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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
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H1B H 0.4781 0.3333 0.6183 0.098 Uiso 1 1 calc R . .
H1C H 0.5656 0.2728 0.6018 0.098 Uiso 1 1 calc R . .
C2 C 0.1600(2) 0.2397(3) 0.7580(2) 0.1017(12) Uani 1 1 d . . .
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H2B H 0.1861 0.2170 0.7104 0.153 Uiso 1 1 calc R . .
H2C H 0.1398 0.2966 0.7447 0.153 Uiso 1 1 calc R . .
C3 C 0.46444(17) 0.30661(16) 0.95561(15) 0.0518(6) Uani 1 1 d . . .
C4 C 0.5735(2) 0.3307(3) 0.9464(2) 0.1042(13) Uani 1 1 d . . .
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H4B H 0.5681 0.3827 0.9150 0.156 Uiso 1 1 calc R . .
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C6 C 0.6455(2) 0.0735(2) 0.58622(17) 0.0788(9) Uani 1 1 d . . .
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H6B H 0.7015 0.1144 0.5953 0.118 Uiso 1 1 calc R . .
H6C H 0.5775 0.1008 0.5780 0.118 Uiso 1 1 calc R . .
C7 C 0.2789(3) 0.14336(17) 0.8589(2) 0.0896(10) Uani 1 1 d . . .
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H7B H 0.3370 0.1365 0.9132 0.134 Uiso 1 1 calc R . .
H7C H 0.3012 0.1248 0.8076 0.134 Uiso 1 1 calc R . .
C9 C 0.8319(3) 0.1762(3) 0.7289(2) 0.1004(11) Uani 1 1 d . . .
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H9B H 0.7774 0.2163 0.7021 0.151 Uiso 1 1 calc R . .
H9C H 0.8338 0.1342 0.6850 0.151 Uiso 1 1 calc R . .
C10 C 0.6856(3) 0.0563(3) 0.95390(18) 0.0934(11) Uani 1 1 d . . .
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H10B H 0.6392 0.1034 0.9505 0.140 Uiso 1 1 calc R . .
H10C H 0.7589 0.0748 0.9675 0.140 Uiso 1 1 calc R . .
C11 C 0.3245(2) 0.40084(14) 0.79229(17) 0.0571(6) Uani 1 1 d . . .
C12 C 0.4784(3) 0.2228(2) 1.0037(2) 0.0964(11) Uani 1 1 d . . .
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H12C H 0.4100 0.2040 1.0089 0.145 Uiso 1 1 calc R . .
C13 C 0.7958(3) 0.2072(2) 0.8742(3) 0.0965(11) Uani 1 1 d . . .
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C14 C 0.1989(2) 0.2595(2) 0.9237(2) 0.0878(10) Uani 1 1 d . . .
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H14B H 0.1760 0.3164 0.9161 0.132 Uiso 1 1 calc R . .
H14C H 0.2522 0.2531 0.9812 0.132 Uiso 1 1 calc R . .
C15 C 0.6555(2) 0.01133(17) 0.86426(17) 0.0608(6) Uani 1 1 d . . .
C16 C 0.2711(3) 0.3933(2) 0.6906(2) 0.0947(11) Uani 1 1 d . . .
H16A H 0.2509 0.4475 0.6655 0.142 Uiso 1 1 calc R . .
H16B H 0.2081 0.3591 0.6804 0.142 Uiso 1 1 calc R . .
H16C H 0.3205 0.3686 0.6619 0.142 Uiso 1 1 calc R . .
C17 C 0.24741(18) 0.23469(16) 0.84695(16) 0.0550(6) Uani 1 1 d . . .
C19 C 0.37614(19) 0.15962(16) 0.61174(16) 0.0599(6) Uani 1 1 d . . .
H19A H 0.3436 0.1157 0.6371 0.090 Uiso 1 1 calc R . .
H19B H 0.4080 0.1370 0.5675 0.090 Uiso 1 1 calc R . .
H19C H 0.3223 0.1996 0.5832 0.090 Uiso 1 1 calc R . .
C20 C 0.7199(3) -0.0694(2) 0.8758(2) 0.0926(10) Uani 1 1 d . . .
H20A H 0.7070 -0.1012 0.9245 0.139 Uiso 1 1 calc R . .
H20B H 0.7952 -0.0568 0.8894 0.139 Uiso 1 1 calc R . .
H20C H 0.6981 -0.1010 0.8206 0.139 Uiso 1 1 calc R . .
C22 C 0.2473(3) 0.4458(2) 0.8359(3) 0.1071(13) Uani 1 1 d . . .
H22A H 0.2283 0.4988 0.8071 0.161 Uiso 1 1 calc R . .
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H22B H 0.2818 0.4539 0.8994 0.161 Uiso 1 1 calc R . .
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C23 C 0.4233(3) 0.45482(18) 0.8022(3) 0.0962(11) Uani 1 1 d . . .
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H23B H 0.4705 0.4287 0.7723 0.144 Uiso 1 1 calc R . .
H23C H 0.4601 0.4618 0.8655 0.144 Uiso 1 1 calc R . .
C24 C 0.7697(3) -0.0333(2) 0.6735(2) 0.0975(11) Uani 1 1 d . . .
H24A H 0.7599 -0.0643 0.6184 0.146 Uiso 1 1 calc R . .
H24B H 0.7837 -0.0707 0.7241 0.146 Uiso 1 1 calc R . .
H24C H 0.8295 0.0040 0.6810 0.146 Uiso 1 1 calc R . .
C25 C 0.5720(3) -0.0415(2) 0.6494(2) 0.0837(9) Uani 1 1 d . . .
H25A H 0.5706 -0.0748 0.5972 0.126 Uiso 1 1 calc R . .
H25B H 0.5068 -0.0097 0.6379 0.126 Uiso 1 1 calc R . .
H25C H 0.5782 -0.0769 0.7010 0.126 Uiso 1 1 calc R . .
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H26B H 0.3637 0.3542 1.0257 0.133 Uiso 1 1 calc R . .
H26C H 0.4268 0.4238 0.9909 0.133 Uiso 1 1 calc R . .
C27 C 0.80611(19) 0.13580(18) 0.81125(19) 0.0656(7) Uani 1 1 d . . .
C28 C 0.5354(2) -0.0076(2) 0.8459(2) 0.0901(10) Uani 1 1 d . . .
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H28B H 0.5091 -0.0335 0.7876 0.135 Uiso 1 1 calc R . .
H28C H 0.4968 0.0432 0.8467 0.135 Uiso 1 1 calc R . .
C29 C 0.66745(19) 0.01684(16) 0.66874(15) 0.0570(6) Uani 1 1 d . . .
C30 C 0.9008(2) 0.0814(2) 0.8588(3) 0.0943(11) Uani 1 1 d . . .
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P2 0.0345(3) 0.0362(3) 0.0363(3) -0.00121(19) 0.0106(2) 0.00340(19)
N1 0.0499(10) 0.0559(11) 0.0484(10) 0.0015(8) 0.0186(8) 0.0158(8)
N2 0.0539(10) 0.0504(11) 0.0458(10) 0.0013(8) 0.0218(9) 0.0148(9)
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C2 0.0616(17) 0.147(3) 0.084(2) -0.019(2) 0.0000(16) -0.036(2)
C3 0.0446(11) 0.0706(15) 0.0376(11) -0.0032(10) 0.0071(9) -0.0011(10)
C4 0.0461(14) 0.183(4) 0.074(2) -0.007(2) 0.0015(13) -0.020(2)
C6 0.0837(19) 0.112(2) 0.0466(14) 0.0038(14) 0.0275(13) 0.0227(17)
C7 0.116(2) 0.0566(17) 0.110(3) -0.0105(16) 0.054(2) -0.0324(17)
C9 0.076(2) 0.118(3) 0.120(3) 0.010(2) 0.047(2) -0.025(2)
C10 0.105(2) 0.134(3) 0.0461(15) 0.0132(17) 0.0282(15) 0.029(2)
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C12 0.109(3) 0.106(3) 0.0606(18) 0.0212(17) 0.0009(17) 0.025(2)
C13 0.0690(18) 0.089(2) 0.124(3) -0.040(2) 0.0137(18) -0.0146(16)
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 are estimated using the full covariance matrix.  The cell esds are taken
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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C11 C 0.3249(3) 0.4039(2) 0.7928(3) 0.0645(11) Uani 1 1 d . . .
