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Refinement of F² 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 $F^2 > 2\text{sigma}(F^2)$ 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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Co1 Co 0.58800(9) 0.76019(6) 0.33210(5) 0.0378(3) Uani 1 1 d . A .
P1 P 0.58284(17) 0.83511(11) 0.23404(10) 0.0471(4) Uani 1 1 d D . .
O1 O 0.4935(5) 0.7810(5) 0.1483(3) 0.0805(19) Uani 1 1 d . A .
C2 C 0.5351(14) 0.7014(8) 0.1196(6) 0.118(4) Uani 1 1 d . . .
H2A H 0.6211 0.7237 0.1048 0.177 Uiso 1 1 calc R A .
H2B H 0.4611 0.6650 0.0744 0.177 Uiso 1 1 calc R . .
H2C H 0.5503 0.6636 0.1611 0.177 Uiso 1 1 calc R . .
O3 O 0.7354(5) 0.8755(4) 0.2274(3) 0.0629(13) Uani 1 1 d . A .
C4 C 0.7655(9) 0.9320(7) 0.1675(5) 0.088(3) Uani 1 1 d . . .
H4A H 0.6782 0.9306 0.1297 0.132 Uiso 1 1 calc R A .
H4B H 0.8232 0.9081 0.1409 0.132 Uiso 1 1 calc R . .
H4C H 0.8154 0.9948 0.1920 0.132 Uiso 1 1 calc R . .

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C6 C 0.5461(13) 0.9882(7) 0.2776(6) 0.069(3) Uani 0.723(7) 1 d PD A 1
H6A H 0.5481 0.9678 0.3284 0.103 Uiso 0.723(7) 1 calc PR A 1
H6B H 0.4827 1.0260 0.2665 0.103 Uiso 0.723(7) 1 calc PR A 1
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O105 O 0.5740(19) 0.9307(7) 0.2711(8) 0.0535(15) Uani 0.277(7) 1 d PD A 2
C106 C 0.536(3) 1.0025(16) 0.2280(17) 0.069(3) Uani 0.277(7) 1 d PD A 2
H10A H 0.5141 0.9830 0.1721 0.103 Uiso 0.277(7) 1 calc PR A 2
H10B H 0.6131 1.0586 0.2436 0.103 Uiso 0.277(7) 1 calc PR A 2
H10C H 0.4536 1.0136 0.2396 0.103 Uiso 0.277(7) 1 calc PR A 2
C7 C 0.8000(8) 0.7637(7) 0.3568(5) 0.080(3) Uani 1 1 d . A .
H7A H 0.8337 0.7290 0.3974 0.120 Uiso 1 1 calc R . .
H7B H 0.8712 0.7850 0.3300 0.120 Uiso 1 1 calc R . .
H7C H 0.7149 0.7246 0.3192 0.120 Uiso 1 1 calc R . .
C8 C 0.7701(9) 0.8428(7) 0.3923(4) 0.084(3) Uani 1 1 d . . .
H8A H 0.8010 0.9010 0.3725 0.100 Uiso 1 1 calc R A .
H8B H 0.7888 0.8500 0.4496 0.100 Uiso 1 1 calc R . .
C9 C 0.3837(6) 0.7440(4) 0.3313(4) 0.0403(13) Uani 1 1 d . . .
C10 C 0.4724(7) 0.7698(4) 0.4095(4) 0.0442(14) Uani 1 1 d . A .
C11 C 0.5415(6) 0.7013(4) 0.4270(3) 0.0399(13) Uani 1 1 d . . .
C12 C 0.4933(6) 0.6323(4) 0.3594(3) 0.0395(13) Uani 1 1 d . A .
C13 C 0.3965(6) 0.6586(4) 0.3006(3) 0.0375(13) Uani 1 1 d . A .
C14 C 0.2803(7) 0.7908(5) 0.2907(5) 0.0616(19) Uani 1 1 d . A .
H14A H 0.1923 0.7672 0.3032 0.092 Uiso 1 1 calc R . .
H14B H 0.2647 0.7791 0.2343 0.092 Uiso 1 1 calc R . .
H14C H 0.3169 0.8565 0.3083 0.092 Uiso 1 1 calc R . .
C15 C 0.4823(9) 0.8508(5) 0.4654(5) 0.071(2) Uani 1 1 d . . .
H15A H 0.4063 0.8352 0.4897 0.106 Uiso 1 1 calc R A .
H15B H 0.4754 0.9025 0.4371 0.106 Uiso 1 1 calc R . .

H15C H 0.5716 0.8672 0.5058 0.106 Uiso 1 1 calc R . . .
C16 C 0.6412(7) 0.6970(5) 0.5030(4) 0.0567(17) Uani 1 1 d . A .
H16A H 0.6835 0.7583 0.5325 0.085 Uiso 1 1 calc R . . .
H16B H 0.7141 0.6726 0.4928 0.085 Uiso 1 1 calc R . . .
H16C H 0.5909 0.6573 0.5332 0.085 Uiso 1 1 calc R . . .
C17 C 0.5353(8) 0.5466(5) 0.3538(5) 0.0592(18) Uani 1 1 d . . .
H17A H 0.4778 0.4999 0.3759 0.089 Uiso 1 1 calc R A .
H17B H 0.6334 0.5589 0.3829 0.089 Uiso 1 1 calc R . . .
H17C H 0.5223 0.5249 0.2991 0.089 Uiso 1 1 calc R . . .
C18 C 0.3097(7) 0.6022(5) 0.2234(4) 0.0536(17) Uani 1 1 d . . .
H18A H 0.3618 0.5647 0.2054 0.080 Uiso 1 1 calc R A .
H18B H 0.2876 0.6426 0.1852 0.080 Uiso 1 1 calc R . . .
H18C H 0.2233 0.5627 0.2296 0.080 Uiso 1 1 calc R . . .
B20 B 0.0527(7) 0.2809(4) 0.2246(4) 0.0338(14) Uani 1 1 d . . .
C21 C 0.2107(6) 0.3098(4) 0.2126(3) 0.0337(12) Uani 1 1 d . . .
C22 C 0.3285(6) 0.2980(4) 0.2650(3) 0.0344(12) Uani 1 1 d . . .
H22 H 0.3183 0.2723 0.3106 0.041 Uiso 1 1 calc R . . .
C23 C 0.4600(6) 0.3225(4) 0.2530(3) 0.0371(13) Uani 1 1 d . . .
C24 C 0.4797(6) 0.3614(4) 0.1874(3) 0.0408(14) Uani 1 1 d . . .
H24 H 0.5686 0.3778 0.1783 0.049 Uiso 1 1 calc R . . .
C25 C 0.3643(7) 0.3757(4) 0.1352(3) 0.0417(14) Uani 1 1 d . . .
C26 C 0.2336(6) 0.3517(4) 0.1483(3) 0.0383(13) Uani 1 1 d . . .
H26 H 0.1581 0.3642 0.1126 0.046 Uiso 1 1 calc R . . .
C27 C 0.5795(6) 0.3059(4) 0.3107(4) 0.0443(14) Uani 1 1 d . . .
C28 C 0.3772(8) 0.4154(5) 0.0620(4) 0.0584(19) Uani 1 1 d . . .
C31 C -0.0677(6) 0.2283(4) 0.1425(3) 0.0374(13) Uani 1 1 d . . .
C32 C -0.0376(7) 0.1902(4) 0.0783(3) 0.0425(14) Uani 1 1 d . . .
H32 H 0.0567 0.1969 0.0802 0.051 Uiso 1 1 calc R . . .

C33 C -0.1416(7) 0.1428(4) 0.0119(3) 0.0473(15) Uani 1 1 d . . .
C34 C -0.2807(7) 0.1301(4) 0.0063(3) 0.0476(15) Uani 1 1 d . . .
H34 H -0.3510 0.0985 -0.0396 0.057 Uiso 1 1 calc R . .
C35 C -0.3146(6) 0.1651(4) 0.0701(3) 0.0438(14) Uani 1 1 d . . .
C36 C -0.2089(6) 0.2136(4) 0.1366(3) 0.0378(13) Uani 1 1 d . . .
H36 H -0.2341 0.2374 0.1791 0.045 Uiso 1 1 calc R . .
C37 C -0.1048(8) 0.1072(5) -0.0580(4) 0.0617(19) Uani 1 1 d . . .
C38 C -0.4644(7) 0.1522(6) 0.0679(4) 0.0602(19) Uani 1 1 d . . .
C41 C 0.0325(5) 0.3770(4) 0.2598(3) 0.0323(12) Uani 1 1 d . . .
C42 C -0.0493(5) 0.4272(4) 0.2181(3) 0.0339(12) Uani 1 1 d . . .
H42 H -0.1013 0.4042 0.1656 0.041 Uiso 1 1 calc R . .
C43 C -0.0565(6) 0.5098(4) 0.2516(3) 0.0361(13) Uani 1 1 d . . .
C44 C 0.0183(6) 0.5468(4) 0.3286(3) 0.0384(13) Uani 1 1 d . . .
H44 H 0.0126 0.6027 0.3514 0.046 Uiso 1 1 calc R . .
C45 C 0.1019(6) 0.4986(4) 0.3708(3) 0.0366(12) Uani 1 1 d . . .
C46 C 0.1086(6) 0.4162(4) 0.3368(3) 0.0364(12) Uani 1 1 d . . .
H46 H 0.1669 0.3853 0.3669 0.044 Uiso 1 1 calc R . .
C47 C -0.1442(7) 0.5623(4) 0.2058(4) 0.0481(15) Uani 1 1 d . . .
C48 C 0.1836(7) 0.5344(4) 0.4542(4) 0.0465(15) Uani 1 1 d . . .
C51 C 0.0382(6) 0.2056(4) 0.2854(3) 0.0322(12) Uani 1 1 d . . .
C52 C -0.0333(6) 0.2064(4) 0.3416(3) 0.0344(12) Uani 1 1 d . . .
H52 H -0.0742 0.2541 0.3466 0.041 Uiso 1 1 calc R . .
C53 C -0.0468(5) 0.1395(4) 0.3907(3) 0.0325(12) Uani 1 1 d . . .
C54 C 0.0138(6) 0.0690(4) 0.3862(3) 0.0349(12) Uani 1 1 d . . .
H54 H 0.0077 0.0246 0.4205 0.042 Uiso 1 1 calc R . .
C55 C 0.0838(6) 0.0657(4) 0.3293(3) 0.0335(12) Uani 1 1 d . . .
C56 C 0.0931(6) 0.1313(4) 0.2798(3) 0.0324(12) Uani 1 1 d . . .
H56 H 0.1382 0.1260 0.2406 0.039 Uiso 1 1 calc R . .
C57 C -0.1281(6) 0.1442(4) 0.4481(3) 0.0423(14) Uani 1 1 d . . .

C58 C 0.1499(6) -0.0084(4) 0.3231(3) 0.0380(13) Uani 1 1 d . . .

F21 F 0.5792(5) 0.3179(6) 0.3812(3) 0.129(3) Uani 1 1 d . . .

F22 F 0.5846(11) 0.2241(5) 0.3010(5) 0.209(6) Uani 1 1 d . . .

F23 F 0.6974(6) 0.3517(7) 0.3083(5) 0.190(5) Uani 1 1 d . . .

F24 F 0.5033(5) 0.4308(4) 0.0535(3) 0.0956(17) Uani 1 1 d . . .

F25 F 0.2946(5) 0.3589(3) -0.0023(2) 0.0786(13) Uani 1 1 d . . .

F26 F 0.3351(7) 0.4905(3) 0.0555(3) 0.1014(19) Uani 1 1 d . . .

F31 F 0.0200(6) 0.0933(5) -0.0404(3) 0.1039(19) Uani 1 1 d . . .

F32 F -0.1004(7) 0.1644(4) -0.1099(3) 0.111(2) Uani 1 1 d . . .

F33 F -0.1911(7) 0.0286(4) -0.0955(4) 0.132(3) Uani 1 1 d . . .

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F35 F -0.5058(5) 0.2264(4) 0.0515(4) 0.1027(19) Uani 1 1 d . . .

F36 F -0.4898(5) 0.1368(6) 0.1339(3) 0.153(4) Uani 1 1 d . . .

F41 F -0.0725(5) 0.6469(3) 0.2027(3) 0.0906(17) Uani 1 1 d . . .

F42 F -0.2123(5) 0.5232(3) 0.1338(3) 0.0861(16) Uani 1 1 d . . .

F43 F -0.2463(5) 0.5713(4) 0.2362(3) 0.0871(15) Uani 1 1 d . . .

F44 F 0.1808(6) 0.6178(3) 0.4775(3) 0.0894(17) Uani 1 1 d . . .

F45 F 0.1369(4) 0.4804(3) 0.5037(2) 0.0632(11) Uani 1 1 d . . .

F46 F 0.3186(3) 0.5367(3) 0.46794(19) 0.0512(9) Uani 1 1 d . . .

F51 F -0.2585(4) 0.1416(4) 0.4141(2) 0.0789(14) Uani 1 1 d . . .

F52 F -0.0755(5) 0.2219(3) 0.4985(3) 0.0775(13) Uani 1 1 d . . .

F53 F -0.1332(6) 0.0771(3) 0.4914(3) 0.0917(18) Uani 1 1 d . . .

F54 F 0.0768(5) -0.0884(3) 0.3347(4) 0.0979(19) Uani 1 1 d . . .

F55 F 0.2686(5) 0.0058(3) 0.3786(3) 0.0969(18) Uani 1 1 d . . .

F56 F 0.1791(8) -0.0208(4) 0.2582(3) 0.128(3) Uani 1 1 d . . .

O61 O 0.0768(8) 0.6007(4) 0.0130(3) 0.087(2) Uani 1 1 d D . .

H63 H 0.033(6) 0.550(3) 0.035(3) 0.035(17) Uiso 1 1 d D . .

H62 H 0.169(2) 0.635(3) 0.023(4) 0.035(17) Uiso 1 1 d D . .

