7 | 1 | 982 | 977 | 27 |
| -1 | 7 | 1 | 284 | 276 | 11 |
| -7 | 8 | 1 | 383 | 385 | 9 |
| -6 | 8 | 1 | 137 | 137 | 20 |
| -5 | 8 | 1 | 632 | 625 | 17 |
| -4 | 8 | 1 | 112 | 114 | -20 |
| -3 | 8 | 1 | 658 | 656 | 22 |
| -2 | 8 | 1 | 187 | 184 | 15 |
| -1 | 8 | 1 | 313 | 299 | 14 |
| -8 | 9 | 1 | 15 | 164 | -14 |
| -7 | 9 | 1 | 362 | 368 | 9 |
| -6 | 9 | 1 | 350 | 342 | 13 |
| -5 | 9 | 1 | 484 | 472 | 16 |
| -4 | 9 | 1 | 444 | 446 | 12 |
| -3 | 9 | 1 | 414 | 403 | 11 |
| -2 | 9 | 1 | 429 | 425 | 11 |
| -1 | 9 | 1 | 135 | 144 | 21 |
| -9 | 10 | 1 | 360 | 367 | 11 |
| -8 | 10 | 1 | 833 | 831 | 16 |
| -7 | 10 | 1 | 291 | 271 | 18 |
| -6 | 10 | 1 | 277 | 292 | 21 |
| -5 | 10 | 1 | 129 | 159 | -24 |
| -4 | 10 | 1 | 222 | 217 | 18 |
| -3 | 10 | 1 | 223 | 231 | 17 |
| -2 | 10 | 1 | 876 | 863 | 24 |
| -1 | 10 | 1 | 488 | 475 | 8 |
| -8 | 11 | 1 | 244 | 254 | 20 |
| -7 | 11 | 1 | 314 | 287 | 15 |
| -6 | 11 | 1 | 875 | 853 | 32 |
| -5 | 11 | 1 | 668 | 657 | 16 |
| -4 | 11 | 1 | 333 | 341 | 12 |
| -3 | 11 | 1 | 324 | 330 | 12 |
| -1 | 1 | 2 | 879 | 863 | 11 |
| 0 | 1 | 2 | 727 | 707 | 7 |
| -2 | 2 | 2 | 1451 | 1414 | 13 |
| -1 | 2 | 2 | 357 | 340 | 16 |
| 0 | 2 | 2 | 1530 | 1472 | 22 |
| -3 | 3 | 2 | 243 | 233 | 12 |
| -2 | 3 | 2 | 1763 | 1706 | 45 |
| -1 | 3 | 2 | 1300 | 1268 | 32 |
| 0 | 3 | 2 | 266 | 243 | 9 |
| -4 | 4 | 2 | 345 | 360 | 15 |
| -3 | 4 | 2 | 342 | 355 | 6 |
| -2 | 4 | 2 | 1357 | 1300 | 38 |
| -1 | 4 | 2 | 452 | 446 | 17 |
| 0 | 4 | 2 | 422 | 429 | 6 |
| -5 | 5 | 2 | 267 | 250 | 9 |
| -4 | 5 | 2 | 662 | 642 | 12 |
| -3 | 5 | 2 | 678 | 653 | 16 |
| -2 | 5 | 2 | 706 | 681 | 9 |
| -1 | 5 | 2 | 722 | 699 | 15 |
| 0 | 5 | 2 | 248 | 223 | 25 |
| -6 | 6 | 2 | 1029 | 1020 | 12 |
| -5 | 6 | 2 | 208 | 210 | 16 |
| -4 | 6 | 2 | 1975 | 1914 | 46 |
| -3 | 6 | 2 | 490 | 466 | 20 |
| -2 | 6 | 2 | 2447 | 2379 | 67 |
| -1 | 6 | 2 | 285 | 275 | 8 |
| 0 | 6 | 2 | 1149 | 1116 | 15 |
| -7 | 7 | 2 | 1782 | 1785 | 22 |
| -6 | 7 | 2 | 689 | 678 | 6 |
| -5 | 7 | 2 | 278 | 274 | 16 |
| -4 | 7 | 2 | 267 | 230 | 10 |
| -3 | 7 | 2 | 262 | 256 | 14 |
| -2 | 7 | 2 | 333 | 324 | 13 |
| -1 | 7 | 2 | 799 | 792 | 13 |
| 0 | 7 | 2 | 1689 | 1694 | 25 |
| -8 | 8 | 2 | 1778 | 1792 | 35 |
| -7 | 8 | 2 | 129 | 146 | -25 |
| -6 | 8 | 2 | 483 | 499 | 16 |
| -5 | 8 | 2 | 760 | 736 | 19 |
| -4 | 8 | 2 | 254 | 229 | 19 |
| -3 | 8 | 2 | 610 | 589 | 20 |
| -2 | 8 | 2 | 566 | 585 | 16 |
| -1 | 8 | 2 | 153 | 166 | 25 |
| 0 | 8 | 2 | 1751 | 1756 | 33 |
| -9 | 9 | 2 | 359 | 353 | 12 |
| -8 | 9 | 2 | 254 | 244 | 22 |
| -7 | 9 | 2 | 232 | 234 | 19 |
| -6 | 9 | 2 | 333 | 323 | 9 |
| -5 | 9 | 2 | 174 | 158 | 23 |
| -4 | 9 | 2 | 181 | 147 | 20 |
| -3 | 9 | 2 | 312 | 308 | 12 |
| -2 | 9 | 2 | 285 | 286 | 11 |
| -1 | 9 | 2 | 244 | 210 | 16 |
| 0 | 9 | 2 | 320 | 335 | 13 |
| -10 | 10 | 2 | 511 | 495 | 11 |
| -9 | 10 | 2 | 775 | 789 | 14 |
| -8 | 10 | 2 | 171 | 144 | 19 |
| -7 | 10 | 2 | 371 | 384 | 11 |
| -6 | 10 | 2 | 968 | 959 | 27 |
| -5 | 10 | 2 | 137 | 85 | -35 |
| -4 | 10 | 2 | 971 | 977 | 21 |
| -3 | 10 | 2 | 406 | 405 | 15 |
| -2 | 10 | 2 | 187 | 186 | 27 |
| -1 | 10 | 2 | 667 | 686 | 17 |
| 0 | 10 | 2 | 445 | 445 | 18 |
| -8 | 11 | 2 | 232 | 235 | 16 |
| -7 | 11 | 2 | 208 | 198 | 17 |
| -6 | 11 | 2 | 515 | 516 | 9 |
| -5 | 11 | 2 | 514 | 506 | 19 |
| -4 | 11 | 2 | 269 | 232 | 19 |
| -3 | 11 | 2 | 295 | 293 | 13 |
| -1 | 2 | 3 | 115 | 36 | -24 |
| -2 | 3 | 3 | 2507 | 2404 | 47 |
| -1 | 3 | 3 | 2035 | 1919 | 45 |
| -3 | 4 | 3 | 710 | 767 | 10 |
| -2 | 4 | 3 | 167 | 173 | 10 |
| -1 | 4 | 3 | 586 | 644 | 10 |
| -4 | 5 | 3 | 2186 | 2101 | 34 |
| -3 | 5 | 3 | 884 | 861 | 15 |
| -2 | 5 | 3 | 892 | 878 | 16 |
| -1 | 5 | 3 | 2259 | 2146 | 49 |
| -5 | 6 | 3 | 1334 | 1312 | 22 |
| -4 | 6 | 3 | 800 | 794 | 19 |
| -3 | 6 | 3 | 261 | 274 | 9 |
| -2 | 6 | 3 | 784 | 762 | 24 |
| -1 | 6 | 3 | 1432 | 1380 | 28 |
| -6 | 7 | 3 | 676 | 675 | 12 |
| -5 | 7 | 3 | 899 | 891 | 21 |
| -4 | 7 | 3 | 1025 | 1011 | 28 |
| -3 | 7 | 3 | 1152 | 1128 | 34 |
| -2 | 7 | 3 | 945 | 940 | 22 |
| -1 | 7 | 3 | 593 | 594 | 11 |
| -8 | 8 | 3 | 242 | 251 | 13 |
| -6 | 8 | 3 | 104 | 134 | -26 |
| -5 | 8 | 3 | 1844 | 1841 | 55 |
| -4 | 8 | 3 | 188 | 190 | 18 |
| -3 | 8 | 3 | 1389 | 1388 | 42 |
| -2 | 8 | 3 | 120 | 100 | -26 |
| -1 | 8 | 3 | 232 | 260 | 17 |
| -8 | 9 | 3 | 240 | 237 | 13 |
| -7 | 9 | 3 | 387 | 390 | 19 |
| -6 | 9 | 3 | 92 | 46 | -27 |
| -5 | 9 | 3 | 606 | 598 | 19 |
| -4 | 9 | 3 | 665 | 664 | 16 |
| -3 | 9 | 3 | 134 | 51 | -32 |
| -2 | 9 | 3 | 311 | 299 | 10 |
| -1 | 9 | 3 | 305 | 309 | 11 |
| -9 | 10 | 3 | 391 | 377 | 10 |
| -8 | 10 | 3 | 428 | 400 | 14 |
| -7 | 10 | 3 | 458 | 457 | 10 |
| -6 | 10 | 3 | 420 | 413 | 15 |
| -5 | 10 | 3 | 150 | 109 | 20 |
| -4 | 10 | 3 | 334 | 316 | 18 |
| -3 | 10 | 3 | 353 | 342 | 16 |
| -2 | 10 | 3 | 410 | 411 | 12 |
| -1 | 10 | 3 | 330 | 344 | 12 |
| -8 | 11 | 3 | 175 | 166 | 27 |
| -7 | 11 | 3 | 256 | 247 | 21 |
| -6 | 11 | 3 | 829 | 831 | 24 |
| -5 | 11 | 3 | 774 | 781 | 23 |
| -4 | 11 | 3 | 360 | 332 | 11 |
| -3 | 11 | 3 | 155 | 125 | 23 |
| 0 | 0 | 4 | 265 | 330 | 18 |
| -1 | 1 | 4 | 525 | 551 | 4 |
| 0 | 1 | 4 | 692 | 715 | 5 |
| -2 | 2 | 4 | 103 | 105 | -57 |
| -1 | 2 | 4 | 230 | 197 | 11 |
| 0 | 2 | 4 | 118 | 101 | 20 |
| -3 | 3 | 4 | 401 | 391 | 6 |
| -2 | 3 | 4 | 510 | 474 | 8 |
| -1 | 3 | 4 | 691 | 637 | 18 |
| 0 | 3 | 4 | 399 | 406 | 7 |
| -4 | 4 | 4 | 1882 | 1780 | 17 |
| -3 | 4 | 4 | 405 | 401 | 7 |
| -2 | 4 | 4 | 1097 | 1136 | 27 |
| -1 | 4 | 4 | 552 | 526 | 7 |
| 0 | 4 | 4 | 1940 | 1815 | 27 |
| -5 | 5 | 4 | 739 | 729 | 9 |
| -4 | 5 | 4 | 1561 | 1537 | 24 |
| -3 | 5 | 4 | 161 | 147 | 13 |
| -2 | 5 | 4 | 187 | 189 | 10 |
| -1 | 5 | 4 | 1503 | 1465 | 29 |
| 0 | 5 | 4 | 695 | 679 | 11 |
| -6 | 6 | 4 | 2369 | 2367 | 28 |
| -5 | 6 | 4 | 863 | 851 | 14 |
| -4 | 6 | 4 | 918 | 906 | 21 |
