Supramolecular bulky phosphines comprising 1,3,5-triaza-7-phosphaadamantane and Zn(salphen)s: structural features and application in hydrosilylation catalysis

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DOI
10.1039/c3dt00078h

Publication date
2013

Document Version
Final published version

Published in
Dalton Transactions

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C54A C 0.4973(3) 0.5897(3) 0.70733(15) 0.0285(11) Uani 1 1 d . . .
H54A H 0.5101 0.6353 0.6965 0.034 Uiso 1 1 calc R . .
C55A C 0.5323(3) 0.5569(3) 0.74451(14) 0.0257(11) Uani 1 1 d . . .
C56A C 0.5100(3) 0.4884(3) 0.76317(14) 0.0250(10) Uani 1 1 d . . .
C57A C 0.7361(3) 0.4132(3) 0.91970(16) 0.0323(12) Uani 1 1 d . . .
C58A C 0.8112(4) 0.4208(3) 0.94500(19) 0.0441(14) Uani 1 1 d . . .
H58A H 0.8087 0.4738 0.9460 0.066 Uiso 1 1 calc R . .
H58B H 0.8689 0.3946 0.9315 0.066 Uiso 1 1 calc R . .
H58C H 0.8032 0.3986 0.9734 0.066 Uiso 1 1 calc R . .
C59A C 0.7484(4) 0.4539(3) 0.87561(18) 0.0465(15) Uani 1 1 d . . .
H59A H 0.7010 0.4515 0.8592 0.070 Uiso 1 1 calc R . .
H59B H 0.8059 0.4292 0.8614 0.070 Uiso 1 1 calc R . .
H59C H 0.7460 0.5063 0.8787 0.070 Uiso 1 1 calc R . .
C60A C 0.6461(4) 0.4546(3) 0.94353(19) 0.0491(16) Uani 1 1 d . . .
H60A H 0.5968 0.4499 0.9291 0.074 Uiso 1 1 calc R . .
H60B H 0.6438 0.5076 0.9443 0.074 Uiso 1 1 calc R . .
H60C H 0.6415 0.4321 0.9720 0.074 Uiso 1 1 calc R . .
C61A C 0.8826(3) 0.1300(3) 0.95011(15) 0.0290(11) Uani 1 1 d . . .
C62A C 0.9757(3) 0.1376(3) 0.92942(17) 0.0331(12) Uani 1 1 d . . .
H62A H 0.9813 0.1292 0.8997 0.050 Uiso 1 1 calc R . .
H62B H 1.0226 0.1004 0.9429 0.050 Uiso 1 1 calc R . .
H62C H 0.9812 0.1879 0.9327 0.050 Uiso 1 1 calc R . .
C63A C 0.8748(3) 0.0499(3) 0.94378(17) 0.0342(12) Uani 1 1 d . . .
H63A H 0.8178 0.0438 0.9572 0.051 Uiso 1 1 calc R . .
H63B H 0.9231 0.0124 0.9562 0.051 Uiso 1 1 calc R . .
H63C H 0.8788 0.0432 0.9139 0.051 Uiso 1 1 calc R . .
C64A C 0.8773(4) 0.1395(3) 0.99810(16) 0.0401(14) Uani 1 1 d . . .
H64A H 0.8818 0.1897 1.0024 0.060 Uiso 1 1 calc R . .
H64B H 0.9260 0.1020 1.0101 0.060 Uiso 1 1 calc R . .
H64C H 0.8206 0.1328 1.0117 0.060 Uiso 1 1 calc R . .
C65A C 0.4105(4) 0.6014(3) 0.64288(15) 0.0338(12) Uani 1 1 d . . .
C66A C 0.3514(4) 0.5615(3) 0.62347(16) 0.0403(13) Uani 1 1 d . . .
H66A H 0.3844 0.5097 0.6190 0.060 Uiso 1 1 calc R . .
H66B H 0.3346 0.5877 0.5968 0.060 Uiso 1 1 calc R . .
H66C H 0.2979 0.5620 0.6425 0.060 Uiso 1 1 calc R . .
C67A C 0.4916(4) 0.6056(3) 0.61118(16) 0.0444(15) Uani 1 1 d . . .
H67A H 0.5314 0.6273 0.6240 0.067 Uiso 1 1 calc R . .
H67B H 0.4713 0.6370 0.5864 0.067 Uiso 1 1 calc R . .
H67C H 0.5234 0.5551 0.6032 0.067 Uiso 1 1 calc R . .
C68A C 0.3534(4) 0.6836(3) 0.65111(17) 0.0420(14) Uani 1 1 d . . .
H68A H 0.3892 0.7104 0.6631 0.063 Uiso 1 1 calc R . .

H68B H 0.3013 0.6815 0.6706 0.063 Uiso 1 1 calc R . .
H68C H 0.3342 0.7098 0.6248 0.063 Uiso 1 1 calc R . .
C69A C 0.5970(3) 0.5892(3) 0.76621(16) 0.0326(12) Uani 1 1 d . . .
C70A C 0.6156(4) 0.6607(3) 0.74159(18) 0.0402(13) Uani 1 1 d . . .
H70A H 0.6428 0.6483 0.7135 0.060 Uiso 1 1 calc R . .
H70B H 0.6558 0.6791 0.7561 0.060 Uiso 1 1 calc R . .
H70C H 0.5597 0.6995 0.7398 0.060 Uiso 1 1 calc R . .
C71A C 0.6884(4) 0.5271(3) 0.76699(19) 0.0424(14) Uani 1 1 d . . .
H71A H 0.6784 0.4812 0.7819 0.064 Uiso 1 1 calc R . .
H71B H 0.7296 0.5450 0.7811 0.064 Uiso 1 1 calc R . .
H71C H 0.7137 0.5166 0.7384 0.064 Uiso 1 1 calc R . .
C72A C 0.5569(2) 0.60484(18) 0.81236(6) 0.0504(16) Uani 1 1 d . . .
H72A H 0.4999 0.6426 0.8122 0.076 Uiso 1 1 calc R . .
H72B H 0.5978 0.6231 0.8265 0.076 Uiso 1 1 calc R . .
H72C H 0.5481 0.5585 0.8271 0.076 Uiso 1 1 calc R . .
P1A P 0.29364(8) 0.51447(8) 0.92938(4) 0.0576(5) Uani 1 1 d RD . .
N5A N 0.40719(9) 0.39813(8) 0.87793(4) 0.0242(9) Uani 1 1 d RD . .
N6A N 0.34120(9) 0.35645(8) 0.94777(4) 0.0245(9) Uani 1 1 d RD . .
N7A N 0.23757(8) 0.40953(8) 0.88801(4) 0.0556(15) Uani 1 1 d RD . .
C73A C 0.41993(9) 0.34325(10) 0.91595(4) 0.0277(11) Uani 1 1 d RD . .
H73A H 0.4324 0.2918 0.9069 0.033 Uiso 1 1 calc R . .
H73B H 0.4721 0.3471 0.9289 0.033 Uiso 1 1 calc R . .
C74A C 0.26192(8) 0.35085(7) 0.92752(4) 0.0392(14) Uani 1 1 d RD . .
H74A H 0.2099 0.3588 0.9486 0.047 Uiso 1 1 calc R . .
H74B H 0.2734 0.2995 0.9184 0.047 Uiso 1 1 calc R . .
C75A C 0.32544(8) 0.39643(7) 0.85815(4) 0.0431(15) Uani 1 1 d RD . .
H75A H 0.3364 0.3473 0.8463 0.052 Uiso 1 1 calc R . .
H75B H 0.3169 0.4352 0.8347 0.052 Uiso 1 1 calc R . .
C76A C 0.39650(8) 0.47510(7) 0.89009(4) 0.0440(14) Uani 1 1 d RD . .
H76A H 0.3926 0.5091 0.8645 0.053 Uiso 1 1 calc R . .
H76B H 0.4505 0.4762 0.9025 0.053 Uiso 1 1 calc R . .
C77A C 0.32627(9) 0.42972(8) 0.96730(4) 0.0478(15) Uani 1 1 d RD . .
H77A H 0.3812 0.4307 0.9789 0.057 Uiso 1 1 calc R . .
H77B H 0.2790 0.4329 0.9907 0.057 Uiso 1 1 calc R . .
C78A C 0.21639(8) 0.47304(9) 0.89869(4) 0.0371(14) Uani 1 1 d RD . .
H78A H 0.1592 0.4792 0.9162 0.045 Uiso 1 1 calc R . .
H78z H 0.2042 0.5063 0.8731 0.045 Uiso 1 1 calc R . .
C1B C 1.0739(3) 0.6472(3) 0.38885(15) 0.0268(11) Uani 1 1 d . . .
C2B C 1.1109(3) 0.5899(3) 0.42138(16) 0.0366(13) Uani 1 1 d . C .
C3B C 1.1311(5) 0.5145(3) 0.41236(18) 0.0548(18) Uani 1 1 d . . .
H3B H 1.1556 0.4781 0.4333 0.066 Uiso 1 1 calc R E .
C4B C 1.1180(5) 0.4882(3) 0.37452(18) 0.061(2) Uani 1 1 d D D .
C5B C 1.0818(4) 0.5423(3) 0.34412(17) 0.0436(15) Uani 1 1 d . . .
H5B H 1.0726 0.5267 0.3184 0.052 Uiso 1 1 calc R E .
C6B C 1.0577(3) 0.6213(3) 0.35061(16) 0.0320(12) Uani 1 1 d . . .
C7B C 1.0163(3) 0.6706(3) 0.31622(15) 0.0287(11) Uani 1 1 d . . .
H7B H 1.0083 0.6474 0.2926 0.034 Uiso 1 1 calc R E .
C8B C 0.9461(3) 0.7870(3) 0.28077(15) 0.0264(11) Uani 1 1 d . . .
C9B C 0.8921(3) 0.7623(3) 0.25653(15) 0.0300(11) Uani 1 1 d . . .
H9B H 0.8844 0.7133 0.2620 0.036 Uiso 1 1 calc R . .
C10B C 0.8497(3) 0.8094(3) 0.22451(17) 0.0353(13) Uani 1 1 d . . .
H10B H 0.8144 0.7921 0.2080 0.042 Uiso 1 1 calc R E .
C11B C 0.8600(3) 0.8830(3) 0.21694(16) 0.0341(12) Uani 1 1 d . . .
H11B H 0.8313 0.9150 0.1953 0.041 Uiso 1 1 calc R . .

C12B C 0.9128(3) 0.9095(3) 0.24133(15) 0.0294(11) Uani 1 1 d . . .
H12B H 0.9182 0.9593 0.2365 0.035 Uiso 1 1 calc R E .
C13B C 0.9570(3) 0.8614(3) 0.27274(14) 0.0233(10) Uani 1 1 d . E .
C14B C 1.0556(3) 0.9328(3) 0.28721(14) 0.0219(10) Uani 1 1 d . . .
H14B H 1.0460 0.9574 0.2605 0.026 Uiso 1 1 calc R E .
C15B C 1.1169(3) 0.9554(3) 0.31080(14) 0.0224(10) Uani 1 1 d . . .
C16B C 1.1585(3) 1.0106(3) 0.28896(14) 0.0252(11) Uani 1 1 d . . .
H16B H 1.1419 1.0309 0.2622 0.030 Uiso 1 1 calc R E .
C17B C 1.2224(3) 1.0349(3) 0.30603(15) 0.0258(11) Uani 1 1 d . . .
C18B C 1.2463(3) 1.0013(3) 0.34625(15) 0.0279(11) Uani 1 1 d . . .
H18B H 1.2903 1.0168 0.3580 0.034 Uiso 1 1 calc R E .
C19B C 1.2097(3) 0.9476(3) 0.36936(14) 0.0237(10) Uani 1 1 d . . .
C20B C 1.1413(3) 0.9221(3) 0.35179(14) 0.0247(10) Uani 1 1 d . . .
C21B C 1.1284(4) 0.6130(3) 0.46357(17) 0.0375(13) Uani 1 1 d . . .
C22B C 1.0381(8) 0.6520(9) 0.4894(5) 0.035(3) Uani 0.75 1 d PDU C 1
H22D H 1.0510 0.6710 0.5145 0.053 Uiso 0.75 1 calc PR C 1
H22E H 1.0035 0.6154 0.4975 0.053 Uiso 0.75 1 calc PR C 1
H22F H 1.0041 0.6936 0.4723 0.053 Uiso 0.75 1 calc PR C 1
C23B C 1.1873(6) 0.6712(6) 0.4582(3) 0.049(2) Uani 0.75 1 d PDU C 1
H23D H 1.2428 0.6506 0.4411 0.073 Uiso 0.75 1 calc PR C 1
H23E H 1.2004 0.6808 0.4856 0.073 Uiso 0.75 1 calc PR C 1
H23F H 1.1549 0.7182 0.4444 0.073 Uiso 0.75 1 calc PR C 1
C24B C 1.1753(14) 0.5474(7) 0.4935(7) 0.072(5) Uani 0.75 1 d PDU C 1
H24D H 1.2324 0.5208 0.4796 0.109 Uiso 0.75 1 calc PR C 1
H24E H 1.1379 0.5127 0.5008 0.109 Uiso 0.75 1 calc PR C 1
H24F H 1.1852 0.5674 0.5188 0.109 Uiso 0.75 1 calc PR C 1
C22" C 1.2126(16) 0.6364(17) 0.4483(9) 0.046(5) Uani 0.25 1 d PDU C 2
H22G H 1.1995 0.6785 0.4274 0.070 Uiso 0.25 1 calc PR C 2
H22H H 1.2568 0.5943 0.4359 0.070 Uiso 0.25 1 calc PR C 2
H22I H 1.2358 0.6516 0.4719 0.070 Uiso 0.25 1 calc PR C 2
C23" C 1.156(4) 0.533(2) 0.491(2) 0.069(9) Uani 0.25 1 d PDU C 2
H23G H 1.1661 0.5417 0.5187 0.103 Uiso 0.25 1 calc PR C 2
H23H H 1.2106 0.5014 0.4771 0.103 Uiso 0.25 1 calc PR C 2
H23I H 1.1084 0.5080 0.4922 0.103 Uiso 0.25 1 calc PR C 2
C24" C 1.057(2) 0.663(3) 0.4810(16) 0.038(6) Uani 0.25 1 d PDU C 2
H24G H 1.0671 0.6714 0.5091 0.057 Uiso 0.25 1 calc PR C 2
H24H H 1.0045 0.6435 0.4824 0.057 Uiso 0.25 1 calc PR C 2
H24I H 1.0466 0.7104 0.4639 0.057 Uiso 0.25 1 calc PR C 2
C25B C 1.1604(7) 0.4031(4) 0.3688(2) 0.0438(17) Uani 0.70 1 d PDU D 1
C26B C 1.1400(6) 0.3821(5) 0.3273(2) 0.0440(19) Uani 0.70 1 d PDU D 1
H26L H 1.1642 0.3282 0.3248 0.066 Uiso 0.70 1 calc PR D 1
H26M H 1.1670 0.4094 0.3043 0.066 Uiso 0.70 1 calc PR D 1
H26N H 1.0757 0.3953 0.3262 0.066 Uiso 0.70 1 calc PR D 1
C27B C 1.2632(6) 0.3800(5) 0.3690(3) 0.0506(17) Uani 0.70 1 d PDU D 1
H27D H 1.2787 0.3892 0.3960 0.076 Uiso 0.70 1 calc PR D 1
H27E H 1.2894 0.4095 0.3469 0.076 Uiso 0.70 1 calc PR D 1
H27F H 1.2861 0.3267 0.3642 0.076 Uiso 0.70 1 calc PR D 1
C28B C 1.1218(7) 0.3579(4) 0.4057(3) 0.0532(17) Uani 0.70 1 d PDU D 1
H28D H 1.0574 0.3781 0.4099 0.080 Uiso 0.70 1 calc PR D 1
H28E H 1.1480 0.3618 0.4311 0.080 Uiso 0.70 1 calc PR D 1
H28F H 1.1357 0.3053 0.3994 0.080 Uiso 0.70 1 calc PR D 1
C25" C 1.1012(11) 0.4071(6) 0.3685(5) 0.050(2) Uani 0.30 1 d PDU D 2
C26" C 1.0978(14) 0.3897(14) 0.3234(4) 0.053(4) Uani 0.30 1 d PDU D 2
H26G H 1.1356 0.4151 0.3045 0.080 Uiso 0.30 1 calc PR D 2

H26H H 1.0367 0.4073 0.3161 0.080 Uiso 0.30 1 calc PR D 2
H26I H 1.1191 0.3356 0.3208 0.080 Uiso 0.30 1 calc PR D 2
C27" C 1.1931(11) 0.3595(11) 0.3814(5) 0.0506(17) Uani 0.30 1 d PDU D 2
H27G H 1.2329 0.3920 0.3811 0.076 Uiso 0.30 1 calc PR D 2
H27H H 1.2186 0.3207 0.3618 0.076 Uiso 0.30 1 calc PR D 2
H27I H 1.1854 0.3360 0.4095 0.076 Uiso 0.30 1 calc PR D 2
C28" C 1.0294(12) 0.3778(10) 0.3973(6) 0.0532(17) Uani 0.30 1 d PDU D 2
H28G H 1.0424 0.3233 0.3964 0.080 Uiso 0.30 1 calc PR D 2
H28H H 0.9710 0.4011 0.3877 0.080 Uiso 0.30 1 calc PR D 2
H28I H 1.0297 0.3904 0.4260 0.080 Uiso 0.30 1 calc PR D 2
C29B C 1.2685(3) 1.0945(3) 0.28297(16) 0.0343(12) Uani 1 1 d . . .
C30B C 1.3690(4) 1.0563(4) 0.2719(2) 0.0611(19) Uani 1 1 d . . .
H30D H 1.3977 1.0396 0.2976 0.092 Uiso 1 1 calc R . .
H30E H 1.3972 1.0922 0.2555 0.092 Uiso 1 1 calc R . .
H30F H 1.3751 1.0130 0.2557 0.092 Uiso 1 1 calc R . .
C31B C 1.2601(4) 1.1593(3) 0.31162(19) 0.0449(14) Uani 1 1 d . . .
H31D H 1.1975 1.1851 0.3178 0.067 Uiso 1 1 calc R . .
H31E H 1.2918 1.1947 0.2974 0.067 Uiso 1 1 calc R . .
H31F H 1.2859 1.1386 0.3377 0.067 Uiso 1 1 calc R . .
C32B C 1.2261(4) 1.1286(4) 0.24247(19) 0.0549(17) Uani 1 1 d . . .
H32D H 1.2325 1.0889 0.2237 0.082 Uiso 1 1 calc R . .
H32E H 1.2560 1.1658 0.2289 0.082 Uiso 1 1 calc R . .
H32F H 1.1631 1.1527 0.2492 0.082 Uiso 1 1 calc R . .
C33B C 1.2422(3) 0.9120(3) 0.41245(16) 0.0325(12) Uani 1 1 d . . .
C34B C 1.1627(4) 0.9238(3) 0.44764(16) 0.0397(13) Uani 1 1 d . . .
H34L H 1.1346 0.9775 0.4493 0.059 Uiso 1 1 calc R . .
H34M H 1.1846 0.9028 0.4744 0.059 Uiso 1 1 calc R . .
H34N H 1.1192 0.8987 0.4411 0.059 Uiso 1 1 calc R . .
C35B C 1.2859(4) 0.8264(3) 0.40910(19) 0.0457(15) Uani 1 1 d . . .
H35L H 1.3091 0.8046 0.4355 0.069 Uiso 1 1 calc R . .
H35M H 1.3344 0.8191 0.3867 0.069 Uiso 1 1 calc R . .
H35N H 1.2414 0.8019 0.4030 0.069 Uiso 1 1 calc R . .
C36B C 1.3122(4) 0.9476(3) 0.42686(18) 0.0447(14) Uani 1 1 d . . .
H36L H 1.2854 1.0008 0.4307 0.067 Uiso 1 1 calc R . .
H36M H 1.3630 0.9421 0.4056 0.067 Uiso 1 1 calc R . .
H36N H 1.3322 0.9221 0.4532 0.067 Uiso 1 1 calc R . .
C37B C 0.7835(3) 1.1061(3) 0.28442(15) 0.0241(10) Uani 1 1 d . . .
C38B C 0.7427(3) 1.0983(3) 0.24725(15) 0.0265(11) Uani 1 1 d . . .
C39B C 0.7930(3) 1.1000(3) 0.20809(15) 0.0302(11) Uani 1 1 d . . .
H39B H 0.7661 1.0948 0.1843 0.036 Uiso 1 1 calc R E .
C40B C 0.8810(3) 1.1090(3) 0.20142(15) 0.0280(11) Uani 1 1 d . . .
C41B C 0.9183(3) 1.1181(3) 0.23708(15) 0.0260(11) Uani 1 1 d . . .
H41B H 0.9761 1.1255 0.2339 0.031 Uiso 1 1 calc R E .
C42B C 0.8727(3) 1.1166(3) 0.27833(14) 0.0237(10) Uani 1 1 d . . .
C43B C 0.9204(3) 1.1284(3) 0.31203(15) 0.0256(11) Uani 1 1 d . . .
H43B H 0.9761 1.1389 0.3043 0.031 Uiso 1 1 calc R E .
C44B C 0.9461(3) 1.1402(3) 0.38225(14) 0.0218(10) Uani 1 1 d . . .
C45B C 1.0397(3) 1.1294(3) 0.37638(15) 0.0253(10) Uani 1 1 d . . .
H45B H 1.0721 1.1114 0.3511 0.030 Uiso 1 1 calc R . .
C46B C 1.0840(3) 1.1456(3) 0.40828(15) 0.0280(11) Uani 1 1 d . . .
H46B H 1.1461 1.1399 0.4040 0.034 Uiso 1 1 calc R E .
C47B C 1.0371(3) 1.1700(3) 0.44617(15) 0.0287(11) Uani 1 1 d . . .
H47B H 1.0675 1.1815 0.4672 0.034 Uiso 1 1 calc R . .
C48B C 0.9446(3) 1.1776(3) 0.45330(15) 0.0256(11) Uani 1 1 d . . .

H48B H 0.9138 1.1919 0.4795 0.031 Uiso 1 1 calc R E .
C49B C 0.8979(3) 1.1638(3) 0.42148(14) 0.0205(10) Uani 1 1 d . E .
C50B C 0.7493(3) 1.2137(3) 0.45146(14) 0.0220(10) Uani 1 1 d . . .
H50B H 0.7743 1.2417 0.4673 0.026 Uiso 1 1 calc R E .
C51B C 0.6538(3) 1.2240(3) 0.45911(14) 0.0218(10) Uani 1 1 d . . .
C52B C 0.6094(3) 1.2781(3) 0.48938(14) 0.0247(10) Uani 1 1 d . . .
H52B H 0.6436 1.3027 0.5024 0.030 Uiso 1 1 calc R E .
C53B C 0.5180(3) 1.2950(3) 0.49993(14) 0.0259(11) Uani 1 1 d . . .
C54B C 0.4705(3) 1.2548(3) 0.47940(15) 0.0268(11) Uani 1 1 d . . .
H54B H 0.4086 1.2642 0.4869 0.032 Uiso 1 1 calc R E .
C55B C 0.5079(3) 1.2031(3) 0.44932(14) 0.0230(10) Uani 1 1 d . . .
C56B C 0.6048(3) 1.1856(3) 0.43820(14) 0.0233(10) Uani 1 1 d . . .
C57B C 0.6455(3) 1.0901(3) 0.25128(15) 0.0316(12) Uani 1 1 d . . .
C58B C 0.6361(3) 1.0206(3) 0.28053(17) 0.0373(13) Uani 1 1 d . . .
H58D H 0.5792 1.0104 0.2778 0.056 Uiso 1 1 calc R . .
H58E H 0.6386 1.0306 0.3094 0.056 Uiso 1 1 calc R . .
H58F H 0.6845 0.9771 0.2727 0.056 Uiso 1 1 calc R . .
C59B C 0.5812(3) 1.1628(3) 0.26905(18) 0.0383(13) Uani 1 1 d . . .
H59D H 0.5847 1.2060 0.2497 0.058 Uiso 1 1 calc R . .
H59E H 0.5983 1.1702 0.2961 0.058 Uiso 1 1 calc R . .
H59F H 0.5204 1.1578 0.2725 0.058 Uiso 1 1 calc R . .
C60B C 0.6163(4) 1.0799(4) 0.20787(18) 0.0480(16) Uani 1 1 d . . .
H60D H 0.6559 1.0348 0.1961 0.072 Uiso 1 1 calc R . .
H60E H 0.6194 1.1236 0.1889 0.072 Uiso 1 1 calc R . .
H60F H 0.5554 1.0750 0.2116 0.072 Uiso 1 1 calc R . .
C61B C 0.9296(4) 1.1067(3) 0.15609(16) 0.0374(13) Uani 1 1 d . . .
C62B C 0.8726(5) 1.1683(4) 0.12711(18) 0.0597(18) Uani 1 1 d . . .
H62D H 0.8138 1.1597 0.1274 0.090 Uiso 1 1 calc R . .
H62E H 0.9017 1.1662 0.0986 0.090 Uiso 1 1 calc R . .
H62F H 0.8663 1.2177 0.1371 0.090 Uiso 1 1 calc R . .
C63B C 1.0244(5) 1.1174(5) 0.15501(19) 0.068(2) Uani 1 1 d . . .
H63D H 1.0544 1.1110 0.1268 0.102 Uiso 1 1 calc R . .
H63E H 1.0580 1.0802 0.1746 0.102 Uiso 1 1 calc R . .
H63F H 1.0204 1.1678 0.1630 0.102 Uiso 1 1 calc R . .
C64B C 0.9377(4) 1.0290(4) 0.13926(18) 0.0483(15) Uani 1 1 d . . .
H64D H 0.8796 1.0182 0.1432 0.072 Uiso 1 1 calc R . .
H64E H 0.9799 0.9901 0.1545 0.072 Uiso 1 1 calc R . .
H64F H 0.9586 1.0300 0.1095 0.072 Uiso 1 1 calc R . .
C65B C 0.4683(3) 1.3526(3) 0.53221(16) 0.0327(12) Uani 1 1 d . . .
C66B C 0.5327(4) 1.3918(4) 0.5490(2) 0.0520(17) Uani 1 1 d . . .
H66D H 0.5755 1.3548 0.5649 0.078 Uiso 1 1 calc R . .
H66E H 0.4985 1.4311 0.5671 0.078 Uiso 1 1 calc R . .
H66F H 0.5644 1.4141 0.5255 0.078 Uiso 1 1 calc R . .
C67B C 0.4267(4) 1.3115(4) 0.57049(17) 0.0464(15) Uani 1 1 d . . .
H67D H 0.3852 1.2870 0.5612 0.070 Uiso 1 1 calc R . .
H67E H 0.3951 1.3479 0.5907 0.070 Uiso 1 1 calc R . .
H67F H 0.4738 1.2738 0.5836 0.070 Uiso 1 1 calc R . .
C68B C 0.3936(4) 1.4136(3) 0.51183(18) 0.0420(14) Uani 1 1 d . . .
H68F H 0.4197 1.4396 0.4880 0.063 Uiso 1 1 calc R . .
H68D H 0.3626 1.4497 0.5323 0.063 Uiso 1 1 calc R . .
H68E H 0.3515 1.3899 0.5024 0.063 Uiso 1 1 calc R . .
C69B C 0.4503(3) 1.1627(3) 0.42918(17) 0.0362(13) Uani 1 1 d . . .
C70B C 0.4748(4) 1.0775(3) 0.4449(3) 0.063(2) Uani 1 1 d . . .
H70D H 0.5386 1.0559 0.4387 0.095 Uiso 1 1 calc R . .

H70E H 0.4422 1.0508 0.4307 0.095 Uiso 1 1 calc R . .
H70F H 0.4589 1.0728 0.4750 0.095 Uiso 1 1 calc R . .
C71B C 0.3489(3) 1.1937(3) 0.44209(17) 0.0377(13) Uani 1 1 d . . .
H71D H 0.3372 1.1871 0.4724 0.057 Uiso 1 1 calc R . .
H71E H 0.3158 1.1663 0.4287 0.057 Uiso 1 1 calc R . .
H71F H 0.3304 1.2470 0.4332 0.057 Uiso 1 1 calc R . .
C72B C 0.4645(4) 1.1712(5) 0.38035(19) 0.063(2) Uani 1 1 d . . .
H72D H 0.4515 1.2244 0.3711 0.094 Uiso 1 1 calc R . .
H72E H 0.4248 1.1479 0.3686 0.094 Uiso 1 1 calc R . .
H72F H 0.5262 1.1465 0.3709 0.094 Uiso 1 1 calc R . .
P1B P 0.73503(18) 0.86523(17) 0.42508(10) 0.0397(7) Uani 0.55 1 d PD E 1
N5B N 0.9111(4) 0.8686(4) 0.3905(2) 0.0213(11) Uani 0.55 1 d PDU E 1
N6B N 0.8014(5) 0.9941(4) 0.4019(2) 0.0225(10) Uani 0.55 1 d PDU E 1
N7B N 0.8600(4) 0.9092(3) 0.46542(17) 0.0318(12) Uani 0.55 1 d PDU E 1
C73B C 0.8781(5) 0.9499(5) 0.3752(2) 0.0217(13) Uani 0.55 1 d PDU E 1
H73C H 0.9275 0.9739 0.3735 0.026 Uiso 0.55 1 calc PR E 1
H73D H 0.8606 0.9520 0.3467 0.026 Uiso 0.55 1 calc PR E 1
C74B C 0.8282(5) 0.9918(3) 0.4456(2) 0.0272(13) Uani 0.55 1 d PDU E 1
H74C H 0.7771 1.0201 0.4635 0.033 Uiso 0.55 1 calc PR E 1
H74D H 0.8767 1.0167 0.4446 0.033 Uiso 0.55 1 calc PR E 1
C75B C 0.9354(4) 0.8663(4) 0.43475(19) 0.0270(14) Uani 0.55 1 d PDU E 1
H75C H 0.9869 0.8875 0.4339 0.032 Uiso 0.55 1 calc PR E 1
H75D H 0.9539 0.8133 0.4456 0.032 Uiso 0.55 1 calc PR E 1
C76B C 0.8429(4) 0.8271(4) 0.3904(2) 0.0257(14) Uani 0.55 1 d PDU E 1
H76C H 0.8683 0.7742 0.3996 0.031 Uiso 0.55 1 calc PR E 1
H76D H 0.8283 0.8282 0.3614 0.031 Uiso 0.55 1 calc PR E 1
C77B C 0.7211(4) 0.9647(3) 0.4018(2) 0.0278(14) Uani 0.55 1 d PDU E 1
H77C H 0.7066 0.9671 0.3727 0.033 Uiso 0.55 1 calc PR E 1
H77D H 0.6702 0.9979 0.4176 0.033 Uiso 0.55 1 calc PR E 1
C78B C 0.7996(5) 0.8783(5) 0.47228(19) 0.0336(19) Uani 0.55 1 d PDU E 1
H78B H 0.7551 0.9068 0.4931 0.040 Uiso 0.55 1 calc PR E 1
H78C H 0.8241 0.8280 0.4857 0.040 Uiso 0.55 1 calc PR E 1
P1" P 0.7984(2) 0.8929(2) 0.47295(9) 0.0285(8) Uani 0.45 1 d PDU E 2
N5" N 0.7956(6) 0.9978(5) 0.4009(2) 0.0231(11) Uani 0.45 1 d PDU E 2
N6" N 0.8978(5) 0.8682(5) 0.3929(2) 0.0204(11) Uani 0.45 1 d PDU E 2
N7" N 0.7291(4) 0.8863(4) 0.39739(15) 0.0273(13) Uani 0.45 1 d PDU E 2
C73" C 0.8840(6) 0.9504(5) 0.3828(3) 0.0204(13) Uani 0.45 1 d PDU E 2
H73E H 0.8888 0.9600 0.3522 0.025 Uiso 0.45 1 calc PR E 2
H73F H 0.9321 0.9663 0.3933 0.025 Uiso 0.45 1 calc PR E 2
C74" C 0.8239(4) 0.8430(4) 0.3775(2) 0.0225(14) Uani 0.45 1 d PDU E 2
H74E H 0.8329 0.7886 0.3846 0.027 Uiso 0.45 1 calc PR E 2
H74F H 0.8266 0.8515 0.3468 0.027 Uiso 0.45 1 calc PR E 2
C75" C 0.7224(5) 0.9703(4) 0.3862(3) 0.0254(14) Uani 0.45 1 d PDU E 2
H75E H 0.7238 0.9797 0.3556 0.031 Uiso 0.45 1 calc PR E 2
H75F H 0.6646 1.0001 0.3986 0.031 Uiso 0.45 1 calc PR E 2
C76" C 0.7884(6) 0.9919(3) 0.4472(2) 0.0237(15) Uani 0.45 1 d PDU E 2
H76E H 0.7306 1.0247 0.4576 0.028 Uiso 0.45 1 calc PR E 2
H76F H 0.8353 1.0114 0.4563 0.028 Uiso 0.45 1 calc PR E 2
C77" C 0.9032(4) 0.8494(5) 0.4390(2) 0.0228(15) Uani 0.45 1 d PDU E 2
H77E H 0.9527 0.8661 0.4474 0.027 Uiso 0.45 1 calc PR E 2
H77F H 0.9171 0.7943 0.4443 0.027 Uiso 0.45 1 calc PR E 2
C78" C 0.71695(13) 0.87168(13) 0.43522(6) 0.032(2) Uani 0.45 1 d PDU E 2
H78D H 0.7195 0.8177 0.4396 0.038 Uiso 0.45 1 calc PR E 2
H78E H 0.6558 0.8995 0.4447 0.038 Uiso 0.45 1 calc PR E 2

N1R N 0.83170(13) 0.10046(13) 0.80867(6) 0.0699(16) Uani 1 1 d RU . .
C1R C 0.85094(13) 0.15565(13) 0.80929(6) 0.0569(16) Uani 1 1 d RU . .
C2R C 0.87433(13) 0.22654(13) 0.81041(6) 0.0591(16) Uani 1 1 d RU . .
H2R1 H 0.8483 0.2617 0.7880 0.089 Uiso 1 1 calc R . .
H2R2 H 0.9389 0.2176 0.8067 0.089 Uiso 1 1 calc R . .
H2R3 H 0.8514 0.2477 0.8373 0.089 Uiso 1 1 calc R . .
N1T N 0.20716(13) 0.74257(13) 0.29376(6) 0.092(2) Uani 0.60 1 d PRDU E 1
C1T C 0.25480(13) 0.78791(13) 0.28497(6) 0.068(2) Uani 0.60 1 d PRDU E 1
C2T C 0.33221(13) 0.83507(13) 0.27093(6) 0.065(2) Uani 0.60 1 d PRDU E 1
H2T1 H 0.3913 0.8002 0.2711 0.097 Uiso 0.60 1 calc PR E 1
H2T2 H 0.3261 0.8733 0.2907 0.097 Uiso 0.60 1 calc PR E 1
H2T3 H 0.3244 0.8591 0.2429 0.097 Uiso 0.60 1 calc PR E 1
N1T' N 0.22253(13) 0.69381(13) 0.28122(6) 0.092(2) Uani 0.40 1 d PRDU E 2
C1T' C 0.26089(13) 0.65310(13) 0.30724(6) 0.089(3) Uani 0.40 1 d PRDU E 2
C2T' C 0.32745(13) 0.59845(13) 0.33682(6) 0.086(4) Uani 0.40 1 d PRDU E 2
H2T4 H 0.3795 0.5706 0.3199 0.129 Uiso 0.40 1 calc PR E 2
H2T5 H 0.2978 0.5633 0.3530 0.129 Uiso 0.40 1 calc PR E 2
H2T6 H 0.3460 0.6278 0.3559 0.129 Uiso 0.40 1 calc PR E 2
N1T'' N 0.55959(13) 0.25750(13) 0.67954(6) 0.117(7) Uani 0.40 1 d PRU . 3
C1T'' C 0.39429(13) 0.77660(13) 0.29914(6) 0.059(3) Uani 0.40 1 d PRDU . 3
C2T'' C 0.33221(13) 0.83507(13) 0.27093(6) 0.061(3) Uani 0.40 1 d PRDU E 3
H2T7 H 0.2905 0.8720 0.2882 0.091 Uiso 0.40 1 calc PR E 3
H2T8 H 0.2993 0.8096 0.2561 0.091 Uiso 0.40 1 calc PR E 3
H2T9 H 0.3678 0.8603 0.2507 0.091 Uiso 0.40 1 calc PR E 3
N1T* N 0.55944(13) 0.29813(13) 0.66592(6) 0.088(5) Uani 0.60 1 d PRU . 4
C1T* C 0.60295(13) 1.35099(13) 0.66070(6) 0.070(4) Uani 0.60 1 d PR . 4
C2T* C 0.32745(13) 0.59845(13) 0.33682(6) 0.087(3) Uani 0.60 1 d PRU . 4
H2TX H 0.3368 0.5574 0.3585 0.131 Uiso 0.60 1 calc PR E 4
H2TY H 0.3373 0.5779 0.3094 0.131 Uiso 0.60 1 calc PR E 4
H2TZ H 0.2666 0.6299 0.3410 0.131 Uiso 0.60 1 calc PR E 4
N1U N 0.80614(13) 0.67717(13) 0.47261(6) 0.0763(18) Uani 1 1 d RDU . .
C1U C 0.82481(13) 0.64171(13) 0.44441(6) 0.0618(17) Uani 1 1 d RDU . .
C2U C 0.84918(13) 0.59115(13) 0.40738(6) 0.085(2) Uani 1 1 d RDU . .
H2U1 H 0.9129 0.5671 0.4051 0.127 Uiso 1 1 calc R . .
H2U2 H 0.8337 0.6215 0.3816 0.127 Uiso 1 1 calc R . .
H2U3 H 0.8164 0.5527 0.4120 0.127 Uiso 1 1 calc R . .
N1V N 0.2795(6) 0.2773(6) 0.6676(2) 0.100(3) Uani 1 1 d U . .
C1V C 0.3425(7) 0.2267(7) 0.6626(2) 0.087(3) Uani 1 1 d U . .
C2V C 0.4229(7) 1.1669(6) 0.6559(3) 0.098(3) Uani 1 1 d . . .
H2V1 H 0.4740 1.1842 0.6610 0.147 Uiso 1 1 calc R . .
H2V2 H 0.4300 1.1526 0.6271 0.147 Uiso 1 1 calc R . .
H2V3 H 0.4190 1.1236 0.6751 0.147 Uiso 1 1 calc R . .
N1W N 0.2585(7) 0.6323(5) 0.8441(2) 0.085(3) Uani 0.70 1 d PD . 1
C1W C -0.2607(9) 0.3468(12) 1.1955(7) 0.080(2) Uani 0.70 1 d PU . 1
C2W C 0.2660(5) 0.6905(5) 0.7638(2) 0.044(2) Uani 0.70 1 d PD . 1
H2W1 H 0.2196 0.6835 0.7482 0.066 Uiso 0.70 1 calc PR . 1
H2W2 H 0.3242 0.6694 0.7489 0.066 Uiso 0.70 1 calc PR . 1
H2W3 H 0.2580 0.7440 0.7663 0.066 Uiso 0.70 1 calc PR . 1
N1W' N -0.3153(14) 0.3128(12) 1.1738(8) 0.086(4) Uani 0.30 1 d PDU F 2
C1W' C -0.275(2) 0.346(3) 1.1901(17) 0.080(2) Uani 0.30 1 d PDU F 2
C2W' C -0.2509(17) 0.4023(14) 1.2185(9) 0.085(4) Uani 0.30 1 d PDU F 2
H2W4 H -0.2863 0.4533 1.2121 0.127 Uiso 0.30 1 calc PR F 2
H2W5 H -0.1878 0.4003 1.2129 0.127 Uiso 0.30 1 calc PR F 2
H2W6 H -0.2641 0.3876 1.2479 0.127 Uiso 0.30 1 calc PR F 2

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_atom_site_aniso_U_12
Zn1A 0.0194(3) 0.0342(3) 0.0173(3) -0.0039(2) -0.0010(2) -0.0002(2)
Zn2A 0.0263(3) 0.0232(3) 0.0166(3) -0.0004(2) -0.0041(2) -0.0054(2)
Zn1B 0.0253(3) 0.0202(3) 0.0255(3) -0.0034(2) -0.0050(2) -0.0016(2)
Zn2B 0.0162(3) 0.0210(3) 0.0225(3) -0.0029(2) 0.0005(2) -0.0036(2)
N1A 0.019(2) 0.037(2) 0.020(2) -0.0056(17) 0.0016(16) -0.0009(17)
N2A 0.021(2) 0.036(2) 0.018(2) -0.0039(17) -0.0022(16) -0.0037(18)
N3A 0.024(2) 0.023(2) 0.0192(19) -0.0019(16) -0.0005(16) -0.0090(17)
N4A 0.031(2) 0.028(2) 0.017(2) -0.0006(17) -0.0040(16) -0.0079(18)
N1B 0.026(2) 0.024(2) 0.023(2) -0.0048(17) -0.0011(16) -0.0043(17)
N2B 0.022(2) 0.024(2) 0.022(2) -0.0057(16) -0.0022(16) -0.0014(17)
N3B 0.0201(19) 0.020(2) 0.025(2) -0.0031(16) -0.0012(16) -0.0050(16)
N4B 0.0188(19) 0.019(2) 0.022(2) -0.0011(16) 0.0009(15) -0.0045(16)
O1A 0.0210(17) 0.062(3) 0.0208(18) -0.0036(17) -0.0008(14) -0.0042(17)
O2A 0.0223(17) 0.038(2) 0.0260(18) -0.0073(15) -0.0037(14) -0.0001(15)
O3A 0.0298(18) 0.0243(18) 0.0237(17) -0.0008(14) -0.0076(14) -0.0027(14)
O4A 0.042(2) 0.0275(19) 0.0222(17) 0.0044(14) -0.0100(15) -0.0126(16)
O1B 0.0363(19) 0.0231(19) 0.0313(19) -0.0024(15) -0.0060(15) -0.0058(15)
O2B 0.0317(18) 0.0289(19) 0.0213(17) -0.0006(14) -0.0055(14) -0.0095(15)
O3B 0.0220(16) 0.0328(19) 0.0228(17) -0.0056(14) 0.0011(13) -0.0091(14)
O4B 0.0168(16) 0.0273(18) 0.0344(19) -0.0093(15) 0.0038(14) -0.0028(14)
C1A 0.023(2) 0.029(3) 0.019(2) 0.001(2) 0.0022(19) 0.003(2)
C2A 0.027(3) 0.030(3) 0.028(3) 0.002(2) 0.002(2) 0.000(2)
C3A 0.025(3) 0.043(3) 0.036(3) -0.011(2) 0.009(2) -0.002(2)
C4A 0.031(3) 0.049(4) 0.034(3) -0.014(3) 0.009(2) -0.005(3)
C5A 0.037(3) 0.045(3) 0.024(3) -0.016(2) 0.004(2) -0.005(3)
C6A 0.026(3) 0.033(3) 0.022(2) -0.007(2) 0.004(2) 0.000(2)
C7A 0.031(3) 0.030(3) 0.023(3) -0.004(2) -0.003(2) -0.004(2)
C8A 0.021(2) 0.031(3) 0.023(2) -0.007(2) -0.0044(19) 0.001(2)
C9A 0.032(3) 0.038(3) 0.028(3) -0.015(2) 0.003(2) -0.003(2)
C10A 0.032(3) 0.046(3) 0.038(3) -0.018(3) -0.008(2) -0.006(3)
C11A 0.027(3) 0.051(4) 0.036(3) -0.015(3) -0.002(2) -0.008(3)
C12A 0.021(3) 0.038(3) 0.039(3) -0.009(2) -0.003(2) -0.002(2)
C13A 0.024(2) 0.035(3) 0.023(3) -0.004(2) -0.0048(19) -0.003(2)
C14A 0.017(2) 0.035(3) 0.019(2) -0.004(2) 0.0013(18) 0.003(2)
C15A 0.025(2) 0.032(3) 0.017(2) -0.004(2) -0.0005(19) -0.005(2)
C16A 0.021(2) 0.032(3) 0.018(2) 0.004(2) -0.0023(18) 0.000(2)
C17A 0.026(3) 0.028(3) 0.019(2) 0.002(2) -0.0008(19) -0.005(2)
C18A 0.036(3) 0.030(3) 0.022(3) 0.000(2) -0.003(2) -0.011(2)
C19A 0.031(3) 0.032(3) 0.018(2) 0.001(2) -0.0025(19) -0.010(2)
C20A 0.025(3) 0.037(3) 0.018(2) 0.001(2) 0.0000(19) -0.004(2)
C21A 0.021(3) 0.094(5) 0.028(3) -0.006(3) -0.002(2) -0.006(3)
C22A 0.046(4) 0.154(7) 0.065(5) 0.039(5) -0.012(3) -0.021(4)
C23A 0.034(3) 0.141(7) 0.114(6) -0.099(5) 0.001(4) -0.011(4)
C24A 0.025(3) 0.067(4) 0.037(3) -0.008(3) 0.001(2) -0.001(3)
C25A 0.042(4) 0.097(6) 0.031(3) -0.026(3) 0.013(3) -0.010(4)
C26A 0.065(6) 0.132(10) 0.046(6) -0.061(7) 0.021(5) -0.023(8)

C27A 0.078(7) 0.118(9) 0.061(6) -0.052(7) 0.018(6) 0.014(7)
C28A 0.053(6) 0.121(9) 0.024(5) -0.018(6) 0.012(4) -0.035(6)
C26' 0.053(7) 0.124(10) 0.045(7) -0.030(8) 0.023(6) -0.017(8)
C27' 0.086(8) 0.123(10) 0.061(7) -0.055(8) 0.027(7) -0.008(8)
C28' 0.088(10) 0.152(14) 0.051(8) -0.032(11) 0.024(8) 0.001(12)
C29A 0.028(3) 0.042(3) 0.034(3) -0.005(2) 0.000(2) -0.010(2)
C30A 0.027(3) 0.069(4) 0.035(3) -0.002(3) -0.005(2) -0.010(3)
C31A 0.031(3) 0.061(4) 0.038(3) 0.002(3) 0.003(2) -0.015(3)
C32A 0.038(3) 0.072(5) 0.068(4) -0.025(4) 0.003(3) -0.028(3)
C33A 0.033(3) 0.024(3) 0.031(3) -0.003(2) -0.004(2) -0.003(2)
C34A 0.046(6) 0.030(6) 0.048(7) -0.019(5) -0.022(5) 0.007(5)
C35A 0.058(7) 0.027(5) 0.048(6) -0.008(4) -0.028(6) -0.004(5)
C36A 0.051(6) 0.040(6) 0.045(6) -0.008(5) 0.006(5) 0.002(5)
C34' 0.041(12) 0.072(18) 0.052(15) -0.037(13) -0.007(10) 0.017(13)
C35' 0.053(13) 0.023(10) 0.048(11) -0.002(8) 0.009(10) 0.005(9)
C36' 0.032(10) 0.039(11) 0.072(14) -0.022(11) 0.021(10) 0.004(8)
C37A 0.022(2) 0.027(3) 0.017(2) -0.0026(19) -0.0016(18) -0.004(2)
C38A 0.027(2) 0.022(2) 0.020(2) -0.0042(19) -0.0028(19) -0.004(2)
C39A 0.023(2) 0.030(3) 0.020(2) -0.006(2) -0.0022(19) -0.005(2)
C40A 0.020(2) 0.030(3) 0.017(2) -0.0009(19) 0.0013(18) -0.003(2)
C41A 0.020(2) 0.027(3) 0.020(2) -0.0036(19) 0.0027(18) -0.002(2)
C42A 0.022(2) 0.024(3) 0.020(2) -0.0008(19) 0.0012(18) -0.0052(19)
C43A 0.026(2) 0.020(2) 0.018(2) -0.0016(18) -0.0004(19) -0.008(2)
C44A 0.021(2) 0.027(3) 0.019(2) -0.0044(19) 0.0023(18) -0.005(2)
C45A 0.029(3) 0.025(3) 0.028(3) 0.000(2) -0.005(2) -0.003(2)
C46A 0.034(3) 0.029(3) 0.034(3) -0.001(2) -0.004(2) -0.012(2)
C47A 0.030(3) 0.039(3) 0.032(3) -0.006(2) -0.002(2) -0.017(2)
C48A 0.032(3) 0.034(3) 0.023(3) 0.002(2) -0.007(2) -0.007(2)
C49A 0.027(2) 0.027(3) 0.018(2) -0.0048(19) 0.0000(19) -0.010(2)
C50A 0.035(3) 0.031(3) 0.023(3) -0.005(2) -0.009(2) -0.007(2)
C51A 0.035(3) 0.030(3) 0.021(2) 0.000(2) -0.007(2) -0.006(2)
C52A 0.041(3) 0.028(3) 0.025(3) -0.003(2) -0.008(2) -0.006(2)
C53A 0.033(3) 0.030(3) 0.020(2) -0.002(2) 0.000(2) -0.001(2)
C54A 0.034(3) 0.024(3) 0.023(3) 0.002(2) 0.002(2) -0.003(2)
C55A 0.028(3) 0.026(3) 0.020(2) -0.005(2) -0.0005(19) -0.003(2)
C56A 0.030(3) 0.022(3) 0.021(2) 0.0015(19) -0.0028(19) -0.005(2)
C57A 0.037(3) 0.026(3) 0.037(3) -0.002(2) -0.016(2) -0.006(2)
C58A 0.054(4) 0.034(3) 0.050(4) -0.004(3) -0.024(3) -0.012(3)
C59A 0.068(4) 0.037(3) 0.043(3) 0.006(3) -0.026(3) -0.023(3)
C60A 0.060(4) 0.036(3) 0.048(4) -0.019(3) -0.025(3) 0.006(3)
C61A 0.022(2) 0.032(3) 0.028(3) 0.001(2) -0.002(2) 0.000(2)
C62A 0.020(2) 0.032(3) 0.043(3) 0.000(2) -0.002(2) -0.002(2)
C63A 0.023(3) 0.030(3) 0.044(3) 0.004(2) -0.004(2) -0.001(2)
C64A 0.037(3) 0.045(3) 0.031(3) 0.000(2) -0.007(2) 0.002(3)
C65A 0.045(3) 0.029(3) 0.023(3) 0.001(2) -0.008(2) -0.001(2)
C66A 0.055(4) 0.039(3) 0.025(3) 0.001(2) -0.012(2) -0.007(3)
C67A 0.050(4) 0.049(4) 0.026(3) 0.007(3) -0.004(2) -0.003(3)
C68A 0.059(4) 0.033(3) 0.030(3) 0.004(2) -0.014(3) -0.003(3)
C69A 0.038(3) 0.029(3) 0.031(3) 0.003(2) -0.008(2) -0.011(2)
C70A 0.045(3) 0.032(3) 0.047(3) 0.005(3) -0.012(3) -0.015(3)
C71A 0.037(3) 0.043(3) 0.050(4) 0.002(3) -0.011(3) -0.014(3)
C72A 0.065(4) 0.051(4) 0.038(3) -0.017(3) -0.013(3) -0.011(3)
P1A 0.0612(11) 0.0478(10) 0.0559(11) -0.0050(8) 0.0064(8) -0.0056(9)
N5A 0.024(2) 0.025(2) 0.021(2) 0.0005(16) -0.0053(16) -0.0007(17)