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O1 0.049(3) 0.120(5) 0.057(3) 0.053(3) 0.004(2) 0.001(3)
C2 0.160(11) 0.101(8) 0.069(6) -0.020(6) 0.056(7) -0.018(8)
O3 0.048(3) 0.082(3) 0.045(3) 0.023(2) 0.012(2) -0.006(2)
C4 0.067(5) 0.120(8) 0.064(5) 0.042(5) 0.026(4) -0.008(5)
O5 0.068(4) 0.048(3) 0.047(4) 0.014(3) 0.016(3) 0.020(3)
C6 0.097(8) 0.052(6) 0.060(7) 0.010(5) 0.029(7) 0.017(5)
O105 0.068(4) 0.048(3) 0.047(4) 0.014(3) 0.016(3) 0.020(3)
C106 0.097(8) 0.052(6) 0.060(7) 0.010(5) 0.029(7) 0.017(5)
C7 0.049(5) 0.120(8) 0.073(5) 0.040(6) 0.019(4) 0.022(5)
C8 0.068(5) 0.096(7) 0.044(4) 0.007(4) 0.006(4) -0.037(5)
C9 0.036(3) 0.039(3) 0.049(3) 0.012(3) 0.016(3) 0.011(3)
C10 0.049(4) 0.039(3) 0.048(4) 0.003(3) 0.020(3) 0.012(3)
C11 0.040(3) 0.042(3) 0.038(3) 0.007(3) 0.015(2) 0.009(3)
C12 0.041(3) 0.037(3) 0.043(3) 0.008(3) 0.014(3) 0.012(3)
C13 0.038(3) 0.035(3) 0.038(3) 0.005(2) 0.012(2) 0.007(3)
C14 0.053(4) 0.056(4) 0.088(5) 0.022(4) 0.026(4) 0.027(4)
C15 0.085(6) 0.059(5) 0.069(5) -0.008(4) 0.028(4) 0.021(4)
C16 0.055(4) 0.069(5) 0.041(4) 0.013(3) 0.012(3) 0.010(4)

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C17 0.075(5) 0.042(4) 0.071(5) 0.017(3) 0.024(4) 0.029(4)
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B20 0.038(3) 0.032(3) 0.032(3) 0.011(3) 0.009(3) 0.009(3)
C21 0.041(3) 0.032(3) 0.029(3) 0.004(2) 0.013(2) 0.009(3)
C22 0.044(3) 0.031(3) 0.029(3) 0.009(2) 0.014(2) 0.008(3)
C23 0.043(3) 0.036(3) 0.035(3) 0.008(2) 0.014(2) 0.012(3)
C24 0.043(3) 0.037(3) 0.042(3) 0.003(3) 0.021(3) 0.002(3)
C25 0.057(4) 0.038(3) 0.033(3) 0.011(2) 0.019(3) 0.013(3)
C26 0.049(4) 0.032(3) 0.035(3) 0.011(2) 0.013(3) 0.012(3)
C27 0.042(4) 0.049(4) 0.045(4) 0.011(3) 0.018(3) 0.013(3)
C28 0.076(5) 0.058(4) 0.054(4) 0.026(4) 0.037(4) 0.018(4)
C31 0.050(4) 0.031(3) 0.031(3) 0.011(2) 0.010(2) 0.012(3)
C32 0.050(4) 0.044(3) 0.033(3) 0.009(3) 0.011(3) 0.013(3)
C33 0.062(4) 0.043(3) 0.032(3) -0.003(3) 0.009(3) 0.013(3)
C34 0.057(4) 0.044(3) 0.034(3) -0.001(3) 0.009(3) 0.007(3)
C35 0.047(4) 0.041(3) 0.036(3) 0.007(3) 0.007(3) 0.005(3)
C36 0.042(3) 0.034(3) 0.031(3) 0.006(2) 0.008(2) 0.003(3)
C37 0.071(5) 0.070(5) 0.039(4) -0.002(3) 0.012(3) 0.016(4)
C38 0.048(4) 0.073(5) 0.036(4) 0.001(3) -0.004(3) -0.003(4)
C41 0.031(3) 0.030(3) 0.033(3) 0.010(2) 0.008(2) 0.005(2)
C42 0.031(3) 0.035(3) 0.031(3) 0.006(2) 0.005(2) 0.006(2)
C43 0.032(3) 0.036(3) 0.041(3) 0.011(2) 0.007(2) 0.012(3)
C44 0.039(3) 0.031(3) 0.043(3) 0.005(2) 0.011(2) 0.009(3)
C45 0.036(3) 0.035(3) 0.035(3) 0.005(2) 0.004(2) 0.010(3)
C46 0.042(3) 0.034(3) 0.032(3) 0.008(2) 0.004(2) 0.015(3)
C47 0.053(4) 0.045(4) 0.052(4) 0.016(3) 0.014(3) 0.022(3)
C48 0.047(4) 0.046(4) 0.042(3) -0.003(3) 0.002(3) 0.020(3)
C51 0.036(3) 0.031(3) 0.026(3) 0.003(2) 0.004(2) 0.008(2)

C52	0.041(3)	0.031(3)	0.033(3)	0.008(2)	0.010(2)	0.013(3)
C53	0.033(3)	0.040(3)	0.026(3)	0.008(2)	0.010(2)	0.009(3)
C54	0.036(3)	0.034(3)	0.034(3)	0.011(2)	0.009(2)	0.007(2)
C55	0.036(3)	0.029(3)	0.035(3)	0.007(2)	0.007(2)	0.010(2)
C56	0.037(3)	0.033(3)	0.028(3)	0.004(2)	0.010(2)	0.010(2)
C57	0.050(4)	0.051(4)	0.039(3)	0.021(3)	0.021(3)	0.024(3)
C58	0.051(4)	0.036(3)	0.030(3)	0.011(2)	0.012(2)	0.015(3)
F21	0.075(3)	0.293(9)	0.039(2)	0.008(4)	0.006(2)	0.100(5)
F22	0.281(11)	0.128(6)	0.153(6)	-0.047(5)	-0.124(7)	0.147(7)
F23	0.047(3)	0.329(12)	0.219(8)	0.205(9)	0.045(4)	0.051(5)
F24	0.079(3)	0.145(5)	0.070(3)	0.056(3)	0.041(3)	0.014(3)
F25	0.105(4)	0.093(3)	0.043(2)	0.026(2)	0.027(2)	0.029(3)
F26	0.192(6)	0.073(3)	0.092(4)	0.055(3)	0.089(4)	0.068(4)
F31	0.109(4)	0.153(5)	0.058(3)	-0.021(3)	0.020(3)	0.065(4)
F32	0.184(6)	0.121(5)	0.063(3)	0.030(3)	0.068(4)	0.066(4)
F33	0.135(5)	0.125(5)	0.097(4)	-0.067(4)	0.056(4)	-0.028(4)
F34	0.051(2)	0.067(3)	0.091(3)	-0.026(2)	-0.013(2)	0.007(2)
F35	0.072(3)	0.078(3)	0.161(5)	-0.023(3)	0.047(3)	0.023(3)
F36	0.048(3)	0.305(10)	0.058(3)	0.053(4)	0.006(2)	-0.027(4)
F41	0.069(3)	0.054(3)	0.131(4)	0.051(3)	-0.006(3)	0.012(2)
F42	0.112(4)	0.074(3)	0.059(3)	0.001(2)	-0.025(2)	0.055(3)
F43	0.082(3)	0.111(4)	0.100(4)	0.040(3)	0.037(3)	0.066(3)
F44	0.122(4)	0.066(3)	0.061(3)	-0.026(2)	-0.028(3)	0.057(3)
F45	0.054(2)	0.097(3)	0.0352(19)	0.006(2)	0.0136(16)	0.015(2)
F46	0.041(2)	0.061(2)	0.0399(19)	0.0031(16)	0.0005(14)	0.0068(17)
F51	0.049(2)	0.149(5)	0.055(2)	0.027(3)	0.0238(19)	0.045(3)
F52	0.084(3)	0.085(3)	0.065(3)	-0.015(2)	0.041(2)	0.016(3)
F53	0.145(4)	0.104(4)	0.100(4)	0.076(3)	0.095(3)	0.088(4)
F54	0.088(3)	0.041(2)	0.195(6)	0.038(3)	0.075(4)	0.029(2)

F55 0.073(3) 0.084(3) 0.117(4) -0.032(3) -0.022(3) 0.053(3)
F56 0.276(8) 0.136(5) 0.076(3) 0.066(3) 0.105(4) 0.170(6)
O61 0.116(5) 0.072(4) 0.043(3) -0.025(3) -0.060(3) 0.066(4)

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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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_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_2
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Co1 C8 1.969(7) . ?

Co1 C9 2.068(6) . ?

Co1 C10 2.078(6) . ?

Co1 C11 2.087(6) . ?

Co1 C13 2.097(6) . ?

Co1 C12 2.105(6) . ?

Co1 P1 2.1637(18) . ?

P1 O3 1.582(5) . ?

P1 O5 1.608(6) . ?
P1 O105 1.608(6) . ?
P1 O1 1.619(6) . ?
O1 C2 1.503(13) . ?
C2 H2A 0.9800 . ?
C2 H2B 0.9800 . ?
C2 H2C 0.9800 . ?
O3 C4 1.469(8) . ?
C4 H4A 0.9800 . ?
C4 H4B 0.9800 . ?
C4 H4C 0.9800 . ?
O5 C6 1.471(11) . ?
C6 H6A 0.9800 . ?
C6 H6B 0.9800 . ?
C6 H6C 0.9800 . ?
O105 C106 1.471(11) . ?
C106 H10A 0.9800 . ?
C106 H10B 0.9800 . ?
C106 H10C 0.9800 . ?
C7 C8 1.477(13) . ?
C7 H7A 0.9800 . ?
C7 H7B 0.9800 . ?
C7 H7C 0.9800 . ?
C8 H8A 0.9900 . ?
C8 H8B 0.9900 . ?
C9 C10 1.433(9) . ?
C9 C13 1.443(8) . ?
C9 C14 1.510(9) . ?
C10 C11 1.432(9) . ?

C10 C15 1.513(9) . ?
C11 C12 1.446(8) . ?
C11 C16 1.505(8) . ?
C12 C13 1.420(8) . ?
C12 C17 1.500(9) . ?
C13 C18 1.510(8) . ?
C14 H14A 0.9800 . ?
C14 H14B 0.9800 . ?
C14 H14C 0.9800 . ?
C15 H15A 0.9800 . ?
C15 H15B 0.9800 . ?
C15 H15C 0.9800 . ?
C16 H16A 0.9800 . ?
C16 H16B 0.9800 . ?
C16 H16C 0.9800 . ?
C17 H17A 0.9800 . ?
C17 H17B 0.9800 . ?
C17 H17C 0.9800 . ?
C18 H18A 0.9800 . ?
C18 H18B 0.9800 . ?
C18 H18C 0.9800 . ?
B20 C51 1.647(8) . ?
B20 C41 1.655(8) . ?
B20 C21 1.659(8) . ?
B20 C31 1.663(8) . ?
C21 C26 1.401(8) . ?
C21 C22 1.403(8) . ?
C22 C23 1.396(8) . ?

C22 H22 0.9500 . ?
C23 C24 1.393(8) . ?
C23 C27 1.492(8) . ?
C24 C25 1.399(9) . ?
C24 H24 0.9500 . ?
C25 C26 1.395(8) . ?
C25 C28 1.507(8) . ?
C26 H26 0.9500 . ?
C27 F23 1.256(8) . ?
C27 F21 1.267(7) . ?
C27 F22 1.275(9) . ?
C28 F24 1.320(8) . ?
C28 F25 1.339(9) . ?
C28 F26 1.341(8) . ?
C31 C36 1.399(8) . ?
C31 C32 1.401(8) . ?
C32 C33 1.391(8) . ?
C32 H32 0.9500 . ?
C33 C34 1.383(9) . ?
C33 C37 1.512(9) . ?
C34 C35 1.397(9) . ?
C34 H34 0.9500 . ?
C35 C36 1.405(8) . ?
C35 C38 1.507(10) . ?
C36 H36 0.9500 . ?
C37 F33 1.317(9) . ?
C37 F32 1.325(9) . ?
C37 F31 1.332(9) . ?
C38 F36 1.302(8) . ?

C38 F34 1.337(8) . ?
C38 F35 1.346(9) . ?
C41 C42 1.405(7) . ?
C41 C46 1.408(8) . ?
C42 C43 1.398(8) . ?
C42 H42 0.9500 . ?
C43 C44 1.399(8) . ?
C43 C47 1.500(8) . ?
C44 C45 1.399(8) . ?
C44 H44 0.9500 . ?
C45 C46 1.396(8) . ?
C45 C48 1.505(8) . ?
C46 H46 0.9500 . ?
C47 F42 1.321(8) . ?
C47 F41 1.330(7) . ?
C47 F43 1.344(8) . ?
C48 F44 1.333(7) . ?
C48 F45 1.349(8) . ?
C48 F46 1.352(7) . ?
C51 C52 1.399(8) . ?
C51 C56 1.414(8) . ?
C52 C53 1.401(7) . ?
C52 H52 0.9500 . ?
C53 C54 1.397(8) . ?
C53 C57 1.501(7) . ?
C54 C55 1.403(8) . ?
C54 H54 0.9500 . ?
C55 C56 1.388(7) . ?

C55 C58 1.489(8) . ?

C56 H56 0.9500 . ?

C57 F51 1.326(7) . ?

C57 F53 1.330(7) . ?

C57 F52 1.346(8) . ?

C58 F56 1.292(7) . ?

C58 F54 1.324(7) . ?

C58 F55 1.329(7) . ?

O61 H63 0.956(10) . ?

O61 H62 0.933(10) . ?

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_geom_angle_atom_site_label_3

_geom_angle

_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

C8 Co1 C9 135.6(4) . . ?

C8 Co1 C10 100.2(3) . . ?

C9 Co1 C10 40.4(2) . . ?

C8 Co1 C11 95.3(3) . . ?

C9 Co1 C11 67.7(2) . . ?

C10 Co1 C11 40.2(2) . . ?

C8 Co1 C13 162.7(3) . . ?

C9 Co1 C13 40.5(2) . . ?

C10 Co1 C13 67.9(2) . . ?

C11 Co1 C13 67.5(2) . . ?

C8 Co1 C12 125.2(3) . . ?

C9 Co1 C12 67.3(2) . . ?

C10 Co1 C12 67.6(2) . . ?

C11 Co1 C12 40.4(2) . . ?

C13 Co1 C12 39.5(2) . . ?

C8 Co1 P1 92.2(2) . . ?

C9 Co1 P1 96.29(17) . . ?

C10 Co1 P1 123.12(18) . . ?

C11 Co1 P1 162.85(18) . . ?

C13 Co1 P1 104.77(16) . . ?

C12 Co1 P1 140.32(17) . . ?

O3 P1 O5 110.1(3) . . ?

O3 P1 O105 94.5(7) . . ?

O5 P1 O105 38.3(6) . . ?

O3 P1 O1 104.8(3) . . ?

O5 P1 O1 87.5(3) . . ?

O105 P1 O1 125.7(6) . . ?

O3 P1 Co1 109.84(19) . . ?

O5 P1 Co1 123.6(2) . . ?

O105 P1 Co1 101.0(5) . . ?

O1 P1 Co1 118.2(2) . . ?

C2 O1 P1 116.9(6) . . ?

O1 C2 H2A 109.5 . . ?

O1 C2 H2B 109.5 . . ?

H2A C2 H2B 109.5 . . ?

O1 C2 H2C 109.5 . . ?

H2A C2 H2C 109.5 . . ?

H2B C2 H2C 109.5 . . ?

C4 O3 P1 122.4(5) . . ?

O3 C4 H4A 109.5 . . ?

O3 C4 H4B 109.5 . . ?

H4A C4 H4B 109.5 . . ?

O3 C4 H4C 109.5 . . ?

H4A C4 H4C 109.5 . . ?

H4B C4 H4C 109.5 . . ?

C6 O5 P1 114.2(6) . . ?

C106 O105 P1 126.3(15) . . ?

O105 C106 H10A 109.5 . . ?

O105 C106 H10B 109.5 . . ?

H10A C106 H10B 109.5 . . ?

O105 C106 H10C 109.5 . . ?

H10A C106 H10C 109.5 . . ?

H10B C106 H10C 109.5 . . ?

C8 C7 H7A 109.5 . . ?

C8 C7 H7B 109.5 . . ?

H7A C7 H7B 109.5 . . ?

C8 C7 H7C 109.5 . . ?

H7A C7 H7C 109.5 . . ?

H7B C7 H7C 109.5 . . ?

C7 C8 Co1 74.4(5) . . ?

C7 C8 H8A 116.1 . . ?

Co1 C8 H8A 116.1 . . ?