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C13 C 0.7990(5) 0.2033(3) 0.8758(5) 0.1048(19) Uani 1 1 d . . .
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H13B H 0.7777 0.1815 0.9275 0.157 Uiso 1 1 calc R . .
H13C H 0.7456 0.2429 0.8426 0.157 Uiso 1 1 calc R . .
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H14B H 0.1745 0.3244 0.9144 0.160 Uiso 1 1 calc R . .
H14C H 0.2516 0.2604 0.9811 0.160 Uiso 1 1 calc R . .
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C16 C 0.2696(5) 0.3980(4) 0.6920(4) 0.116(2) Uani 1 1 d . . .
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H16C H 0.3179 0.3729 0.6612 0.174 Uiso 1 1 calc R . .
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C17 C 0.2420(3) 0.2399(3) 0.8452(3) 0.0643(11) Uani 1 1 d . . .
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H19C H 0.3171 0.1953 0.5716 0.101 Uiso 1 1 calc R . .
C20 C 0.7190(5) -0.0711(3) 0.8768(4) 0.107(2) Uani 1 1 d . . .
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H20B H 0.7951 -0.0584 0.8910 0.161 Uiso 1 1 calc R . .
H20C H 0.6968 -0.1028 0.8203 0.161 Uiso 1 1 calc R . .
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H22A H 0.2343 0.5041 0.8087 0.174 Uiso 1 1 calc R . .
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H24C H 0.8298 0.0004 0.6837 0.145 Uiso 1 1 calc R . .
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H25A H 0.5697 -0.0762 0.5966 0.132 Uiso 1 1 calc R . .
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H26C H 0.4293 0.4221 0.9924 0.155 Uiso 1 1 calc R . .
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H28B H 0.5093 -0.0337 0.7862 0.156 Uiso 1 1 calc R . .
H28C H 0.4980 0.0438 0.8471 0.156 Uiso 1 1 calc R . .
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C30 C 0.9014(4) 0.0772(3) 0.8616(4) 0.1002(17) Uani 1 1 d . . .
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P2 0.0393(5) 0.0436(5) 0.0374(5) -0.0010(3) 0.0079(4) 0.0058(3)
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C3 0.049(2) 0.085(3) 0.044(2) -0.004(2) 0.0021(19) -0.0022(18)
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C9 0.078(4) 0.119(4) 0.110(5) 0.008(4) 0.039(3) -0.026(3)
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C13 0.078(4) 0.101(4) 0.125(5) -0.048(3) 0.011(4) -0.021(3)
C14 0.092(4) 0.128(4) 0.123(5) -0.040(4) 0.069(4) -0.044(3)
C15 0.075(3) 0.080(3) 0.055(3) 0.013(2) 0.025(2) 0.010(2)
C16 0.147(6) 0.106(4) 0.078(4) 0.036(3) 0.004(4) 0.044(4)
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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P2 P 0.35647(8) 0.30238(6) 0.83292(7) 0.0478(2) Uani 1 1 d . . .
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N2 N 0.3971(4) 0.2549(3) 0.7660(3) 0.0950(16) Uani 1 1 d . . .
C1 C 0.5388(5) 0.3083(4) 0.6251(4) 0.0942(19) Uani 1 1 d . . .
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C2 C 0.1451(6) 0.2633(8) 0.7502(6) 0.179(5) Uani 1 1 d . . .
H2A H 0.0824 0.2339 0.7511 0.268 Uiso 1 1 calc R . .
H2B H 0.1713 0.2427 0.7025 0.268 Uiso 1 1 calc R . .
H2C H 0.1286 0.3201 0.7404 0.268 Uiso 1 1 calc R . .
C3 C 0.4540(4) 0.3038(4) 0.9483(3) 0.0833(16) Uani 1 1 d . . .
C4 C 0.5619(5) 0.3235(9) 0.9398(6) 0.199(6) Uani 1 1 d . . .

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H4B H 0.5591 0.3740 0.9078 0.298 Uiso 1 1 calc R . .
H4C H 0.5847 0.2807 0.9073 0.298 Uiso 1 1 calc R . .
C6 C 0.6475(5) 0.0671(4) 0.5910(3) 0.0939(18) Uani 1 1 d . . .
H6A H 0.6458 0.0345 0.5390 0.141 Uiso 1 1 calc R . .
H6B H 0.7029 0.1069 0.5999 0.141 Uiso 1 1 calc R . .
H6C H 0.5806 0.0942 0.5817 0.141 Uiso 1 1 calc R . .
C7 C 0.2487(8) 0.1611(5) 0.8506(7) 0.161(4) Uani 1 1 d . . .
H7A H 0.1852 0.1346 0.8547 0.241 Uiso 1 1 calc R . .
H7B H 0.3053 0.1501 0.9043 0.241 Uiso 1 1 calc R . .
H7C H 0.2675 0.1409 0.7990 0.241 Uiso 1 1 calc R . .
C9 C 0.8337(6) 0.1666(5) 0.7315(5) 0.133(3) Uani 1 1 d . . .
H9A H 0.9012 0.1934 0.7506 0.199 Uiso 1 1 calc R . .
H9B H 0.7800 0.2055 0.7033 0.199 Uiso 1 1 calc R . .
H9C H 0.8359 0.1243 0.6892 0.199 Uiso 1 1 calc R . .
C10 C 0.6878(6) 0.0584(6) 0.9580(4) 0.133(3) Uani 1 1 d . . .
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H10B H 0.6423 0.1048 0.9539 0.200 Uiso 1 1 calc R . .
H10C H 0.7599 0.0762 0.9703 0.200 Uiso 1 1 calc R . .
C11 C 0.3253(5) 0.4112(3) 0.7941(4) 0.0846(16) Uani 1 1 d . . .
C12 C 0.4632(9) 0.2180(6) 0.9869(6) 0.181(5) Uani 1 1 d . . .
H12A H 0.5107 0.2182 1.0469 0.272 Uiso 1 1 calc R . .
H12B H 0.4900 0.1822 0.9494 0.272 Uiso 1 1 calc R . .
H12C H 0.3946 0.1995 0.9886 0.272 Uiso 1 1 calc R . .
C13 C 0.8001(6) 0.2008(4) 0.8755(6) 0.123(3) Uani 1 1 d . . .
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H13A H 0.8678 0.2271 0.8967 0.185 Uiso 1 1 calc R . .
H13B H 0.7790 0.1806 0.9260 0.185 Uiso 1 1 calc R . .
H13C H 0.7485 0.2393 0.8426 0.185 Uiso 1 1 calc R . .
C14 C 0.1857(6) 0.2815(5) 0.9154(6) 0.145(4) Uani 1 1 d . . .
H14A H 0.1255 0.2489 0.9163 0.218 Uiso 1 1 calc R . .
H14B H 0.1644 0.3374 0.9048 0.218 Uiso 1 1 calc R . .
H14C H 0.2390 0.2769 0.9725 0.218 Uiso 1 1 calc R . .
C15 C 0.6559(5) 0.0116(4) 0.8687(4) 0.0839(16) Uani 1 1 d . . .
C16 C 0.2669(9) 0.4094(6) 0.6940(5) 0.171(4) Uani 1 1 d . . .