N6A 0.025(2) 0.027(2) 0.020(2) -0.0057(16) -0.0005(16) -0.0014(17)
N7A 0.033(3) 0.097(5) 0.037(3) 0.001(3) 0.007(2) -0.025(3)
C73A 0.023(2) 0.030(3) 0.026(3) 0.001(2) -0.002(2) -0.001(2)
C74A 0.026(3) 0.053(4) 0.033(3) 0.014(3) -0.004(2) -0.005(3)
C75A 0.027(3) 0.068(4) 0.026(3) 0.002(3) -0.006(2) 0.001(3)
C76A 0.056(4) 0.032(3) 0.037(3) -0.005(2) 0.014(3) -0.007(3)
C77A 0.067(4) 0.039(3) 0.033(3) -0.012(3) 0.001(3) -0.007(3)
C78A 0.015(2) 0.066(4) 0.026(3) 0.028(3) -0.010(2) -0.012(3)
C1B 0.024(2) 0.022(3) 0.030(3) -0.003(2) 0.004(2) 0.000(2)
C2B 0.035(3) 0.029(3) 0.034(3) -0.004(2) 0.006(2) 0.008(2)
C3B 0.090(5) 0.022(3) 0.031(3) 0.001(2) 0.007(3) 0.016(3)
C4B 0.115(6) 0.023(3) 0.028(3) -0.002(2) 0.018(3) 0.001(3)
C5B 0.071(4) 0.022(3) 0.029(3) -0.007(2) 0.010(3) -0.003(3)
C6B 0.035(3) 0.023(3) 0.030(3) -0.002(2) 0.009(2) 0.000(2)
C7B 0.035(3) 0.031(3) 0.022(2) -0.007(2) 0.006(2) -0.014(2)
C8B 0.020(2) 0.027(3) 0.030(3) -0.006(2) 0.003(2) -0.002(2)
C9B 0.028(3) 0.032(3) 0.032(3) -0.007(2) 0.000(2) -0.011(2)
C10B 0.026(3) 0.045(3) 0.038(3) -0.014(3) -0.007(2) -0.009(2)
C11B 0.030(3) 0.040(3) 0.032(3) -0.002(2) -0.013(2) -0.003(2)
C12B 0.026(3) 0.030(3) 0.030(3) -0.005(2) -0.004(2) -0.001(2)
C13B 0.018(2) 0.029(3) 0.023(2) -0.009(2) -0.0001(18) -0.004(2)
C14B 0.019(2) 0.024(3) 0.019(2) -0.0037(19) 0.0019(18) 0.000(2)
C15B 0.021(2) 0.023(2) 0.021(2) -0.0044(19) 0.0011(18) -0.0015(19)
C16B 0.020(2) 0.030(3) 0.020(2) -0.004(2) 0.0030(18) 0.001(2)
C17B 0.021(2) 0.026(3) 0.030(3) -0.006(2) 0.0040(19) -0.005(2)
C18B 0.018(2) 0.029(3) 0.036(3) -0.011(2) -0.002(2) -0.002(2)
C19B 0.023(2) 0.021(2) 0.026(3) -0.007(2) -0.0042(19) -0.001(2)
C20B 0.020(2) 0.026(3) 0.025(2) -0.003(2) -0.0014(19) 0.000(2)
C21B 0.036(3) 0.033(3) 0.038(3) 0.005(2) -0.010(2) 0.002(2)
C22B 0.043(6) 0.041(6) 0.019(7) -0.002(4) 0.005(4) -0.007(4)
C23B 0.033(5) 0.062(7) 0.047(5) -0.025(5) -0.003(4) 0.003(4)
C24B 0.117(11) 0.034(6) 0.051(6) -0.013(5) -0.038(7) 0.022(6)
C22" 0.032(10) 0.055(12) 0.050(10) -0.013(10) -0.007(9) -0.004(9)
C23" 0.114(15) 0.033(11) 0.049(10) -0.006(11) -0.036(12) 0.012(11)
C24" 0.045(11) 0.048(11) 0.022(13) 0.001(10) -0.007(9) -0.014(10)
C25B 0.059(4) 0.019(3) 0.039(3) -0.002(3) 0.001(3) 0.012(3)
C26B 0.056(5) 0.017(4) 0.050(3) -0.008(3) 0.003(3) 0.005(4)
C27B 0.067(3) 0.031(3) 0.041(3) -0.013(3) 0.000(3) 0.010(3)
C28B 0.081(4) 0.024(3) 0.051(3) -0.006(3) 0.001(3) -0.010(3)
C25" 0.069(4) 0.023(4) 0.044(4) -0.002(3) -0.001(4) 0.007(4)
C26" 0.074(8) 0.024(7) 0.047(4) -0.002(6) -0.004(5) 0.012(8)
C27" 0.067(3) 0.031(3) 0.041(3) -0.013(3) 0.000(3) 0.010(3)
C28" 0.081(4) 0.024(3) 0.051(3) -0.006(3) 0.001(3) -0.010(3)
C29B 0.027(3) 0.043(3) 0.033(3) -0.003(2) 0.007(2) -0.015(2)
C30B 0.036(3) 0.067(5) 0.079(5) -0.013(4) 0.024(3) -0.021(3)
C31B 0.049(4) 0.041(3) 0.048(4) -0.001(3) 0.004(3) -0.023(3)
C32B 0.058(4) 0.073(5) 0.042(4) 0.017(3) -0.005(3) -0.040(4)
C33B 0.038(3) 0.031(3) 0.030(3) -0.002(2) -0.014(2) -0.006(2)
C34B 0.058(4) 0.039(3) 0.024(3) 0.005(2) -0.007(2) -0.018(3)
C35B 0.052(4) 0.035(3) 0.052(4) -0.003(3) -0.029(3) -0.004(3)
C36B 0.051(4) 0.050(4) 0.042(3) 0.002(3) -0.026(3) -0.020(3)
C37B 0.023(2) 0.021(2) 0.027(3) -0.003(2) -0.003(2) -0.0020(19)
C38B 0.024(2) 0.027(3) 0.025(3) -0.007(2) -0.003(2) 0.000(2)
C39B 0.031(3) 0.032(3) 0.024(3) -0.006(2) -0.003(2) -0.002(2)

C40B 0.030(3) 0.028(3) 0.023(3) 0.000(2) 0.001(2) -0.005(2)
C41B 0.023(2) 0.025(3) 0.029(3) -0.001(2) 0.001(2) -0.005(2)
C42B 0.021(2) 0.021(2) 0.026(3) -0.0015(19) -0.0019(19) -0.0019(19)
C43B 0.019(2) 0.020(2) 0.034(3) 0.002(2) 0.003(2) -0.0027(19)
C44B 0.021(2) 0.021(2) 0.025(2) -0.0014(19) -0.0050(19) -0.0047(19)
C45B 0.020(2) 0.029(3) 0.026(3) -0.005(2) 0.0030(19) -0.005(2)
C46B 0.013(2) 0.035(3) 0.036(3) -0.001(2) -0.002(2) -0.005(2)
C47B 0.021(2) 0.035(3) 0.029(3) -0.002(2) -0.009(2) -0.004(2)
C48B 0.019(2) 0.032(3) 0.024(2) -0.003(2) 0.0003(19) -0.004(2)
C49B 0.015(2) 0.023(2) 0.023(2) 0.0016(19) -0.0009(18) -0.0061(19)
C50B 0.021(2) 0.027(3) 0.018(2) 0.0014(19) -0.0064(18) -0.006(2)
C51B 0.020(2) 0.023(2) 0.020(2) 0.0017(19) 0.0013(18) -0.0033(19)
C52B 0.025(2) 0.027(3) 0.020(2) 0.0001(19) -0.0043(19) -0.003(2)
C53B 0.025(3) 0.027(3) 0.020(2) 0.001(2) 0.0008(19) 0.000(2)
C54B 0.020(2) 0.028(3) 0.028(3) 0.007(2) 0.0040(19) -0.005(2)
C55B 0.019(2) 0.023(3) 0.026(2) 0.003(2) 0.0015(19) -0.0063(19)
C56B 0.021(2) 0.021(2) 0.024(2) 0.003(2) 0.0019(19) -0.0013(19)
C57B 0.023(3) 0.045(3) 0.028(3) -0.013(2) -0.002(2) -0.005(2)
C58B 0.029(3) 0.041(3) 0.045(3) -0.012(3) -0.001(2) -0.013(2)
C59B 0.024(3) 0.046(3) 0.043(3) -0.007(3) -0.005(2) -0.004(2)
C60B 0.031(3) 0.079(5) 0.038(3) -0.016(3) -0.010(2) -0.013(3)
C61B 0.038(3) 0.046(3) 0.026(3) -0.001(2) 0.002(2) -0.011(3)
C62B 0.081(5) 0.064(4) 0.028(3) 0.000(3) 0.006(3) -0.014(4)
C63B 0.068(5) 0.118(7) 0.032(3) -0.014(4) 0.015(3) -0.053(5)
C64B 0.037(3) 0.064(4) 0.039(3) -0.018(3) 0.003(3) -0.003(3)
C65B 0.025(3) 0.037(3) 0.032(3) -0.010(2) 0.004(2) -0.002(2)
C66B 0.034(3) 0.060(4) 0.061(4) -0.039(3) 0.007(3) -0.004(3)
C67B 0.042(3) 0.055(4) 0.036(3) -0.011(3) 0.007(3) -0.004(3)
C68B 0.036(3) 0.029(3) 0.051(4) -0.011(3) 0.001(3) 0.008(2)
C69B 0.021(3) 0.043(3) 0.046(3) -0.014(3) 0.008(2) -0.011(2)
C70B 0.031(3) 0.037(4) 0.122(6) -0.017(4) 0.012(4) -0.014(3)
C71B 0.025(3) 0.047(3) 0.042(3) -0.008(3) 0.002(2) -0.009(2)
C72B 0.030(3) 0.119(6) 0.050(4) -0.041(4) 0.006(3) -0.029(4)
P1B 0.0233(13) 0.0294(16) 0.065(2) -0.0056(14) -0.0024(13) -0.0051(12)
N5B 0.019(2) 0.0202(19) 0.0225(19) 0.0009(18) 0.0011(18) -0.0032(17)
N6B 0.0187(19) 0.023(2) 0.0242(19) -0.0010(18) -0.0008(18) -0.0032(17)
N7B 0.027(2) 0.034(2) 0.024(2) 0.000(2) 0.001(2) 0.007(2)
C73B 0.019(2) 0.021(2) 0.023(2) 0.001(2) -0.001(2) -0.003(2)
C74B 0.024(3) 0.029(2) 0.025(2) -0.003(2) -0.002(2) 0.001(2)
C75B 0.023(3) 0.029(3) 0.022(2) 0.002(2) 0.002(2) 0.002(2)
C76B 0.023(3) 0.024(3) 0.029(3) -0.002(3) 0.002(3) -0.006(2)
C77B 0.021(2) 0.023(3) 0.035(3) 0.004(2) -0.003(2) -0.002(2)
C78B 0.029(3) 0.034(3) 0.023(3) 0.003(3) 0.005(3) 0.012(3)
P1" 0.0249(15) 0.0300(17) 0.0197(14) 0.0015(12) 0.0030(12) 0.0082(13)
N5" 0.019(2) 0.023(2) 0.024(2) -0.0007(19) -0.0001(19) -0.0024(18)
N6" 0.017(2) 0.020(2) 0.022(2) 0.0003(19) 0.0023(19) -0.0036(19)
N7" 0.019(2) 0.020(3) 0.039(3) 0.001(3) -0.009(2) 0.002(2)
C73" 0.019(2) 0.020(2) 0.021(2) 0.000(2) -0.002(2) -0.003(2)
C74" 0.018(3) 0.019(3) 0.029(3) 0.000(3) -0.005(2) -0.003(2)
C75" 0.021(2) 0.023(2) 0.029(3) 0.002(2) -0.002(2) -0.002(2)
C76" 0.018(3) 0.026(3) 0.025(3) -0.003(2) 0.003(3) -0.004(3)
C77" 0.016(3) 0.026(3) 0.022(2) 0.002(2) 0.004(2) -0.002(2)
C78" 0.019(4) 0.018(4) 0.055(4) 0.002(4) -0.005(3) 0.002(4)
N1R 0.083(4) 0.070(4) 0.049(3) -0.019(3) 0.018(3) -0.013(3)

C1R 0.056(4) 0.064(4) 0.042(3) -0.011(3) 0.010(3) -0.006(3)
C2R 0.056(4) 0.067(4) 0.049(4) -0.010(3) 0.015(3) -0.013(3)
N1T 0.075(4) 0.071(5) 0.126(5) -0.004(4) -0.018(4) -0.011(4)
C1T 0.066(5) 0.048(5) 0.080(5) -0.006(5) -0.013(5) 0.008(4)
C2T 0.064(5) 0.053(5) 0.065(5) -0.012(5) 0.003(5) 0.005(4)
N1T' 0.075(4) 0.071(5) 0.126(5) -0.004(4) -0.018(4) -0.011(4)
C1T' 0.083(6) 0.071(6) 0.108(6) 0.001(5) -0.005(5) -0.014(5)
C2T' 0.098(8) 0.063(7) 0.083(7) -0.003(6) 0.010(6) -0.006(6)
N1T'' 0.078(8) 0.170(16) 0.094(11) -0.043(12) -0.005(8) -0.006(10)
C1T'' 0.052(7) 0.055(7) 0.065(7) -0.014(6) 0.002(6) -0.007(6)
C2T'' 0.059(6) 0.050(6) 0.067(6) -0.011(5) 0.004(5) -0.004(5)
N1T* 0.055(6) 0.143(13) 0.066(7) -0.063(9) -0.011(5) -0.002(6)
C1T* 0.071(8) 0.078(9) 0.025(5) -0.016(6) -0.008(5) 0.047(7)
C2T* 0.102(7) 0.063(6) 0.083(7) -0.009(6) 0.019(6) -0.010(6)
N1U 0.061(4) 0.058(4) 0.107(5) 0.014(3) -0.014(4) -0.017(3)
C1U 0.040(3) 0.067(4) 0.077(4) 0.030(3) -0.010(3) -0.023(3)
C2U 0.069(5) 0.101(6) 0.075(5) 0.020(3) 0.005(4) -0.022(4)
N1V 0.087(5) 0.185(9) 0.039(3) 0.006(5) 0.006(4) -0.062(5)
C1V 0.084(6) 0.167(10) 0.030(4) 0.000(5) -0.012(4) -0.065(6)
C2V 0.124(8) 0.124(8) 0.060(5) 0.006(5) -0.029(5) -0.052(7)
N1W 0.118(8) 0.078(7) 0.061(6) 0.035(5) -0.030(6) -0.031(6)
C1W 0.050(4) 0.063(4) 0.134(5) 0.009(4) -0.036(4) -0.020(4)
C2W 0.045(5) 0.060(6) 0.019(4) 0.005(4) 0.007(3) -0.008(4)
N1W' 0.061(7) 0.072(7) 0.130(8) 0.003(7) -0.043(7) -0.012(6)
C1W' 0.050(4) 0.063(4) 0.134(5) 0.009(4) -0.036(4) -0.020(4)
C2W' 0.057(7) 0.069(8) 0.130(9) -0.005(7) -0.025(7) -0.014(7)
_geom_special_details
;
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.
;
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
Zn1A O2A 1.970(3) . ?
Zn1A O1A 1.981(3) . ?
Zn1A N2A 2.094(4) . ?
Zn1A N1A 2.102(4) . ?
Zn1A N6A 2.1560(14) . ?
Zn2A O4A 1.945(3) . ?
Zn2A O3A 1.981(3) . ?
Zn2A N3A 2.077(4) . ?
Zn2A N4A 2.099(4) . ?
Zn2A N5A 2.1574(13) . ?
Zn1B O2B 1.967(3) . ?
Zn1B O1B 1.976(3) . ?
Zn1B N1B 2.091(4) . ?

Zn1B N2B 2.099(4) . ?
Zn1B N5B 2.103(6) . ?
Zn1B N6" 2.279(7) . ?
Zn2B O3B 1.958(3) . ?
Zn2B O4B 1.986(3) . ?
Zn2B N4B 2.080(4) . ?
Zn2B N5" 2.102(7) . ?
Zn2B N3B 2.108(4) . ?
Zn2B N6B 2.172(7) . ?
N1A C7A 1.299(6) . ?
N1A C8A 1.418(6) . ?
N2A C14A 1.287(6) . ?
N2A C13A 1.434(6) . ?
N3A C43A 1.293(6) . ?
N3A C44A 1.419(6) . ?
N4A C50A 1.293(6) . ?
N4A C49A 1.412(6) . ?
N1B C7B 1.290(6) . ?
N1B C8B 1.414(6) . ?
N2B C14B 1.294(6) . ?
N2B C13B 1.415(6) . ?
N3B C43B 1.295(6) . ?
N3B C44B 1.409(6) . ?
N4B C50B 1.290(6) . ?
N4B C49B 1.409(5) . ?
O1A C1A 1.295(5) . ?
O2A C20A 1.304(6) . ?
O3A C37A 1.297(5) . ?
O4A C56A 1.293(5) . ?
O1B C1B 1.296(6) . ?
O2B C20B 1.291(6) . ?
O3B C37B 1.309(5) . ?
O4B C56B 1.296(5) . ?
C1A C6A 1.428(7) . ?
C1A C2A 1.442(7) . ?
C2A C3A 1.386(7) . ?
C2A C21A 1.508(7) . ?
C3A C4A 1.397(8) . ?
C4A C5A 1.363(7) . ?
C4A C25A 1.529(7) . ?
C5A C6A 1.423(6) . ?
C6A C7A 1.423(7) . ?
C8A C9A 1.376(7) . ?
C8A C13A 1.401(6) . ?
C9A C10A 1.380(7) . ?
C10A C11A 1.383(7) . ?
C11A C12A 1.379(7) . ?
C12A C13A 1.384(7) . ?
C14A C15A 1.427(7) . ?
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N6" C74" 1.488(5) . ?
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N2A C14A C15A 126.8(4) . . ?
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C76A N5A C75A 108.6 . . ?
C76A N5A C73A 110.0 . . ?
C75A N5A C73A 110.6 . . ?
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C73A N6A C77A 111.7 . . ?
C73A N6A C74A 108.5 . . ?
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C73A N6A Zn1A 111.8 . . ?
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C78A N7A C75A 109.8 . . ?
C78A N7A C74A 110.4 . . ?
C75A N7A C74A 104.5 . . ?
N6A C73A N5A 113.2 . . ?
N6A C74A N7A 114.7 . . ?
N5A C75A N7A 115.5 . . ?
N5A C76A P1A 115.9 . . ?
N6A C77A P1A 113.3 . . ?
N7A C78A P1A 122.9 . . ?
O1B C1B C6B 123.0(4) . . ?
O1B C1B C2B 119.5(4) . . ?
C6B C1B C2B 117.5(4) . . ?
C3B C2B C1B 117.8(5) . . ?
C3B C2B C21B 121.5(5) . . ?
C1B C2B C21B 120.7(5) . . ?
C2B C3B C4B 125.4(5) . . ?
C5B C4B C3B 116.7(5) . . ?
C5B C4B C25B 126.7(6) . . ?
C3B C4B C25B 115.7(6) . . ?
C5B C4B C25" 111.7(8) . . ?
C3B C4B C25" 126.6(7) . . ?
C25B C4B C25" 33.2(5) . . ?
C4B C5B C6B 122.1(5) . . ?
C5B C6B C1B 120.5(5) . . ?
C5B C6B C7B 115.1(5) . . ?
C1B C6B C7B 124.4(4) . . ?
N1B C7B C6B 125.4(5) . . ?

C9B C8B C13B 119.6(4) . . ?
C9B C8B N1B 124.8(5) . . ?
C13B C8B N1B 115.5(4) . . ?
C10B C9B C8B 120.7(5) . . ?
C9B C10B C11B 119.5(5) . . ?
C10B C11B C12B 120.7(5) . . ?
C13B C12B C11B 119.6(5) . . ?
C12B C13B C8B 119.9(4) . . ?
C12B C13B N2B 125.0(4) . . ?
C8B C13B N2B 115.1(4) . . ?
N2B C14B C15B 126.2(4) . . ?
C16B C15B C20B 120.8(4) . . ?
C16B C15B C14B 114.8(4) . . ?
C20B C15B C14B 124.3(4) . . ?
C17B C16B C15B 122.0(4) . . ?
C16B C17B C18B 116.7(4) . . ?
C16B C17B C29B 123.0(4) . . ?
C18B C17B C29B 120.3(4) . . ?
C19B C18B C17B 125.0(5) . . ?
C18B C19B C20B 118.8(4) . . ?
C18B C19B C33B 121.5(4) . . ?
C20B C19B C33B 119.7(4) . . ?
O2B C20B C15B 122.9(4) . . ?
O2B C20B C19B 120.4(4) . . ?
C15B C20B C19B 116.7(4) . . ?
C24" C21B C22" 120(2) . . ?
C24" C21B C2B 112(3) . . ?
C22" C21B C2B 97.4(12) . . ?
C24" C21B C24B 116(2) . . ?
C22" C21B C24B 94.1(16) . . ?
C2B C21B C24B 115.4(8) . . ?
C24" C21B C22B 15(2) . . ?
C22" C21B C22B 133.9(13) . . ?
C2B C21B C22B 110.9(8) . . ?
C24B C21B C22B 104.8(9) . . ?
C24" C21B C23B 93(2) . . ?
C22" C21B C23B 27.4(10) . . ?
C2B C21B C23B 112.7(5) . . ?
C24B C21B C23B 105.9(8) . . ?
C22B C21B C23B 106.4(8) . . ?
C24" C21B C23" 114(2) . . ?
C22" C21B C23" 108(2) . . ?
C2B C21B C23" 103(3) . . ?
C24B C21B C23" 17(3) . . ?
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C23B C21B C23" 123(2) . . ?
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C26B C25B C27B 107.1(6) . . ?
C28B C25B C27B 107.5(6) . . ?
C26B C25B C4B 110.3(6) . . ?
C28B C25B C4B 108.1(6) . . ?
C27B C25B C4B 113.3(7) . . ?
C26" C25" C28" 109.1(9) . . ?
C26" C25" C27" 106.1(9) . . ?

C28" C25" C27" 106.8(9) . . ?
C26" C25" C4B 115.9(13) . . ?
C28" C25" C4B 121.0(11) . . ?
C27" C25" C4B 95.7(12) . . ?
C32B C29B C31B 108.3(5) . . ?
C32B C29B C30B 109.1(5) . . ?
C31B C29B C30B 108.7(5) . . ?
C32B C29B C17B 111.4(4) . . ?
C31B C29B C17B 110.3(4) . . ?
C30B C29B C17B 109.1(4) . . ?
C35B C33B C36B 107.9(4) . . ?
C35B C33B C19B 109.4(4) . . ?
C36B C33B C19B 112.7(4) . . ?
C35B C33B C34B 109.6(5) . . ?
C36B C33B C34B 106.4(4) . . ?
C19B C33B C34B 110.8(4) . . ?
O3B C37B C42B 123.1(4) . . ?
O3B C37B C38B 119.3(4) . . ?
C42B C37B C38B 117.6(4) . . ?
C39B C38B C37B 118.0(4) . . ?
C39B C38B C57B 121.6(4) . . ?
C37B C38B C57B 120.4(4) . . ?
C38B C39B C40B 125.4(5) . . ?
C41B C40B C39B 115.9(4) . . ?
C41B C40B C61B 124.7(4) . . ?
C39B C40B C61B 119.4(4) . . ?
C40B C41B C42B 122.8(4) . . ?
C41B C42B C37B 120.2(4) . . ?
C41B C42B C43B 115.8(4) . . ?
C37B C42B C43B 123.9(4) . . ?
N3B C43B C42B 126.3(4) . . ?
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C45B C44B C49B 119.8(4) . . ?
N3B C44B C49B 115.2(4) . . ?
C46B C45B C44B 119.7(4) . . ?
C47B C46B C45B 120.6(4) . . ?
C46B C47B C48B 120.4(4) . . ?
C49B C48B C47B 120.2(4) . . ?
C48B C49B N4B 125.3(4) . . ?
C48B C49B C44B 119.2(4) . . ?
N4B C49B C44B 115.5(4) . . ?
N4B C50B C51B 127.0(4) . . ?
C56B C51B C52B 121.3(4) . . ?
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C52B C51B C50B 114.7(4) . . ?
C53B C52B C51B 121.9(4) . . ?
C52B C53B C54B 116.0(4) . . ?
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C54B C53B C65B 120.8(4) . . ?
C55B C54B C53B 125.7(4) . . ?
C54B C55B C56B 118.0(4) . . ?
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C56B C55B C69B 120.6(4) . . ?
O4B C56B C51B 122.7(4) . . ?

O4B C56B C55B 120.1(4) . . ?
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C58B C57B C38B 111.1(4) . . ?
C58B C57B C59B 109.8(4) . . ?
C38B C57B C59B 108.7(4) . . ?
C58B C57B C60B 107.1(5) . . ?
C38B C57B C60B 111.8(4) . . ?
C59B C57B C60B 108.2(4) . . ?
C63B C61B C64B 108.2(5) . . ?
C63B C61B C62B 110.6(5) . . ?
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C64B C61B C40B 108.9(4) . . ?
C62B C61B C40B 109.1(4) . . ?
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C53B C65B C66B 111.7(4) . . ?
C68B C65B C66B 108.8(5) . . ?
C67B C65B C66B 107.3(5) . . ?
C55B C69B C71B 112.7(4) . . ?
C55B C69B C72B 111.3(4) . . ?
C71B C69B C72B 107.2(4) . . ?
C55B C69B C70B 108.9(5) . . ?
C71B C69B C70B 106.2(4) . . ?
C72B C69B C70B 110.3(5) . . ?
C77B P1B C76B 93.5(3) . . ?
C77B P1B C78B 94.7(3) . . ?
C76B P1B C78B 93.1(3) . . ?
C76B N5B C73B 111.8(5) . . ?
C76B N5B C75B 109.3(5) . . ?
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C75B N5B Zn1B 105.3(4) . . ?
C73B N6B C77B 110.7(5) . . ?
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C74B N6B Zn2B 106.2(4) . . ?
C78B N7B C75B 111.2(6) . . ?
C78B N7B C74B 112.3(6) . . ?
C75B N7B C74B 106.9(4) . . ?
N6B C73B N5B 114.5(4) . . ?
N6B C74B N7B 112.3(4) . . ?
N5B C75B N7B 114.6(4) . . ?
N5B C76B P1B 114.7(4) . . ?
N6B C77B P1B 114.3(4) . . ?
N7B C78B P1B 119.7(5) . . ?
C77" P1" C76" 94.0(3) . . ?
C77" P1" C78" 94.3(3) . . ?
C76" P1" C78" 92.4(3) . . ?
C76" N5" C73" 111.2(6) . . ?

C76" N5" C75" 109.4(5) . . ?
C73" N5" C75" 108.1(5) . . ?
C76" N5" Zn2B 109.2(5) . . ?
C73" N5" Zn2B 114.9(5) . . ?
C75" N5" Zn2B 103.7(4) . . ?
C73" N6" C77" 110.8(5) . . ?
C73" N6" C74" 109.4(5) . . ?
C77" N6" C74" 111.7(5) . . ?
C73" N6" Zn1B 106.4(5) . . ?
C77" N6" Zn1B 110.5(4) . . ?
C74" N6" Zn1B 108.0(4) . . ?
C78" N7" C75" 112.7(5) . . ?
C78" N7" C74" 113.0(5) . . ?
C75" N7" C74" 105.5(5) . . ?
N6" C73" N5" 114.3(4) . . ?
N6" C74" N7" 112.1(5) . . ?
N5" C75" N7" 114.5(5) . . ?
N5" C76" P1" 115.5(4) . . ?
N6" C77" P1" 114.5(4) . . ?
N7" C78" P1" 119.2(3) . . ?
N1R C1R C2R 179.2 . . ?
N1T C1T C2T 170.1 . . ?
N1T' C1T' C2T' 170.0 . . ?
N1T" C1T" C2T" 171.7(3) 2_666 . ?
N1T* C1T* C2T* 164.88(15) 1_565 2_676 ?
N1U C1U C2U 177.7 . . ?
N1V C1V C2V 177.1(12) . 1_545 ?
N1W C1W C2W 167.7(15) 2_567 2_567 ?
N1W' C1W' C2W' 162(3) . . ?
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_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
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_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
O2A Zn1A N1A C7A -91.1(5) . . . . ?
O1A Zn1A N1A C7A 17.4(4) . . . . ?
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N6A Zn1A N1A C7A 109.6(4) . . . . ?
O2A Zn1A N1A C8A 76.4(5) . . . . ?
O1A Zn1A N1A C8A -175.1(3) . . . . ?
N2A Zn1A N1A C8A 15.2(3) . . . . ?
N6A Zn1A N1A C8A -82.9(3) . . . . ?
O2A Zn1A N2A C14A -3.8(4) . . . . ?
O1A Zn1A N2A C14A 118.6(5) . . . . ?
N1A Zn1A N2A C14A 153.0(4) . . . . ?
N6A Zn1A N2A C14A -101.8(4) . . . . ?
O2A Zn1A N2A C13A -173.5(3) . . . . ?
O1A Zn1A N2A C13A -51.1(7) . . . . ?

N1A Zn1A N2A C13A -16.6(3) . . . . ?
N6A Zn1A N2A C13A 88.5(3) . . . . ?
O4A Zn2A N3A C43A 93.3(4) . . . . ?
O3A Zn2A N3A C43A -9.4(4) . . . . ?
N4A Zn2A N3A C43A 157.6(4) . . . . ?
N5A Zn2A N3A C43A -104.2(4) . . . . ?
O4A Zn2A N3A C44A -82.0(4) . . . . ?
O3A Zn2A N3A C44A 175.2(3) . . . . ?
N4A Zn2A N3A C44A -17.7(3) . . . . ?
N5A Zn2A N3A C44A 80.5(3) . . . . ?
O4A Zn2A N4A C50A -6.9(4) . . . . ?
O3A Zn2A N4A C50A -115.9(5) . . . . ?
N3A Zn2A N4A C50A -160.9(4) . . . . ?
N5A Zn2A N4A C50A 99.9(4) . . . . ?
O4A Zn2A N4A C49A 171.5(3) . . . . ?
O3A Zn2A N4A C49A 62.6(6) . . . . ?
N3A Zn2A N4A C49A 17.6(3) . . . . ?
N5A Zn2A N4A C49A -81.6(3) . . . . ?
O2B Zn1B N1B C7B 92.7(5) . . . . ?
O1B Zn1B N1B C7B -24.0(4) . . . . ?
N2B Zn1B N1B C7B 147.4(4) . . . . ?
N5B Zn1B N1B C7B -119.5(4) . . . . ?
N6" Zn1B N1B C7B -118.0(4) . . . . ?
O2B Zn1B N1B C8B -73.4(5) . . . . ?
O1B Zn1B N1B C8B 169.9(3) . . . . ?
N2B Zn1B N1B C8B -18.7(3) . . . . ?
N5B Zn1B N1B C8B 74.4(4) . . . . ?
N6" Zn1B N1B C8B 75.9(4) . . . . ?
O2B Zn1B N2B C14B 9.3(4) . . . . ?
O1B Zn1B N2B C14B -121.6(5) . . . . ?
N1B Zn1B N2B C14B -151.6(4) . . . . ?
N5B Zn1B N2B C14B 103.8(4) . . . . ?
N6" Zn1B N2B C14B 106.9(4) . . . . ?
O2B Zn1B N2B C13B -179.4(3) . . . . ?
O1B Zn1B N2B C13B 49.8(6) . . . . ?
N1B Zn1B N2B C13B 19.8(3) . . . . ?
N5B Zn1B N2B C13B -84.8(3) . . . . ?
N6" Zn1B N2B C13B -81.8(3) . . . . ?
O3B Zn2B N3B C43B 3.3(4) . . . . ?
O4B Zn2B N3B C43B -116.0(5) . . . . ?
N4B Zn2B N3B C43B -154.1(4) . . . . ?
N5" Zn2B N3B C43B 102.3(4) . . . . ?
N6B Zn2B N3B C43B 103.2(4) . . . . ?
O3B Zn2B N3B C44B 176.1(3) . . . . ?
O4B Zn2B N3B C44B 56.9(6) . . . . ?
N4B Zn2B N3B C44B 18.7(3) . . . . ?
N5" Zn2B N3B C44B -84.9(4) . . . . ?
N6B Zn2B N3B C44B -84.0(3) . . . . ?
O3B Zn2B N4B C50B 94.4(4) . . . . ?
O4B Zn2B N4B C50B -15.3(4) . . . . ?
N5" Zn2B N4B C50B -107.4(4) . . . . ?
N3B Zn2B N4B C50B 153.2(4) . . . . ?
N6B Zn2B N4B C50B -109.1(4) . . . . ?
O3B Zn2B N4B C49B -77.7(4) . . . . ?

O4B Zn2B N4B C49B 172.7(3) . . . . ?
N5" Zn2B N4B C49B 80.5(4) . . . . ?
N3B Zn2B N4B C49B -18.9(3) . . . . ?
N6B Zn2B N4B C49B 78.9(3) . . . . ?
O2A Zn1A O1A C1A 135.5(5) . . . . ?
N2A Zn1A O1A C1A 14.8(8) . . . . ?
N1A Zn1A O1A C1A -18.8(5) . . . . ?
N6A Zn1A O1A C1A -125.6(5) . . . . ?
O1A Zn1A O2A C20A -158.3(4) . . . . ?
N2A Zn1A O2A C20A 5.9(4) . . . . ?
N1A Zn1A O2A C20A -53.0(6) . . . . ?
N6A Zn1A O2A C20A 107.0(4) . . . . ?
O4A Zn2A O3A C37A -139.8(4) . . . . ?
N3A Zn2A O3A C37A 11.6(4) . . . . ?
N4A Zn2A O3A C37A -32.2(7) . . . . ?
N5A Zn2A O3A C37A 112.5(4) . . . . ?
O3A Zn2A O4A C56A 167.7(4) . . . . ?
N3A Zn2A O4A C56A 67.2(5) . . . . ?
N4A Zn2A O4A C56A 5.3(4) . . . . ?
N5A Zn2A O4A C56A -94.8(4) . . . . ?
O2B Zn1B O1B C1B -134.6(4) . . . . ?
N1B Zn1B O1B C1B 23.8(4) . . . . ?
N2B Zn1B O1B C1B -5.4(7) . . . . ?
N5B Zn1B O1B C1B 129.2(4) . . . . ?
N6" Zn1B O1B C1B 126.5(4) . . . . ?
O1B Zn1B O2B C20B 153.4(4) . . . . ?
N1B Zn1B O2B C20B 39.4(6) . . . . ?
N2B Zn1B O2B C20B -13.4(4) . . . . ?
N5B Zn1B O2B C20B -109.5(4) . . . . ?
N6" Zn1B O2B C20B -110.3(4) . . . . ?
O4B Zn2B O3B C37B 163.2(4) . . . . ?
N4B Zn2B O3B C37B 56.6(5) . . . . ?
N5" Zn2B O3B C37B -102.2(5) . . . . ?
N3B Zn2B O3B C37B -0.1(4) . . . . ?
N6B Zn2B O3B C37B -100.4(4) . . . . ?
O3B Zn2B O4B C56B -136.1(4) . . . . ?
N4B Zn2B O4B C56B 18.4(4) . . . . ?
N5" Zn2B O4B C56B 124.0(4) . . . . ?
N3B Zn2B O4B C56B -18.7(7) . . . . ?
N6B Zn2B O4B C56B 122.8(4) . . . . ?
Zn1A O1A C1A C6A 13.8(7) . . . . ?
Zn1A O1A C1A C2A -166.6(3) . . . . ?
O1A C1A C2A C3A 179.5(5) . . . . ?
C6A C1A C2A C3A -0.9(7) . . . . ?
O1A C1A C2A C21A -2.1(8) . . . . ?
C6A C1A C2A C21A 177.5(5) . . . . ?
C1A C2A C3A C4A 0.3(8) . . . . ?
C21A C2A C3A C4A -178.1(6) . . . . ?
C2A C3A C4A C5A 0.2(9) . . . . ?
C2A C3A C4A C25A 179.5(6) . . . . ?
C3A C4A C5A C6A 0.0(9) . . . . ?
C25A C4A C5A C6A -179.3(6) . . . . ?
C4A C5A C6A C7A -179.7(5) . . . . ?
C4A C5A C6A C1A -0.7(8) . . . . ?

O1A C1A C6A C7A -0.4(8) . . . . ?
C2A C1A C6A C7A -180.0(5) . . . . ?
O1A C1A C6A C5A -179.3(5) . . . . ?
C2A C1A C6A C5A 1.1(7) . . . . ?
C8A N1A C7A C6A -180.0(5) . . . . ?
Zn1A N1A C7A C6A -13.2(7) . . . . ?
C5A C6A C7A N1A -179.8(5) . . . . ?
C1A C6A C7A N1A 1.3(8) . . . . ?
C7A N1A C8A C9A -23.8(8) . . . . ?
Zn1A N1A C8A C9A 168.2(4) . . . . ?
C7A N1A C8A C13A 156.6(5) . . . . ?
Zn1A N1A C8A C13A -11.4(5) . . . . ?
C13A C8A C9A C10A -0.2(8) . . . . ?
N1A C8A C9A C10A -179.8(5) . . . . ?
C8A C9A C10A C11A 2.1(9) . . . . ?
C9A C10A C11A C12A -1.1(9) . . . . ?
C10A C11A C12A C13A -1.9(8) . . . . ?
C11A C12A C13A C8A 3.8(8) . . . . ?
C11A C12A C13A N2A -176.4(5) . . . . ?
C9A C8A C13A C12A -2.7(8) . . . . ?
N1A C8A C13A C12A 176.9(4) . . . . ?
C9A C8A C13A N2A 177.5(4) . . . . ?
N1A C8A C13A N2A -2.9(6) . . . . ?
C14A N2A C13A C12A 25.9(7) . . . . ?
Zn1A N2A C13A C12A -163.9(4) . . . . ?
C14A N2A C13A C8A -154.3(5) . . . . ?
Zn1A N2A C13A C8A 15.9(5) . . . . ?
C13A N2A C14A C15A 173.9(4) . . . . ?
Zn1A N2A C14A C15A 4.9(7) . . . . ?
N2A C14A C15A C20A -6.2(8) . . . . ?
N2A C14A C15A C16A 178.5(5) . . . . ?
C20A C15A C16A C17A 0.5(7) . . . . ?
C14A C15A C16A C17A 176.0(4) . . . . ?
C15A C16A C17A C18A -4.1(7) . . . . ?
C15A C16A C17A C33A 179.0(4) . . . . ?
C16A C17A C18A C19A 3.1(7) . . . . ?
C33A C17A C18A C19A -180.0(4) . . . . ?
C17A C18A C19A C20A 1.5(7) . . . . ?
C17A C18A C19A C29A -176.8(4) . . . . ?
Zn1A O2A C20A C15A -8.8(7) . . . . ?
Zn1A O2A C20A C19A 170.0(3) . . . . ?
C16A C15A C20A O2A -177.1(4) . . . . ?
C14A C15A C20A O2A 7.8(7) . . . . ?
C16A C15A C20A C19A 4.1(7) . . . . ?
C14A C15A C20A C19A -171.0(4) . . . . ?
C18A C19A C20A O2A 176.2(4) . . . . ?
C29A C19A C20A O2A -5.5(7) . . . . ?
C18A C19A C20A C15A -5.0(6) . . . . ?
C29A C19A C20A C15A 173.3(4) . . . . ?
C3A C2A C21A C23A -126.2(6) . . . . ?
C1A C2A C21A C23A 55.5(8) . . . . ?
C3A C2A C21A C24A -3.9(8) . . . . ?
C1A C2A C21A C24A 177.8(5) . . . . ?
C3A C2A C21A C22A 110.8(6) . . . . ?

C1A C2A C21A C22A -67.5(7) . . . . ?
C5A C4A C25A C26' -179.3(12) . . . . ?
C3A C4A C25A C26' 1.4(14) . . . . ?
C5A C4A C25A C26A 1.4(12) . . . . ?
C3A C4A C25A C26A -178.0(10) . . . . ?
C5A C4A C25A C28' -48.0(14) . . . . ?
C3A C4A C25A C28' 132.7(12) . . . . ?
C5A C4A C25A C27A 123.6(9) . . . . ?
C3A C4A C25A C27A -55.7(10) . . . . ?
C5A C4A C25A C28A -120.0(7) . . . . ?
C3A C4A C25A C28A 60.7(8) . . . . ?
C5A C4A C25A C27' 64.3(11) . . . . ?
C3A C4A C25A C27' -115.0(10) . . . . ?
C18A C19A C29A C31A 120.6(5) . . . . ?
C20A C19A C29A C31A -57.6(6) . . . . ?
C18A C19A C29A C32A 2.3(7) . . . . ?
C20A C19A C29A C32A -175.9(5) . . . . ?
C18A C19A C29A C30A -118.1(5) . . . . ?
C20A C19A C29A C30A 63.8(6) . . . . ?
C16A C17A C33A C34' -141.8(12) . . . . ?
C18A C17A C33A C34' 41.4(13) . . . . ?
C16A C17A C33A C35A 61.4(7) . . . . ?
C18A C17A C33A C35A -115.4(7) . . . . ?
C16A C17A C33A C35' 95.7(10) . . . . ?
C18A C17A C33A C35' -81.1(10) . . . . ?
C16A C17A C33A C36' -19.0(11) . . . . ?
C18A C17A C33A C36' 164.2(10) . . . . ?
C16A C17A C33A C36A -58.6(7) . . . . ?
C18A C17A C33A C36A 124.6(6) . . . . ?
C16A C17A C33A C34A -176.9(6) . . . . ?
C18A C17A C33A C34A 6.3(8) . . . . ?
Zn2A O3A C37A C42A -10.2(6) . . . . ?
Zn2A O3A C37A C38A 168.9(3) . . . . ?
O3A C37A C38A C39A -179.8(4) . . . . ?
C42A C37A C38A C39A -0.6(6) . . . . ?
O3A C37A C38A C57A -0.8(7) . . . . ?
C42A C37A C38A C57A 178.4(4) . . . . ?
C37A C38A C39A C40A -0.5(7) . . . . ?
C57A C38A C39A C40A -179.5(4) . . . . ?
C38A C39A C40A C41A 1.2(7) . . . . ?
C38A C39A C40A C61A 179.5(4) . . . . ?
C39A C40A C41A C42A -0.7(6) . . . . ?
C61A C40A C41A C42A -179.0(4) . . . . ?
O3A C37A C42A C41A -179.8(4) . . . . ?
C38A C37A C42A C41A 1.0(6) . . . . ?
O3A C37A C42A C43A 2.6(7) . . . . ?
C38A C37A C42A C43A -176.6(4) . . . . ?
C40A C41A C42A C37A -0.3(7) . . . . ?
C40A C41A C42A C43A 177.5(4) . . . . ?
C44A N3A C43A C42A -178.2(4) . . . . ?
Zn2A N3A C43A C42A 6.9(6) . . . . ?
C37A C42A C43A N3A -1.5(7) . . . . ?
C41A C42A C43A N3A -179.2(4) . . . . ?
C43A N3A C44A C45A 21.9(6) . . . . ?

Zn2A N3A C44A C45A -162.6(4) . . . . ?
C43A N3A C44A C49A -159.9(4) . . . . ?
Zn2A N3A C44A C49A 15.7(5) . . . . ?
C49A C44A C45A C46A 1.7(7) . . . . ?
N3A C44A C45A C46A 179.9(4) . . . . ?
C44A C45A C46A C47A -2.0(7) . . . . ?
C45A C46A C47A C48A 0.6(7) . . . . ?
C46A C47A C48A C49A 1.1(7) . . . . ?
C47A C48A C49A C44A -1.3(7) . . . . ?
C47A C48A C49A N4A -178.9(4) . . . . ?
C45A C44A C49A C48A -0.1(7) . . . . ?
N3A C44A C49A C48A -178.4(4) . . . . ?
C45A C44A C49A N4A 177.7(4) . . . . ?
N3A C44A C49A N4A -0.6(6) . . . . ?
C50A N4A C49A C48A -18.5(7) . . . . ?
Zn2A N4A C49A C48A 163.0(4) . . . . ?
C50A N4A C49A C44A 163.8(4) . . . . ?
Zn2A N4A C49A C44A -14.6(5) . . . . ?
C49A N4A C50A C51A -176.7(5) . . . . ?
Zn2A N4A C50A C51A 1.6(7) . . . . ?
N4A C50A C51A C52A -177.9(5) . . . . ?
N4A C50A C51A C56A 8.5(8) . . . . ?
C50A C51A C52A C53A -172.9(5) . . . . ?
C56A C51A C52A C53A 0.9(8) . . . . ?
C51A C52A C53A C54A 2.8(7) . . . . ?
C51A C52A C53A C65A 179.8(5) . . . . ?
C52A C53A C54A C55A -1.7(7) . . . . ?
C65A C53A C54A C55A -178.8(4) . . . . ?
C53A C54A C55A C56A -3.0(7) . . . . ?
C53A C54A C55A C69A 175.0(4) . . . . ?
Zn2A O4A C56A C51A 1.9(7) . . . . ?
Zn2A O4A C56A C55A -176.4(3) . . . . ?
C52A C51A C56A O4A 176.1(4) . . . . ?
C50A C51A C56A O4A -10.6(8) . . . . ?
C52A C51A C56A C55A -5.5(7) . . . . ?
C50A C51A C56A C55A 167.7(4) . . . . ?
C54A C55A C56A O4A -175.2(4) . . . . ?
C69A C55A C56A O4A 6.8(7) . . . . ?
C54A C55A C56A C51A 6.5(6) . . . . ?
C69A C55A C56A C51A -171.6(4) . . . . ?
C39A C38A C57A C58A 0.1(7) . . . . ?
C37A C38A C57A C58A -178.9(4) . . . . ?
C39A C38A C57A C59A 119.8(5) . . . . ?
C37A C38A C57A C59A -59.1(6) . . . . ?
C39A C38A C57A C60A -118.8(5) . . . . ?
C37A C38A C57A C60A 62.2(6) . . . . ?
C41A C40A C61A C63A -3.4(6) . . . . ?
C39A C40A C61A C63A 178.5(4) . . . . ?
C41A C40A C61A C64A -124.6(5) . . . . ?
C39A C40A C61A C64A 57.2(6) . . . . ?
C41A C40A C61A C62A 116.5(5) . . . . ?
C39A C40A C61A C62A -61.7(6) . . . . ?
C52A C53A C65A C67A -116.3(6) . . . . ?
C54A C53A C65A C67A 60.6(6) . . . . ?

C52A C53A C65A C66A 4.7(7) . . . . ?
C54A C53A C65A C66A -178.4(4) . . . . ?
C52A C53A C65A C68A 124.3(5) . . . . ?
C54A C53A C65A C68A -58.8(6) . . . . ?
C54A C55A C69A C70A 0.4(7) . . . . ?
C56A C55A C69A C70A 178.4(4) . . . . ?
C54A C55A C69A C72A 124.4(5) . . . . ?
C56A C55A C69A C72A -57.6(5) . . . . ?
C54A C55A C69A C71A -117.9(5) . . . . ?
C56A C55A C69A C71A 60.1(6) . . . . ?
O4A Zn2A N5A C76A -33.32(10) . . . . ?
O3A Zn2A N5A C76A 66.02(9) . . . . ?
N3A Zn2A N5A C76A 155.49(10) . . . . ?
N4A Zn2A N5A C76A -124.71(11) . . . . ?
O4A Zn2A N5A C75A 85.99(11) . . . . ?
O3A Zn2A N5A C75A -174.67(10) . . . . ?
N3A Zn2A N5A C75A -85.20(11) . . . . ?
N4A Zn2A N5A C75A -5.40(12) . . . . ?
O4A Zn2A N5A C73A -152.99(10) . . . . ?
O3A Zn2A N5A C73A -53.66(10) . . . . ?
N3A Zn2A N5A C73A 35.82(11) . . . . ?
N4A Zn2A N5A C73A 115.62(11) . . . . ?
O2A Zn1A N6A C73A -65.66(9) . . . . ?
O1A Zn1A N6A C73A -167.15(11) . . . . ?
N2A Zn1A N6A C73A 24.64(11) . . . . ?
N1A Zn1A N6A C73A 105.11(10) . . . . ?
O2A Zn1A N6A C77A 170.26(9) . . . . ?
O1A Zn1A N6A C77A 68.77(11) . . . . ?
N2A Zn1A N6A C77A -99.44(11) . . . . ?
N1A Zn1A N6A C77A -18.97(11) . . . . ?
O2A Zn1A N6A C74A 50.33(9) . . . . ?
O1A Zn1A N6A C74A -51.17(11) . . . . ?
N2A Zn1A N6A C74A 140.62(11) . . . . ?
N1A Zn1A N6A C74A -138.90(10) . . . . ?
C77A N6A C73A N5A -66.7 . . . . ?
C74A N6A C73A N5A 58.3 . . . . ?
Zn1A N6A C73A N5A 170.68(7) . . . . ?
C76A N5A C73A N6A 63.8 . . . . ?
C75A N5A C73A N6A -56.2 . . . . ?
Zn2A N5A C73A N6A -177.00(6) . . . . ?
C73A N6A C74A N7A -59.2 . . . . ?
C77A N6A C74A N7A 65.1 . . . . ?
Zn1A N6A C74A N7A -177.6 . . . . ?
C78A N7A C74A N6A -63.6 . . . . ?
C75A N7A C74A N6A 54.4 . . . . ?
C76A N5A C75A N7A -66.5 . . . . ?
C73A N5A C75A N7A 54.3 . . . . ?
Zn2A N5A C75A N7A 173.8 . . . . ?
C78A N7A C75A N5A 67.1 . . . . ?
C74A N7A C75A N5A -51.4 . . . . ?
C75A N5A C76A P1A 59.2 . . . . ?
C73A N5A C76A P1A -62.1 . . . . ?
Zn2A N5A C76A P1A 179.5 . . . . ?
C77A P1A C76A N5A 53.3 . . . . ?

C78A P1A C76A N5A -42.9 . . . . ?
C73A N6A C77A P1A 66.3 . . . . ?
C74A N6A C77A P1A -56.2 . . . . ?
Zn1A N6A C77A P1A -169.55(7) . . . . ?
C76A P1A C77A N6A -53.0 . . . . ?
C78A P1A C77A N6A 38.3 . . . . ?
C75A N7A C78A P1A -59.7 . . . . ?
C74A N7A C78A P1A 55.0 . . . . ?
C77A P1A C78A N7A -44.1 . . . . ?
C76A P1A C78A N7A 47.6 . . . . ?
Zn1B O1B C1B C6B -15.2(7) . . . . ?
Zn1B O1B C1B C2B 165.8(3) . . . . ?
O1B C1B C2B C3B -178.4(5) . . . . ?
C6B C1B C2B C3B 2.6(7) . . . . ?
O1B C1B C2B C21B 0.3(7) . . . . ?
C6B C1B C2B C21B -178.8(5) . . . . ?
C1B C2B C3B C4B -0.8(10) . . . . ?
C21B C2B C3B C4B -179.5(6) . . . . ?
C2B C3B C4B C5B -0.2(11) . . . . ?
C2B C3B C4B C25B 169.9(7) . . . . ?
C2B C3B C4B C25" -153.1(9) . . . . ?
C3B C4B C5B C6B -0.6(10) . . . . ?
C25B C4B C5B C6B -169.4(7) . . . . ?
C25" C4B C5B C6B 156.2(8) . . . . ?
C4B C5B C6B C1B 2.4(9) . . . . ?
C4B C5B C6B C7B -177.1(6) . . . . ?
O1B C1B C6B C5B 177.7(5) . . . . ?
C2B C1B C6B C5B -3.3(7) . . . . ?
O1B C1B C6B C7B -2.9(8) . . . . ?
C2B C1B C6B C7B 176.1(5) . . . . ?
C8B N1B C7B C6B -177.5(4) . . . . ?
Zn1B N1B C7B C6B 17.4(7) . . . . ?
C5B C6B C7B N1B -179.9(5) . . . . ?
C1B C6B C7B N1B 0.6(8) . . . . ?
C7B N1B C8B C9B 31.6(7) . . . . ?
Zn1B N1B C8B C9B -161.8(4) . . . . ?
C7B N1B C8B C13B -151.6(4) . . . . ?
Zn1B N1B C8B C13B 14.9(5) . . . . ?
C13B C8B C9B C10B 0.6(7) . . . . ?
N1B C8B C9B C10B 177.2(4) . . . . ?
C8B C9B C10B C11B -1.2(7) . . . . ?
C9B C10B C11B C12B 0.1(8) . . . . ?
C10B C11B C12B C13B 1.5(7) . . . . ?
C11B C12B C13B C8B -2.0(7) . . . . ?
C11B C12B C13B N2B -179.9(4) . . . . ?
C9B C8B C13B C12B 1.0(7) . . . . ?
N1B C8B C13B C12B -175.9(4) . . . . ?
C9B C8B C13B N2B 179.1(4) . . . . ?
N1B C8B C13B N2B 2.2(6) . . . . ?
C14B N2B C13B C12B -28.5(6) . . . . ?
Zn1B N2B C13B C12B 159.8(4) . . . . ?
C14B N2B C13B C8B 153.6(4) . . . . ?
Zn1B N2B C13B C8B -18.1(5) . . . . ?
C13B N2B C14B C15B -176.9(4) . . . . ?

Zn1B N2B C14B C15B -6.2(6) . . . . ?
N2B C14B C15B C16B 177.2(4) . . . . ?
N2B C14B C15B C20B 1.9(7) . . . . ?
C20B C15B C16B C17B -0.8(7) . . . . ?
C14B C15B C16B C17B -176.3(4) . . . . ?
C15B C16B C17B C18B 1.1(7) . . . . ?
C15B C16B C17B C29B 180.0(4) . . . . ?
C16B C17B C18B C19B -0.9(7) . . . . ?
C29B C17B C18B C19B -179.8(4) . . . . ?
C17B C18B C19B C20B 0.3(7) . . . . ?
C17B C18B C19B C33B 177.9(4) . . . . ?
Zn1B O2B C20B C15B 13.4(6) . . . . ?
Zn1B O2B C20B C19B -166.7(3) . . . . ?
C16B C15B C20B O2B -179.9(4) . . . . ?
C14B C15B C20B O2B -4.9(7) . . . . ?
C16B C15B C20B C19B 0.1(6) . . . . ?
C14B C15B C20B C19B 175.1(4) . . . . ?
C18B C19B C20B O2B -179.8(4) . . . . ?
C33B C19B C20B O2B 2.5(6) . . . . ?
C18B C19B C20B C15B 0.1(6) . . . . ?
C33B C19B C20B C15B -177.5(4) . . . . ?
C3B C2B C21B C24" -131(2) . . . . ?
C1B C2B C21B C24" 50(2) . . . . ?
C3B C2B C21B C22" 102.1(13) . . . . ?
C1B C2B C21B C22" -76.6(12) . . . . ?
C3B C2B C21B C24B 3.9(12) . . . . ?
C1B C2B C21B C24B -174.7(10) . . . . ?
C3B C2B C21B C22B -115.0(8) . . . . ?
C1B C2B C21B C22B 66.4(8) . . . . ?
C3B C2B C21B C23B 125.8(6) . . . . ?
C1B C2B C21B C23B -52.9(7) . . . . ?
C3B C2B C21B C23" -8(2) . . . . ?
C1B C2B C21B C23" 173(2) . . . . ?
C5B C4B C25B C26B -12.0(12) . . . . ?
C3B C4B C25B C26B 179.0(7) . . . . ?
C25" C4B C25B C26B 60.9(11) . . . . ?
C5B C4B C25B C28B -132.9(8) . . . . ?
C3B C4B C25B C28B 58.1(10) . . . . ?
C25" C4B C25B C28B -60.0(12) . . . . ?
C5B C4B C25B C27B 108.0(9) . . . . ?
C3B C4B C25B C27B -60.9(9) . . . . ?
C25" C4B C25B C27B -179.1(12) . . . . ?
C5B C4B C25" C26" 31.6(14) . . . . ?
C3B C4B C25" C26" -174.4(10) . . . . ?
C25B C4B C25" C26" -92.8(13) . . . . ?
C5B C4B C25" C28" -104.0(13) . . . . ?
C3B C4B C25" C28" 50.0(17) . . . . ?
C25B C4B C25" C28" 131.6(18) . . . . ?
C5B C4B C25" C27" 142.6(8) . . . . ?
C3B C4B C25" C27" -63.4(12) . . . . ?
C25B C4B C25" C27" 18.2(10) . . . . ?
C16B C17B C29B C32B 6.8(7) . . . . ?
C18B C17B C29B C32B -174.4(5) . . . . ?
C16B C17B C29B C31B 127.1(5) . . . . ?