C7 C8 H8B 116.1 . . ?

Co1 C8 H8B 116.1 . . ?

H8A C8 H8B 113.1 . . ?

C10 C9 C13 108.3(5) . . ?

C10 C9 C14 126.3(6) . . ?

C13 C9 C14 124.9(6) . . ?
C10 C9 Co1 70.1(3) . . ?
C13 C9 Co1 70.8(3) . . ?
C14 C9 Co1 130.7(4) . . ?
C11 C10 C9 107.7(5) . . ?
C11 C10 C15 126.1(6) . . ?
C9 C10 C15 126.0(6) . . ?
C11 C10 Co1 70.2(3) . . ?
C9 C10 Co1 69.4(3) . . ?
C15 C10 Co1 129.4(5) . . ?
C10 C11 C12 107.9(5) . . ?
C10 C11 C16 127.2(6) . . ?
C12 C11 C16 124.8(6) . . ?
C10 C11 Co1 69.5(3) . . ?
C12 C11 Co1 70.5(3) . . ?
C16 C11 Co1 127.9(4) . . ?
C13 C12 C11 108.3(5) . . ?
C13 C12 C17 126.2(6) . . ?
C11 C12 C17 125.5(6) . . ?
C13 C12 Co1 69.9(3) . . ?
C11 C12 Co1 69.2(3) . . ?
C17 C12 Co1 128.1(4) . . ?
C12 C13 C9 107.8(5) . . ?
C12 C13 C18 126.2(5) . . ?
C9 C13 C18 125.6(5) . . ?
C12 C13 Co1 70.6(3) . . ?
C9 C13 Co1 68.7(3) . . ?
C18 C13 Co1 131.6(4) . . ?

C9 C14 H14A 109.5 . . ?
C9 C14 H14B 109.5 . . ?
H14A C14 H14B 109.5 . . ?
C9 C14 H14C 109.5 . . ?
H14A C14 H14C 109.5 . . ?
H14B C14 H14C 109.5 . . ?
C10 C15 H15A 109.5 . . ?
C10 C15 H15B 109.5 . . ?
H15A C15 H15B 109.5 . . ?
C10 C15 H15C 109.5 . . ?
H15A C15 H15C 109.5 . . ?
H15B C15 H15C 109.5 . . ?
C11 C16 H16A 109.5 . . ?
C11 C16 H16B 109.5 . . ?
H16A C16 H16B 109.5 . . ?
C11 C16 H16C 109.5 . . ?
H16A C16 H16C 109.5 . . ?
H16B C16 H16C 109.5 . . ?
C12 C17 H17A 109.5 . . ?
C12 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
C12 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
C13 C18 H18A 109.5 . . ?
C13 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
C13 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?

H18B C18 H18C 109.5 . . ?
C51 B20 C41 110.9(4) . . ?
C51 B20 C21 111.3(4) . . ?
C41 B20 C21 105.0(4) . . ?
C51 B20 C31 104.0(4) . . ?
C41 B20 C31 114.1(4) . . ?
C21 B20 C31 111.7(5) . . ?
C26 C21 C22 115.8(5) . . ?
C26 C21 B20 120.0(5) . . ?
C22 C21 B20 124.1(5) . . ?
C23 C22 C21 122.8(5) . . ?
C23 C22 H22 118.6 . . ?
C21 C22 H22 118.6 . . ?
C24 C23 C22 120.4(5) . . ?
C24 C23 C27 120.1(5) . . ?
C22 C23 C27 119.5(5) . . ?
C23 C24 C25 117.8(5) . . ?
C23 C24 H24 121.1 . . ?
C25 C24 H24 121.1 . . ?
C26 C25 C24 121.2(5) . . ?
C26 C25 C28 118.1(6) . . ?
C24 C25 C28 120.7(6) . . ?
C25 C26 C21 121.9(5) . . ?
C25 C26 H26 119.1 . . ?
C21 C26 H26 119.1 . . ?
F23 C27 F21 106.2(7) . . ?
F23 C27 F22 102.9(8) . . ?
F21 C27 F22 103.2(7) . . ?

F23 C27 C23 114.9(5) . . ?
F21 C27 C23 115.3(5) . . ?
F22 C27 C23 113.0(6) . . ?
F24 C28 F25 104.4(6) . . ?
F24 C28 F26 110.4(6) . . ?
F25 C28 F26 103.1(6) . . ?
F24 C28 C25 112.9(6) . . ?
F25 C28 C25 112.2(6) . . ?
F26 C28 C25 113.0(6) . . ?
C36 C31 C32 115.9(5) . . ?
C36 C31 B20 120.3(5) . . ?
C32 C31 B20 123.6(5) . . ?
C33 C32 C31 122.0(6) . . ?
C33 C32 H32 119.0 . . ?
C31 C32 H32 119.0 . . ?
C34 C33 C32 121.5(6) . . ?
C34 C33 C37 118.0(6) . . ?
C32 C33 C37 120.5(6) . . ?
C33 C34 C35 118.0(6) . . ?
C33 C34 H34 121.0 . . ?
C35 C34 H34 121.0 . . ?
C34 C35 C36 120.1(6) . . ?
C34 C35 C38 120.5(6) . . ?
C36 C35 C38 119.4(6) . . ?
C31 C36 C35 122.4(6) . . ?
C31 C36 H36 118.8 . . ?
C35 C36 H36 118.8 . . ?
F33 C37 F32 106.4(7) . . ?
F33 C37 F31 104.7(7) . . ?

F32 C37 F31 104.6(7) . . ?
F33 C37 C33 114.1(6) . . ?
F32 C37 C33 112.6(7) . . ?
F31 C37 C33 113.6(6) . . ?
F36 C38 F34 109.3(7) . . ?
F36 C38 F35 104.4(8) . . ?
F34 C38 F35 103.7(6) . . ?
F36 C38 C35 113.6(6) . . ?
F34 C38 C35 112.6(6) . . ?
F35 C38 C35 112.6(6) . . ?
C42 C41 C46 115.7(5) . . ?
C42 C41 B20 125.7(5) . . ?
C46 C41 B20 118.5(5) . . ?
C43 C42 C41 122.0(5) . . ?
C43 C42 H42 119.0 . . ?
C41 C42 H42 119.0 . . ?
C42 C43 C44 121.4(5) . . ?
C42 C43 C47 121.1(5) . . ?
C44 C43 C47 117.6(5) . . ?
C45 C44 C43 117.6(5) . . ?
C45 C44 H44 121.2 . . ?
C43 C44 H44 121.2 . . ?
C46 C45 C44 120.6(5) . . ?
C46 C45 C48 119.4(5) . . ?
C44 C45 C48 120.0(5) . . ?
C45 C46 C41 122.8(5) . . ?
C45 C46 H46 118.6 . . ?
C41 C46 H46 118.6 . . ?

F42 C47 F41 107.6(5) . . ?
F42 C47 F43 103.0(6) . . ?
F41 C47 F43 105.3(6) . . ?
F42 C47 C43 114.3(5) . . ?
F41 C47 C43 113.2(5) . . ?
F43 C47 C43 112.6(5) . . ?
F44 C48 F45 106.6(5) . . ?
F44 C48 F46 107.3(5) . . ?
F45 C48 F46 104.5(5) . . ?
F44 C48 C45 113.7(5) . . ?
F45 C48 C45 112.0(5) . . ?
F46 C48 C45 112.1(5) . . ?
C52 C51 C56 115.7(5) . . ?
C52 C51 B20 124.2(5) . . ?
C56 C51 B20 120.0(5) . . ?
C51 C52 C53 122.4(5) . . ?
C51 C52 H52 118.8 . . ?
C53 C52 H52 118.8 . . ?
C54 C53 C52 120.7(5) . . ?
C54 C53 C57 120.3(5) . . ?
C52 C53 C57 119.0(5) . . ?
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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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C1 C 0.72159(19) 0.18544(18) 0.62858(12) 0.0359(8) Uani 1 1 d . . .
H1A H 0.7284 0.2363 0.6291 0.043 Uiso 1 1 calc R . .
H1B H 0.6708 0.1715 0.6195 0.043 Uiso 1 1 calc R . .
C2 C 0.75487(19) 0.14724(19) 0.66850(12) 0.0369(9) Uani 1 1 d . . .
H2A H 0.7913 0.1144 0.6559 0.055 Uiso 1 1 calc R . .
H2B H 0.7163 0.1220 0.6860 0.055 Uiso 1 1 calc R . .
H2C H 0.7794 0.1797 0.6904 0.055 Uiso 1 1 calc R . .
C3 C 0.66334(18) 0.02076(19) 0.62234(13) 0.0378(8) Uani 1 1 d . . .
H3A H 0.6297 -0.0142 0.6092 0.057 Uiso 1 1 calc R . .
H3B H 0.6345 0.0584 0.6367 0.057 Uiso 1 1 calc R . .
H3C H 0.6947 -0.0003 0.6470 0.057 Uiso 1 1 calc R . .
C4 C 0.65394(18) 0.08725(19) 0.53088(13) 0.0388(9) Uani 1 1 d . . .
H4A H 0.6790 0.0984 0.5006 0.058 Uiso 1 1 calc R . .
H4B H 0.6303 0.1290 0.5437 0.058 Uiso 1 1 calc R . .
H4C H 0.6164 0.0517 0.5250 0.058 Uiso 1 1 calc R . .
C5 C 0.7519(2) -0.02400(17) 0.54556(12) 0.0350(8) Uani 1 1 d . . .
H5A H 0.7856 -0.0487 0.5672 0.052 Uiso 1 1 calc R . .
H5B H 0.7778 -0.0128 0.5155 0.052 Uiso 1 1 calc R . .
H5C H 0.7092 -0.0534 0.5384 0.052 Uiso 1 1 calc R . .
C6 C 0.85328(16) 0.15202(16) 0.53467(11) 0.0230(7) Uani 1 1 d . . .
C7 C 0.89801(15) 0.10354(16) 0.56200(10) 0.0237(7) Uani 1 1 d . . .
C8 C 0.91710(15) 0.13583(17) 0.60551(10) 0.0255(7) Uani 1 1 d . . .
C9 C 0.88569(17) 0.20395(17) 0.60599(11) 0.0288(7) Uani 1 1 d . . .
C10 C 0.84750(16) 0.21446(16) 0.56189(11) 0.0262(7) Uani 1 1 d . . .
C11 C 0.82852(18) 0.14171(17) 0.48370(11) 0.0296(7) Uani 1 1 d . . .
H11A H 0.7867 0.1723 0.4769 0.044 Uiso 1 1 calc R . .

H11B H 0.8134 0.0935 0.4791 0.044 Uiso 1 1 calc R . . .
H11C H 0.8693 0.1526 0.4618 0.044 Uiso 1 1 calc R . . .
C12 C 0.92720(17) 0.03556(17) 0.54477(12) 0.0326(8) Uani 1 1 d . . .
H12A H 0.9795 0.0405 0.5363 0.049 Uiso 1 1 calc R . . .
H12B H 0.8992 0.0207 0.5164 0.049 Uiso 1 1 calc R . . .
H12C H 0.9220 0.0010 0.5704 0.049 Uiso 1 1 calc R . . .
C13 C 0.96511(17) 0.1055(2) 0.64428(12) 0.0378(9) Uani 1 1 d . . .
H13A H 0.9602 0.0550 0.6442 0.057 Uiso 1 1 calc R . . .
H13B H 0.9497 0.1237 0.6757 0.057 Uiso 1 1 calc R . . .
H13C H 1.0168 0.1181 0.6383 0.057 Uiso 1 1 calc R . . .
C14 C 0.8961(2) 0.25622(19) 0.64533(13) 0.0428(9) Uani 1 1 d . . .
H14A H 0.9423 0.2816 0.6399 0.064 Uiso 1 1 calc R . . .
H14B H 0.8984 0.2325 0.6765 0.064 Uiso 1 1 calc R . . .
H14C H 0.8546 0.2887 0.6453 0.064 Uiso 1 1 calc R . . .
C15 C 0.81110(19) 0.27978(16) 0.54533(13) 0.0355(8) Uani 1 1 d . . .
H15A H 0.7912 0.3047 0.5732 0.053 Uiso 1 1 calc R . . .
H15B H 0.7708 0.2685 0.5231 0.053 Uiso 1 1 calc R . . .
H15C H 0.8474 0.3089 0.5288 0.053 Uiso 1 1 calc R . . .
B20 B 0.73031(17) 0.27894(17) 0.83167(11) 0.0176(7) Uani 1 1 d . . .
C21 C 0.78723(15) 0.34494(14) 0.83000(10) 0.0181(6) Uani 1 1 d . . .
C22 C 0.78634(15) 0.40147(15) 0.86127(10) 0.0191(6) Uani 1 1 d . . .
H22 H 0.7510 0.4023 0.8866 0.023 Uiso 1 1 calc R . . .
C23 C 0.83544(15) 0.45686(15) 0.85673(10) 0.0203(6) Uani 1 1 d . . .
C24 C 0.88679(15) 0.45804(16) 0.81967(11) 0.0226(7) Uani 1 1 d . . .
H24 H 0.9194 0.4961 0.8159 0.027 Uiso 1 1 calc R . . .
C25 C 0.88939(15) 0.40253(15) 0.78836(10) 0.0215(6) Uani 1 1 d . . .
C26 C 0.84158(15) 0.34661(15) 0.79425(11) 0.0213(7) Uani 1 1 d . . .
H26 H 0.8461 0.3082 0.7732 0.026 Uiso 1 1 calc R . . .

C27 C 0.83435(16) 0.51521(16) 0.89142(11) 0.0239(7) Uani 1 1 d . . .
C28 C 0.94013(17) 0.40450(16) 0.74582(12) 0.0286(7) Uani 1 1 d . . .
F29 F 0.77117(10) 0.51958(9) 0.91693(7) 0.0360(5) Uani 1 1 d . . .
F30 F 0.84409(10) 0.57703(9) 0.87054(6) 0.0333(4) Uani 1 1 d . . .
F31 F 0.88859(10) 0.50986(9) 0.92475(6) 0.0354(5) Uani 1 1 d . . .
F32 F 0.90442(13) 0.42384(16) 0.70610(8) 0.0789(9) Uani 1 1 d . . .
F33 F 0.99652(13) 0.44694(13) 0.75130(10) 0.0749(9) Uani 1 1 d . . .
F34 F 0.96896(10) 0.34316(10) 0.73480(7) 0.0393(5) Uani 1 1 d . . .
C36 C 0.78136(14) 0.20954(15) 0.83766(10) 0.0181(6) Uani 1 1 d . . .
C37 C 0.83022(15) 0.20505(16) 0.87704(10) 0.0217(6) Uani 1 1 d . . .
H37 H 0.8329 0.2426 0.8991 0.026 Uiso 1 1 calc R . .
C38 C 0.87442(16) 0.14767(16) 0.88467(11) 0.0244(7) Uani 1 1 d . . .
C39 C 0.87308(15) 0.09178(16) 0.85334(10) 0.0233(7) Uani 1 1 d . . .
H39 H 0.9033 0.0524 0.8588 0.028 Uiso 1 1 calc R . .
C40 C 0.82660(15) 0.09514(15) 0.81408(10) 0.0199(6) Uani 1 1 d . . .
C41 C 0.78200(14) 0.15322(14) 0.80650(10) 0.0186(6) Uani 1 1 d . . .
H41 H 0.7509 0.1542 0.7789 0.022 Uiso 1 1 calc R . .
C42 C 0.92335(18) 0.14388(18) 0.92806(12) 0.0346(8) Uani 1 1 d . . .
C43 C 0.82685(16) 0.03881(15) 0.77773(11) 0.0245(7) Uani 1 1 d . . .
F44 F 0.93594(12) 0.20518(11) 0.94851(8) 0.0535(6) Uani 1 1 d . . .
F45 F 0.98884(10) 0.11411(12) 0.91890(7) 0.0500(6) Uani 1 1 d . . .
F46 F 0.89368(12) 0.10482(11) 0.96364(7) 0.0483(6) Uani 1 1 d . . .
F47 F 0.86534(10) 0.05537(9) 0.73789(6) 0.0358(5) Uani 1 1 d . . .
F48 F 0.85571(11) -0.02051(9) 0.79400(7) 0.0375(5) Uani 1 1 d . . .
F49 F 0.75813(9) 0.02304(9) 0.76183(7) 0.0340(5) Uani 1 1 d . . .
C50 C 0.67041(15) 0.28525(14) 0.87613(10) 0.0178(6) Uani 1 1 d . . .
C51 C 0.66287(15) 0.23729(15) 0.91354(10) 0.0193(6) Uani 1 1 d . . .
H51 H 0.6952 0.1986 0.9145 0.023 Uiso 1 1 calc R . .
C52 C 0.60945(15) 0.24448(15) 0.94942(10) 0.0191(6) Uani 1 1 d . . .