H16A H 0.2488 0.4640 0.6728 0.257 Uiso 1 1 calc R . .
H16B H 0.2034 0.3777 0.6844 0.257 Uiso 1 1 calc R . .
H16C H 0.3116 0.3854 0.6615 0.257 Uiso 1 1 calc R . .
C17 C 0.2301(4) 0.2521(4) 0.8411(4) 0.0797(15) Uani 1 1 d . . .
C19 C 0.3599(4) 0.1475(3) 0.5841(3) 0.0777(14) Uani 1 1 d . . .
H19A H 0.3298 0.1048 0.6115 0.116 Uiso 1 1 calc R . .
H19B H 0.3937 0.1241 0.5425 0.116 Uiso 1 1 calc R . .
H19C H 0.3049 0.1840 0.5524 0.116 Uiso 1 1 calc R . .
C20 C 0.7199(7) -0.0686(5) 0.8830(5) 0.144(3) Uani 1 1 d . . .
H20A H 0.7059 -0.0988 0.9315 0.216 Uiso 1 1 calc R . .
H20B H 0.7942 -0.0563 0.8977 0.216 Uiso 1 1 calc R . .
H20C H 0.6995 -0.1004 0.8287 0.216 Uiso 1 1 calc R . .
C22 C 0.2626(8) 0.4596(4) 0.8435(7) 0.159(4) Uani 1 1 d . . .
H22A H 0.2444 0.5115 0.8146 0.238 Uiso 1 1 calc R . .
H22B H 0.3042 0.4676 0.9049 0.238 Uiso 1 1 calc R . .
H22C H 0.1990 0.4305 0.8425 0.238 Uiso 1 1 calc R . .
C23 C 0.4300(7) 0.4552(4) 0.8024(7) 0.156(4) Uani 1 1 d . . .
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H23B H 0.4699 0.4256 0.7696 0.234 Uiso 1 1 calc R . .
H23C H 0.4700 0.4584 0.8649 0.234 Uiso 1 1 calc R . .
C24 C 0.7647(5) -0.0408(4) 0.6808(4) 0.108(2) Uani 1 1 d . . .
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H24B H 0.7749 -0.0778 0.7307 0.162 Uiso 1 1 calc R . .
H24C H 0.8262 -0.0067 0.6898 0.162 Uiso 1 1 calc R . .
C25 C 0.5717(5) -0.0436(4) 0.6550(4) 0.0981(19) Uani 1 1 d . . .
H25A H 0.5696 -0.0770 0.6035 0.147 Uiso 1 1 calc R . .
H25B H 0.5085 -0.0111 0.6427 0.147 Uiso 1 1 calc R . .
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C26 C 0.4312(6) 0.3614(6) 1.0160(4) 0.145(3) Uani 1 1 d . . .
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H26B H 0.3653 0.3467 1.0268 0.217 Uiso 1 1 calc R . .
H26C H 0.4265 0.4160 0.9929 0.217 Uiso 1 1 calc R . .
C27 C 0.8080(4) 0.1295(4) 0.8132(4) 0.0796(15) Uani 1 1 d . . .
C28 C 0.5380(6) -0.0061(6) 0.8506(5) 0.141(3) Uani 1 1 d . . .
H28A H 0.5275 -0.0420 0.8964 0.212 Uiso 1 1 calc R . .
H28B H 0.5114 -0.0314 0.7925 0.212 Uiso 1 1 calc R . .
H28C H 0.5006 0.0440 0.8516 0.212 Uiso 1 1 calc R . .
C29 C 0.6682(4) 0.0120(3) 0.6747(3) 0.0644(12) Uani 1 1 d . . .
C30 C 0.9011(4) 0.0745(5) 0.8629(5) 0.119(3) Uani 1 1 d . . .
H30A H 0.9650 0.1063 0.8809 0.178 Uiso 1 1 calc R . .
H30B H 0.9095 0.0315 0.8234 0.178 Uiso 1 1 calc R . .
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N2 0.111(4) 0.107(4) 0.081(3) -0.008(3) 0.049(3) 0.049(3)
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C3 0.064(3) 0.120(5) 0.057(3) -0.010(3) 0.004(2) 0.003(3)
C4 0.051(4) 0.391(18) 0.137(7) 0.008(10) -0.001(4) -0.018(7)
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C7 0.217(10) 0.090(5) 0.203(10) -0.025(6) 0.104(8) -0.061(6)
C9 0.103(5) 0.161(7) 0.147(7) -0.003(6) 0.057(5) -0.056(5)
C10 0.150(7) 0.198(9) 0.058(3) 0.003(4) 0.041(4) 0.015(6)
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C14 0.119(6) 0.170(8) 0.185(9) -0.065(6) 0.105(6) -0.060(5)
C15 0.091(4) 0.106(4) 0.064(3) 0.013(3) 0.037(3) 0.009(3)
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_cell_angle_gamma                 83.628(13)
_cell_volume                      3994(4)
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_diffrn_radiation_type            MoK\a
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_reflns_number_total              11423
_reflns_number_gt                 4880
_reflns_threshold_expression      >2sigma(I)
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_scheme       calc
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P1 P 1.02380(16) 1.25768(12) 0.62539(12) 0.0627(6) Uani 1 1 d . . .
P2 P 0.58103(16) 1.31849(12) 0.71211(12) 0.0652(6) Uani 1 1 d . . .
P3 P 0.44656(17) 0.81443(13) 0.75962(14) 0.0748(7) Uani 1 1 d . . .
P4 P -0.00252(16) 0.76630(12) 0.90833(12) 0.0638(6) Uani 1 1 d . . .
N1 N 0.9120(4) 1.2312(3) 0.6794(3) 0.0717(18) Uani 1 1 d . . .
N2 N 0.6778(4) 1.2714(3) 0.6776(3) 0.0656(17) Uani 1 1 d . . .
N3 N 0.3457(4) 0.7702(3) 0.7794(3) 0.0757(19) Uani 1 1 d . . .
N4 N 0.1093(4) 0.7372(3) 0.8995(3) 0.0695(18) Uani 1 1 d . . .
C1 C 1.1184(6) 1.1741(5) 0.6495(6) 0.081(3) Uani 1 1 d . . .
C2 C 1.0713(7) 1.0959(5) 0.6580(6) 0.127(4) Uani 1 1 d . . .
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H4C H 1.2618 1.2319 0.5887 0.203 Uiso 1 1 calc R . .
H4D H 1.2322 1.1904 0.5373 0.203 Uiso 1 1 calc R . .
C5 C 1.0441(7) 1.2929(6) 0.5132(5) 0.087(3) Uani 1 1 d . . .
C6 C 0.9463(7) 1.3383(6) 0.4980(5) 0.127(4) Uani 1 1 d . . .
H6A H 0.9551 1.3565 0.4407 0.190 Uiso 1 1 calc R . .
H6B H 0.9363 1.3832 0.5163 0.190 Uiso 1 1 calc R . .
H6C H 0.8867 1.3036 0.5274 0.190 Uiso 1 1 calc R . .
C7 C 1.0471(7) 1.2205(6) 0.4853(5) 0.132(4) Uani 1 1 d . . .
H7A H 1.0570 1.2390 0.4278 0.198 Uiso 1 1 calc R . .
H7B H 0.9826 1.1914 0.5144 0.198 Uiso 1 1 calc R . .
H7C H 1.1035 1.1864 0.4963 0.198 Uiso 1 1 calc R . .
C8 C 1.1415(6) 1.3436(5) 0.4557(5) 0.119(4) Uani 1 1 d . . .
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H8A H 1.1427 1.3577 0.4003 0.179 Uiso 1 1 calc R . .
H8B H 1.2027 1.3138 0.4625 0.179 Uiso 1 1 calc R . .