| -3 | 6 | 4 | 790 | 752 | 24 |
| -2 | 6 | 4 | 863 | 839 | 25 |
| -1 | 6 | 4 | 1133 | 1091 | 29 |
| 0 | 6 | 4 | 2209 | 2185 | 35 |
| -7 | 7 | 4 | 401 | 393 | 10 |
| -6 | 7 | 4 | 723 | 728 | 17 |
| -5 | 7 | 4 | 704 | 696 | 24 |
| -4 | 7 | 4 | 459 | 436 | 11 |
| -3 | 7 | 4 | 551 | 532 | 15 |
| -2 | 7 | 4 | 597 | 598 | 15 |
| -1 | 7 | 4 | 560 | 562 | 11 |
| 0 | 7 | 4 | 326 | 305 | 22 |
| -8 | 8 | 4 | 484 | 489 | 21 |
| -7 | 8 | 4 | 349 | 347 | 9 |
| -6 | 8 | 4 | 965 | 957 | 21 |
| -5 | 8 | 4 | 373 | 347 | 17 |
| -4 | 8 | 4 | 1221 | 1208 | 34 |
| -3 | 8 | 4 | 451 | 424 | 10 |
| -2 | 8 | 4 | 896 | 870 | 23 |
| -1 | 8 | 4 | 403 | 407 | 9 |
| 0 | 8 | 4 | 605 | 613 | 8 |
| -9 | 9 | 4 | 761 | 758 | 12 |
| -8 | 9 | 4 | 276 | 279 | 20 |
| -7 | 9 | 4 | 239 | 251 | 12 |
| -6 | 9 | 4 | 1278 | 1259 | 39 |
| -5 | 9 | 4 | 273 | 289 | 11 |
| -4 | 9 | 4 | 331 | 344 | 14 |
| -3 | 9 | 4 | 1409 | 1385 | 40 |
| -2 | 9 | 4 | 246 | 240 | 25 |
| -1 | 9 | 4 | 380 | 373 | 9 |
| 0 | 9 | 4 | 743 | 743 | 7 |
| -9 | 10 | 4 | 366 | 370 | 12 |
| -8 | 10 | 4 | 501 | 498 | 12 |
| -7 | 10 | 4 | 296 | 276 | 12 |
| -6 | 10 | 4 | 486 | 481 | 14 |
| -5 | 10 | 4 | 176 | 141 | 23 |
| -4 | 10 | 4 | 559 | 572 | 13 |
| -3 | 10 | 4 | 379 | 371 | 16 |
| -2 | 10 | 4 | 570 | 561 | 9 |
| -1 | 10 | 4 | 276 | 275 | 13 |
| -8 | 11 | 4 | 211 | 210 | 19 |
| -7 | 11 | 4 | 446 | 440 | 15 |
| -6 | 11 | 4 | 172 | 176 | 19 |
| -5 | 11 | 4 | 133 | 132 | -27 |
| -4 | 11 | 4 | 451 | 419 | 14 |
| -3 | 11 | 4 | 134 | 157 | -25 |
| -1 | 2 | 5 | 106 | 93 | -24 |
| -2 | 3 | 5 | 2023 | 1994 | 29 |
| -1 | 3 | 5 | 1729 | 1696 | 29 |
| -3 | 4 | 5 | 674 | 627 | 12 |
| -2 | 4 | 5 | 285 | 286 | 6 |
| -1 | 4 | 5 | 511 | 479 | 12 |
| -4 | 5 | 5 | 1136 | 1137 | 20 |
| -3 | 5 | 5 | 148 | 176 | 18 |
| -2 | 5 | 5 | 246 | 230 | 16 |
| -1 | 5 | 5 | 1266 | 1246 | 23 |
| -5 | 6 | 5 | 844 | 848 | 18 |
| -4 | 6 | 5 | 695 | 664 | 16 |
| -3 | 6 | 5 | 944 | 926 | 23 |
| -2 | 6 | 5 | 910 | 889 | 24 |
| -1 | 6 | 5 | 844 | 842 | 15 |
| -6 | 7 | 5 | 288 | 287 | 11 |
| -5 | 7 | 5 | 1093 | 1087 | 27 |
| -4 | 7 | 5 | 883 | 884 | 22 |
| -3 | 7 | 5 | 712 | 709 | 18 |
| -2 | 7 | 5 | 1084 | 1079 | 30 |
| -1 | 7 | 5 | 395 | 381 | 7 |
| -7 | 8 | 5 | 392 | 403 | 8 |
| -6 | 8 | 5 | 296 | 296 | 10 |
| -5 | 8 | 5 | 480 | 468 | 8 |
| -4 | 8 | 5 | 662 | 662 | 21 |
| -3 | 8 | 5 | 638 | 623 | 23 |
| -2 | 8 | 5 | 276 | 266 | 10 |
| -1 | 8 | 5 | 378 | 379 | 8 |
| -8 | 9 | 5 | 312 | 321 | 10 |
| -7 | 9 | 5 | 310 | 320 | 10 |
| -6 | 9 | 5 | 2062 | 2044 | 48 |
| -5 | 9 | 5 | 860 | 861 | 23 |
| -4 | 9 | 5 | 696 | 700 | 25 |
| -3 | 9 | 5 | 1888 | 1890 | 56 |
| -2 | 9 | 5 | 336 | 341 | 9 |
| -1 | 9 | 5 | 291 | 288 | 11 |
| -9 | 10 | 5 | 345 | 343 | 11 |
| -8 | 10 | 5 | 1122 | 1124 | 20 |
| -7 | 10 | 5 | 603 | 597 | 11 |
| -6 | 10 | 5 | 185 | 198 | -36 |
| -5 | 10 | 5 | 316 | 333 | 17 |
| -4 | 10 | 5 | 157 | 168 | -31 |
| -3 | 10 | 5 | 513 | 520 | 15 |
| -2 | 10 | 5 | 1123 | 1136 | 30 |
| -1 | 10 | 5 | 428 | 408 | 9 |
| -8 | 11 | 5 | 267 | 238 | 14 |
| -7 | 11 | 5 | 982 | 951 | 33 |
| -6 | 11 | 5 | 239 | 207 | 15 |
| -5 | 11 | 5 | 181 | 162 | 20 |
| -4 | 11 | 5 | 901 | 879 | 25 |
| -3 | 11 | 5 | 275 | 261 | 17 |
| 0 | 0 | 6 | 1454 | 1447 | 13 |
| -1 | 1 | 6 | 1201 | 1217 | 16 |
| 0 | 1 | 6 | 919 | 923 | 17 |
| -2 | 2 | 6 | 3028 | 3000 | 20 |
| -1 | 2 | 6 | 1446 | 1409 | 9 |
| 0 | 2 | 6 | 3171 | 3147 | 32 |
| -3 | 3 | 6 | 258 | 222 | 10 |
| -2 | 3 | 6 | 3296 | 3284 | 34 |
| -1 | 3 | 6 | 2458 | 2442 | 34 |
| 0 | 3 | 6 | 248 | 215 | 18 |
| -4 | 4 | 6 | 1467 | 1471 | 15 |
| -3 | 4 | 6 | 602 | 594 | 10 |
| -2 | 4 | 6 | 750 | 678 | 15 |
| -1 | 4 | 6 | 796 | 765 | 23 |
| 0 | 4 | 6 | 1435 | 1403 | 16 |
| -5 | 5 | 6 | 150 | 131 | -34 |
| -4 | 5 | 6 | 1389 | 1366 | 18 |
| -3 | 5 | 6 | 399 | 382 | 11 |
| -2 | 5 | 6 | 364 | 347 | 13 |
| -1 | 5 | 6 | 1392 | 1336 | 30 |
| 0 | 5 | 6 | 160 | 150 | 16 |
| -6 | 6 | 6 | 1372 | 1362 | 25 |
| -5 | 6 | 6 | 1141 | 1138 | 19 |
| -4 | 6 | 6 | 1378 | 1365 | 30 |
| -3 | 6 | 6 | 1146 | 1076 | 21 |
| -2 | 6 | 6 | 1314 | 1318 | 23 |
| -1 | 6 | 6 | 865 | 860 | 17 |
| 0 | 6 | 6 | 1512 | 1487 | 28 |
| -7 | 7 | 6 | 1988 | 1998 | 32 |
| -6 | 7 | 6 | 432 | 433 | 7 |
| -5 | 7 | 6 | 670 | 678 | 15 |
| -4 | 7 | 6 | 485 | 463 | 13 |
| -3 | 7 | 6 | 363 | 358 | 7 |
| -2 | 7 | 6 | 568 | 565 | 14 |
| -1 | 7 | 6 | 411 | 410 | 7 |
| 0 | 7 | 6 | 1528 | 1507 | 28 |
| -8 | 8 | 6 | 759 | 764 | 17 |
| -7 | 8 | 6 | 525 | 526 | 7 |
| -6 | 8 | 6 | 1018 | 1025 | 19 |
| -5 | 8 | 6 | 1180 | 1172 | 31 |
| -4 | 8 | 6 | 1197 | 1167 | 33 |
| -3 | 8 | 6 | 1584 | 1576 | 40 |
| -2 | 8 | 6 | 1165 | 1163 | 26 |
| -1 | 8 | 6 | 425 | 413 | 8 |
| 0 | 8 | 6 | 897 | 911 | 16 |
| -9 | 9 | 6 | 785 | 789 | 8 |
| -8 | 9 | 6 | 360 | 389 | 11 |
| -7 | 9 | 6 | 595 | 574 | 19 |
| -6 | 9 | 6 | 545 | 534 | 19 |
| -5 | 9 | 6 | 26 | 227 | -25 |
| -4 | 9 | 6 | 270 | 298 | 13 |
| -3 | 9 | 6 | 593 | 569 | 23 |
| -2 | 9 | 6 | 677 | 662 | 17 |
| -1 | 9 | 6 | 308 | 295 | 10 |
| 0 | 9 | 6 | 607 | 607 | 9 |
| -9 | 10 | 6 | 683 | 690 | 12 |
| -8 | 10 | 6 | 1861 | 1859 | 34 |
| -7 | 10 | 6 | 440 | 436 | 20 |
| -6 | 10 | 6 | 430 | 427 | 14 |
| -5 | 10 | 6 | 319 | 325 | 11 |
| -4 | 10 | 6 | 382 | 378 | 13 |
| -3 | 10 | 6 | 338 | 325 | 11 |
| -2 | 10 | 6 | 2010 | 1983 | 42 |
| -1 | 10 | 6 | 885 | 869 | 21 |
| -8 | 11 | 6 | 215 | 230 | 20 |
| -7 | 11 | 6 | 266 | 239 | 13 |
| -6 | 11 | 6 | 782 | 791 | 19 |
| -5 | 11 | 6 | 694 | 683 | 26 |
| -4 | 11 | 6 | 295 | 289 | 21 |
| -3 | 11 | 6 | 307 | 301 | 19 |
| -1 | 2 | 7 | 282 | 287 | 7 |
| -2 | 3 | 7 | 1511 | 1527 | 15 |
| -1 | 3 | 7 | 1519 | 1573 | 21 |
| -3 | 4 | 7 | 1336 | 1238 | 11 |
| -2 | 4 | 7 | 131 | 114 | 18 |
| -1 | 4 | 7 | 1703 | 1564 | 29 |
| -4 | 5 | 7 | 700 | 685 | 7 |
| -3 | 5 | 7 | 308 | 297 | 7 |
| -2 | 5 | 7 | 367 | 350 | 13 |
| -1 | 5 | 7 | 822 | 813 | 17 |