C53 C 0.56146(15) 0.30035(15) 0.94960(10) 0.0216(6) Uani 1 1 d . . .
H53 H 0.5253 0.3054 0.9742 0.026 Uiso 1 1 calc R . . .
C54 C 0.56772(15) 0.34849(15) 0.91294(10) 0.0200(6) Uani 1 1 d . . .
C55 C 0.62066(15) 0.34078(15) 0.87684(10) 0.0196(6) Uani 1 1 d . . .
H55 H 0.6231 0.3743 0.8519 0.024 Uiso 1 1 calc R . . .
C56 C 0.60236(17) 0.19302(16) 0.98916(11) 0.0263(7) Uani 1 1 d . . .
C57 C 0.51893(17) 0.41066(17) 0.91339(11) 0.0260(7) Uani 1 1 d . . .
F58 F 0.65026(13) 0.14067(10) 0.98621(7) 0.0501(6) Uani 1 1 d . . .
F59 F 0.61446(13) 0.22102(10) 1.03243(7) 0.0467(5) Uani 1 1 d . . .
F60 F 0.53518(11) 0.16559(13) 0.99210(9) 0.0638(7) Uani 1 1 d . . .
F61 F 0.45168(12) 0.39714(12) 0.93045(10) 0.0753(9) Uani 1 1 d . . .
F62 F 0.54572(15) 0.46103(12) 0.94078(9) 0.0746(9) Uani 1 1 d . . .
F63 F 0.50915(10) 0.43928(10) 0.87066(6) 0.0379(5) Uani 1 1 d . . .
C64 C 0.68121(14) 0.27713(14) 0.78168(10) 0.0171(6) Uani 1 1 d . . .
C65 C 0.62981(14) 0.22370(15) 0.77415(10) 0.0195(6) Uani 1 1 d . . .
H65 H 0.6239 0.1895 0.7984 0.023 Uiso 1 1 calc R . . .
C66 C 0.58754(15) 0.21906(15) 0.73271(10) 0.0207(6) Uani 1 1 d . . .
C67 C 0.59248(15) 0.26891(15) 0.69691(10) 0.0221(7) Uani 1 1 d . . .
H67 H 0.5634 0.2658 0.6685 0.026 Uiso 1 1 calc R . . .
C68 C 0.64094(16) 0.32329(16) 0.70385(10) 0.0231(7) Uani 1 1 d . . .
C69 C 0.68482(15) 0.32685(15) 0.74535(10) 0.0193(6) Uani 1 1 d . . .
H69 H 0.7182 0.3645 0.7489 0.023 Uiso 1 1 calc R . . .
C70 C 0.53478(16) 0.16053(17) 0.72559(11) 0.0276(7) Uani 1 1 d . . .
C71 C 0.6484(2) 0.37736(18) 0.66582(12) 0.0337(8) Uani 1 1 d . . .
F72 F 0.55017(10) 0.10547(9) 0.75322(7) 0.0376(5) Uani 1 1 d . . .
F73 F 0.46463(9) 0.17848(10) 0.73609(7) 0.0375(5) Uani 1 1 d . . .
F74 F 0.53352(10) 0.13798(10) 0.67983(6) 0.0384(5) Uani 1 1 d . . .
F75 F 0.6444(6) 0.4383(4) 0.6796(3) 0.060(4) Uani 0.50 1 d P . .

F76 F 0.6105(5) 0.3681(4) 0.6282(2) 0.057(2) Uani 0.50 1 d P . .

 F77 F 0.7218(3) 0.3747(3) 0.6470(2) 0.0515(15) Uani 0.50 1 d P . .

 F78 F 0.6825(8) 0.4320(6) 0.6779(4) 0.123(6) Uani 0.50 1 d P . .

 F79 F 0.5799(4) 0.4069(6) 0.6572(5) 0.140(4) Uani 0.50 1 d P . .

 F80 F 0.6646(11) 0.3574(4) 0.6251(3) 0.140(6) Uani 0.50 1 d P . .

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 P1 0.0157(4) 0.0291(4) 0.0286(4) 0.0015(4) -0.0021(3) -0.0026(3)
 C1 0.0308(18) 0.036(2) 0.041(2) -0.0043(16) 0.0140(16) 0.0017(16)
 C2 0.0314(18) 0.052(2) 0.0273(18) -0.0094(16) 0.0108(15) -0.0093(17)
 C3 0.0257(18) 0.044(2) 0.044(2) 0.0018(17) 0.0062(16) -0.0168(16)
 C4 0.0223(17) 0.049(2) 0.045(2) 0.0040(18) -0.0124(15) -0.0016(16)
 C5 0.0384(19) 0.0301(19) 0.0364(19) -0.0010(15) -0.0008(16) -0.0028(16)
 C6 0.0157(14) 0.0286(17) 0.0246(16) 0.0003(13) 0.0034(12) -0.0011(13)
 C7 0.0125(14) 0.0345(17) 0.0241(16) 0.0016(13) 0.0051(12) -0.0008(13)
 C8 0.0117(13) 0.0420(19) 0.0229(16) -0.0011(14) 0.0024(12) -0.0039(14)
 C9 0.0210(15) 0.0369(19) 0.0285(17) -0.0053(15) 0.0057(13) -0.0089(14)
 C10 0.0205(16) 0.0280(17) 0.0300(17) -0.0013(14) 0.0075(13) -0.0042(13)
 C11 0.0276(16) 0.0377(19) 0.0234(16) 0.0025(14) -0.0001(13) 0.0034(15)
 C12 0.0227(17) 0.043(2) 0.0321(18) -0.0006(16) 0.0051(14) 0.0113(15)
 C13 0.0176(16) 0.065(3) 0.0310(19) 0.0007(17) -0.0047(14) -0.0009(16)

C14 0.043(2) 0.048(2) 0.037(2) -0.0134(17) 0.0046(17) -0.0203(19)
 C15 0.039(2) 0.0259(18) 0.041(2) 0.0032(15) 0.0091(16) -0.0013(16)
 B20 0.0119(15) 0.0200(17) 0.0209(17) 0.0000(14) 0.0007(13) -0.0013(13)
 C21 0.0126(14) 0.0224(15) 0.0192(15) 0.0019(12) -0.0040(11) 0.0008(12)
 C22 0.0121(14) 0.0255(16) 0.0198(15) 0.0035(12) -0.0037(11) 0.0004(12)
 C23 0.0150(14) 0.0220(16) 0.0239(16) 0.0005(13) -0.0066(12) 0.0019(12)
 C24 0.0126(14) 0.0245(16) 0.0305(17) 0.0046(13) -0.0038(12) -0.0026(13)
 C25 0.0120(14) 0.0278(17) 0.0247(16) 0.0023(13) 0.0008(12) -0.0009(13)
 C26 0.0147(15) 0.0229(16) 0.0264(16) -0.0019(13) -0.0020(12) 0.0000(12)
 C27 0.0189(15) 0.0247(17) 0.0281(17) 0.0012(13) -0.0061(13) -0.0027(13)
 C28 0.0189(15) 0.0288(18) 0.0381(19) -0.0005(15) 0.0063(14) -0.0020(14)
 F29 0.0287(10) 0.0371(11) 0.0422(11) -0.0149(9) 0.0077(8) -0.0064(9)
 F30 0.0400(11) 0.0212(10) 0.0386(11) -0.0004(8) -0.0034(9) -0.0005(8)
 F31 0.0355(11) 0.0359(11) 0.0349(10) -0.0046(9) -0.0178(9) -0.0026(9)
 F32 0.0514(14) 0.139(2) 0.0467(14) 0.0502(15) 0.0253(12) 0.0473(16)
 F33 0.0540(15) 0.0666(16) 0.104(2) -0.0414(15) 0.0531(14) -0.0411(13)
 F34 0.0344(11) 0.0388(11) 0.0445(12) -0.0032(9) 0.0160(9) 0.0026(9)
 C36 0.0105(13) 0.0219(15) 0.0218(15) 0.0016(12) 0.0020(11) -0.0028(12)
 C37 0.0167(14) 0.0258(16) 0.0225(15) -0.0020(13) 0.0008(12) -0.0006(13)
 C38 0.0160(15) 0.0320(18) 0.0250(16) 0.0032(13) -0.0009(12) 0.0018(13)
 C39 0.0150(15) 0.0273(17) 0.0275(16) 0.0059(13) 0.0072(12) 0.0035(13)
 C40 0.0145(14) 0.0197(16) 0.0254(16) 0.0012(13) 0.0065(12) -0.0018(12)
 C41 0.0103(13) 0.0251(16) 0.0203(15) 0.0031(12) 0.0013(11) -0.0039(12)
 C42 0.0291(18) 0.040(2) 0.0347(19) -0.0056(17) -0.0080(15) 0.0121(16)
 C43 0.0185(15) 0.0224(17) 0.0326(17) 0.0017(14) 0.0025(13) 0.0007(13)
 F44 0.0549(14) 0.0479(13) 0.0576(14) -0.0067(11) -0.0364(11) 0.0055(11)
 F45 0.0254(10) 0.0843(17) 0.0402(12) -0.0022(11) -0.0098(9) 0.0215(11)
 F46 0.0549(14) 0.0623(14) 0.0277(11) 0.0075(10) -0.0028(10) 0.0146(12)

F47 0.0385(11) 0.0354(11) 0.0336(11) -0.0075(8) 0.0177(9) -0.0091(9)
F48 0.0422(11) 0.0229(10) 0.0473(12) -0.0029(9) -0.0006(9) 0.0085(9)
F49 0.0210(9) 0.0347(11) 0.0463(11) -0.0128(9) 0.0014(8) -0.0039(8)
C50 0.0133(13) 0.0197(15) 0.0205(15) -0.0016(12) -0.0027(12) -0.0030(12)
C51 0.0158(14) 0.0179(15) 0.0242(15) -0.0030(12) -0.0020(12) -0.0022(12)
C52 0.0155(14) 0.0209(15) 0.0209(15) 0.0006(12) -0.0013(12) -0.0048(12)
C53 0.0149(14) 0.0292(17) 0.0208(15) -0.0023(13) 0.0029(12) -0.0030(13)
C54 0.0123(14) 0.0223(16) 0.0255(16) -0.0030(12) -0.0018(11) -0.0011(12)
C55 0.0149(14) 0.0222(16) 0.0218(15) 0.0011(12) -0.0020(12) -0.0029(12)
C56 0.0229(16) 0.0273(17) 0.0286(17) 0.0011(14) 0.0002(13) -0.0020(14)
C57 0.0226(16) 0.0297(18) 0.0257(17) 0.0010(14) 0.0031(13) 0.0023(14)
F58 0.0687(15) 0.0367(12) 0.0450(12) 0.0172(10) 0.0188(11) 0.0229(11)
F59 0.0714(15) 0.0444(12) 0.0243(10) 0.0064(9) -0.0013(10) -0.0028(11)
F60 0.0338(12) 0.0784(17) 0.0793(17) 0.0490(14) -0.0146(11) -0.0297(12)
F61 0.0408(13) 0.0626(15) 0.123(2) 0.0490(15) 0.0526(14) 0.0309(12)
F62 0.104(2) 0.0418(13) 0.0777(17) -0.0294(12) -0.0552(16) 0.0406(14)
F63 0.0327(10) 0.0497(12) 0.0313(10) 0.0088(9) 0.0002(8) 0.0208(9)
C64 0.0098(13) 0.0201(15) 0.0214(15) -0.0010(12) 0.0026(11) 0.0032(11)
C65 0.0126(14) 0.0226(16) 0.0233(15) 0.0002(12) 0.0030(12) 0.0016(12)
C66 0.0125(13) 0.0249(16) 0.0247(16) -0.0051(13) 0.0043(12) -0.0005(12)
C67 0.0165(14) 0.0302(17) 0.0195(15) -0.0028(13) -0.0027(12) 0.0018(13)
C68 0.0213(15) 0.0262(17) 0.0219(15) 0.0011(13) 0.0008(12) 0.0029(13)
C69 0.0126(14) 0.0216(15) 0.0237(15) -0.0024(13) 0.0006(11) -0.0016(12)
C70 0.0183(15) 0.0367(19) 0.0278(18) -0.0033(15) 0.0000(13) -0.0037(14)
C71 0.042(2) 0.034(2) 0.0249(18) 0.0037(15) -0.0050(15) -0.0005(17)
F72 0.0370(11) 0.0299(10) 0.0459(12) 0.0032(9) -0.0088(9) -0.0128(9)
F73 0.0137(9) 0.0501(12) 0.0485(12) -0.0068(10) 0.0031(8) -0.0088(9)
F74 0.0364(11) 0.0494(12) 0.0295(10) -0.0133(9) 0.0006(8) -0.0176(10)
F75 0.138(9) 0.012(3) 0.029(4) -0.004(2) 0.023(5) 0.024(5)

F76 0.087(5) 0.062(5) 0.023(3) 0.014(3) -0.033(3) -0.039(4)
F77 0.048(3) 0.049(4) 0.057(4) 0.028(3) 0.028(2) 0.005(2)
F78 0.212(13) 0.089(9) 0.067(7) 0.051(6) -0.073(8) -0.112(9)
F79 0.051(4) 0.166(9) 0.204(10) 0.149(8) 0.009(6) 0.031(5)
F80 0.341(18) 0.035(4) 0.044(5) 0.006(3) 0.096(9) 0.032(10)

_geom_special_details

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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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_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Co1 C1 1.961(3) . ?

Co1 C6 2.057(3) . ?

Co1 C9 2.069(3) . ?

Co1 C10 2.075(3) . ?

Co1 C8 2.096(3) . ?

Co1 C7 2.097(3) . ?

Co1 P1 2.1976(9) . ?

P1 C5 1.810(3) . ?

P1 C4 1.818(3) . ?

P1 C3 1.822(3) . ?

C1 C2 1.462(5) . ?

C1 H1A 0.9900 . ?