C18B C17B C29B C31B -54.1(6) . . . . ?
C16B C17B C29B C30B -113.6(5) . . . . ?
C18B C17B C29B C30B 65.2(6) . . . . ?
C18B C19B C33B C35B -115.7(5) . . . . ?
C20B C19B C33B C35B 61.9(6) . . . . ?
C18B C19B C33B C36B 4.3(6) . . . . ?
C20B C19B C33B C36B -178.1(4) . . . . ?
C18B C19B C33B C34B 123.4(5) . . . . ?
C20B C19B C33B C34B -59.0(6) . . . . ?
Zn2B O3B C37B C42B -0.6(7) . . . . ?
Zn2B O3B C37B C38B -179.4(3) . . . . ?
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TWINABS Version 2008/0 Bruker-Nonius
Blessing, Acta Cryst. (1995) A51 33-38
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they should be multiplied by a factor of 2 to 10
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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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N3 N 0.1777(2) 0.74600(12) 0.03516(16) 0.0191(8) Uani 1 1 d . . .
N4 N 0.1738(2) 0.82530(12) -0.00019(16) 0.0195(8) Uani 1 1 d . . .
N5 N -0.1989(2) 0.79340(11) 0.02731(16) 0.0178(8) Uani 1 1 d . . .
N6 N -0.0973(2) 0.74779(12) -0.00592(16) 0.0174(8) Uani 1 1 d . . .
N7 N 0.0188(2) 0.87591(11) 0.10888(15) 0.0150(8) Uani 1 1 d . . .
N8 N 0.1147(2) 0.81964(11) 0.11160(15) 0.0158(8) Uani 1 1 d . . .
N9 N -0.0181(2) 0.80069(11) 0.10931(15) 0.0147(8) Uani 1 1 d . . .
O1 O 0.02692(17) 0.97449(10) 0.13349(13) 0.0212(7) Uani 1 1 d . . .
O2 O -0.12284(17) 0.93490(10) 0.09402(13) 0.0222(7) Uani 1 1 d . . .
O3 O 0.27049(18) 0.76878(9) 0.14267(13) 0.0220(7) Uani 1 1 d . . .
O4 O 0.26719(17) 0.85598(9) 0.10082(14) 0.0211(7) Uani 1 1 d . . .
O5 O -0.15591(17) 0.75483(10) 0.13437(13) 0.0198(7) Uani 1 1 d . . .
O6 O -0.04523(18) 0.70367(9) 0.09483(13) 0.0207(7) Uani 1 1 d . . .
F1 F 0.07535(17) 1.02097(10) 0.22315(12) 0.0336(7) Uani 1 1 d . . .
F2 F 0.30088(16) 1.05845(10) 0.17673(12) 0.0335(7) Uani 1 1 d . . .
F3 F 0.36665(17) 0.73759(9) 0.23341(12) 0.0340(7) Uani 1 1 d . . .
F4 F 0.2888(2) 0.59821(9) 0.18315(14) 0.0401(8) Uani 1 1 d . . .
F5 F -0.18960(15) 0.74858(9) 0.23018(11) 0.0268(6) Uani 1 1 d . . .
F6 F -0.38129(16) 0.85253(9) 0.17951(12) 0.0314(7) Uani 1 1 d . . .
C1 C 0.0923(3) 0.99398(14) 0.1403(2) 0.0216(11) Uani 1 1 d . . .
C2 C 0.1211(3) 1.01801(15) 0.1886(2) 0.0225(11) Uani 1 1 d . . .
C3 C 0.1886(3) 1.03944(15) 0.2019(2) 0.0247(11) Uani 1 1 d . . .
H3 H 0.2051 1.0552 0.2351 0.030 Uiso 1 1 calc R . .
C4 C 0.2326(3) 1.03700(15) 0.1639(2) 0.0253(11) Uani 1 1 d . . .
C5 C 0.2106(3) 1.01510(15) 0.1166(2) 0.0229(11) Uani 1 1 d . . .
H5 H 0.2424 1.0142 0.0923 0.027 Uiso 1 1 calc R . .
C6 C 0.1392(3) 0.99314(14) 0.1032(2) 0.0200(10) Uani 1 1 d . . .
C7 C 0.1166(3) 0.97506(13) 0.0495(2) 0.0199(10) Uani 1 1 d . . .
H7 H 0.1513 0.9774 0.0274 0.024 Uiso 1 1 calc R . .
C8 C 0.0324(3) 0.94019(14) -0.02663(19) 0.0190(10) Uani 1 1 d . . .
C9 C 0.0752(3) 0.94655(14) -0.0645(2) 0.0221(11) Uani 1 1 d . . .
H9 H 0.1204 0.9632 -0.0547 0.027 Uiso 1 1 calc R . .
C10 C 0.0517(3) 0.92862(15) -0.1165(2) 0.0251(11) Uani 1 1 d . . .
H10 H 0.0807 0.9331 -0.1422 0.030 Uiso 1 1 calc R . .
C11 C -0.0145(3) 0.90395(15) -0.1310(2) 0.0246(11) Uani 1 1 d . . .
H11 H -0.0290 0.8905 -0.1660 0.030 Uiso 1 1 calc R . .
C12 C -0.0589(3) 0.89898(15) -0.0947(2) 0.0225(11) Uani 1 1 d . . .
H12 H -0.1042 0.8824 -0.1049 0.027 Uiso 1 1 calc R . .
C13 C -0.0377(3) 0.91809(14) -0.0433(2) 0.0207(10) Uani 1 1 d . . .
C14 C -0.1573(3) 0.91553(13) -0.0235(2) 0.0192(10) Uani 1 1 d . . .
H14 H -0.1768 0.9085 -0.0613 0.023 Uiso 1 1 calc R . .
C15 C -0.2124(2) 0.92148(13) 0.00702(19) 0.0173(10) Uani 1 1 d . . .
C16 C -0.2901(3) 0.91882(14) -0.0241(2) 0.0217(11) Uani 1 1 d . . .
H16 H -0.3019 0.9127 -0.0623 0.026 Uiso 1 1 calc R . .
C17 C -0.3478(3) 0.92496(14) 0.0004(2) 0.0235(11) Uani 1 1 d . . .

H17 H -0.3997 0.9215 -0.0198 0.028 Uiso 1 1 calc R . .
C18 C -0.3285(3) 0.93650(15) 0.0565(2) 0.0233(11) Uani 1 1 d . . .
H18 H -0.3689 0.9417 0.0730 0.028 Uiso 1 1 calc R . .
C19 C -0.2553(3) 0.94061(14) 0.0884(2) 0.0209(10) Uani 1 1 d . . .
C20 C -0.1935(2) 0.93239(14) 0.0638(2) 0.0200(10) Uani 1 1 d . . .
C21 C -0.2380(3) 0.95682(15) 0.1478(2) 0.0220(10) Uani 1 1 d . . .
C22 C -0.1910(3) 0.92445(16) 0.1893(2) 0.0298(12) Uani 1 1 d . . .
H22A H -0.2209 0.8984 0.1881 0.045 Uiso 1 1 calc R . .
H22B H -0.1790 0.9365 0.2264 0.045 Uiso 1 1 calc R . .
H22C H -0.1435 0.9179 0.1796 0.045 Uiso 1 1 calc R . .
C23 C -0.1920(3) 0.99867(15) 0.1522(2) 0.0298(12) Uani 1 1 d . . .
H23A H -0.1437 0.9933 0.1429 0.045 Uiso 1 1 calc R . .
H23B H -0.1812 1.0096 0.1898 0.045 Uiso 1 1 calc R . .
H23C H -0.2219 1.0196 0.1266 0.045 Uiso 1 1 calc R . .
C24 C -0.3114(3) 0.96675(19) 0.1649(2) 0.0333(13) Uani 1 1 d . . .
H24A H -0.3439 0.9857 0.1377 0.050 Uiso 1 1 calc R . .
H24B H -0.2981 0.9805 0.2010 0.050 Uiso 1 1 calc R . .
H24C H -0.3390 0.9403 0.1668 0.050 Uiso 1 1 calc R . .
C25 C 0.2724(3) 0.72802(15) 0.1492(2) 0.0233(11) Uani 1 1 d . . .
C26 C 0.3219(3) 0.71030(16) 0.1975(2) 0.0262(11) Uani 1 1 d . . .
C27 C 0.3279(3) 0.66789(16) 0.2093(2) 0.0305(12) Uani 1 1 d . . .
H27 H 0.3617 0.6576 0.2423 0.037 Uiso 1 1 calc R . .
C28 C 0.2832(3) 0.64057(16) 0.1715(2) 0.0307(12) Uani 1 1 d . . .
C29 C 0.2342(3) 0.65405(16) 0.1236(2) 0.0254(11) Uani 1 1 d . . .
H29 H 0.2036 0.6342 0.0990 0.030 Uiso 1 1 calc R . .
C30 C 0.2294(3) 0.69760(15) 0.1111(2) 0.0217(10) Uani 1 1 d . . .
C31 C 0.1842(2) 0.70844(14) 0.0568(2) 0.0195(10) Uani 1 1 d . . .
H31 H 0.1568 0.6861 0.0348 0.023 Uiso 1 1 calc R . .
C32 C 0.1369(2) 0.75254(15) -0.0207(2) 0.0196(10) Uani 1 1 d . . .
C33 C 0.1066(3) 0.72148(15) -0.0590(2) 0.0241(11) Uani 1 1 d . . .
H33 H 0.1150 0.6925 -0.0489 0.029 Uiso 1 1 calc R . .
C34 C 0.0644(3) 0.73163(16) -0.1115(2) 0.0260(11) Uani 1 1 d . . .
H34 H 0.0433 0.7098 -0.1370 0.031 Uiso 1 1 calc R . .
C35 C 0.0530(3) 0.77379(17) -0.1270(2) 0.0259(11) Uani 1 1 d . . .
H35 H 0.0225 0.7808 -0.1628 0.031 Uiso 1 1 calc R . .
C36 C 0.0860(3) 0.80572(16) -0.0907(2) 0.0237(11) Uani 1 1 d . . .
H36 H 0.0784 0.8346 -0.1016 0.028 Uiso 1 1 calc R . .
C37 C 0.1305(3) 0.79529(14) -0.0378(2) 0.0203(10) Uani 1 1 d . . .
C38 C 0.1952(3) 0.86047(14) -0.0173(2) 0.0194(10) Uani 1 1 d . . .
H38 H 0.1758 0.8665 -0.0554 0.023 Uiso 1 1 calc R . .
C39 C 0.2453(3) 0.89151(14) 0.0152(2) 0.0191(10) Uani 1 1 d . . .
C40 C 0.2621(3) 0.92692(14) -0.0147(2) 0.0220(11) Uani 1 1 d . . .
H40 H 0.2401 0.9286 -0.0533 0.026 Uiso 1 1 calc R . .
C41 C 0.3095(3) 0.95827(15) 0.0115(2) 0.0272(12) Uani 1 1 d . . .
H41 H 0.3206 0.9818 -0.0085 0.033 Uiso 1 1 calc R . .
C42 C 0.3418(3) 0.95525(15) 0.0688(2) 0.0264(12) Uani 1 1 d . . .
H42 H 0.3742 0.9775 0.0866 0.032 Uiso 1 1 calc R . .
C43 C 0.3290(3) 0.92186(14) 0.1002(2) 0.0229(11) Uani 1 1 d . . .
C44 C 0.2788(2) 0.88819(14) 0.0722(2) 0.0192(10) Uani 1 1 d . . .
C45 C 0.3662(3) 0.91944(16) 0.1618(2) 0.0313(13) Uani 1 1 d . . .
C46 C 0.3039(3) 0.91733(17) 0.1933(2) 0.0334(13) Uani 1 1 d . . .
H46A H 0.2708 0.9423 0.1842 0.050 Uiso 1 1 calc R . .
H46B H 0.3282 0.9167 0.2329 0.050 Uiso 1 1 calc R . .
H46C H 0.2732 0.8916 0.1825 0.050 Uiso 1 1 calc R . .

C47 C 0.4176(3) 0.87963(19) 0.1761(3) 0.0466(17) Uani 1 1 d . . .
H47A H 0.4406 0.8785 0.2158 0.070 Uiso 1 1 calc R . .
H47B H 0.4580 0.8810 0.1571 0.070 Uiso 1 1 calc R . .
H47C H 0.3866 0.8542 0.1643 0.070 Uiso 1 1 calc R . .
C48 C 0.4164(4) 0.95895(18) 0.1833(3) 0.0432(15) Uani 1 1 d . . .
H48A H 0.3838 0.9841 0.1794 0.065 Uiso 1 1 calc R . .
H48B H 0.4538 0.9628 0.1620 0.065 Uiso 1 1 calc R . .
H48C H 0.4432 0.9549 0.2222 0.065 Uiso 1 1 calc R . .
C49 C -0.2093(2) 0.77933(13) 0.14208(19) 0.0168(10) Uani 1 1 d . . .
C50 C -0.2290(3) 0.77718(14) 0.19274(19) 0.0208(10) Uani 1 1 d . . .
C51 C -0.2844(2) 0.80075(15) 0.2064(2) 0.0208(10) Uani 1 1 d . . .
H51 H -0.2945 0.7979 0.2413 0.025 Uiso 1 1 calc R . .
C52 C -0.3254(3) 0.82912(15) 0.1672(2) 0.0218(11) Uani 1 1 d . . .
C53 C -0.3105(3) 0.83400(14) 0.1174(2) 0.0207(10) Uani 1 1 d . . .
H53 H -0.3387 0.8540 0.0918 0.025 Uiso 1 1 calc R . .
C54 C -0.2526(2) 0.80910(14) 0.1036(2) 0.0195(10) Uani 1 1 d . . .
C55 C -0.2460(2) 0.81422(13) 0.04883(19) 0.0179(10) Uani 1 1 d . . .
H55 H -0.2785 0.8345 0.0262 0.021 Uiso 1 1 calc R . .
C56 C -0.1977(2) 0.79909(14) -0.02789(19) 0.0184(10) Uani 1 1 d . . .
C57 C -0.2502(3) 0.82357(14) -0.0669(2) 0.0233(11) Uani 1 1 d . . .
H57 H -0.2911 0.8372 -0.0568 0.028 Uiso 1 1 calc R . .
C58 C -0.2430(3) 0.82804(14) -0.11965(19) 0.0214(11) Uani 1 1 d . . .
H58 H -0.2789 0.8447 -0.1456 0.026 Uiso 1 1 calc R . .
C59 C -0.1836(3) 0.80826(15) -0.1350(2) 0.0238(11) Uani 1 1 d . . .
H59 H -0.1778 0.8122 -0.1709 0.029 Uiso 1 1 calc R . .
C60 C -0.1329(3) 0.78286(15) -0.0978(2) 0.0216(10) Uani 1 1 d . . .
H60 H -0.0921 0.7696 -0.1084 0.026 Uiso 1 1 calc R . .
C61 C -0.1410(3) 0.77654(14) -0.04500(19) 0.0196(10) Uani 1 1 d . . .
C62 C -0.0653(2) 0.71557(14) -0.0230(2) 0.0191(10) Uani 1 1 d . . .
H62 H -0.0685 0.7149 -0.0612 0.023 Uiso 1 1 calc R . .
C63 C -0.0256(2) 0.68099(15) 0.0091(2) 0.0200(10) Uani 1 1 d . . .
C64 C 0.0020(3) 0.64944(14) -0.0204(2) 0.0202(10) Uani 1 1 d . . .
H64 H -0.0064 0.6523 -0.0590 0.024 Uiso 1 1 calc R . .
C65 C 0.0405(3) 0.61502(15) 0.0056(2) 0.0244(11) Uani 1 1 d . . .
H65 H 0.0602 0.5944 -0.0143 0.029 Uiso 1 1 calc R . .
C66 C 0.0506(3) 0.61062(14) 0.0623(2) 0.0206(10) Uani 1 1 d . . .
H66 H 0.0780 0.5866 0.0801 0.025 Uiso 1 1 calc R . .
C67 C 0.0228(3) 0.63925(14) 0.0939(2) 0.0204(10) Uani 1 1 d . . .
C68 C -0.0168(3) 0.67612(14) 0.0667(2) 0.0210(11) Uani 1 1 d . . .
C69 C 0.0311(3) 0.63173(15) 0.1555(2) 0.0250(11) Uani 1 1 d . . .
C70 C 0.0741(3) 0.66896(16) 0.1898(2) 0.0288(12) Uani 1 1 d . . .
H70A H 0.0443 0.6950 0.1799 0.043 Uiso 1 1 calc R . .
H70B H 0.1241 0.6724 0.1824 0.043 Uiso 1 1 calc R . .
H70C H 0.0814 0.6630 0.2290 0.043 Uiso 1 1 calc R . .
C71 C -0.0487(3) 0.62695(17) 0.1640(2) 0.0300(12) Uani 1 1 d . . .
H71A H -0.0443 0.6194 0.2023 0.045 Uiso 1 1 calc R . .
H71B H -0.0765 0.6046 0.1398 0.045 Uiso 1 1 calc R . .
H71C H -0.0764 0.6538 0.1552 0.045 Uiso 1 1 calc R . .
C72 C 0.0764(3) 0.59101(16) 0.1758(2) 0.0323(12) Uani 1 1 d . . .
H72A H 0.0832 0.5879 0.2154 0.048 Uiso 1 1 calc R . .
H72B H 0.1266 0.5927 0.1682 0.048 Uiso 1 1 calc R . .
H72C H 0.0484 0.5665 0.1566 0.048 Uiso 1 1 calc R . .
C73 C 0.0871(3) 0.86250(14) 0.09144(19) 0.0174(10) Uani 1 1 d . . .
H73A H 0.0745 0.8627 0.0508 0.021 Uiso 1 1 calc R . .

H73B H 0.1287 0.8832 0.1053 0.021 Uiso 1 1 calc R . .
C74 C 0.0509(2) 0.78934(14) 0.09221(19) 0.0161(9) Uani 1 1 d . . .
H74A H 0.0376 0.7879 0.0516 0.019 Uiso 1 1 calc R . .
H74B H 0.0681 0.7608 0.1066 0.019 Uiso 1 1 calc R . .
C75 C -0.0425(2) 0.84384(13) 0.08917(19) 0.0152(9) Uani 1 1 d . . .
H75A H -0.0878 0.8520 0.1017 0.018 Uiso 1 1 calc R . .
H75B H -0.0577 0.8437 0.0485 0.018 Uiso 1 1 calc R . .
C76 C 0.0365(3) 0.88142(14) 0.16983(19) 0.0188(10) Uani 1 1 d . . .
H76A H -0.0103 0.8911 0.1792 0.023 Uiso 1 1 calc RD . .
H76B H 0.0755 0.9040 0.1811 0.023 Uiso 1 1 calc RD . .
C77 C 0.1433(3) 0.81902(14) 0.17267(19) 0.0189(10) Uani 1 1 d . . .
H77A H 0.1868 0.8390 0.1838 0.023 Uiso 1 1 calc R . .
H77B H 0.1630 0.7903 0.1843 0.023 Uiso 1 1 calc R . .
C78 C -0.0041(3) 0.79727(14) 0.17041(18) 0.0182(10) Uani 1 1 d . . .
H78A H 0.0102 0.7677 0.1816 0.022 Uiso 1 1 calc R . .
H78B H -0.0522 0.8037 0.1801 0.022 Uiso 1 1 calc R . .
O1W O 0.0084 0.9464 0.2542 0.031 Uani 0.25 1 d PU A -1
H1W1 H -0.0053 0.9631 0.2265 0.047 Uiso 0.25 1 d PD B -1
H1W2 H 0.0251 0.9632 0.2816 0.047 Uiso 0.25 1 d P C -1
loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Zn1 0.0173(3) 0.0195(3) 0.0159(3) 0.0003(2) 0.0037(2) -0.0003(2)
Zn2 0.0189(3) 0.0196(3) 0.0154(3) 0.0004(2) 0.0064(2) 0.0005(2)
Zn3 0.0192(3) 0.0187(3) 0.0139(3) -0.0009(2) 0.0044(2) -0.0002(2)
P1 0.0199(6) 0.0219(6) 0.0128(6) -0.0006(5) 0.0040(5) 0.0000(4)
N1 0.020(2) 0.0188(19) 0.015(2) -0.0012(16) 0.0014(16) 0.0001(14)
N2 0.024(2) 0.0191(19) 0.017(2) -0.0019(16) 0.0070(17) 0.0003(15)
N3 0.0166(19) 0.0219(19) 0.020(2) -0.0049(16) 0.0063(15) 0.0008(15)
N4 0.021(2) 0.023(2) 0.017(2) -0.0018(16) 0.0086(16) -0.0004(15)
N5 0.0193(19) 0.0179(18) 0.014(2) -0.0001(15) 0.0005(15) -0.0006(15)
N6 0.0184(19) 0.0208(19) 0.014(2) 0.0001(16) 0.0052(15) 0.0006(14)
N7 0.0164(19) 0.0186(18) 0.010(2) 0.0003(15) 0.0044(15) -0.0026(14)
N8 0.0201(19) 0.0191(18) 0.009(2) 0.0016(15) 0.0044(15) 0.0007(14)
N9 0.0162(18) 0.0194(18) 0.009(2) -0.0036(15) 0.0035(14) 0.0003(14)
O1 0.0214(17) 0.0213(16) 0.0214(19) 0.0011(13) 0.0065(13) -0.0024(12)
O2 0.0196(16) 0.0313(17) 0.0165(18) 0.0012(14) 0.0061(13) -0.0010(13)
O3 0.0252(17) 0.0207(16) 0.0199(19) 0.0027(13) 0.0054(14) 0.0006(13)
O4 0.0223(16) 0.0173(15) 0.0232(19) 0.0007(14) 0.0048(14) -0.0026(12)
O5 0.0206(16) 0.0221(16) 0.0181(18) 0.0009(13) 0.0078(13) 0.0006(13)
O6 0.0277(17) 0.0202(16) 0.0169(18) -0.0039(13) 0.0103(14) 0.0029(13)
F1 0.0374(17) 0.0477(18) 0.0169(16) -0.0028(13) 0.0096(13) -0.0100(13)
F2 0.0286(15) 0.0412(17) 0.0303(18) -0.0074(14) 0.0072(13) -0.0164(13)
F3 0.0417(17) 0.0338(16) 0.0221(16) -0.0014(13) 0.0008(13) 0.0134(13)
F4 0.063(2) 0.0240(15) 0.037(2) 0.0122(13) 0.0193(16) 0.0111(14)
F5 0.0328(15) 0.0292(14) 0.0181(16) 0.0039(12) 0.0066(12) 0.0048(11)
F6 0.0288(15) 0.0384(16) 0.0305(18) 0.0012(13) 0.0143(13) 0.0088(12)
C1 0.025(2) 0.019(2) 0.020(3) 0.0056(19) 0.004(2) 0.0003(18)
C2 0.031(3) 0.024(2) 0.013(3) 0.0012(19) 0.007(2) -0.0002(19)

C3 0.028(3) 0.028(3) 0.015(3) -0.002(2) 0.002(2) -0.001(2)
C4 0.020(2) 0.026(2) 0.026(3) 0.003(2) 0.000(2) -0.0048(19)
C5 0.024(2) 0.024(2) 0.020(3) -0.001(2) 0.006(2) -0.0002(19)
C6 0.021(2) 0.019(2) 0.020(3) 0.0028(19) 0.006(2) -0.0011(17)
C7 0.023(2) 0.016(2) 0.023(3) 0.0001(19) 0.010(2) 0.0007(17)
C8 0.020(2) 0.018(2) 0.017(3) 0.0016(19) 0.0019(19) 0.0032(17)
C9 0.025(2) 0.021(2) 0.018(3) 0.0021(19) 0.003(2) 0.0032(18)
C10 0.027(3) 0.025(2) 0.026(3) 0.003(2) 0.011(2) 0.0039(19)
C11 0.030(3) 0.023(2) 0.018(3) -0.003(2) 0.003(2) 0.0010(19)
C12 0.025(2) 0.025(2) 0.018(3) 0.000(2) 0.005(2) -0.0011(18)
C13 0.021(2) 0.019(2) 0.024(3) 0.007(2) 0.010(2) 0.0002(18)
C14 0.026(3) 0.016(2) 0.014(3) -0.0003(18) 0.004(2) -0.0004(17)
C15 0.016(2) 0.017(2) 0.017(3) 0.0035(18) 0.0017(19) -0.0017(16)
C16 0.021(2) 0.021(2) 0.020(3) 0.001(2) 0.002(2) -0.0018(18)
C17 0.018(2) 0.023(2) 0.027(3) 0.005(2) 0.000(2) -0.0014(17)
C18 0.025(3) 0.021(2) 0.028(3) 0.002(2) 0.015(2) -0.0020(19)
C19 0.028(3) 0.021(2) 0.015(3) 0.0045(19) 0.008(2) 0.0020(18)
C20 0.018(2) 0.019(2) 0.019(3) 0.0052(19) -0.002(2) -0.0013(17)
C21 0.023(2) 0.028(2) 0.017(3) -0.003(2) 0.009(2) -0.0022(19)
C22 0.029(3) 0.032(3) 0.025(3) 0.000(2) 0.001(2) -0.005(2)
C23 0.035(3) 0.026(3) 0.030(3) -0.003(2) 0.011(2) -0.003(2)
C24 0.029(3) 0.051(3) 0.024(3) 0.002(3) 0.015(2) 0.004(2)
C25 0.024(2) 0.028(3) 0.021(3) 0.001(2) 0.012(2) 0.0068(19)
C26 0.034(3) 0.028(3) 0.019(3) -0.006(2) 0.011(2) 0.007(2)
C27 0.043(3) 0.034(3) 0.020(3) 0.007(2) 0.018(2) 0.015(2)
C28 0.044(3) 0.024(3) 0.031(3) 0.006(2) 0.023(3) 0.007(2)
C29 0.032(3) 0.024(2) 0.025(3) 0.004(2) 0.016(2) 0.003(2)
C30 0.020(2) 0.026(2) 0.021(3) 0.001(2) 0.0093(19) 0.0041(18)
C31 0.016(2) 0.019(2) 0.025(3) 0.0008(19) 0.0092(19) 0.0023(17)
C32 0.017(2) 0.026(2) 0.018(3) -0.002(2) 0.0090(19) 0.0004(18)
C33 0.027(3) 0.025(2) 0.024(3) -0.004(2) 0.014(2) -0.0059(19)
C34 0.023(3) 0.036(3) 0.023(3) -0.012(2) 0.014(2) -0.009(2)
C35 0.023(3) 0.041(3) 0.015(3) -0.002(2) 0.008(2) -0.004(2)
C36 0.023(2) 0.032(3) 0.017(3) 0.002(2) 0.0065(19) -0.0006(19)
C37 0.023(2) 0.023(2) 0.019(3) -0.0025(19) 0.013(2) 0.0004(18)
C38 0.020(2) 0.027(2) 0.014(3) -0.0005(19) 0.0089(19) 0.0049(18)
C39 0.019(2) 0.020(2) 0.021(3) -0.0008(19) 0.0098(19) 0.0016(17)
C40 0.027(3) 0.022(2) 0.021(3) 0.0023(19) 0.013(2) 0.0061(18)
C41 0.028(3) 0.021(2) 0.037(3) 0.005(2) 0.017(2) 0.0033(19)
C42 0.021(2) 0.019(2) 0.038(3) -0.002(2) 0.006(2) -0.0012(18)
C43 0.021(2) 0.022(2) 0.029(3) -0.002(2) 0.011(2) 0.0011(18)
C44 0.013(2) 0.022(2) 0.023(3) -0.001(2) 0.0064(19) 0.0015(17)
C45 0.030(3) 0.028(3) 0.027(3) -0.003(2) -0.006(2) -0.004(2)
C46 0.050(3) 0.034(3) 0.014(3) -0.004(2) 0.004(2) 0.001(2)
C47 0.032(3) 0.044(3) 0.050(4) -0.001(3) -0.014(3) 0.006(2)
C48 0.048(3) 0.037(3) 0.034(3) -0.007(3) -0.009(3) -0.008(3)
C49 0.019(2) 0.017(2) 0.015(3) -0.0016(18) 0.0059(19) -0.0078(17)
C50 0.023(2) 0.022(2) 0.015(3) -0.0005(19) 0.0002(19) -0.0041(18)
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C53 0.020(2) 0.021(2) 0.021(3) 0.0005(19) 0.005(2) -0.0032(17)
C54 0.019(2) 0.020(2) 0.018(3) -0.0001(19) 0.0027(19) -0.0036(17)
C55 0.019(2) 0.015(2) 0.019(3) -0.0001(18) 0.0046(19) -0.0036(17)
C56 0.019(2) 0.021(2) 0.014(3) -0.0022(18) 0.0020(18) -0.0040(17)

C57 0.027(3) 0.019(2) 0.018(3) -0.0027(19) -0.003(2) -0.0008(18)
C58 0.025(3) 0.021(2) 0.016(3) 0.0058(19) 0.0004(19) -0.0050(18)
C59 0.030(3) 0.024(2) 0.017(3) -0.004(2) 0.005(2) -0.0086(19)
C60 0.023(2) 0.025(2) 0.018(3) -0.002(2) 0.008(2) -0.0030(18)
C61 0.023(2) 0.019(2) 0.015(3) -0.0013(18) 0.0032(19) -0.0055(17)
C62 0.019(2) 0.022(2) 0.016(3) -0.0038(19) 0.0041(18) -0.0061(18)
C63 0.017(2) 0.023(2) 0.019(3) -0.0032(19) 0.0033(19) -0.0011(17)
C64 0.024(2) 0.022(2) 0.016(3) -0.0034(19) 0.0074(19) -0.0042(18)
C65 0.020(2) 0.025(2) 0.028(3) -0.007(2) 0.006(2) -0.0028(18)
C66 0.023(2) 0.019(2) 0.021(3) -0.0004(19) 0.008(2) 0.0013(17)
C67 0.017(2) 0.023(2) 0.022(3) 0.001(2) 0.0059(19) 0.0009(17)
C68 0.018(2) 0.023(2) 0.021(3) -0.002(2) 0.0051(19) -0.0048(18)
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C70 0.032(3) 0.035(3) 0.019(3) 0.000(2) 0.006(2) 0.007(2)
C71 0.033(3) 0.033(3) 0.026(3) 0.000(2) 0.012(2) 0.001(2)
C72 0.044(3) 0.031(3) 0.021(3) 0.003(2) 0.008(2) 0.006(2)
C73 0.019(2) 0.020(2) 0.013(2) 0.0016(18) 0.0044(18) 0.0011(17)
C74 0.021(2) 0.019(2) 0.010(2) -0.0016(18) 0.0086(18) 0.0009(17)
C75 0.014(2) 0.016(2) 0.017(3) 0.0004(18) 0.0061(18) -0.0028(16)
C76 0.023(2) 0.022(2) 0.011(2) -0.0030(18) 0.0042(18) 0.0000(18)
C77 0.024(2) 0.022(2) 0.010(2) 0.0020(18) 0.0019(18) -0.0001(18)
C78 0.024(2) 0.019(2) 0.013(3) 0.0022(18) 0.0068(19) -0.0010(17)
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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.
;
loop_
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Zn1 N1 2.107(4) . ?
Zn1 N7 2.194(4) . ?
Zn2 O4 1.960(3) . ?
Zn2 O3 1.966(3) . ?
Zn2 N4 2.082(4) . ?
Zn2 N3 2.111(4) . ?
Zn2 N8 2.201(4) . ?
Zn3 O5 1.959(3) . ?
Zn3 O6 1.969(3) . ?
Zn3 N6 2.071(4) . ?
Zn3 N5 2.123(4) . ?
Zn3 N9 2.200(3) . ?
P1 C76 1.845(5) . ?

P1 C77 1.845(5) . ?
P1 C78 1.853(4) . ?
N1 C7 1.304(6) . ?
N1 C8 1.425(6) . ?
N2 C14 1.293(6) . ?
N2 C13 1.428(7) . ?
N3 C31 1.296(6) . ?
N3 C32 1.423(6) . ?
N4 C38 1.288(6) . ?
N4 C37 1.420(6) . ?
N5 C55 1.306(6) . ?
N5 C56 1.411(6) . ?
N6 C62 1.300(6) . ?
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N7 C73 1.485(6) . ?
N7 C75 1.487(5) . ?
N7 C76 1.495(6) . ?
N8 C74 1.481(6) . ?
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C35 C36 1.386(7) . ?
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C67 C69 1.541(7) . ?
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C69 C72 1.538(7) . ?
C69 C70 1.543(7) . ?
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N5 Zn3 N9 103.24(13) . . ?
C76 P1 C77 96.4(2) . . ?
C76 P1 C78 96.4(2) . . ?
C77 P1 C78 96.0(2) . . ?
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C7 N1 Zn1 124.5(3) . . ?
C8 N1 Zn1 113.6(3) . . ?
C14 N2 C13 119.8(4) . . ?
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C31 N3 C32 121.0(4) . . ?
C31 N3 Zn2 124.4(3) . . ?
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C38 N4 C37 120.8(4) . . ?
C38 N4 Zn2 124.8(3) . . ?
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F1 C2 C3 118.1(4) . . ?
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C3 C2 C1 125.6(5) . . ?
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C5 C4 C3 123.0(4) . . ?
F2 C4 C3 117.0(4) . . ?
C4 C5 C6 119.8(5) . . ?
C1 C6 C7 124.1(4) . . ?
C1 C6 C5 119.9(4) . . ?
C7 C6 C5 115.7(4) . . ?
N1 C7 C6 125.2(5) . . ?
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C12 C11 C10 120.2(5) . . ?
C11 C12 C13 120.4(4) . . ?
C12 C13 C8 119.7(5) . . ?
C12 C13 N2 124.3(4) . . ?
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N2 C14 C15 127.3(4) . . ?