| -5 | 6 | 7 | 742 | 755 | 11 |
| -4 | 6 | 7 | 1155 | 1151 | 23 |
| -3 | 6 | 7 | 686 | 685 | 19 |
| -2 | 6 | 7 | 1551 | 1540 | 35 |
| -1 | 6 | 7 | 1016 | 1014 | 15 |
| -6 | 7 | 7 | 425 | 435 | 7 |
| -5 | 7 | 7 | 512 | 512 | 16 |
| -4 | 7 | 7 | 623 | 625 | 15 |
| -3 | 7 | 7 | 784 | 793 | 19 |
| -2 | 7 | 7 | 412 | 418 | 15 |
| -1 | 7 | 7 | 470 | 471 | 10 |
| -7 | 8 | 7 | 515 | 527 | 11 |
| -6 | 8 | 7 | 333 | 322 | 9 |
| -5 | 8 | 7 | 1860 | 1865 | 43 |
| -4 | 8 | 7 | 375 | 377 | 9 |
| -3 | 8 | 7 | 2159 | 2182 | 46 |
| -2 | 8 | 7 | 299 | 294 | 10 |
| -1 | 8 | 7 | 427 | 422 | 10 |
| -8 | 9 | 7 | 284 | 278 | 15 |
| -7 | 9 | 7 | 658 | 673 | 14 |
| -6 | 9 | 7 | 96 | 67 | -26 |
| -5 | 9 | 7 | 153 | 175 | 21 |
| -4 | 9 | 7 | 245 | 235 | 14 |
| -3 | 9 | 7 | 134 | 78 | 20 |
| -2 | 9 | 7 | 580 | 581 | 15 |
| -1 | 9 | 7 | 172 | 208 | 16 |
| -9 | 10 | 7 | 819 | 829 | 14 |
| -8 | 10 | 7 | 116 | 92 | -33 |
| -7 | 10 | 7 | 101 | 75 | -42 |
| -6 | 10 | 7 | 10 | 100 | -9 |
| -5 | 10 | 7 | 105 | 115 | -32 |
| -4 | 10 | 7 | 110 | 100 | -27 |
| -3 | 10 | 7 | 126 | 56 | -37 |
| -2 | 10 | 7 | 7 | 75 | -7 |
| -1 | 10 | 7 | 1013 | 1020 | 18 |
| -8 | 11 | 7 | 136 | 115 | -29 |
| -7 | 11 | 7 | 13 | 67 | -13 |
| -6 | 11 | 7 | 539 | 533 | 11 |

Table 5 Observed and calculated structure factors for 1



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -5 | 11 | 7 | 475 | 488 | 18 |
| -4 | 11 | 7 | 120 | 72 | -24 |
| -3 | 11 | 7 | 104 | 102 | -35 |
| 0 | 0 | 8 | 1810 | 1785 | 8 |
| -1 | 1 | 8 | 1273 | 1265 | 6 |
| 0 | 1 | 8 | 1714 | 1701 | 7 |
| -2 | 2 | 8 | 3013 | 3035 | 10 |
| -1 | 2 | 8 | 1643 | 1636 | 15 |
| 0 | 2 | 8 | 2472 | 2489 | 19 |
| -3 | 3 | 8 | 651 | 673 | 11 |
| -2 | 3 | 8 | 1349 | 1378 | 11 |
| -1 | 3 | 8 | 1480 | 1535 | 26 |
| 0 | 3 | 8 | 546 | 553 | 6 |
| -4 | 4 | 8 | 1075 | 1076 | 12 |
| -3 | 4 | 8 | 805 | 782 | 13 |
| -2 | 4 | 8 | 1212 | 1179 | 19 |
| -1 | 4 | 8 | 705 | 664 | 17 |
| 0 | 4 | 8 | 1166 | 1167 | 10 |
| -5 | 5 | 8 | 614 | 614 | 10 |
| -4 | 5 | 8 | 1055 | 1048 | 11 |
| -3 | 5 | 8 | 455 | 452 | 10 |
| -2 | 5 | 8 | 569 | 569 | 14 |
| -1 | 5 | 8 | 1328 | 1297 | 27 |
| 0 | 5 | 8 | 496 | 485 | 6 |
| -6 | 6 | 8 | 2194 | 2196 | 37 |
| -5 | 6 | 8 | 796 | 794 | 9 |
| -4 | 6 | 8 | 1037 | 1046 | 20 |
| -3 | 6 | 8 | 983 | 948 | 19 |
| -2 | 6 | 8 | 1330 | 1323 | 30 |
| -1 | 6 | 8 | 1074 | 1066 | 28 |
| 0 | 6 | 8 | 1909 | 1905 | 29 |
| -7 | 7 | 8 | 1390 | 1414 | 24 |
| -6 | 7 | 8 | 401 | 405 | 11 |
| -5 | 7 | 8 | 325 | 318 | 10 |
| -4 | 7 | 8 | 280 | 249 | 17 |
| -3 | 7 | 8 | 236 | 189 | 16 |
| -2 | 7 | 8 | 269 | 250 | 14 |
| -1 | 7 | 8 | 432 | 420 | 11 |
| 0 | 7 | 8 | 1349 | 1345 | 30 |
| -8 | 8 | 8 | 793 | 808 | 21 |
| -7 | 8 | 8 | 464 | 455 | 10 |
| -6 | 8 | 8 | 744 | 730 | 11 |
| -5 | 8 | 8 | 1269 | 1269 | 30 |
| -4 | 8 | 8 | 1635 | 1609 | 44 |
| -3 | 8 | 8 | 1036 | 1047 | 27 |
| -2 | 8 | 8 | 700 | 692 | 14 |
| -1 | 8 | 8 | 419 | 413 | 12 |
| 0 | 8 | 8 | 600 | 604 | 10 |
| -9 | 9 | 8 | 354 | 343 | 21 |
| -8 | 9 | 8 | 344 | 326 | 9 |
| -7 | 9 | 8 | 218 | 193 | 15 |
| -6 | 9 | 8 | 465 | 467 | 11 |
| -5 | 9 | 8 | 24 | 157 | -23 |
| -4 | 9 | 8 | 232 | 210 | 12 |
| -3 | 9 | 8 | 496 | 492 | 16 |
| -2 | 9 | 8 | 245 | 251 | 12 |
| -1 | 9 | 8 | 379 | 377 | 13 |
| 0 | 9 | 8 | 386 | 387 | 16 |
| -9 | 10 | 8 | 570 | 583 | 12 |
| -8 | 10 | 8 | 1593 | 1639 | 32 |
| -7 | 10 | 8 | 775 | 772 | 19 |
| -6 | 10 | 8 | 325 | 311 | 13 |
| -5 | 10 | 8 | 322 | 311 | 19 |
| -4 | 10 | 8 | 404 | 416 | 14 |
| -3 | 10 | 8 | 972 | 959 | 29 |
| -2 | 10 | 8 | 1535 | 1553 | 32 |
| -1 | 10 | 8 | 660 | 662 | 11 |
| -7 | 11 | 8 | 343 | 339 | 12 |
| -6 | 11 | 8 | 493 | 499 | 10 |
| -5 | 11 | 8 | 479 | 488 | 14 |
| -4 | 11 | 8 | 21 | 252 | -20 |
| -1 | 2 | 9 | 831 | 903 | 10 |
| -2 | 3 | 9 | 807 | 841 | 6 |
| -1 | 3 | 9 | 870 | 927 | 9 |
| -3 | 4 | 9 | 747 | 742 | 7 |
| -2 | 4 | 9 | 1099 | 1083 | 15 |
| -1 | 4 | 9 | 801 | 795 | 8 |
| -4 | 5 | 9 | 1116 | 1130 | 9 |
| -3 | 5 | 9 | 443 | 435 | 11 |
| -2 | 5 | 9 | 592 | 573 | 9 |
| -1 | 5 | 9 | 834 | 841 | 13 |
| -5 | 6 | 9 | 799 | 804 | 13 |
| -4 | 6 | 9 | 540 | 542 | 9 |
| -3 | 6 | 9 | 515 | 511 | 11 |
| -2 | 6 | 9 | 484 | 478 | 9 |
| -1 | 6 | 9 | 1095 | 1082 | 17 |
| -6 | 7 | 9 | 230 | 236 | 20 |
| -5 | 7 | 9 | 426 | 434 | 12 |
| -4 | 7 | 9 | 778 | 780 | 11 |
| -3 | 7 | 9 | 969 | 971 | 19 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -2 | 7 | 9 | 453 | 474 | 7 |
| -1 | 7 | 9 | 270 | 267 | 10 |
| -7 | 8 | 9 | 473 | 482 | 7 |
| -6 | 8 | 9 | 347 | 365 | 11 |
| -5 | 8 | 9 | 205 | 228 | 18 |
| -4 | 8 | 9 | 293 | 292 | 13 |
| -3 | 8 | 9 | 167 | 170 | 17 |
| -2 | 8 | 9 | 476 | 484 | 11 |
| -1 | 8 | 9 | 360 | 362 | 16 |
| -8 | 9 | 9 | 296 | 280 | 10 |
| -7 | 9 | 9 | 117 | 135 | -27 |
| -6 | 9 | 9 | 846 | 831 | 20 |
| -5 | 9 | 9 | 226 | 227 | 13 |
| -4 | 9 | 9 | 168 | 181 | 20 |
| -3 | 9 | 9 | 844 | 824 | 20 |
| -2 | 9 | 9 | 12 | 181 | -11 |
| -1 | 9 | 9 | 278 | 285 | 11 |
| -9 | 10 | 9 | 416 | 432 | 12 |
| -8 | 10 | 9 | 704 | 706 | 16 |
| -7 | 10 | 9 | 121 | 99 | -27 |
| -6 | 10 | 9 | 129 | 111 | -23 |
| -5 | 10 | 9 | 166 | 119 | 20 |
| -4 | 10 | 9 | 109 | 121 | -30 |
| -3 | 10 | 9 | 13 | 75 | -12 |
| -2 | 10 | 9 | 611 | 609 | 13 |
| -1 | 10 | 9 | 407 | 393 | 15 |
| -7 | 11 | 9 | 332 | 340 | 14 |
| -6 | 11 | 9 | 511 | 512 | 14 |
| -5 | 11 | 9 | 604 | 608 | 10 |
| -4 | 11 | 9 | 385 | 394 | 14 |
| 0 | 0 | 10 | 5182 | 5272 | 8 |
| -1 | 1 | 10 | 1464 | 1532 | 16 |
| 0 | 1 | 10 | 1087 | 1149 | 8 |
| -2 | 2 | 10 | 2166 | 2167 | 9 |
| -1 | 2 | 10 | 1126 | 1159 | 14 |
| 0 | 2 | 10 | 2757 | 2758 | 22 |
| -3 | 3 | 10 | 1042 | 1055 | 7 |
| -2 | 3 | 10 | 1182 | 1127 | 10 |
| -1 | 3 | 10 | 885 | 846 | 7 |
| 0 | 3 | 10 | 1180 | 1192 | 22 |
| -4 | 4 | 10 | 488 | 486 | 9 |
| -3 | 4 | 10 | 1180 | 1156 | 11 |
| -2 | 4 | 10 | 1334 | 1299 | 15 |
| -1 | 4 | 10 | 1249 | 1244 | 24 |