C1 H1B 0.9900 . ?

C2 H2A 0.9800 . ?

C2 H2B 0.9800 . ?

C2 H2C 0.9800 . ?

C3 H3A 0.9800 . ?

C3 H3B 0.9800 . ?

C3 H3C 0.9800 . ?

C4 H4A 0.9800 . ?

C4 H4B 0.9800 . ?

C4 H4C 0.9800 . ?

C5 H5A 0.9800 . ?

C5 H5B 0.9800 . ?

C5 H5C 0.9800 . ?

C6 C10 1.428(4) . ?

C6 C7 1.452(4) . ?

C6 C11 1.498(4) . ?

C7 C8 1.403(4) . ?

C7 C12 1.495(4) . ?

C8 C9 1.434(5) . ?

C8 C13 1.503(4) . ?

C9 C10 1.421(4) . ?

C9 C14 1.500(4) . ?

C10 C15 1.496(4) . ?

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C11 H11B 0.9800 . ?
C11 H11C 0.9800 . ?
C12 H12A 0.9800 . ?
C12 H12B 0.9800 . ?
C12 H12C 0.9800 . ?
C13 H13A 0.9800 . ?
C13 H13B 0.9800 . ?
C13 H13C 0.9800 . ?
C14 H14A 0.9800 . ?
C14 H14B 0.9800 . ?
C14 H14C 0.9800 . ?
C15 H15A 0.9800 . ?
C15 H15B 0.9800 . ?
C15 H15C 0.9800 . ?
B20 C36 1.637(4) . ?
B20 C21 1.640(4) . ?
B20 C64 1.649(4) . ?
B20 C50 1.648(4) . ?
C21 C22 1.396(4) . ?
C21 C26 1.398(4) . ?
C22 C23 1.397(4) . ?
C22 H22 0.9500 . ?
C23 C24 1.387(4) . ?
C23 C27 1.483(4) . ?
C24 C25 1.382(4) . ?
C24 H24 0.9500 . ?
C25 C26 1.394(4) . ?

C25 C28 1.497(4) . ?

C26 H26 0.9500 . ?

C27 F30 1.340(3) . ?

C27 F29 1.348(3) . ?

C27 F31 1.353(3) . ?

C28 F33 1.318(4) . ?

C28 F34 1.331(4) . ?

C28 F32 1.332(4) . ?

C36 C41 1.391(4) . ?

C36 C37 1.409(4) . ?

C37 C38 1.384(4) . ?

C37 H37 0.9500 . ?

C38 C39 1.387(4) . ?

C38 C42 1.497(4) . ?

C39 C40 1.379(4) . ?

C39 H39 0.9500 . ?

C40 C41 1.399(4) . ?

C40 C43 1.485(4) . ?

C41 H41 0.9500 . ?

C42 F44 1.333(4) . ?

C42 F45 1.342(4) . ?

C42 F46 1.355(4) . ?

C43 F48 1.338(3) . ?

C43 F47 1.346(3) . ?

C43 F49 1.355(3) . ?

C50 C51 1.399(4) . ?

C50 C55 1.401(4) . ?

C51 C52 1.395(4) . ?

C51 H51 0.9500 . ?

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C52 C56 1.491(4) . ?
C53 C54 1.384(4) . ?
C53 H53 0.9500 . ?
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C54 C57 1.491(4) . ?
C55 H55 0.9500 . ?
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C56 F58 1.335(4) . ?
C56 F59 1.336(4) . ?
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C57 F62 1.327(4) . ?
C57 F61 1.332(4) . ?
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C64 C65 1.406(4) . ?
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C65 H65 0.9500 . ?
C66 C67 1.387(4) . ?
C66 C70 1.494(4) . ?
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C67 H67 0.9500 . ?
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C68 C71 1.492(4) . ?
C69 H69 0.9500 . ?
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C70 F74 1.344(4) . ?
C70 F73 1.348(3) . ?
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C71 F75 1.241(7) . ?

C71 F76 1.263(6) . ?

C71 F78 1.269(10) . ?

C71 F79 1.386(7) . ?

C71 F77 1.428(6) . ?

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F76 F79 1.232(11) . ?

F77 F80 1.245(16) . ?

F77 F78 1.572(14) . ?

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C1 Co1 C10 95.56(13) . . ?

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C10 Co1 C7 67.92(12) . . ?
C8 Co1 C7 39.10(11) . . ?
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C9 Co1 P1 166.48(9) . . ?
C10 Co1 P1 128.85(9) . . ?
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C7 Co1 P1 102.72(9) . . ?
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C5 P1 C3 101.11(17) . . ?
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C3 P1 Co1 113.22(12) . . ?
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Co1 C1 H1A 116.0 . . ?
C2 C1 H1B 116.0 . . ?
Co1 C1 H1B 116.0 . . ?
H1A C1 H1B 113.0 . . ?
C1 C2 H2A 109.5 . . ?
C1 C2 H2B 109.5 . . ?
H2A C2 H2B 109.5 . . ?
C1 C2 H2C 109.5 . . ?

H2A C2 H2C 109.5 . . ?

H2B C2 H2C 109.5 . . ?

P1 C3 H3A 109.5 . . ?

P1 C3 H3B 109.5 . . ?

H3A C3 H3B 109.5 . . ?

P1 C3 H3C 109.5 . . ?

H3A C3 H3C 109.5 . . ?

H3B C3 H3C 109.5 . . ?

P1 C4 H4A 109.5 . . ?

P1 C4 H4B 109.5 . . ?

H4A C4 H4B 109.5 . . ?

P1 C4 H4C 109.5 . . ?

H4A C4 H4C 109.5 . . ?

H4B C4 H4C 109.5 . . ?

P1 C5 H5A 109.5 . . ?

P1 C5 H5B 109.5 . . ?

H5A C5 H5B 109.5 . . ?

P1 C5 H5C 109.5 . . ?

H5A C5 H5C 109.5 . . ?

H5B C5 H5C 109.5 . . ?

C10 C6 C7 108.0(3) . . ?

C10 C6 C11 126.2(3) . . ?

C7 C6 C11 125.1(3) . . ?

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C7 C6 Co1 71.05(16) . . ?

C11 C6 Co1 131.5(2) . . ?

C8 C7 C6 107.5(3) . . ?

C8 C7 C12 125.4(3) . . ?

C6 C7 C12 126.6(3) . . ?

C8 C7 Co1 70.39(16) . . ?
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C12 C7 Co1 132.9(2) . . ?
C7 C8 C9 108.6(3) . . ?
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C7 C8 Co1 70.51(16) . . ?
C9 C8 Co1 68.87(16) . . ?
C13 C8 Co1 128.4(2) . . ?
C10 C9 C8 108.4(3) . . ?
C10 C9 C14 126.4(3) . . ?
C8 C9 C14 125.1(3) . . ?
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C8 C9 Co1 70.86(17) . . ?
C14 C9 Co1 127.8(2) . . ?
C9 C10 C6 107.4(3) . . ?
C9 C10 C15 126.8(3) . . ?
C6 C10 C15 125.6(3) . . ?
C9 C10 Co1 69.74(18) . . ?
C6 C10 Co1 69.10(17) . . ?
C15 C10 Co1 128.8(2) . . ?
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C6 C11 H11B 109.5 . . ?
H11A C11 H11B 109.5 . . ?
C6 C11 H11C 109.5 . . ?
H11A C11 H11C 109.5 . . ?
H11B C11 H11C 109.5 . . ?
C7 C12 H12A 109.5 . . ?

C7 C12 H12B 109.5 . . ?
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H12B C12 H12C 109.5 . . ?
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H14B C14 H14C 109.5 . . ?
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C10 C15 H15B 109.5 . . ?
H15A C15 H15B 109.5 . . ?
C10 C15 H15C 109.5 . . ?
H15A C15 H15C 109.5 . . ?
H15B C15 H15C 109.5 . . ?
C36 B20 C21 106.6(2) . . ?
C36 B20 C64 111.9(2) . . ?
C21 B20 C64 109.4(2) . . ?
C36 B20 C50 110.8(2) . . ?
C21 B20 C50 112.1(2) . . ?
C64 B20 C50 106.1(2) . . ?

C22 C21 C26 115.6(3) . . ?
C22 C21 B20 125.7(2) . . ?
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C23 C22 H22 118.8 . . ?
C24 C23 C22 120.4(3) . . ?
C24 C23 C27 118.6(3) . . ?
C22 C23 C27 121.0(3) . . ?
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C25 C24 H24 120.8 . . ?
C23 C24 H24 120.8 . . ?
C24 C25 C26 120.5(3) . . ?
C24 C25 C28 119.9(3) . . ?
C26 C25 C28 119.6(3) . . ?
C25 C26 C21 122.6(3) . . ?
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C21 C26 H26 118.7 . . ?
F30 C27 F29 106.4(2) . . ?
F30 C27 F31 105.6(2) . . ?
F29 C27 F31 105.1(2) . . ?
F30 C27 C23 113.3(2) . . ?
F29 C27 C23 113.6(2) . . ?
F31 C27 C23 112.1(2) . . ?
F33 C28 F34 106.1(3) . . ?
F33 C28 F32 107.3(3) . . ?
F34 C28 F32 104.5(3) . . ?
F33 C28 C25 113.6(3) . . ?

F34 C28 C25 113.5(3) . . ?
F32 C28 C25 111.3(2) . . ?
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C37 C38 C42 120.3(3) . . ?
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C40 C39 H39 121.0 . . ?
C38 C39 H39 121.0 . . ?
C39 C40 C41 120.6(3) . . ?
C39 C40 C43 120.1(3) . . ?
C41 C40 C43 119.2(3) . . ?
C36 C41 C40 122.6(3) . . ?
C36 C41 H41 118.7 . . ?
C40 C41 H41 118.7 . . ?
F44 C42 F45 108.1(3) . . ?
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F45 C42 F46 104.4(3) . . ?
F44 C42 C38 113.6(3) . . ?
F45 C42 C38 113.0(3) . . ?
F46 C42 C38 112.3(3) . . ?
F48 C43 F47 106.2(2) . . ?
F48 C43 F49 106.0(2) . . ?
F47 C43 F49 105.1(2) . . ?

F48 C43 C40 113.6(3) . . ?
F47 C43 C40 112.7(2) . . ?
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C51 C50 C55 115.8(3) . . ?
C51 C50 B20 124.9(2) . . ?
C55 C50 B20 119.3(2) . . ?
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C53 C52 C51 121.0(3) . . ?
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C51 C52 C56 121.4(3) . . ?
C54 C53 C52 118.0(3) . . ?
C54 C53 H53 121.0 . . ?
C52 C53 H53 121.0 . . ?
C53 C54 C55 120.9(3) . . ?
C53 C54 C57 119.2(3) . . ?
C55 C54 C57 119.9(3) . . ?
C54 C55 C50 122.2(3) . . ?
C54 C55 H55 118.9 . . ?
C50 C55 H55 118.9 . . ?
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F58 C56 F59 104.8(2) . . ?
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F58 C56 C52 113.8(2) . . ?
F59 C56 C52 112.4(3) . . ?
F63 C57 F62 104.9(3) . . ?

F63 C57 F61 106.2(3) . . ?
F62 C57 F61 105.9(3) . . ?
F63 C57 C54 114.2(2) . . ?
F62 C57 C54 112.3(2) . . ?
F61 C57 C54 112.7(3) . . ?
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C65 C64 B20 119.8(2) . . ?
C66 C65 C64 122.5(3) . . ?
C66 C65 H65 118.8 . . ?
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C65 C66 C67 121.0(3) . . ?
C65 C66 C70 120.8(3) . . ?
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C66 C67 H67 121.0 . . ?
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C64 C69 H69 118.9 . . ?
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F74 C70 F73 105.8(2) . . ?
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F74 C70 C66 112.4(2) . . ?
F73 C70 C66 112.2(3) . . ?

F80 C71 F75 126.5(6) . . ?
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F80 C71 F78 112.8(8) . . ?
F76 C71 F78 126.9(6) . . ?
F80 C71 F79 100.6(8) . . ?
F75 C71 F79 67.0(7) . . ?
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C1 Co1 P1 C4 63.92(17) ?

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C9 Co1 P1 C4 -64.7(4) ?
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C6 Co1 C1 C2 -158.87(18) ?
C9 Co1 C1 C2 -90.4(2) ?
C10 Co1 C1 C2 -130.7(2) ?
C8 Co1 C1 C2 -66.6(3) ?
C7 Co1 C1 C2 -121.2(4) ?
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C9 Co1 C6 C10 -37.58(18) ?
C8 Co1 C6 C10 -81.34(19) ?
C7 Co1 C6 C10 -118.0(2) ?
P1 Co1 C6 C10 142.78(16) ?
C1 Co1 C6 C7 164.38(19) ?
C9 Co1 C6 C7 80.39(19) ?
C10 Co1 C6 C7 118.0(2) ?
C8 Co1 C6 C7 36.63(18) ?
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C1 Co1 C6 C11 -75.1(3) ?

C9 Co1 C6 C11 -159.1(3) ?
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C7 Co1 C6 C11 120.5(4) ?
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Co1 C6 C7 C8 -59.6(2) ?
C10 C6 C7 C12 -171.0(3) ?
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Co1 C6 C7 C12 127.9(3) ?
C10 C6 C7 Co1 61.1(2) ?
C11 C6 C7 Co1 -127.9(3) ?
C1 Co1 C7 C8 70.8(5) ?
C6 Co1 C7 C8 119.2(3) ?
C9 Co1 C7 C8 37.44(19) ?
C10 Co1 C7 C8 81.0(2) ?
P1 Co1 C7 C8 -151.96(17) ?
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C9 Co1 C7 C6 -81.73(19) ?
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C8 Co1 C7 C6 -119.2(3) ?
P1 Co1 C7 C6 88.87(16) ?
C1 Co1 C7 C12 -168.6(4) ?
C6 Co1 C7 C12 -120.2(4) ?
C9 Co1 C7 C12 158.0(3) ?
C10 Co1 C7 C12 -158.4(3) ?
C8 Co1 C7 C12 120.6(4) ?
P1 Co1 C7 C12 -31.4(3) ?

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C12 C7 C8 C9 172.2(3) ?
Co1 C7 C8 C9 -58.5(2) ?
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C12 C7 C8 C13 -5.4(5) ?
Co1 C7 C8 C13 123.9(3) ?
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C1 Co1 C8 C9 -38.1(3) ?
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Co1 C8 C9 C10 -60.4(2) ?
C7 C8 C9 C14 -177.2(3) ?

C13 C8 C9 C14 0.4(5) ?
Co1 C8 C9 C14 123.3(3) ?
C7 C8 C9 Co1 59.5(2) ?
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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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'calc w=1/[s^2^(Fo^2^)(0.1090P)^2^.4957P] where P=(Fo^2^ - ^2^)/3'

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loop_

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H1B H 0.6627 0.9739 0.2710 0.053 Uiso 1 1 calc R . .

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H2B H 0.6431 0.8778 0.3088 0.069 Uiso 1 1 calc R . .

C3 C 0.7731(4) 0.8440(3) 0.2720(3) 0.0389(12) Uani 1 1 d U A .

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C6 C 0.8144(5) 0.7399(3) 0.2426(4) 0.0512(15) Uani 1 1 d U A .

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H6B H 0.7930 0.6963 0.2507 0.077 Uiso 1 1 calc R . .