C16 C15 C20 120.5(4) . . ?
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F3 C26 C25 117.0(4) . . ?
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O6 C68 C67 119.8(4) . . ?
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'-x, y, -z+1/2'
'x+1/2, y+1/2, z'
'-x+1/2, y+1/2, -z+1/2'
'-x, -y, -z'
'x, -y, z-1/2'
'-x+1/2, -y+1/2, -z'
'x+1/2, -y+1/2, z-1/2'
_cell_length_a                 30.798(2)
_cell_length_b                 13.5677(9)
_cell_length_c                 29.886(2)
_cell_angle_alpha               90.00
_cell_angle_beta                101.815(2)
_cell_angle_gamma               90.00
_cell_volume                   12223.7(14)
_cell_formula_units_Z           8
_cell_measurement_temperature    100(2)
_cell_measurement_reflns_used    9798
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_cell_measurement_theta_max      28.06
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_exptl_crystal_colour            orange
_exptl_crystal_size_max          0.20
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_exptl_crystal_size_min          0.15
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.434
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             5488
_exptl_absorpt_coefficient_mu    1.041
_exptl_absorpt_correction_type   empirical
_exptl_absorpt_correction_T_min  0.8188
_exptl_absorpt_correction_T_max  0.8595
_exptl_absorpt_process_details
;
SADABS Version 2008/1 Bruker-Nonius
Blessing, Acta Cryst. (1995) A51 33-38
```

;
_exptl_special_details
;
It should be noted that the esd's of the cell dimensions are probably too low;
they should be multiplied by a factor of 2 to 10
;
_diffrn_ambient_temperature 100(2)
_diffrn_measurement_specimen_suppport 'magnetic support whith MicroMount'
_diffrn_radiation_wavelength 0.71073
_diffrn_radiation_type MoK\a
_diffrn_source 'Micorfocus source E025 IuS'
_diffrn_source_type 'Bruker APEX DUO'
_diffrn_source_power 50
_diffrn_source_current 0.6
_diffrn_source_size '0.2 mm x 0.2 mm fine focus'
_diffrn_radiation_monochromator 'Quazar MX Multilayer Optics'
_diffrn_detector_type '4K CCD area detector APEX II'
_diffrn_measurement_device_type 'APEX DUO Kappa 4-axis goniometer'
_diffrn_measurement_method
;
Fullsphere data collection, phi and omega scans
;
_diffrn_detector_area_resol_mean 512
_diffrn_reflns_number 211665
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_diffrn_reflns_av_sigmaI/netI 0.0229
_diffrn_reflns_limit_h_min -40
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_diffrn_reflns_limit_l_min -39
_diffrn_reflns_limit_l_max 39
_diffrn_reflns_theta_min 1.35
_diffrn_reflns_theta_max 28.20
_reflns_number_total 15010
_reflns_number_gt 12760
_reflns_threshold_expression >2sigma(I)
_computing_data_collection 'Bruker APEX2 v2011.4-0'
_computing_cell_refinement 'Bruker APEX2 v2011.4-0'
_computing_data_reduction 'Bruker SAINT V7.60A'
_computing_structure_solution Sir2011
_computing_structure_refinement 'SHELXS-97 (Sheldrick, 2008)'
_computing_molecular_graphics 'Bruker SHELXTL'
_computing_publication_material 'Bruker SHELXTL'
_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.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0266P)^2^+22.9438P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment noref
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_number_reflns 15010
_refine_ls_number_parameters 855
_refine_ls_number_restraints 237
_refine_ls_R_factor_all 0.0408
_refine_ls_R_factor_gt 0.0310
_refine_ls_wR_factor_ref 0.0753
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_refine_ls_goodness_of_fit_ref 1.060
_refine_ls_restrained_S_all 1.059
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_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Zn1 Zn 0.891776(6) 0.947604(15) 0.505822(6) 0.01495(5) Uani 1 1 d . . .
Zn2 Zn 0.914352(6) 0.815517(14) 0.693561(6) 0.01366(5) Uani 1 1 d . . .
Cl1 Cl 0.83001(2) 1.42749(4) 0.54321(2) 0.04877(16) Uani 1 1 d . . .
Cl2 Cl 0.92621(2) 1.40912(4) 0.605325(19) 0.03540(12) Uani 1 1 d . . .
Cl3 Cl 1.103982(14) 0.60653(3) 0.643225(15) 0.02239(9) Uani 1 1 d . . .
Cl4 Cl 1.053918(16) 0.42355(3) 0.67354(2) 0.03329(12) Uani 1 1 d . . .
N1 N 0.85012(5) 1.06944(11) 0.49062(5) 0.0197(3) Uani 1 1 d . . .
N2 N 0.92984(5) 1.05421(10) 0.54406(5) 0.0160(3) Uani 1 1 d . A .
N3 N 0.97814(5) 0.82281(10) 0.68157(5) 0.0153(3) Uani 1 1 d . . .
N4 N 0.93554(5) 0.66940(10) 0.70539(5) 0.0154(3) Uani 1 1 d . A .
O1 O 0.86466(4) 0.89007(10) 0.44697(4) 0.0216(3) Uani 1 1 d . . .
O2 O 0.94188(4) 0.85428(9) 0.51992(4) 0.0167(2) Uani 1 1 d . . .
O3 O 0.91095(4) 0.96109(9) 0.69078(4) 0.0172(2) Uani 1 1 d . . .
O4 O 0.87727(4) 0.79577(9) 0.73871(4) 0.0171(2) Uani 1 1 d . . .
C1 C 0.82769(6) 0.91070(15) 0.41908(6) 0.0231(4) Uani 1 1 d . . .
C2 C 0.81334(7) 0.84815(17) 0.37975(6) 0.0287(5) Uani 1 1 d . . .
C3 C 0.77340(7) 0.86917(19) 0.35100(7) 0.0376(6) Uani 1 1 d . . .
H3 H 0.7638 0.8283 0.3250 0.045 Uiso 1 1 calc R A .

C4 C 0.74643(7) 0.94748(19) 0.35821(8) 0.0426(6) Uani 1 1 d . . .
H4 H 0.7185 0.9574 0.3382 0.051 Uiso 1 1 calc R . .
C5 C 0.76022(7) 1.01003(18) 0.39415(8) 0.0362(5) Uani 1 1 d . . .
H5 H 0.7422 1.0647 0.3984 0.043 Uiso 1 1 calc R A .
C6 C 0.80110(6) 0.99444(15) 0.42523(6) 0.0254(4) Uani 1 1 d . . .
C7 C 0.81463(6) 1.07060(15) 0.45839(7) 0.0245(4) Uani 1 1 d . . .
H7 H 0.7960 1.1269 0.4567 0.029 Uiso 1 1 calc R A .
C8 C 0.86460(6) 1.15213(14) 0.51847(6) 0.0210(4) Uani 1 1 d . . .
C9 C 0.84086(7) 1.23948(15) 0.51906(7) 0.0285(4) Uani 1 1 d . . .
H9 H 0.8117 1.2448 0.5012 0.034 Uiso 1 1 calc R . .
C10 C 0.85935(7) 1.31824(15) 0.54538(7) 0.0310(5) Uani 1 1 d . . .
C11 C 0.90149(7) 1.31013(14) 0.57300(7) 0.0266(4) Uani 1 1 d . . .
C12 C 0.92493(6) 1.22287(13) 0.57424(6) 0.0215(4) Uani 1 1 d . . .
H12 H 0.9531 1.2166 0.5942 0.026 Uiso 1 1 calc R A .
C13 C 0.90744(6) 1.14421(13) 0.54641(6) 0.0185(3) Uani 1 1 d . A .
C14 C 0.97261(6) 1.04779(13) 0.55791(6) 0.0169(3) Uani 1 1 d . . .
H14 H 0.9875 1.1060 0.5703 0.020 Uiso 1 1 calc R A .
C15 C 0.99953(5) 0.96276(12) 0.55647(6) 0.0153(3) Uani 1 1 d . . .
C16 C 1.04537(6) 0.97594(13) 0.57476(6) 0.0182(3) Uani 1 1 d . . .
H16 H 1.0558 1.0383 0.5869 0.022 Uiso 1 1 calc R A .
C17 C 1.07488(6) 0.90056(13) 0.57529(6) 0.0186(3) Uani 1 1 d . . .
H17 H 1.1055 0.9099 0.5879 0.022 Uiso 1 1 calc R . .
C18 C 1.05919(6) 0.80918(13) 0.55688(6) 0.0174(3) Uani 1 1 d . . .
H18 H 1.0799 0.7571 0.5574 0.021 Uiso 1 1 calc R A .
C19 C 1.01508(6) 0.79081(12) 0.53794(6) 0.0155(3) Uani 1 1 d . . .
C20 C 0.98350(5) 0.86943(12) 0.53744(5) 0.0141(3) Uani 1 1 d . . .
C21 C 0.84232(7) 0.76166(18) 0.37078(7) 0.0332(5) Uani 1 1 d . . .
C22 C 0.82221(9) 0.7060(2) 0.32655(8) 0.0546(8) Uani 1 1 d . . .
H22A H 0.7939 0.6763 0.3295 0.082 Uiso 1 1 calc R . .
H22B H 0.8427 0.6541 0.3212 0.082 Uiso 1 1 calc R . .
H22C H 0.8172 0.7521 0.3008 0.082 Uiso 1 1 calc R . .
C23 C 0.88824(7) 0.79986(19) 0.36574(7) 0.0389(6) Uani 1 1 d . . .
H23A H 0.8845 0.8534 0.3433 0.058 Uiso 1 1 calc R . .
H23B H 0.9050 0.7461 0.3554 0.058 Uiso 1 1 calc R . .
H23C H 0.9044 0.8244 0.3953 0.058 Uiso 1 1 calc R . .
C24 C 0.84842(7) 0.68656(17) 0.40972(8) 0.0338(5) Uani 1 1 d . . .
H24A H 0.8642 0.7175 0.4380 0.051 Uiso 1 1 calc R . .
H24B H 0.8656 0.6304 0.4023 0.051 Uiso 1 1 calc R . .
H24C H 0.8193 0.6637 0.4138 0.051 Uiso 1 1 calc R . .
C25 C 0.99945(6) 0.68851(13) 0.51914(6) 0.0187(3) Uani 1 1 d . . .
C26 C 0.96859(6) 0.64375(13) 0.54841(6) 0.0220(4) Uani 1 1 d . . .
H26A H 0.9849 0.6361 0.5800 0.033 Uiso 1 1 calc R . .
H26B H 0.9581 0.5792 0.5361 0.033 Uiso 1 1 calc R . .
H26C H 0.9432 0.6875 0.5478 0.033 Uiso 1 1 calc R . .
C27 C 0.97476(6) 0.69474(14) 0.46894(6) 0.0226(4) Uani 1 1 d . . .
H27A H 0.9498 0.7407 0.4664 0.034 Uiso 1 1 calc R . .
H27B H 0.9636 0.6293 0.4584 0.034 Uiso 1 1 calc R . .
H27C H 0.9951 0.7182 0.4500 0.034 Uiso 1 1 calc R . .
C28 C 1.03867(6) 0.61770(14) 0.52099(7) 0.0248(4) Uani 1 1 d . . .
H28A H 1.0598 0.6463 0.5042 0.037 Uiso 1 1 calc R . .
H28B H 1.0278 0.5546 0.5071 0.037 Uiso 1 1 calc R . .
H28C H 1.0534 0.6069 0.5529 0.037 Uiso 1 1 calc R . .
C29 C 0.94075(6) 1.02759(12) 0.68884(5) 0.0146(3) Uani 1 1 d . . .
C30 C 0.93034(6) 1.13093(13) 0.69199(6) 0.0168(3) Uani 1 1 d . . .

C31 C 0.96313(6) 1.19923(13) 0.69027(6) 0.0219(4) Uani 1 1 d . . .
H31 H 0.9564 1.2671 0.6928 0.026 Uiso 1 1 calc R A .
C32 C 1.00599(6) 1.17385(14) 0.68497(7) 0.0242(4) Uani 1 1 d . . .
H32 H 1.0274 1.2235 0.6836 0.029 Uiso 1 1 calc R . .
C33 C 1.01638(6) 1.07692(14) 0.68185(6) 0.0213(4) Uani 1 1 d . . .
H33 H 1.0454 1.0592 0.6784 0.026 Uiso 1 1 calc R A .
C34 C 0.98478(6) 1.00230(12) 0.68362(6) 0.0165(3) Uani 1 1 d . . .
C35 C 1.00043(6) 0.90391(13) 0.68109(6) 0.0177(3) Uani 1 1 d . . .
H35 H 1.0306 0.8969 0.6788 0.021 Uiso 1 1 calc R A .
C36 C 0.99845(5) 0.73012(12) 0.67892(6) 0.0155(3) Uani 1 1 d . . .
C37 C 1.03801(6) 0.71592(13) 0.66394(6) 0.0171(3) Uani 1 1 d . . .
H37 H 1.0533 0.7709 0.6549 0.021 Uiso 1 1 calc R . .
C38 C 1.05510(6) 0.62218(13) 0.66220(6) 0.0182(3) Uani 1 1 d . . .
C39 C 1.03288(6) 0.54111(13) 0.67512(6) 0.0202(4) Uani 1 1 d . . .
C40 C 0.99322(6) 0.55382(13) 0.68940(6) 0.0192(3) Uani 1 1 d . . .
H40 H 0.9781 0.4982 0.6980 0.023 Uiso 1 1 calc R A .
C41 C 0.97547(5) 0.64762(13) 0.69125(6) 0.0158(3) Uani 1 1 d . A .
C42 C 0.91151(6) 0.60220(12) 0.71933(6) 0.0161(3) Uani 1 1 d . . .
H42 H 0.9212 0.5359 0.7186 0.019 Uiso 1 1 calc R A .
C43 C 0.87165(6) 0.61922(13) 0.73571(6) 0.0161(3) Uani 1 1 d . . .
C44 C 0.84813(6) 0.53427(13) 0.74430(6) 0.0184(3) Uani 1 1 d . . .
H44 H 0.8588 0.4710 0.7382 0.022 Uiso 1 1 calc R A .
C45 C 0.81038(6) 0.54163(14) 0.76113(6) 0.0208(4) Uani 1 1 d . . .
H45 H 0.7942 0.4843 0.7659 0.025 Uiso 1 1 calc R . .
C46 C 0.79572(6) 0.63531(14) 0.77132(6) 0.0198(4) Uani 1 1 d . . .
H46 H 0.7692 0.6395 0.7829 0.024 Uiso 1 1 calc R A .
C47 C 0.81766(5) 0.72184(13) 0.76550(6) 0.0163(3) Uani 1 1 d . . .
C48 C 0.85661(5) 0.71563(13) 0.74582(5) 0.0150(3) Uani 1 1 d . . .
C49 C 0.88381(6) 1.16313(13) 0.69726(6) 0.0195(4) Uani 1 1 d . . .
C50 C 0.87211(6) 1.11591(15) 0.73992(6) 0.0246(4) Uani 1 1 d . . .
H50A H 0.8927 1.1397 0.7673 0.037 Uiso 1 1 calc R . .
H50B H 0.8745 1.0441 0.7380 0.037 Uiso 1 1 calc R . .
H50C H 0.8417 1.1338 0.7418 0.037 Uiso 1 1 calc R . .
C51 C 0.88056(7) 1.27528(14) 0.70301(8) 0.0311(5) Uani 1 1 d . . .
H51A H 0.9025 1.2966 0.7298 0.047 Uiso 1 1 calc R . .
H51B H 0.8507 1.2924 0.7072 0.047 Uiso 1 1 calc R . .
H51C H 0.8863 1.3084 0.6757 0.047 Uiso 1 1 calc R . .
C52 C 0.84931(6) 1.13435(15) 0.65454(6) 0.0243(4) Uani 1 1 d . . .
H52A H 0.8196 1.1523 0.6589 0.036 Uiso 1 1 calc R . .
H52B H 0.8506 1.0631 0.6496 0.036 Uiso 1 1 calc R . .
H52C H 0.8556 1.1693 0.6279 0.036 Uiso 1 1 calc R . .
C53 C 0.80278(6) 0.82152(13) 0.78152(6) 0.0178(3) Uani 1 1 d . . .
C54 C 0.75959(6) 0.81194(15) 0.79930(7) 0.0247(4) Uani 1 1 d . . .
H54A H 0.7506 0.8770 0.8084 0.037 Uiso 1 1 calc R . .
H54B H 0.7644 0.7676 0.8257 0.037 Uiso 1 1 calc R . .
H54C H 0.7362 0.7852 0.7751 0.037 Uiso 1 1 calc R . .
C55 C 0.83891(6) 0.86015(15) 0.82116(6) 0.0236(4) Uani 1 1 d . . .
H55A H 0.8664 0.8712 0.8102 0.035 Uiso 1 1 calc R . .
H55B H 0.8442 0.8115 0.8459 0.035 Uiso 1 1 calc R . .
H55C H 0.8291 0.9223 0.8325 0.035 Uiso 1 1 calc R . .
C56 C 0.79462(6) 0.89845(14) 0.74305(6) 0.0219(4) Uani 1 1 d . . .
H56A H 0.8219 0.9082 0.7316 0.033 Uiso 1 1 calc R . .
H56B H 0.7857 0.9610 0.7549 0.033 Uiso 1 1 calc R . .
H56C H 0.7710 0.8753 0.7181 0.033 Uiso 1 1 calc R . .

P1 P 0.81476(2) 0.68346(5) 0.55711(2) 0.01689(14) Uani 0.75 1 d PDU A 1
N5 N 0.85566(4) 0.86774(10) 0.55014(5) 0.0145(3) Uani 0.75 1 d PDU A 1
N6 N 0.86694(4) 0.79749(10) 0.62837(5) 0.0145(3) Uani 0.75 1 d PDU A 1
N7 N 0.79406(9) 0.8669(2) 0.59078(11) 0.0160(6) Uani 0.75 1 d PDU A 1
C57 C 0.84266(11) 0.7723(2) 0.52579(10) 0.0168(6) Uani 0.75 1 d PDU A 1
H57A H 0.8697 0.7409 0.5192 0.020 Uiso 0.75 1 calc PR A 1
H57B H 0.8227 0.7870 0.4961 0.020 Uiso 0.75 1 calc PR A 1
C58 C 0.85540(12) 0.6938(2) 0.61253(11) 0.0162(6) Uani 0.75 1 d PDU A 1
H58A H 0.8432 0.6592 0.6364 0.019 Uiso 0.75 1 calc PR A 1
H58B H 0.8830 0.6594 0.6096 0.019 Uiso 0.75 1 calc PR A 1
C59 C 0.77391(8) 0.77373(18) 0.57079(8) 0.0167(4) Uani 0.75 1 d PDU A 1
H59A H 0.7520 0.7890 0.5425 0.020 Uiso 0.75 1 calc PR A 1
H59B H 0.7577 0.7430 0.5925 0.020 Uiso 0.75 1 calc PR A 1
C60 C 0.88670(10) 0.8514(2) 0.59438(9) 0.0142(5) Uani 0.75 1 d PDU A 1
H60A H 0.9126 0.8139 0.5888 0.017 Uiso 0.75 1 calc PR A 1
H60B H 0.8975 0.9161 0.6074 0.017 Uiso 0.75 1 calc PR A 1
C61 C 0.81572(10) 0.9201(2) 0.55939(12) 0.0149(6) Uani 0.75 1 d PDU A 1
H61A H 0.8247 0.9860 0.5723 0.018 Uiso 0.75 1 calc PR A 1
H61B H 0.7943 0.9300 0.5302 0.018 Uiso 0.75 1 calc PR A 1
C62 C 0.82513(10) 0.8497(3) 0.63322(10) 0.0151(6) Uani 0.75 1 d PDU A 1
H62A H 0.8102 0.8103 0.6535 0.018 Uiso 0.75 1 calc PR A 1
H62B H 0.8332 0.9140 0.6483 0.018 Uiso 0.75 1 calc PR A 1
P1' P 0.77991(9) 0.8480(3) 0.58806(12) 0.0287(7) Uani 0.25 1 d PDU A 2
N5' N 0.83234(19) 0.6960(4) 0.5628(2) 0.0230(13) Uani 0.25 1 d PDU A 2
N6' N 0.86694(4) 0.79749(10) 0.62837(5) 0.0145(3) Uani 0.25 1 d PDU A 2
N7' N 0.85566(4) 0.86774(10) 0.55014(5) 0.0145(3) Uani 0.25 1 d PDU A 2
C57' C 0.78606(19) 0.7239(4) 0.5655(2) 0.0274(13) Uani 0.25 1 d PDU A 2
H57C H 0.7748 0.6754 0.5850 0.033 Uiso 0.25 1 calc PR A 2
H57D H 0.7672 0.7193 0.5344 0.033 Uiso 0.25 1 calc PR A 2
C58' C 0.8250(2) 0.8361(8) 0.6396(2) 0.0172(17) Uani 0.25 1 d PDU A 2
H58C H 0.8309 0.9014 0.6544 0.021 Uiso 0.25 1 calc PR A 2
H58D H 0.8153 0.7911 0.6617 0.021 Uiso 0.25 1 calc PR A 2
C59' C 0.8122(2) 0.9130(6) 0.5511(3) 0.0156(17) Uani 0.25 1 d PDU A 2
H59C H 0.7943 0.9149 0.5196 0.019 Uiso 0.25 1 calc PR A 2
H59D H 0.8170 0.9819 0.5619 0.019 Uiso 0.25 1 calc PR A 2
C60' C 0.8617(3) 0.6973(4) 0.6088(3) 0.0188(16) Uani 0.25 1 d PDU A 2
H60C H 0.8491 0.6537 0.6294 0.023 Uiso 0.25 1 calc PR A 2
H60D H 0.8912 0.6711 0.6066 0.023 Uiso 0.25 1 calc PR A 2
C61' C 0.8505(3) 0.7669(5) 0.5328(3) 0.0195(15) Uani 0.25 1 d PDU A 2
H61C H 0.8797 0.7426 0.5288 0.023 Uiso 0.25 1 calc PR A 2
H61D H 0.8304 0.7677 0.5024 0.023 Uiso 0.25 1 calc PR A 2
C62' C 0.8832(3) 0.8653(6) 0.5957(2) 0.0142(5) Uani 0.25 1 d PDU A 2
H62C H 0.8852 0.9328 0.6085 0.017 Uiso 0.25 1 calc PR A 2
H62D H 0.9135 0.8448 0.5934 0.017 Uiso 0.25 1 calc PR A 2
N1S N 0.7469(2) 0.2088(4) 0.5743(2) 0.0511(14) Uani 0.65 1 d PDU B 1
C1S C 0.7326(3) 0.1381(4) 0.5844(3) 0.0398(14) Uani 0.65 1 d PDU B 1
C2S C 0.71445(19) 0.0517(4) 0.6018(3) 0.0518(15) Uani 0.65 1 d PDU B 1
H2S1 H 0.7358 -0.0025 0.6043 0.078 Uiso 0.65 1 calc PR B 1
H2S2 H 0.6868 0.0328 0.5810 0.078 Uiso 0.65 1 calc PR B 1
H2S3 H 0.7083 0.0660 0.6321 0.078 Uiso 0.65 1 calc PR B 1
N1S' N 0.7522(5) 0.1816(10) 0.5618(5) 0.078(4) Uani 0.35 1 d PDU C 2
C1S' C 0.7302(7) 0.1348(15) 0.5788(8) 0.073(4) Uani 0.35 1 d PDU C 2
C2S' C 0.6999(4) 0.0657(12) 0.5927(6) 0.085(5) Uani 0.35 1 d PDU C 2
H2S4 H 0.6867 0.0243 0.5666 0.128 Uiso 0.35 1 calc PR C 2

H2S5 H 0.6764 0.1018 0.6034 0.128 Uiso 0.35 1 calc PR C 2
H2S6 H 0.7160 0.0242 0.6174 0.128 Uiso 0.35 1 calc PR C 2
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_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Zn1 0.01285(9) 0.02076(10) 0.01111(9) -0.00060(7) 0.00220(7) -0.00003(7)
Zn2 0.01293(9) 0.01453(9) 0.01399(9) 0.00068(7) 0.00384(7) 0.00032(7)
Cl1 0.0599(4) 0.0348(3) 0.0537(4) 0.0029(3) 0.0166(3) 0.0284(3)
Cl2 0.0547(3) 0.0190(2) 0.0367(3) -0.0053(2) 0.0191(3) 0.0019(2)
Cl3 0.01549(19) 0.0291(2) 0.0236(2) -0.00094(17) 0.00647(17) 0.00536(17)
Cl4 0.0247(2) 0.0186(2) 0.0588(3) -0.0015(2) 0.0138(2) 0.00619(18)
N1 0.0180(7) 0.0271(8) 0.0149(7) 0.0061(6) 0.0052(6) 0.0030(6)
N2 0.0182(7) 0.0174(7) 0.0127(7) 0.0016(5) 0.0039(6) 0.0015(6)
N3 0.0149(7) 0.0168(7) 0.0144(7) 0.0001(5) 0.0035(6) 0.0011(5)
N4 0.0139(7) 0.0172(7) 0.0152(7) 0.0007(5) 0.0031(6) 0.0003(5)
O1 0.0159(6) 0.0350(7) 0.0130(6) -0.0038(5) 0.0007(5) -0.0032(5)
O2 0.0129(6) 0.0189(6) 0.0180(6) -0.0029(5) 0.0027(5) -0.0006(5)
O3 0.0157(6) 0.0155(6) 0.0207(6) -0.0011(5) 0.0046(5) -0.0011(5)
O4 0.0177(6) 0.0166(6) 0.0184(6) -0.0003(5) 0.0071(5) -0.0008(5)
C1 0.0169(9) 0.0395(11) 0.0128(8) 0.0072(7) 0.0027(7) -0.0099(8)
C2 0.0252(10) 0.0463(12) 0.0132(8) 0.0049(8) 0.0007(7) -0.0215(9)
C3 0.0350(12) 0.0527(14) 0.0201(10) 0.0125(10) -0.0061(9) -0.0261(11)
C4 0.0268(11) 0.0603(16) 0.0319(12) 0.0269(11) -0.0148(9) -0.0240(11)
C5 0.0209(10) 0.0468(13) 0.0370(12) 0.0261(10) -0.0032(9) -0.0069(9)
C6 0.0188(9) 0.0372(11) 0.0186(9) 0.0127(8) 0.0000(7) -0.0062(8)
C7 0.0181(9) 0.0316(10) 0.0244(9) 0.0143(8) 0.0058(8) 0.0025(8)
C8 0.0230(9) 0.0245(9) 0.0179(8) 0.0060(7) 0.0098(7) 0.0052(7)
C9 0.0279(10) 0.0314(11) 0.0277(10) 0.0078(8) 0.0096(8) 0.0124(8)
C10 0.0402(12) 0.0248(10) 0.0322(11) 0.0067(8) 0.0176(9) 0.0155(9)
C11 0.0376(11) 0.0208(9) 0.0253(10) 0.0006(8) 0.0159(9) 0.0032(8)
C12 0.0267(9) 0.0206(9) 0.0194(9) 0.0016(7) 0.0103(8) 0.0029(7)
C13 0.0229(9) 0.0189(8) 0.0159(8) 0.0036(7) 0.0095(7) 0.0029(7)
C14 0.0195(8) 0.0176(8) 0.0135(8) -0.0003(6) 0.0036(7) -0.0025(7)
C15 0.0160(8) 0.0169(8) 0.0132(8) 0.0011(6) 0.0032(6) -0.0008(6)
C16 0.0184(8) 0.0204(8) 0.0158(8) 0.0001(7) 0.0036(7) -0.0038(7)
C17 0.0140(8) 0.0256(9) 0.0156(8) 0.0028(7) 0.0017(7) -0.0024(7)
C18 0.0166(8) 0.0198(8) 0.0164(8) 0.0036(7) 0.0051(7) 0.0026(7)
C19 0.0176(8) 0.0163(8) 0.0134(8) 0.0010(6) 0.0048(7) -0.0007(6)
C20 0.0152(8) 0.0177(8) 0.0099(7) 0.0014(6) 0.0041(6) -0.0012(6)
C21 0.0293(11) 0.0539(14) 0.0177(9) -0.0152(9) 0.0079(8) -0.0252(10)
C22 0.0496(15) 0.083(2) 0.0322(13) -0.0282(13) 0.0097(11) -0.0391(15)
C23 0.0349(12) 0.0588(15) 0.0284(11) -0.0203(10) 0.0190(10) -0.0266(11)
C24 0.0307(11) 0.0392(12) 0.0350(11) -0.0130(10) 0.0153(9) -0.0115(9)
C25 0.0193(8) 0.0176(8) 0.0204(9) -0.0020(7) 0.0072(7) 0.0002(7)
C26 0.0255(9) 0.0179(8) 0.0243(9) -0.0010(7) 0.0092(8) -0.0019(7)
C27 0.0256(9) 0.0222(9) 0.0209(9) -0.0052(7) 0.0068(8) -0.0023(7)
C28 0.0254(10) 0.0203(9) 0.0298(10) -0.0048(8) 0.0082(8) 0.0017(7)
C29 0.0174(8) 0.0171(8) 0.0086(7) -0.0003(6) 0.0007(6) -0.0004(6)
C30 0.0200(8) 0.0177(8) 0.0126(8) -0.0014(6) 0.0028(7) 0.0004(7)

C31 0.0264(9) 0.0159(8) 0.0229(9) -0.0019(7) 0.0038(8) -0.0007(7)
C32 0.0240(9) 0.0200(9) 0.0291(10) -0.0010(7) 0.0063(8) -0.0076(7)
C33 0.0175(8) 0.0235(9) 0.0232(9) 0.0000(7) 0.0048(7) -0.0031(7)
C34 0.0170(8) 0.0177(8) 0.0149(8) 0.0000(6) 0.0038(7) -0.0020(6)
C35 0.0150(8) 0.0223(9) 0.0162(8) -0.0005(7) 0.0044(7) -0.0005(7)
C36 0.0144(8) 0.0188(8) 0.0127(8) -0.0005(6) 0.0014(6) 0.0012(6)
C37 0.0145(8) 0.0202(8) 0.0164(8) -0.0007(7) 0.0026(7) -0.0009(6)
C38 0.0128(8) 0.0242(9) 0.0175(8) -0.0012(7) 0.0028(7) 0.0027(7)
C39 0.0175(8) 0.0184(8) 0.0234(9) -0.0023(7) 0.0013(7) 0.0041(7)
C40 0.0168(8) 0.0174(8) 0.0230(9) -0.0005(7) 0.0036(7) -0.0002(7)
C41 0.0140(8) 0.0194(8) 0.0137(8) -0.0009(6) 0.0018(6) 0.0005(6)
C42 0.0168(8) 0.0165(8) 0.0141(8) -0.0004(6) 0.0010(7) 0.0002(6)
C43 0.0153(8) 0.0192(8) 0.0129(8) -0.0004(6) 0.0007(6) -0.0019(6)
C44 0.0179(8) 0.0181(8) 0.0179(8) -0.0016(7) 0.0007(7) -0.0032(7)
C45 0.0173(8) 0.0232(9) 0.0210(9) -0.0005(7) 0.0021(7) -0.0075(7)
C46 0.0137(8) 0.0290(9) 0.0169(8) -0.0017(7) 0.0036(7) -0.0044(7)
C47 0.0137(8) 0.0223(8) 0.0120(8) -0.0007(6) 0.0006(6) 0.0000(6)
C48 0.0136(8) 0.0197(8) 0.0108(7) 0.0002(6) 0.0003(6) -0.0006(6)
C49 0.0224(9) 0.0164(8) 0.0204(9) -0.0017(7) 0.0056(7) 0.0011(7)
C50 0.0266(10) 0.0283(10) 0.0210(9) -0.0041(8) 0.0094(8) 0.0017(8)
C51 0.0313(11) 0.0204(9) 0.0434(12) -0.0053(9) 0.0120(10) 0.0038(8)
C52 0.0221(9) 0.0269(10) 0.0226(9) 0.0003(8) 0.0018(8) 0.0039(7)
C53 0.0143(8) 0.0242(9) 0.0155(8) -0.0032(7) 0.0043(7) -0.0006(7)
C54 0.0213(9) 0.0320(10) 0.0234(9) -0.0039(8) 0.0104(8) -0.0001(8)
C55 0.0221(9) 0.0283(10) 0.0194(9) -0.0069(7) 0.0018(7) -0.0001(8)
C56 0.0176(8) 0.0275(9) 0.0210(9) -0.0016(7) 0.0051(7) 0.0047(7)
P1 0.0159(3) 0.0186(3) 0.0157(3) -0.0023(2) 0.0021(3) -0.0040(3)
N5 0.0124(6) 0.0188(7) 0.0125(6) -0.0013(5) 0.0026(5) -0.0008(5)
N6 0.0144(6) 0.0160(6) 0.0140(6) 0.0005(5) 0.0046(5) 0.0000(5)
N7 0.0106(13) 0.0211(12) 0.0165(11) -0.0014(9) 0.0033(11) 0.0005(10)
C57 0.0135(14) 0.0231(13) 0.0142(13) -0.0053(10) 0.0038(11) -0.0027(10)
C58 0.0160(13) 0.0167(12) 0.0158(12) 0.0001(10) 0.0031(10) 0.0002(10)
C59 0.0133(10) 0.0195(11) 0.0173(11) -0.0005(9) 0.0033(9) -0.0025(9)
C60 0.0117(8) 0.0167(11) 0.0143(8) 0.0012(7) 0.0033(6) 0.0008(8)
C61 0.0135(12) 0.0206(13) 0.0106(13) 0.0022(10) 0.0023(10) 0.0024(10)
C62 0.0145(12) 0.0202(13) 0.0119(11) 0.0017(10) 0.0056(9) 0.0011(10)
P1' 0.0150(14) 0.051(2) 0.0201(12) 0.0099(12) 0.0029(11) 0.0015(13)
N5' 0.022(3) 0.026(2) 0.021(2) -0.004(2) 0.005(2) -0.007(2)
N6' 0.0144(6) 0.0160(6) 0.0140(6) 0.0005(5) 0.0046(5) 0.0000(5)
N7' 0.0124(6) 0.0188(7) 0.0125(6) -0.0013(5) 0.0026(5) -0.0008(5)
C57' 0.023(3) 0.038(3) 0.018(3) 0.001(3) -0.001(3) -0.015(3)
C58' 0.013(3) 0.023(4) 0.014(3) 0.001(3) 0.002(2) 0.000(3)
C59' 0.011(3) 0.025(3) 0.012(3) -0.002(3) 0.003(2) -0.001(3)
C60' 0.019(3) 0.020(3) 0.018(3) 0.000(2) 0.006(3) -0.006(3)
C61' 0.017(3) 0.024(3) 0.017(3) -0.004(2) 0.000(3) -0.004(2)
C62' 0.0117(8) 0.0167(11) 0.0143(8) 0.0012(7) 0.0033(6) 0.0008(8)
N1S 0.049(3) 0.040(2) 0.055(3) 0.0144(19) -0.011(2) 0.0064(18)
C1S 0.037(3) 0.029(2) 0.048(3) 0.003(2) -0.005(2) 0.0109(19)
C2S 0.045(3) 0.035(2) 0.078(4) 0.001(2) 0.018(3) 0.005(2)
N1S' 0.042(5) 0.118(9) 0.072(8) 0.043(7) 0.003(5) -0.017(6)
C1S' 0.041(6) 0.101(9) 0.074(8) 0.030(6) 0.005(6) -0.018(6)
C2S' 0.067(8) 0.103(9) 0.085(8) 0.018(7) 0.013(7) -0.035(6)
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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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Zn1 O1 1.9490(12) . ?
Zn1 O2 1.9738(12) . ?
Zn1 N2 2.0552(15) . ?
Zn1 N1 2.0847(15) . ?
Zn1 N5 2.1838(13) . ?
Zn2 O4 1.9566(11) . ?
Zn2 O3 1.9788(12) . ?
Zn2 N3 2.0703(14) . ?
Zn2 N4 2.0944(14) . ?
Zn2 N6 2.1962(14) . ?
Cl1 C10 1.730(2) . ?
Cl2 C11 1.737(2) . ?
Cl3 C38 1.7271(17) . ?
Cl4 C39 1.7259(18) . ?
N1 C7 1.301(2) . ?
N1 C8 1.414(2) . ?
N2 C14 1.300(2) . ?
N2 C13 1.411(2) . ?
N3 C35 1.299(2) . ?
N3 C36 1.414(2) . ?
N4 C42 1.296(2) . ?
N4 C41 1.411(2) . ?
O1 C1 1.296(2) . ?
O2 C20 1.298(2) . ?
O3 C29 1.297(2) . ?
O4 C48 1.299(2) . ?
C1 C6 1.434(3) . ?
C1 C2 1.444(3) . ?
C2 C3 1.378(3) . ?
C2 C21 1.531(3) . ?
C3 C4 1.393(4) . ?
C4 C5 1.366(4) . ?
C5 C6 1.419(3) . ?
C6 C7 1.433(3) . ?
C8 C9 1.395(3) . ?
C8 C13 1.414(3) . ?
C9 C10 1.379(3) . ?
C10 C11 1.392(3) . ?
C11 C12 1.383(3) . ?
C12 C13 1.392(3) . ?
C14 C15 1.427(2) . ?

C15 C16 1.417(2) . ?
C15 C20 1.434(2) . ?
C16 C17 1.366(2) . ?
C17 C18 1.402(2) . ?
C18 C19 1.383(2) . ?
C19 C20 1.442(2) . ?
C19 C25 1.537(2) . ?
C21 C24 1.529(3) . ?
C21 C22 1.538(3) . ?
C21 C23 1.542(3) . ?
C25 C28 1.535(2) . ?
C25 C27 1.539(3) . ?
C25 C26 1.542(2) . ?
C29 C34 1.438(2) . ?
C29 C30 1.446(2) . ?
C30 C31 1.379(2) . ?
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C32 C33 1.361(3) . ?
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C36 C37 1.395(2) . ?
C36 C41 1.413(2) . ?
C37 C38 1.381(2) . ?
C38 C39 1.391(3) . ?
C39 C40 1.385(2) . ?
C40 C41 1.391(2) . ?
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C43 C44 1.412(2) . ?
C43 C48 1.440(2) . ?
C44 C45 1.362(2) . ?
C45 C46 1.403(3) . ?
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C47 C48 1.443(2) . ?
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C49 C50 1.534(2) . ?
C49 C52 1.535(3) . ?
C49 C51 1.537(3) . ?
C53 C56 1.535(3) . ?
C53 C54 1.536(2) . ?
C53 C55 1.542(2) . ?
P1 C57 1.844(3) . ?
P1 C59 1.860(3) . ?
P1 C58 1.866(3) . ?
N5 C60 1.481(3) . ?
N5 C61 1.495(3) . ?
N5 C57 1.499(3) . ?
N6 C60 1.480(3) . ?
N6 C62 1.503(3) . ?
N6 C58 1.503(3) . ?
N7 C62 1.443(4) . ?
N7 C61 1.450(4) . ?
N7 C59 1.479(3) . ?
P1' C57' 1.838(5) . ?

P1' C59' 1.852(5) . ?
P1' C58' 1.859(5) . ?
N5' C60' 1.482(5) . ?
N5' C57' 1.493(5) . ?
N5' C61' 1.497(5) . ?
N1S C1S 1.123(4) . ?
C1S C2S 1.440(5) . ?
N1S' C1S' 1.123(6) . ?
C1S' C2S' 1.442(6) . ?
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O1 Zn1 O2 96.18(5) . . ?
O1 Zn1 N2 150.91(6) . . ?
O2 Zn1 N2 90.04(5) . . ?
O1 Zn1 N1 89.43(6) . . ?
O2 Zn1 N1 167.04(6) . . ?
N2 Zn1 N1 79.55(6) . . ?
O1 Zn1 N5 99.86(5) . . ?
O2 Zn1 N5 91.45(5) . . ?
N2 Zn1 N5 108.38(5) . . ?
N1 Zn1 N5 99.12(5) . . ?
O4 Zn2 O3 97.60(5) . . ?
O4 Zn2 N3 146.57(5) . . ?
O3 Zn2 N3 89.37(5) . . ?
O4 Zn2 N4 87.69(5) . . ?
O3 Zn2 N4 164.55(5) . . ?
N3 Zn2 N4 78.49(5) . . ?
O4 Zn2 N6 102.74(5) . . ?
O3 Zn2 N6 93.10(5) . . ?
N3 Zn2 N6 109.51(5) . . ?
N4 Zn2 N6 99.90(5) . . ?
C7 N1 C8 122.84(16) . . ?
C7 N1 Zn1 123.87(14) . . ?
C8 N1 Zn1 113.28(11) . . ?
C14 N2 C13 121.05(15) . . ?
C14 N2 Zn1 123.73(12) . . ?
C13 N2 Zn1 114.05(11) . . ?
C35 N3 C36 120.81(14) . . ?
C35 N3 Zn2 124.39(12) . . ?
C36 N3 Zn2 114.43(10) . . ?
C42 N4 C41 122.63(15) . . ?
C42 N4 Zn2 122.79(12) . . ?
C41 N4 Zn2 114.09(11) . . ?
C1 O1 Zn1 130.65(13) . . ?
C20 O2 Zn1 130.46(11) . . ?
C29 O3 Zn2 131.65(11) . . ?
C48 O4 Zn2 127.01(10) . . ?
O1 C1 C6 122.54(17) . . ?

O1 C1 C2 118.61(19) . . ?
C6 C1 C2 118.84(17) . . ?
C3 C2 C1 118.1(2) . . ?
C3 C2 C21 121.8(2) . . ?
C1 C2 C21 120.05(17) . . ?
C2 C3 C4 123.1(2) . . ?
C5 C4 C3 119.8(2) . . ?
C4 C5 C6 120.9(2) . . ?
C5 C6 C7 116.0(2) . . ?
C5 C6 C1 119.2(2) . . ?
C7 C6 C1 124.54(17) . . ?
N1 C7 C6 125.77(18) . . ?
C9 C8 N1 125.38(18) . . ?
C9 C8 C13 119.05(18) . . ?
N1 C8 C13 115.53(15) . . ?
C10 C9 C8 120.62(19) . . ?
C9 C10 C11 120.19(18) . . ?
C9 C10 Cl1 119.40(17) . . ?
C11 C10 Cl1 120.41(17) . . ?
C12 C11 C10 120.10(19) . . ?
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C11 C12 C13 120.29(18) . . ?
C12 C13 N2 124.05(17) . . ?
C12 C13 C8 119.65(16) . . ?
N2 C13 C8 116.29(16) . . ?
N2 C14 C15 127.00(16) . . ?
C16 C15 C14 115.19(15) . . ?
C16 C15 C20 119.97(15) . . ?
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C18 C19 C25 121.33(15) . . ?
C20 C19 C25 120.29(15) . . ?
O2 C20 C15 122.10(15) . . ?
O2 C20 C19 119.70(15) . . ?
C15 C20 C19 118.20(15) . . ?
C24 C21 C2 111.27(16) . . ?
C24 C21 C22 107.0(2) . . ?
C2 C21 C22 112.4(2) . . ?
C24 C21 C23 109.03(19) . . ?
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C22 C21 C23 107.28(17) . . ?
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C19 C25 C26 109.36(14) . . ?
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_exptl_absorpt_coefficient_mu    0.985
_exptl_absorpt_correction_type   empirical
_exptl_absorpt_correction_T_min  0.8274
_exptl_absorpt_correction_T_max  0.9524
_exptl_absorpt_process_details
;
SADABS Version 2008/1 Bruker-Nonius
Blessing, Acta Cryst. (1995) A51 33-38
;
_exptl_special_details
;
It should be noted that the esd's of the cell dimensions are probably too low;
they should be multiplied by a factor of 2 to 10
;
_diffrn_ambient_temperature      100(2)
_diffrn_measurement_specimen_suppport 'magnetic support whith MicroMount'
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\a
```

```
_diffrn_source                 'Micorfocus source E025 IuS'
_diffrn_source_type            'Bruker APEX DUO'
_diffrn_source_power           50
_diffrn_source_current         0.6
_diffrn_source_size            '0.2 mm x 0.2 mm fine focus'
_diffrn_radiation_monochromator  'Quazar MX Multilayer Optics'
_diffrn_detector_type          '4K CCD area detector APEX II'
_diffrn_measurement_device_type  'APEX DUO Kappa 4-axis goniometer'
_diffrn_measurement_method
;
Fullsphere data collection, phi and omega scans
;
_diffrn_detector_area_resol_mean 512
_diffrn_reflns_number          128388
_diffrn_reflns_av_R_equivalents  0.0453
_diffrn_reflns_av_sigmaI/netI    0.0554
_diffrn_reflns_limit_h_min       -37
_diffrn_reflns_limit_h_max       36
_diffrn_reflns_limit_k_min       -21
_diffrn_reflns_limit_k_max       21
_diffrn_reflns_limit_l_min       -42
_diffrn_reflns_limit_l_max       42
_diffrn_reflns_theta_min         1.42
_diffrn_reflns_theta_max         26.82
_reflns_number_total             34428
_reflns_number_gt                29211
_reflns_threshold_expression     >2sigma(I)
_computing_data_collection       'Bruker APEX2 v2011.4-0'
_computing_cell_refinement       'Bruker APEX2 v2011.4-0'
_computing_data_reduction        'Bruker SAINT V7.60A'
_computing_structure_solution    Sir2011
_computing_structure_refinement  'SHELXS-97 (Sheldrick, 2008)'
_computing_molecular_graphics    'Bruker SHELXTL'
_computing_publication_material  'Bruker SHELXTL'
_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.
;
_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0470P)^2^+25.8373P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    noref
_refine_ls_extinction_method     none
```

_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details 'Flack H D (1983), Acta Cryst. A39, 876-881'
_chemical_absolute_configuration ad
_refine_ls_abs_structure_Flack 0.022(6)
_refine_ls_number_reflns 34428
_refine_ls_number_parameters 2383
_refine_ls_number_restraints 403
_refine_ls_R_factor_all 0.0571
_refine_ls_R_factor_gt 0.0435
_refine_ls_wR_factor_ref 0.1064
_refine_ls_wR_factor_gt 0.1002
_refine_ls_goodness_of_fit_ref 1.017
_refine_ls_restrained_S_all 1.022
_refine_ls_shift/su_max 0.001
_refine_ls_shift/su_mean 0.000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Zn1A Zn 0.755979(16) 0.54025(2) 0.482663(13) 0.02512(10) Uani 1 1 d . . .
Zn2A Zn 0.610681(16) 0.29017(2) 0.484028(14) 0.02455(10) Uani 1 1 d . . .
Zn3A Zn 0.806296(19) 0.19421(3) 0.478220(19) 0.04169(14) Uani 1 1 d . . .
Zn1B Zn 0.471459(15) 0.38850(3) 0.317459(13) 0.02198(9) Uani 1 1 d . . .
Zn2B Zn 0.270487(15) 0.48027(2) 0.310382(13) 0.02008(9) Uani 1 1 d . . .
Zn3B Zn 0.324552(15) 0.13973(2) 0.319986(14) 0.02410(10) Uani 1 1 d . . .
P1A P 0.74895(4) 0.33849(6) 0.57974(3) 0.0289(2) Uani 1 1 d . . .
N7A N 0.74520(10) 0.42175(17) 0.50668(9) 0.0198(6) Uani 1 1 d . . .
N8A N 0.76395(10) 0.28028(17) 0.50534(9) 0.0215(7) Uani 1 1 d . . .
N9A N 0.68356(10) 0.32265(16) 0.50694(8) 0.0169(6) Uani 1 1 d . . .
O1A O 0.69994(9) 0.58422(15) 0.49968(7) 0.0282(6) Uani 1 1 d D . .
C1A C 0.66265(12) 0.6150(2) 0.47913(10) 0.0264(8) Uani 1 1 d D . .
C2A C 0.63161(13) 0.6590(2) 0.49919(11) 0.0298(9) Uani 1 1 d D . .
C3A C 0.59293(14) 0.6933(2) 0.47659(12) 0.0378(10) Uani 1 1 d D . .
H3A H 0.5732 0.7241 0.4900 0.045 Uiso 1 1 calc R . .
C4A C 0.58135(16) 0.6846(3) 0.43423(13) 0.0447(12) Uani 1 1 d D . .
H4A H 0.5540 0.7086 0.4195 0.054 Uiso 1 1 calc R . .
C5A C 0.60908(15) 0.6424(3) 0.41466(12) 0.0414(12) Uani 1 1 d D . .
H5A H 0.6012 0.6372 0.3860 0.050 Uiso 1 1 calc R . .
C6A C 0.64992(14) 0.6054(2) 0.43580(10) 0.0335(10) Uani 1 1 d D . .
C7A C 0.64394(13) 0.6695(2) 0.54583(11) 0.0340(10) Uani 1 1 d D . .
C8A C 0.64682(18) 0.5900(3) 0.56733(13) 0.0435(12) Uani 1 1 d D . .
H8A1 H 0.6687 0.5559 0.5566 0.065 Uiso 1 1 calc R . .
H8A2 H 0.6160 0.5655 0.5627 0.065 Uiso 1 1 calc R . .
H8A3 H 0.6577 0.5977 0.5965 0.065 Uiso 1 1 calc R . .

C9A C 0.69044(15) 0.7132(3) 0.55663(17) 0.0618(17) Uani 1 1 d D . .
H9A1 H 0.7012 0.7120 0.5861 0.093 Uiso 1 1 calc R . .
H9A2 H 0.6863 0.7680 0.5475 0.093 Uiso 1 1 calc R . .
H9A3 H 0.7135 0.6876 0.5432 0.093 Uiso 1 1 calc R . .
C10A C 0.60694(16) 0.7184(3) 0.56205(15) 0.0470(12) Uani 1 1 d D . .
H10A H 0.5767 0.6920 0.5552 0.071 Uiso 1 1 calc R . .
H10B H 0.6048 0.7709 0.5496 0.071 Uiso 1 1 calc R . .
H10C H 0.6157 0.7235 0.5916 0.071 Uiso 1 1 calc R . .
C11A C 0.67786(14) 0.5638(2) 0.41177(11) 0.0352(11) Uani 1 1 d D . .
H11A H 0.6662 0.5612 0.3834 0.042 Uiso 1 1 calc R . .
N1A N 0.71720(11) 0.52963(18) 0.42481(9) 0.0289(7) Uani 1 1 d D . .
C12A C 0.74264(15) 0.4965(2) 0.39637(11) 0.0329(10) Uani 1 1 d D . .
C13A C 0.72231(17) 0.4697(2) 0.35740(11) 0.0378(11) Uani 1 1 d D . .
H13A H 0.6894 0.4693 0.3492 0.045 Uiso 1 1 calc R . .
C14A C 0.75020(19) 0.4439(2) 0.33121(12) 0.0440(13) Uani 1 1 d D . .
H14A H 0.7364 0.4244 0.3052 0.053 Uiso 1 1 calc R . .
C15A C 0.7979(2) 0.4461(2) 0.34243(13) 0.0462(13) Uani 1 1 d D . .
H15A H 0.8169 0.4313 0.3236 0.055 Uiso 1 1 calc R . .
C16A C 0.81818(17) 0.4701(2) 0.38143(13) 0.0433(12) Uani 1 1 d D . .
H16A H 0.8511 0.4706 0.3892 0.052 Uiso 1 1 calc R . .
C17A C 0.79093(15) 0.4932(2) 0.40918(12) 0.0340(10) Uani 1 1 d D . .
N2A N 0.80728(12) 0.5179(2) 0.44947(10) 0.0333(8) Uani 1 1 d D . .
C18A C 0.85143(15) 0.5199(2) 0.46505(12) 0.0333(10) Uani 1 1 d D . .
H18A H 0.8719 0.4996 0.4486 0.040 Uiso 1 1 calc R . .
C19A C 0.87267(14) 0.5492(2) 0.50420(12) 0.0313(9) Uani 1 1 d D . .
C20A C 0.92179(14) 0.5503(2) 0.51196(13) 0.0354(10) Uani 1 1 d D . .
H20A H 0.9383 0.5278 0.4929 0.043 Uiso 1 1 calc R . .
C21A C 0.94546(16) 0.5835(3) 0.54657(14) 0.0455(12) Uani 1 1 d D . .
H21A H 0.9785 0.5836 0.5518 0.055 Uiso 1 1 calc R . .
C22A C 0.92119(15) 0.6176(3) 0.57447(13) 0.0390(10) Uani 1 1 d D . .
H22A H 0.9386 0.6409 0.5983 0.047 Uiso 1 1 calc R . .
C23A C 0.87325(13) 0.6191(2) 0.56915(11) 0.0283(9) Uani 1 1 d D . .
C24A C 0.84722(13) 0.5836(2) 0.53263(11) 0.0279(9) Uani 1 1 d D . .
O2A O 0.80204(9) 0.58366(16) 0.52681(8) 0.0309(6) Uani 1 1 d D . .
C25A C 0.84855(14) 0.6591(2) 0.59990(11) 0.0296(9) Uani 1 1 d D . .
C26A C 0.81454(19) 0.6031(3) 0.61571(14) 0.0542(15) Uani 1 1 d D . .
H26A H 0.7903 0.5864 0.5931 0.081 Uiso 1 1 calc R . .
H26B H 0.8002 0.6305 0.6360 0.081 Uiso 1 1 calc R . .
H26C H 0.8315 0.5568 0.6281 0.081 Uiso 1 1 calc R . .
C27A C 0.82108(14) 0.7305(2) 0.58035(11) 0.0309(9) Uani 1 1 d D . .
H27A H 0.8426 0.7693 0.5726 0.046 Uiso 1 1 calc R . .
H27B H 0.8040 0.7543 0.5998 0.046 Uiso 1 1 calc R . .
H27C H 0.7991 0.7136 0.5562 0.046 Uiso 1 1 calc R . .
C28A C 0.88336(16) 0.6889(3) 0.63743(13) 0.0451(12) Uani 1 1 d D . .
H28A H 0.9015 0.6444 0.6506 0.068 Uiso 1 1 calc R . .
H28B H 0.8662 0.7136 0.6566 0.068 Uiso 1 1 calc R . .
H28C H 0.9044 0.7276 0.6288 0.068 Uiso 1 1 calc R . .
O3A O 0.58111(9) 0.32760(15) 0.52771(8) 0.0274(6) Uani 1 1 d . . .
C29A C 0.56028(14) 0.3933(2) 0.53223(12) 0.0272(9) Uani 1 1 d . . .
C30A C 0.54200(15) 0.4059(3) 0.56910(12) 0.0319(9) Uani 1 1 d . . .
C31A C 0.52067(17) 0.4757(3) 0.57361(14) 0.0423(11) Uani 1 1 d . . .
H31A H 0.5094 0.4843 0.5981 0.051 Uiso 1 1 calc R . .
C32A C 0.51423(17) 0.5357(3) 0.54435(15) 0.0403(11) Uani 1 1 d . . .
H32A H 0.4989 0.5832 0.5489 0.048 Uiso 1 1 calc R . .

C33A C 0.53053(15) 0.5241(2) 0.50920(13) 0.0319(9) Uani 1 1 d . . .
H33A H 0.5261 0.5638 0.4889 0.038 Uiso 1 1 calc R . .
C34A C 0.55400(13) 0.4539(2) 0.50254(11) 0.0235(8) Uani 1 1 d . . .
C35A C 0.56680(13) 0.4480(2) 0.46337(11) 0.0235(8) Uani 1 1 d . . .
H35A H 0.5610 0.4927 0.4461 0.028 Uiso 1 1 calc R . .
C36A C 0.54689(16) 0.3413(3) 0.60172(13) 0.0415(11) Uani 1 1 d . . .
C37A C 0.59858(17) 0.3197(4) 0.61690(15) 0.0532(14) Uani 1 1 d . . .
H37A H 0.6010 0.2833 0.6399 0.080 Uiso 1 1 calc R . .
H37B H 0.6164 0.3676 0.6256 0.080 Uiso 1 1 calc R . .
H37C H 0.6111 0.2946 0.5949 0.080 Uiso 1 1 calc R . .
C38A C 0.51913(16) 0.2695(3) 0.58451(15) 0.0455(12) Uani 1 1 d . . .
H38A H 0.5221 0.2282 0.6053 0.068 Uiso 1 1 calc R . .
H38B H 0.5310 0.2500 0.5609 0.068 Uiso 1 1 calc R . .
H38C H 0.4863 0.2840 0.5763 0.068 Uiso 1 1 calc R . .
C39A C 0.5277(2) 0.3689(4) 0.63909(15) 0.0589(15) Uani 1 1 d . . .
H39A H 0.4950 0.3841 0.6308 0.088 Uiso 1 1 calc R . .
H39B H 0.5457 0.4143 0.6514 0.088 Uiso 1 1 calc R . .
H39C H 0.5301 0.3260 0.6589 0.088 Uiso 1 1 calc R . .
N3A N 0.58545(11) 0.38747(18) 0.44933(9) 0.0218(7) Uani 1 1 d . . .
C40A C 0.59334(14) 0.3841(3) 0.40876(11) 0.0287(9) Uani 1 1 d . . .
C41A C 0.58353(14) 0.4440(3) 0.38028(12) 0.0352(10) Uani 1 1 d . . .
H41A H 0.5705 0.4923 0.3872 0.042 Uiso 1 1 calc R . .
C42A C 0.59291(15) 0.4325(3) 0.34171(13) 0.0428(12) Uani 1 1 d . . .
H42A H 0.5857 0.4729 0.3219 0.051 Uiso 1 1 calc R . .
C43A C 0.61269(16) 0.3630(4) 0.33153(14) 0.0499(14) Uani 1 1 d . . .
H43A H 0.6199 0.3565 0.3052 0.060 Uiso 1 1 calc R . .
C44A C 0.62173(16) 0.3038(3) 0.35947(14) 0.0481(13) Uani 1 1 d . . .
H44A H 0.6356 0.2564 0.3525 0.058 Uiso 1 1 calc R . .
C45A C 0.61107(14) 0.3118(3) 0.39785(13) 0.0359(11) Uani 1 1 d . . .
N4A N 0.61594(12) 0.2507(2) 0.42677(11) 0.0351(9) Uani 1 1 d . . .
C46A C 0.61436(16) 0.1756(3) 0.41695(16) 0.0537(15) Uani 1 1 d . . .
H46A H 0.6118 0.1637 0.3889 0.064 Uiso 1 1 calc R . .
C47A C 0.61612(17) 0.1099(3) 0.4440(2) 0.0561(16) Uani 1 1 d . . .
C48A C 0.6121(2) 0.0344(4) 0.4231(2) 0.086(3) Uani 1 1 d . . .
H48A H 0.6101 0.0310 0.3945 0.103 Uiso 1 1 calc R . .
C49A C 0.6116(2) -0.0317(3) 0.4467(3) 0.080(2) Uani 1 1 d . . .
H49A H 0.6075 -0.0817 0.4338 0.095 Uiso 1 1 calc R . .
C50A C 0.6167(2) -0.0279(3) 0.4880(3) 0.083(2) Uani 1 1 d . . .
H50A H 0.6178 -0.0761 0.5025 0.099 Uiso 1 1 calc R . .
C51A C 0.62033(17) 0.0408(3) 0.5099(2) 0.0606(18) Uani 1 1 d . . .
C52A C 0.61956(15) 0.1140(3) 0.48618(18) 0.0465(13) Uani 1 1 d . . .
O4A O 0.62134(11) 0.18050(16) 0.50383(10) 0.0404(7) Uani 1 1 d . . .
C53A C 0.6274(2) 0.0437(3) 0.5553(2) 0.0680(19) Uani 1 1 d . . .
C54A C 0.6278(2) -0.0410(3) 0.5736(3) 0.093(3) Uani 1 1 d . . .
H54A H 0.5990 -0.0685 0.5617 0.140 Uiso 1 1 calc R . .
H54B H 0.6300 -0.0374 0.6031 0.140 Uiso 1 1 calc R . .
H54C H 0.6546 -0.0703 0.5676 0.140 Uiso 1 1 calc R . .
C55A C 0.5861(3) 0.0864(4) 0.5679(3) 0.115(4) Uani 1 1 d . . .
H55A H 0.5865 0.1419 0.5599 0.172 Uiso 1 1 calc R . .
H55B H 0.5886 0.0827 0.5973 0.172 Uiso 1 1 calc R . .
H55C H 0.5570 0.0620 0.5543 0.172 Uiso 1 1 calc R . .
C56A C 0.6732(2) 0.0813(3) 0.57331(18) 0.0564(14) Uani 1 1 d . . .
H56A H 0.6988 0.0479 0.5680 0.085 Uiso 1 1 calc R . .
H56B H 0.6753 0.0872 0.6027 0.085 Uiso 1 1 calc R . .

H56C H 0.6754 0.1332 0.5610 0.085 Uiso 1 1 calc R . .
O5A O 0.81923(10) 0.11871(14) 0.52196(8) 0.0310(6) Uani 1 1 d D . .
C57A C 0.79896(12) 0.0539(2) 0.52893(10) 0.0247(8) Uani 1 1 d D . .
C58A C 0.81600(13) 0.0103(2) 0.56536(10) 0.0290(9) Uani 1 1 d D . .
C59A C 0.79393(15) -0.0576(2) 0.57272(13) 0.0412(11) Uani 1 1 d D . .
H59A H 0.8048 -0.0854 0.5972 0.049 Uiso 1 1 calc R A .
C60A C 0.75570(16) -0.0878(3) 0.54530(15) 0.0485(13) Uani 1 1 d D . .
H60A H 0.7414 -0.1356 0.5512 0.058 Uiso 1 1 calc R . .
C61A C 0.73952(15) -0.0489(2) 0.51068(14) 0.0391(11) Uani 1 1 d D . .
H61A H 0.7138 -0.0697 0.4922 0.047 Uiso 1 1 calc R A .
C62A C 0.76005(12) 0.0225(2) 0.50123(10) 0.0253(8) Uani 1 1 d D . .
C63A C 0.85964(13) 0.0389(2) 0.59504(11) 0.0387(11) Uani 1 1 d D . .
C64A C 0.8701(2) -0.0125(4) 0.63296(15) 0.0711(18) Uani 1 1 d D . .
H64A H 0.8715 -0.0679 0.6250 0.107 Uiso 1 1 calc R . .
H64B H 0.8455 -0.0057 0.6490 0.107 Uiso 1 1 calc R . .
H64C H 0.9001 0.0030 0.6493 0.107 Uiso 1 1 calc R . .
C65A C 0.90167(14) 0.0360(3) 0.57395(13) 0.0399(11) Uani 1 1 d D . .
H65A H 0.9287 0.0589 0.5918 0.060 Uiso 1 1 calc R . .
H65B H 0.8949 0.0660 0.5486 0.060 Uiso 1 1 calc R . .
H65C H 0.9084 -0.0189 0.5680 0.060 Uiso 1 1 calc R . .
C66A C 0.85358(18) 0.1243(3) 0.60890(16) 0.0608(16) Uani 1 1 d D . .
H66A H 0.8258 0.1278 0.6213 0.091 Uiso 1 1 calc R . .
H66B H 0.8501 0.1596 0.5854 0.091 Uiso 1 1 calc R . .
H66C H 0.8810 0.1399 0.6288 0.091 Uiso 1 1 calc R . .
C67A C 0.74250(15) 0.0536(2) 0.46193(11) 0.0333(10) Uani 1 1 d D . .
H67A H 0.7177 0.0255 0.4458 0.040 Uiso 1 1 calc R A .
N5A N 0.75669(13) 0.11601(19) 0.44587(9) 0.0404(10) Uani 1 1 d D A .
C68A C 0.7342(3) 0.1303(5) 0.40409(18) 0.021(2) Uani 0.50 1 d PD A 1
C69A C 0.6984(3) 0.0872(4) 0.37975(17) 0.0208(17) Uani 0.50 1 d PD A 1
H69A H 0.6852 0.0433 0.3910 0.025 Uiso 0.50 1 calc PR A 1
C70A C 0.6821(3) 0.1077(5) 0.3397(2) 0.038(2) Uani 0.50 1 d PD A 1
H70A H 0.6585 0.0771 0.3235 0.046 Uiso 0.50 1 calc PR A 1
C71A C 0.7001(3) 0.1729(5) 0.32345(19) 0.028(2) Uani 0.50 1 d PD A 1
H71A H 0.6885 0.1879 0.2962 0.034 Uiso 0.50 1 calc PR A 1
C72A C 0.7353(4) 0.2165(6) 0.3472(2) 0.029(2) Uani 0.50 1 d PD A 1
H72A H 0.7474 0.2614 0.3359 0.035 Uiso 0.50 1 calc PR A 1
C73A C 0.7529(2) 0.1953(4) 0.38700(17) 0.0203(17) Uani 0.50 1 d PD A 1
N6A N 0.7917(2) 0.2298(5) 0.41252(17) 0.021(2) Uani 0.50 1 d PDU A 1
C74A C 0.8214(2) 0.2693(4) 0.39592(19) 0.0285(18) Uani 0.50 1 d PD A 1
H74A H 0.8135 0.2781 0.3675 0.034 Uiso 0.50 1 calc PR A 1
C75A C 0.8647(3) 0.3006(5) 0.4165(2) 0.026(2) Uani 0.50 1 d PD A 1
C76A C 0.8899(3) 0.3434(4) 0.3915(2) 0.046(2) Uani 0.50 1 d PD A 1
H76A H 0.8777 0.3490 0.3633 0.055 Uiso 0.50 1 calc PR A 1
C77A C 0.9314(3) 0.3766(4) 0.4076(2) 0.048(3) Uani 0.50 1 d PD A 1
H77A H 0.9472 0.4086 0.3913 0.058 Uiso 0.50 1 calc PR A 1
C78A C 0.9506(4) 0.3631(8) 0.4483(3) 0.054(4) Uani 0.50 1 d PDU A 1
H78A H 0.9813 0.3817 0.4581 0.065 Uiso 0.50 1 calc PR A 1
C79A C 0.92796(18) 0.3247(4) 0.47515(18) 0.033(2) Uani 0.50 1 d PD A 1
C80A C 0.8830(2) 0.2901(5) 0.4589(2) 0.023(2) Uani 0.50 1 d PDU A 1
O6A O 0.86135(16) 0.2519(3) 0.48327(16) 0.0259(12) Uani 0.50 1 d PD A 1
C81A C 0.9516(2) 0.3096(4) 0.5188(2) 0.039(3) Uani 0.50 1 d PDU A 1
C82A C 0.9990(2) 0.3518(4) 0.5297(3) 0.054(3) Uani 0.50 1 d PD A 1
H82A H 1.0192 0.3349 0.5110 0.082 Uiso 0.50 1 calc PR A 1
H82B H 1.0136 0.3386 0.5576 0.082 Uiso 0.50 1 calc PR A 1

H82C H 0.9942 0.4089 0.5274 0.082 Uiso 0.50 1 calc PR A 1
C83A C 0.9602(3) 0.2209(4) 0.5249(3) 0.053(3) Uani 0.50 1 d PD A 1
H83A H 0.9791 0.2019 0.5056 0.080 Uiso 0.50 1 calc PR A 1
H83B H 0.9303 0.1932 0.5203 0.080 Uiso 0.50 1 calc PR A 1
H83C H 0.9766 0.2111 0.5527 0.080 Uiso 0.50 1 calc PR A 1
C84A C 0.9217(3) 0.3388(5) 0.5494(2) 0.040(2) Uani 0.50 1 d PD A 1
H84A H 0.8913 0.3128 0.5438 0.060 Uiso 0.50 1 calc PR A 1
H84B H 0.9175 0.3959 0.5468 0.060 Uiso 0.50 1 calc PR A 1
H84C H 0.9374 0.3260 0.5771 0.060 Uiso 0.50 1 calc PR A 1
C68' C 0.7511(4) 0.1527(6) 0.4086(2) 0.036(3) Uani 0.50 1 d PD A 2
C69' C 0.7168(3) 0.1174(5) 0.3790(2) 0.035(2) Uani 0.50 1 d PD A 2
H69C H 0.7008 0.0721 0.3858 0.042 Uiso 0.50 1 calc PR A 2
C70' C 0.7062(4) 0.1479(6) 0.3402(2) 0.052(4) Uani 0.50 1 d PD A 2
H70C H 0.6829 0.1239 0.3205 0.063 Uiso 0.50 1 calc PR A 2
C71' C 0.7297(5) 0.2133(8) 0.3305(2) 0.050(4) Uani 0.50 1 d PD A 2
H71C H 0.7218 0.2357 0.3041 0.060 Uiso 0.50 1 calc PR A 2
C72' C 0.7650(3) 0.2469(5) 0.3590(2) 0.044(2) Uani 0.50 1 d PD A 2
H72C H 0.7809 0.2919 0.3518 0.053 Uiso 0.50 1 calc PR A 2
C73' C 0.7771(3) 0.2155(6) 0.3977(2) 0.029(3) Uani 0.50 1 d PD A 2
N6' N 0.8137(2) 0.2418(4) 0.42817(18) 0.0296(18) Uani 0.50 1 d PD A 2
C74' C 0.8496(3) 0.2778(5) 0.4188(2) 0.032(3) Uani 0.50 1 d PD A 2
H74C H 0.8494 0.2855 0.3907 0.039 Uiso 0.50 1 calc PR A 2
C75' C 0.8893(3) 0.3067(7) 0.4463(2) 0.039(3) Uani 0.50 1 d PD A 2
C76' C 0.9240(3) 0.3433(5) 0.4284(2) 0.051(3) Uani 0.50 1 d PD A 2
H76C H 0.9204 0.3463 0.3997 0.061 Uiso 0.50 1 calc PR A 2
C77' C 0.9624(4) 0.3739(9) 0.4521(3) 0.046(2) Uani 0.50 1 d PD A 2
H77B H 0.9839 0.4036 0.4402 0.055 Uiso 0.50 1 calc PR A 2
C78' C 0.9706(3) 0.3620(5) 0.4941(2) 0.054(3) Uani 0.50 1 d PD A 2
H78B H 0.9996 0.3783 0.5096 0.064 Uiso 0.50 1 calc PR A 2
C79' C 0.9385(2) 0.3279(5) 0.51411(19) 0.038(3) Uani 0.50 1 d PDU A 2
C80' C 0.8966(2) 0.2960(4) 0.48946(19) 0.033(2) Uani 0.50 1 d PD A 2
O6' O 0.86646(17) 0.2611(3) 0.50746(16) 0.0285(13) Uani 0.50 1 d PD A 2
C81' C 0.9468(2) 0.3241(4) 0.56019(19) 0.046(3) Uani 0.50 1 d PD A 2
C82' C 0.9933(3) 0.3613(5) 0.5806(3) 0.066(3) Uani 0.50 1 d PD A 2
H82D H 0.9944 0.4163 0.5719 0.098 Uiso 0.50 1 calc PR A 2
H82E H 1.0191 0.3320 0.5727 0.098 Uiso 0.50 1 calc PR A 2
H82F H 0.9960 0.3594 0.6101 0.098 Uiso 0.50 1 calc PR A 2
C83' C 0.9078(3) 0.3675(5) 0.5761(3) 0.043(2) Uani 0.50 1 d PD A 2
H83D H 0.9067 0.4224 0.5670 0.064 Uiso 0.50 1 calc PR A 2
H83E H 0.9139 0.3659 0.6058 0.064 Uiso 0.50 1 calc PR A 2
H83F H 0.8780 0.3420 0.5656 0.064 Uiso 0.50 1 calc PR A 2
C84' C 0.9475(4) 0.2378(4) 0.5754(3) 0.071(4) Uani 0.50 1 d PD A 2
H84D H 0.9182 0.2118 0.5636 0.106 Uiso 0.50 1 calc PR A 2
H84E H 0.9513 0.2373 0.6051 0.106 Uiso 0.50 1 calc PR A 2
H84F H 0.9735 0.2096 0.5672 0.106 Uiso 0.50 1 calc PR A 2
C85A C 0.75755(14) 0.4297(2) 0.55147(11) 0.0239(8) Uani 1 1 d . . .
H85A H 0.7385 0.4722 0.5602 0.029 Uiso 1 1 calc R . .
H85B H 0.7906 0.4458 0.5588 0.029 Uiso 1 1 calc R . .
C86A C 0.69549(12) 0.4020(2) 0.49374(11) 0.0188(7) Uani 1 1 d . . .
H86A H 0.6874 0.4050 0.4638 0.023 Uiso 1 1 calc R . .
H86B H 0.6765 0.4416 0.5050 0.023 Uiso 1 1 calc R . .
C87A C 0.77368(13) 0.3605(2) 0.49176(12) 0.0243(8) Uani 1 1 d . . .
H87A H 0.8070 0.3727 0.5014 0.029 Uiso 1 1 calc R A .
H87B H 0.7677 0.3617 0.4617 0.029 Uiso 1 1 calc R . .