H8C H 1.1401 1.3911 0.4684 0.179 Uiso 1 1 calc R . .
C9 C 1.0559(7) 1.3441(5) 0.6502(6) 0.086(3) Uani 1 1 d . . .
C10 C 1.1721(7) 1.3650(5) 0.6221(6) 0.121(4) Uani 1 1 d . . .
H10A H 1.1802 1.4088 0.6379 0.181 Uiso 1 1 calc R . .
H10B H 1.2001 1.3795 0.5639 0.181 Uiso 1 1 calc R . .
H10C H 1.2085 1.3197 0.6471 0.181 Uiso 1 1 calc R . .
C11 C 1.0102(7) 1.3261(5) 0.7426(6) 0.123(4) Uani 1 1 d . . .
H11A H 1.0252 1.3697 0.7559 0.185 Uiso 1 1 calc R . .
H11B H 1.0406 1.2784 0.7703 0.185 Uiso 1 1 calc R . .
H11C H 0.9361 1.3190 0.7594 0.185 Uiso 1 1 calc R . .
C12 C 0.9989(8) 1.4183(5) 0.6135(6) 0.140(4) Uani 1 1 d . . .
H12A H 1.0142 1.4616 0.6270 0.210 Uiso 1 1 calc R . .
H12B H 0.9253 1.4079 0.6351 0.210 Uiso 1 1 calc R . .
H12C H 1.0213 1.4320 0.5553 0.210 Uiso 1 1 calc R . .
C13A C 0.4562(16) 1.2497(12) 0.7753(13) 0.113(7) Uiso 0.50 1 d P . .
C13 C 0.4518(16) 1.2667(12) 0.7069(13) 0.119(7) Uiso 0.50 1 d P . .
C14 C 0.4909(9) 1.2190(6) 0.8771(7) 0.152(4) Uiso 1 1 d . . .
C15 C 0.4658(7) 1.1831(6) 0.7429(6) 0.116(3) Uiso 1 1 d . . .
C16 C 0.3506(9) 1.3006(6) 0.7742(6) 0.150(4) Uiso 1 1 d . . .
C17A C 0.6253(14) 1.3777(10) 0.7739(10) 0.090(5) Uiso 0.50 1 d P . .
C17 C 0.5592(14) 1.3118(10) 0.8248(10) 0.093(5) Uiso 0.50 1 d P . .
C18 C 0.5002(9) 1.3969(6) 0.8366(6) 0.140(4) Uiso 1 1 d . . .
C19 C 0.6717(7) 1.3175(5) 0.8300(5) 0.098(3) Uiso 1 1 d . . .
C20 C 0.6935(12) 1.4515(9) 0.7081(9) 0.076(5) Uiso 0.50 1 d P . .
C21A C 0.5630(14) 1.4066(10) 0.6238(10) 0.089(5) Uiso 0.50 1 d P . .
C21 C 0.6597(18) 1.4598(13) 0.6576(13) 0.316(11) Uiso 1 1 d . . .
C22 C 0.6523(8) 1.4312(5) 0.5522(6) 0.113(3) Uiso 1 1 d . . .
C23 C 0.4844(8) 1.4721(6) 0.6461(6) 0.131(4) Uiso 1 1 d . . .
C24 C 0.4851(11) 1.3270(8) 0.5977(8) 0.191(5) Uiso 1 1 d . . .
C25 C 0.7821(6) 1.1210(4) 0.6179(4) 0.058(2) Uiso 1 1 d . . .
C26 C 0.7424(6) 1.1540(5) 0.5551(5) 0.087(3) Uiso 1 1 d . . .
H26A H 0.7074 1.2021 0.5500 0.104 Uiso 1 1 calc R . .
C27 C 0.7537(9) 1.1164(7) 0.4984(5) 0.118(4) Uani 1 1 d . . .
H27A H 0.7267 1.1398 0.4556 0.142 Uiso 1 1 calc R . .
C28 C 0.8045(10) 1.0450(7) 0.5054(7) 0.120(4) Uani 1 1 d . . .
H28A H 0.8153 1.0219 0.4658 0.144 Uiso 1 1 calc R . .
C29 C 0.8387(8) 1.0087(6) 0.5695(7) 0.112(4) Uani 1 1 d . . .
H29A H 0.8680 0.9584 0.5767 0.134 Uiso 1 1 calc R . .
C30 C 0.8300(6) 1.0472(5) 0.6258(5) 0.086(3) Uani 1 1 d . . .
H30A H 0.8565 1.0229 0.6687 0.103 Uiso 1 1 calc R . .
C31 C 0.7376(6) 1.1023(4) 0.8214(4) 0.056(2) Uani 1 1 d . . .
C32 C 0.6632(6) 1.0438(4) 0.8513(5) 0.068(2) Uani 1 1 d . . .
H32A H 0.6327 1.0354 0.8168 0.082 Uiso 1 1 calc R . .
C33 C 0.6338(7) 0.9971(5) 0.9338(6) 0.083(3) Uani 1 1 d . . .
H33A H 0.5835 0.9575 0.9540 0.099 Uiso 1 1 calc R . .
C34 C 0.6777(8) 1.0089(6) 0.9854(5) 0.087(3) Uani 1 1 d . . .
H34A H 0.6562 0.9782 1.0405 0.104 Uiso 1 1 calc R . .
C35 C 0.7509(7) 1.0639(5) 0.9567(5) 0.082(3) Uani 1 1 d . . .
H35A H 0.7820 1.0704 0.9917 0.098 Uiso 1 1 calc R . .
C36 C 0.7825(6) 1.1123(4) 0.8750(5) 0.068(2) Uani 1 1 d . . .
H36A H 0.8334 1.1512 0.8561 0.082 Uiso 1 1 calc R . .
C37 C 0.5598(8) 0.7705(8) 0.6965(9) 0.146(5) Uani 1 1 d . . .
C38 C 0.5426(11) 0.7979(10) 0.6093(8) 0.269(10) Uani 1 1 d . . .
H38A H 0.5957 0.7753 0.5740 0.403 Uiso 1 1 calc R . .
H38B H 0.5463 0.8549 0.5859 0.403 Uiso 1 1 calc R . .
H38C H 0.4754 0.7799 0.6158 0.403 Uiso 1 1 calc R . .
C39 C 0.5486(8) 0.6828(8) 0.7267(8) 0.174(5) Uani 1 1 d . . .
H39A H 0.6050 0.6609 0.6928 0.262 Uiso 1 1 calc R . .
H39B H 0.4837 0.6689 0.7249 0.262 Uiso 1 1 calc R . .
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H39C H 0.5499 0.6616 0.7818 0.262 Uiso 1 1 calc R . .
C40 C 0.6695(8) 0.7978(8) 0.6885(9) 0.229(8) Uani 1 1 d . . .
H40A H 0.7228 0.7720 0.6567 0.344 Uiso 1 1 calc R . .
H40B H 0.6761 0.7836 0.7417 0.344 Uiso 1 1 calc R . .
H40C H 0.6765 0.8544 0.6620 0.344 Uiso 1 1 calc R . .
C41 C 0.4308(9) 0.9230(6) 0.7053(8) 0.137(4) Uani 1 1 d . . .
C42 C 0.5363(8) 0.9723(6) 0.6542(7) 0.194(6) Uani 1 1 d . . .
H42A H 0.5208 1.0268 0.6284 0.291 Uiso 1 1 calc R . .
H42B H 0.5771 0.9502 0.6133 0.291 Uiso 1 1 calc R . .
H42C H 0.5747 0.9697 0.6900 0.291 Uiso 1 1 calc R . .
C43 C 0.3550(9) 0.9582(6) 0.7730(8) 0.181(6) Uani 1 1 d . . .
H43A H 0.3431 1.0136 0.7476 0.272 Uiso 1 1 calc R . .