H6C H 0.8907 0.7443 0.2567 0.077 Uiso 1 1 calc R . .

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H16C H 0.8024 1.1397 0.1737 0.092 Uiso 0.740(7) 1 calc PR A 1
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H17A H 1.0364 1.0602 0.1918 0.098 Uiso 0.740(7) 1 calc PR A 1
H17B H 1.0197 1.0584 0.1100 0.098 Uiso 0.740(7) 1 calc PR A 1
H17C H 1.0635 0.9970 0.1531 0.098 Uiso 0.740(7) 1 calc PR A 1
C108 C 0.7958(16) 0.9559(9) 0.1163(11) 0.066(5) Uani 0.260(7) 1 d PDU A 2
C109 C 0.7111(12) 0.9852(10) 0.1451(14) 0.055(4) Uani 0.260(7) 1 d PDU A 2
C110 C 0.7483(12) 1.0395(9) 0.1788(12) 0.056(6) Uani 0.260(7) 1 d PDU A 2
C111 C 0.8585(13) 1.0452(7) 0.1767(11) 0.058(4) Uani 0.260(7) 1 d PDU A 2
C112 C 0.8890(11) 0.9919(9) 0.1388(11) 0.063(4) Uani 0.260(7) 1 d PDU A 2
C113 C 0.789(2) 0.8960(10) 0.0764(13) 0.123(13) Uani 0.260(7) 1 d PDU A 2
H13D H 0.8586 0.8758 0.0817 0.185 Uiso 0.260(7) 1 calc PR A 2
H13E H 0.7652 0.9054 0.0280 0.185 Uiso 0.260(7) 1 calc PR A 2
H13F H 0.7385 0.8673 0.0932 0.185 Uiso 0.260(7) 1 calc PR A 2
C114 C 0.5995(12) 0.9603(9) 0.1368(14) 0.080(9) Uani 0.260(7) 1 d PDU A 2
H14D H 0.5916 0.9255 0.1035 0.120 Uiso 0.260(7) 1 calc PR A 2
H14E H 0.5503 0.9945 0.1204 0.120 Uiso 0.260(7) 1 calc PR A 2
H14F H 0.5842 0.9448 0.1809 0.120 Uiso 0.260(7) 1 calc PR A 2
C115 C 0.6820(16) 1.0865(8) 0.2137(14) 0.079(9) Uani 0.260(7) 1 d PDU A 2
H15D H 0.6231 1.0638 0.2292 0.118 Uiso 0.260(7) 1 calc PR A 2
H15E H 0.6543 1.1196 0.1811 0.118 Uiso 0.260(7) 1 calc PR A 2
H15F H 0.7261 1.1059 0.2531 0.118 Uiso 0.260(7) 1 calc PR A 2
C116 C 0.9275(16) 1.0997(9) 0.2034(12) 0.086(10) Uani 0.260(7) 1 d PDU A 2
H16D H 0.9778 1.1086 0.1719 0.129 Uiso 0.260(7) 1 calc PR A 2
H16E H 0.9660 1.0890 0.2485 0.129 Uiso 0.260(7) 1 calc PR A 2

H16F H 0.8838 1.1373 0.2071 0.129 Uiso 0.260(7) 1 calc PR A 2
C117 C 0.9957(15) 0.9794(16) 0.1178(17) 0.142(15) Uani 0.260(7) 1 d PDU A 2
H17D H 1.0514 0.9925 0.1547 0.213 Uiso 0.260(7) 1 calc PR A 2
H17E H 1.0021 1.0037 0.0764 0.213 Uiso 0.260(7) 1 calc PR A 2
H17F H 1.0028 0.9340 0.1087 0.213 Uiso 0.260(7) 1 calc PR A 2
O18 O 0.9702(3) 1.03842(18) 0.3317(2) 0.0525(11) Uani 1 1 d U . .
C19 C 1.0667(5) 1.0711(3) 0.3623(4) 0.069(2) Uani 1 1 d U A .
H19A H 1.0499 1.1016 0.3965 0.103 Uiso 1 1 calc R . .
H19B H 1.0971 1.0937 0.3265 0.103 Uiso 1 1 calc R . .
H19C H 1.1177 1.0400 0.3843 0.103 Uiso 1 1 calc R . .
O20 O 1.0776(3) 0.95791(18) 0.2882(2) 0.0467(9) Uani 1 1 d U . .
C21 C 1.1023(5) 0.8967(3) 0.2622(4) 0.0534(16) Uani 1 1 d U A .
H21A H 1.1141 0.8661 0.2999 0.080 Uiso 1 1 calc R . .
H21B H 1.1662 0.9001 0.2408 0.080 Uiso 1 1 calc R . .
H21C H 1.0434 0.8824 0.2281 0.080 Uiso 1 1 calc R . .
O22 O 0.9505(3) 0.92362(19) 0.3653(2) 0.0502(10) Uani 1 1 d U . .
C23 C 1.0263(6) 0.9251(3) 0.4273(3) 0.0604(18) Uani 1 1 d U A .
H23A H 1.0979 0.9246 0.4156 0.091 Uiso 1 1 calc R . .
H23B H 1.0163 0.8879 0.4554 0.091 Uiso 1 1 calc R . .
H23C H 1.0163 0.9639 0.4530 0.091 Uiso 1 1 calc R . .
B30 B 0.3949(4) 0.7223(2) 0.8781(3) 0.0218(9) Uani 1 1 d U . .
C31 C 0.5173(3) 0.7412(2) 0.9057(2) 0.0197(8) Uani 1 1 d U . .
C32 C 0.5863(3) 0.7033(2) 0.9499(2) 0.0195(9) Uani 1 1 d U . .
H32 H 0.5631 0.6627 0.9625 0.023 Uiso 1 1 calc R . .
C33 C 0.6884(3) 0.7231(2) 0.9760(2) 0.0223(9) Uani 1 1 d U . .
C34 C 0.7256(3) 0.7813(2) 0.9579(2) 0.0223(9) Uani 1 1 d U B .
H34 H 0.7951 0.7948 0.9757 0.027 Uiso 1 1 calc R . .
C35 C 0.6598(3) 0.8196(2) 0.9134(2) 0.0218(9) Uani 1 1 d U . .

C36 C 0.5579(4) 0.7997(2) 0.8884(2) 0.0227(9) Uani 1 1 d U B .
H36 H 0.5138 0.8270 0.8584 0.027 Uiso 1 1 calc R . .
C37 C 0.7588(4) 0.6807(2) 1.0227(2) 0.0268(10) Uani 1 1 d U . .
F31 F 0.7073(2) 0.64488(14) 1.06217(16) 0.0417(8) Uani 1 1 d U . .
F32 F 0.8311(2) 0.71309(14) 1.06663(17) 0.0444(8) Uani 1 1 d U . .
F33 F 0.8148(2) 0.64111(15) 0.98988(17) 0.0488(8) Uani 1 1 d U . .
C38 C 0.6966(4) 0.8821(2) 0.8909(3) 0.0303(8) Uani 0.788(10) 1 d PU B .
F34 F 0.7833(4) 0.9053(3) 0.9320(4) 0.0483(15) Uani 0.788(10) 1 d PU . .
F35 F 0.6268(5) 0.9279(4) 0.8866(4) 0.0539(18) Uani 0.788(10) 1 d PU . .
F36 F 0.7298(6) 0.8794(2) 0.8295(3) 0.0616(18) Uani 0.788(10) 1 d PU . .
C381 C 0.6966(4) 0.8821(2) 0.8909(3) 0.0303(8) Uani 0.212(10) 1 d PU B 3
F341 F 0.7897(16) 0.8903(12) 0.9012(13) 0.044(3) Uani 0.212(10) 1 d PU B 3
F351 F 0.642(2) 0.9269(15) 0.9183(14) 0.053(3) Uani 0.212(10) 1 d PU B 3
F361 F 0.658(2) 0.8893(11) 0.8238(9) 0.063(3) Uani 0.212(10) 1 d PU B 3
C41 C 0.3679(3) 0.73711(19) 0.7947(2) 0.0205(9) Uani 1 1 d U . .
C42 C 0.4458(4) 0.7401(2) 0.7526(2) 0.0249(9) Uani 1 1 d U C .
H42 H 0.5172 0.7340 0.7728 0.030 Uiso 1 1 calc R . .
C43 C 0.4247(4) 0.7514(2) 0.6828(2) 0.0290(10) Uani 1 1 d U . .
C44 C 0.3222(4) 0.7582(2) 0.6503(3) 0.0303(10) Uani 1 1 d U C .
H44 H 0.3070 0.7652 0.6024 0.036 Uiso 1 1 calc R . .
C45 C 0.2421(4) 0.7544(2) 0.6902(3) 0.0293(10) Uani 1 1 d U . .
C46 C 0.2648(4) 0.7441(2) 0.7600(2) 0.0252(9) Uani 1 1 d U C .
H46 H 0.2079 0.7417 0.7855 0.030 Uiso 1 1 calc R . .
C47 C 0.5127(5) 0.7584(3) 0.6432(3) 0.0471(11) Uani 0.821(6) 1 d PU C .
F41 F 0.5821(4) 0.7101(3) 0.6548(3) 0.0673(14) Uani 0.821(6) 1 d PU . .
F42 F 0.5739(4) 0.8089(3) 0.6645(3) 0.0709(15) Uani 0.821(6) 1 d PU . .
F43 F 0.4844(4) 0.7634(5) 0.5775(3) 0.096(3) Uani 0.821(6) 1 d PU . .
C471 C 0.5127(5) 0.7584(3) 0.6432(3) 0.0471(11) Uani 0.179(6) 1 d PU C 4
F411 F 0.6046(16) 0.7491(15) 0.6701(11) 0.056(3) Uani 0.179(6) 1 d PU C 4

F421 F 0.513(2) 0.8122(15) 0.6084(17) 0.090(4) Uani 0.179(6) 1 d PU C 4
 F431 F 0.500(2) 0.7110(19) 0.5863(13) 0.095(4) Uani 0.179(6) 1 d PU C 4
 C48 C 0.1301(4) 0.7596(3) 0.6551(3) 0.0399(11) Uani 1 1 d U C .
 F44 F 0.1167(3) 0.8065(2) 0.6096(2) 0.0746(12) Uani 1 1 d U ..
 F45 F 0.0974(3) 0.70722(18) 0.62139(19) 0.0608(10) Uani 1 1 d U ..
 F46 F 0.0615(2) 0.7702(2) 0.69772(18) 0.0623(10) Uani 1 1 d U ..
 C51 C 0.3746(3) 0.6469(2) 0.8907(2) 0.0201(9) Uani 1 1 d U ..
 C52 C 0.3772(4) 0.6009(2) 0.8400(2) 0.0246(10) Uani 1 1 d U ..
 H52 H 0.3880 0.6140 0.7956 0.030 Uiso 1 1 calc R ..
 C53 C 0.3645(4) 0.5362(2) 0.8525(3) 0.0283(10) Uani 1 1 d U ..
 C54 C 0.3476(4) 0.5153(2) 0.9163(3) 0.0321(11) Uani 1 1 d U D .
 H54 H 0.3376 0.4715 0.9245 0.039 Uiso 1 1 calc R ..
 C55 C 0.3456(4) 0.5596(2) 0.9679(3) 0.0287(10) Uani 1 1 d U ..
 C56 C 0.3581(3) 0.6242(2) 0.9549(2) 0.0239(9) Uani 1 1 d U D .
 H56 H 0.3552 0.6538 0.9908 0.029 Uiso 1 1 calc R ..
 C57 C 0.3663(5) 0.4897(2) 0.7957(3) 0.0416(12) Uani 1 1 d U ..
 F51 F 0.4605(4) 0.4768(3) 0.7848(3) 0.1083(19) Uani 1 1 d U ..
 F52 F 0.3208(4) 0.43573(17) 0.8061(2) 0.0889(15) Uani 1 1 d U ..
 F53 F 0.3142(4) 0.51006(18) 0.73655(19) 0.0837(14) Uani 1 1 d U ..
 C58 C 0.3238(4) 0.5380(2) 1.0359(3) 0.0366(9) Uani 0.916(6) 1 d PU D .
 F54 F 0.3710(4) 0.4830(2) 1.0551(2) 0.0606(13) Uani 0.916(6) 1 d PU ..
 F55 F 0.3575(7) 0.5780(2) 1.0864(2) 0.095(2) Uani 0.916(6) 1 d PU ..
 F56 F 0.2230(3) 0.5267(4) 1.0373(3) 0.0852(18) Uani 0.916(6) 1 d PU ..
 C581 C 0.3238(4) 0.5380(2) 1.0359(3) 0.0366(9) Uani 0.084(6) 1 d PU D 5
 F541 F 0.296(5) 0.482(2) 1.039(3) 0.059(4) Uani 0.084(6) 1 d PU D 5
 F551 F 0.400(4) 0.542(4) 1.079(2) 0.072(4) Uani 0.084(6) 1 d PU D 5
 F561 F 0.257(8) 0.573(4) 1.059(3) 0.093(4) Uani 0.084(6) 1 d PU D 5
 C61 C 0.3162(3) 0.7649(2) 0.9186(2) 0.0213(9) Uani 1 1 d U ..

C62 C 0.2085(4) 0.7492(2) 0.9142(2) 0.0249(9) Uani 1 1 d U E .
 H62 H 0.1839 0.7113 0.8912 0.030 Uiso 1 1 calc R . .
 C63 C 0.1373(4) 0.7864(2) 0.9419(3) 0.0327(10) Uani 1 1 d U . .
 C64 C 0.1699(4) 0.8401(2) 0.9792(3) 0.0376(11) Uani 1 1 d U E .
 H64 H 0.1208 0.8657 0.9983 0.045 Uiso 1 1 calc R . .
 C65 C 0.2764(4) 0.8557(2) 0.9880(3) 0.0337(10) Uani 1 1 d U . .
 C66 C 0.3470(4) 0.8195(2) 0.9573(2) 0.0261(10) Uani 1 1 d U E .
 H66 H 0.4189 0.8321 0.9628 0.031 Uiso 1 1 calc R . .
 C67 C 0.0223(4) 0.7688(3) 0.9304(3) 0.0428(10) Uani 0.734(5) 1 d PU E .
 F61 F -0.0059(3) 0.7249(3) 0.8775(3) 0.0615(14) Uani 0.734(5) 1 d PU . .
 F62 F -0.0143(4) 0.7425(4) 0.9825(3) 0.0644(16) Uani 0.734(5) 1 d PU . .
 F63 F -0.0430(4) 0.8166(2) 0.9073(4) 0.0655(15) Uani 0.734(5) 1 d PU . .
 C671 C 0.0223(4) 0.7688(3) 0.9304(3) 0.0428(10) Uani 0.266(5) 1 d PU E 6
 F611 F -0.0135(11) 0.7826(9) 0.8776(8) 0.063(2) Uani 0.266(5) 1 d PU E 6
 F621 F -0.0194(9) 0.8103(8) 0.9811(9) 0.071(3) Uani 0.266(5) 1 d PU E 6
 F631 F 0.0157(13) 0.7183(8) 0.9567(10) 0.062(2) Uani 0.266(5) 1 d PU E 6
 C68 C 0.3150(5) 0.9108(3) 1.0313(3) 0.0499(13) Uani 1 1 d U E .
 F64 F 0.3915(3) 0.94278(17) 1.0090(2) 0.0679(11) Uani 1 1 d U . .
 F65 F 0.3509(5) 0.8952(2) 1.0938(2) 0.1095(19) Uani 1 1 d U . .
 F66 F 0.2402(4) 0.9544(2) 1.0338(3) 0.1159(19) Uani 1 1 d U . .