C88A C 0.77865(14) 0.2713(2) 0.54958(12) 0.0300(9) Uani 1 1 d . . .
H88A H 0.8126 0.2806 0.5567 0.036 Uiso 1 1 calc R A .
H88B H 0.7727 0.2164 0.5571 0.036 Uiso 1 1 calc R . .
C89A C 0.71346(13) 0.2639(2) 0.49209(11) 0.0211(8) Uani 1 1 d . . .
H89A H 0.7061 0.2628 0.4621 0.025 Uiso 1 1 calc R A .
H89B H 0.7064 0.2112 0.5020 0.025 Uiso 1 1 calc R . .
C90A C 0.68898(13) 0.3193(2) 0.55197(11) 0.0236(8) Uani 1 1 d . . .
H90A H 0.6792 0.2665 0.5597 0.028 Uiso 1 1 calc R A .
H90B H 0.6678 0.3584 0.5607 0.028 Uiso 1 1 calc R . .
P1B P 0.33745(4) 0.32764(6) 0.21781(3) 0.0238(2) Uani 1 1 d . . .
N7B N 0.39914(10) 0.35411(17) 0.29178(9) 0.0188(6) Uani 1 1 d . . .
N8B N 0.33776(10) 0.25439(17) 0.29285(9) 0.0194(6) Uani 1 1 d . . .
N9B N 0.31768(10) 0.39580(16) 0.28922(8) 0.0163(6) Uani 1 1 d . . .
O1B O 0.50297(9) 0.35540(16) 0.27373(8) 0.0264(6) Uani 1 1 d . . .
C1B C 0.52276(13) 0.2900(2) 0.26768(11) 0.0242(8) Uani 1 1 d . . .
C2B C 0.54211(14) 0.2796(2) 0.23115(12) 0.0273(9) Uani 1 1 d . . .
C3B C 0.56320(16) 0.2096(3) 0.22563(13) 0.0365(10) Uani 1 1 d . . .
H3B H 0.5754 0.2026 0.2015 0.044 Uiso 1 1 calc R . .
C4B C 0.56785(18) 0.1474(3) 0.25379(16) 0.0455(12) Uani 1 1 d . . .
H4B H 0.5835 0.1003 0.2490 0.055 Uiso 1 1 calc R . .
C5B C 0.54952(16) 0.1558(3) 0.28801(14) 0.0361(10) Uani 1 1 d . . .
H5B H 0.5514 0.1132 0.3066 0.043 Uiso 1 1 calc R . .
C6B C 0.52793(13) 0.2261(2) 0.29647(12) 0.0269(8) Uani 1 1 d . . .
C7B C 0.54078(14) 0.3472(3) 0.20062(12) 0.0304(9) Uani 1 1 d . . .
C8B C 0.56107(18) 0.3236(3) 0.16335(14) 0.0440(11) Uani 1 1 d . . .
H8B1 H 0.5613 0.3695 0.1456 0.066 Uiso 1 1 calc R . .
H8B2 H 0.5420 0.2819 0.1485 0.066 Uiso 1 1 calc R . .
H8B3 H 0.5929 0.3044 0.1721 0.066 Uiso 1 1 calc R . .
C9B C 0.56993(16) 0.4162(2) 0.22091(13) 0.0340(10) Uani 1 1 d . . .
H9B1 H 0.6025 0.3998 0.2285 0.051 Uiso 1 1 calc R . .
H9B2 H 0.5583 0.4324 0.2453 0.051 Uiso 1 1 calc R . .
H9B3 H 0.5677 0.4605 0.2019 0.051 Uiso 1 1 calc R . .
C10B C 0.49079(16) 0.3779(3) 0.18459(14) 0.0462(12) Uani 1 1 d . . .
H10F H 0.4916 0.4176 0.1635 0.069 Uiso 1 1 calc R . .
H10G H 0.4783 0.4017 0.2070 0.069 Uiso 1 1 calc R . .
H10H H 0.4709 0.3340 0.1732 0.069 Uiso 1 1 calc R . .
N1B N 0.49681(11) 0.2899(2) 0.35075(9) 0.0288(8) Uani 1 1 d . . .
C11B C 0.51528(13) 0.2304(2) 0.33550(11) 0.0268(8) Uani 1 1 d . . .
H11B H 0.5210 0.1848 0.3521 0.032 Uiso 1 1 calc R . .
C12B C 0.48973(13) 0.2902(2) 0.39151(11) 0.0301(9) Uani 1 1 d D . .
C13B C 0.50093(15) 0.2301(3) 0.41947(12) 0.0387(11) Uani 1 1 d D . .
H13B H 0.5147 0.1833 0.4116 0.046 Uiso 1 1 calc R . .
C14B C 0.49251(16) 0.2368(3) 0.45873(12) 0.0478(13) Uani 1 1 d D . .
H14B H 0.5013 0.1957 0.4778 0.057 Uiso 1 1 calc R . .
C15B C 0.47115(16) 0.3042(3) 0.46982(13) 0.0483(13) Uani 1 1 d D . .
H15B H 0.4641 0.3082 0.4963 0.058 Uiso 1 1 calc R . .
C16B C 0.46010(14) 0.3654(3) 0.44286(11) 0.0376(11) Uani 1 1 d D . .
H16B H 0.4451 0.4109 0.4507 0.045 Uiso 1 1 calc R . .
C17B C 0.47085(13) 0.3609(3) 0.40398(11) 0.0328(10) Uani 1 1 d D . .
N2B N 0.46442(11) 0.4223(2) 0.37557(9) 0.0289(7) Uani 1 1 d D . .
C18B C 0.46552(14) 0.4951(2) 0.38799(12) 0.0335(10) Uani 1 1 d D . .
H18B H 0.4677 0.5031 0.4163 0.040 Uiso 1 1 calc R . .
C19B C 0.46375(14) 0.5646(2) 0.36330(12) 0.0337(10) Uani 1 1 d D . .
C20B C 0.46661(16) 0.6367(3) 0.38442(15) 0.0478(14) Uani 1 1 d D . .

H20B H 0.4684 0.6363 0.4130 0.057 Uiso 1 1 calc R . .
C21B C 0.46687(17) 0.7057(3) 0.36509(16) 0.0536(15) Uani 1 1 d D . .
H21B H 0.4685 0.7536 0.3799 0.064 Uiso 1 1 calc R . .
C22B C 0.46477(15) 0.7071(2) 0.32294(16) 0.0447(12) Uani 1 1 d D . .
H22B H 0.4648 0.7564 0.3096 0.054 Uiso 1 1 calc R . .
C23B C 0.46257(13) 0.6377(2) 0.29974(13) 0.0330(10) Uani 1 1 d D . .
C24B C 0.46252(13) 0.5640(2) 0.32062(12) 0.0285(9) Uani 1 1 d D . .
O2B O 0.46164(10) 0.49834(14) 0.30010(8) 0.0283(6) Uani 1 1 d D . .
C25B C 0.46165(14) 0.6405(2) 0.25433(13) 0.0371(11) Uani 1 1 d D . .
C26B C 0.46182(19) 0.7244(2) 0.23792(18) 0.0534(14) Uani 1 1 d D . .
H26F H 0.4640 0.7228 0.2091 0.080 Uiso 1 1 calc R . .
H26G H 0.4885 0.7532 0.2531 0.080 Uiso 1 1 calc R . .
H26H H 0.4330 0.7512 0.2411 0.080 Uiso 1 1 calc R . .
C27B C 0.50686(19) 0.5993(3) 0.24645(19) 0.0632(18) Uani 1 1 d D . .
H27F H 0.5096 0.5472 0.2593 0.095 Uiso 1 1 calc R . .
H27G H 0.5340 0.6313 0.2579 0.095 Uiso 1 1 calc R . .
H27H H 0.5054 0.5934 0.2172 0.095 Uiso 1 1 calc R . .
C28B C 0.41859(17) 0.5990(2) 0.23079(13) 0.0406(11) Uani 1 1 d D . .
H28F H 0.4207 0.5424 0.2367 0.061 Uiso 1 1 calc R . .
H28G H 0.4168 0.6074 0.2016 0.061 Uiso 1 1 calc R . .
H28H H 0.3906 0.6205 0.2390 0.061 Uiso 1 1 calc R . .
O3B O 0.26038(9) 0.55644(14) 0.26642(7) 0.0231(5) Uani 1 1 d . . .
C29B C 0.28151(13) 0.6218(2) 0.26135(11) 0.0204(7) Uani 1 1 d . . .
C30B C 0.26703(14) 0.6658(2) 0.22435(12) 0.0256(8) Uani 1 1 d . . .
C31B C 0.29041(15) 0.7339(2) 0.21953(13) 0.0327(9) Uani 1 1 d . . .
H31B H 0.2813 0.7626 0.1950 0.039 Uiso 1 1 calc R . .
C32B C 0.32699(16) 0.7638(2) 0.24850(13) 0.0345(10) Uani 1 1 d . . .
H32B H 0.3419 0.8116 0.2436 0.041 Uiso 1 1 calc R . .
C33B C 0.34086(14) 0.7236(2) 0.28384(12) 0.0291(9) Uani 1 1 d . . .
H33B H 0.3655 0.7437 0.3037 0.035 Uiso 1 1 calc R . .
C34B C 0.31894(13) 0.6519(2) 0.29124(11) 0.0227(8) Uani 1 1 d . . .
C35B C 0.22631(15) 0.6367(2) 0.19271(12) 0.0297(9) Uani 1 1 d . . .
C36B C 0.21697(18) 0.6896(3) 0.15524(13) 0.0437(11) Uani 1 1 d . . .
H36A H 0.2449 0.6923 0.1431 0.066 Uiso 1 1 calc R . .
H36B H 0.2088 0.7425 0.1631 0.066 Uiso 1 1 calc R . .
H36C H 0.1912 0.6678 0.1354 0.066 Uiso 1 1 calc R . .
C37B C 0.23497(18) 0.5537(3) 0.17787(13) 0.0410(11) Uani 1 1 d . . .
H37F H 0.2092 0.5384 0.1562 0.062 Uiso 1 1 calc R . .
H37G H 0.2372 0.5165 0.2005 0.062 Uiso 1 1 calc R . .
H37H H 0.2641 0.5530 0.1674 0.062 Uiso 1 1 calc R . .
C38B C 0.18200(15) 0.6374(2) 0.21088(13) 0.0344(9) Uani 1 1 d . . .
H38F H 0.1751 0.6914 0.2181 0.052 Uiso 1 1 calc R . .
H38G H 0.1865 0.6042 0.2352 0.052 Uiso 1 1 calc R . .
H38H H 0.1560 0.6168 0.1909 0.052 Uiso 1 1 calc R . .
C39E C 0.33369(13) 0.6188(2) 0.33064(11) 0.0235(8) Uani 1 1 d . . .
H39F H 0.3581 0.6453 0.3481 0.028 Uiso 1 1 calc R . .
N3B N 0.31729(11) 0.55631(17) 0.34514(9) 0.0206(6) Uani 1 1 d . . .
C40B C 0.33176(13) 0.5320(2) 0.38556(11) 0.0222(8) Uani 1 1 d . . .
C41B C 0.36620(15) 0.5674(2) 0.41433(11) 0.0283(8) Uani 1 1 d . . .
H41B H 0.3817 0.6131 0.4073 0.034 Uiso 1 1 calc R . .
C42B C 0.37790(15) 0.5364(3) 0.45314(12) 0.0328(10) Uani 1 1 d . . .
H42B H 0.4012 0.5610 0.4726 0.039 Uiso 1 1 calc R . .
C43B C 0.35567(16) 0.4696(3) 0.46352(12) 0.0353(10) Uani 1 1 d . . .
H43B H 0.3645 0.4475 0.4899 0.042 Uiso 1 1 calc R . .

C44B C 0.32100(16) 0.4352(2) 0.43604(12) 0.0338(10) Uani 1 1 d . . .
H44B H 0.3062 0.3891 0.4435 0.041 Uiso 1 1 calc R . .
C45B C 0.30705(14) 0.4668(2) 0.39718(11) 0.0265(8) Uani 1 1 d . . .
N4B N 0.27029(12) 0.43766(18) 0.36775(9) 0.0250(7) Uani 1 1 d . . .
C46B C 0.23525(15) 0.4009(2) 0.37842(12) 0.0308(9) Uani 1 1 d . . .
H46B H 0.2371 0.3917 0.4066 0.037 Uiso 1 1 calc R . .
C47B C 0.19417(15) 0.3730(2) 0.35179(13) 0.0328(9) Uani 1 1 d . . .
C48B C 0.15954(18) 0.3382(3) 0.37107(15) 0.0461(12) Uani 1 1 d . . .
H48B H 0.1650 0.3336 0.3998 0.055 Uiso 1 1 calc R . .
C49B C 0.11900(18) 0.3117(3) 0.34900(16) 0.0472(12) Uani 1 1 d . . .
H49B H 0.0960 0.2894 0.3623 0.057 Uiso 1 1 calc R . .
C50B C 0.11100(16) 0.3169(3) 0.30707(15) 0.0398(11) Uani 1 1 d . . .
H50B H 0.0826 0.2967 0.2921 0.048 Uiso 1 1 calc R . .
C51B C 0.14248(15) 0.3502(2) 0.28608(13) 0.0316(9) Uani 1 1 d . . .
C52B C 0.18545(14) 0.3809(2) 0.30885(12) 0.0268(9) Uani 1 1 d . . .
O4B O 0.21521(9) 0.41487(15) 0.28991(8) 0.0250(6) Uani 1 1 d . . .
C53B C 0.13235(15) 0.3544(2) 0.23895(14) 0.0353(10) Uani 1 1 d . . .
C54B C 0.08511(15) 0.3171(3) 0.22065(16) 0.0444(12) Uani 1 1 d . . .
H54F H 0.0795 0.3227 0.1910 0.067 Uiso 1 1 calc R . .
H54G H 0.0603 0.3437 0.2315 0.067 Uiso 1 1 calc R . .
H54H H 0.0855 0.2611 0.2278 0.067 Uiso 1 1 calc R . .
C55B C 0.13052(17) 0.4413(3) 0.22567(16) 0.0447(12) Uani 1 1 d . . .
H55F H 0.1606 0.4663 0.2359 0.067 Uiso 1 1 calc R . .
H55G H 0.1061 0.4686 0.2367 0.067 Uiso 1 1 calc R . .
H55H H 0.1237 0.4443 0.1960 0.067 Uiso 1 1 calc R . .
C56B C 0.17023(15) 0.3105(3) 0.22192(13) 0.0342(10) Uani 1 1 d . . .
H56F H 0.1634 0.3128 0.1922 0.051 Uiso 1 1 calc R . .
H56G H 0.1711 0.2554 0.2307 0.051 Uiso 1 1 calc R . .
H56H H 0.2005 0.3351 0.2320 0.051 Uiso 1 1 calc R . .
O5B O 0.28000(9) 0.09452(15) 0.27558(7) 0.0232(5) Uani 1 1 d . . .
C57B C 0.23481(13) 0.0962(2) 0.26801(11) 0.0200(7) Uani 1 1 d . . .
C58B C 0.21059(13) 0.0604(2) 0.23094(11) 0.0229(8) Uani 1 1 d . . .
C59B C 0.16265(15) 0.0626(2) 0.22273(12) 0.0310(9) Uani 1 1 d . . .
H59B H 0.1468 0.0397 0.1982 0.037 Uiso 1 1 calc R B .
C60B C 0.13610(15) 0.0974(3) 0.24917(14) 0.0354(10) Uani 1 1 d . . .
H60B H 0.1031 0.0980 0.2426 0.042 Uiso 1 1 calc R . .
C61B C 0.15889(14) 0.1298(2) 0.28425(13) 0.0297(9) Uani 1 1 d . . .
H61B H 0.1412 0.1533 0.3022 0.036 Uiso 1 1 calc R B .
C62B C 0.20784(13) 0.1301(2) 0.29498(11) 0.0222(8) Uani 1 1 d . . .
C63B C 0.23798(14) 0.0195(2) 0.20154(11) 0.0259(8) Uani 1 1 d . . .
C64B C 0.27408(16) 0.0748(2) 0.18847(12) 0.0339(9) Uani 1 1 d . . .
H64F H 0.2878 0.0493 0.1672 0.051 Uiso 1 1 calc R . .
H64G H 0.2986 0.0863 0.2119 0.051 Uiso 1 1 calc R . .
H64H H 0.2589 0.1239 0.1779 0.051 Uiso 1 1 calc R . .
C65B C 0.26275(16) -0.0529(2) 0.22267(13) 0.0330(10) Uani 1 1 d . . .
H65F H 0.2396 -0.0908 0.2285 0.049 Uiso 1 1 calc R . .
H65G H 0.2827 -0.0367 0.2482 0.049 Uiso 1 1 calc R . .
H65H H 0.2818 -0.0773 0.2049 0.049 Uiso 1 1 calc R . .
C66B C 0.20595(18) -0.0087(3) 0.16291(13) 0.0417(11) Uani 1 1 d . . .
H66F H 0.2241 -0.0389 0.1463 0.063 Uiso 1 1 calc R . .
H66G H 0.1918 0.0369 0.1474 0.063 Uiso 1 1 calc R . .
H66H H 0.1815 -0.0422 0.1702 0.063 Uiso 1 1 calc R . .
C67B C 0.22713(14) 0.1616(2) 0.33402(11) 0.0245(8) Uani 1 1 d . . .
H67B H 0.2058 0.1814 0.3497 0.029 Uiso 1 1 calc R B .

N5B N 0.27017(11) 0.16573(17) 0.34982(9) 0.0235(7) Uani 1 1 d . B .
C68B C 0.2806(3) 0.1943(10) 0.3914(3) 0.023(2) Uani 0.60 1 d PD B 1
C69B C 0.2505(3) 0.2182(10) 0.4164(3) 0.027(2) Uani 0.60 1 d PD B 1
H69B H 0.2179 0.2177 0.4063 0.032 Uiso 0.60 1 calc PR B 1
C70B C 0.2669(3) 0.2427(8) 0.4560(3) 0.034(3) Uani 0.60 1 d PD B 1
H70B H 0.2459 0.2571 0.4732 0.041 Uiso 0.60 1 calc PR B 1
C71B C 0.3145(3) 0.2457(6) 0.4700(2) 0.042(3) Uani 0.60 1 d PD B 1
H71B H 0.3260 0.2658 0.4963 0.050 Uiso 0.60 1 calc PR B 1
C72B C 0.3453(3) 0.2201(8) 0.4464(3) 0.040(3) Uani 0.60 1 d PD B 1
H72B H 0.3777 0.2203 0.4571 0.048 Uiso 0.60 1 calc PR B 1
C73B C 0.3291(3) 0.1939(6) 0.4069(2) 0.028(2) Uani 0.60 1 d PD B 1
N6B N 0.3574(3) 0.1605(8) 0.3818(2) 0.0260(19) Uani 0.60 1 d PD B 1
C74B C 0.3973(3) 0.1299(6) 0.3974(2) 0.031(2) Uani 0.60 1 d PD B 1
H74B H 0.4075 0.1372 0.4257 0.038 Uiso 0.60 1 calc PR B 1
C75B C 0.4280(2) 0.0864(5) 0.3767(2) 0.031(2) Uani 0.60 1 d PD B 1
C76B C 0.4697(2) 0.0607(5) 0.4015(2) 0.051(2) Uani 0.60 1 d PD B 1
H76B H 0.4755 0.0727 0.4297 0.061 Uiso 0.60 1 calc PR B 1
C77B C 0.5013(3) 0.0196(6) 0.3859(3) 0.068(4) Uani 0.60 1 d PD B 1
H77C H 0.5292 0.0027 0.4029 0.081 Uiso 0.60 1 calc PR B 1
C78B C 0.4932(3) 0.0015(6) 0.3443(3) 0.056(3) Uani 0.60 1 d PD B 1
H78C H 0.5166 -0.0254 0.3335 0.068 Uiso 0.60 1 calc PR B 1
C79B C 0.45145(19) 0.0220(4) 0.31821(19) 0.0341(17) Uani 0.60 1 d PDU B 1
C80B C 0.4183(2) 0.0678(5) 0.3347(2) 0.027(2) Uani 0.60 1 d PD B 1
O6B O 0.3801(3) 0.0909(10) 0.3108(2) 0.0295(18) Uani 0.60 1 d PD B 1
C81B C 0.4423(2) -0.0033(3) 0.2741(2) 0.039(2) Uani 0.60 1 d PD B 1
C82B C 0.4331(3) 0.0655(5) 0.2446(3) 0.044(3) Uani 0.60 1 d PD B 1
H82G H 0.4603 0.1002 0.2485 0.066 Uiso 0.60 1 calc PR B 1
H82H H 0.4060 0.0951 0.2497 0.066 Uiso 0.60 1 calc PR B 1
H82I H 0.4270 0.0455 0.2167 0.066 Uiso 0.60 1 calc PR B 1
C83B C 0.3987(3) -0.0585(5) 0.2673(3) 0.064(3) Uani 0.60 1 d PD B 1
H83G H 0.3721 -0.0299 0.2741 0.096 Uiso 0.60 1 calc PR B 1
H83H H 0.4052 -0.1049 0.2848 0.096 Uiso 0.60 1 calc PR B 1
H83I H 0.3916 -0.0750 0.2388 0.096 Uiso 0.60 1 calc PR B 1
C84B C 0.4836(3) -0.0501(5) 0.2635(3) 0.073(4) Uani 0.60 1 d PD B 1
H84G H 0.5113 -0.0166 0.2674 0.109 Uiso 0.60 1 calc PR B 1
H84H H 0.4761 -0.0672 0.2351 0.109 Uiso 0.60 1 calc PR B 1
H84I H 0.4895 -0.0964 0.2812 0.109 Uiso 0.60 1 calc PR B 1
C68" C 0.2930(4) 0.1865(14) 0.3901(4) 0.018(3) Uani 0.40 1 d PDU B 2
C69" C 0.2666(3) 0.2119(18) 0.4179(5) 0.034(4) Uani 0.40 1 d PD B 2
H69D H 0.2338 0.2154 0.4099 0.041 Uiso 0.40 1 calc PR B 2
C70" C 0.2871(4) 0.2325(12) 0.4573(4) 0.028(4) Uani 0.40 1 d PD B 2
H70D H 0.2687 0.2503 0.4761 0.034 Uiso 0.40 1 calc PR B 2
C71" C 0.3350(4) 0.2266(8) 0.4685(3) 0.027(3) Uani 0.40 1 d PD B 2
H71D H 0.3494 0.2391 0.4956 0.033 Uiso 0.40 1 calc PR B 2
C72" C 0.3622(3) 0.2031(11) 0.4414(4) 0.033(4) Uani 0.40 1 d PD B 2
H72D H 0.3952 0.2055 0.4488 0.040 Uiso 0.40 1 calc PR B 2
C73" C 0.3415(3) 0.1757(8) 0.4030(3) 0.017(3) Uani 0.40 1 d PDU B 2
N6" N 0.3659(5) 0.1449(13) 0.3743(3) 0.025(3) Uani 0.40 1 d PD B 2
C74" C 0.4050(4) 0.1082(8) 0.3855(3) 0.022(3) Uani 0.40 1 d PD B 2
H74D H 0.4177 0.1091 0.4137 0.027 Uiso 0.40 1 calc PR B 2
C75" C 0.4315(3) 0.0666(8) 0.3602(2) 0.026(3) Uani 0.40 1 d PD B 2
C77" C 0.4719(3) 0.0287(6) 0.3812(3) 0.038(3) Uani 0.40 1 d PD B 2
H77D H 0.4798 0.0331 0.4099 0.046 Uiso 0.40 1 calc PR B 2
C76" C 0.4990(4) -0.0135(9) 0.3611(3) 0.044(4) Uani 0.40 1 d PDU B 2

H76D H 0.5252 -0.0410 0.3756 0.053 Uiso 0.40 1 calc PR B 2
C78" C 0.4886(3) -0.0171(6) 0.3186(3) 0.044(4) Uani 0.40 1 d PD B 2
H78D H 0.5095 -0.0441 0.3047 0.052 Uiso 0.40 1 calc PR B 2
C79" C 0.4486(3) 0.0178(5) 0.2956(2) 0.024(2) Uani 0.40 1 d PDU B 2
C80" C 0.4189(4) 0.0610(9) 0.3173(2) 0.023(3) Uani 0.40 1 d PD B 2
O6" O 0.3797(5) 0.0898(13) 0.2973(3) 0.023(3) Uani 0.40 1 d PD B 2
C81" C 0.4370(2) 0.0094(5) 0.2498(2) 0.030(3) Uani 0.40 1 d PDU B 2
C83" C 0.3908(3) -0.0334(7) 0.2365(4) 0.055(4) Uani 0.40 1 d PD B 2
H83J H 0.3929 -0.0864 0.2483 0.083 Uiso 0.40 1 calc PR B 2
H83K H 0.3839 -0.0372 0.2068 0.083 Uiso 0.40 1 calc PR B 2
H83L H 0.3659 -0.0041 0.2459 0.083 Uiso 0.40 1 calc PR B 2
C82" C 0.4330(5) 0.0934(6) 0.2305(4) 0.044(4) Uani 0.40 1 d PD B 2
H82J H 0.4093 0.1237 0.2410 0.066 Uiso 0.40 1 calc PR B 2
H82K H 0.4243 0.0889 0.2009 0.066 Uiso 0.40 1 calc PR B 2
H82L H 0.4630 0.1204 0.2375 0.066 Uiso 0.40 1 calc PR B 2
C84" C 0.4746(3) -0.0368(7) 0.2333(4) 0.052(4) Uani 0.40 1 d PD B 2
H84J H 0.4772 -0.0898 0.2451 0.079 Uiso 0.40 1 calc PR B 2
H84K H 0.5045 -0.0095 0.2406 0.079 Uiso 0.40 1 calc PR B 2
H84L H 0.4661 -0.0406 0.2037 0.079 Uiso 0.40 1 calc PR B 2
C85B C 0.39637(13) 0.3519(2) 0.24707(11) 0.0214(8) Uani 1 1 d . . .
H85C H 0.4188 0.3123 0.2407 0.026 Uiso 1 1 calc R . .
H85D H 0.4059 0.4038 0.2380 0.026 Uiso 1 1 calc R . .
C86B C 0.38703(12) 0.2760(2) 0.30700(11) 0.0194(7) Uani 1 1 d . . .
H86C H 0.4071 0.2353 0.2979 0.023 Uiso 1 1 calc R B .
H86D H 0.3936 0.2767 0.3371 0.023 Uiso 1 1 calc R . .
C87B C 0.36766(12) 0.4140(2) 0.30363(11) 0.0181(7) Uani 1 1 d . . .
H87C H 0.3748 0.4657 0.2925 0.022 Uiso 1 1 calc R B .
H87D H 0.3736 0.4185 0.3336 0.022 Uiso 1 1 calc R . .
C88B C 0.32744(14) 0.2409(2) 0.24826(11) 0.0235(8) Uani 1 1 d . . .
H88C H 0.2945 0.2245 0.2403 0.028 Uiso 1 1 calc R B .
H88D H 0.3470 0.1970 0.2417 0.028 Uiso 1 1 calc R . .
C89B C 0.30750(13) 0.3169(2) 0.30435(11) 0.0195(7) Uani 1 1 d . . .
H89C H 0.3114 0.3188 0.3343 0.023 Uiso 1 1 calc R B .
H89D H 0.2746 0.3034 0.2934 0.023 Uiso 1 1 calc R . .
C90B C 0.30562(14) 0.3991(2) 0.24417(11) 0.0213(8) Uani 1 1 d . . .
H90C H 0.3120 0.4528 0.2352 0.026 Uiso 1 1 calc R B .
H90D H 0.2718 0.3894 0.2358 0.026 Uiso 1 1 calc R . .
C1S C 0.8711(4) 0.3319(6) 0.6469(4) 0.066(3) Uani 0.50 1 d P C 1
H1S1 H 0.8567 0.2933 0.6262 0.079 Uiso 0.50 1 calc PR C 1
H1S2 H 0.8509 0.3367 0.6674 0.079 Uiso 0.50 1 calc PR C 1
Cl1S Cl 0.92626(10) 0.29681(15) 0.67056(9) 0.0613(7) Uani 0.50 1 d P C 1
Cl2S Cl 0.87445(10) 0.42390(16) 0.62340(9) 0.0604(7) Uani 0.50 1 d P C 1
C1T C 0.0018(6) 0.4543(15) 0.6469(7) 0.168(11) Uani 0.50 1 d P . .
H1T1 H -0.0065 0.4285 0.6711 0.201 Uiso 0.50 1 calc PR . .
H1T2 H -0.0236 0.4450 0.6234 0.201 Uiso 0.50 1 calc PR . .
Cl1T Cl 0.05395(15) 0.4159(2) 0.63706(11) 0.0919(12) Uani 0.50 1 d P . .
Cl2T Cl 0.01015(12) 0.5594(2) 0.65583(11) 0.0838(10) Uani 0.50 1 d P . .
loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13

_atom_site_aniso_U_12
Zn1A 0.0281(3) 0.0251(2) 0.0237(2) -0.00384(17) 0.00882(18) -0.01133(19)
Zn2A 0.0174(2) 0.0220(2) 0.0341(2) -0.00397(18) 0.00427(19) -0.00358(18)
Zn3A 0.0384(3) 0.0203(2) 0.0769(4) 0.0116(2) 0.0383(3) 0.0069(2)
Zn1B 0.0155(2) 0.0281(2) 0.0231(2) -0.00590(17) 0.00558(17) -0.00054(18)
Zn2B 0.0180(2) 0.0194(2) 0.0237(2) 0.00232(16) 0.00611(16) 0.00044(17)
Zn3B 0.0170(2) 0.0203(2) 0.0326(2) 0.00542(17) -0.00163(18) -0.00349(17)
P1A 0.0321(6) 0.0261(5) 0.0260(5) -0.0034(4) -0.0016(4) 0.0028(4)
N7A 0.0159(16) 0.0201(15) 0.0234(15) -0.0009(12) 0.0033(12) -0.0058(12)
N8A 0.0142(16) 0.0151(14) 0.0354(17) 0.0030(12) 0.0053(13) -0.0004(12)
N9A 0.0139(15) 0.0185(14) 0.0181(14) -0.0019(11) 0.0022(12) -0.0023(12)
O1A 0.0266(16) 0.0317(15) 0.0253(14) -0.0057(11) 0.0023(12) -0.0048(12)
C1A 0.028(2) 0.0174(17) 0.033(2) 0.0031(15) 0.0041(17) -0.0093(16)
C2A 0.026(2) 0.0230(19) 0.042(2) 0.0021(17) 0.0086(18) -0.0081(17)
C3A 0.028(2) 0.035(2) 0.052(3) 0.011(2) 0.011(2) -0.0011(19)
C4A 0.037(3) 0.038(3) 0.055(3) 0.018(2) -0.002(2) -0.003(2)
C5A 0.046(3) 0.044(3) 0.031(2) 0.011(2) -0.003(2) -0.013(2)
C6A 0.038(3) 0.029(2) 0.031(2) 0.0074(17) 0.0001(19) -0.0122(19)
C7A 0.015(2) 0.043(2) 0.043(2) -0.0177(19) 0.0041(18) -0.0026(18)
C8A 0.042(3) 0.063(3) 0.025(2) 0.000(2) 0.0055(19) 0.016(2)
C9A 0.026(3) 0.080(4) 0.080(4) -0.056(3) 0.012(3) -0.016(3)
C10A 0.030(3) 0.052(3) 0.062(3) -0.011(2) 0.017(2) 0.003(2)
C11A 0.054(3) 0.031(2) 0.0201(19) 0.0021(16) 0.0052(19) -0.019(2)
N1A 0.036(2) 0.0239(16) 0.0273(17) 0.0011(13) 0.0078(15) -0.0095(15)
C12A 0.055(3) 0.023(2) 0.0227(19) -0.0034(15) 0.0143(19) -0.0146(19)
C13A 0.066(3) 0.025(2) 0.0213(19) 0.0027(15) 0.004(2) -0.011(2)
C14A 0.088(4) 0.022(2) 0.023(2) -0.0018(16) 0.013(2) -0.005(2)
C15A 0.090(4) 0.023(2) 0.032(2) -0.0027(17) 0.028(3) -0.012(2)
C16A 0.066(3) 0.029(2) 0.042(2) -0.0124(18) 0.031(2) -0.024(2)
C17A 0.049(3) 0.024(2) 0.032(2) -0.0054(16) 0.016(2) -0.0197(19)
N2A 0.040(2) 0.0328(18) 0.0309(18) -0.0081(14) 0.0164(16) -0.0180(17)
C18A 0.045(3) 0.0195(19) 0.041(2) -0.0020(17) 0.023(2) -0.0096(18)
C19A 0.038(3) 0.0208(19) 0.038(2) 0.0055(16) 0.0141(19) -0.0043(17)
C20A 0.030(3) 0.032(2) 0.046(3) 0.0065(18) 0.011(2) 0.0046(19)
C21A 0.031(3) 0.047(3) 0.057(3) -0.003(2) 0.003(2) 0.008(2)
C22A 0.037(3) 0.033(2) 0.043(3) -0.0023(19) -0.005(2) 0.004(2)
C23A 0.028(2) 0.0209(18) 0.035(2) 0.0009(15) 0.0026(17) -0.0012(16)
C24A 0.035(2) 0.0154(17) 0.035(2) 0.0004(15) 0.0114(18) -0.0088(16)
O2A 0.0273(16) 0.0382(16) 0.0284(14) -0.0102(12) 0.0086(12) -0.0167(13)
C25A 0.035(2) 0.027(2) 0.025(2) 0.0007(16) 0.0016(17) -0.0076(18)
C26A 0.076(4) 0.054(3) 0.038(3) -0.009(2) 0.025(3) -0.035(3)
C27A 0.030(2) 0.035(2) 0.028(2) -0.0035(16) 0.0069(17) -0.0033(18)
C28A 0.040(3) 0.058(3) 0.035(2) -0.016(2) 0.000(2) -0.007(2)
O3A 0.0219(15) 0.0280(14) 0.0333(15) 0.0011(11) 0.0083(12) 0.0015(12)
C29A 0.017(2) 0.039(2) 0.026(2) -0.0051(16) 0.0054(16) -0.0102(17)
C30A 0.021(2) 0.050(3) 0.027(2) -0.0020(18) 0.0092(17) -0.0063(19)
C31A 0.034(3) 0.054(3) 0.046(3) -0.013(2) 0.024(2) -0.010(2)
C32A 0.036(3) 0.035(2) 0.055(3) -0.015(2) 0.022(2) -0.001(2)
C33A 0.031(2) 0.027(2) 0.040(2) -0.0063(17) 0.0129(19) -0.0043(18)
C34A 0.0176(19) 0.0226(18) 0.031(2) -0.0081(15) 0.0054(16) -0.0076(15)
C35A 0.0140(19) 0.0242(19) 0.032(2) 0.0000(15) 0.0035(15) -0.0061(15)
C36A 0.032(3) 0.063(3) 0.033(2) 0.005(2) 0.017(2) -0.004(2)
C37A 0.036(3) 0.086(4) 0.039(3) 0.017(3) 0.009(2) -0.007(3)
C38A 0.028(3) 0.060(3) 0.050(3) 0.017(2) 0.011(2) -0.002(2)

C39A 0.059(4) 0.087(4) 0.039(3) 0.009(3) 0.030(3) 0.000(3)
N3A 0.0137(16) 0.0304(17) 0.0205(15) -0.0049(12) 0.0013(12) -0.0050(13)
C40A 0.015(2) 0.047(2) 0.0222(19) -0.0070(17) -0.0007(16) -0.0047(17)
C41A 0.017(2) 0.059(3) 0.030(2) -0.0071(19) 0.0030(17) -0.0069(19)
C42A 0.022(2) 0.082(4) 0.022(2) 0.007(2) -0.0018(17) -0.009(2)
C43A 0.019(2) 0.103(4) 0.028(2) -0.016(3) 0.0045(19) -0.001(3)
C44A 0.025(2) 0.083(4) 0.033(2) -0.025(2) -0.0028(19) 0.008(2)
C45A 0.014(2) 0.058(3) 0.033(2) -0.023(2) -0.0032(17) 0.000(2)
N4A 0.0210(19) 0.038(2) 0.042(2) -0.0170(16) -0.0056(15) 0.0055(16)
C46A 0.023(2) 0.070(4) 0.060(3) -0.044(3) -0.014(2) 0.006(2)
C47A 0.030(3) 0.025(2) 0.100(5) -0.011(3) -0.024(3) 0.004(2)
C48A 0.058(4) 0.049(4) 0.128(6) -0.040(4) -0.038(4) 0.010(3)
C49A 0.062(4) 0.028(3) 0.130(6) -0.012(3) -0.032(4) 0.010(3)
C50A 0.046(4) 0.022(3) 0.166(8) -0.009(3) -0.020(4) -0.003(2)
C51A 0.018(2) 0.022(2) 0.132(6) 0.009(3) -0.009(3) -0.0034(18)
C52A 0.016(2) 0.031(2) 0.084(4) -0.008(2) -0.012(2) -0.0059(18)
O4A 0.0293(17) 0.0243(15) 0.071(2) 0.0028(14) 0.0183(15) -0.0039(13)
C53A 0.041(3) 0.039(3) 0.129(6) 0.038(3) 0.033(4) 0.007(2)
C54A 0.040(3) 0.051(4) 0.186(8) 0.060(4) 0.017(4) 0.002(3)
C55A 0.074(5) 0.085(5) 0.210(9) 0.091(6) 0.093(6) 0.044(4)
C56A 0.059(4) 0.038(3) 0.080(4) 0.016(2) 0.033(3) 0.008(2)
O5A 0.0280(16) 0.0242(13) 0.0420(16) -0.0007(11) 0.0095(13) -0.0060(12)
C57A 0.021(2) 0.0264(19) 0.028(2) 0.0028(15) 0.0088(16) 0.0051(16)
C58A 0.026(2) 0.036(2) 0.027(2) 0.0040(16) 0.0117(17) 0.0039(18)
C59A 0.033(3) 0.046(3) 0.047(3) 0.018(2) 0.013(2) 0.011(2)
C60A 0.038(3) 0.031(2) 0.079(4) 0.023(2) 0.015(3) -0.005(2)
C61A 0.028(2) 0.026(2) 0.061(3) 0.005(2) 0.002(2) -0.0023(18)
C62A 0.019(2) 0.0242(19) 0.033(2) 0.0016(16) 0.0058(16) -0.0002(16)
C63A 0.031(2) 0.057(3) 0.027(2) 0.0000(19) 0.0020(18) 0.012(2)
C64A 0.046(3) 0.119(5) 0.044(3) 0.017(3) -0.004(3) 0.014(3)
C65A 0.023(2) 0.055(3) 0.039(2) -0.015(2) 0.0002(19) 0.007(2)
C66A 0.038(3) 0.079(4) 0.059(3) -0.038(3) -0.008(2) 0.017(3)
C67A 0.041(3) 0.0226(19) 0.034(2) -0.0058(16) 0.0009(19) 0.0127(18)
N5A 0.064(3) 0.035(2) 0.0253(18) 0.0065(15) 0.0162(18) 0.0244(19)
C68A 0.046(8) 0.008(5) 0.006(4) -0.002(3) -0.003(4) 0.005(4)
C69A 0.018(5) 0.025(4) 0.018(4) -0.008(3) -0.001(3) 0.009(3)
C70A 0.039(6) 0.039(5) 0.038(5) -0.009(4) 0.010(4) 0.013(4)
C71A 0.037(6) 0.039(5) 0.011(4) -0.002(4) 0.008(4) 0.017(4)
C72A 0.027(6) 0.030(5) 0.030(7) 0.004(5) 0.009(5) 0.004(4)
C73A 0.024(5) 0.023(4) 0.017(4) 0.007(3) 0.012(4) 0.013(4)
N6A 0.014(5) 0.030(4) 0.021(5) 0.013(4) 0.006(4) 0.004(4)
C74A 0.042(5) 0.023(4) 0.025(4) 0.002(3) 0.018(4) 0.004(4)
C75A 0.026(6) 0.011(5) 0.045(6) 0.005(4) 0.019(4) -0.005(4)
C76A 0.054(5) 0.019(3) 0.077(6) -0.002(3) 0.043(4) 0.000(3)
C77A 0.051(6) 0.013(4) 0.098(8) -0.004(4) 0.059(6) -0.003(4)
C78A 0.048(7) 0.016(5) 0.103(8) -0.016(5) 0.027(6) -0.021(4)
C79A 0.006(4) 0.012(3) 0.084(7) -0.002(4) 0.012(4) -0.002(3)
C80A 0.016(4) 0.012(4) 0.043(5) 0.010(4) 0.014(4) 0.006(3)
O6A 0.015(3) 0.023(3) 0.038(3) 0.010(3) 0.003(3) -0.002(2)
C81A 0.013(5) 0.023(5) 0.074(6) 0.011(4) -0.006(4) 0.000(4)
C82A 0.022(5) 0.026(4) 0.112(9) -0.004(5) 0.003(5) -0.004(4)
C83A 0.027(5) 0.025(4) 0.099(9) 0.012(5) -0.009(5) 0.000(4)
C84A 0.028(5) 0.029(5) 0.058(6) 0.015(4) -0.002(5) -0.011(4)
C68' 0.043(8) 0.028(7) 0.036(6) -0.025(5) 0.003(5) 0.006(5)

C69' 0.021(6) 0.029(6) 0.059(7) -0.007(5) 0.017(5) 0.005(4)
C70' 0.060(9) 0.079(10) 0.018(6) 0.001(6) 0.008(6) 0.041(8)
C71' 0.057(9) 0.054(8) 0.039(8) 0.007(7) 0.008(7) 0.039(7)
C72' 0.070(8) 0.033(5) 0.033(5) 0.004(4) 0.020(5) 0.025(5)
C73' 0.029(8) 0.032(6) 0.025(7) 0.006(5) 0.003(6) 0.006(5)
N6' 0.030(5) 0.028(4) 0.031(4) 0.003(3) 0.004(4) 0.009(4)
C74' 0.058(9) 0.011(5) 0.037(6) 0.006(4) 0.034(6) 0.002(5)
C75' 0.048(7) 0.026(6) 0.052(7) 0.005(5) 0.034(6) 0.004(5)
C76' 0.065(8) 0.022(5) 0.081(8) 0.005(5) 0.054(7) 0.014(5)
C77' 0.054(5) 0.019(3) 0.077(6) -0.002(3) 0.043(4) 0.000(3)
C78' 0.024(5) 0.033(5) 0.108(10) -0.011(5) 0.024(6) -0.006(4)
C79' 0.015(5) 0.019(4) 0.079(7) -0.004(4) 0.001(5) 0.000(4)
C80' 0.026(5) 0.016(4) 0.058(6) 0.002(4) 0.014(4) 0.007(3)
O6' 0.018(3) 0.034(3) 0.031(3) 0.009(3) -0.001(3) 0.000(2)
C81' 0.020(5) 0.024(5) 0.084(8) 0.011(5) -0.014(5) 0.006(4)
C82' 0.046(7) 0.032(5) 0.110(10) 0.005(6) -0.009(6) 0.002(5)
C83' 0.038(6) 0.038(5) 0.050(6) 0.010(4) 0.001(5) -0.006(4)
C84' 0.053(7) 0.032(5) 0.112(10) 0.008(6) -0.028(7) -0.004(5)
C85A 0.023(2) 0.0229(18) 0.0236(18) -0.0058(14) -0.0009(15) 0.0009(16)
C86A 0.0163(19) 0.0151(16) 0.0251(18) -0.0001(13) 0.0038(14) -0.0027(14)
C87A 0.0169(19) 0.0196(18) 0.038(2) -0.0030(15) 0.0104(16) -0.0066(15)
C88A 0.022(2) 0.0237(19) 0.040(2) 0.0007(16) -0.0050(17) 0.0038(16)
C89A 0.0167(19) 0.0186(17) 0.0281(19) 0.0002(14) 0.0046(15) -0.0070(15)
C90A 0.021(2) 0.0265(19) 0.0240(19) 0.0030(14) 0.0065(15) -0.0058(16)
P1B 0.0257(5) 0.0248(5) 0.0217(5) 0.0003(4) 0.0069(4) -0.0032(4)
N7B 0.0155(16) 0.0200(15) 0.0213(15) -0.0003(11) 0.0046(12) 0.0008(12)
N8B 0.0152(16) 0.0177(14) 0.0262(16) 0.0009(12) 0.0063(12) 0.0013(12)
N9B 0.0110(15) 0.0177(14) 0.0207(15) 0.0028(11) 0.0042(12) -0.0002(12)
O1B 0.0201(14) 0.0367(15) 0.0246(13) -0.0036(11) 0.0101(11) 0.0041(12)
C1B 0.0121(19) 0.033(2) 0.0266(19) -0.0058(15) 0.0023(15) -0.0047(15)
C2B 0.017(2) 0.033(2) 0.033(2) -0.0119(16) 0.0071(16) -0.0076(16)
C3B 0.038(3) 0.037(2) 0.040(2) -0.0114(19) 0.020(2) -0.006(2)
C4B 0.047(3) 0.027(2) 0.070(3) -0.012(2) 0.031(3) 0.001(2)
C5B 0.032(3) 0.032(2) 0.047(3) -0.0038(19) 0.013(2) -0.0015(19)
C6B 0.016(2) 0.030(2) 0.036(2) -0.0026(16) 0.0074(16) 0.0004(16)
C7B 0.020(2) 0.045(2) 0.028(2) -0.0059(17) 0.0092(16) 0.0002(18)
C8B 0.047(3) 0.054(3) 0.035(2) -0.008(2) 0.018(2) 0.001(2)
C9B 0.032(2) 0.032(2) 0.037(2) 0.0013(17) 0.0049(19) -0.0026(18)
C10B 0.028(2) 0.079(4) 0.032(2) 0.003(2) 0.0074(19) 0.001(2)
N1B 0.0161(18) 0.045(2) 0.0255(17) -0.0004(14) 0.0046(14) 0.0028(15)
C11B 0.0144(19) 0.035(2) 0.029(2) 0.0020(16) -0.0010(16) -0.0006(16)
C12B 0.011(2) 0.053(3) 0.027(2) -0.0025(18) 0.0039(16) -0.0027(18)
C13B 0.018(2) 0.064(3) 0.035(2) 0.006(2) 0.0069(18) -0.001(2)
C14B 0.022(2) 0.090(4) 0.030(2) 0.011(2) -0.0011(18) -0.015(2)
C15B 0.029(3) 0.089(4) 0.028(2) -0.011(2) 0.0081(19) -0.020(3)
C16B 0.021(2) 0.069(3) 0.024(2) -0.015(2) 0.0084(17) -0.015(2)
C17B 0.013(2) 0.057(3) 0.028(2) -0.0068(19) 0.0020(16) -0.0089(19)
N2B 0.0166(17) 0.046(2) 0.0249(17) -0.0104(15) 0.0066(13) -0.0024(15)
C18B 0.013(2) 0.055(3) 0.032(2) -0.0205(19) 0.0034(16) -0.0009(18)
C19B 0.016(2) 0.043(2) 0.041(2) -0.0178(19) 0.0027(17) -0.0020(18)
C20B 0.020(2) 0.059(3) 0.060(3) -0.035(3) -0.004(2) 0.010(2)
C21B 0.028(3) 0.047(3) 0.080(4) -0.046(3) -0.008(2) 0.008(2)
C22B 0.017(2) 0.034(2) 0.080(4) -0.023(2) -0.001(2) 0.0031(18)
C23B 0.011(2) 0.030(2) 0.059(3) -0.0164(19) 0.0106(18) 0.0000(16)

C24B 0.0119(19) 0.0260(19) 0.048(2) -0.0149(17) 0.0076(17) -0.0027(15)
O2B 0.0271(16) 0.0272(14) 0.0344(15) -0.0114(11) 0.0157(12) -0.0085(12)
C25B 0.033(3) 0.0188(19) 0.069(3) -0.0004(19) 0.033(2) -0.0001(17)
C26B 0.044(3) 0.027(2) 0.095(4) 0.010(2) 0.029(3) 0.002(2)
C27B 0.067(4) 0.037(3) 0.104(5) 0.022(3) 0.065(4) 0.022(3)
C28B 0.065(3) 0.023(2) 0.035(2) -0.0012(17) 0.014(2) -0.006(2)
O3B 0.0244(14) 0.0166(12) 0.0272(13) 0.0044(9) 0.0019(11) 0.0023(10)
C29B 0.0186(19) 0.0184(17) 0.0260(18) -0.0002(13) 0.0089(15) 0.0003(14)
C30B 0.025(2) 0.0205(18) 0.032(2) 0.0022(15) 0.0076(17) 0.0031(15)
C31B 0.032(2) 0.026(2) 0.041(2) 0.0133(17) 0.0084(19) 0.0008(17)
C32B 0.033(2) 0.026(2) 0.046(3) 0.0117(18) 0.010(2) -0.0066(18)
C33B 0.020(2) 0.030(2) 0.038(2) -0.0004(17) 0.0075(17) -0.0038(17)
C34B 0.019(2) 0.0247(18) 0.0253(19) 0.0022(14) 0.0070(15) 0.0038(15)
C35B 0.032(2) 0.026(2) 0.031(2) 0.0047(16) 0.0062(17) 0.0055(17)
C36B 0.049(3) 0.043(3) 0.035(2) 0.0127(19) -0.004(2) 0.002(2)
C37B 0.052(3) 0.040(2) 0.028(2) -0.0034(18) -0.001(2) 0.014(2)
C38B 0.026(2) 0.028(2) 0.047(3) 0.0019(17) 0.0007(19) 0.0012(17)
C39E 0.0169(19) 0.0233(18) 0.031(2) -0.0025(15) 0.0066(15) 0.0005(15)
N3B 0.0208(17) 0.0210(15) 0.0209(15) -0.0001(12) 0.0065(12) 0.0048(13)
C40B 0.0176(19) 0.0242(18) 0.0258(18) 0.0013(14) 0.0067(15) 0.0077(15)
C41B 0.029(2) 0.030(2) 0.027(2) -0.0026(16) 0.0075(17) 0.0058(17)
C42B 0.032(2) 0.041(2) 0.024(2) -0.0057(17) 0.0031(17) 0.0115(19)
C43B 0.041(3) 0.045(2) 0.0215(19) 0.0039(17) 0.0083(18) 0.013(2)
C44B 0.042(3) 0.034(2) 0.029(2) 0.0033(17) 0.0153(19) 0.0065(19)
C45B 0.031(2) 0.0285(19) 0.0224(18) 0.0011(15) 0.0107(16) 0.0086(17)
N4B 0.0299(19) 0.0219(16) 0.0261(16) 0.0003(12) 0.0125(14) 0.0000(14)
C46B 0.037(3) 0.028(2) 0.031(2) 0.0006(16) 0.0164(19) 0.0029(18)
C47B 0.030(2) 0.029(2) 0.045(2) -0.0013(18) 0.020(2) -0.0043(18)
C48B 0.050(3) 0.049(3) 0.048(3) -0.002(2) 0.031(2) -0.011(2)
C49B 0.039(3) 0.046(3) 0.066(3) -0.005(2) 0.034(3) -0.016(2)
C50B 0.026(2) 0.034(2) 0.064(3) -0.005(2) 0.019(2) -0.008(2)
C51B 0.026(2) 0.0217(19) 0.050(3) -0.0033(17) 0.0139(19) 0.0013(17)
C52B 0.022(2) 0.0191(18) 0.043(2) 0.0002(16) 0.0159(18) 0.0019(15)
O4B 0.0181(14) 0.0255(13) 0.0323(14) 0.0004(11) 0.0076(11) -0.0020(11)
C53B 0.024(2) 0.031(2) 0.049(3) 0.0008(19) 0.0031(19) -0.0061(18)
C54B 0.020(2) 0.046(3) 0.066(3) -0.011(2) 0.005(2) -0.009(2)
C55B 0.034(3) 0.036(2) 0.058(3) 0.005(2) -0.007(2) -0.003(2)
C56B 0.026(2) 0.036(2) 0.040(2) -0.0043(18) 0.0071(19) -0.0087(19)
O5B 0.0203(14) 0.0259(13) 0.0235(13) 0.0008(10) 0.0046(11) 0.0001(11)
C57B 0.018(2) 0.0154(16) 0.0256(18) 0.0027(13) 0.0018(15) -0.0018(14)
C58B 0.023(2) 0.0187(17) 0.0263(19) 0.0001(14) 0.0020(15) -0.0011(15)
C59B 0.027(2) 0.031(2) 0.032(2) -0.0080(17) -0.0032(17) -0.0034(18)
C60B 0.015(2) 0.039(2) 0.049(3) -0.005(2) -0.0019(19) -0.0016(18)
C61B 0.025(2) 0.025(2) 0.042(2) -0.0061(17) 0.0132(18) 0.0009(17)
C62B 0.021(2) 0.0199(18) 0.0267(19) -0.0015(14) 0.0078(16) -0.0023(15)
C63B 0.025(2) 0.029(2) 0.0221(19) -0.0058(15) 0.0016(16) 0.0002(17)
C64B 0.046(3) 0.028(2) 0.031(2) 0.0000(16) 0.0172(19) 0.0017(19)
C65B 0.041(3) 0.025(2) 0.036(2) -0.0043(16) 0.0153(19) 0.0058(18)
C66B 0.042(3) 0.049(3) 0.031(2) -0.0120(19) -0.002(2) 0.005(2)
C67B 0.026(2) 0.0190(18) 0.031(2) 0.0002(15) 0.0112(17) -0.0062(16)
N5B 0.0264(19) 0.0170(15) 0.0281(16) -0.0004(12) 0.0074(14) -0.0059(13)
C68B 0.019(4) 0.030(5) 0.021(4) 0.001(3) 0.004(4) -0.009(5)
C69B 0.043(6) 0.021(4) 0.019(4) -0.005(3) 0.013(4) -0.016(6)
C70B 0.048(8) 0.025(5) 0.029(4) -0.001(3) 0.010(5) -0.014(6)

C71B 0.069(11) 0.028(6) 0.028(5) 0.009(4) 0.006(6) -0.013(6)
C72B 0.053(7) 0.049(8) 0.015(4) 0.002(4) -0.002(5) -0.028(7)
C73B 0.040(6) 0.013(5) 0.031(4) 0.010(3) 0.011(4) -0.001(4)
N6B 0.022(4) 0.023(6) 0.030(4) 0.005(4) -0.003(4) -0.011(3)
C74B 0.024(5) 0.031(6) 0.034(5) 0.009(4) -0.005(4) -0.014(4)
C75B 0.018(5) 0.026(6) 0.046(6) 0.017(5) -0.003(5) -0.005(4)
C76B 0.019(4) 0.050(6) 0.079(7) 0.035(5) -0.003(4) -0.008(4)
C77B 0.017(5) 0.071(7) 0.111(10) 0.058(7) 0.001(6) 0.004(5)
C78B 0.023(5) 0.049(7) 0.101(11) 0.033(7) 0.023(7) 0.002(5)
C79B 0.019(3) 0.031(3) 0.053(4) 0.011(3) 0.010(3) -0.006(3)
C80B 0.014(4) 0.015(4) 0.051(7) 0.006(6) 0.007(5) 0.001(3)
O6B 0.009(3) 0.029(3) 0.047(5) -0.006(5) -0.005(3) 0.002(2)
C81B 0.015(4) 0.035(4) 0.067(7) -0.012(5) 0.012(4) 0.001(3)
C82B 0.026(5) 0.040(6) 0.070(8) -0.016(5) 0.018(5) -0.001(4)
C83B 0.037(5) 0.048(5) 0.113(9) -0.028(6) 0.031(6) -0.002(4)
C84B 0.053(7) 0.041(5) 0.141(11) -0.011(7) 0.062(8) 0.007(5)
C68" 0.017(5) 0.018(5) 0.020(5) 0.007(3) 0.010(4) -0.003(4)
C69" 0.018(7) 0.034(9) 0.051(10) -0.001(6) 0.007(7) -0.016(8)
C70" 0.038(12) 0.032(8) 0.016(6) 0.004(5) 0.009(7) -0.013(9)
C71" 0.041(10) 0.009(6) 0.025(7) 0.002(5) -0.011(7) -0.002(5)
C72" 0.035(8) 0.039(9) 0.027(7) 0.018(5) 0.010(6) -0.010(7)
C73" 0.021(6) 0.006(6) 0.019(5) 0.000(4) -0.007(5) 0.000(5)
N6" 0.025(7) 0.023(8) 0.027(5) -0.002(5) 0.006(5) -0.002(4)
C74" 0.021(7) 0.015(8) 0.028(7) 0.006(5) -0.005(6) -0.001(5)
C75" 0.025(7) 0.029(7) 0.023(7) -0.007(6) -0.001(6) 0.002(5)
C77" 0.032(8) 0.010(5) 0.070(9) -0.003(5) 0.002(7) 0.006(5)
C76" 0.026(6) 0.048(8) 0.054(8) -0.005(7) -0.003(6) -0.003(6)
C78" 0.015(6) 0.027(6) 0.084(10) -0.030(7) -0.003(6) -0.001(4)
C79" 0.013(4) 0.024(4) 0.033(4) -0.007(4) -0.001(4) -0.006(3)
C80" 0.022(7) 0.019(5) 0.029(7) -0.008(6) 0.006(5) -0.010(5)
O6" 0.015(5) 0.014(4) 0.035(6) -0.012(6) -0.005(4) 0.003(3)
C81" 0.028(5) 0.022(5) 0.038(6) -0.025(5) 0.006(5) -0.002(4)
C83" 0.020(6) 0.062(9) 0.084(10) -0.049(8) 0.011(7) -0.010(6)
C82" 0.019(7) 0.050(10) 0.064(10) -0.011(7) 0.014(7) -0.005(7)
C84" 0.030(7) 0.053(8) 0.078(10) -0.039(8) 0.023(7) -0.011(6)
C85B 0.020(2) 0.0211(18) 0.0245(18) -0.0003(14) 0.0079(15) -0.0018(15)
C86B 0.0147(18) 0.0188(17) 0.0238(18) 0.0003(13) 0.0009(14) 0.0007(14)
C87B 0.0150(18) 0.0185(17) 0.0219(17) 0.0006(13) 0.0064(14) 0.0000(14)
C88B 0.020(2) 0.0219(18) 0.0288(19) -0.0046(15) 0.0062(15) -0.0041(15)
C89B 0.0153(19) 0.0194(17) 0.0245(18) 0.0027(14) 0.0055(14) 0.0004(15)
C90B 0.021(2) 0.0218(18) 0.0205(18) 0.0018(14) 0.0026(15) -0.0003(15)
C1S 0.030(6) 0.045(6) 0.121(11) 0.021(6) 0.008(6) 0.002(5)
Cl1S 0.0525(17) 0.0458(14) 0.0787(19) 0.0075(12) -0.0059(14) 0.0043(12)
Cl2S 0.0485(16) 0.0562(15) 0.0788(19) 0.0197(13) 0.0181(14) 0.0135(12)
C1T 0.077(12) 0.28(3) 0.158(17) -0.123(18) 0.065(12) -0.118(16)
Cl1T 0.109(3) 0.088(2) 0.085(2) 0.0368(19) 0.035(2) 0.025(2)
Cl2T 0.067(2) 0.087(2) 0.083(2) -0.0077(18) -0.0234(18) 0.0073(18)
_geom_special_details
;
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.
;
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
Zn1A O2A 1.952(2) . ?
Zn1A O1A 1.979(3) . ?
Zn1A N2A 2.062(3) . ?
Zn1A N1A 2.066(3) . ?
Zn1A N7A 2.211(3) . ?
Zn2A O3A 1.940(3) . ?
Zn2A O4A 1.982(3) . ?
Zn2A N4A 2.065(4) . ?
Zn2A N3A 2.076(3) . ?
Zn2A N9A 2.199(3) . ?
Zn3A O6A 1.866(4) . ?
Zn3A N6' 1.909(6) . ?
Zn3A O5A 1.932(3) . ?
Zn3A N5A 2.113(4) . ?
Zn3A O6' 2.171(5) . ?
Zn3A N8A 2.216(3) . ?
Zn3A N6A 2.247(5) . ?
Zn1B O1B 1.952(2) . ?
Zn1B O2B 1.959(3) . ?
Zn1B N1B 2.072(3) . ?
Zn1B N2B 2.077(3) . ?
Zn1B N7B 2.210(3) . ?
Zn2B O3B 1.942(2) . ?
Zn2B O4B 1.977(3) . ?
Zn2B N4B 2.055(3) . ?
Zn2B N3B 2.076(3) . ?
Zn2B N9B 2.197(3) . ?
Zn3B O6B 1.899(5) . ?
Zn3B O5B 1.946(3) . ?
Zn3B N6" 1.991(10) . ?
Zn3B N5B 2.076(3) . ?
Zn3B O6" 2.087(8) . ?
Zn3B N6B 2.146(7) . ?
Zn3B N8B 2.213(3) . ?
P1A C88A 1.844(4) . ?
P1A C85A 1.857(4) . ?
P1A C90A 1.857(4) . ?
N7A C87A 1.476(5) . ?
N7A C86A 1.477(5) . ?
N7A C85A 1.484(4) . ?
N8A C88A 1.473(5) . ?
N8A C87A 1.480(4) . ?
N8A C89A 1.488(5) . ?
N9A C89A 1.473(5) . ?
N9A C86A 1.480(4) . ?
N9A C90A 1.489(4) . ?