H43B H 0.3867 0.9521 0.8139 0.272 Uiso 1 1 calc R . .
H43C H 0.2897 0.9298 0.7980 0.272 Uiso 1 1 calc R . .
C44 C 0.3764(10) 0.9293(6) 0.6433(6) 0.167(5) Uani 1 1 d . . .
H44A H 0.3661 0.9844 0.6152 0.251 Uiso 1 1 calc R . .
H44B H 0.3102 0.9024 0.6711 0.251 Uiso 1 1 calc R . .
H44C H 0.4187 0.9052 0.6046 0.251 Uiso 1 1 calc R . .
C45 C 0.4819(10) 0.8018(8) 0.8557(7) 0.134(4) Uani 1 1 d . . .
C46 C 0.5261(10) 0.7163(6) 0.8881(8) 0.197(7) Uani 1 1 d . . .
H46A H 0.5419 0.7103 0.9367 0.295 Uiso 1 1 calc R . .
H46B H 0.5883 0.7093 0.8472 0.295 Uiso 1 1 calc R . .
H46C H 0.4751 0.6771 0.9003 0.295 Uiso 1 1 calc R . .
C47 C 0.5613(9) 0.8662(6) 0.8415(7) 0.187(6) Uani 1 1 d . . .
H47A H 0.5744 0.8580 0.8917 0.281 Uiso 1 1 calc R . .
H47B H 0.5330 0.9182 0.8235 0.281 Uiso 1 1 calc R . .
H47C H 0.6254 0.8617 0.8008 0.281 Uiso 1 1 calc R . .
C48 C 0.3755(9) 0.8144(7) 0.9178(6) 0.155(5) Uani 1 1 d . . .
H48A H 0.3858 0.8093 0.9682 0.233 Uiso 1 1 calc R . .
H48B H 0.3259 0.7751 0.9276 0.233 Uiso 1 1 calc R . .
H48C H 0.3498 0.8666 0.8955 0.233 Uiso 1 1 calc R . .
C49 C -0.0224(8) 0.8444(6) 0.9600(7) 0.108(3) Uani 1 1 d . . .
C50 C 0.0341(8) 0.9232(5) 0.8939(7) 0.160(5) Uani 1 1 d . . .
H50A H 0.0265 0.9632 0.9185 0.241 Uiso 1 1 calc R . .
H50B H 0.0035 0.9414 0.8509 0.241 Uiso 1 1 calc R . .
H50C H 0.1067 0.9129 0.8718 0.241 Uiso 1 1 calc R . .
C51 C 0.0326(8) 0.8168(6) 1.0249(6) 0.126(4) Uani 1 1 d . . .
H51A H 0.0233 0.8556 1.0512 0.189 Uiso 1 1 calc R . .
H51B H 0.1056 0.8107 0.9994 0.189 Uiso 1 1 calc R . .
H51C H 0.0035 0.7667 1.0646 0.189 Uiso 1 1 calc R . .
C52 C -0.1379(7) 0.8629(6) 1.0001(6) 0.147(4) Uani 1 1 d . . .
H52A H -0.1406 0.9016 1.0255 0.221 Uiso 1 1 calc R . .
H52B H -0.1727 0.8150 1.0406 0.221 Uiso 1 1 calc R . .
H52C H -0.1716 0.8835 0.9591 0.221 Uiso 1 1 calc R . .
C53 C -0.0297(9) 0.8143(7) 0.8099(6) 0.121(4) Uani 1 1 d . . .
C54 C 0.0662(8) 0.8597(6) 0.7470(5) 0.143(4) Uani 1 1 d . . .
H54A H 0.0531 0.8855 0.6961 0.214 Uiso 1 1 calc R . .
H54B H 0.1231 0.8235 0.7400 0.214 Uiso 1 1 calc R . .
H54C H 0.0837 0.8990 0.7649 0.214 Uiso 1 1 calc R . .
C55 C -0.0412(8) 0.7444(7) 0.7779(6) 0.158(5) Uani 1 1 d . . .
H55A H -0.0544 0.7672 0.7266 0.237 Uiso 1 1 calc R . .
H55B H -0.0981 0.7098 0.8170 0.237 Uiso 1 1 calc R . .
H55C H 0.0220 0.7144 0.7709 0.237 Uiso 1 1 calc R . .
C56 C -0.1292(9) 0.8690(6) 0.8105(6) 0.169(5) Uani 1 1 d . . .
H56A H -0.1333 0.8917 0.7562 0.254 Uiso 1 1 calc R . .
H56B H -0.1239 0.9109 0.8299 0.254 Uiso 1 1 calc R . .
H56C H -0.1906 0.8376 0.8458 0.254 Uiso 1 1 calc R . .
C57 C -0.0996(8) 0.6817(5) 0.9752(7) 0.107(3) Uani 1 1 d . . .
C58 C -0.0994(8) 0.6618(5) 1.0667(5) 0.136(4) Uani 1 1 d . . .
H58A H -0.1470 0.6186 1.1028 0.204 Uiso 1 1 calc R . .
H58B H -0.1205 0.7079 1.0827 0.204 Uiso 1 1 calc R . .
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H58C H -0.0306 0.6469 1.0694 0.204 Uiso 1 1 calc R . .
C59 C -0.2128(7) 0.6984(6) 0.9727(6) 0.144(4) Uani 1 1 d . . .
H59A H -0.2554 0.6521 1.0076 0.216 Uiso 1 1 calc R . .
H59B H -0.2131 0.7112 0.9179 0.216 Uiso 1 1 calc R . .
H59C H -0.2398 0.7424 0.9913 0.216 Uiso 1 1 calc R . .
C60 C -0.0596(7) 0.6091(5) 0.9502(6) 0.121(4) Uani 1 1 d . . .
H60A H -0.1078 0.5656 0.9832 0.181 Uiso 1 1 calc R . .
H60B H 0.0070 0.5945 0.9579 0.181 Uiso 1 1 calc R . .
H60C H -0.0527 0.6213 0.8939 0.181 Uiso 1 1 calc R . .
C61 C 0.2260(6) 0.6330(5) 0.7677(5) 0.064(2) Uani 1 1 d . . .
C62 C 0.2597(7) 0.6716(5) 0.6845(5) 0.088(3) Uani 1 1 d . . .
H62A H 0.2919 0.7211 0.6643 0.106 Uiso 1 1 calc R . .
C63 C 0.2482(8) 0.6404(6) 0.6305(6) 0.112(4) Uani 1 1 d . . .
H63A H 0.2706 0.6691 0.5748 0.135 Uiso 1 1 calc R . .
C64 C 0.2046(9) 0.5689(7) 0.6579(6) 0.110(4) Uani 1 1 d . . .
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C66 C 0.1809(8) 0.5586(5) 0.7928(5) 0.104(3) Uani 1 1 d . . .
H66A H 0.1561 0.5295 0.8482 0.125 Uiso 1 1 calc R . .
C67 C 0.2708(6) 0.5984(4) 0.9513(5) 0.063(2) Uani 1 1 d . . .
C68 C 0.2112(7) 0.5954(5) 1.0302(6) 0.084(3) Uani 1 1 d . . .
H68A H 0.1596 0.6330 1.0373 0.101 Uiso 1 1 calc R . .
C69 C 0.2274(9) 0.5378(7) 1.0978(6) 0.116(4) Uani 1 1 d . . .
H69A H 0.1870 0.5375 1.1496 0.139 Uiso 1 1 calc R . .
C70 C 0.3018(11) 0.4811(7) 1.0900(7) 0.122(4) Uani 1 1 d . . .
H70A H 0.3119 0.4422 1.1359 0.147 Uiso 1 1 calc R . .
C71 C 0.3606(8) 0.4826(5) 1.0142(8) 0.106(3) Uani 1 1 d . . .
H71A H 0.4125 0.4450 1.0087 0.128 Uiso 1 1 calc R . .