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Co1	0.0371(4)	0.0310(4)	0.0321(4)	0.0038(3)	0.0045(3)	-0.0002(3)
P1	0.0382(8)	0.0327(8)	0.0390(8)	0.0008(6)	-0.0034(6)	0.0001(6)
C1	0.040(3)	0.054(3)	0.041(3)	0.007(2)	0.010(2)	0.011(2)
C2	0.074(4)	0.054(3)	0.052(4)	-0.001(3)	0.032(3)	-0.013(3)
C3	0.047(3)	0.039(2)	0.030(3)	0.005(2)	0.005(2)	-0.010(2)
O4	0.0375(19)	0.0341(16)	0.0304(19)	0.0015(14)	0.0040(15)	-0.0060(14)
C6	0.050(4)	0.033(3)	0.068(4)	0.004(3)	0.002(3)	-0.007(2)
O7	0.059(3)	0.0402(19)	0.042(2)	0.0073(17)	0.0093(19)	-0.0148(17)
C8	0.032(3)	0.034(3)	0.033(2)	0.006(2)	0.007(3)	0.001(2)
C9	0.030(3)	0.037(3)	0.032(2)	0.003(2)	0.002(2)	0.001(2)
C10	0.040(3)	0.044(4)	0.033(4)	0.000(3)	0.009(3)	0.006(2)
C11	0.055(3)	0.033(2)	0.030(4)	0.003(2)	0.002(3)	0.003(3)
C12	0.036(3)	0.041(3)	0.033(3)	0.007(3)	0.000(3)	-0.007(2)
C13	0.043(4)	0.062(5)	0.038(4)	-0.004(4)	0.004(4)	0.017(4)
C14	0.043(4)	0.064(5)	0.036(4)	-0.007(4)	-0.003(3)	-0.011(3)
C15	0.051(4)	0.087(7)	0.034(5)	0.012(4)	0.009(4)	0.036(4)
C16	0.101(8)	0.024(3)	0.055(6)	0.008(3)	-0.002(5)	0.005(4)
C17	0.048(4)	0.086(7)	0.058(6)	0.026(5)	-0.001(4)	-0.034(4)
C108	0.109(13)	0.058(8)	0.028(3)	0.008(4)	-0.002(5)	0.020(10)
C109	0.065(7)	0.054(8)	0.040(6)	0.009(7)	-0.014(5)	-0.003(6)
C110	0.054(9)	0.043(10)	0.064(19)	0.003(8)	-0.013(12)	0.011(7)
C111	0.061(9)	0.051(5)	0.058(10)	0.029(6)	-0.006(6)	-0.005(6)
C112	0.073(9)	0.070(9)	0.046(5)	0.047(8)	0.015(5)	0.027(9)
C113	0.27(4)	0.067(14)	0.027(9)	-0.001(10)	0.01(2)	0.030(17)
C114	0.071(8)	0.052(15)	0.10(2)	0.044(15)	-0.047(10)	-0.009(10)
C115	0.106(19)	0.025(11)	0.11(2)	0.029(11)	0.026(17)	0.029(12)
C116	0.108(19)	0.075(12)	0.067(17)	0.057(11)	-0.009(16)	-0.047(15)
C117	0.114(15)	0.25(5)	0.08(3)	0.04(3)	0.069(17)	0.04(2)

O18 0.044(2) 0.037(2) 0.070(3) -0.0060(19) -0.014(2) -0.0016(16)
 C19 0.061(4) 0.040(3) 0.091(6) -0.008(4) -0.033(4) -0.005(3)
 O20 0.0352(19) 0.044(2) 0.057(3) -0.0037(19) -0.0042(18) -0.0010(16)
 C21 0.042(3) 0.051(3) 0.064(4) -0.006(3) -0.003(3) 0.008(3)
 O22 0.057(3) 0.050(2) 0.038(2) 0.0100(18) -0.0108(18) -0.0062(19)
 C23 0.070(4) 0.061(4) 0.041(3) 0.003(3) -0.019(3) -0.002(3)
 B30 0.025(2) 0.019(2) 0.021(2) 0.0023(19) 0.0020(18) 0.0035(18)
 C31 0.0243(19) 0.018(2) 0.017(2) -0.0031(17) 0.0051(16) 0.0002(15)
 C32 0.023(2) 0.019(2) 0.018(2) 0.0003(17) 0.0071(17) 0.0007(16)
 C33 0.022(2) 0.023(2) 0.022(2) 0.0021(17) 0.0046(17) 0.0048(16)
 C34 0.020(2) 0.025(2) 0.023(2) 0.0000(17) 0.0044(18) -0.0009(16)
 C35 0.024(2) 0.0217(18) 0.020(2) 0.0002(16) 0.0055(18) 0.0005(15)
 C36 0.029(2) 0.021(2) 0.018(2) 0.0005(18) 0.0024(19) 0.0034(16)
 C37 0.022(2) 0.029(2) 0.028(3) 0.0056(18) 0.0001(18) 0.0025(17)
 F31 0.0299(15) 0.0444(17) 0.0498(19) 0.0296(15) 0.0027(14) 0.0024(12)
 F32 0.0408(17) 0.0390(17) 0.0460(19) 0.0119(14) -0.0173(14) -0.0066(13)
 F33 0.0449(18) 0.054(2) 0.0464(19) 0.0047(15) 0.0044(15) 0.0299(15)
 C38 0.031(2) 0.028(2) 0.0303(19) 0.0052(18) 0.0012(17) -0.0006(14)
 F34 0.045(2) 0.035(3) 0.058(3) 0.018(3) -0.014(3) -0.0190(19)
 F35 0.037(2) 0.0248(19) 0.099(5) 0.022(4) 0.007(3) 0.0019(16)
 F36 0.107(5) 0.041(3) 0.045(2) 0.004(2) 0.036(3) -0.022(3)
 C381 0.031(2) 0.028(2) 0.0303(19) 0.0052(18) 0.0012(17) -0.0006(14)
 F341 0.032(2) 0.035(11) 0.068(8) 0.027(9) 0.011(5) -0.005(3)
 F351 0.056(6) 0.019(4) 0.089(6) 0.003(11) 0.031(7) 0.000(8)
 F361 0.086(6) 0.068(10) 0.031(3) 0.023(3) -0.004(5) -0.057(8)
 C41 0.025(2) 0.015(2) 0.021(2) 0.0003(17) 0.0024(16) 0.0004(17)
 C42 0.024(2) 0.027(2) 0.022(2) -0.002(2) -0.0006(17) -0.0010(18)
 C43 0.032(2) 0.035(3) 0.021(2) 0.002(2) 0.0047(18) -0.0062(18)
 C44 0.036(2) 0.034(3) 0.018(2) 0.003(2) -0.0031(18) -0.004(2)

C45 0.030(2) 0.030(3) 0.025(2) 0.002(2) -0.0029(17) 0.0025(19)
 C46 0.026(2) 0.024(2) 0.025(2) 0.002(2) 0.0043(18) 0.0035(18)
 C47 0.036(2) 0.080(3) 0.0252(18) 0.004(2) 0.0042(19) -0.0111(17)
 F41 0.055(3) 0.092(3) 0.063(3) -0.010(3) 0.035(2) 0.008(2)
 F42 0.060(3) 0.085(3) 0.073(3) 0.003(3) 0.028(3) -0.034(2)
 F43 0.045(3) 0.219(8) 0.0242(18) 0.019(4) 0.0075(18) -0.028(4)
 C471 0.036(2) 0.080(3) 0.0252(18) 0.004(2) 0.0042(19) -0.0111(17)
 F411 0.032(3) 0.106(5) 0.031(7) -0.002(8) 0.010(4) -0.004(7)
 F421 0.047(13) 0.134(5) 0.093(12) 0.067(6) 0.025(7) -0.014(8)
 F431 0.072(14) 0.186(7) 0.038(10) -0.050(8) 0.043(5) -0.064(11)
 C48 0.034(2) 0.053(3) 0.031(3) 0.000(2) -0.001(2) 0.000(2)
 F44 0.047(2) 0.098(3) 0.072(3) 0.048(2) -0.0160(19) 0.008(2)
 F45 0.0379(18) 0.080(2) 0.058(2) -0.0249(19) -0.0139(17) -0.0046(17)
 F46 0.0297(17) 0.115(3) 0.0398(19) -0.0102(19) -0.0030(15) 0.0179(18)
 C51 0.017(2) 0.0207(19) 0.021(2) 0.0014(16) -0.0022(18) 0.0012(16)
 C52 0.029(2) 0.024(2) 0.021(2) 0.0027(17) 0.005(2) 0.0019(18)
 C53 0.029(2) 0.025(2) 0.031(2) -0.0027(18) 0.002(2) 0.0024(19)
 C54 0.042(3) 0.020(2) 0.033(2) 0.0048(18) 0.003(2) -0.003(2)
 C55 0.032(3) 0.027(2) 0.0261(19) 0.0058(16) 0.001(2) -0.0022(19)
 C56 0.026(2) 0.024(2) 0.021(2) 0.0009(17) 0.000(2) 0.0000(18)
 C57 0.062(3) 0.026(2) 0.040(3) -0.002(2) 0.016(3) 0.002(2)
 F51 0.068(3) 0.142(4) 0.121(4) -0.091(4) 0.034(2) 0.002(2)
 F52 0.173(4) 0.037(2) 0.065(3) -0.0229(18) 0.049(3) -0.034(2)
 F53 0.158(4) 0.046(2) 0.040(2) -0.0185(17) -0.008(2) 0.023(2)
 C58 0.050(2) 0.028(2) 0.031(2) 0.0081(16) 0.003(2) -0.0061(18)
 F54 0.085(3) 0.053(2) 0.046(2) 0.0287(18) 0.016(3) 0.023(2)
 F55 0.211(6) 0.050(2) 0.027(2) -0.003(2) 0.025(4) -0.048(3)
 F56 0.0474(19) 0.156(6) 0.056(3) 0.058(3) 0.018(2) 0.009(2)

C581 0.050(2) 0.028(2) 0.031(2) 0.0081(16) 0.003(2) -0.0061(18)
 F541 0.076(8) 0.048(5) 0.064(16) -0.004(9) 0.05(2) -0.041(6)
 F551 0.076(5) 0.132(15) 0.006(10) -0.024(19) 0.005(8) -0.048(5)
 F561 0.169(13) 0.091(12) 0.03(3) 0.041(17) 0.052(19) 0.077(12)
 C61 0.025(2) 0.022(2) 0.017(2) 0.0052(17) 0.0015(18) 0.0031(17)
 C62 0.028(2) 0.024(2) 0.023(2) 0.0068(19) 0.005(2) 0.0025(17)
 C63 0.0321(18) 0.037(3) 0.032(3) 0.012(2) 0.0141(19) 0.0079(16)
 C64 0.046(2) 0.036(3) 0.036(3) 0.008(2) 0.023(2) 0.0139(19)
 C65 0.051(3) 0.026(2) 0.028(3) 0.0020(19) 0.019(2) 0.0077(18)
 C66 0.033(2) 0.023(2) 0.023(2) 0.0012(18) 0.006(2) 0.0029(17)
 C67 0.035(2) 0.050(3) 0.046(2) 0.0126(17) 0.0158(19) 0.0112(16)
 F61 0.026(2) 0.084(3) 0.074(3) -0.018(2) 0.007(2) 0.001(2)
 F62 0.033(3) 0.106(5) 0.055(3) 0.024(3) 0.008(2) -0.020(3)
 F63 0.028(2) 0.049(3) 0.116(5) 0.020(2) 0.002(3) 0.0064(19)
 C671 0.035(2) 0.050(3) 0.046(2) 0.0126(17) 0.0158(19) 0.0112(16)
 F611 0.046(6) 0.087(4) 0.054(3) 0.017(4) -0.006(4) 0.003(6)
 F621 0.011(5) 0.105(5) 0.099(4) -0.049(5) 0.014(6) -0.007(6)
 F631 0.040(7) 0.058(4) 0.087(4) 0.026(4) 0.003(6) -0.012(4)
 C68 0.076(4) 0.034(3) 0.044(3) -0.010(2) 0.023(3) 0.004(2)
 F64 0.104(3) 0.045(2) 0.060(2) -0.0219(18) 0.027(2) -0.0237(19)
 F65 0.226(6) 0.064(3) 0.034(2) -0.0103(19) 0.005(3) -0.046(3)
 F66 0.108(3) 0.066(3) 0.179(5) -0.074(3) 0.037(3) 0.018(2)

_geom_special_details

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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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loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Co1 O4 1.974(3) . ?

Co1 C1 2.013(6) . ?

Co1 C11 2.037(8) . ?

Co1 C112 2.037(19) . ?

Co1 C108 2.06(2) . ?

Co1 C10 2.077(9) . ?

Co1 C109 2.08(3) . ?

Co1 C111 2.116(19) . ?

Co1 C9 2.117(8) . ?

Co1 C12 2.123(8) . ?

Co1 P1 2.1339(16) . ?

Co1 C8 2.135(7) . ?

P1 O18 1.552(4) . ?

P1 O22 1.588(4) . ?

P1 O20 1.608(4) . ?

C1 C2 1.511(8) . ?

C2 C3 1.488(8) . ?

C3 O4 1.232(6) . ?

C3 O7 1.310(6) . ?
C6 O7 1.447(7) . ?
C8 C12 1.428(10) . ?
C8 C9 1.439(10) . ?
C8 C13 1.483(10) . ?
C9 C10 1.374(12) . ?
C9 C14 1.508(10) . ?
C10 C11 1.426(12) . ?
C10 C15 1.535(10) . ?
C11 C12 1.436(10) . ?
C11 C16 1.496(10) . ?
C12 C17 1.512(10) . ?
C108 C112 1.429(10) . ?
C108 C109 1.439(10) . ?
C108 C113 1.483(10) . ?
C109 C110 1.374(12) . ?
C109 C114 1.508(10) . ?
C110 C111 1.426(12) . ?
C110 C115 1.534(10) . ?
C111 C112 1.436(10) . ?
C111 C116 1.496(10) . ?
C112 C117 1.512(10) . ?
O18 C19 1.464(7) . ?
O20 C21 1.440(7) . ?
O22 C23 1.446(7) . ?
B30 C31 1.631(7) . ?
B30 C51 1.635(6) . ?
B30 C61 1.646(7) . ?
B30 C41 1.664(7) . ?

C31 C32 1.396(6) . ?
C31 C36 1.400(6) . ?
C32 C33 1.396(6) . ?
C33 C34 1.383(6) . ?
C33 C37 1.487(6) . ?
C34 C35 1.383(6) . ?
C35 C36 1.389(6) . ?
C35 C38 1.489(6) . ?
C37 F31 1.330(5) . ?
C37 F33 1.333(5) . ?
C37 F32 1.355(6) . ?
C38 F341 1.19(2) . ?
C38 F35 1.309(8) . ?
C38 F351 1.34(2) . ?
C38 F36 1.348(7) . ?
C38 F361 1.353(18) . ?
C38 F34 1.364(7) . ?
C41 C42 1.396(7) . ?
C41 C46 1.402(6) . ?
C42 C43 1.385(7) . ?
C43 C44 1.381(7) . ?
C43 C47 1.475(7) . ?
C44 C45 1.389(7) . ?
C45 C46 1.384(7) . ?
C45 C48 1.500(7) . ?
C47 F411 1.23(2) . ?
C47 F43 1.300(7) . ?
C47 F421 1.33(2) . ?