O1A C1A 1.289(4) . ?
C1A C2A 1.436(4) . ?
C1A C6A 1.440(4) . ?
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C2A C7A 1.548(5) . ?
C3A C4A 1.405(5) . ?
C4A C5A 1.341(5) . ?
C5A C6A 1.418(5) . ?
C6A C11A 1.434(5) . ?
C7A C8A 1.525(5) . ?
C7A C9A 1.533(5) . ?
C7A C10A 1.541(5) . ?
C11A N1A 1.291(5) . ?
N1A C12A 1.428(4) . ?
C12A C17A 1.400(6) . ?
C12A C13A 1.408(5) . ?
C13A C14A 1.375(5) . ?
C14A C15A 1.377(7) . ?
C15A C16A 1.393(6) . ?
C16A C17A 1.388(5) . ?
C17A N2A 1.411(5) . ?
N2A C18A 1.301(5) . ?
C18A C19A 1.434(5) . ?
C19A C20A 1.413(5) . ?
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C40A C45A 1.407(6) . ?
C41A C42A 1.384(6) . ?
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C44A C45A 1.385(6) . ?

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C81A C84A 1.548(6) . ?
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C81' C82' 1.542(6) . ?
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N6' Zn3A N8A 104.1(2) . . ?
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O3A C29A C34A 123.1(3) . . ?
O3A C29A C30A 118.9(4) . . ?

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C35A N3A C40A 122.3(3) . . ?
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C50A C49A C48A 122.2(6) . . ?
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C50A C51A C52A 115.9(7) . . ?
C50A C51A C53A 123.7(6) . . ?
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O4A C52A C47A 120.2(5) . . ?
O4A C52A C51A 120.2(5) . . ?
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C52A O4A Zn2A 133.5(3) . . ?
C51A C53A C56A 111.6(5) . . ?
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C82' C81' C84' 106.5(5) . . ?
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N7A C86A N9A 113.1(3) . . ?
N7A C87A N8A 113.1(3) . . ?
N8A C88A P1A 114.1(3) . . ?
N9A C89A N8A 113.0(3) . . ?
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C6B C1B C2B 117.6(3) . . ?
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C11B C6B C1B 124.3(4) . . ?
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N8B C89B N9B 113.1(3) . . ?
N9B C90B P1B 114.5(2) . . ?
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Cl1T C1T Cl2T 107.6(8) . . ?
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N5A Zn3A N8A C88A 117.6(2) . . . . ?
O6' Zn3A N8A C88A -62.4(3) . . . . ?
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O6A Zn3A N8A C87A 39.8(3) . . . . ?
N6' Zn3A N8A C87A -29.4(3) . . . . ?
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N5A Zn3A N8A C87A -122.6(2) . . . . ?
O6' Zn3A N8A C87A 57.4(3) . . . . ?
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N6' Zn3A N8A C89A 89.8(3) . . . . ?
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O6' Zn3A N8A C89A 176.7(3) . . . . ?
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O3A Zn2A N9A C86A -90.9(2) . . . . ?
O4A Zn2A N9A C86A 171.7(2) . . . . ?
N4A Zn2A N9A C86A 82.9(2) . . . . ?

N3A Zn2A N9A C86A 1.6(2) . . . . ?
O3A Zn2A N9A C90A 29.7(2) . . . . ?
O4A Zn2A N9A C90A -67.7(2) . . . . ?
N4A Zn2A N9A C90A -156.5(2) . . . . ?
N3A Zn2A N9A C90A 122.2(2) . . . . ?
O2A Zn1A O1A C1A 139.3(3) . . . . ?
N2A Zn1A O1A C1A 23.8(6) . . . . ?
N1A Zn1A O1A C1A -19.2(3) . . . . ?
N7A Zn1A O1A C1A -119.0(3) . . . . ?
Zn1A O1A C1A C2A -165.5(3) . . . . ?
Zn1A O1A C1A C6A 15.9(5) . . . . ?
O1A C1A C2A C3A 177.9(4) . . . . ?
C6A C1A C2A C3A -3.4(5) . . . . ?
O1A C1A C2A C7A 0.5(5) . . . . ?
C6A C1A C2A C7A 179.2(3) . . . . ?
C1A C2A C3A C4A 2.4(6) . . . . ?
C7A C2A C3A C4A 179.7(4) . . . . ?
C2A C3A C4A C5A -1.0(7) . . . . ?
C3A C4A C5A C6A 0.6(7) . . . . ?
C4A C5A C6A C11A -178.0(4) . . . . ?
C4A C5A C6A C1A -1.7(6) . . . . ?
O1A C1A C6A C5A -178.3(4) . . . . ?
C2A C1A C6A C5A 3.0(5) . . . . ?
O1A C1A C6A C11A -2.2(6) . . . . ?
C2A C1A C6A C11A 179.1(4) . . . . ?
C3A C2A C7A C8A 121.7(4) . . . . ?
C1A C2A C7A C8A -61.0(4) . . . . ?
C3A C2A C7A C9A -116.6(4) . . . . ?
C1A C2A C7A C9A 60.7(5) . . . . ?
C3A C2A C7A C10A 2.5(5) . . . . ?
C1A C2A C7A C10A 179.8(3) . . . . ?
C5A C6A C11A N1A 176.4(4) . . . . ?
C1A C6A C11A N1A 0.2(7) . . . . ?
C6A C11A N1A C12A -174.6(4) . . . . ?
C6A C11A N1A Zn1A -10.3(6) . . . . ?
O2A Zn1A N1A C11A -89.5(4) . . . . ?
O1A Zn1A N1A C11A 15.6(3) . . . . ?
N2A Zn1A N1A C11A -151.8(3) . . . . ?
N7A Zn1A N1A C11A 108.5(3) . . . . ?
O2A Zn1A N1A C12A 75.6(4) . . . . ?
O1A Zn1A N1A C12A -179.4(3) . . . . ?
N2A Zn1A N1A C12A 13.3(3) . . . . ?
N7A Zn1A N1A C12A -86.4(3) . . . . ?
C11A N1A C12A C17A 152.4(4) . . . . ?
Zn1A N1A C12A C17A -13.7(4) . . . . ?
C11A N1A C12A C13A -26.4(6) . . . . ?
Zn1A N1A C12A C13A 167.6(3) . . . . ?
C17A C12A C13A C14A -3.3(6) . . . . ?
N1A C12A C13A C14A 175.4(4) . . . . ?
C12A C13A C14A C15A -1.7(6) . . . . ?
C13A C14A C15A C16A 3.9(6) . . . . ?
C14A C15A C16A C17A -1.1(6) . . . . ?
C15A C16A C17A C12A -3.8(6) . . . . ?
C15A C16A C17A N2A 179.4(4) . . . . ?

C13A C12A C17A C16A 6.0(6) . . . . ?
N1A C12A C17A C16A -172.8(4) . . . . ?
C13A C12A C17A N2A -176.9(3) . . . . ?
N1A C12A C17A N2A 4.3(5) . . . . ?
C16A C17A N2A C18A -1.3(6) . . . . ?
C12A C17A N2A C18A -178.1(4) . . . . ?
C16A C17A N2A Zn1A -175.9(3) . . . . ?
C12A C17A N2A Zn1A 7.2(4) . . . . ?
O2A Zn1A N2A C18A 13.6(3) . . . . ?
O1A Zn1A N2A C18A 130.2(4) . . . . ?
N1A Zn1A N2A C18A 174.2(3) . . . . ?
N7A Zn1A N2A C18A -87.8(3) . . . . ?
O2A Zn1A N2A C17A -171.8(3) . . . . ?
O1A Zn1A N2A C17A -55.2(5) . . . . ?
N1A Zn1A N2A C17A -11.2(3) . . . . ?
N7A Zn1A N2A C17A 86.8(3) . . . . ?
C17A N2A C18A C19A 174.8(4) . . . . ?
Zn1A N2A C18A C19A -11.0(6) . . . . ?
N2A C18A C19A C20A -174.8(4) . . . . ?
N2A C18A C19A C24A -1.5(6) . . . . ?
C18A C19A C20A C21A 174.0(4) . . . . ?
C24A C19A C20A C21A 0.5(6) . . . . ?
C19A C20A C21A C22A -0.8(7) . . . . ?
C20A C21A C22A C23A 0.6(7) . . . . ?
C21A C22A C23A C24A -0.2(6) . . . . ?
C21A C22A C23A C25A -178.2(4) . . . . ?
C20A C19A C24A O2A -179.7(4) . . . . ?
C18A C19A C24A O2A 7.3(6) . . . . ?
C20A C19A C24A C23A 0.0(5) . . . . ?
C18A C19A C24A C23A -173.0(3) . . . . ?
C22A C23A C24A O2A 179.6(4) . . . . ?
C25A C23A C24A O2A -2.3(5) . . . . ?
C22A C23A C24A C19A -0.1(5) . . . . ?
C25A C23A C24A C19A 177.9(3) . . . . ?
C19A C24A O2A Zn1A 1.2(5) . . . . ?
C23A C24A O2A Zn1A -178.5(3) . . . . ?
O1A Zn1A O2A C24A -173.0(3) . . . . ?
N2A Zn1A O2A C24A -9.4(3) . . . . ?
N1A Zn1A O2A C24A -69.8(5) . . . . ?
N7A Zn1A O2A C24A 92.2(3) . . . . ?
C22A C23A C25A C27A 114.5(4) . . . . ?
C24A C23A C25A C27A -63.5(4) . . . . ?
C22A C23A C25A C26A -125.0(4) . . . . ?
C24A C23A C25A C26A 57.0(5) . . . . ?
C22A C23A C25A C28A -4.9(5) . . . . ?
C24A C23A C25A C28A 177.1(4) . . . . ?
O4A Zn2A O3A C29A -171.6(3) . . . . ?
N4A Zn2A O3A C29A -68.7(5) . . . . ?
N3A Zn2A O3A C29A -7.9(3) . . . . ?
N9A Zn2A O3A C29A 94.9(3) . . . . ?
Zn2A O3A C29A C34A 1.9(6) . . . . ?
Zn2A O3A C29A C30A -178.7(3) . . . . ?
O3A C29A C30A C31A 179.2(4) . . . . ?
C34A C29A C30A C31A -1.3(6) . . . . ?

O3A C29A C30A C36A -0.9(6) . . . . ?
C34A C29A C30A C36A 178.5(4) . . . . ?
C29A C30A C31A C32A 1.6(7) . . . . ?
C36A C30A C31A C32A -178.3(4) . . . . ?
C30A C31A C32A C33A -0.5(7) . . . . ?
C31A C32A C33A C34A -0.9(7) . . . . ?
C32A C33A C34A C29A 1.1(6) . . . . ?
C32A C33A C34A C35A 176.6(4) . . . . ?
O3A C29A C34A C33A 179.4(4) . . . . ?
C30A C29A C34A C33A 0.0(6) . . . . ?
O3A C29A C34A C35A 4.4(6) . . . . ?
C30A C29A C34A C35A -175.0(4) . . . . ?
C33A C34A C35A N3A -174.9(4) . . . . ?
C29A C34A C35A N3A 0.4(6) . . . . ?
C31A C30A C36A C38A 115.4(5) . . . . ?
C29A C30A C36A C38A -64.5(5) . . . . ?
C31A C30A C36A C39A -3.4(6) . . . . ?
C29A C30A C36A C39A 176.7(4) . . . . ?
C31A C30A C36A C37A -122.0(5) . . . . ?
C29A C30A C36A C37A 58.1(6) . . . . ?
C34A C35A N3A C40A 174.4(4) . . . . ?
C34A C35A N3A Zn2A -9.9(5) . . . . ?
O3A Zn2A N3A C35A 11.5(3) . . . . ?
O4A Zn2A N3A C35A 124.7(4) . . . . ?
N4A Zn2A N3A C35A 172.1(3) . . . . ?
N9A Zn2A N3A C35A -89.9(3) . . . . ?
O3A Zn2A N3A C40A -172.5(3) . . . . ?
O4A Zn2A N3A C40A -59.3(5) . . . . ?
N4A Zn2A N3A C40A -11.9(2) . . . . ?
N9A Zn2A N3A C40A 86.1(2) . . . . ?
C35A N3A C40A C41A 1.7(6) . . . . ?
Zn2A N3A C40A C41A -174.4(3) . . . . ?
C35A N3A C40A C45A -176.0(3) . . . . ?
Zn2A N3A C40A C45A 7.9(4) . . . . ?
C45A C40A C41A C42A -2.2(6) . . . . ?
N3A C40A C41A C42A -179.8(4) . . . . ?
C40A C41A C42A C43A -1.2(6) . . . . ?
C41A C42A C43A C44A 2.1(7) . . . . ?
C42A C43A C44A C45A 0.6(7) . . . . ?
C43A C44A C45A C40A -4.0(7) . . . . ?
C43A C44A C45A N4A 174.5(4) . . . . ?
C41A C40A C45A C44A 4.8(6) . . . . ?
N3A C40A C45A C44A -177.4(4) . . . . ?
C41A C40A C45A N4A -173.8(4) . . . . ?
N3A C40A C45A N4A 4.0(5) . . . . ?
C44A C45A N4A C46A -25.6(7) . . . . ?
C40A C45A N4A C46A 152.9(4) . . . . ?
C44A C45A N4A Zn2A 167.5(3) . . . . ?
C40A C45A N4A Zn2A -14.0(5) . . . . ?
O3A Zn2A N4A C46A -90.7(5) . . . . ?
O4A Zn2A N4A C46A 13.9(3) . . . . ?
N3A Zn2A N4A C46A -153.2(4) . . . . ?
N9A Zn2A N4A C46A 105.7(3) . . . . ?
O3A Zn2A N4A C45A 76.3(5) . . . . ?

O4A Zn2A N4A C45A -179.2(3) . . . . ?
N3A Zn2A N4A C45A 13.8(3) . . . . ?
N9A Zn2A N4A C45A -87.3(3) . . . . ?
C45A N4A C46A C47A -175.9(4) . . . . ?
Zn2A N4A C46A C47A -10.3(7) . . . . ?
N4A C46A C47A C52A 0.5(8) . . . . ?
N4A C46A C47A C48A 178.3(5) . . . . ?
C52A C47A C48A C49A 0.5(9) . . . . ?
C46A C47A C48A C49A -177.4(5) . . . . ?
C47A C48A C49A C50A -3.1(10) . . . . ?
C48A C49A C50A C51A 3.6(11) . . . . ?
C49A C50A C51A C52A -1.4(9) . . . . ?
C49A C50A C51A C53A -178.0(6) . . . . ?
C46A C47A C52A O4A 0.1(8) . . . . ?
C48A C47A C52A O4A -177.5(5) . . . . ?
C46A C47A C52A C51A 179.1(5) . . . . ?
C48A C47A C52A C51A 1.5(7) . . . . ?
C50A C51A C52A O4A 177.9(5) . . . . ?
C53A C51A C52A O4A -5.4(7) . . . . ?
C50A C51A C52A C47A -1.1(7) . . . . ?
C53A C51A C52A C47A 175.6(5) . . . . ?
C47A C52A O4A Zn2A 11.2(7) . . . . ?
C51A C52A O4A Zn2A -167.8(3) . . . . ?
O3A Zn2A O4A C52A 142.9(4) . . . . ?
N4A Zn2A O4A C52A -15.8(4) . . . . ?
N3A Zn2A O4A C52A 30.6(7) . . . . ?
N9A Zn2A O4A C52A -115.7(4) . . . . ?
C50A C51A C53A C56A 116.6(6) . . . . ?
C52A C51A C53A C56A -59.8(6) . . . . ?
C50A C51A C53A C55A -119.0(6) . . . . ?
C52A C51A C53A C55A 64.6(7) . . . . ?
C50A C51A C53A C54A -2.6(8) . . . . ?
C52A C51A C53A C54A -179.0(4) . . . . ?
O6A Zn3A O5A C57A -163.4(4) . . . . ?
N6' Zn3A O5A C57A -97.4(6) . . . . ?
N5A Zn3A O5A C57A -9.3(3) . . . . ?
O6' Zn3A O5A C57A -179.0(4) . . . . ?
N8A Zn3A O5A C57A 94.9(3) . . . . ?
N6A Zn3A O5A C57A -50.9(6) . . . . ?
Zn3A O5A C57A C62A 2.7(5) . . . . ?
Zn3A O5A C57A C58A -178.2(3) . . . . ?
O5A C57A C58A C59A 179.1(4) . . . . ?
C62A C57A C58A C59A -1.8(5) . . . . ?
O5A C57A C58A C63A -2.7(5) . . . . ?
C62A C57A C58A C63A 176.4(3) . . . . ?
C57A C58A C59A C60A 1.8(7) . . . . ?
C63A C58A C59A C60A -176.4(4) . . . . ?
C58A C59A C60A C61A -0.7(8) . . . . ?
C59A C60A C61A C62A -0.3(8) . . . . ?
C60A C61A C62A C67A 174.2(4) . . . . ?
C60A C61A C62A C57A 0.3(7) . . . . ?
O5A C57A C62A C61A 179.9(4) . . . . ?
C58A C57A C62A C61A 0.8(6) . . . . ?
O5A C57A C62A C67A 6.6(6) . . . . ?

C58A C57A C62A C67A -172.5(4) . . . . ?
C59A C58A C63A C64A -5.5(5) . . . . ?
C57A C58A C63A C64A 176.4(4) . . . . ?
C59A C58A C63A C65A 114.3(4) . . . . ?
C57A C58A C63A C65A -63.8(4) . . . . ?
C59A C58A C63A C66A -125.9(4) . . . . ?
C57A C58A C63A C66A 56.0(5) . . . . ?
C61A C62A C67A N5A -177.3(4) . . . . ?
C57A C62A C67A N5A -3.8(7) . . . . ?
C62A C67A N5A C68' 169.0(9) . . . . ?
C62A C67A N5A C68A 176.0(6) . . . . ?
C62A C67A N5A Zn3A -6.7(6) . . . . ?
O6A Zn3A N5A C67A 129.0(4) . . . . ?
N6' Zn3A N5A C67A 166.2(4) . . . . ?
O5A Zn3A N5A C67A 10.8(3) . . . . ?
O6' Zn3A N5A C67A 90.5(9) . . . . ?
N8A Zn3A N5A C67A -89.4(3) . . . . ?
N6A Zn3A N5A C67A 172.7(4) . . . . ?
O6A Zn3A N5A C68' -48.2(7) . . . . ?
N6' Zn3A N5A C68' -11.0(6) . . . . ?
O5A Zn3A N5A C68' -166.4(6) . . . . ?
O6' Zn3A N5A C68' -86.6(11) . . . . ?
N8A Zn3A N5A C68' 93.5(6) . . . . ?
N6A Zn3A N5A C68' -4.5(6) . . . . ?
O6A Zn3A N5A C68A -53.9(7) . . . . ?
N6' Zn3A N5A C68A -16.7(6) . . . . ?
O5A Zn3A N5A C68A -172.1(6) . . . . ?
O6' Zn3A N5A C68A -92.3(11) . . . . ?
N8A Zn3A N5A C68A 87.8(6) . . . . ?
N6A Zn3A N5A C68A -10.2(6) . . . . ?
C67A N5A C68A C73A -175.8(7) . . . . ?
C68' N5A C68A C73A -6.6(15) . . . . ?
Zn3A N5A C68A C73A 6.8(11) . . . . ?
C67A N5A C68A C69A 2.5(14) . . . . ?
C68' N5A C68A C69A 172(3) . . . . ?
Zn3A N5A C68A C69A -174.9(8) . . . . ?
C73A C68A C69A C70A 0.5(15) . . . . ?
N5A C68A C69A C70A -177.7(9) . . . . ?
C68A C69A C70A C71A -1.9(14) . . . . ?
C69A C70A C71A C72A 1.4(14) . . . . ?
C70A C71A C72A C73A 0.4(17) . . . . ?
C71A C72A C73A C68A -1.8(17) . . . . ?
C71A C72A C73A N6A 173.0(10) . . . . ?
C69A C68A C73A C72A 1.3(15) . . . . ?
N5A C68A C73A C72A 179.8(9) . . . . ?
C69A C68A C73A N6A -174.1(9) . . . . ?
N5A C68A C73A N6A 4.4(12) . . . . ?
C72A C73A N6A C74A -19.8(16) . . . . ?
C68A C73A N6A C74A 155.2(8) . . . . ?
C72A C73A N6A Zn3A 172.0(9) . . . . ?
C68A C73A N6A Zn3A -13.1(11) . . . . ?
O6A Zn3A N6A C74A 5.1(7) . . . . ?
N6' Zn3A N6A C74A 4.7(8) . . . . ?
O5A Zn3A N6A C74A -110.8(6) . . . . ?

N5A Zn3A N6A C74A -155.5(8) . . . . ?
O6' Zn3A N6A C74A 13.7(8) . . . . ?
N8A Zn3A N6A C74A 103.6(7) . . . . ?
O6A Zn3A N6A C73A 172.8(7) . . . . ?
N6' Zn3A N6A C73A 172.4(15) . . . . ?
O5A Zn3A N6A C73A 56.9(10) . . . . ?
N5A Zn3A N6A C73A 12.3(7) . . . . ?
O6' Zn3A N6A C73A -178.5(7) . . . . ?
N8A Zn3A N6A C73A -88.6(7) . . . . ?
C73A N6A C74A C75A -172.9(9) . . . . ?
Zn3A N6A C74A C75A -5.1(13) . . . . ?
N6A C74A C75A C76A -178.1(9) . . . . ?
N6A C74A C75A C80A 2.8(16) . . . . ?
C74A C75A C76A C77A 179.5(8) . . . . ?
C80A C75A C76A C77A -1.4(14) . . . . ?
C75A C76A C77A C78A 4.7(14) . . . . ?
C76A C77A C78A C79A -7(2) . . . . ?
C77A C78A C79A C80A 5.8(19) . . . . ?
C77A C78A C79A C81A 177.8(11) . . . . ?
C76A C75A C80A O6A 179.5(9) . . . . ?
C74A C75A C80A O6A -1.4(16) . . . . ?
C76A C75A C80A C79A 0.0(14) . . . . ?
C74A C75A C80A C79A 179.1(9) . . . . ?
C78A C79A C80A O6A 178.4(11) . . . . ?
C81A C79A C80A O6A 6.3(12) . . . . ?
C78A C79A C80A C75A -2.1(14) . . . . ?
C81A C79A C80A C75A -174.2(8) . . . . ?
C75A C80A O6A Zn3A 4.0(16) . . . . ?
C79A C80A O6A Zn3A -176.6(5) . . . . ?
N6' Zn3A O6A C80A -4.7(9) . . . . ?
O5A Zn3A O6A C80A 151.1(9) . . . . ?
N5A Zn3A O6A C80A 36.1(11) . . . . ?
O6' Zn3A O6A C80A -161.7(13) . . . . ?
N8A Zn3A O6A C80A -106.3(9) . . . . ?
N6A Zn3A O6A C80A -4.8(9) . . . . ?
C78A C79A C81A C83A -111.5(10) . . . . ?
C80A C79A C81A C83A 60.2(8) . . . . ?
C78A C79A C81A C82A 8.2(11) . . . . ?
C80A C79A C81A C82A 179.9(7) . . . . ?
C78A C79A C81A C84A 128.0(10) . . . . ?
C80A C79A C81A C84A -60.2(8) . . . . ?
C67A N5A C68' C73' -168.5(9) . . . . ?
C68A N5A C68' C73' 176(3) . . . . ?
Zn3A N5A C68' C73' 7.9(14) . . . . ?
C67A N5A C68' C69' 7.4(17) . . . . ?
C68A N5A C68' C69' -7.7(14) . . . . ?
Zn3A N5A C68' C69' -176.3(9) . . . . ?
N5A C68' C69' C70' 178.7(9) . . . . ?
C73' C68' C69' C70' -5.1(18) . . . . ?
C68' C69' C70' C71' 0.3(18) . . . . ?
C69' C70' C71' C72' 2(2) . . . . ?
C70' C71' C72' C73' 0(2) . . . . ?
C71' C72' C73' C68' -4.5(18) . . . . ?
C71' C72' C73' N6' 176.4(12) . . . . ?

N5A C68' C73' C72' -177.4(10) . . . . ?
C69' C68' C73' C72' 7.0(18) . . . . ?
N5A C68' C73' N6' 1.8(19) . . . . ?
C69' C68' C73' N6' -173.8(11) . . . . ?
C72' C73' N6' C74' -25.8(18) . . . . ?
C68' C73' N6' C74' 155.1(10) . . . . ?
C72' C73' N6' Zn3A 167.4(9) . . . . ?
C68' C73' N6' Zn3A -11.7(13) . . . . ?
O6A Zn3A N6' C74' 9.3(8) . . . . ?
O5A Zn3A N6' C74' -64.3(11) . . . . ?
N5A Zn3A N6' C74' -152.4(8) . . . . ?
O6' Zn3A N6' C74' 17.5(8) . . . . ?
N8A Zn3A N6' C74' 103.3(8) . . . . ?
N6A Zn3A N6' C74' -171.2(15) . . . . ?
O6A Zn3A N6' C73' 174.5(8) . . . . ?
O5A Zn3A N6' C73' 100.9(8) . . . . ?
N5A Zn3A N6' C73' 12.8(7) . . . . ?
O6' Zn3A N6' C73' -177.3(8) . . . . ?
N8A Zn3A N6' C73' -91.5(7) . . . . ?
N6A Zn3A N6' C73' -5.9(10) . . . . ?
C73' N6' C74' C75' -179.2(11) . . . . ?
Zn3A N6' C74' C75' -15.6(16) . . . . ?
N6' C74' C75' C76' 179.5(10) . . . . ?
N6' C74' C75' C80' 3.7(19) . . . . ?
C74' C75' C76' C77' 178.6(12) . . . . ?
C80' C75' C76' C77' -5.4(18) . . . . ?
C75' C76' C77' C78' 7(2) . . . . ?
C76' C77' C78' C79' -8(2) . . . . ?
C77' C78' C79' C80' 6.5(16) . . . . ?
C77' C78' C79' C81' -173.5(10) . . . . ?
C76' C75' C80' O6' -178.2(9) . . . . ?
C74' C75' C80' O6' -2.6(17) . . . . ?
C76' C75' C80' C79' 4.0(15) . . . . ?
C74' C75' C80' C79' 179.7(10) . . . . ?
C78' C79' C80' O6' 177.7(8) . . . . ?
C81' C79' C80' O6' -2.4(12) . . . . ?
C78' C79' C80' C75' -4.5(14) . . . . ?
C81' C79' C80' C75' 175.5(9) . . . . ?
C75' C80' O6' Zn3A 11.5(12) . . . . ?
C79' C80' O6' Zn3A -170.7(6) . . . . ?
O6A Zn3A O6' C80' 5.2(6) . . . . ?
N6' Zn3A O6' C80' -15.9(6) . . . . ?
O5A Zn3A O6' C80' 139.8(6) . . . . ?
N5A Zn3A O6' C80' 59.9(12) . . . . ?
N8A Zn3A O6' C80' -120.2(6) . . . . ?
N6A Zn3A O6' C80' -18.9(7) . . . . ?
C78' C79' C81' C83' 120.3(9) . . . . ?
C80' C79' C81' C83' -59.6(9) . . . . ?
C78' C79' C81' C82' 0.0(11) . . . . ?
C80' C79' C81' C82' -179.9(8) . . . . ?
C78' C79' C81' C84' -120.1(9) . . . . ?
C80' C79' C81' C84' 60.0(9) . . . . ?
C87A N7A C85A P1A -60.1(3) . . . . ?
C86A N7A C85A P1A 61.5(3) . . . . ?

Zn1A N7A C85A P1A 177.36(18) . . . . ?
C88A P1A C85A N7A 48.0(3) . . . . ?
C90A P1A C85A N7A -49.2(3) . . . . ?
C87A N7A C86A N9A 55.7(4) . . . . ?
C85A N7A C86A N9A -67.1(4) . . . . ?
Zn1A N7A C86A N9A 178.5(2) . . . . ?
C89A N9A C86A N7A -55.7(4) . . . . ?
C90A N9A C86A N7A 66.6(4) . . . . ?
Zn2A N9A C86A N7A -176.0(2) . . . . ?
C86A N7A C87A N8A -56.4(4) . . . . ?
C85A N7A C87A N8A 66.4(4) . . . . ?
Zn1A N7A C87A N8A -175.7(2) . . . . ?
C88A N8A C87A N7A -67.0(4) . . . . ?
C89A N8A C87A N7A 56.5(4) . . . . ?
Zn3A N8A C87A N7A 177.1(2) . . . . ?
C87A N8A C88A P1A 60.8(4) . . . . ?
C89A N8A C88A P1A -60.8(4) . . . . ?
Zn3A N8A C88A P1A 179.01(19) . . . . ?
C85A P1A C88A N8A -48.2(3) . . . . ?
C90A P1A C88A N8A 48.1(3) . . . . ?
C86A N9A C89A N8A 56.1(4) . . . . ?
C90A N9A C89A N8A -66.0(4) . . . . ?
Zn2A N9A C89A N8A 179.3(2) . . . . ?
C88A N8A C89A N9A 67.0(4) . . . . ?
C87A N8A C89A N9A -56.4(4) . . . . ?
Zn3A N8A C89A N9A -176.0(2) . . . . ?
C89A N9A C90A P1A 60.0(3) . . . . ?
C86A N9A C90A P1A -61.3(3) . . . . ?
Zn2A N9A C90A P1A 176.49(17) . . . . ?
C88A P1A C90A N9A -47.9(3) . . . . ?
C85A P1A C90A N9A 49.4(3) . . . . ?
O1B Zn1B N7B C87B -143.3(2) . . . . ?
O2B Zn1B N7B C87B -45.9(2) . . . . ?
N1B Zn1B N7B C87B 124.4(2) . . . . ?
N2B Zn1B N7B C87B 43.6(2) . . . . ?
O1B Zn1B N7B C85B -23.6(2) . . . . ?
O2B Zn1B N7B C85B 73.8(2) . . . . ?
N1B Zn1B N7B C85B -115.9(2) . . . . ?
N2B Zn1B N7B C85B 163.3(2) . . . . ?
O1B Zn1B N7B C86B 96.8(2) . . . . ?
O2B Zn1B N7B C86B -165.8(2) . . . . ?
N1B Zn1B N7B C86B 4.4(2) . . . . ?
N2B Zn1B N7B C86B -76.4(2) . . . . ?
O6B Zn3B N8B C89B -164.2(3) . . . . ?
O5B Zn3B N8B C89B 94.3(2) . . . . ?
N6" Zn3B N8B C89B -86.4(3) . . . . ?
N5B Zn3B N8B C89B 2.8(3) . . . . ?
O6" Zn3B N8B C89B -174.7(4) . . . . ?
N6B Zn3B N8B C89B -74.2(3) . . . . ?
O6B Zn3B N8B C86B -43.5(3) . . . . ?
O5B Zn3B N8B C86B -144.9(2) . . . . ?
N6" Zn3B N8B C86B 34.3(3) . . . . ?
N5B Zn3B N8B C86B 123.6(2) . . . . ?
O6" Zn3B N8B C86B -54.0(4) . . . . ?

N6B Zn3B N8B C86B 46.6(3) . . . . ?
O6B Zn3B N8B C88B 75.9(3) . . . . ?
O5B Zn3B N8B C88B -25.5(2) . . . . ?
N6" Zn3B N8B C88B 153.7(3) . . . . ?
N5B Zn3B N8B C88B -117.1(2) . . . . ?
O6" Zn3B N8B C88B 65.4(4) . . . . ?
N6B Zn3B N8B C88B 166.0(3) . . . . ?
O3B Zn2B N9B C89B -147.6(2) . . . . ?
O4B Zn2B N9B C89B -50.5(2) . . . . ?
N4B Zn2B N9B C89B 39.0(2) . . . . ?
N3B Zn2B N9B C89B 119.8(2) . . . . ?
O3B Zn2B N9B C87B 91.8(2) . . . . ?
O4B Zn2B N9B C87B -171.2(2) . . . . ?
N4B Zn2B N9B C87B -81.7(2) . . . . ?
N3B Zn2B N9B C87B -0.9(2) . . . . ?
O3B Zn2B N9B C90B -29.5(2) . . . . ?
O4B Zn2B N9B C90B 67.6(2) . . . . ?
N4B Zn2B N9B C90B 157.1(2) . . . . ?
N3B Zn2B N9B C90B -122.1(2) . . . . ?
O2B Zn1B O1B C1B 174.0(3) . . . . ?
N1B Zn1B O1B C1B 11.5(3) . . . . ?
N2B Zn1B O1B C1B 70.6(5) . . . . ?
N7B Zn1B O1B C1B -91.4(3) . . . . ?
Zn1B O1B C1B C6B -4.5(5) . . . . ?
Zn1B O1B C1B C2B 177.3(3) . . . . ?
O1B C1B C2B C3B 179.6(4) . . . . ?
C6B C1B C2B C3B 1.3(5) . . . . ?
O1B C1B C2B C7B 2.4(5) . . . . ?
C6B C1B C2B C7B -175.9(3) . . . . ?
C1B C2B C3B C4B -1.0(7) . . . . ?
C7B C2B C3B C4B 176.1(4) . . . . ?
C2B C3B C4B C5B 1.7(8) . . . . ?
C3B C4B C5B C6B -2.7(7) . . . . ?
C4B C5B C6B C11B -172.8(4) . . . . ?
C4B C5B C6B C1B 3.0(7) . . . . ?
O1B C1B C6B C5B 179.4(4) . . . . ?
C2B C1B C6B C5B -2.3(6) . . . . ?
O1B C1B C6B C11B -5.1(6) . . . . ?
C2B C1B C6B C11B 173.1(4) . . . . ?
C3B C2B C7B C8B 5.2(6) . . . . ?
C1B C2B C7B C8B -177.7(4) . . . . ?
C3B C2B C7B C9B -113.7(4) . . . . ?
C1B C2B C7B C9B 63.4(5) . . . . ?
C3B C2B C7B C10B 126.1(4) . . . . ?
C1B C2B C7B C10B -56.8(5) . . . . ?
O1B Zn1B N1B C11B -13.7(3) . . . . ?
O2B Zn1B N1B C11B -124.7(4) . . . . ?
N2B Zn1B N1B C11B -174.4(3) . . . . ?
N7B Zn1B N1B C11B 87.1(3) . . . . ?
O1B Zn1B N1B C12B 170.1(3) . . . . ?
O2B Zn1B N1B C12B 59.1(5) . . . . ?
N2B Zn1B N1B C12B 9.5(3) . . . . ?
N7B Zn1B N1B C12B -89.1(3) . . . . ?
C12B N1B C11B C6B -173.9(4) . . . . ?

Zn1B N1B C11B C6B 10.2(6) . . . . ?
C5B C6B C11B N1B 177.0(4) . . . . ?
C1B C6B C11B N1B 1.4(6) . . . . ?
C11B N1B C12B C13B 0.0(6) . . . . ?
Zn1B N1B C12B C13B 176.3(3) . . . . ?
C11B N1B C12B C17B 177.6(4) . . . . ?
Zn1B N1B C12B C17B -6.1(4) . . . . ?
C17B C12B C13B C14B 2.3(6) . . . . ?
N1B C12B C13B C14B 179.9(4) . . . . ?
C12B C13B C14B C15B 1.9(7) . . . . ?
C13B C14B C15B C16B -2.7(7) . . . . ?
C14B C15B C16B C17B -0.9(7) . . . . ?
C15B C16B C17B N2B -174.7(4) . . . . ?
C15B C16B C17B C12B 5.2(6) . . . . ?
C13B C12B C17B C16B -5.8(6) . . . . ?
N1B C12B C17B C16B 176.4(3) . . . . ?
C13B C12B C17B N2B 174.0(4) . . . . ?
N1B C12B C17B N2B -3.8(5) . . . . ?
C16B C17B N2B C18B 27.3(6) . . . . ?
C12B C17B N2B C18B -152.6(4) . . . . ?
C16B C17B N2B Zn1B -168.3(3) . . . . ?
C12B C17B N2B Zn1B 11.8(4) . . . . ?
O1B Zn1B N2B C18B 91.1(4) . . . . ?
O2B Zn1B N2B C18B -13.7(3) . . . . ?
N1B Zn1B N2B C18B 152.2(3) . . . . ?
N7B Zn1B N2B C18B -106.9(3) . . . . ?
O1B Zn1B N2B C17B -72.5(4) . . . . ?
O2B Zn1B N2B C17B -177.3(3) . . . . ?
N1B Zn1B N2B C17B -11.4(3) . . . . ?
N7B Zn1B N2B C17B 89.5(3) . . . . ?
C17B N2B C18B C19B 174.0(4) . . . . ?
Zn1B N2B C18B C19B 11.3(6) . . . . ?
N2B C18B C19B C20B -178.6(4) . . . . ?
N2B C18B C19B C24B -2.9(7) . . . . ?
C24B C19B C20B C21B 1.9(7) . . . . ?
C18B C19B C20B C21B 177.8(4) . . . . ?
C19B C20B C21B C22B -0.7(7) . . . . ?
C20B C21B C22B C23B -0.3(7) . . . . ?
C21B C22B C23B C24B 0.0(6) . . . . ?
C21B C22B C23B C25B -178.3(4) . . . . ?
C20B C19B C24B O2B 177.4(4) . . . . ?
C18B C19B C24B O2B 1.9(6) . . . . ?
C20B C19B C24B C23B -2.2(6) . . . . ?
C18B C19B C24B C23B -177.7(4) . . . . ?
C22B C23B C24B O2B -178.3(4) . . . . ?
C25B C23B C24B O2B 0.0(5) . . . . ?
C22B C23B C24B C19B 1.2(5) . . . . ?
C25B C23B C24B C19B 179.5(3) . . . . ?
C19B C24B O2B Zn1B -11.2(5) . . . . ?
C23B C24B O2B Zn1B 168.4(3) . . . . ?
O1B Zn1B O2B C24B -143.9(3) . . . . ?
N1B Zn1B O2B C24B -33.9(6) . . . . ?
N2B Zn1B O2B C24B 14.5(3) . . . . ?
N7B Zn1B O2B C24B 115.1(3) . . . . ?

C22B C23B C25B C26B -1.8(5) . . . . ?
C24B C23B C25B C26B 179.9(4) . . . . ?
C22B C23B C25B C28B -122.9(4) . . . . ?
C24B C23B C25B C28B 58.8(5) . . . . ?
C22B C23B C25B C27B 116.3(4) . . . . ?
C24B C23B C25B C27B -62.0(5) . . . . ?
O4B Zn2B O3B C29B 173.2(3) . . . . ?
N4B Zn2B O3B C29B 70.7(5) . . . . ?
N3B Zn2B O3B C29B 8.9(3) . . . . ?
N9B Zn2B O3B C29B -92.9(3) . . . . ?
Zn2B O3B C29B C34B -1.8(5) . . . . ?
Zn2B O3B C29B C30B 178.1(2) . . . . ?
O3B C29B C30B C31B -179.0(3) . . . . ?
C34B C29B C30B C31B 1.0(5) . . . . ?
O3B C29B C30B C35B 2.2(5) . . . . ?
C34B C29B C30B C35B -177.9(3) . . . . ?
C29B C30B C31B C32B -1.0(6) . . . . ?
C35B C30B C31B C32B 177.8(4) . . . . ?
C30B C31B C32B C33B 0.3(7) . . . . ?
C31B C32B C33B C34B 0.5(6) . . . . ?
C32B C33B C34B C39E -174.8(4) . . . . ?
C32B C33B C34B C29B -0.5(6) . . . . ?
O3B C29B C34B C33B 179.7(3) . . . . ?
C30B C29B C34B C33B -0.2(5) . . . . ?
O3B C29B C34B C39E -6.6(6) . . . . ?
C30B C29B C34B C39E 173.5(3) . . . . ?
C31B C30B C35B C36B 2.8(6) . . . . ?
C29B C30B C35B C36B -178.4(4) . . . . ?
C31B C30B C35B C38B -115.5(4) . . . . ?
C29B C30B C35B C38B 63.4(4) . . . . ?
C31B C30B C35B C37B 122.8(4) . . . . ?
C29B C30B C35B C37B -58.4(5) . . . . ?
C33B C34B C39E N3B 176.3(4) . . . . ?
C29B C34B C39E N3B 2.3(6) . . . . ?
C34B C39E N3B C40B -174.8(3) . . . . ?
C34B C39E N3B Zn2B 8.7(5) . . . . ?
O3B Zn2B N3B C39E -11.8(3) . . . . ?
O4B Zn2B N3B C39E -124.8(4) . . . . ?
N4B Zn2B N3B C39E -171.0(3) . . . . ?
N9B Zn2B N3B C39E 90.4(3) . . . . ?
O3B Zn2B N3B C40B 171.5(2) . . . . ?
O4B Zn2B N3B C40B 58.4(5) . . . . ?
N4B Zn2B N3B C40B 12.3(2) . . . . ?
N9B Zn2B N3B C40B -86.3(2) . . . . ?
C39E N3B C40B C41B -3.4(6) . . . . ?
Zn2B N3B C40B C41B 173.3(3) . . . . ?
C39E N3B C40B C45B 174.4(3) . . . . ?
Zn2B N3B C40B C45B -8.9(4) . . . . ?
N3B C40B C41B C42B -178.6(4) . . . . ?
C45B C40B C41B C42B 3.7(5) . . . . ?
C40B C41B C42B C43B 0.4(6) . . . . ?
C41B C42B C43B C44B -2.1(6) . . . . ?
C42B C43B C44B C45B -0.5(6) . . . . ?
C43B C44B C45B N4B -176.7(4) . . . . ?

C43B C44B C45B C40B 4.6(6) . . . . ?
C41B C40B C45B C44B -6.1(5) . . . . ?
N3B C40B C45B C44B 175.9(3) . . . . ?
C41B C40B C45B N4B 175.0(3) . . . . ?
N3B C40B C45B N4B -2.9(5) . . . . ?
C44B C45B N4B C46B 27.8(6) . . . . ?
C40B C45B N4B C46B -153.5(4) . . . . ?
C44B C45B N4B Zn2B -165.4(3) . . . . ?
C40B C45B N4B Zn2B 13.4(4) . . . . ?
O3B Zn2B N4B C46B 88.7(4) . . . . ?
O4B Zn2B N4B C46B -15.2(3) . . . . ?
N3B Zn2B N4B C46B 152.6(3) . . . . ?
N9B Zn2B N4B C46B -107.6(3) . . . . ?
O3B Zn2B N4B C45B -77.6(4) . . . . ?
O4B Zn2B N4B C45B 178.5(3) . . . . ?
N3B Zn2B N4B C45B -13.7(2) . . . . ?
N9B Zn2B N4B C45B 86.1(3) . . . . ?
C45B N4B C46B C47B 175.6(4) . . . . ?
Zn2B N4B C46B C47B 10.2(6) . . . . ?
N4B C46B C47B C52B 0.4(7) . . . . ?
N4B C46B C47B C48B -176.7(4) . . . . ?
C52B C47B C48B C49B 1.1(7) . . . . ?
C46B C47B C48B C49B 178.4(4) . . . . ?
C47B C48B C49B C50B 1.0(8) . . . . ?
C48B C49B C50B C51B -1.5(8) . . . . ?
C49B C50B C51B C52B -0.1(7) . . . . ?
C49B C50B C51B C53B 179.6(4) . . . . ?
C48B C47B C52B O4B 177.4(4) . . . . ?
C46B C47B C52B O4B 0.4(6) . . . . ?
C48B C47B C52B C51B -2.7(6) . . . . ?
C46B C47B C52B C51B -179.7(4) . . . . ?
C50B C51B C52B O4B -177.8(4) . . . . ?
C53B C51B C52B O4B 2.4(5) . . . . ?
C50B C51B C52B C47B 2.2(6) . . . . ?
C53B C51B C52B C47B -177.5(4) . . . . ?
C47B C52B O4B Zn2B -13.2(5) . . . . ?
C51B C52B O4B Zn2B 166.9(3) . . . . ?
O3B Zn2B O4B C52B -139.5(3) . . . . ?
N4B Zn2B O4B C52B 17.7(3) . . . . ?
N3B Zn2B O4B C52B -27.4(6) . . . . ?
N9B Zn2B O4B C52B 118.2(3) . . . . ?
C50B C51B C53B C56B -120.8(4) . . . . ?
C52B C51B C53B C56B 58.9(5) . . . . ?
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SADABS Version 2008/1 Bruker-Nonius
Blessing, Acta Cryst. (1995) A51 33-38
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they should be multiplied by a factor of 2 to 10
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
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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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N2 N 0.28837(17) 0.56356(18) 0.45319(9) 0.0173(6) Uani 1 1 d . B .
N3 N 0.22832(18) 1.1050(2) 0.44975(10) 0.0210(7) Uani 1 1 d . . .
N4 N 0.11805(19) 0.9771(2) 0.44213(10) 0.0225(7) Uani 1 1 d . A .
O1 O 0.24244(14) 0.73948(16) 0.35273(8) 0.0231(6) Uani 1 1 d . . .
O2 O 0.36630(15) 0.60674(16) 0.37227(8) 0.0236(6) Uani 1 1 d . . .
O3 O 0.25071(15) 1.07303(16) 0.54569(8) 0.0226(6) Uani 1 1 d . . .
O4 O 0.15104(14) 0.91221(16) 0.53217(8) 0.0224(6) Uani 1 1 d . . .
C1 C 0.1694(2) 0.7634(2) 0.33756(12) 0.0211(8) Uani 1 1 d . . .