| 0 | 4 | 10 | 365 | 373 | 8 |
| -5 | 5 | 10 | 175 | 158 | 18 |
| -4 | 5 | 10 | 741 | 747 | 8 |
| -3 | 5 | 10 | 162 | 161 | 13 |
| -2 | 5 | 10 | 198 | 194 | 12 |
| -1 | 5 | 10 | 1009 | 995 | 18 |
| 0 | 5 | 10 | 198 | 208 | 16 |
| -6 | 6 | 10 | 1284 | 1303 | 23 |
| -5 | 6 | 10 | 644 | 663 | 8 |
| -4 | 6 | 10 | 1545 | 1535 | 11 |
| -3 | 6 | 10 | 1120 | 1092 | 17 |
| -2 | 6 | 10 | 1774 | 1761 | 31 |
| -1 | 6 | 10 | 480 | 493 | 9 |
| 0 | 6 | 10 | 1653 | 1641 | 36 |
| -7 | 7 | 10 | 2031 | 2066 | 22 |
| -6 | 7 | 10 | 97 | 77 | -28 |
| -5 | 7 | 10 | 542 | 556 | 6 |
| -4 | 7 | 10 | 465 | 471 | 9 |
| -3 | 7 | 10 | 597 | 595 | 16 |
| -2 | 7 | 10 | 722 | 734 | 16 |
| -1 | 7 | 10 | 156 | 93 | 21 |
| 0 | 7 | 10 | 1599 | 1588 | 32 |
| -8 | 8 | 10 | 133 | 98 | -28 |
| -7 | 8 | 10 | 314 | 310 | 10 |
| -6 | 8 | 10 | 568 | 574 | 6 |
| -5 | 8 | 10 | 108 | 97 | -30 |
| -4 | 8 | 10 | 1567 | 1544 | 38 |
| -3 | 8 | 10 | 91 | 87 | -29 |
| -2 | 8 | 10 | 623 | 607 | 16 |
| -1 | 8 | 10 | 305 | 312 | 10 |
| 0 | 8 | 10 | 147 | 125 | -31 |
| -9 | 9 | 10 | 527 | 524 | 10 |
| -8 | 9 | 10 | 588 | 613 | 7 |
| -7 | 9 | 10 | 156 | 143 | 19 |
| -6 | 9 | 10 | 628 | 633 | 15 |
| -5 | 9 | 10 | 326 | 334 | 10 |
| -4 | 9 | 10 | 366 | 366 | 12 |
| -3 | 9 | 10 | 762 | 768 | 15 |
| -2 | 9 | 10 | 12 | 143 | -12 |
| -1 | 9 | 10 | 531 | 546 | 16 |
| 0 | 9 | 10 | 455 | 474 | 11 |
| -9 | 10 | 10 | 427 | 448 | 10 |
| -8 | 10 | 10 | 623 | 642 | 8 |
| -7 | 10 | 10 | 763 | 776 | 20 |
| -6 | 10 | 10 | 346 | 338 | 12 |
| -5 | 10 | 10 | 597 | 592 | 22 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -4 | 10 | 10 | 267 | 257 | 17 |
| -3 | 10 | 10 | 585 | 577 | 19 |
| -2 | 10 | 10 | 743 | 741 | 14 |
| -1 | 10 | 10 | 587 | 581 | 8 |
| -7 | 11 | 10 | 124 | 160 | -27 |
| -6 | 11 | 10 | 648 | 653 | 21 |
| -5 | 11 | 10 | 482 | 490 | 9 |
| -4 | 11 | 10 | 131 | 161 | -26 |
| -1 | 2 | 11 | 403 | 474 | 13 |
| -2 | 3 | 11 | 2041 | 1994 | 8 |
| -1 | 3 | 11 | 1585 | 1571 | 11 |
| -3 | 4 | 11 | 743 | 736 | 4 |
| -2 | 4 | 11 | 631 | 646 | 9 |
| -1 | 4 | 11 | 833 | 829 | 8 |
| -4 | 5 | 11 | 1374 | 1397 | 12 |
| -3 | 5 | 11 | 823 | 810 | 12 |
| -2 | 5 | 11 | 880 | 870 | 14 |
| -1 | 5 | 11 | 1144 | 1157 | 16 |
| -5 | 6 | 11 | 1369 | 1383 | 17 |
| -4 | 6 | 11 | 1156 | 1168 | 15 |
| -3 | 6 | 11 | 730 | 716 | 14 |
| -2 | 6 | 11 | 1522 | 1535 | 29 |
| -1 | 6 | 11 | 1038 | 1038 | 15 |
| -6 | 7 | 11 | 229 | 258 | 18 |
| -5 | 7 | 11 | 620 | 628 | 8 |
| -4 | 7 | 11 | 949 | 951 | 18 |
| -3 | 7 | 11 | 830 | 815 | 15 |
| -2 | 7 | 11 | 836 | 841 | 21 |
| -1 | 7 | 11 | 165 | 192 | 18 |
| -7 | 8 | 11 | 230 | 219 | 12 |
| -6 | 8 | 11 | 777 | 797 | 17 |
| -5 | 8 | 11 | 1340 | 1346 | 29 |
| -4 | 8 | 11 | 137 | 13 | -28 |
| -3 | 8 | 11 | 1733 | 1750 | 43 |
| -2 | 8 | 11 | 597 | 593 | 22 |
| -1 | 8 | 11 | 14 | 166 | -14 |
| -8 | 9 | 11 | 382 | 371 | 9 |
| -7 | 9 | 11 | 271 | 281 | 15 |
| -6 | 9 | 11 | 311 | 306 | 10 |
| -5 | 9 | 11 | 151 | 119 | 25 |
| -4 | 9 | 11 | 131 | 110 | -24 |
| -3 | 9 | 11 | 404 | 401 | 9 |
| -2 | 9 | 11 | 354 | 359 | 12 |
| -1 | 9 | 11 | 448 | 458 | 12 |
| -9 | 10 | 11 | 299 | 304 | 16 |
| -8 | 10 | 11 | 271 | 281 | 23 |
| -7 | 10 | 11 | 380 | 386 | 10 |
| -6 | 10 | 11 | 306 | 297 | 22 |
| -5 | 10 | 11 | 15 | 126 | -15 |
| -4 | 10 | 11 | 403 | 390 | 13 |
| -3 | 10 | 11 | 327 | 313 | 20 |
| -2 | 10 | 11 | 268 | 230 | 18 |
| -1 | 10 | 11 | 392 | 389 | 11 |
| -6 | 11 | 11 | 922 | 908 | 16 |
| -5 | 11 | 11 | 689 | 688 | 13 |
| -4 | 11 | 11 | 650 | 626 | 19 |
| 0 | 0 | 12 | 295 | 82 | -21 |
| -1 | 1 | 12 | 1033 | 1086 | 13 |
| 0 | 1 | 12 | 855 | 888 | 15 |
| -2 | 2 | 12 | 1178 | 1181 | 7 |
| -1 | 2 | 12 | 284 | 289 | 10 |
| 0 | 2 | 12 | 918 | 930 | 6 |
| -3 | 3 | 12 | 338 | 328 | 11 |
| -2 | 3 | 12 | 1600 | 1600 | 16 |
| -1 | 3 | 12 | 1223 | 1215 | 13 |
| 0 | 3 | 12 | 375 | 379 | 8 |
| -4 | 4 | 12 | 1482 | 1511 | 12 |
| -3 | 4 | 12 | 559 | 562 | 5 |
| -2 | 4 | 12 | 1039 | 1033 | 9 |
| -1 | 4 | 12 | 438 | 434 | 11 |
| 0 | 4 | 12 | 1642 | 1651 | 14 |
| -5 | 5 | 12 | 390 | 376 | 8 |
| -4 | 5 | 12 | 418 | 402 | 6 |
| -3 | 5 | 12 | 161 | 139 | 13 |
| -2 | 5 | 12 | 185 | 168 | 11 |
| -1 | 5 | 12 | 313 | 300 | 10 |
| 0 | 5 | 12 | 329 | 312 | 13 |
| -6 | 6 | 12 | 574 | 580 | 7 |
| -5 | 6 | 12 | 516 | 522 | 9 |
| -4 | 6 | 12 | 1505 | 1506 | 18 |
| -3 | 6 | 12 | 11 | 72 | -11 |
| -2 | 6 | 12 | 1126 | 1122 | 16 |
| -1 | 6 | 12 | 566 | 560 | 10 |
| 0 | 6 | 12 | 523 | 509 | 11 |
| -7 | 7 | 12 | 1958 | 1972 | 16 |
| -6 | 7 | 12 | 651 | 668 | 7 |
| -5 | 7 | 12 | 479 | 486 | 10 |
| -4 | 7 | 12 | 531 | 524 | 15 |
| -3 | 7 | 12 | 578 | 572 | 13 |
| -2 | 7 | 12 | 595 | 588 | 10 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -1 | 7 | 12 | 484 | 499 | 12 |
| 0 | 7 | 12 | 1865 | 1869 | 36 |
| -8 | 8 | 12 | 454 | 461 | 10 |
| -7 | 8 | 12 | 475 | 459 | 8 |
| -6 | 8 | 12 | 692 | 695 | 16 |
| -5 | 8 | 12 | 532 | 534 | 16 |
| -4 | 8 | 12 | 893 | 892 | 16 |
| -3 | 8 | 12 | 618 | 597 | 20 |
| -2 | 8 | 12 | 589 | 586 | 9 |
| -1 | 8 | 12 | 391 | 382 | 16 |
| 0 | 8 | 12 | 556 | 561 | 13 |
| -9 | 9 | 12 | 110 | 82 | -44 |
| -8 | 9 | 12 | 396 | 415 | 10 |
| -7 | 9 | 12 | 350 | 340 | 10 |
| -6 | 9 | 12 | 188 | 187 | 16 |
| -5 | 9 | 12 | 392 | 385 | 13 |
| -4 | 9 | 12 | 329 | 338 | 10 |
| -3 | 9 | 12 | 185 | 178 | 27 |
| -2 | 9 | 12 | 326 | 302 | 13 |
| -1 | 9 | 12 | 436 | 440 | 12 |
| 0 | 9 | 12 | 129 | 66 | -33 |
| -9 | 10 | 12 | 698 | 719 | 9 |
| -8 | 10 | 12 | 712 | 718 | 11 |
| -7 | 10 | 12 | 253 | 223 | 14 |
| -6 | 10 | 12 | 650 | 639 | 21 |
| -5 | 10 | 12 | 279 | 250 | 20 |
| -4 | 10 | 12 | 809 | 816 | 16 |
| -3 | 10 | 12 | 172 | 190 | 22 |
| -2 | 10 | 12 | 553 | 564 | 8 |
| -1 | 10 | 12 | 884 | 882 | 13 |
| -6 | 11 | 12 | 846 | 849 | 18 |
| -5 | 11 | 12 | 653 | 654 | 17 |
| -1 | 2 | 13 | 501 | 482 | 4 |
| -2 | 3 | 13 | 1447 | 1452 | 7 |