C47 F41 1.348(8) . ?

C47 F42 1.351(8) . ?

C47 F431 1.49(3) . ?

C48 F45 1.323(6) . ?

C48 F46 1.328(6) . ?

C48 F44 1.328(7) . ?

C51 C52 1.398(6) . ?

C51 C56 1.402(6) . ?

C52 C53 1.397(6) . ?

C53 C54 1.383(7) . ?

C53 C57 1.493(7) . ?

C54 C55 1.387(7) . ?

C55 C56 1.398(7) . ?

C55 C58 1.486(7) . ?

C57 F51 1.288(7) . ?

C57 F52 1.309(7) . ?

C57 F53 1.328(7) . ?

C58 F551 1.20(5) . ?

C58 F541 1.23(4) . ?

C58 F561 1.26(5) . ?

C58 F56 1.318(7) . ?

C58 F55 1.329(7) . ?

C58 F54 1.336(6) . ?

C61 C66 1.403(7) . ?

C61 C62 1.410(6) . ?

C62 C63 1.377(7) . ?

C63 C64 1.380(8) . ?

C63 C67 1.504(8) . ?

C64 C65 1.389(8) . ?

C65 C66 1.392(7) . ?
C65 C68 1.482(8) . ?
C67 F611 1.113(15) . ?
C67 F631 1.194(16) . ?
C67 F62 1.319(8) . ?
C67 F63 1.343(7) . ?
C67 F61 1.402(8) . ?
C67 F621 1.489(14) . ?
C68 F65 1.296(8) . ?
C68 F64 1.319(7) . ?
C68 F66 1.334(7) . ?

loop_

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_geom_angle_atom_site_label_3
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O4 Co1 C1 84.9(2) . . ?
O4 Co1 C11 158.5(2) . . ?
C1 Co1 C11 107.5(3) . . ?
O4 Co1 C112 116.7(5) . . ?
C1 Co1 C112 153.8(5) . . ?
C11 Co1 C112 47.4(5) . . ?
O4 Co1 C108 94.7(5) . . ?
C1 Co1 C108 128.7(6) . . ?

C11 Co1 C108 63.9(6) . . ?

C112 Co1 C108 40.8(5) . . ?

O4 Co1 C10 124.0(3) . . ?

C1 Co1 C10 91.6(3) . . ?

C11 Co1 C10 40.6(3) . . ?

C112 Co1 C10 64.4(5) . . ?

C108 Co1 C10 47.3(6) . . ?

O4 Co1 C109 109.6(5) . . ?

C1 Co1 C109 91.4(6) . . ?

C11 Co1 C109 54.0(5) . . ?

C112 Co1 C109 68.2(7) . . ?

C108 Co1 C109 40.7(5) . . ?

C10 Co1 C109 14.5(5) . . ?

O4 Co1 C111 157.1(5) . . ?

C1 Co1 C111 117.0(5) . . ?

C11 Co1 C111 13.9(4) . . ?

C112 Co1 C111 40.4(4) . . ?

C108 Co1 C111 67.0(6) . . ?

C10 Co1 C111 53.3(5) . . ?

C109 Co1 C111 65.9(6) . . ?

O4 Co1 C9 92.6(2) . . ?

C1 Co1 C9 112.1(3) . . ?

C11 Co1 C9 66.6(3) . . ?

C112 Co1 C9 55.7(5) . . ?

C108 Co1 C9 16.6(5) . . ?

C10 Co1 C9 38.2(3) . . ?

C109 Co1 C9 27.6(4) . . ?

C111 Co1 C9 73.6(5) . . ?

O4 Co1 C12 127.2(3) . . ?

C1 Co1 C12 147.3(3) . . ?
C11 Co1 C12 40.3(3) . . ?
C112 Co1 C12 13.0(5) . . ?
C108 Co1 C12 52.4(6) . . ?
C10 Co1 C12 66.6(3) . . ?
C109 Co1 C12 73.5(7) . . ?
C111 Co1 C12 30.4(5) . . ?
C9 Co1 C12 66.0(3) . . ?
O4 Co1 P1 94.49(11) . . ?
C1 Co1 P1 88.76(19) . . ?
C11 Co1 P1 103.1(2) . . ?
C112 Co1 P1 103.2(5) . . ?
C108 Co1 P1 142.1(5) . . ?
C10 Co1 P1 141.4(3) . . ?
C109 Co1 P1 155.9(5) . . ?
C111 Co1 P1 92.7(5) . . ?
C9 Co1 P1 158.5(2) . . ?
C12 Co1 P1 93.8(2) . . ?
O4 Co1 C8 93.6(2) . . ?
C1 Co1 C8 151.6(3) . . ?
C11 Co1 C8 67.1(3) . . ?
C112 Co1 C8 26.2(5) . . ?
C108 Co1 C8 23.0(5) . . ?
C10 Co1 C8 65.8(3) . . ?
C109 Co1 C8 62.4(6) . . ?
C111 Co1 C8 64.1(5) . . ?
C9 Co1 C8 39.6(3) . . ?
C12 Co1 C8 39.2(3) . . ?

P1 C₀₁ C₈ 119.6(2) . . ?
O₁₈ P₁ O₂₂ 107.4(2) . . ?
O₁₈ P₁ O₂₀ 100.1(2) . . ?
O₂₂ P₁ O₂₀ 103.1(2) . . ?
O₁₈ P₁ C₀₁ 114.36(16) . . ?
O₂₂ P₁ C₀₁ 111.71(16) . . ?
O₂₀ P₁ C₀₁ 118.79(17) . . ?
C₂ C₁ C₀₁ 108.4(4) . . ?
C₃ C₂ C₁ 110.5(5) . . ?
O₄ C₃ O₇ 121.6(5) . . ?
O₄ C₃ C₂ 121.6(5) . . ?
O₇ C₃ C₂ 116.7(5) . . ?
C₃ O₄ C₀₁ 114.2(3) . . ?
C₃ O₇ C₆ 116.8(4) . . ?
C₁₂ C₈ C₉ 107.2(7) . . ?
C₁₂ C₈ C₁₃ 126.7(7) . . ?
C₉ C₈ C₁₃ 126.1(7) . . ?
C₁₂ C₈ C₀₁ 69.9(4) . . ?
C₉ C₈ C₀₁ 69.5(4) . . ?
C₁₃ C₈ C₀₁ 127.1(5) . . ?
C₁₀ C₉ C₈ 108.8(7) . . ?
C₁₀ C₉ C₁₄ 126.5(8) . . ?
C₈ C₉ C₁₄ 124.6(8) . . ?
C₁₀ C₉ C₀₁ 69.3(5) . . ?
C₈ C₉ C₀₁ 70.9(4) . . ?
C₁₄ C₉ C₀₁ 126.8(6) . . ?
C₉ C₁₀ C₁₁ 109.1(7) . . ?
C₉ C₁₀ C₁₅ 125.3(8) . . ?
C₁₁ C₁₀ C₁₅ 125.3(8) . . ?

C9 C10 Co1 72.5(5) . . ?
C11 C10 Co1 68.2(4) . . ?
C15 C10 Co1 130.2(6) . . ?
C10 C11 C12 107.4(6) . . ?
C10 C11 C16 125.9(8) . . ?
C12 C11 C16 126.1(9) . . ?
C10 C11 Co1 71.2(5) . . ?
C12 C11 Co1 73.1(4) . . ?
C16 C11 Co1 127.5(6) . . ?
C8 C12 C11 107.2(6) . . ?
C8 C12 C17 124.9(8) . . ?
C11 C12 C17 127.5(8) . . ?
C8 C12 Co1 70.9(4) . . ?
C11 C12 Co1 66.6(4) . . ?
C17 C12 Co1 132.5(6) . . ?
C112 C108 C109 107.2(7) . . ?
C112 C108 C113 126.6(7) . . ?
C109 C108 C113 126.0(8) . . ?
C112 C108 Co1 68.6(10) . . ?
C109 C108 Co1 70.2(12) . . ?
C113 C108 Co1 122.1(16) . . ?
C110 C109 C108 108.8(7) . . ?
C110 C109 C114 126.6(8) . . ?
C108 C109 C114 124.6(8) . . ?
C110 C109 Co1 73.8(13) . . ?
C108 C109 Co1 69.1(12) . . ?
C114 C109 Co1 124.4(19) . . ?
C109 C110 C111 109.1(7) . . ?

C109 C110 C115 125.5(8) . . ?
C111 C110 C115 125.4(9) . . ?
C109 C110 Co1 68.3(14) . . ?
C111 C110 Co1 69.2(10) . . ?
C115 C110 Co1 128.4(18) . . ?
C110 C111 C112 107.5(7) . . ?
C110 C111 C116 126.1(9) . . ?
C112 C111 C116 126.2(9) . . ?
C110 C111 Co1 71.7(10) . . ?
C112 C111 Co1 66.9(8) . . ?
C116 C111 Co1 130.8(14) . . ?
C108 C112 C111 107.2(6) . . ?
C108 C112 C117 124.9(8) . . ?
C111 C112 C117 127.5(9) . . ?
C108 C112 Co1 70.6(10) . . ?
C111 C112 Co1 72.8(9) . . ?
C117 C112 Co1 127.7(15) . . ?
C19 O18 P1 127.8(4) . . ?
C21 O20 P1 118.0(4) . . ?
C23 O22 P1 121.8(4) . . ?
C31 B30 C51 110.7(4) . . ?
C31 B30 C61 109.5(4) . . ?
C51 B30 C61 109.4(4) . . ?
C31 B30 C41 109.3(4) . . ?
C51 B30 C41 108.6(4) . . ?
C61 B30 C41 109.3(3) . . ?
C32 C31 C36 115.6(4) . . ?
C32 C31 B30 123.8(4) . . ?
C36 C31 B30 120.5(4) . . ?

C33 C32 C31 122.0(4) . . ?
C34 C33 C32 120.6(4) . . ?
C34 C33 C37 119.5(4) . . ?
C32 C33 C37 119.8(4) . . ?
C33 C34 C35 118.8(4) . . ?
C34 C35 C36 120.0(4) . . ?
C34 C35 C38 121.0(4) . . ?
C36 C35 C38 119.0(4) . . ?
C35 C36 C31 122.9(4) . . ?
F31 C37 F33 106.4(4) . . ?
F31 C37 F32 105.2(4) . . ?
F33 C37 F32 105.1(4) . . ?
F31 C37 C33 113.4(4) . . ?
F33 C37 C33 113.2(4) . . ?
F32 C37 C33 112.9(4) . . ?
F341 C38 F351 113.7(18) . . ?
F35 C38 F36 106.2(5) . . ?
F341 C38 F361 111.2(14) . . ?
F351 C38 F361 100.5(16) . . ?
F35 C38 F34 105.2(6) . . ?
F36 C38 F34 102.3(5) . . ?
F35 C38 C35 115.2(5) . . ?
F36 C38 C35 112.9(4) . . ?
F34 C38 C35 113.8(5) . . ?
F351 F35 F361 134(3) . . ?
F361 F36 F341 115.2(15) . . ?
C42 C41 C46 114.2(4) . . ?
C42 C41 B30 122.7(4) . . ?

C46 C41 B30 123.0(4) . . ?
C43 C42 C41 123.5(4) . . ?
C44 C43 C42 120.7(4) . . ?
C44 C43 C47 119.5(5) . . ?
C42 C43 C47 119.8(5) . . ?
C43 C44 C45 117.6(4) . . ?
C46 C45 C44 120.9(4) . . ?
C46 C45 C48 121.0(5) . . ?
C44 C45 C48 118.0(4) . . ?
C45 C46 C41 123.0(4) . . ?
F411 C47 F421 106.3(18) . . ?
F43 C47 F41 108.0(7) . . ?
F43 C47 F42 108.0(6) . . ?
F41 C47 F42 101.7(5) . . ?
F43 C47 C43 114.8(5) . . ?
F41 C47 C43 111.9(5) . . ?
F42 C47 C43 111.6(5) . . ?
F411 C47 F431 101.9(18) . . ?
F421 C47 F431 101(2) . . ?
F45 C48 F46 105.6(5) . . ?
F45 C48 F44 106.3(5) . . ?
F46 C48 F44 106.0(5) . . ?
F45 C48 C45 112.3(5) . . ?
F46 C48 C45 113.4(4) . . ?
F44 C48 C45 112.6(5) . . ?
C52 C51 C56 116.0(4) . . ?
C52 C51 B30 122.8(4) . . ?
C56 C51 B30 121.2(4) . . ?
C53 C52 C51 122.1(4) . . ?

C54 C53 C52 120.7(4) . . ?
C54 C53 C57 120.0(4) . . ?
C52 C53 C57 119.3(5) . . ?
C53 C54 C55 118.7(4) . . ?
C54 C55 C56 120.2(4) . . ?
C54 C55 C58 119.2(4) . . ?
C56 C55 C58 120.5(4) . . ?
C55 C56 C51 122.4(4) . . ?
F51 C57 F52 107.1(5) . . ?
F51 C57 F53 106.3(5) . . ?
F52 C57 F53 104.0(5) . . ?
F51 C57 C53 112.8(5) . . ?
F52 C57 C53 113.2(5) . . ?
F53 C57 C53 112.9(4) . . ?
F551 C58 F541 104(4) . . ?
F551 C58 F561 104(5) . . ?
F541 C58 F561 108(5) . . ?
F56 C58 F55 107.9(6) . . ?
F56 C58 F54 103.9(5) . . ?
F55 C58 F54 104.8(5) . . ?
F56 C58 C55 113.2(5) . . ?
F55 C58 C55 113.7(4) . . ?
F54 C58 C55 112.6(5) . . ?
C66 C61 C62 114.7(4) . . ?
C66 C61 B30 124.6(4) . . ?
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C62 C63 C64 120.9(5) . . ?

C62 C63 C67 119.6(5) . . ?
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C64 C65 C68 119.6(5) . . ?
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C65 C66 C61 122.6(5) . . ?
F611 C67 F631 126.5(15) . . ?
F62 C67 F63 107.7(5) . . ?
F62 C67 F61 102.9(6) . . ?
F63 C67 F61 99.4(5) . . ?
F611 C67 F621 109.9(12) . . ?
F631 C67 F621 99.9(13) . . ?
F611 C67 C63 109.5(9) . . ?
F631 C67 C63 106.6(9) . . ?
F62 C67 C63 116.3(5) . . ?
F63 C67 C63 114.4(5) . . ?
F61 C67 C63 114.3(4) . . ?
F621 C67 C63 101.4(6) . . ?
F65 C68 F64 105.9(6) . . ?
F65 C68 F66 107.1(6) . . ?
F64 C68 F66 103.6(5) . . ?
F65 C68 C65 113.1(5) . . ?
F64 C68 C65 114.0(5) . . ?
F66 C68 C65 112.4(6) . . ?

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O22 P1 O20 C21 67.4(5) ?
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C61 B30 C31 C36 -71.9(5) ?
C41 B30 C31 C36 47.8(5) ?
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C31 C32 C33 C37 -179.9(4) ?

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