C2 C 0.1594(2) 0.8084(2) 0.29394(12) 0.0231(8) Uani 1 1 d . . .
C3 C 0.0810(2) 0.8309(3) 0.27779(13) 0.0283(9) Uani 1 1 d . . .
H3 H 0.0740 0.8592 0.2487 0.034 Uiso 1 1 calc R B .
C4 C 0.0116(2) 0.8143(3) 0.30208(13) 0.0299(9) Uani 1 1 d . . .
H4 H -0.0411 0.8313 0.2897 0.036 Uiso 1 1 calc R . .
C5 C 0.0203(2) 0.7731(3) 0.34393(13) 0.0286(9) Uani 1 1 d . . .
H5 H -0.0268 0.7621 0.3607 0.034 Uiso 1 1 calc R B .
C6 C 0.0980(2) 0.7469(2) 0.36264(12) 0.0226(8) Uani 1 1 d . . .
C7 C 0.0995(2) 0.7010(2) 0.40558(12) 0.0217(8) Uani 1 1 d . . .
H7 H 0.0485 0.6945 0.4194 0.026 Uiso 1 1 calc R B .
C8 C 0.1561(2) 0.6188(2) 0.46894(11) 0.0176(8) Uani 1 1 d . . .
C9 C 0.0899(2) 0.6238(2) 0.49685(12) 0.0209(8) Uani 1 1 d . . .
H9 H 0.0458 0.6629 0.4889 0.025 Uiso 1 1 calc R . .
C10 C 0.0878(2) 0.5726(2) 0.53597(12) 0.0217(8) Uani 1 1 d . . .
H10 H 0.0418 0.5767 0.5543 0.026 Uiso 1 1 calc R B .
C11 C 0.1513(2) 0.5151(2) 0.54926(11) 0.0170(7) Uani 1 1 d . . .
C12 C 0.2184(2) 0.5118(2) 0.52208(11) 0.0183(8) Uani 1 1 d . . .
H12 H 0.2629 0.4738 0.5308 0.022 Uiso 1 1 calc R B .
C13 C 0.2220(2) 0.5629(2) 0.48239(11) 0.0159(7) Uani 1 1 d . B .
C14 C 0.3529(2) 0.5139(2) 0.46018(12) 0.0190(8) Uani 1 1 d . . .
H14 H 0.3558 0.4786 0.4872 0.023 Uiso 1 1 calc R B .
C15 C 0.4200(2) 0.5076(2) 0.43077(12) 0.0210(8) Uani 1 1 d . . .
C16 C 0.4854(2) 0.4523(3) 0.44596(13) 0.0257(9) Uani 1 1 d . . .
H16 H 0.4852 0.4258 0.4755 0.031 Uiso 1 1 calc R B .
C17 C 0.5491(2) 0.4363(3) 0.41885(14) 0.0309(9) Uani 1 1 d . . .
H17 H 0.5946 0.4019 0.4301 0.037 Uiso 1 1 calc R . .
C18 C 0.5466(2) 0.4710(3) 0.37448(14) 0.0319(10) Uani 1 1 d . . .
H18 H 0.5906 0.4579 0.3557 0.038 Uiso 1 1 calc R B .
C19 C 0.4835(2) 0.5235(2) 0.35640(12) 0.0232(8) Uani 1 1 d . . .
C20 C 0.4203(2) 0.5494(2) 0.38645(12) 0.0196(8) Uani 1 1 d . . .
C21 C 0.2349(2) 0.8293(3) 0.26692(13) 0.0293(9) Uani 1 1 d . . .
C22 C 0.2958(2) 0.8855(3) 0.29628(14) 0.0344(10) Uani 1 1 d . . .
H22A H 0.2681 0.9388 0.3068 0.052 Uiso 1 1 calc R . .
H22B H 0.3414 0.9028 0.2778 0.052 Uiso 1 1 calc R . .
H22C H 0.3167 0.8510 0.3230 0.052 Uiso 1 1 calc R . .
C23 C 0.2753(3) 0.7433(3) 0.25192(14) 0.0419(11) Uani 1 1 d . . .
H23A H 0.2904 0.7072 0.2791 0.063 Uiso 1 1 calc R . .
H23B H 0.3245 0.7573 0.2357 0.063 Uiso 1 1 calc R . .
H23C H 0.2367 0.7102 0.2314 0.063 Uiso 1 1 calc R . .
C24 C 0.2121(3) 0.8830(3) 0.22319(13) 0.0372(10) Uani 1 1 d . . .
H24A H 0.1724 0.8497 0.2035 0.056 Uiso 1 1 calc R . .
H24B H 0.2615 0.8939 0.2065 0.056 Uiso 1 1 calc R . .
H24C H 0.1880 0.9397 0.2317 0.056 Uiso 1 1 calc R . .
C25 C 0.1505(2) 0.4566(2) 0.59233(11) 0.0200(8) Uani 1 1 d . . .
C26 C 0.0764(2) 0.4751(3) 0.62055(13) 0.0302(10) Uani 1 1 d . . .
H26A H 0.0776 0.5371 0.6307 0.045 Uiso 1 1 calc R . .
H26B H 0.0781 0.4362 0.6475 0.045 Uiso 1 1 calc R . .
H26C H 0.0259 0.4641 0.6016 0.045 Uiso 1 1 calc R . .
C27 C 0.2285(2) 0.4728(3) 0.62287(12) 0.0299(9) Uani 1 1 d . . .
H27A H 0.2765 0.4577 0.6058 0.045 Uiso 1 1 calc R . .
H27B H 0.2276 0.4359 0.6505 0.045 Uiso 1 1 calc R . .
H27C H 0.2313 0.5354 0.6318 0.045 Uiso 1 1 calc R . .
C28 C 0.1477(2) 0.3592(2) 0.57721(13) 0.0251(9) Uani 1 1 d . . .
H28A H 0.0979 0.3485 0.5576 0.038 Uiso 1 1 calc R . .

H28B H 0.1476 0.3210 0.6044 0.038 Uiso 1 1 calc R . .
H28C H 0.1959 0.3458 0.5600 0.038 Uiso 1 1 calc R . .
C29 C 0.4774(2) 0.5514(3) 0.30601(13) 0.0331(10) Uani 1 1 d . . .
C30 C 0.5450(3) 0.5076(4) 0.27890(15) 0.0633(16) Uani 1 1 d . . .
H30A H 0.5988 0.5283 0.2910 0.095 Uiso 1 1 calc R . .
H30B H 0.5372 0.5235 0.2463 0.095 Uiso 1 1 calc R . .
H30C H 0.5419 0.4431 0.2822 0.095 Uiso 1 1 calc R . .
C31 C 0.3957(3) 0.5201(3) 0.28326(14) 0.0390(11) Uani 1 1 d . . .
H31A H 0.3926 0.4554 0.2850 0.059 Uiso 1 1 calc R . .
H31B H 0.3918 0.5387 0.2509 0.059 Uiso 1 1 calc R . .
H31C H 0.3505 0.5462 0.2993 0.059 Uiso 1 1 calc R . .
C32 C 0.4844(3) 0.6519(3) 0.30130(15) 0.0455(12) Uani 1 1 d . . .
H32A H 0.4428 0.6806 0.3191 0.068 Uiso 1 1 calc R . .
H32B H 0.4759 0.6685 0.2688 0.068 Uiso 1 1 calc R . .
H32C H 0.5390 0.6710 0.3129 0.068 Uiso 1 1 calc R . .
C33 C 0.2893(2) 1.1479(2) 0.54656(12) 0.0216(8) Uani 1 1 d . . .
C34 C 0.3223(2) 1.1819(2) 0.59021(13) 0.0232(8) Uani 1 1 d . . .
C35 C 0.3655(2) 1.2611(2) 0.59051(13) 0.0242(8) Uani 1 1 d . . .
H35 H 0.3878 1.2832 0.6191 0.029 Uiso 1 1 calc R B .
C36 C 0.3778(2) 1.3100(2) 0.55031(13) 0.0240(8) Uani 1 1 d . . .
H36 H 0.4087 1.3633 0.5518 0.029 Uiso 1 1 calc R . .
C37 C 0.3448(2) 1.2799(2) 0.50932(13) 0.0236(8) Uani 1 1 d . . .
H37 H 0.3514 1.3138 0.4823 0.028 Uiso 1 1 calc R B .
C38 C 0.3012(2) 1.1996(2) 0.50595(12) 0.0212(8) Uani 1 1 d . . .
C39 C 0.2667(2) 1.1768(2) 0.46092(12) 0.0235(8) Uani 1 1 d . . .
H39 H 0.2729 1.2190 0.4371 0.028 Uiso 1 1 calc R B .
C40 C 0.1920(2) 1.0905(2) 0.40497(12) 0.0227(8) Uani 1 1 d . . .
C41 C 0.2120(2) 1.1373(3) 0.36567(12) 0.0284(9) Uani 1 1 d . A .
H41 H 0.2528 1.1822 0.3683 0.034 Uiso 1 1 calc R . .
C42 C 0.1736(3) 1.1196(3) 0.32306(13) 0.0326(10) Uani 1 1 d . . .
C43 C 0.1166(3) 1.0507(3) 0.31978(13) 0.0335(10) Uani 1 1 d . A .
H43 H 0.0905 1.0367 0.2907 0.040 Uiso 1 1 calc R . .
C44 C 0.0973(2) 1.0027(3) 0.35784(12) 0.0293(9) Uani 1 1 d . . .
H44 H 0.0590 0.9554 0.3546 0.035 Uiso 1 1 calc R A .
C45 C 0.1334(2) 1.0229(2) 0.40110(12) 0.0243(9) Uani 1 1 d . A .
C46 C 0.0515(2) 0.9323(3) 0.44612(12) 0.0251(9) Uani 1 1 d . . .
H46 H 0.0130 0.9328 0.4204 0.030 Uiso 1 1 calc R B .
C47 C 0.0298(2) 0.8821(3) 0.48518(12) 0.0235(8) Uani 1 1 d . . .
C48 C -0.0462(2) 0.8368(3) 0.48062(13) 0.0291(9) Uani 1 1 d . . .
H48 H -0.0789 0.8411 0.4526 0.035 Uiso 1 1 calc R B .
C49 C -0.0730(2) 0.7873(3) 0.51568(14) 0.0300(9) Uani 1 1 d . . .
H49 H -0.1228 0.7550 0.5117 0.036 Uiso 1 1 calc R . .
C50 C -0.0273(2) 0.7840(3) 0.55749(13) 0.0278(9) Uani 1 1 d . . .
H50 H -0.0482 0.7512 0.5821 0.033 Uiso 1 1 calc R B .
C51 C 0.0475(2) 0.8266(2) 0.56472(12) 0.0239(8) Uani 1 1 d . . .
C52 C 0.0790(2) 0.8753(2) 0.52724(12) 0.0206(8) Uani 1 1 d . . .
C53 C 0.3063(2) 1.1319(3) 0.63465(13) 0.0275(9) Uani 1 1 d . . .
C54 C 0.3498(3) 1.1757(3) 0.67659(13) 0.0422(11) Uani 1 1 d . . .
H54A H 0.4092 1.1734 0.6737 0.063 Uiso 1 1 calc R . .
H54B H 0.3358 1.1443 0.7045 0.063 Uiso 1 1 calc R . .
H54C H 0.3322 1.2376 0.6784 0.063 Uiso 1 1 calc R . .
C55 C 0.3385(3) 1.0358(3) 0.63340(13) 0.0313(9) Uani 1 1 d . . .
H55A H 0.3059 1.0019 0.6102 0.047 Uiso 1 1 calc R . .
H55B H 0.3342 1.0084 0.6637 0.047 Uiso 1 1 calc R . .

H55C H 0.3960 1.0362 0.6255 0.047 Uiso 1 1 calc R . .
C56 C 0.2142(2) 1.1315(3) 0.64227(14) 0.0326(10) Uani 1 1 d . . .
H56A H 0.1956 1.1923 0.6469 0.049 Uiso 1 1 calc R . .
H56B H 0.2040 1.0959 0.6695 0.049 Uiso 1 1 calc R . .
H56C H 0.1843 1.1061 0.6153 0.049 Uiso 1 1 calc R . .
C57 C 0.1973(3) 1.1720(3) 0.28078(13) 0.0411(9) Uani 0.75 1 d PDU A 1
C58 C 0.1872(5) 1.2724(4) 0.2906(5) 0.0459(18) Uani 0.75 1 d PDU A 1
H58A H 0.1296 1.2852 0.2957 0.069 Uiso 0.75 1 calc PR A 1
H58B H 0.2043 1.3067 0.2643 0.069 Uiso 0.75 1 calc PR A 1
H58C H 0.2213 1.2886 0.3182 0.069 Uiso 0.75 1 calc PR A 1
C59 C 0.1444(6) 1.1492(8) 0.2373(3) 0.0454(19) Uani 0.75 1 d PDU A 1
H59A H 0.1510 1.0864 0.2300 0.068 Uiso 0.75 1 calc PR A 1
H59B H 0.1617 1.1853 0.2116 0.068 Uiso 0.75 1 calc PR A 1
H59C H 0.0868 1.1615 0.2424 0.068 Uiso 0.75 1 calc PR A 1
C60 C 0.2867(4) 1.1499(6) 0.2718(4) 0.0476(19) Uani 0.75 1 d PDU A 1
H60A H 0.3223 1.1682 0.2983 0.071 Uiso 0.75 1 calc PR A 1
H60B H 0.3025 1.1816 0.2443 0.071 Uiso 0.75 1 calc PR A 1
H60C H 0.2921 1.0860 0.2670 0.071 Uiso 0.75 1 calc PR A 1
C57' C 0.1973(3) 1.1720(3) 0.28078(13) 0.0411(9) Uani 0.25 1 d PDU A 2
C58' C 0.2080(17) 1.2722(7) 0.2915(14) 0.043(3) Uani 0.25 1 d PDU A 2
H58D H 0.1579 1.2952 0.3041 0.064 Uiso 0.25 1 calc PR A 2
H58E H 0.2185 1.3041 0.2631 0.064 Uiso 0.25 1 calc PR A 2
H58F H 0.2543 1.2806 0.3140 0.064 Uiso 0.25 1 calc PR A 2
C59' C 0.1327(16) 1.162(2) 0.2410(9) 0.042(3) Uani 0.25 1 d PDU A 2
H59D H 0.1297 1.0993 0.2315 0.063 Uiso 0.25 1 calc PR A 2
H59E H 0.1478 1.1982 0.2150 0.063 Uiso 0.25 1 calc PR A 2
H59F H 0.0792 1.1805 0.2510 0.063 Uiso 0.25 1 calc PR A 2
C60' C 0.2778(9) 1.1321(19) 0.2655(11) 0.043(3) Uani 0.25 1 d PDU A 2
H60D H 0.3198 1.1356 0.2909 0.065 Uiso 0.25 1 calc PR A 2
H60E H 0.2961 1.1652 0.2390 0.065 Uiso 0.25 1 calc PR A 2
H60F H 0.2689 1.0700 0.2568 0.065 Uiso 0.25 1 calc PR A 2
C61 C 0.0964(2) 0.8197(3) 0.61138(12) 0.0255(9) Uani 1 1 d . . .
C62 C 0.1182(2) 0.9122(3) 0.62989(13) 0.0301(9) Uani 1 1 d . . .
H62A H 0.1482 0.9447 0.6071 0.045 Uiso 1 1 calc R . .
H62B H 0.1525 0.9068 0.6585 0.045 Uiso 1 1 calc R . .
H62C H 0.0679 0.9443 0.6359 0.045 Uiso 1 1 calc R . .
C63 C 0.0479(3) 0.7732(3) 0.64794(14) 0.0350(10) Uani 1 1 d . . .
H63A H -0.0039 0.8044 0.6513 0.052 Uiso 1 1 calc R . .
H63B H 0.0801 0.7735 0.6774 0.052 Uiso 1 1 calc R . .
H63C H 0.0367 0.7119 0.6385 0.052 Uiso 1 1 calc R . .
C64 C 0.1753(2) 0.7657(3) 0.60545(13) 0.0303(9) Uani 1 1 d . . .
H64A H 0.1608 0.7053 0.5957 0.046 Uiso 1 1 calc R . .
H64B H 0.2079 0.7638 0.6348 0.046 Uiso 1 1 calc R . .
H64C H 0.2073 0.7939 0.5821 0.046 Uiso 1 1 calc R . .
P1 P 0.46495(7) 0.90076(8) 0.44799(5) 0.0240(3) Uani 0.85 1 d PDU B 1
N5 N 0.33956(16) 0.77217(18) 0.44532(9) 0.0168(5) Uani 0.85 1 d PDU B 1
N6 N 0.30675(15) 0.91706(18) 0.47955(9) 0.0176(5) Uani 0.85 1 d PDU B 1
N7 N 0.3999(2) 0.8125(2) 0.52238(11) 0.0172(6) Uani 0.85 1 d PDU B 1
C65 C 0.4776(3) 0.8513(3) 0.50540(15) 0.0270(7) Uani 0.85 1 d PDU B 1
H65A H 0.5195 0.8041 0.5049 0.032 Uiso 0.85 1 calc PR B 1
H65B H 0.4983 0.8972 0.5274 0.032 Uiso 0.85 1 calc PR B 1
C66 C 0.3726(2) 0.9673(3) 0.45840(15) 0.0208(8) Uani 0.85 1 d PDU B 1
H66A H 0.3888 1.0176 0.4787 0.025 Uiso 0.85 1 calc PR B 1
H66B H 0.3505 0.9921 0.4287 0.025 Uiso 0.85 1 calc PR B 1

C67 C 0.4106(2) 0.8045(3) 0.42038(15) 0.0191(8) Uani 0.85 1 d PDU B 1
H67A H 0.3912 0.8213 0.3887 0.023 Uiso 0.85 1 calc PR B 1
H67B H 0.4502 0.7552 0.4180 0.023 Uiso 0.85 1 calc PR B 1
C68 C 0.2775(2) 0.8428(3) 0.45041(14) 0.0144(7) Uani 0.85 1 d PDU B 1
H68A H 0.2602 0.8659 0.4195 0.017 Uiso 0.85 1 calc PR B 1
H68B H 0.2287 0.8166 0.4637 0.017 Uiso 0.85 1 calc PR B 1
C69 C 0.3369(2) 0.8805(3) 0.52539(14) 0.0175(8) Uani 0.85 1 d PDU B 1
H69A H 0.3593 0.9296 0.5448 0.021 Uiso 0.85 1 calc PR B 1
H69B H 0.2899 0.8549 0.5408 0.021 Uiso 0.85 1 calc PR B 1
C70 C 0.3679(2) 0.7421(3) 0.49274(13) 0.0167(7) Uani 0.85 1 d PDU B 1
H70A H 0.3213 0.7139 0.5073 0.020 Uiso 0.85 1 calc PR B 1
H70B H 0.4109 0.6966 0.4901 0.020 Uiso 0.85 1 calc PR B 1
P1' P 0.4471(4) 0.8292(5) 0.5174(2) 0.0270(7) Uani 0.15 1 d PDU B 2
N5' N 0.30675(15) 0.91706(18) 0.47955(9) 0.0176(5) Uani 0.15 1 d PDU B 2
N6' N 0.33956(16) 0.77217(18) 0.44532(9) 0.0168(5) Uani 0.15 1 d PDU B 2
N7' N 0.4254(6) 0.9038(6) 0.4297(3) 0.0240(3) Uani 0.15 1 d PDU B 2
C65' C 0.4880(6) 0.8868(9) 0.4687(4) 0.0240(3) Uani 0.15 1 d PDU B 2
H65C H 0.5113 0.9442 0.4794 0.029 Uiso 0.15 1 calc PR B 2
H65D H 0.5332 0.8512 0.4570 0.029 Uiso 0.15 1 calc PR B 2
C66' C 0.3919(7) 0.7400(6) 0.4849(3) 0.0189(9) Uani 0.15 1 d PDU B 2
H66C H 0.4324 0.6977 0.4737 0.023 Uiso 0.15 1 calc PR B 2
H66D H 0.3573 0.7074 0.5061 0.023 Uiso 0.15 1 calc PR B 2
C67' C 0.3568(6) 0.9028(7) 0.5231(3) 0.0182(13) Uani 0.15 1 d PDU B 2
H67C H 0.3215 0.8769 0.5461 0.022 Uiso 0.15 1 calc PR B 2
H67D H 0.3763 0.9610 0.5350 0.022 Uiso 0.15 1 calc PR B 2
C68' C 0.2752(4) 0.8327(6) 0.4591(4) 0.0166(12) Uani 0.15 1 d PDU B 2
H68C H 0.2420 0.8022 0.4817 0.020 Uiso 0.15 1 calc PR B 2
H68D H 0.2385 0.8464 0.4318 0.020 Uiso 0.15 1 calc PR B 2
C69' C 0.3907(7) 0.8204(7) 0.4120(3) 0.0195(13) Uani 0.15 1 d PDU B 2
H69C H 0.4360 0.7811 0.4037 0.023 Uiso 0.15 1 calc PR B 2
H69D H 0.3564 0.8327 0.3836 0.023 Uiso 0.15 1 calc PR B 2
C70' C 0.3591(7) 0.9589(7) 0.4446(4) 0.0189(9) Uani 0.15 1 d PDU B 2
H70C H 0.3235 0.9753 0.4173 0.023 Uiso 0.15 1 calc PR B 2
H70D H 0.3829 1.0142 0.4578 0.023 Uiso 0.15 1 calc PR B 2
O1S O 0.9629(4) 0.5561(4) 0.70344(18) 0.0518(13) Uani 0.75 1 d PDU C 1
C1S C 0.9049(5) 0.5114(7) 0.6965(3) 0.0480(11) Uani 0.75 1 d PDU C 1
C2S C 0.8498(4) 0.5127(6) 0.6555(2) 0.0579(18) Uani 0.75 1 d PDU C 1
H2S1 H 0.8686 0.5570 0.6339 0.087 Uiso 0.75 1 calc PR C 1
H2S2 H 0.7944 0.5277 0.6640 0.087 Uiso 0.75 1 calc PR C 1
H2S3 H 0.8493 0.4541 0.6409 0.087 Uiso 0.75 1 calc PR C 1
C3S C 0.8829(5) 0.4446(6) 0.7348(3) 0.0736(17) Uani 0.75 1 d PDU C 1
H3S1 H 0.8936 0.3841 0.7246 0.110 Uiso 0.75 1 calc PR C 1
H3S2 H 0.8248 0.4507 0.7408 0.110 Uiso 0.75 1 calc PR C 1
H3S3 H 0.9165 0.4571 0.7630 0.110 Uiso 0.75 1 calc PR C 1
O1S' O 0.9261(9) 0.4474(11) 0.7305(6) 0.0736(17) Uani 0.25 1 d PDU D 2
C1S' C 0.9033(14) 0.5001(17) 0.7025(9) 0.0480(11) Uani 0.25 1 d PDU D 2
C2S' C 0.8316(12) 0.4941(19) 0.6705(7) 0.059(3) Uani 0.25 1 d PDU D 2
H2S4 H 0.8401 0.5304 0.6433 0.088 Uiso 0.25 1 calc PR D 2
H2S5 H 0.7833 0.5156 0.6855 0.088 Uiso 0.25 1 calc PR D 2
H2S6 H 0.8230 0.4323 0.6611 0.088 Uiso 0.25 1 calc PR D 2
C3S' C 0.9659(16) 0.5723(17) 0.6897(10) 0.051(3) Uani 0.25 1 d PDU D 2
H3S4 H 0.9588 0.6250 0.7087 0.076 Uiso 0.25 1 calc PR D 2
H3S5 H 0.9567 0.5879 0.6572 0.076 Uiso 0.25 1 calc PR D 2
H3S6 H 1.0217 0.5495 0.6953 0.076 Uiso 0.25 1 calc PR D 2

O1T O 0.5835(6) 0.8514(6) 0.6085(4) 0.095(2) Uani 0.50 1 d PDU E 1
C1T C 0.5444(9) 0.8054(12) 0.6320(8) 0.0784(19) Uani 0.50 1 d PDU E 1
C2T C 0.4589(6) 0.8138(8) 0.6427(4) 0.077(3) Uani 0.50 1 d PDU E 1
H2T1 H 0.4353 0.8667 0.6276 0.116 Uiso 0.50 1 calc PR E 1
H2T2 H 0.4553 0.8190 0.6760 0.116 Uiso 0.50 1 calc PR E 1
H2T3 H 0.4286 0.7613 0.6316 0.116 Uiso 0.50 1 calc PR E 1
C3T C 0.5837(8) 0.7143(7) 0.6456(5) 0.088(2) Uani 0.50 1 d PDU E 1
H3T1 H 0.6324 0.7047 0.6282 0.132 Uiso 0.50 1 calc PR E 1
H3T2 H 0.5440 0.6669 0.6387 0.132 Uiso 0.50 1 calc PR E 1
H3T3 H 0.5995 0.7141 0.6786 0.132 Uiso 0.50 1 calc PR E 1
O1T' O 0.5934(6) 0.7973(6) 0.6074(3) 0.089(2) Uani 0.50 1 d PDU F 2
C1T' C 0.5442(11) 0.7891(11) 0.6353(7) 0.0774(19) Uani 0.50 1 d PDU F 2
C2T' C 0.5400(8) 0.7214(7) 0.6706(4) 0.080(3) Uani 0.50 1 d PDU F 2
H2T4 H 0.4855 0.6942 0.6686 0.120 Uiso 0.50 1 calc PR F 2
H2T5 H 0.5501 0.7484 0.7010 0.120 Uiso 0.50 1 calc PR F 2
H2T6 H 0.5815 0.6760 0.6660 0.120 Uiso 0.50 1 calc PR F 2
C3T' C 0.4829(8) 0.8669(8) 0.6399(4) 0.087(3) Uani 0.50 1 d PDU F 2
H3T4 H 0.5063 0.9212 0.6276 0.130 Uiso 0.50 1 calc PR F 2
H3T5 H 0.4727 0.8757 0.6725 0.130 Uiso 0.50 1 calc PR F 2
H3T6 H 0.4313 0.8531 0.6227 0.130 Uiso 0.50 1 calc PR F 2
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_atom_site_aniso_U_12
Zn1 0.0195(2) 0.0156(2) 0.0165(2) 0.00158(17) 0.00438(15) 0.00075(17)
Zn2 0.0209(2) 0.0188(2) 0.0170(2) 0.00062(18) 0.00298(16) 0.00507(18)
N1 0.0163(15) 0.0163(16) 0.0207(15) 0.0002(13) 0.0024(12) -0.0017(13)
N2 0.0187(15) 0.0131(16) 0.0206(15) 0.0000(12) 0.0067(12) -0.0002(13)
N3 0.0243(16) 0.0191(18) 0.0201(16) -0.0003(13) 0.0046(13) 0.0076(14)
N4 0.0279(17) 0.0228(18) 0.0167(15) -0.0017(13) 0.0021(13) 0.0088(14)
O1 0.0215(13) 0.0273(15) 0.0210(13) 0.0080(11) 0.0040(10) 0.0017(11)
O2 0.0299(14) 0.0216(14) 0.0201(13) 0.0018(11) 0.0088(11) 0.0047(12)
O3 0.0305(14) 0.0166(14) 0.0209(13) 0.0000(11) 0.0020(11) 0.0000(12)
O4 0.0191(13) 0.0273(15) 0.0207(13) 0.0045(11) 0.0007(10) 0.0003(11)
C1 0.028(2) 0.017(2) 0.0181(18) 0.0000(15) -0.0017(15) -0.0011(16)
C2 0.032(2) 0.017(2) 0.0199(18) -0.0005(15) -0.0002(16) -0.0002(16)
C3 0.039(2) 0.023(2) 0.0227(19) 0.0025(17) -0.0055(17) 0.0003(18)
C4 0.026(2) 0.033(2) 0.030(2) 0.0053(18) -0.0092(17) 0.0004(18)
C5 0.024(2) 0.033(2) 0.029(2) 0.0052(18) 0.0000(16) 0.0000(18)
C6 0.026(2) 0.023(2) 0.0184(18) 0.0034(16) -0.0023(15) -0.0020(16)
C7 0.0197(19) 0.021(2) 0.0241(19) 0.0022(16) 0.0024(15) -0.0036(16)
C8 0.0215(18) 0.0158(19) 0.0159(17) 0.0012(14) 0.0031(14) -0.0036(15)
C9 0.0213(19) 0.019(2) 0.0231(19) 0.0022(16) 0.0029(15) 0.0035(15)
C10 0.0202(19) 0.025(2) 0.0206(18) -0.0034(16) 0.0078(15) -0.0003(16)
C11 0.0257(19) 0.0098(19) 0.0158(17) -0.0031(14) 0.0031(14) -0.0014(15)
C12 0.0207(18) 0.0147(19) 0.0196(18) -0.0016(15) 0.0017(14) 0.0027(15)
C13 0.0189(18) 0.0142(19) 0.0150(17) -0.0024(14) 0.0045(14) -0.0026(15)
C14 0.0242(19) 0.014(2) 0.0196(18) 0.0024(15) 0.0047(14) 0.0004(15)
C15 0.0217(19) 0.018(2) 0.0242(19) -0.0002(16) 0.0053(15) 0.0001(16)
C16 0.030(2) 0.023(2) 0.024(2) 0.0019(17) 0.0071(16) 0.0028(17)

C17 0.022(2) 0.032(2) 0.038(2) 0.0006(19) 0.0020(17) 0.0065(18)
C18 0.024(2) 0.040(3) 0.033(2) -0.0041(19) 0.0141(17) 0.0011(18)
C19 0.0196(19) 0.026(2) 0.0243(19) -0.0052(16) 0.0058(15) -0.0009(16)
C20 0.0201(19) 0.016(2) 0.0232(19) -0.0046(15) 0.0042(15) -0.0030(16)
C21 0.039(2) 0.026(2) 0.0226(19) 0.0071(17) 0.0064(17) 0.0025(19)
C22 0.034(2) 0.038(3) 0.032(2) 0.0144(19) 0.0042(18) -0.002(2)
C23 0.056(3) 0.038(3) 0.033(2) 0.011(2) 0.015(2) 0.014(2)
C24 0.050(3) 0.035(3) 0.027(2) 0.0130(19) 0.0053(19) 0.005(2)
C25 0.0247(19) 0.018(2) 0.0173(18) 0.0017(15) 0.0038(15) 0.0011(16)
C26 0.035(2) 0.031(2) 0.026(2) 0.0072(17) 0.0150(17) 0.0037(18)
C27 0.039(2) 0.033(2) 0.0172(19) 0.0013(17) 0.0023(17) -0.0063(19)
C28 0.031(2) 0.016(2) 0.030(2) 0.0042(16) 0.0099(17) -0.0018(16)
C29 0.024(2) 0.052(3) 0.024(2) -0.0026(19) 0.0116(17) 0.003(2)
C30 0.054(3) 0.108(5) 0.029(3) 0.002(3) 0.019(2) 0.026(3)
C31 0.046(3) 0.044(3) 0.027(2) -0.013(2) 0.0028(19) 0.001(2)
C32 0.047(3) 0.058(3) 0.032(2) 0.007(2) 0.004(2) -0.019(2)
C33 0.0211(19) 0.015(2) 0.029(2) -0.0016(16) 0.0042(15) 0.0075(16)
C34 0.025(2) 0.015(2) 0.030(2) 0.0005(16) 0.0026(16) 0.0054(16)
C35 0.025(2) 0.021(2) 0.027(2) -0.0054(16) 0.0031(16) 0.0051(17)
C36 0.022(2) 0.016(2) 0.035(2) 0.0000(17) 0.0069(16) 0.0026(16)
C37 0.026(2) 0.019(2) 0.027(2) 0.0026(16) 0.0090(16) 0.0069(16)
C38 0.0201(19) 0.020(2) 0.0235(19) -0.0003(16) 0.0051(15) 0.0074(16)
C39 0.029(2) 0.019(2) 0.0240(19) 0.0043(16) 0.0104(16) 0.0112(17)
C40 0.029(2) 0.022(2) 0.0167(18) 0.0003(15) 0.0037(15) 0.0138(17)
C41 0.039(2) 0.021(2) 0.025(2) 0.0009(17) 0.0062(17) 0.0133(18)
C42 0.052(3) 0.029(2) 0.018(2) 0.0002(17) 0.0068(18) 0.023(2)
C43 0.050(3) 0.032(3) 0.018(2) -0.0024(18) 0.0012(18) 0.017(2)
C44 0.037(2) 0.026(2) 0.025(2) -0.0036(18) -0.0005(17) 0.0124(19)
C45 0.033(2) 0.021(2) 0.0195(19) 0.0001(15) 0.0055(16) 0.0134(17)
C46 0.022(2) 0.030(2) 0.0233(19) -0.0085(17) -0.0021(15) 0.0106(17)
C47 0.0213(19) 0.026(2) 0.0236(19) -0.0073(17) 0.0017(15) 0.0075(16)
C48 0.0169(19) 0.040(3) 0.030(2) -0.0136(19) -0.0011(16) 0.0074(18)
C49 0.018(2) 0.035(2) 0.038(2) -0.0122(19) 0.0105(17) 0.0012(17)
C50 0.027(2) 0.026(2) 0.032(2) -0.0045(18) 0.0126(17) -0.0001(17)
C51 0.0198(19) 0.023(2) 0.030(2) -0.0073(17) 0.0076(15) 0.0017(16)
C52 0.0166(18) 0.022(2) 0.0233(19) -0.0071(16) 0.0029(15) 0.0063(15)
C53 0.040(2) 0.020(2) 0.023(2) -0.0058(16) -0.0004(17) 0.0009(18)
C54 0.068(3) 0.034(3) 0.024(2) -0.0019(19) 0.000(2) -0.011(2)
C55 0.040(2) 0.027(2) 0.026(2) 0.0048(18) -0.0028(18) 0.0060(19)
C56 0.044(3) 0.026(2) 0.029(2) -0.0009(18) 0.0101(19) 0.0043(19)
C57 0.071(2) 0.0317(18) 0.0212(16) 0.0077(16) 0.0117(16) 0.0178(18)
C58 0.075(5) 0.034(3) 0.029(3) 0.005(2) 0.007(4) 0.008(3)
C59 0.084(4) 0.033(4) 0.019(3) 0.004(2) 0.009(3) 0.022(3)
C60 0.072(3) 0.044(4) 0.029(4) 0.012(3) 0.021(3) 0.011(3)
C57' 0.071(2) 0.0317(18) 0.0212(16) 0.0077(16) 0.0117(16) 0.0178(18)
C58' 0.073(6) 0.034(4) 0.023(5) 0.007(4) 0.015(5) 0.013(4)
C59' 0.076(5) 0.031(6) 0.019(5) 0.003(5) 0.012(4) 0.022(5)
C60' 0.069(4) 0.035(6) 0.027(6) 0.005(5) 0.015(5) 0.011(5)
C61 0.027(2) 0.026(2) 0.0242(19) 0.0023(17) 0.0062(16) -0.0030(17)
C62 0.040(2) 0.030(2) 0.021(2) 0.0000(17) 0.0060(17) -0.0032(19)
C63 0.040(3) 0.033(3) 0.033(2) 0.0042(19) 0.0088(19) -0.002(2)
C64 0.027(2) 0.032(2) 0.032(2) 0.0067(18) 0.0019(17) 0.0008(18)
P1 0.0137(5) 0.0177(6) 0.0415(7) -0.0026(5) 0.0084(5) -0.0011(5)
N5 0.0147(11) 0.0148(11) 0.0214(11) 0.0016(10) 0.0052(9) 0.0023(9)

N6 0.0166(11) 0.0147(11) 0.0219(11) 0.0000(10) 0.0035(9) -0.0002(9)
N7 0.0095(13) 0.0172(15) 0.0250(14) -0.0028(12) 0.0015(12) 0.0001(12)
C65 0.0248(11) 0.0261(11) 0.0302(10) -0.0017(8) 0.0036(8) 0.0000(8)
C66 0.0175(16) 0.0137(16) 0.0314(18) -0.0015(14) 0.0047(15) -0.0028(13)
C67 0.0135(16) 0.0168(17) 0.0276(17) 0.0014(14) 0.0063(14) 0.0044(14)
C68 0.0148(15) 0.0136(16) 0.0153(15) 0.0018(13) 0.0043(12) 0.0012(13)
C69 0.0146(16) 0.0160(17) 0.0215(16) -0.0048(14) -0.0021(14) -0.0033(14)
C70 0.0124(16) 0.0160(16) 0.0221(16) -0.0006(14) 0.0038(14) 0.0044(13)
P1' 0.0248(11) 0.0261(11) 0.0302(10) -0.0017(8) 0.0036(8) 0.0000(8)
N5' 0.0166(11) 0.0147(11) 0.0219(11) 0.0000(10) 0.0035(9) -0.0002(9)
N6' 0.0147(11) 0.0148(11) 0.0214(11) 0.0016(10) 0.0052(9) 0.0023(9)
N7' 0.0137(5) 0.0177(6) 0.0415(7) -0.0026(5) 0.0084(5) -0.0011(5)
C65' 0.0137(5) 0.0177(6) 0.0415(7) -0.0026(5) 0.0084(5) -0.0011(5)
C66' 0.0152(18) 0.0158(17) 0.0259(18) -0.0003(16) 0.0038(16) 0.0002(15)
C67' 0.015(2) 0.017(3) 0.023(2) -0.002(2) 0.002(2) -0.002(2)
C68' 0.016(2) 0.015(2) 0.020(2) 0.001(2) 0.004(2) 0.0014(19)
C69' 0.014(3) 0.016(2) 0.029(2) 0.001(2) 0.007(2) 0.003(2)
C70' 0.0152(18) 0.0158(17) 0.0259(18) -0.0003(16) 0.0038(16) 0.0002(15)
O1S 0.044(2) 0.057(3) 0.056(3) -0.018(2) 0.020(2) -0.022(2)
C1S 0.043(2) 0.043(2) 0.059(2) -0.0180(19) 0.0172(19) -0.0082(18)
C2S 0.056(4) 0.056(4) 0.062(4) -0.028(3) 0.006(3) -0.001(3)
C3S 0.065(4) 0.072(3) 0.086(3) 0.006(3) 0.018(3) -0.018(3)
O1S' 0.065(4) 0.072(3) 0.086(3) 0.006(3) 0.018(3) -0.018(3)
C1S' 0.043(2) 0.043(2) 0.059(2) -0.0180(19) 0.0172(19) -0.0082(18)
C2S' 0.057(5) 0.053(6) 0.067(6) -0.023(5) 0.011(5) -0.012(5)
C3S' 0.045(5) 0.051(5) 0.058(6) -0.012(5) 0.019(5) -0.009(4)
O1T 0.105(5) 0.094(6) 0.083(4) 0.017(5) -0.013(4) -0.026(5)
C1T 0.093(4) 0.077(5) 0.064(4) -0.002(4) -0.006(3) -0.014(4)
C2T 0.101(5) 0.075(6) 0.055(5) -0.011(5) -0.004(4) 0.002(5)
C3T 0.099(5) 0.077(5) 0.087(5) -0.002(5) -0.011(5) -0.007(4)
O1T' 0.094(5) 0.099(6) 0.073(4) -0.005(5) 0.004(3) 0.001(5)
C1T' 0.091(4) 0.076(5) 0.064(4) -0.004(4) -0.007(3) -0.011(4)
C2T' 0.098(6) 0.067(5) 0.074(5) -0.006(4) 0.001(5) -0.015(5)
C3T' 0.101(6) 0.090(6) 0.068(5) -0.009(5) -0.010(5) 0.010(5)
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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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Zn1 O2 1.959(2) . ?
Zn1 N1 2.063(3) . ?
Zn1 N2 2.089(3) . ?
Zn1 N5 2.175(3) . ?

Zn2 O3 1.947(2) . ?
Zn2 O4 1.972(2) . ?
Zn2 N4 2.053(3) . ?
Zn2 N3 2.086(3) . ?
Zn2 N6 2.182(3) . ?
N1 C7 1.300(4) . ?
N1 C8 1.415(4) . ?
N2 C14 1.300(4) . ?
N2 C13 1.417(4) . ?
N3 C39 1.285(5) . ?
N3 C40 1.417(4) . ?
N4 C46 1.292(5) . ?
N4 C45 1.416(5) . ?
O1 C1 1.300(4) . ?
O2 C20 1.288(4) . ?
O3 C33 1.294(4) . ?
O4 C52 1.304(4) . ?
C1 C6 1.434(5) . ?
C1 C2 1.440(5) . ?
C2 C3 1.382(5) . ?
C2 C21 1.534(5) . ?
C3 C4 1.394(5) . ?
C4 C5 1.367(5) . ?
C5 C6 1.410(5) . ?
C6 C7 1.428(5) . ?
C8 C9 1.393(5) . ?
C8 C13 1.407(5) . ?
C9 C10 1.378(5) . ?
C10 C11 1.391(5) . ?
C11 C12 1.390(5) . ?
C11 C25 1.535(5) . ?
C12 C13 1.393(5) . ?
C14 C15 1.435(5) . ?
C15 C16 1.406(5) . ?
C15 C20 1.436(5) . ?
C16 C17 1.365(5) . ?
C17 C18 1.392(5) . ?
C18 C19 1.381(5) . ?
C19 C20 1.445(5) . ?
C19 C29 1.524(5) . ?
C21 C22 1.530(6) . ?
C21 C23 1.533(6) . ?
C21 C24 1.537(5) . ?
C25 C26 1.529(5) . ?
C25 C27 1.531(5) . ?
C25 C28 1.536(5) . ?
C29 C32 1.528(6) . ?
C29 C31 1.531(6) . ?
C29 C30 1.544(5) . ?
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C36 C37 1.358(5) . ?
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C40 C41 1.400(5) . ?
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C51 C52 1.436(5) . ?
C51 C61 1.538(5) . ?
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C53 C55 1.544(5) . ?
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C57 C60 1.536(7) . ?
C57 C58 1.554(6) . ?
C61 C62 1.532(5) . ?
C61 C63 1.534(5) . ?
C61 C64 1.543(5) . ?
P1 C65 1.831(5) . ?
P1 C66 1.853(4) . ?
P1 C67 1.862(4) . ?
N5 C68 1.485(5) . ?
N5 C67 1.488(5) . ?
N5 C70 1.500(5) . ?
N6 C68 1.469(5) . ?
N6 C66 1.480(5) . ?
N6 C69 1.501(5) . ?
N7 C70 1.448(5) . ?
N7 C69 1.460(5) . ?
N7 C65 1.508(5) . ?
P1' C65' 1.825(7) . ?
P1' C66' 1.851(6) . ?
P1' C67' 1.862(6) . ?
N7' C70' 1.452(7) . ?
N7' C69' 1.463(7) . ?
N7' C65' 1.506(7) . ?
O1S C1S 1.172(7) . ?
C1S C2S 1.454(7) . ?
C1S C3S 1.560(11) . ?
O1S' C1S' 1.185(8) . ?
C1S' C2S' 1.457(8) . ?
C1S' C3S' 1.554(12) . ?
O1T C1T 1.186(7) . ?
C1T C2T 1.455(8) . ?
C1T C3T 1.559(12) . ?

O1T' C1T' 1.183(7) . ?
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C1T' C3T' 1.555(12) . ?
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O1 Zn1 O2 94.87(10) . . ?
O1 Zn1 N1 89.17(10) . . ?
O2 Zn1 N1 149.66(11) . . ?
O1 Zn1 N2 161.23(11) . . ?
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N1 Zn1 N2 79.13(11) . . ?
O1 Zn1 N5 96.60(10) . . ?
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N1 Zn1 N5 102.34(10) . . ?
N2 Zn1 N5 100.19(11) . . ?
O3 Zn2 O4 97.12(10) . . ?
O3 Zn2 N4 152.95(11) . . ?
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O3 Zn2 N6 101.88(10) . . ?
O4 Zn2 N6 94.25(10) . . ?
N4 Zn2 N6 103.93(11) . . ?
N3 Zn2 N6 97.67(11) . . ?
C7 N1 C8 121.2(3) . . ?
C7 N1 Zn1 125.3(2) . . ?
C8 N1 Zn1 113.2(2) . . ?
C14 N2 C13 123.0(3) . . ?
C14 N2 Zn1 123.4(2) . . ?
C13 N2 Zn1 112.9(2) . . ?
C39 N3 C40 122.4(3) . . ?
C39 N3 Zn2 125.3(2) . . ?
C40 N3 Zn2 112.2(2) . . ?
C46 N4 C45 121.6(3) . . ?
C46 N4 Zn2 124.9(2) . . ?
C45 N4 Zn2 113.1(2) . . ?
C1 O1 Zn1 131.8(2) . . ?
C20 O2 Zn1 130.5(2) . . ?
C33 O3 Zn2 131.6(2) . . ?
C52 O4 Zn2 131.0(2) . . ?
O1 C1 C6 122.5(3) . . ?
O1 C1 C2 119.0(3) . . ?
C6 C1 C2 118.5(3) . . ?
C3 C2 C1 118.1(3) . . ?
C3 C2 C21 122.2(3) . . ?
C1 C2 C21 119.8(3) . . ?
C2 C3 C4 123.3(3) . . ?

C5 C4 C3 119.3(4) . . ?
C4 C5 C6 121.0(4) . . ?
C5 C6 C7 116.3(3) . . ?
C5 C6 C1 119.8(3) . . ?
C7 C6 C1 123.9(3) . . ?
N1 C7 C6 126.6(3) . . ?
C9 C8 C13 118.6(3) . . ?
C9 C8 N1 125.0(3) . . ?
C13 C8 N1 116.3(3) . . ?
C10 C9 C8 120.6(3) . . ?
C9 C10 C11 121.7(3) . . ?
C12 C11 C10 117.7(3) . . ?
C12 C11 C25 119.3(3) . . ?
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C11 C12 C13 121.7(3) . . ?
C12 C13 C8 119.6(3) . . ?
C12 C13 N2 124.9(3) . . ?
C8 C13 N2 115.5(3) . . ?
N2 C14 C15 126.0(3) . . ?
C16 C15 C14 116.5(3) . . ?
C16 C15 C20 120.0(3) . . ?
C14 C15 C20 123.3(3) . . ?
C17 C16 C15 121.0(4) . . ?
C16 C17 C18 119.2(4) . . ?
C19 C18 C17 123.4(3) . . ?
C18 C19 C20 118.0(3) . . ?
C18 C19 C29 122.0(3) . . ?
C20 C19 C29 120.0(3) . . ?
O2 C20 C15 123.0(3) . . ?
O2 C20 C19 119.3(3) . . ?
C15 C20 C19 117.7(3) . . ?
C22 C21 C23 110.6(3) . . ?
C22 C21 C2 110.2(3) . . ?
C23 C21 C2 110.1(3) . . ?
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C23 C21 C24 107.4(3) . . ?
C2 C21 C24 111.8(3) . . ?
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C26 C25 C11 112.3(3) . . ?
C27 C25 C11 109.5(3) . . ?
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C32 C29 C30 108.7(4) . . ?
C31 C29 C30 106.2(4) . . ?
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O3 C33 C34 119.0(3) . . ?
C38 C33 C34 117.9(3) . . ?
C35 C34 C33 118.4(3) . . ?
C35 C34 C53 122.1(3) . . ?

C33 C34 C53 119.5(3) . . ?
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C36 C37 C38 121.5(3) . . ?
C37 C38 C39 116.0(3) . . ?
C37 C38 C33 120.1(3) . . ?
C39 C38 C33 123.7(3) . . ?
N3 C39 C38 126.3(3) . . ?
C41 C40 C45 119.6(3) . . ?
C41 C40 N3 124.6(4) . . ?
C45 C40 N3 115.8(3) . . ?
C42 C41 C40 121.3(4) . . ?
C41 C42 C43 118.1(4) . . ?
C41 C42 C57 119.9(4) . . ?
C43 C42 C57 121.9(4) . . ?
C44 C43 C42 121.4(4) . . ?
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C44 C45 N4 124.7(4) . . ?
C40 C45 N4 116.3(3) . . ?
N4 C46 C47 126.8(3) . . ?
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C48 C47 C46 116.0(3) . . ?
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C48 C49 C50 119.8(4) . . ?
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C50 C51 C61 120.7(3) . . ?
C52 C51 C61 121.0(3) . . ?
O4 C52 C47 121.6(3) . . ?
O4 C52 C51 119.8(3) . . ?
C47 C52 C51 118.6(3) . . ?
C54 C53 C34 111.5(3) . . ?
C54 C53 C56 107.5(3) . . ?
C34 C53 C56 109.9(3) . . ?
C54 C53 C55 106.4(3) . . ?
C34 C53 C55 111.6(3) . . ?
C56 C53 C55 109.8(3) . . ?
C59 C57 C42 113.1(6) . . ?
C59 C57 C60 107.9(4) . . ?
C42 C57 C60 108.2(5) . . ?
C59 C57 C58 108.1(4) . . ?
C42 C57 C58 108.7(6) . . ?
C60 C57 C58 110.8(5) . . ?
C62 C61 C63 107.0(3) . . ?
C62 C61 C51 110.3(3) . . ?
C63 C61 C51 112.4(3) . . ?
C62 C61 C64 110.0(3) . . ?
C63 C61 C64 107.8(3) . . ?
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C65 P1 C66 97.0(2) . . ?
C65 P1 C67 95.8(2) . . ?
C66 P1 C67 96.97(19) . . ?

C68 N5 C67 111.8(3) . . ?
C68 N5 C70 107.5(3) . . ?
C67 N5 C70 109.9(3) . . ?
C68 N5 Zn1 107.3(2) . . ?
C67 N5 Zn1 108.2(2) . . ?
C70 N5 Zn1 112.1(2) . . ?
C68 N6 C66 111.8(3) . . ?
C68 N6 C69 108.1(3) . . ?
C66 N6 C69 110.4(3) . . ?
C68 N6 Zn2 109.8(2) . . ?
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C69 N6 Zn2 104.7(2) . . ?
C70 N7 C69 108.6(3) . . ?
C70 N7 C65 111.9(3) . . ?
C69 N7 C65 110.9(3) . . ?
N7 C65 P1 113.9(3) . . ?
N6 C66 P1 114.2(3) . . ?
N5 C67 P1 114.3(3) . . ?
N6 C68 N5 113.9(3) . . ?
N7 C69 N6 113.7(3) . . ?
N7 C70 N5 114.0(3) . . ?
C65' P1' C66' 98.0(5) . . ?
C65' P1' C67' 96.5(5) . . ?
C66' P1' C67' 96.6(4) . . ?
C70' N7' C69' 108.6(6) . . ?
C70' N7' C65' 111.0(7) . . ?
C69' N7' C65' 110.5(7) . . ?
N7' C65' P1' 113.8(5) . . ?
O1S C1S C2S 126.1(8) . . ?
O1S C1S C3S 117.9(6) . . ?
C2S C1S C3S 116.0(6) . . ?
O1S' C1S' C2S' 127.4(11) . . ?
O1S' C1S' C3S' 116.8(10) . . ?
C2S' C1S' C3S' 114.1(9) . . ?
O1T C1T C2T 128.9(10) . . ?
O1T C1T C3T 115.8(8) . . ?
C2T C1T C3T 114.1(8) . . ?
O1T' C1T' C2T' 128.4(10) . . ?
O1T' C1T' C3T' 116.6(8) . . ?
C2T' C1T' C3T' 114.4(8) . . ?
loop_
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_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
O1 Zn1 N1 C7 5.9(3) . . . . ?
O2 Zn1 N1 C7 -92.3(3) . . . . ?
N2 Zn1 N1 C7 -159.3(3) . . . . ?

N5 Zn1 N1 C7 102.5(3) . . . . ?
O1 Zn1 N1 C8 -179.8(2) . . . . ?
O2 Zn1 N1 C8 81.9(3) . . . . ?
N2 Zn1 N1 C8 14.9(2) . . . . ?
N5 Zn1 N1 C8 -83.3(2) . . . . ?
O1 Zn1 N2 C14 123.0(4) . . . . ?
O2 Zn1 N2 C14 23.1(3) . . . . ?
N1 Zn1 N2 C14 175.3(3) . . . . ?
N5 Zn1 N2 C14 -83.9(3) . . . . ?
O1 Zn1 N2 C13 -66.6(4) . . . . ?
O2 Zn1 N2 C13 -166.6(2) . . . . ?
N1 Zn1 N2 C13 -14.3(2) . . . . ?
N5 Zn1 N2 C13 86.4(2) . . . . ?
O3 Zn2 N3 C39 4.7(3) . . . . ?
O4 Zn2 N3 C39 120.5(4) . . . . ?
N4 Zn2 N3 C39 160.0(3) . . . . ?
N6 Zn2 N3 C39 -97.2(3) . . . . ?
O3 Zn2 N3 C40 -170.8(2) . . . . ?
O4 Zn2 N3 C40 -54.9(5) . . . . ?
N4 Zn2 N3 C40 -15.5(2) . . . . ?
N6 Zn2 N3 C40 87.3(2) . . . . ?
O3 Zn2 N4 C46 -90.6(4) . . . . ?
O4 Zn2 N4 C46 13.0(3) . . . . ?
N3 Zn2 N4 C46 -157.5(3) . . . . ?
N6 Zn2 N4 C46 107.1(3) . . . . ?
O3 Zn2 N4 C45 82.2(3) . . . . ?
O4 Zn2 N4 C45 -174.2(2) . . . . ?
N3 Zn2 N4 C45 15.3(2) . . . . ?
N6 Zn2 N4 C45 -80.1(2) . . . . ?
O2 Zn1 O1 C1 140.7(3) . . . . ?
N1 Zn1 O1 C1 -9.2(3) . . . . ?
N2 Zn1 O1 C1 41.9(5) . . . . ?
N5 Zn1 O1 C1 -111.5(3) . . . . ?
O1 Zn1 O2 C20 177.2(3) . . . . ?
N1 Zn1 O2 C20 -86.1(4) . . . . ?
N2 Zn1 O2 C20 -21.4(3) . . . . ?
N5 Zn1 O2 C20 78.7(3) . . . . ?
O4 Zn2 O3 C33 -174.0(3) . . . . ?
N4 Zn2 O3 C33 -72.2(4) . . . . ?
N3 Zn2 O3 C33 -7.6(3) . . . . ?
N6 Zn2 O3 C33 90.1(3) . . . . ?
O3 Zn2 O4 C52 137.2(3) . . . . ?
N4 Zn2 O4 C52 -16.3(3) . . . . ?
N3 Zn2 O4 C52 22.3(6) . . . . ?
N6 Zn2 O4 C52 -120.2(3) . . . . ?
Zn1 O1 C1 C6 8.5(5) . . . . ?
Zn1 O1 C1 C2 -171.5(2) . . . . ?
O1 C1 C2 C3 178.1(3) . . . . ?
C6 C1 C2 C3 -1.9(5) . . . . ?
O1 C1 C2 C21 -1.7(5) . . . . ?
C6 C1 C2 C21 178.3(3) . . . . ?
C1 C2 C3 C4 1.6(6) . . . . ?
C21 C2 C3 C4 -178.6(4) . . . . ?
C2 C3 C4 C5 -0.4(6) . . . . ?