| -1 | 3 | 13 | 1602 | 1592 | 15 |
| -3 | 4 | 13 | 927 | 942 | 6 |
| -2 | 4 | 13 | 126 | 85 | 20 |
| -1 | 4 | 13 | 731 | 746 | 7 |
| -4 | 5 | 13 | 1144 | 1145 | 10 |
| -3 | 5 | 13 | 378 | 381 | 6 |
| -2 | 5 | 13 | 462 | 474 | 9 |
| -1 | 5 | 13 | 1216 | 1212 | 17 |
| -5 | 6 | 13 | 453 | 435 | 7 |
| -4 | 6 | 13 | 691 | 690 | 6 |
| -3 | 6 | 13 | 1289 | 1329 | 15 |
| -2 | 6 | 13 | 598 | 606 | 7 |
| -1 | 6 | 13 | 542 | 555 | 10 |
| -6 | 7 | 13 | 268 | 265 | 10 |
| -5 | 7 | 13 | 953 | 964 | 10 |
| -4 | 7 | 13 | 747 | 765 | 12 |
| -3 | 7 | 13 | 829 | 841 | 16 |
| -2 | 7 | 13 | 758 | 757 | 13 |
| -1 | 7 | 13 | 333 | 346 | 9 |
| -7 | 8 | 13 | 552 | 565 | 7 |
| -6 | 8 | 13 | 219 | 189 | 18 |
| -5 | 8 | 13 | 960 | 964 | 25 |
| -4 | 8 | 13 | 683 | 691 | 12 |
| -3 | 8 | 13 | 710 | 716 | 19 |
| -2 | 8 | 13 | 144 | 167 | 20 |
| -1 | 8 | 13 | 487 | 491 | 7 |
| -8 | 9 | 13 | 389 | 399 | 11 |
| -7 | 9 | 13 | 336 | 344 | 12 |
| -6 | 9 | 13 | 524 | 531 | 11 |
| -5 | 9 | 13 | 492 | 488 | 9 |
| -4 | 9 | 13 | 622 | 610 | 12 |
| -3 | 9 | 13 | 653 | 666 | 10 |
| -2 | 9 | 13 | 259 | 260 | 14 |
| -1 | 9 | 13 | 546 | 535 | 12 |
| -8 | 10 | 13 | 140 | 134 | -28 |
| -7 | 10 | 13 | 194 | 175 | 20 |
| -6 | 10 | 13 | 650 | 639 | 17 |
| -5 | 10 | 13 | 617 | 634 | 16 |
| -4 | 10 | 13 | 457 | 480 | 9 |
| -3 | 10 | 13 | 172 | 160 | 20 |
| -2 | 10 | 13 | 169 | 120 | 21 |
| 0 | 0 | 14 | 2283 | 2476 | 10 |
| -1 | 1 | 14 | 573 | 565 | 10 |
| 0 | 1 | 14 | 535 | 540 | 6 |
| -2 | 2 | 14 | 1047 | 1019 | 10 |
| -1 | 2 | 14 | 231 | 93 | 37 |
| 0 | 2 | 14 | 890 | 875 | 9 |
| -3 | 3 | 14 | 1348 | 1325 | 15 |
| -2 | 3 | 14 | 1247 | 1266 | 23 |
| -1 | 3 | 14 | 947 | 944 | 10 |
| 0 | 3 | 14 | 1009 | 986 | 11 |
| -4 | 4 | 14 | 339 | 346 | 8 |
| -3 | 4 | 14 | 679 | 687 | 4 |
| -2 | 4 | 14 | 3204 | 3228 | 19 |
| -1 | 4 | 14 | 912 | 910 | 9 |
| 0 | 4 | 14 | 331 | 329 | 13 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -5 | 5 | 14 | 346 | 336 | 9 |
| -4 | 5 | 14 | 661 | 656 | 8 |
| -3 | 5 | 14 | 626 | 620 | 15 |
| -2 | 5 | 14 | 519 | 509 | 6 |
| -1 | 5 | 14 | 756 | 746 | 8 |
| 0 | 5 | 14 | 386 | 391 | 8 |
| -6 | 6 | 14 | 970 | 961 | 14 |
| -5 | 6 | 14 | 707 | 712 | 9 |
| -4 | 6 | 14 | 267 | 244 | 10 |
| -3 | 6 | 14 | 329 | 340 | 8 |
| -2 | 6 | 14 | 273 | 279 | 9 |
| -1 | 6 | 14 | 878 | 873 | 8 |
| 0 | 6 | 14 | 802 | 796 | 13 |
| -7 | 7 | 14 | 1278 | 1279 | 21 |
| -6 | 7 | 14 | 699 | 703 | 10 |
| -5 | 7 | 14 | 876 | 877 | 7 |
| -4 | 7 | 14 | 698 | 691 | 10 |
| -3 | 7 | 14 | 538 | 537 | 10 |
| -2 | 7 | 14 | 1143 | 1157 | 25 |
| -1 | 7 | 14 | 702 | 697 | 14 |
| 0 | 7 | 14 | 1337 | 1318 | 21 |
| -8 | 8 | 14 | 1385 | 1406 | 16 |
| -7 | 8 | 14 | 586 | 586 | 7 |
| -6 | 8 | 14 | 299 | 307 | 10 |
| -5 | 8 | 14 | 831 | 823 | 21 |
| -4 | 8 | 14 | 1154 | 1153 | 17 |
| -3 | 8 | 14 | 1005 | 1002 | 24 |
| -2 | 8 | 14 | 414 | 406 | 9 |
| -1 | 8 | 14 | 606 | 602 | 10 |
| 0 | 8 | 14 | 1055 | 1056 | 15 |
| -9 | 9 | 14 | 914 | 914 | 16 |
| -8 | 9 | 14 | 398 | 377 | 9 |
| -7 | 9 | 14 | 756 | 756 | 10 |
| -6 | 9 | 14 | 1110 | 1136 | 15 |
| -5 | 9 | 14 | 546 | 563 | 11 |
| -4 | 9 | 14 | 542 | 537 | 8 |
| -3 | 9 | 14 | 1241 | 1263 | 25 |
| -2 | 9 | 14 | 615 | 604 | 11 |
| -1 | 9 | 14 | 384 | 378 | 10 |
| 0 | 9 | 14 | 1145 | 1143 | 32 |
| -8 | 10 | 14 | 1047 | 1075 | 13 |
| -7 | 10 | 14 | 223 | 227 | 16 |
| -6 | 10 | 14 | 1082 | 1070 | 23 |
| -5 | 10 | 14 | 147 | 154 | 24 |
| -4 | 10 | 14 | 846 | 848 | 20 |
| -3 | 10 | 14 | 174 | 170 | 31 |
| -2 | 10 | 14 | 1253 | 1254 | 24 |
| -1 | 2 | 15 | 864 | 874 | 13 |
| -2 | 3 | 15 | 855 | 896 | 34 |
| -1 | 3 | 15 | 801 | 785 | 10 |
| -3 | 4 | 15 | 922 | 947 | 8 |
| -2 | 4 | 15 | 476 | 490 | 23 |
| -1 | 4 | 15 | 1184 | 1228 | 7 |
| -4 | 5 | 15 | 238 | 244 | 10 |
| -3 | 5 | 15 | 645 | 641 | 11 |
| -2 | 5 | 15 | 653 | 657 | 8 |
| -1 | 5 | 15 | 325 | 305 | 7 |
| -5 | 6 | 15 | 529 | 530 | 6 |
| -4 | 6 | 15 | 863 | 872 | 8 |
| -3 | 6 | 15 | 1251 | 1277 | 7 |
| -2 | 6 | 15 | 1145 | 1172 | 16 |
| -1 | 6 | 15 | 435 | 437 | 7 |
| -6 | 7 | 15 | 398 | 403 | 8 |
| -5 | 7 | 15 | 492 | 493 | 8 |
| -4 | 7 | 15 | 1058 | 1071 | 13 |
| -3 | 7 | 15 | 818 | 828 | 14 |
| -2 | 7 | 15 | 580 | 591 | 13 |
| -1 | 7 | 15 | 326 | 322 | 10 |
| -7 | 8 | 15 | 340 | 337 | 9 |
| -6 | 8 | 15 | 322 | 319 | 10 |
| -5 | 8 | 15 | 134 | 146 | 21 |
| -4 | 8 | 15 | 1047 | 1058 | 16 |
| -3 | 8 | 15 | 186 | 162 | 16 |
| -2 | 8 | 15 | 242 | 240 | 20 |
| -1 | 8 | 15 | 447 | 453 | 8 |
| -8 | 9 | 15 | 419 | 430 | 9 |
| -7 | 9 | 15 | 264 | 259 | 12 |
| -6 | 9 | 15 | 588 | 607 | 7 |
| -5 | 9 | 15 | 295 | 317 | 14 |
| -4 | 9 | 15 | 244 | 237 | 13 |
| -3 | 9 | 15 | 495 | 507 | 11 |
| -2 | 9 | 15 | 355 | 347 | 10 |
| -1 | 9 | 15 | 418 | 420 | 9 |
| -8 | 10 | 15 | 503 | 507 | 9 |
| -7 | 10 | 15 | 128 | 107 | -34 |
| -6 | 10 | 15 | 294 | 293 | 14 |
| -5 | 10 | 15 | 458 | 454 | 12 |
| -4 | 10 | 15 | 372 | 371 | 11 |
| -3 | 10 | 15 | 172 | 143 | 26 |
| -2 | 10 | 15 | 430 | 437 | 10 |

Table 5 Observed and calculated structure factors for 1



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 0 | 0 | 16 | 2073 | 2060 | 11 |
| -1 | 1 | 16 | 437 | 420 | 14 |
| 0 | 1 | 16 | 499 | 518 | 9 |
| -2 | 2 | 16 | 1075 | 1143 | 13 |
| -1 | 2 | 16 | 642 | 649 | 24 |
| 0 | 2 | 16 | 962 | 1008 | 11 |
| -3 | 3 | 16 | 777 | 744 | 6 |
| -2 | 3 | 16 | 1822 | 1889 | 17 |
| -1 | 3 | 16 | 1480 | 1522 | 10 |
| 0 | 3 | 16 | 1016 | 993 | 15 |
| -4 | 4 | 16 | 548 | 550 | 7 |
| -3 | 4 | 16 | 322 | 336 | 11 |
| -2 | 4 | 16 | 2247 | 2231 | 9 |
| -1 | 4 | 16 | 246 | 251 | 17 |
| 0 | 4 | 16 | 723 | 715 | 6 |
| -5 | 5 | 16 | 197 | 174 | 20 |
| -4 | 5 | 16 | 204 | 199 | 12 |
| -3 | 5 | 16 | 1087 | 1114 | 15 |
| -2 | 5 | 16 | 891 | 908 | 5 |
| -1 | 5 | 16 | 218 | 211 | 11 |
| 0 | 5 | 16 | 175 | 214 | 30 |
| -6 | 6 | 16 | 155 | 124 | -29 |
| -5 | 6 | 16 | 898 | 912 | 9 |