C72 C 0.3457(7) 0.5384(5) 0.9448(6) 0.082(3) Uani 1 1 d . . .
H72A H 0.3853 0.5364 0.8937 0.098 Uiso 1 1 calc R . .

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P3 0.0524(15) 0.0781(16) 0.0948(17) -0.0419(14) -0.0079(13) -0.0097(13)
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N2 0.047(4) 0.082(4) 0.065(4) -0.030(4) -0.012(3) 0.011(3)
N3 0.064(5) 0.080(5) 0.082(5) -0.027(4) -0.014(4) -0.026(4)
N4 0.051(4) 0.085(5) 0.071(4) -0.027(4) -0.020(4) 0.013(4)
C1 0.059(6) 0.067(6) 0.095(7) -0.016(5) -0.014(5) 0.009(5)
C2 0.119(9) 0.053(6) 0.187(11) -0.028(6) -0.039(8) 0.013(6)
C3 0.104(9) 0.100(8) 0.144(10) 0.002(7) -0.060(8) 0.014(6)
C4 0.069(7) 0.120(8) 0.168(10) -0.031(7) -0.003(7) 0.025(6)
C5 0.076(7) 0.089(7) 0.075(6) -0.014(5) -0.010(6) -0.004(6)
C6 0.091(8) 0.151(9) 0.084(7) 0.022(6) -0.021(6) -0.018(7)
C7 0.123(9) 0.188(11) 0.068(7) -0.040(7) 0.004(6) -0.055(8)
C8 0.085(7) 0.131(8) 0.089(7) 0.002(6) 0.008(6) -0.033(6)
C9 0.079(7) 0.073(6) 0.100(7) -0.034(6) -0.015(6) -0.008(5)
C10 0.090(8) 0.114(8) 0.158(9) -0.047(7) -0.024(7) -0.046(6)
C11 0.124(9) 0.124(8) 0.147(10) -0.082(8) -0.031(8) -0.021(7)
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C12 0.165(11) 0.066(7) 0.187(11) -0.046(7) -0.057(9) 0.023(7)
C27 0.194(12) 0.110(9) 0.076(7) -0.038(7) -0.067(7) 0.001(8)
C28 0.155(12) 0.103(9) 0.078(8) -0.045(7) 0.016(8) -0.026(8)
C29 0.145(10) 0.079(8) 0.104(9) -0.044(7) -0.014(8) -0.009(7)
C30 0.084(7) 0.082(7) 0.090(7) -0.035(6) -0.019(5) 0.000(5)
C31 0.053(5) 0.054(5) 0.059(5) -0.023(4) -0.005(4) -0.014(4)
C32 0.071(6) 0.059(5) 0.073(6) -0.020(5) -0.021(5) -0.011(5)
C33 0.081(7) 0.056(6) 0.092(7) -0.021(6) 0.001(6) -0.025(5)
C34 0.097(8) 0.077(7) 0.072(7) -0.013(6) -0.019(6) -0.009(6)
C35 0.091(8) 0.080(7) 0.074(7) -0.022(5) -0.033(6) 0.012(6)
C36 0.073(6) 0.057(5) 0.072(6) -0.014(5) -0.025(5) -0.012(4)
C37 0.088(9) 0.126(10) 0.217(14) -0.097(10) 0.004(9) -0.007(8)
C38 0.200(16) 0.46(3) 0.127(12) -0.161(16) 0.066(12) -0.097(17)
C39 0.111(10) 0.205(14) 0.240(15) -0.165(13) -0.025(10) 0.075(10)
C40 0.044(8) 0.281(17) 0.35(2) -0.159(15) 0.018(10) -0.019(9)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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 'N'  'N'   0.0061   0.0033
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 'P'  'P'   0.1023   0.0942
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 'Sn'  'Sn'  -0.6537   1.4246
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 'Cl'  'Cl'   0.1484   0.1585
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_exptl_absorpt_coefficient_mu     1.597
_exptl_absorpt_correction_type    sadabs
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_reflns_number_total              2619
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_reflns_threshold_expression      >2sigma(I)
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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 'calc w=1/[\s^2^(Fo^2^)+(0.1000P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
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 'Flack H D (1983), Acta Cryst. A39, 876-881'
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P1 P 0.27829(10) 1.47213(7) 0.10976(6) 0.0531(2) Uani 1 1 d . . .
Cl Cl 0.0739(2) 1.96218(10) 0.21362(11) 0.1072(5) Uani 1 1 d . . .
N1 N 0.1980(4) 1.5653(3) 0.1614(2) 0.0597(8) Uani 1 1 d . . .
H1A H 0.1530 1.5310 0.1991 0.072 Uiso 1 1 calc R . .
C2 C 0.2126(7) 1.7277(4) 0.3013(3) 0.0861(14) Uani 1 1 d . . .
H2A H 0.2480 1.6539 0.3102 0.129 Uiso 1 1 calc R . .
H2B H 0.1290 1.7411 0.3348 0.129 Uiso 1 1 calc R . .
H2C H 0.2887 1.7798 0.3139 0.129 Uiso 1 1 calc R . .
C3 C 0.2998(6) 1.8121(4) 0.0942(4) 0.0958(17) Uani 1 1 d . . .
H3A H 0.3508 1.7527 0.0682 0.144 Uiso 1 1 calc R . .
H3B H 0.3693 1.8591 0.1207 0.144 Uiso 1 1 calc R . .
H3C H 0.2466 1.8544 0.0554 0.144 Uiso 1 1 calc R . .
C5 C 0.3138(11) 1.2369(4) 0.1286(5) 0.142(3) Uani 1 1 d . . .
H5A H 0.3124 1.1793 0.1680 0.213 Uiso 1 1 calc R . .
H5B H 0.4085 1.2392 0.1036 0.213 Uiso 1 1 calc R . .
H5C H 0.2400 1.2224 0.0892 0.213 Uiso 1 1 calc R . .
C10 C 0.1710(7) 1.4362(5) 0.0178(3) 0.0885(14) Uani 1 1 d . . .
H10A H 0.2190 1.3731 -0.0081 0.106 Uiso 1 1 calc R . .
C9 C 0.5517(7) 1.5690(6) 0.1430(5) 0.128(3) Uani 1 1 d . . .
H9A H 0.6434 1.5949 0.1219 0.192 Uiso 1 1 calc R . .
H9B H 0.5697 1.5113 0.1811 0.192 Uiso 1 1 calc R . .
H9C H 0.5014 1.6291 0.1686 0.192 Uiso 1 1 calc R . .
C1 C -0.0689(5) 1.7224(5) 0.1429(3) 0.0896(15) Uani 1 1 d . . .
H1B H -0.0818 1.6474 0.1253 0.134 Uiso 1 1 calc R . .
H1C H -0.0913 1.7721 0.1000 0.134 Uiso 1 1 calc R . .
H1D H -0.1333 1.7368 0.1869 0.134 Uiso 1 1 calc R . .
C6 C 0.3826(8) 1.3640(6) 0.2442(3) 0.117(2) Uani 1 1 d . . .
H6A H 0.3863 1.2972 0.2751 0.176 Uiso 1 1 calc R . .
H6B H 0.3410 1.4224 0.2758 0.176 Uiso 1 1 calc R . .
H6C H 0.4801 1.3843 0.2281 0.176 Uiso 1 1 calc R . .
C7 C 0.4530(5) 1.5221(4) 0.0725(3) 0.0805(12) Uani 1 1 d . . .
H7A H 0.4308 1.5852 0.0378 0.097 Uiso 1 1 calc R . .
C12 C 0.0153(7) 1.3983(7) 0.0465(5) 0.141(3) Uani 1 1 d . . .
H12A H -0.0436 1.3790 0.0011 0.212 Uiso 1 1 calc R . .