| -4 | 6 | 16 | 1199 | 1205 | 13 |
| -3 | 6 | 16 | 226 | 220 | 16 |
| -2 | 6 | 16 | 1584 | 1595 | 24 |
| -1 | 6 | 16 | 681 | 684 | 8 |
| 0 | 6 | 16 | 163 | 139 | 25 |
| -7 | 7 | 16 | 1291 | 1322 | 22 |
| -6 | 7 | 16 | 428 | 443 | 7 |
| -5 | 7 | 16 | 765 | 774 | 5 |
| -4 | 7 | 16 | 526 | 523 | 10 |
| -3 | 7 | 16 | 426 | 422 | 8 |
| -2 | 7 | 16 | 578 | 578 | 11 |
| -1 | 7 | 16 | 398 | 397 | 8 |
| 0 | 7 | 16 | 1212 | 1220 | 20 |
| -8 | 8 | 16 | 2074 | 2087 | 29 |
| -7 | 8 | 16 | 536 | 553 | 7 |
| -6 | 8 | 16 | 176 | 183 | 24 |
| -5 | 8 | 16 | 831 | 833 | 17 |
| -4 | 8 | 16 | 894 | 898 | 18 |
| -3 | 8 | 16 | 741 | 759 | 17 |
| -2 | 8 | 16 | 172 | 180 | 17 |
| -1 | 8 | 16 | 554 | 538 | 7 |
| 0 | 8 | 16 | 2490 | 2464 | 40 |
| -9 | 9 | 16 | 609 | 596 | 13 |
| -8 | 9 | 16 | 267 | 277 | 14 |
| -7 | 9 | 16 | 688 | 699 | 7 |
| -6 | 9 | 16 | 314 | 318 | 11 |
| -5 | 9 | 16 | 292 | 299 | 11 |
| -4 | 9 | 16 | 306 | 331 | 11 |
| -3 | 9 | 16 | 244 | 237 | 13 |
| -2 | 9 | 16 | 922 | 905 | 12 |
| -1 | 9 | 16 | 216 | 206 | 17 |
| 0 | 9 | 16 | 443 | 445 | 12 |
| -8 | 10 | 16 | 437 | 436 | 14 |
| -7 | 10 | 16 | 325 | 322 | 12 |
| -6 | 10 | 16 | 983 | 967 | 16 |
| -5 | 10 | 16 | 104 | 154 | -33 |
| -4 | 10 | 16 | 1060 | 1061 | 20 |
| -3 | 10 | 16 | 267 | 274 | 14 |
| -2 | 10 | 16 | 306 | 325 | 13 |
| -1 | 2 | 17 | 428 | 250 | -112 |
| -2 | 3 | 17 | 853 | 918 | 25 |
| -1 | 3 | 17 | 1019 | 1081 | 18 |
| -3 | 4 | 17 | 1489 | 1506 | 7 |
| -2 | 4 | 17 | 342 | 124 | -103 |
| -1 | 4 | 17 | 1680 | 1698 | 15 |
| -4 | 5 | 17 | 351 | 359 | 8 |
| -3 | 5 | 17 | 775 | 777 | 6 |
| -2 | 5 | 17 | 776 | 779 | 5 |
| -1 | 5 | 17 | 470 | 483 | 6 |
| -5 | 6 | 17 | 287 | 301 | 10 |
| -4 | 6 | 17 | 852 | 866 | 5 |
| -3 | 6 | 17 | 836 | 842 | 6 |
| -2 | 6 | 17 | 802 | 818 | 10 |
| -1 | 6 | 17 | 266 | 278 | 11 |
| -6 | 7 | 17 | 521 | 521 | 7 |
| -5 | 7 | 17 | 265 | 276 | 12 |
| -4 | 7 | 17 | 452 | 460 | 7 |
| -3 | 7 | 17 | 445 | 446 | 9 |
| -2 | 7 | 17 | 222 | 212 | 12 |
| -1 | 7 | 17 | 382 | 396 | 13 |
| -7 | 8 | 17 | 403 | 403 | 9 |
| -6 | 8 | 17 | 15 | 153 | -14 |
| -5 | 8 | 17 | 697 | 695 | 14 |
| -4 | 8 | 17 | 382 | 387 | 11 |
| -3 | 8 | 17 | 575 | 576 | 15 |
| -2 | 8 | 17 | 138 | 132 | 22 |
| -1 | 8 | 17 | 356 | 358 | 12 |
| -8 | 9 | 17 | 414 | 395 | 9 |
| -7 | 9 | 17 | 222 | 225 | 22 |
| -6 | 9 | 17 | 186 | 185 | 18 |
| -5 | 9 | 17 | 358 | 348 | 10 |
| -4 | 9 | 17 | 291 | 272 | 16 |
| -3 | 9 | 17 | 141 | 138 | 25 |
| -2 | 9 | 17 | 163 | 177 | 20 |
| -1 | 9 | 17 | 490 | 472 | 8 |
| -7 | 10 | 17 | 271 | 265 | 14 |
| -6 | 10 | 17 | 610 | 613 | 16 |
| -5 | 10 | 17 | 190 | 202 | 21 |
| -4 | 10 | 17 | 599 | 597 | 14 |
| -3 | 10 | 17 | 320 | 314 | 17 |
| 0 | 0 | 18 | 3665 | 3621 | 16 |
| -1 | 1 | 18 | 658 | 655 | 9 |
| 0 | 1 | 18 | 851 | 860 | 10 |
| -2 | 2 | 18 | 1779 | 1813 | 20 |
| -1 | 2 | 18 | 988 | 1045 | 49 |
| 0 | 2 | 18 | 1354 | 1383 | 15 |
| -3 | 3 | 18 | 620 | 621 | 7 |
| -2 | 3 | 18 | 532 | 552 | 8 |
| -1 | 3 | 18 | 644 | 680 | 20 |
| 0 | 3 | 18 | 804 | 828 | 15 |
| -4 | 4 | 18 | 833 | 835 | 7 |
| -3 | 4 | 18 | 322 | 310 | 17 |
| -2 | 4 | 18 | 2606 | 2632 | 14 |
| -1 | 4 | 18 | 234 | 231 | 13 |
| 0 | 4 | 18 | 686 | 687 | 9 |
| -5 | 5 | 18 | 268 | 254 | 19 |
| -4 | 5 | 18 | 507 | 518 | 6 |
| -3 | 5 | 18 | 952 | 976 | 10 |
| -2 | 5 | 18 | 1255 | 1279 | 10 |
| -1 | 5 | 18 | 603 | 606 | 12 |
| 0 | 5 | 18 | 201 | 197 | 17 |
| -6 | 6 | 18 | 838 | 868 | 9 |
| -5 | 6 | 18 | 140 | 123 | 20 |
| -4 | 6 | 18 | 1605 | 1613 | 10 |
| -3 | 6 | 18 | 525 | 521 | 7 |
| -2 | 6 | 18 | 1279 | 1286 | 13 |
| -1 | 6 | 18 | 168 | 165 | 21 |
| 0 | 6 | 18 | 958 | 970 | 16 |
| -7 | 7 | 18 | 711 | 720 | 7 |
| -6 | 7 | 18 | 942 | 952 | 7 |
| -5 | 7 | 18 | 948 | 966 | 10 |
| -4 | 7 | 18 | 841 | 848 | 9 |
| -3 | 7 | 18 | 1130 | 1135 | 24 |
| -2 | 7 | 18 | 769 | 776 | 8 |
| -1 | 7 | 18 | 738 | 730 | 10 |
| 0 | 7 | 18 | 886 | 878 | 17 |
| -8 | 8 | 18 | 1024 | 1047 | 8 |
| -7 | 8 | 18 | 289 | 302 | 11 |
| -6 | 8 | 18 | 642 | 660 | 9 |
| -5 | 8 | 18 | 735 | 741 | 6 |
| -4 | 8 | 18 | 676 | 683 | 6 |
| -3 | 8 | 18 | 570 | 562 | 7 |
| -2 | 8 | 18 | 540 | 554 | 10 |
| -1 | 8 | 18 | 251 | 234 | 13 |
| 0 | 8 | 18 | 997 | 1014 | 17 |
| -8 | 9 | 18 | 418 | 402 | 10 |
| -7 | 9 | 18 | 424 | 421 | 9 |
| -6 | 9 | 18 | 348 | 353 | 11 |
| -5 | 9 | 18 | 602 | 599 | 10 |
| -4 | 9 | 18 | 768 | 762 | 6 |
| -3 | 9 | 18 | 353 | 363 | 11 |
| -2 | 9 | 18 | 348 | 356 | 11 |
| -1 | 9 | 18 | 529 | 531 | 10 |
| -7 | 10 | 18 | 116 | 117 | -32 |
| -6 | 10 | 18 | 637 | 645 | 8 |
| -5 | 10 | 18 | 321 | 324 | 12 |
| -4 | 10 | 18 | 785 | 780 | 17 |
| -3 | 10 | 18 | 180 | 155 | 32 |
| -1 | 2 | 19 | 1002 | 1065 | 75 |
| -2 | 3 | 19 | 708 | 729 | 14 |
| -1 | 3 | 19 | 903 | 935 | 19 |
| -3 | 4 | 19 | 734 | 731 | 5 |
| -2 | 4 | 19 | 1046 | 1076 | 39 |
| -1 | 4 | 19 | 799 | 796 | 6 |
| -4 | 5 | 19 | 481 | 490 | 7 |
| -3 | 5 | 19 | 501 | 513 | 6 |
| -2 | 5 | 19 | 672 | 687 | 10 |
| -1 | 5 | 19 | 632 | 645 | 6 |
| -5 | 6 | 19 | 686 | 695 | 6 |
| -4 | 6 | 19 | 460 | 462 | 7 |
| -3 | 6 | 19 | 282 | 273 | 11 |
| -2 | 6 | 19 | 406 | 410 | 8 |
| -1 | 6 | 19 | 908 | 919 | 11 |
| -6 | 7 | 19 | 331 | 339 | 9 |
| -5 | 7 | 19 | 529 | 522 | 7 |
| -4 | 7 | 19 | 823 | 847 | 11 |
| -3 | 7 | 19 | 1073 | 1083 | 10 |
| -2 | 7 | 19 | 481 | 485 | 7 |
| -1 | 7 | 19 | 260 | 259 | 12 |
| -7 | 8 | 19 | 195 | 199 | 16 |
| -6 | 8 | 19 | 456 | 470 | 8 |
| -5 | 8 | 19 | 525 | 530 | 12 |
| -4 | 8 | 19 | 469 | 475 | 8 |
| -3 | 8 | 19 | 603 | 608 | 10 |
| -2 | 8 | 19 | 477 | 481 | 9 |
| -1 | 8 | 19 | 177 | 165 | 18 |
| -8 | 9 | 19 | 111 | 60 | -33 |
| -7 | 9 | 19 | 127 | 54 | -34 |
| -6 | 9 | 19 | 1216 | 1203 | 15 |
| -5 | 9 | 19 | 541 | 545 | 15 |
| -4 | 9 | 19 | 459 | 462 | 14 |
| -3 | 9 | 19 | 1113 | 1094 | 19 |
| -2 | 9 | 19 | 84 | 41 | -53 |
| -1 | 9 | 19 | 173 | 68 | -22 |
| -6 | 10 | 19 | 191 | 189 | 27 |
| -5 | 10 | 19 | 882 | 907 | 10 |
| -4 | 10 | 19 | 148 | 141 | 23 |
| 0 | 0 | 20 | 1331 | 1320 | 21 |
| -1 | 1 | 20 | 634 | 622 | 12 |
| 0 | 1 | 20 | 485 | 475 | 7 |
| -2 | 2 | 20 | 1613 | 1629 | 17 |
| -1 | 2 | 20 | 611 | 616 | 14 |
| 0 | 2 | 20 | 1292 | 1324 | 13 |
| -3 | 3 | 20 | 967 | 987 | 10 |
| -2 | 3 | 20 | 1216 | 1243 | 45 |
| -1 | 3 | 20 | 928 | 960 | 32 |
| 0 | 3 | 20 | 981 | 1016 | 11 |
| -4 | 4 | 20 | 1459 | 1468 | 9 |
| -3 | 4 | 20 | 496 | 526 | 10 |
| -2 | 4 | 20 | 536 | 528 | 25 |
| -1 | 4 | 20 | 675 | 697 | 5 |
| 0 | 4 | 20 | 1708 | 1716 | 21 |
| -5 | 5 | 20 | 541 | 549 | 8 |
| -4 | 5 | 20 | 574 | 576 | 9 |
| -3 | 5 | 20 | 754 | 755 | 5 |
| -2 | 5 | 20 | 559 | 579 | 10 |
| -1 | 5 | 20 | 698 | 683 | 10 |
| 0 | 5 | 20 | 431 | 417 | 9 |
| -6 | 6 | 20 | 1034 | 1047 | 13 |
| -5 | 6 | 20 | 308 | 300 | 14 |
| -4 | 6 | 20 | 1139 | 1150 | 10 |
| -3 | 6 | 20 | 8 | 145 | -7 |
| -2 | 6 | 20 | 946 | 945 | 9 |
| -1 | 6 | 20 | 278 | 223 | 18 |
| 0 | 6 | 20 | 1110 | 1117 | 13 |
| -7 | 7 | 20 | 678 | 686 | 10 |
| -6 | 7 | 20 | 633 | 648 | 6 |
| -5 | 7 | 20 | 912 | 933 | 5 |
| -4 | 7 | 20 | 983 | 990 | 9 |
| -3 | 7 | 20 | 800 | 813 | 8 |
| -2 | 7 | 20 | 698 | 706 | 11 |
| -1 | 7 | 20 | 848 | 863 | 13 |
| 0 | 7 | 20 | 658 | 641 | 16 |
| -8 | 8 | 20 | 619 | 639 | 9 |
| -7 | 8 | 20 | 356 | 369 | 10 |
| -6 | 8 | 20 | 620 | 616 | 7 |
| -5 | 8 | 20 | 382 | 372 | 9 |
| -4 | 8 | 20 | 581 | 576 | 7 |
| -3 | 8 | 20 | 486 | 482 | 11 |
| -2 | 8 | 20 | 793 | 789 | 13 |
| -1 | 8 | 20 | 439 | 443 | 9 |
| 0 | 8 | 20 | 503 | 475 | 10 |
| -8 | 9 | 20 | 445 | 448 | 10 |
| -7 | 9 | 20 | 409 | 417 | 14 |
| -6 | 9 | 20 | 212 | 209 | 30 |
| -5 | 9 | 20 | 603 | 606 | 15 |
| -4 | 9 | 20 | 481 | 478 | 10 |
| -3 | 9 | 20 | 283 | 261 | 13 |
| -2 | 9 | 20 | 410 | 400 | 10 |
| -1 | 9 | 20 | 416 | 410 | 10 |
| -5 | 10 | 20 | 238 | 236 | 29 |
| -1 | 2 | 21 | 590 | 607 | 41 |
| -2 | 3 | 21 | 1199 | 1243 | 62 |
| -1 | 3 | 21 | 1539 | 1607 | 49 |
| -3 | 4 | 21 | 855 | 864 | 5 |
| -2 | 4 | 21 | 545 | 541 | 22 |
| -1 | 4 | 21 | 791 | 791 | 6 |
| -4 | 5 | 21 | 1104 | 1102 | 7 |
| -3 | 5 | 21 | 692 | 711 | 6 |
| -2 | 5 | 21 | 606 | 621 | 8 |
| -1 | 5 | 21 | 898 | 901 | 9 |
| -5 | 6 | 21 | 1833 | 1849 | 12 |
| -4 | 6 | 21 | 582 | 589 | 11 |
| -3 | 6 | 21 | 204 | 224 | 13 |
| -2 | 6 | 21 | 659 | 669 | 8 |
| -1 | 6 | 21 | 1725 | 1741 | 28 |
| -6 | 7 | 21 | 387 | 381 | 9 |
| -5 | 7 | 21 | 412 | 437 | 9 |
| -4 | 7 | 21 | 1111 | 1102 | 15 |
| -3 | 7 | 21 | 1116 | 1121 | 9 |
| -2 | 7 | 21 | 558 | 555 | 8 |
| -1 | 7 | 21 | 286 | 288 | 11 |
| -7 | 8 | 21 | 149 | 91 | -29 |
| -6 | 8 | 21 | 775 | 776 | 6 |
| -5 | 8 | 21 | 635 | 632 | 10 |
| -4 | 8 | 21 | 231 | 216 | 16 |
| -3 | 8 | 21 | 828 | 848 | 11 |
| -2 | 8 | 21 | 614 | 606 | 7 |
| -1 | 8 | 21 | 167 | 113 | 22 |
| -7 | 9 | 21 | 130 | 138 | -34 |
| -6 | 9 | 21 | 161 | 201 | 24 |
| -5 | 9 | 21 | 369 | 358 | 11 |
| -4 | 9 | 21 | 326 | 331 | 12 |
| -3 | 9 | 21 | 272 | 253 | 16 |
| -2 | 9 | 21 | 12 | 121 | -12 |
| 0 | 0 | 22 | 2225 | 2192 | 12 |
| -1 | 1 | 22 | 719 | 708 | 6 |
| 0 | 1 | 22 | 667 | 668 | 10 |
| -2 | 2 | 22 | 1273 | 1319 | 13 |
| -1 | 2 | 22 | 511 | 490 | 28 |
| 0 | 2 | 22 | 1402 | 1429 | 10 |
| -3 | 3 | 22 | 753 | 767 | 10 |
| -2 | 3 | 22 | 1057 | 1107 | 48 |
| -1 | 3 | 22 | 1403 | 1473 | 66 |
| 0 | 3 | 22 | 760 | 753 | 12 |
| -4 | 4 | 22 | 884 | 910 | 8 |
| -3 | 4 | 22 | 187 | 204 | 16 |
| -2 | 4 | 22 | 1495 | 1502 | 8 |
| -1 | 4 | 22 | 219 | 215 | 18 |
| 0 | 4 | 22 | 775 | 803 | 10 |
| -5 | 5 | 22 | 1235 | 1234 | 9 |
| -4 | 5 | 22 | 626 | 628 | 15 |
| -3 | 5 | 22 | 284 | 283 | 19 |
| -2 | 5 | 22 | 273 | 271 | 21 |
| -1 | 5 | 22 | 562 | 562 | 7 |
| 0 | 5 | 22 | 1034 | 1046 | 7 |
| -6 | 6 | 22 | 1232 | 1242 | 11 |
| -5 | 6 | 22 | 734 | 748 | 15 |
| -4 | 6 | 22 | 851 | 870 | 5 |
| -3 | 6 | 22 | 407 | 416 | 9 |
| -2 | 6 | 22 | 639 | 648 | 6 |
| -1 | 6 | 22 | 723 | 719 | 10 |
| 0 | 6 | 22 | 1269 | 1259 | 14 |
| -7 | 7 | 22 | 973 | 986 | 9 |
| -6 | 7 | 22 | 696 | 708 | 6 |
| -5 | 7 | 22 | 424 | 432 | 8 |
| -4 | 7 | 22 | 192 | 176 | 18 |
| -3 | 7 | 22 | 157 | 148 | 20 |
| -2 | 7 | 22 | 485 | 483 | 11 |
| -1 | 7 | 22 | 664 | 664 | 6 |
| 0 | 7 | 22 | 1320 | 1317 | 21 |
| -8 | 8 | 22 | 284 | 266 | 16 |
| -7 | 8 | 22 | 401 | 398 | 10 |
| -6 | 8 | 22 | 980 | 978 | 8 |
| -5 | 8 | 22 | 766 | 767 | 8 |
| -4 | 8 | 22 | 1427 | 1430 | 15 |
| -3 | 8 | 22 | 577 | 577 | 9 |
| -2 | 8 | 22 | 902 | 897 | 10 |
| -1 | 8 | 22 | 366 | 349 | 11 |
| 0 | 8 | 22 | 245 | 220 | 18 |
| -7 | 9 | 22 | 522 | 523 | 9 |
| -6 | 9 | 22 | 216 | 257 | 28 |
| -5 | 9 | 22 | 27 | 269 | -27 |
| -4 | 9 | 22 | 376 | 357 | 10 |
| -3 | 9 | 22 | 340 | 333 | 11 |
| -2 | 9 | 22 | 500 | 514 | 14 |
| -1 | 2 | 23 | 738 | 764 | 98 |
| -2 | 3 | 23 | 930 | 969 | 46 |
| -1 | 3 | 23 | 1250 | 1304 | 51 |
| -3 | 4 | 23 | 462 | 460 | 7 |
| -2 | 4 | 23 | 432 | 118 | -135 |
| -1 | 4 | 23 | 369 | 363 | 8 |
| -4 | 5 | 23 | 1264 | 1268 | 12 |
| -3 | 5 | 23 | 532 | 535 | 7 |
| -2 | 5 | 23 | 403 | 399 | 8 |
| -1 | 5 | 23 | 1018 | 1020 | 7 |
| -5 | 6 | 23 | 390 | 378 | 10 |
| -4 | 6 | 23 | 199 | 214 | 20 |
| -3 | 6 | 23 | 496 | 498 | 19 |
| -2 | 6 | 23 | 286 | 286 | 11 |
| -1 | 6 | 23 | 424 | 421 | 8 |
| -6 | 7 | 23 | 168 | 128 | 19 |
| -5 | 7 | 23 | 681 | 687 | 9 |
| -4 | 7 | 23 | 480 | 484 | 8 |
| -3 | 7 | 23 | 489 | 503 | 8 |
| -2 | 7 | 23 | 569 | 564 | 8 |
| -1 | 7 | 23 | 194 | 160 | 15 |
| -7 | 8 | 23 | 122 | 100 | -28 |
| -6 | 8 | 23 | 33 | 281 | -32 |
| -5 | 8 | 23 | 315 | 312 | 12 |
| -4 | 8 | 23 | 531 | 528 | 12 |
| -3 | 8 | 23 | 415 | 400 | 9 |
| -2 | 8 | 23 | 331 | 327 | 14 |
| -1 | 8 | 23 | 97 | 106 | -39 |
| -6 | 9 | 23 | 263 | 260 | 17 |
| -5 | 9 | 23 | 206 | 228 | 22 |
| -4 | 9 | 23 | 246 | 237 | 19 |
| -3 | 9 | 23 | 291 | 308 | 13 |
| 0 | 0 | 24 | 2686 | 2675 | 12 |
| -1 | 1 | 24 | 670 | 665 | 7 |