H12B H -0.0310 1.4575 0.0751 0.212 Uiso 1 1 calc R . .
H12C H 0.0249 1.3351 0.0807 0.212 Uiso 1 1 calc R . .
C11 C 0.1733(9) 1.5344(6) -0.0404(4) 0.126(2) Uani 1 1 d . . .
H11A H 0.1184 1.5158 -0.0873 0.189 Uiso 1 1 calc R . .
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H11B H 0.2729 1.5509 -0.0548 0.189 Uiso 1 1 calc R . .
H11C H 0.1301 1.5980 -0.0153 0.189 Uiso 1 1 calc R . .
C8 C 0.5341(7) 1.4367(5) 0.0202(4) 0.112(2) Uani 1 1 d . . .
H8A H 0.6254 1.4676 0.0023 0.168 Uiso 1 1 calc R . .
H8B H 0.4744 1.4183 -0.0250 0.168 Uiso 1 1 calc R . .
H8C H 0.5530 1.3711 0.0508 0.168 Uiso 1 1 calc R . .
C4 C 0.2838(8) 1.3446(4) 0.1673(3) 0.0908(16) Uani 1 1 d . . .
H4A H 0.1840 1.3369 0.1884 0.109 Uiso 1 1 calc R . .

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P1 0.0574(5) 0.0512(5) 0.0505(5) -0.0036(4) 0.0026(4) -0.0011(4)
Cl 0.1345(12) 0.0605(7) 0.1266(11) -0.0082(7) 0.0551(10) 0.0130(7)
N1 0.065(2) 0.0535(17) 0.0609(17) -0.0005(14) 0.0142(16) -0.0016(15)
C2 0.108(4) 0.085(3) 0.065(2) -0.011(2) -0.003(3) -0.006(3)
C3 0.106(4) 0.068(3) 0.113(4) 0.006(3) 0.056(4) -0.002(3)
C5 0.234(9) 0.060(3) 0.132(5) -0.005(3) 0.018(6) 0.016(5)
C10 0.100(4) 0.100(4) 0.065(3) -0.006(3) -0.012(3) 0.001(3)
C9 0.060(3) 0.140(6) 0.184(7) -0.042(5) -0.006(4) -0.019(3)
C1 0.065(3) 0.102(4) 0.102(3) -0.007(3) -0.022(3) 0.020(3)
C6 0.128(5) 0.149(6) 0.075(3) 0.030(4) -0.010(4) 0.034(5)
C7 0.068(3) 0.076(3) 0.097(3) -0.007(2) 0.019(2) -0.001(2)
C12 0.096(4) 0.198(8) 0.129(6) -0.062(6) -0.011(4) -0.053(5)
C11 0.151(6) 0.153(6) 0.075(3) 0.028(4) -0.038(4) -0.003(5)
C8 0.093(4) 0.112(4) 0.131(5) -0.024(4) 0.050(4) 0.000(3)
C4 0.124(4) 0.061(2) 0.087(3) 0.007(2) 0.012(3) 0.015(3)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
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 used when they are defined by crystal symmetry.  An approximate (isotropic)
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Sn1 C2 2.138(5) . ?
Sn1 N1 2.246(3) . ?
Sn1 Cl 2.7650(17) . ?
P1 N1 1.598(3) . ?
P1 C7 1.814(5) . ?
P1 C4 1.820(5) . ?
P1 C10 1.877(5) . ?
C5 C4 1.479(7) . ?
C10 C11 1.537(8) . ?
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C9 C7 1.590(9) . ?
C6 C4 1.591(8) . ?
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C1 Sn1 C2 120.8(2) . . ?
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C3 Sn1 N1 98.85(16) . . ?
C2 Sn1 N1 88.61(17) . . ?
C1 Sn1 Cl 87.05(15) . . ?
C3 Sn1 Cl 86.96(14) . . ?
C2 Sn1 Cl 87.95(16) . . ?
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N1 P1 C7 110.8(2) . . ?
N1 P1 C4 108.7(2) . . ?
C7 P1 C4 116.2(3) . . ?
N1 P1 C10 111.8(2) . . ?
C7 P1 C10 104.5(3) . . ?
C4 P1 C10 104.8(3) . . ?
P1 N1 Sn1 147.7(2) . . ?
C11 C10 C12 115.7(6) . . ?
C11 C10 P1 109.7(4) . . ?
C12 C10 P1 106.7(4) . . ?
C8 C7 C9 113.0(5) . . ?
C8 C7 P1 113.2(4) . . ?
C9 C7 P1 111.0(4) . . ?
C5 C4 C6 112.4(6) . . ?
C5 C4 P1 121.1(4) . . ?
C6 C4 P1 108.7(4) . . ?

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'B'  'B'   0.0013   0.0007
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'N'  'N'   0.0061   0.0033
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'F'  'F'   0.0171   0.0103
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Si'  'Si'   0.0817   0.0704
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'P'  'P'   0.1023   0.0942
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_cell_angle_gamma                 69.860(10)
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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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P1 P 0.94759(16) 0.03465(15) 0.25719(8) 0.0517(5) Uani 1 1 d . . .
N1 N 0.8068(4) -0.0270(4) 0.2335(2) 0.0428(9) Uani 1 1 d . . .
Si1 Si 0.65357(17) 0.09958(14) 0.17149(9) 0.0509(5) Uani 1 1 d . . .
C1 C 0.7828(6) -0.2591(5) 0.1672(3) 0.0462(11) Uani 1 1 d . . .
C2 C 0.9011(8) -0.2686(6) 0.1119(3) 0.0609(16) Uani 1 1 d . . .
C3 C 0.9012(12) -0.3128(7) 0.0361(4) 0.089(3) Uani 1 1 d . . .
C4 C 0.7779(14) -0.3535(8) 0.0110(4) 0.099(3) Uani 1 1 d . . .
C5 C 0.6570(11) -0.3485(7) 0.0617(4) 0.083(2) Uani 1 1 d . . .
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C6 C 0.6633(8) -0.3019(6) 0.1376(4) 0.0691(17) Uani 1 1 d . . .
C7 C 0.9473(5) -0.3100(5) 0.3079(3) 0.0400(10) Uani 1 1 d . . .
C8 C 1.0452(6) -0.4535(5) 0.2879(3) 0.0453(12) Uani 1 1 d . . .
C9 C 1.1505(6) -0.5558(5) 0.3395(3) 0.0507(13) Uani 1 1 d . . .
C10 C 1.1630(6) -0.5189(6) 0.4156(3) 0.0529(13) Uani 1 1 d . . .
C11 C 1.0688(6) -0.3804(6) 0.4391(3) 0.0506(13) Uani 1 1 d . . .
C12 C 0.9666(5) -0.2821(5) 0.3863(3) 0.0399(10) Uani 1 1 d . . .
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C15 C 0.5152(7) -0.3379(7) 0.3906(4) 0.0616(15) Uani 1 1 d . . .
C16 C 0.4249(6) -0.2148(7) 0.4282(3) 0.0613(15) Uani 1 1 d . . .
C17 C 0.4437(6) -0.0796(7) 0.4126(3) 0.0547(13) Uani 1 1 d . . .
C18 C 0.5557(6) -0.0688(5) 0.3575(3) 0.0451(11) Uani 1 1 d . . .
C19 C 0.9983(8) 0.1421(8) 0.1766(3) 0.0697(17) Uani 1 1 d . . .
H19A H 0.9057 0.2230 0.1591 0.105 Uiso 1 1 calc R . .
H19B H 1.0412 0.0778 0.1337 0.105 Uiso 1 1 calc R . .
H19C H 1.0750 0.1826 0.1943 0.105 Uiso 1 1 calc R . .
C20 C 1.1376(7) -0.1041(8) 0.2791(4) 0.0773(19) Uani 1 1 d . . .