| 0 | 1 | 24 | 569 | 555 | 8 |
| -2 | 2 | 24 | 1982 | 1975 | 17 |
| -1 | 2 | 24 | 1248 | 1421 | 84 |
| 0 | 2 | 24 | 2220 | 2219 | 18 |
| -3 | 3 | 24 | 760 | 765 | 7 |
| -2 | 3 | 24 | 610 | 614 | 65 |
| -1 | 3 | 24 | 610 | 587 | 60 |
| 0 | 3 | 24 | 966 | 969 | 7 |
| -4 | 4 | 24 | 987 | 1006 | 7 |
| -3 | 4 | 24 | 417 | 424 | 11 |
| -2 | 4 | 24 | 152 | 159 | 24 |
| -1 | 4 | 24 | 514 | 500 | 10 |
| 0 | 4 | 24 | 1159 | 1168 | 8 |
| -5 | 5 | 24 | 209 | 192 | 25 |
| -4 | 5 | 24 | 404 | 402 | 18 |
| -3 | 5 | 24 | 26 | 265 | -26 |
| -2 | 5 | 24 | 290 | 302 | 19 |
| -1 | 5 | 24 | 408 | 396 | 9 |
| 0 | 5 | 24 | 208 | 238 | 23 |
| -6 | 6 | 24 | 1447 | 1458 | 11 |
| -5 | 6 | 24 | 574 | 566 | 11 |
| -4 | 6 | 24 | 635 | 633 | 6 |
| -3 | 6 | 24 | 1210 | 1190 | 13 |
| -2 | 6 | 24 | 509 | 515 | 7 |
| -1 | 6 | 24 | 623 | 604 | 16 |
| 0 | 6 | 24 | 1844 | 1842 | 13 |
| -7 | 7 | 24 | 277 | 290 | 16 |
| -6 | 7 | 24 | 323 | 319 | 11 |
| -5 | 7 | 24 | 557 | 554 | 7 |
| -4 | 7 | 24 | 212 | 220 | 16 |
| -3 | 7 | 24 | 274 | 245 | 24 |
| -2 | 7 | 24 | 749 | 742 | 6 |
| -1 | 7 | 24 | 388 | 398 | 9 |
| 0 | 7 | 24 | 273 | 264 | 17 |
| -7 | 8 | 24 | 436 | 442 | 10 |
| -6 | 8 | 24 | 711 | 696 | 7 |
| -5 | 8 | 24 | 431 | 422 | 10 |
| -4 | 8 | 24 | 1305 | 1301 | 15 |
| -3 | 8 | 24 | 520 | 515 | 14 |
| -2 | 8 | 24 | 723 | 721 | 7 |
| -1 | 8 | 24 | 578 | 593 | 8 |
| -6 | 9 | 24 | 544 | 544 | 9 |
| -5 | 9 | 24 | 10 | 116 | -9 |
| -4 | 9 | 24 | 129 | 109 | -27 |
| -3 | 9 | 24 | 687 | 667 | 7 |
| -1 | 2 | 25 | 907 | 993 | 38 |
| -2 | 3 | 25 | 945 | 980 | 24 |
| -1 | 3 | 25 | 747 | 769 | 20 |
| -3 | 4 | 25 | 494 | 504 | 7 |
| -2 | 4 | 25 | 421 | 409 | 8 |
| -1 | 4 | 25 | 620 | 625 | 6 |
| -4 | 5 | 25 | 869 | 856 | 10 |
| -3 | 5 | 25 | 632 | 642 | 11 |
| -2 | 5 | 25 | 485 | 483 | 13 |
| -1 | 5 | 25 | 648 | 637 | 6 |
| -5 | 6 | 25 | 638 | 646 | 7 |
| -4 | 6 | 25 | 328 | 331 | 14 |
| -3 | 6 | 25 | 526 | 522 | 27 |
| -2 | 6 | 25 | 408 | 415 | 12 |
| -1 | 6 | 25 | 478 | 489 | 12 |
| -6 | 7 | 25 | 543 | 551 | 8 |
| -5 | 7 | 25 | 482 | 490 | 8 |
| -4 | 7 | 25 | 165 | 163 | 19 |
| -3 | 7 | 25 | 146 | 157 | -30 |
| -2 | 7 | 25 | 407 | 409 | 9 |
| -1 | 7 | 25 | 444 | 433 | 10 |
| -7 | 8 | 25 | 288 | 306 | 14 |
| -6 | 8 | 25 | 264 | 284 | 15 |
| -5 | 8 | 25 | 517 | 517 | 12 |
| -4 | 8 | 25 | 622 | 624 | 8 |
| -3 | 8 | 25 | 385 | 388 | 10 |
| -2 | 8 | 25 | 190 | 212 | 26 |
| -1 | 8 | 25 | 374 | 367 | 11 |
| 0 | 0 | 26 | 756 | 792 | 12 |
| -1 | 1 | 26 | 714 | 716 | 15 |
| 0 | 1 | 26 | 642 | 638 | 7 |
| -2 | 2 | 26 | 405 | 403 | 12 |

Table 5 Observed and calculated structure factors for 1



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -1 | 2 | 26 | 607 | 202 | -151 |
| 0 | 2 | 26 | 326 | 330 | 11 |
| -3 | 3 | 26 | 600 | 603 | 8 |
| -2 | 3 | 26 | 526 | 506 | 82 |
| -1 | 3 | 26 | 469 | 450 | 63 |
| 0 | 3 | 26 | 808 | 811 | 15 |
| -4 | 4 | 26 | 1731 | 1724 | 30 |
| -3 | 4 | 26 | 341 | 304 | 61 |
| -2 | 4 | 26 | 174 | 179 | 23 |
| -1 | 4 | 26 | 378 | 369 | 13 |
| 0 | 4 | 26 | 1674 | 1674 | 10 |
| -5 | 5 | 26 | 319 | 317 | 13 |
| -4 | 5 | 26 | 353 | 376 | 22 |
| -3 | 5 | 26 | 464 | 468 | 19 |
| -2 | 5 | 26 | 417 | 416 | 11 |
| -1 | 5 | 26 | 303 | 286 | 22 |
| 0 | 5 | 26 | 339 | 344 | 12 |
| -6 | 6 | 26 | 1010 | 1004 | 7 |
| -5 | 6 | 26 | 500 | 499 | 8 |
| -4 | 6 | 26 | 906 | 902 | 7 |
| -3 | 6 | 26 | 452 | 464 | 8 |
| -2 | 6 | 26 | 874 | 875 | 6 |
| -1 | 6 | 26 | 531 | 544 | 8 |
| 0 | 6 | 26 | 815 | 823 | 9 |
| -7 | 7 | 26 | 484 | 503 | 13 |
| -6 | 7 | 26 | 427 | 410 | 15 |
| -5 | 7 | 26 | 530 | 513 | 12 |
| -4 | 7 | 26 | 741 | 740 | 8 |
| -3 | 7 | 26 | 733 | 712 | 12 |
| -2 | 7 | 26 | 385 | 406 | 10 |
| -1 | 7 | 26 | 524 | 517 | 11 |
| 0 | 7 | 26 | 596 | 594 | 11 |
| -7 | 8 | 26 | 222 | 229 | 16 |
| -6 | 8 | 26 | 1083 | 1069 | 12 |
| -5 | 8 | 26 | 421 | 421 | 10 |
| -4 | 8 | 26 | 552 | 524 | 9 |
| -3 | 8 | 26 | 475 | 465 | 9 |
| -2 | 8 | 26 | 999 | 1000 | 10 |
| -1 | 8 | 26 | 290 | 302 | 14 |
| -1 | 2 | 27 | 431 | 137 | -89 |
| -2 | 3 | 27 | 639 | 667 | 28 |
| -1 | 3 | 27 | 680 | 716 | 19 |
| -3 | 4 | 27 | 1539 | 1546 | 8 |
| -2 | 4 | 27 | 332 | 289 | 51 |
| -1 | 4 | 27 | 1571 | 1551 | 12 |
| -4 | 5 | 27 | 569 | 584 | 7 |
| -3 | 5 | 27 | 1239 | 1235 | 10 |
| -2 | 5 | 27 | 1171 | 1162 | 10 |
| -1 | 5 | 27 | 709 | 708 | 8 |
| -5 | 6 | 27 | 360 | 362 | 10 |
| -4 | 6 | 27 | 224 | 177 | -50 |
| -3 | 6 | 27 | 252 | 225 | 18 |
| -2 | 6 | 27 | 213 | 220 | 15 |
| -1 | 6 | 27 | 308 | 299 | 11 |
| -6 | 7 | 27 | 485 | 487 | 13 |
| -5 | 7 | 27 | 225 | 236 | 19 |
| -4 | 7 | 27 | 294 | 286 | 17 |
| -3 | 7 | 27 | 351 | 344 | 17 |
| -2 | 7 | 27 | 306 | 285 | 15 |
| -1 | 7 | 27 | 471 | 458 | 9 |
| -6 | 8 | 27 | 300 | 321 | 15 |
| -5 | 8 | 27 | 463 | 461 | 10 |
| -4 | 8 | 27 | 113 | 70 | -28 |
| -3 | 8 | 27 | 440 | 397 | 17 |
| -2 | 8 | 27 | 343 | 337 | 14 |
| 0 | 0 | 28 | 1374 | 1423 | 14 |
| -1 | 1 | 28 | 1350 | 1323 | 16 |
| 0 | 1 | 28 | 1254 | 1235 | 16 |
| -2 | 2 | 28 | 1398 | 1371 | 19 |
| -1 | 2 | 28 | 641 | 648 | 22 |
| 0 | 2 | 28 | 1250 | 1212 | 12 |
| -3 | 3 | 28 | 432 | 432 | 10 |
| -2 | 3 | 28 | 414 | 436 | 27 |
| -1 | 3 | 28 | 386 | 396 | 42 |
| 0 | 3 | 28 | 404 | 408 | 13 |
| -4 | 4 | 28 | 289 | 265 | 15 |
| -3 | 4 | 28 | 651 | 696 | 48 |
| -2 | 4 | 28 | 722 | 763 | 28 |
| -1 | 4 | 28 | 895 | 924 | 25 |
| 0 | 4 | 28 | 313 | 334 | 13 |
| -5 | 5 | 28 | 492 | 478 | 10 |
| -4 | 5 | 28 | 633 | 623 | 14 |
| -3 | 5 | 28 | 619 | 607 | 37 |
| -2 | 5 | 28 | 477 | 466 | 19 |
| -1 | 5 | 28 | 757 | 754 | 8 |
| 0 | 5 | 28 | 519 | 517 | 11 |
| -6 | 6 | 28 | 1229 | 1256 | 21 |
| -5 | 6 | 28 | 619 | 622 | 7 |
| -4 | 6 | 28 | 412 | 419 | 9 |
| -3 | 6 | 28 | 537 | 529 | 8 |
| -2 | 6 | 28 | 436 | 422 | 8 |
| -1 | 6 | 28 | 466 | 473 | 9 |
| 0 | 6 | 28 | 1016 | 1034 | 8 |
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