H20A H 1.1695 -0.1719 0.2367 0.116 Uiso 1 1 calc R . .
H20B H 1.1316 -0.1597 0.3274 0.116 Uiso 1 1 calc R . .
H20C H 1.2132 -0.0549 0.2849 0.116 Uiso 1 1 calc R . .
C21 C 0.9005(9) 0.1547(8) 0.3393(4) 0.0777(18) Uani 1 1 d . . .
H21A H 0.7997 0.2318 0.3308 0.117 Uiso 1 1 calc R . .
H21B H 0.9793 0.2005 0.3441 0.117 Uiso 1 1 calc R . .
H21C H 0.8974 0.0963 0.3869 0.117 Uiso 1 1 calc R . .
C22 C 0.5950(9) 0.2986(6) 0.2015(5) 0.0756(18) Uani 1 1 d . . .
H22A H 0.5629 0.3040 0.2559 0.113 Uiso 1 1 calc R . .
H22B H 0.5091 0.3612 0.1691 0.113 Uiso 1 1 calc R . .
H22C H 0.6829 0.3330 0.1947 0.113 Uiso 1 1 calc R . .
C23 C 0.7154(9) 0.0880(8) 0.0641(4) 0.0766(18) Uani 1 1 d . . .
H23A H 0.7453 -0.0145 0.0490 0.115 Uiso 1 1 calc R . .
H23B H 0.8032 0.1223 0.0569 0.115 Uiso 1 1 calc R . .
H23C H 0.6292 0.1502 0.0319 0.115 Uiso 1 1 calc R . .
C24 C 0.4639(7) 0.0602(6) 0.1740(4) 0.0655(15) Uani 1 1 d . . .
H24A H 0.4251 0.0643 0.2274 0.098 Uiso 1 1 calc R . .
H24B H 0.4818 -0.0381 0.1550 0.098 Uiso 1 1 calc R . .
H24C H 0.3879 0.1343 0.1410 0.098 Uiso 1 1 calc R . .
F1 F 1.0287(4) -0.2333(4) 0.13204(19) 0.0701(10) Uani 1 1 d . . .
F2 F 1.0193(7) -0.3176(5) -0.0145(2) 0.115(2) Uani 1 1 d . . .
F3 F 0.7758(10) -0.3967(5) -0.0629(3) 0.153(3) Uani 1 1 d . . .
F4 F 0.5377(7) -0.3902(5) 0.0399(3) 0.125(2) Uani 1 1 d . . .
F5 F 0.5348(4) -0.2961(4) 0.1829(2) 0.0749(10) Uani 1 1 d . . .
F6 F 1.0393(4) -0.5061(3) 0.21560(18) 0.0670(10) Uani 1 1 d . . .
F7 F 1.2362(4) -0.6935(4) 0.3148(2) 0.0753(10) Uani 1 1 d . . .
F8 F 1.2617(4) -0.6172(4) 0.4663(2) 0.0779(11) Uani 1 1 d . . .
F9 F 1.0762(4) -0.3418(4) 0.51389(17) 0.0665(9) Uani 1 1 d . . .
F10 F 0.8796(4) -0.1458(3) 0.41324(16) 0.0537(8) Uani 1 1 d . . .
F11 F 0.7144(4) -0.4515(3) 0.30188(19) 0.0607(8) Uani 1 1 d . . .
F12 F 0.4987(5) -0.4737(4) 0.4049(3) 0.0892(12) Uani 1 1 d . . .
F13 F 0.3147(5) -0.2257(6) 0.4808(2) 0.0998(14) Uani 1 1 d . . .
F14 F 0.3542(4) 0.0426(4) 0.4502(2) 0.0775(11) Uani 1 1 d . . .
F15 F 0.5696(4) 0.0687(3) 0.34861(19) 0.0605(9) Uani 1 1 d . . .

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N1 0.046(2) 0.044(2) 0.042(2) -0.0022(16) 0.0131(17) -0.0217(17)
Si1 0.0567(9) 0.0427(8) 0.0552(9) 0.0029(6) 0.0012(7) -0.0204(6)
C1 0.068(3) 0.040(2) 0.031(2) -0.0035(19) 0.001(2) -0.018(2)
C2 0.094(4) 0.047(3) 0.034(3) -0.006(2) 0.015(3) -0.015(3)
C3 0.145(8) 0.057(4) 0.045(4) -0.002(3) 0.027(5) -0.009(4)
C4 0.172(9) 0.058(4) 0.040(4) -0.008(3) -0.013(5) -0.004(5)
C5 0.146(7) 0.054(3) 0.047(4) -0.016(3) -0.037(4) -0.026(4)
C6 0.089(4) 0.041(3) 0.074(4) -0.002(3) -0.003(3) -0.019(3)
C7 0.044(2) 0.050(2) 0.030(2) -0.0050(19) 0.0144(18) -0.023(2)
C8 0.050(3) 0.047(2) 0.037(3) -0.006(2) 0.015(2) -0.015(2)
C9 0.049(3) 0.050(3) 0.050(3) 0.000(2) 0.013(2) -0.014(2)
C10 0.047(3) 0.061(3) 0.052(3) 0.016(2) 0.004(2) -0.023(2)
C11 0.056(3) 0.072(3) 0.035(3) 0.005(2) 0.010(2) -0.038(3)
C12 0.047(2) 0.051(3) 0.028(2) -0.0077(19) 0.0112(19) -0.026(2)
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C14 0.050(3) 0.053(3) 0.047(3) 0.000(2) 0.003(2) -0.025(2)
C15 0.062(3) 0.074(4) 0.061(4) 0.018(3) 0.001(3) -0.043(3)
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C18 0.046(3) 0.053(3) 0.042(3) -0.007(2) 0.007(2) -0.024(2)
C19 0.085(4) 0.094(4) 0.048(3) 0.016(3) -0.003(3) -0.058(4)
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C24 0.055(3) 0.054(3) 0.086(4) 0.003(3) -0.002(3) -0.019(2)
F1 0.082(2) 0.079(2) 0.0482(19) -0.0067(15) 0.0307(17) -0.0263(18)
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F4 0.169(5) 0.083(3) 0.132(4) -0.016(3) -0.077(4) -0.046(3)
F5 0.080(2) 0.073(2) 0.084(3) -0.0028(18) -0.0192(19) -0.0413(18)
F6 0.087(2) 0.0539(16) 0.0452(18) -0.0146(13) 0.0171(16) -0.0038(15)
F7 0.072(2) 0.0557(18) 0.079(2) -0.0050(16) 0.0098(18) 0.0025(15)
F8 0.071(2) 0.087(2) 0.071(2) 0.0293(19) -0.0188(17) -0.0250(18)
F9 0.086(2) 0.096(2) 0.0328(16) 0.0028(15) 0.0027(14) -0.0513(19)
F10 0.0685(18) 0.0559(16) 0.0403(16) -0.0170(12) 0.0127(13) -0.0248(14)
F11 0.076(2) 0.0454(15) 0.068(2) -0.0058(14) 0.0065(16) -0.0301(14)
F12 0.102(3) 0.094(3) 0.095(3) 0.024(2) 0.007(2) -0.069(2)
F13 0.082(3) 0.154(4) 0.079(3) 0.007(3) 0.039(2) -0.064(3)
F14 0.061(2) 0.103(3) 0.062(2) -0.0249(19) 0.0271(17) -0.0174(18)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Si1 C24 1.876(6) . ?
Si1 C23 1.889(6) . ?
C1 C6 1.389(9) . ?
C1 C2 1.390(8) . ?
C2 F1 1.362(8) . ?
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C3 F2 1.346(9) . ?
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C14 F11 1.350(6) . ?
C14 C15 1.381(7) . ?
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C15 F12 1.355(7) . ?
C16 F13 1.352(6) . ?
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