C3 C4 C5 C6 -0.5(6) . . . . ?
C4 C5 C6 C7 -177.3(4) . . . . ?
C4 C5 C6 C1 0.1(6) . . . . ?
O1 C1 C6 C5 -178.9(3) . . . . ?
C2 C1 C6 C5 1.1(5) . . . . ?
O1 C1 C6 C7 -1.7(6) . . . . ?
C2 C1 C6 C7 178.3(3) . . . . ?
C8 N1 C7 C6 -176.5(3) . . . . ?
Zn1 N1 C7 C6 -2.7(5) . . . . ?
C5 C6 C7 N1 176.3(4) . . . . ?
C1 C6 C7 N1 -0.9(6) . . . . ?
C7 N1 C8 C9 -20.0(5) . . . . ?
Zn1 N1 C8 C9 165.5(3) . . . . ?
C7 N1 C8 C13 161.0(3) . . . . ?
Zn1 N1 C8 C13 -13.5(4) . . . . ?
C13 C8 C9 C10 -2.3(5) . . . . ?
N1 C8 C9 C10 178.7(3) . . . . ?
C8 C9 C10 C11 0.6(6) . . . . ?
C9 C10 C11 C12 1.1(5) . . . . ?
C9 C10 C11 C25 -179.4(3) . . . . ?
C10 C11 C12 C13 -1.0(5) . . . . ?
C25 C11 C12 C13 179.4(3) . . . . ?
C11 C12 C13 C8 -0.7(5) . . . . ?
C11 C12 C13 N2 179.5(3) . . . . ?
C9 C8 C13 C12 2.3(5) . . . . ?
N1 C8 C13 C12 -178.6(3) . . . . ?
C9 C8 C13 N2 -177.9(3) . . . . ?
N1 C8 C13 N2 1.2(4) . . . . ?
C14 N2 C13 C12 1.7(5) . . . . ?
Zn1 N2 C13 C12 -168.7(3) . . . . ?
C14 N2 C13 C8 -178.1(3) . . . . ?
Zn1 N2 C13 C8 11.5(4) . . . . ?
C13 N2 C14 C15 176.3(3) . . . . ?
Zn1 N2 C14 C15 -14.3(5) . . . . ?
N2 C14 C15 C16 177.4(3) . . . . ?
N2 C14 C15 C20 -6.9(6) . . . . ?
C14 C15 C16 C17 174.8(4) . . . . ?
C20 C15 C16 C17 -1.2(6) . . . . ?
C15 C16 C17 C18 -3.9(6) . . . . ?
C16 C17 C18 C19 1.8(6) . . . . ?
C17 C18 C19 C20 5.2(6) . . . . ?
C17 C18 C19 C29 -172.6(4) . . . . ?
Zn1 O2 C20 C15 9.0(5) . . . . ?
Zn1 O2 C20 C19 -172.6(2) . . . . ?
C16 C15 C20 O2 -173.6(3) . . . . ?
C14 C15 C20 O2 10.8(6) . . . . ?
C16 C15 C20 C19 8.0(5) . . . . ?
C14 C15 C20 C19 -167.6(3) . . . . ?
C18 C19 C20 O2 171.7(3) . . . . ?
C29 C19 C20 O2 -10.4(5) . . . . ?
C18 C19 C20 C15 -9.9(5) . . . . ?
C29 C19 C20 C15 168.1(3) . . . . ?
C3 C2 C21 C22 122.7(4) . . . . ?
C1 C2 C21 C22 -57.5(4) . . . . ?

C3 C2 C21 C23 -115.0(4) . . . . ?
C1 C2 C21 C23 64.8(4) . . . . ?
C3 C2 C21 C24 4.3(5) . . . . ?
C1 C2 C21 C24 -176.0(3) . . . . ?
C12 C11 C25 C26 174.4(3) . . . . ?
C10 C11 C25 C26 -5.1(5) . . . . ?
C12 C11 C25 C27 53.8(4) . . . . ?
C10 C11 C25 C27 -125.8(4) . . . . ?
C12 C11 C25 C28 -65.5(4) . . . . ?
C10 C11 C25 C28 115.0(4) . . . . ?
C18 C19 C29 C32 -116.6(4) . . . . ?
C20 C19 C29 C32 65.5(5) . . . . ?
C18 C19 C29 C31 122.0(4) . . . . ?
C20 C19 C29 C31 -55.8(5) . . . . ?
C18 C19 C29 C30 4.7(6) . . . . ?
C20 C19 C29 C30 -173.1(4) . . . . ?
Zn2 O3 C33 C38 4.3(5) . . . . ?
Zn2 O3 C33 C34 -175.7(2) . . . . ?
O3 C33 C34 C35 178.3(3) . . . . ?
C38 C33 C34 C35 -1.7(5) . . . . ?
O3 C33 C34 C53 -3.9(5) . . . . ?
C38 C33 C34 C53 176.1(3) . . . . ?
C33 C34 C35 C36 0.6(5) . . . . ?
C53 C34 C35 C36 -177.1(3) . . . . ?
C34 C35 C36 C37 1.3(5) . . . . ?
C35 C36 C37 C38 -2.2(5) . . . . ?
C36 C37 C38 C39 177.7(3) . . . . ?
C36 C37 C38 C33 1.1(5) . . . . ?
O3 C33 C38 C37 -179.1(3) . . . . ?
C34 C33 C38 C37 0.9(5) . . . . ?
O3 C33 C38 C39 4.6(5) . . . . ?
C34 C33 C38 C39 -175.4(3) . . . . ?
C40 N3 C39 C38 176.1(3) . . . . ?
Zn2 N3 C39 C38 1.1(5) . . . . ?
C37 C38 C39 N3 176.3(3) . . . . ?
C33 C38 C39 N3 -7.2(6) . . . . ?
C39 N3 C40 C41 18.9(5) . . . . ?
Zn2 N3 C40 C41 -165.4(3) . . . . ?
C39 N3 C40 C45 -162.2(3) . . . . ?
Zn2 N3 C40 C45 13.4(4) . . . . ?
C45 C40 C41 C42 1.5(5) . . . . ?
N3 C40 C41 C42 -179.7(3) . . . . ?
C40 C41 C42 C43 -2.8(6) . . . . ?
C40 C41 C42 C57 -179.8(3) . . . . ?
C41 C42 C43 C44 1.4(6) . . . . ?
C57 C42 C43 C44 178.4(4) . . . . ?
C42 C43 C44 C45 1.3(6) . . . . ?
C43 C44 C45 C40 -2.6(5) . . . . ?
C43 C44 C45 N4 -179.4(3) . . . . ?
C41 C40 C45 C44 1.2(5) . . . . ?
N3 C40 C45 C44 -177.7(3) . . . . ?
C41 C40 C45 N4 178.4(3) . . . . ?
N3 C40 C45 N4 -0.5(5) . . . . ?
C46 N4 C45 C44 -22.9(5) . . . . ?

Zn2 N4 C45 C44 164.1(3) . . . . ?
C46 N4 C45 C40 160.2(3) . . . . ?
Zn2 N4 C45 C40 -12.9(4) . . . . ?
C45 N4 C46 C47 178.7(3) . . . . ?
Zn2 N4 C46 C47 -9.1(5) . . . . ?
N4 C46 C47 C48 -178.5(3) . . . . ?
N4 C46 C47 C52 1.5(6) . . . . ?
C52 C47 C48 C49 0.2(5) . . . . ?
C46 C47 C48 C49 -179.8(3) . . . . ?
C47 C48 C49 C50 3.0(6) . . . . ?
C48 C49 C50 C51 -2.9(6) . . . . ?
C49 C50 C51 C52 -0.5(6) . . . . ?
C49 C50 C51 C61 -179.0(3) . . . . ?
Zn2 O4 C52 C47 14.2(5) . . . . ?
Zn2 O4 C52 C51 -165.7(2) . . . . ?
C48 C47 C52 O4 176.6(3) . . . . ?
C46 C47 C52 O4 -3.4(6) . . . . ?
C48 C47 C52 C51 -3.5(5) . . . . ?
C46 C47 C52 C51 176.5(3) . . . . ?
C50 C51 C52 O4 -176.4(3) . . . . ?
C61 C51 C52 O4 2.0(5) . . . . ?
C50 C51 C52 C47 3.7(5) . . . . ?
C61 C51 C52 C47 -177.9(3) . . . . ?
C35 C34 C53 C54 -5.1(5) . . . . ?
C33 C34 C53 C54 177.1(3) . . . . ?
C35 C34 C53 C56 114.0(4) . . . . ?
C33 C34 C53 C56 -63.8(4) . . . . ?
C35 C34 C53 C55 -123.9(4) . . . . ?
C33 C34 C53 C55 58.3(4) . . . . ?
C41 C42 C57 C59 -175.5(5) . . . . ?
C43 C42 C57 C59 7.6(6) . . . . ?
C41 C42 C57 C60 65.1(5) . . . . ?
C43 C42 C57 C60 -111.9(5) . . . . ?
C41 C42 C57 C58 -55.3(6) . . . . ?
C43 C42 C57 C58 127.7(5) . . . . ?
C50 C51 C61 C62 -126.9(4) . . . . ?
C52 C51 C61 C62 54.7(4) . . . . ?
C50 C51 C61 C63 -7.6(5) . . . . ?
C52 C51 C61 C63 174.0(3) . . . . ?
C50 C51 C61 C64 112.0(4) . . . . ?
C52 C51 C61 C64 -66.4(4) . . . . ?
O1 Zn1 N5 C68 54.4(2) . . . . ?
O2 Zn1 N5 C68 151.6(2) . . . . ?
N1 Zn1 N5 C68 -36.2(2) . . . . ?
N2 Zn1 N5 C68 -117.1(2) . . . . ?
O1 Zn1 N5 C67 -66.3(2) . . . . ?
O2 Zn1 N5 C67 30.8(2) . . . . ?
N1 Zn1 N5 C67 -156.9(2) . . . . ?
N2 Zn1 N5 C67 122.1(2) . . . . ?
O1 Zn1 N5 C70 172.3(2) . . . . ?
O2 Zn1 N5 C70 -90.5(2) . . . . ?
N1 Zn1 N5 C70 81.7(2) . . . . ?
N2 Zn1 N5 C70 0.7(2) . . . . ?
O3 Zn2 N6 C68 164.9(2) . . . . ?

O4 Zn2 N6 C68 66.7(2) . . . . ?
N4 Zn2 N6 C68 -23.2(3) . . . . ?
N3 Zn2 N6 C68 -104.1(2) . . . . ?
O3 Zn2 N6 C66 -70.5(2) . . . . ?
O4 Zn2 N6 C66 -168.7(2) . . . . ?
N4 Zn2 N6 C66 101.4(2) . . . . ?
N3 Zn2 N6 C66 20.5(3) . . . . ?
O3 Zn2 N6 C69 49.0(2) . . . . ?
O4 Zn2 N6 C69 -49.2(2) . . . . ?
N4 Zn2 N6 C69 -139.1(2) . . . . ?
N3 Zn2 N6 C69 140.0(2) . . . . ?
C70 N7 C65 P1 60.9(4) . . . . ?
C69 N7 C65 P1 -60.6(4) . . . . ?
C66 P1 C65 N7 48.4(3) . . . . ?
C67 P1 C65 N7 -49.4(3) . . . . ?
C68 N6 C66 P1 -60.3(4) . . . . ?
C69 N6 C66 P1 60.1(4) . . . . ?
Zn2 N6 C66 P1 176.18(18) . . . . ?
C65 P1 C66 N6 -49.1(3) . . . . ?
C67 P1 C66 N6 47.6(3) . . . . ?
C68 N5 C67 P1 58.2(4) . . . . ?
C70 N5 C67 P1 -61.1(3) . . . . ?
Zn1 N5 C67 P1 176.22(18) . . . . ?
C65 P1 C67 N5 51.0(3) . . . . ?
C66 P1 C67 N5 -46.8(3) . . . . ?
C66 N6 C68 N5 66.3(4) . . . . ?
C69 N6 C68 N5 -55.5(4) . . . . ?
Zn2 N6 C68 N5 -169.1(2) . . . . ?
C67 N5 C68 N6 -65.3(4) . . . . ?
C70 N5 C68 N6 55.5(4) . . . . ?
Zn1 N5 C68 N6 176.3(2) . . . . ?
C70 N7 C69 N6 -56.7(4) . . . . ?
C65 N7 C69 N6 66.7(4) . . . . ?
C68 N6 C69 N7 55.8(4) . . . . ?
C66 N6 C69 N7 -66.8(4) . . . . ?
Zn2 N6 C69 N7 172.8(3) . . . . ?
C69 N7 C70 N5 57.2(4) . . . . ?
C65 N7 C70 N5 -65.6(4) . . . . ?
C68 N5 C70 N7 -56.3(4) . . . . ?
C67 N5 C70 N7 65.6(4) . . . . ?
Zn1 N5 C70 N7 -174.0(2) . . . . ?
C70' N7' C65' P1' 60.7(9) . . . . ?
C69' N7' C65' P1' -59.8(8) . . . . ?
C66' P1' C65' N7' 47.9(8) . . . . ?
C67' P1' C65' N7' -49.8(8) . . . . ?
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_diffrn_reflns_theta_full 25.91
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data_mo_da635_0m

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;
?
;
_chemical_name_common           ?
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_chemical_formula_moiety        ?
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_chemical_formula_weight        1294.64
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Zn Zn 0.2839 1.4301 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl 0.1484 0.1585 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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_symmetry_space_group_name_H-M   P2(1)/c
loop_
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'x, y, z'
'-x, y+1/2, -z+1/2'
'-x, -y, -z'
'x, -y-1/2, z-1/2'
_cell_length_a                  14.3779(7)
_cell_length_b                  30.8290(15)
_cell_length_c                  17.5123(8)
_cell_angle_alpha               90.00
_cell_angle_beta                110.964(2)
_cell_angle_gamma               90.00
_cell_volume                    7248.6(6)
_cell_formula_units_Z           4
_cell_measurement_temperature   100(2)
_cell_measurement_reflns_used   9983
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_exptl_absorpt_process_details
;
SADABS Version 2008/1 Bruker-Nonius
Blessing, Acta Cryst. (1995) A51 33-38
;
_exptl_special_details
;
It should be noted that the esd's of the cell dimensions are probably too low;
they should be multiplied by a factor of 2 to 10
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_diffrn_ambient_temperature      100(2)
_diffrn_measurement_specimen_suppport 'magnetic support whith MicroMount'
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\a
_diffrn_source                   'Micorfocus source E025 IuS'
_diffrn_source_type              'Bruker APEX DUO'
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_diffrn_source_current           0.6
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_diffrn_radiation_monochromator  'Quazar MX Multilayer Optics'
_diffrn_detector_type            '4K CCD area detector APEX II'
_diffrn_measurement_device_type  'APEX DUO Kappa 4-axis goniometer'
_diffrn_measurement_method
;
Fullsphere data collection, phi and omega scans
;
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_diffrn_reflns_av_sigmaI/netI    0.0396
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_diffrn_reflns_limit_k_max       39
_diffrn_reflns_limit_l_min       -20
_diffrn_reflns_limit_l_max       21
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_diffrn_reflns_theta_max         26.80
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_reflns_number_gt                11757
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_computing_publication_material  'Bruker SHELXTL'
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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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_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.1170P)^2^+7.3184P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
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_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_number_reflns 15211
_refine_ls_number_parameters 944
_refine_ls_number_restraints 515
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_refine_ls_R_factor_gt 0.0588
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_refine_ls_wR_factor_gt 0.1798
_refine_ls_goodness_of_fit_ref 1.045
_refine_ls_restrained_S_all 1.053
_refine_ls_shift/su_max 0.000
_refine_ls_shift/su_mean 0.000
SQUEEZE RESULTS (APPEND TO CIF)
Note: Data are Listed for all Voids in the P1 Unit Cell
i.e. Centre of Gravity, Solvent Accessible Volume,
Recovered number of Electrons in the Void and
Details about the Squeezed Material
loop_
_platon_squeeze_void_nr
_platon_squeeze_void_average_x
_platon_squeeze_void_average_y
_platon_squeeze_void_average_z
_platon_squeeze_void_volume
_platon_squeeze_void_count_electrons
_platon_squeeze_void_content
1 0.500 0.000 1.000 381 87 ' '
2 0.500 0.500 0.500 381 87 ' '
_platon_squeeze_details
;
;
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Zn1 Zn 0.16840(3) 0.177904(12) 0.24194(2) 0.02236(11) Uani 1 1 d . . .
Zn2 Zn -0.02897(3) 0.157831(12) -0.10759(2) 0.02674(12) Uani 1 1 d . . .
N1 N 0.0669(2) 0.16960(9) 0.30065(17) 0.0243(6) Uani 1 1 d . . .
N2 N 0.0779(2) 0.23118(9) 0.19959(16) 0.0258(6) Uani 1 1 d . B .
N3 N 0.0576(2) 0.21270(9) -0.08423(16) 0.0262(6) Uani 1 1 d . . .
N4 N 0.0650(2) 0.14283(10) -0.17000(18) 0.0327(7) Uani 1 1 d . B .
O1 O 0.26830(16) 0.14769(8) 0.33192(14) 0.0273(5) Uani 1 1 d . . .
O2 O 0.25842(17) 0.20019(7) 0.18836(14) 0.0276(5) Uani 1 1 d . . .
O3 O -0.12280(18) 0.18583(7) -0.06524(15) 0.0294(5) Uani 1 1 d . . .
O4 O -0.12838(19) 0.11895(8) -0.18081(15) 0.0355(6) Uani 1 1 d . . .
C1 C 0.2570(2) 0.12172(10) 0.38596(19) 0.0230(7) Uani 1 1 d . . .
C2 C 0.3401(2) 0.09645(10) 0.43669(19) 0.0234(7) Uani 1 1 d . . .
C3 C 0.3274(2) 0.06929(11) 0.4945(2) 0.0282(7) Uani 1 1 d . . .
H3 H 0.3832 0.0527 0.5270 0.034 Uiso 1 1 calc R B .
C4 C 0.2384(3) 0.06428(11) 0.5089(2) 0.0289(7) Uani 1 1 d . A .
C5 C 0.1656(2) 0.11718(10) 0.4000(2) 0.0246(7) Uani 1 1 d . . .
C6 C 0.0785(2) 0.14289(11) 0.3596(2) 0.0258(7) Uani 1 1 d . . .
H6 H 0.0244 0.1398 0.3782 0.031 Uiso 1 1 calc R B .
C7 C -0.0187(2) 0.19610(11) 0.2683(2) 0.0254(7) Uani 1 1 d . . .
C8 C -0.1059(3) 0.19102(12) 0.2841(2) 0.0312(8) Uani 1 1 d . . .
H8 H -0.1129 0.1671 0.3159 0.037 Uiso 1 1 calc R . .
C9 C -0.1833(3) 0.22069(14) 0.2537(2) 0.0367(9) Uani 1 1 d . . .
H9 H -0.2418 0.2177 0.2664 0.044 Uiso 1 1 calc R B .
C10 C -0.1748(3) 0.25472(13) 0.2045(2) 0.0402(9) Uani 1 1 d . . .
H10 H -0.2272 0.2752 0.1841 0.048 Uiso 1 1 calc R . .
C11 C -0.0904(3) 0.25868(12) 0.1855(2) 0.0347(8) Uani 1 1 d . . .
H11 H -0.0861 0.2814 0.1503 0.042 Uiso 1 1 calc R B .
C12 C -0.0110(2) 0.22995(11) 0.2169(2) 0.0261(7) Uani 1 1 d . B .
C13 C 0.1029(3) 0.26548(11) 0.1682(2) 0.0293(7) Uani 1 1 d . . .
H13 H 0.0591 0.2896 0.1582 0.035 Uiso 1 1 calc R B .
C14 C 0.1897(3) 0.27052(11) 0.1474(2) 0.0317(8) Uani 1 1 d . . .
C15 C 0.2005(3) 0.31180(12) 0.1151(2) 0.0364(8) Uani 1 1 d . . .
H15 H 0.1497 0.3329 0.1064 0.044 Uiso 1 1 calc R B .
C16 C 0.2817(3) 0.32156(13) 0.0966(2) 0.0412(9) Uani 1 1 d . . .
H16 H 0.2878 0.3492 0.0751 0.049 Uiso 1 1 calc R . .
C17 C 0.3568(3) 0.29027(13) 0.1097(2) 0.0411(9) Uani 1 1 d . . .
H17 H 0.4136 0.2974 0.0966 0.049 Uiso 1 1 calc R B .
C18 C 0.3514(3) 0.24951(12) 0.1410(2) 0.0339(8) Uani 1 1 d . . .
C19 C 0.2647(3) 0.23849(12) 0.1595(2) 0.0299(7) Uani 1 1 d . . .
C20 C 0.4426(2) 0.10154(10) 0.4281(2) 0.0255(7) Uani 1 1 d . . .
C21 C 0.4811(3) 0.14775(11) 0.4543(2) 0.0323(8) Uani 1 1 d . . .
H21A H 0.4342 0.1688 0.4190 0.048 Uiso 1 1 calc R . .
H21B H 0.5464 0.1514 0.4493 0.048 Uiso 1 1 calc R . .
H21C H 0.4872 0.1525 0.5112 0.048 Uiso 1 1 calc R . .
C22 C 0.4368(3) 0.09293(12) 0.3404(2) 0.0318(8) Uani 1 1 d . . .
H22A H 0.4135 0.0632 0.3248 0.048 Uiso 1 1 calc R . .

H22B H 0.5030 0.0966 0.3372 0.048 Uiso 1 1 calc R . .
H22C H 0.3903 0.1135 0.3033 0.048 Uiso 1 1 calc R . .
C23 C 0.5192(3) 0.06983(12) 0.4831(2) 0.0329(8) Uani 1 1 d . . .
H23A H 0.5230 0.0734 0.5397 0.049 Uiso 1 1 calc R . .
H23B H 0.5846 0.0758 0.4797 0.049 Uiso 1 1 calc R . .
H23C H 0.4992 0.0401 0.4650 0.049 Uiso 1 1 calc R . .
C24 C 0.2298(3) 0.03520(12) 0.5777(2) 0.0379(8) Uani 0.60 1 d PDU A 1
C25 C 0.1395(5) 0.0053(3) 0.5425(6) 0.0481(19) Uani 0.60 1 d PDU A 1
H25A H 0.0795 0.0228 0.5170 0.072 Uiso 0.60 1 calc PR A 1
H25B H 0.1318 -0.0122 0.5866 0.072 Uiso 0.60 1 calc PR A 1
H25C H 0.1495 -0.0139 0.5015 0.072 Uiso 0.60 1 calc PR A 1
C26 C 0.2131(6) 0.0632(2) 0.6441(4) 0.0443(16) Uani 0.60 1 d PDU A 1
H26A H 0.2681 0.0838 0.6656 0.066 Uiso 0.60 1 calc PR A 1
H26B H 0.2103 0.0445 0.6885 0.066 Uiso 0.60 1 calc PR A 1
H26C H 0.1502 0.0791 0.6206 0.066 Uiso 0.60 1 calc PR A 1
C27 C 0.3221(5) 0.0075(2) 0.6195(5) 0.0398(16) Uani 0.60 1 d PDU A 1
H27A H 0.3394 -0.0085 0.5780 0.060 Uiso 0.60 1 calc PR A 1
H27B H 0.3085 -0.0130 0.6569 0.060 Uiso 0.60 1 calc PR A 1
H27C H 0.3779 0.0263 0.6503 0.060 Uiso 0.60 1 calc PR A 1
C24' C 0.2298(3) 0.03520(12) 0.5777(2) 0.0379(8) Uani 0.40 1 d PDU A 2
C25' C 0.1238(5) 0.0185(4) 0.5582(9) 0.049(3) Uani 0.40 1 d PDU A 2
H25D H 0.0796 0.0429 0.5571 0.074 Uiso 0.40 1 calc PR A 2
H25E H 0.1229 -0.0022 0.6004 0.074 Uiso 0.40 1 calc PR A 2
H25F H 0.1008 0.0041 0.5048 0.074 Uiso 0.40 1 calc PR A 2
C26' C 0.2598(10) 0.0617(4) 0.6569(6) 0.053(2) Uani 0.40 1 d PDU A 2
H26D H 0.3267 0.0737 0.6689 0.079 Uiso 0.40 1 calc PR A 2
H26E H 0.2598 0.0428 0.7020 0.079 Uiso 0.40 1 calc PR A 2
H26F H 0.2123 0.0854 0.6504 0.079 Uiso 0.40 1 calc PR A 2
C27' C 0.3013(8) -0.0029(3) 0.5919(8) 0.050(2) Uani 0.40 1 d PDU A 2
H27D H 0.2785 -0.0224 0.5446 0.074 Uiso 0.40 1 calc PR A 2
H27E H 0.3034 -0.0187 0.6410 0.074 Uiso 0.40 1 calc PR A 2
H27F H 0.3681 0.0078 0.5991 0.074 Uiso 0.40 1 calc PR A 2
C28 C 0.4353(3) 0.21604(14) 0.1546(2) 0.0414(9) Uani 1 1 d . . .
C29 C 0.5217(3) 0.23528(18) 0.1335(3) 0.0612(14) Uani 1 1 d . . .
H29A H 0.4977 0.2436 0.0756 0.092 Uiso 1 1 calc R . .
H29B H 0.5747 0.2136 0.1439 0.092 Uiso 1 1 calc R . .
H29C H 0.5479 0.2609 0.1674 0.092 Uiso 1 1 calc R . .
C30 C 0.4772(3) 0.20206(16) 0.2446(3) 0.0504(11) Uani 1 1 d . . .
H30A H 0.5018 0.2276 0.2793 0.076 Uiso 1 1 calc R . .
H30B H 0.5321 0.1816 0.2529 0.076 Uiso 1 1 calc R . .
H30C H 0.4246 0.1881 0.2590 0.076 Uiso 1 1 calc R . .
C31 C 0.3964(3) 0.17693(15) 0.0994(3) 0.0509(11) Uani 1 1 d . . .
H31A H 0.3467 0.1617 0.1158 0.076 Uiso 1 1 calc R . .
H31B H 0.4518 0.1573 0.1042 0.076 Uiso 1 1 calc R . .
H31C H 0.3658 0.1866 0.0425 0.076 Uiso 1 1 calc R . .
C32 C -0.1296(3) 0.22638(10) -0.04731(19) 0.0265(7) Uani 1 1 d . . .
C33 C -0.2205(3) 0.24167(11) -0.0385(2) 0.0280(7) Uani 1 1 d . . .
C34 C -0.2267(3) 0.28462(11) -0.0213(2) 0.0291(7) Uani 1 1 d . . .
H34 H -0.2876 0.2947 -0.0180 0.035 Uiso 1 1 calc R B .
C35 C -0.1493(3) 0.31511(11) -0.0080(2) 0.0281(7) Uani 1 1 d . . .
C36 C -0.0636(3) 0.30023(11) -0.0162(2) 0.0271(7) Uani 1 1 d . . .
H36 H -0.0099 0.3199 -0.0075 0.033 Uiso 1 1 calc R B .
C37 C -0.0521(2) 0.25691(10) -0.0369(2) 0.0253(7) Uani 1 1 d . . .
C38 C 0.0349(3) 0.24834(11) -0.0559(2) 0.0271(7) Uani 1 1 d . . .

H38 H 0.0814 0.2714 -0.0467 0.033 Uiso 1 1 calc R B .
C39 C 0.1418(3) 0.20951(11) -0.1079(2) 0.0289(7) Uani 1 1 d . . .
C40 C 0.2173(3) 0.24001(12) -0.0904(2) 0.0330(8) Uani 1 1 d . . .
H40 H 0.2148 0.2650 -0.0595 0.040 Uiso 1 1 calc R . .
C41 C 0.2962(3) 0.23463(14) -0.1171(2) 0.0397(9) Uani 1 1 d . . .
H41 H 0.3470 0.2560 -0.1052 0.048 Uiso 1 1 calc R B .
C42 C 0.3009(3) 0.19773(15) -0.1615(3) 0.0453(10) Uani 1 1 d . . .
H42 H 0.3548 0.1940 -0.1802 0.054 Uiso 1 1 calc R . .
C43 C 0.2276(3) 0.16666(14) -0.1782(3) 0.0436(10) Uani 1 1 d . . .
H43 H 0.2322 0.1412 -0.2073 0.052 Uiso 1 1 calc R B .
C44 C 0.1466(3) 0.17202(12) -0.1528(2) 0.0337(8) Uani 1 1 d . B .
C45 C 0.0557(3) 0.10783(12) -0.2138(2) 0.0367(9) Uani 1 1 d . . .
H45 H 0.1080 0.1014 -0.2331 0.044 Uiso 1 1 calc R B .
C46 C -0.0255(3) 0.07834(12) -0.2351(2) 0.0378(9) Uani 1 1 d . . .
C47 C -0.1156(3) 0.08573(11) -0.2207(2) 0.0350(9) Uani 1 1 d . . .
C48 C -0.1972(3) 0.05570(12) -0.2541(2) 0.0397(9) Uani 1 1 d . . .
C49 C -0.1816(4) 0.01974(12) -0.2959(2) 0.0451(11) Uani 1 1 d . . .
H49 H -0.2346 -0.0004 -0.3174 0.054 Uiso 1 1 calc R B .
C50 C -0.0941(4) 0.01166(13) -0.3079(2) 0.0505(12) Uani 1 1 d . . .
H50 H -0.0867 -0.0139 -0.3355 0.061 Uiso 1 1 calc R . .
C51 C -0.0168(4) 0.04105(13) -0.2796(2) 0.0459(10) Uani 1 1 d . . .
H51 H 0.0429 0.0362 -0.2899 0.055 Uiso 1 1 calc R B .
C52 C -0.3071(3) 0.21047(12) -0.0497(3) 0.0382(9) Uani 1 1 d . . .
C53 C -0.2734(4) 0.17390(14) 0.0141(3) 0.0519(11) Uani 1 1 d . . .
H53A H -0.2192 0.1575 0.0060 0.078 Uiso 1 1 calc R . .
H53B H -0.3295 0.1544 0.0076 0.078 Uiso 1 1 calc R . .
H53C H -0.2500 0.1864 0.0691 0.078 Uiso 1 1 calc R . .
C54 C -0.3430(3) 0.19116(14) -0.1372(3) 0.0460(10) Uani 1 1 d . . .
H54A H -0.3573 0.2148 -0.1773 0.069 Uiso 1 1 calc R . .
H54B H -0.4035 0.1740 -0.1466 0.069 Uiso 1 1 calc R . .
H54C H -0.2908 0.1725 -0.1432 0.069 Uiso 1 1 calc R . .
C55 C -0.3958(3) 0.23310(15) -0.0392(3) 0.0499(11) Uani 1 1 d . . .
H55A H -0.3758 0.2454 0.0160 0.075 Uiso 1 1 calc R . .
H55B H -0.4496 0.2121 -0.0471 0.075 Uiso 1 1 calc R . .
H55C H -0.4191 0.2564 -0.0797 0.075 Uiso 1 1 calc R . .
C56 C -0.1678(3) 0.36233(11) 0.0087(3) 0.0363(9) Uani 1 1 d . . .
C57 C -0.2446(4) 0.38143(14) -0.0703(3) 0.0540(12) Uani 1 1 d . . .
H57A H -0.2177 0.3802 -0.1144 0.081 Uiso 1 1 calc R . .
H57B H -0.2585 0.4117 -0.0607 0.081 Uiso 1 1 calc R . .
H57C H -0.3063 0.3645 -0.0859 0.081 Uiso 1 1 calc R . .
C58 C -0.2082(3) 0.36605(12) 0.0777(3) 0.0393(9) Uani 1 1 d . . .
H58A H -0.2177 0.3967 0.0878 0.059 Uiso 1 1 calc R . .
H58B H -0.1609 0.3530 0.1275 0.059 Uiso 1 1 calc R . .
H58C H -0.2722 0.3509 0.0623 0.059 Uiso 1 1 calc R . .
C59 C -0.0716(4) 0.38866(13) 0.0331(4) 0.0593(14) Uani 1 1 d . . .
H59A H -0.0521 0.3925 -0.0147 0.089 Uiso 1 1 calc R . .
H59B H -0.0187 0.3732 0.0760 0.089 Uiso 1 1 calc R . .
H59C H -0.0823 0.4171 0.0536 0.089 Uiso 1 1 calc R . .
C60 C -0.2971(3) 0.06442(12) -0.2438(2) 0.0423(10) Uani 1 1 d . . .
C61 C -0.2855(3) 0.06786(14) -0.1533(2) 0.0446(10) Uani 1 1 d . . .
H61A H -0.2558 0.0411 -0.1248 0.067 Uiso 1 1 calc R . .
H61B H -0.3511 0.0722 -0.1491 0.067 Uiso 1 1 calc R . .
H61C H -0.2423 0.0925 -0.1282 0.067 Uiso 1 1 calc R . .
C62 C -0.3422(3) 0.10667(13) -0.2875(2) 0.0436(10) Uani 1 1 d . . .

H62A H -0.2987 0.1310 -0.2614 0.065 Uiso 1 1 calc R . .
H62B H -0.4080 0.1111 -0.2839 0.065 Uiso 1 1 calc R . .
H62C H -0.3489 0.1049 -0.3451 0.065 Uiso 1 1 calc R . .
C63 C -0.3730(4) 0.02795(14) -0.2809(3) 0.0563(12) Uani 1 1 d . . .
H63A H -0.3802 0.0235 -0.3381 0.084 Uiso 1 1 calc R . .
H63B H -0.4375 0.0361 -0.2780 0.084 Uiso 1 1 calc R . .
H63C H -0.3495 0.0011 -0.2501 0.084 Uiso 1 1 calc R . .
P1 P -0.00582(17) 0.05137(6) 0.09172(12) 0.0466(5) Uani 0.60 1 d PDU B 1
N5 N 0.1117(5) 0.12565(18) 0.1510(6) 0.0265(8) Uani 0.60 1 d PDU B 1
N6 N 0.0386(5) 0.1181(2) 0.0012(7) 0.0313(9) Uani 0.60 1 d PDU B 1
N7 N 0.1799(3) 0.07129(17) 0.0797(3) 0.0399(10) Uani 0.60 1 d PDU B 1
C64 C 0.0743(13) 0.1484(5) 0.0713(7) 0.0276(12) Uani 0.60 1 d PDU B 1
H64A H 0.0190 0.1679 0.0701 0.033 Uiso 0.60 1 calc PR B 1
H64B H 0.1283 0.1665 0.0658 0.033 Uiso 0.60 1 calc PR B 1
C65 C 0.1188(6) 0.0888(2) -0.0028(4) 0.0388(12) Uani 0.60 1 d PDU B 1
H65A H 0.1626 0.1049 -0.0255 0.047 Uiso 0.60 1 calc PR B 1
H65B H 0.0886 0.0644 -0.0402 0.047 Uiso 0.60 1 calc PR B 1
C66 C 0.2003(5) 0.1015(2) 0.1499(4) 0.0297(12) Uani 0.60 1 d PDU B 1
H66A H 0.2280 0.0846 0.2013 0.036 Uiso 0.60 1 calc PR B 1
H66B H 0.2516 0.1226 0.1487 0.036 Uiso 0.60 1 calc PR B 1
C67 C 0.0405(5) 0.09555(17) 0.1665(4) 0.0300(11) Uani 0.60 1 d PDU B 1
H67A H -0.0173 0.1125 0.1679 0.036 Uiso 0.60 1 calc PR B 1
H67B H 0.0731 0.0825 0.2214 0.036 Uiso 0.60 1 calc PR B 1
C68 C -0.0391(5) 0.08655(18) 0.0010(3) 0.0355(12) Uani 0.60 1 d PDU B 1
H68A H -0.0547 0.0680 -0.0481 0.043 Uiso 0.60 1 calc PR B 1
H68B H -0.1004 0.1027 -0.0037 0.043 Uiso 0.60 1 calc PR B 1
C69 C 0.1175(4) 0.03568(18) 0.0896(4) 0.0418(12) Uani 0.60 1 d PDU B 1
H69A H 0.1546 0.0203 0.1412 0.050 Uiso 0.60 1 calc PR B 1
H69B H 0.1070 0.0149 0.0442 0.050 Uiso 0.60 1 calc PR B 1
P1' P 0.1686(3) 0.05251(10) 0.08777(18) 0.0531(9) Uani 0.40 1 d PDU B 2
N5' N 0.0355(7) 0.1172(4) 0.0011(10) 0.0321(11) Uani 0.40 1 d PDU B 2
N6' N 0.1108(8) 0.1267(3) 0.1531(9) 0.0266(10) Uani 0.40 1 d PDU B 2
N7' N -0.0191(4) 0.0726(2) 0.0951(4) 0.0420(12) Uani 0.40 1 d PDU B 2
C64' C 0.066(2) 0.1472(7) 0.0717(10) 0.0279(13) Uani 0.40 1 d PDU B 2
H64C H 0.0067 0.1639 0.0707 0.033 Uiso 0.40 1 calc PR B 2
H64D H 0.1145 0.1681 0.0647 0.033 Uiso 0.40 1 calc PR B 2
C65' C 0.0224(8) 0.1050(3) 0.1604(6) 0.0313(13) Uani 0.40 1 d PDU B 2
H65C H 0.0414 0.0906 0.2144 0.038 Uiso 0.40 1 calc PR B 2
H65D H -0.0290 0.1270 0.1571 0.038 Uiso 0.40 1 calc PR B 2
C66' C -0.0487(8) 0.0958(3) 0.0163(5) 0.0359(14) Uani 0.40 1 d PDU B 2
H66C H -0.0990 0.1180 0.0150 0.043 Uiso 0.40 1 calc PR B 2
H66D H -0.0805 0.0749 -0.0284 0.043 Uiso 0.40 1 calc PR B 2
C67' C 0.1313(8) 0.0959(3) 0.0084(6) 0.0380(13) Uani 0.40 1 d PDU B 2
H67C H 0.1844 0.1182 0.0221 0.046 Uiso 0.40 1 calc PR B 2
H67D H 0.1250 0.0832 -0.0451 0.046 Uiso 0.40 1 calc PR B 2
C68' C 0.1935(8) 0.0956(3) 0.1661(5) 0.0318(14) Uani 0.40 1 d PDU B 2
H68C H 0.2090 0.0817 0.2202 0.038 Uiso 0.40 1 calc PR B 2
H68D H 0.2534 0.1119 0.1674 0.038 Uiso 0.40 1 calc PR B 2
C69' C 0.0500(5) 0.0363(2) 0.0976(6) 0.0507(15) Uani 0.40 1 d PDU B 2
H69C H 0.0155 0.0158 0.0530 0.061 Uiso 0.40 1 calc PR B 2
H69D H 0.0649 0.0206 0.1500 0.061 Uiso 0.40 1 calc PR B 2
C70 C 0.1587(3) 0.08865(11) 0.4610(2) 0.0293(7) Uani 1 1 d . . .
C1X C -0.2351(8) 0.4078(5) -0.3241(9) 0.061(4) Uani 0.25 1 d PDU C 1
H1X1 H -0.2054 0.3811 -0.3373 0.073 Uiso 0.25 1 calc PR C 1

H1X2 H -0.2556 0.4268 -0.3728 0.073 Uiso 0.25 1 calc PR C 1
Cl1X Cl -0.1445(17) 0.4350(8) -0.2406(12) 0.0559(7) Uani 0.25 1 d PDU C 1
Cl2X Cl -0.3425(6) 0.3936(3) -0.3000(5) 0.121(3) Uani 0.25 1 d PDU C 1
C1Z C -0.1906(14) 0.4668(5) -0.3277(8) 0.061(3) Uani 0.25 1 d PDU D 2
H1Z1 H -0.2397 0.4874 -0.3206 0.073 Uiso 0.25 1 calc PR D 2
H1Z2 H -0.1364 0.4840 -0.3355 0.073 Uiso 0.25 1 calc PR D 2
Cl1Z Cl -0.2493(6) 0.4348(3) -0.4163(5) 0.122(3) Uani 0.25 1 d PDU D 2
Cl2Z Cl -0.1399(17) 0.4344(8) -0.2371(12) 0.0559(7) Uani 0.25 1 d PDU D 2
loop_
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_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Zn1 0.02120(19) 0.0268(2) 0.0183(2) 0.00253(14) 0.00605(15) 0.00031(14)
Zn2 0.0337(2) 0.0255(2) 0.0185(2) -0.00037(14) 0.00626(16) 0.00597(15)
N1 0.0211(13) 0.0297(14) 0.0204(14) 0.0019(11) 0.0054(11) 0.0005(11)
N2 0.0258(14) 0.0298(14) 0.0214(14) 0.0000(11) 0.0079(11) 0.0017(11)
N3 0.0317(15) 0.0266(14) 0.0212(14) 0.0046(11) 0.0105(12) 0.0080(11)
N4 0.0398(17) 0.0330(15) 0.0241(15) 0.0000(12) 0.0100(13) 0.0098(13)
O1 0.0214(11) 0.0349(12) 0.0227(12) 0.0072(10) 0.0044(9) -0.0010(9)
O2 0.0278(12) 0.0311(12) 0.0260(12) 0.0048(10) 0.0122(10) -0.0005(9)
O3 0.0368(13) 0.0242(11) 0.0280(13) 0.0015(9) 0.0128(11) 0.0040(9)
O4 0.0378(14) 0.0317(13) 0.0286(13) -0.0066(11) 0.0015(11) 0.0026(11)
C1 0.0229(15) 0.0257(15) 0.0184(15) -0.0004(12) 0.0048(12) -0.0015(12)
C2 0.0218(15) 0.0257(15) 0.0217(16) -0.0006(13) 0.0066(13) -0.0019(12)
C3 0.0263(17) 0.0279(16) 0.0276(18) 0.0022(14) 0.0065(14) 0.0016(13)
C4 0.0317(18) 0.0271(16) 0.0302(18) 0.0026(14) 0.0139(15) 0.0012(13)
C5 0.0231(16) 0.0272(16) 0.0222(16) 0.0003(13) 0.0066(13) -0.0006(12)
C6 0.0246(16) 0.0307(16) 0.0223(17) 0.0002(13) 0.0085(13) -0.0028(13)
C7 0.0219(16) 0.0323(17) 0.0189(16) -0.0021(13) 0.0036(13) 0.0034(13)
C8 0.0252(17) 0.0424(19) 0.0250(18) 0.0042(15) 0.0077(14) 0.0025(14)
C9 0.0259(18) 0.058(2) 0.0281(19) 0.0065(17) 0.0113(15) 0.0097(16)
C10 0.0322(19) 0.049(2) 0.038(2) 0.0083(18) 0.0098(17) 0.0164(17)
C11 0.0334(19) 0.0377(19) 0.033(2) 0.0100(16) 0.0123(16) 0.0087(15)
C12 0.0242(16) 0.0323(17) 0.0210(16) -0.0012(13) 0.0072(13) 0.0036(13)
C13 0.0309(17) 0.0258(16) 0.0277(18) 0.0019(14) 0.0062(14) 0.0007(13)
C14 0.0323(18) 0.0330(18) 0.0272(18) 0.0036(14) 0.0076(15) -0.0029(14)
C15 0.042(2) 0.0323(18) 0.034(2) 0.0048(15) 0.0125(17) -0.0025(15)
C16 0.048(2) 0.036(2) 0.036(2) 0.0086(17) 0.0117(18) -0.0120(17)
C17 0.040(2) 0.050(2) 0.035(2) 0.0082(18) 0.0148(17) -0.0101(18)
C18 0.0319(18) 0.042(2) 0.0279(18) 0.0074(15) 0.0108(15) -0.0036(15)
C19 0.0301(18) 0.0368(18) 0.0213(17) 0.0002(14) 0.0074(14) -0.0065(14)
C20 0.0203(15) 0.0261(15) 0.0267(17) 0.0002(13) 0.0043(13) -0.0006(12)
C21 0.0228(17) 0.0285(17) 0.039(2) -0.0030(15) 0.0030(15) -0.0014(13)
C22 0.0268(17) 0.0407(19) 0.0286(18) -0.0056(15) 0.0108(14) -0.0049(14)
C23 0.0253(17) 0.0355(18) 0.035(2) 0.0043(15) 0.0072(15) 0.0033(14)
C24 0.0457(17) 0.0330(16) 0.0393(17) 0.0127(13) 0.0203(14) 0.0042(13)
C25 0.051(3) 0.042(4) 0.048(4) 0.014(3) 0.015(3) -0.005(3)
C26 0.060(4) 0.040(3) 0.037(3) 0.014(2) 0.022(3) 0.013(3)
C27 0.045(3) 0.034(3) 0.041(4) 0.012(3) 0.017(3) 0.002(3)
C24' 0.0457(17) 0.0330(16) 0.0393(17) 0.0127(13) 0.0203(14) 0.0042(13)

C25' 0.053(3) 0.046(5) 0.051(5) 0.016(4) 0.021(4) -0.002(3)
C26' 0.069(5) 0.040(4) 0.044(4) 0.010(3) 0.014(4) 0.003(4)
C27' 0.059(4) 0.037(4) 0.055(5) 0.017(4) 0.022(4) 0.008(4)
C28 0.0305(19) 0.058(2) 0.039(2) 0.0168(19) 0.0164(17) 0.0035(17)
C29 0.041(2) 0.080(3) 0.071(3) 0.035(3) 0.030(2) 0.011(2)
C30 0.029(2) 0.070(3) 0.047(3) 0.022(2) 0.0073(18) -0.0033(19)
C31 0.049(3) 0.059(3) 0.051(3) 0.009(2) 0.026(2) 0.018(2)
C32 0.0362(18) 0.0262(16) 0.0167(15) 0.0031(12) 0.0088(14) 0.0021(13)
C33 0.0321(18) 0.0304(17) 0.0228(17) 0.0012(13) 0.0113(14) 0.0024(14)
C34 0.0313(18) 0.0323(17) 0.0270(18) 0.0020(14) 0.0144(14) 0.0047(14)
C35 0.0341(18) 0.0266(16) 0.0269(18) 0.0023(13) 0.0151(15) 0.0059(13)
C36 0.0312(17) 0.0248(16) 0.0280(18) 0.0025(13) 0.0139(14) 0.0007(13)
C37 0.0311(17) 0.0244(15) 0.0207(16) 0.0032(12) 0.0096(13) 0.0052(13)
C38 0.0320(17) 0.0252(16) 0.0239(17) 0.0031(13) 0.0096(14) 0.0033(13)
C39 0.0320(18) 0.0328(17) 0.0218(17) 0.0057(14) 0.0096(14) 0.0108(14)
C40 0.0339(19) 0.0348(18) 0.0294(19) 0.0034(15) 0.0100(15) 0.0103(15)
C41 0.033(2) 0.047(2) 0.039(2) 0.0051(18) 0.0137(17) 0.0082(16)
C42 0.037(2) 0.062(3) 0.042(2) -0.002(2) 0.0194(18) 0.0133(19)
C43 0.043(2) 0.051(2) 0.040(2) -0.0056(19) 0.0185(19) 0.0088(18)
C44 0.0348(19) 0.0396(19) 0.0263(18) 0.0037(15) 0.0104(15) 0.0124(15)
C45 0.051(2) 0.0353(19) 0.0244(18) 0.0014(15) 0.0146(17) 0.0131(17)
C46 0.058(2) 0.0309(18) 0.0211(17) 0.0011(14) 0.0105(17) 0.0091(17)
C47 0.054(2) 0.0278(17) 0.0161(16) 0.0016(13) 0.0033(15) 0.0066(16)
C48 0.060(3) 0.0280(17) 0.0206(18) 0.0039(14) 0.0017(17) -0.0008(17)
C49 0.077(3) 0.0263(18) 0.0259(19) -0.0009(15) 0.011(2) -0.0040(19)
C50 0.091(4) 0.0298(19) 0.030(2) -0.0003(16) 0.022(2) 0.003(2)
C51 0.076(3) 0.034(2) 0.031(2) -0.0015(16) 0.023(2) 0.010(2)
C52 0.036(2) 0.0363(19) 0.045(2) -0.0048(17) 0.0172(17) -0.0035(15)
C53 0.062(3) 0.041(2) 0.062(3) 0.005(2) 0.034(2) -0.011(2)
C54 0.038(2) 0.046(2) 0.049(3) -0.0130(19) 0.0109(19) -0.0028(17)
C55 0.039(2) 0.051(2) 0.069(3) -0.017(2) 0.030(2) -0.0115(19)
C56 0.038(2) 0.0260(17) 0.051(2) -0.0028(16) 0.0241(18) 0.0022(15)
C57 0.074(3) 0.044(2) 0.059(3) 0.018(2) 0.042(3) 0.026(2)
C58 0.044(2) 0.0315(19) 0.046(2) -0.0065(16) 0.0205(19) 0.0006(16)
C59 0.057(3) 0.029(2) 0.108(4) -0.019(2) 0.048(3) -0.0067(19)
C60 0.052(2) 0.0331(19) 0.029(2) 0.0017(16) -0.0011(17) -0.0033(17)
C61 0.049(2) 0.042(2) 0.035(2) 0.0036(17) 0.0054(18) -0.0013(18)
C62 0.048(2) 0.037(2) 0.032(2) 0.0043(16) -0.0027(17) -0.0035(17)
C63 0.073(3) 0.040(2) 0.043(2) -0.0023(19) 0.005(2) -0.013(2)
P1 0.0611(12) 0.0392(10) 0.0299(9) -0.0007(8) 0.0046(9) -0.0092(9)
N5 0.0326(16) 0.0267(15) 0.0172(15) 0.0048(13) 0.0052(14) 0.0029(13)
N6 0.0424(17) 0.0262(15) 0.0191(15) -0.0029(14) 0.0035(15) 0.0044(14)
N7 0.0589(18) 0.030(2) 0.0222(18) 0.0008(17) 0.0039(16) 0.0067(17)
C64 0.037(2) 0.0261(17) 0.0166(17) 0.0020(14) 0.0060(17) 0.0048(17)
C65 0.055(2) 0.035(2) 0.019(2) -0.0040(18) 0.0037(19) 0.0155(19)
C66 0.039(2) 0.029(2) 0.018(2) 0.0038(18) 0.0065(18) 0.0089(17)
C67 0.038(2) 0.025(2) 0.0212(19) 0.0034(17) 0.0035(17) -0.0010(18)
C68 0.048(2) 0.025(2) 0.024(2) -0.0002(18) 0.0011(19) 0.0010(18)
C69 0.069(3) 0.026(2) 0.017(2) -0.0017(18) 0.000(2) 0.015(2)
P1' 0.091(2) 0.0301(16) 0.0190(12) 0.0003(12) -0.0033(14) 0.0315(15)
N5' 0.0436(19) 0.0261(18) 0.0194(17) -0.0022(16) 0.0024(17) 0.0060(16)
N6' 0.0340(18) 0.0260(18) 0.0172(17) 0.0035(16) 0.0059(17) 0.0044(16)
N7' 0.057(2) 0.027(2) 0.026(2) 0.0028(19) -0.0033(18) -0.0046(19)
C64' 0.037(2) 0.026(2) 0.0173(19) 0.0022(17) 0.0058(19) 0.0037(19)

C65' 0.040(2) 0.026(2) 0.020(2) 0.005(2) 0.002(2) -0.003(2)
C66' 0.048(2) 0.027(2) 0.022(2) 0.000(2) -0.001(2) -0.002(2)
C67' 0.051(2) 0.031(2) 0.022(2) -0.007(2) 0.002(2) 0.010(2)
C68' 0.042(2) 0.029(2) 0.019(2) 0.003(2) 0.006(2) 0.010(2)
C69' 0.073(3) 0.030(2) 0.027(3) -0.001(2) -0.008(3) 0.006(2)
C70 0.0329(18) 0.0274(16) 0.0283(18) 0.0018(14) 0.0116(15) 0.0013(13)
C1X 0.049(8) 0.033(8) 0.093(14) -0.001(7) 0.016(6) 0.027(6)
Cl1X 0.0676(18) 0.0488(12) 0.0763(17) -0.0124(12) 0.0560(12) -0.0077(12)
Cl2X 0.093(5) 0.158(8) 0.095(5) -0.019(5) 0.015(4) -0.073(5)
C1Z 0.060(6) 0.058(5) 0.064(4) -0.021(3) 0.022(4) 0.001(4)
Cl1Z 0.091(5) 0.172(8) 0.115(4) -0.110(5) 0.050(4) -0.045(5)
Cl2Z 0.0676(18) 0.0488(12) 0.0763(17) -0.0124(12) 0.0560(12) -0.0077(12)
_geom_special_details
;
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_distance
_geom_bond_site_symmetry_2
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Zn1 O1 1.948(2) . ?
Zn1 O2 1.974(2) . ?
Zn1 N2 2.062(3) . ?
Zn1 N1 2.079(3) . ?
Zn1 N6' 2.163(8) . ?
Zn1 N5 2.206(6) . ?
Zn2 O4 1.953(2) . ?
Zn2 O3 1.957(2) . ?
Zn2 N3 2.053(3) . ?
Zn2 N4 2.071(3) . ?
Zn2 N6 2.179(6) . ?
Zn2 N5' 2.189(9) . ?
N1 C6 1.284(4) . ?
N1 C7 1.416(4) . ?
N2 C13 1.301(4) . ?
N2 C12 1.415(4) . ?
N3 C38 1.294(4) . ?
N3 C39 1.417(4) . ?
N4 C45 1.302(5) . ?
N4 C44 1.423(5) . ?
O1 C1 1.293(4) . ?
O2 C19 1.300(4) . ?
O3 C32 1.301(4) . ?
O4 C47 1.289(4) . ?
C1 C5 1.427(5) . ?
C1 C2 1.437(4) . ?
C2 C3 1.375(5) . ?

C2 C20 1.542(4) . ?
C3 C4 1.399(5) . ?
C4 C70 1.376(5) . ?
C4 C24 1.541(5) . ?
C5 C70 1.414(5) . ?
C5 C6 1.437(4) . ?
C7 C8 1.388(5) . ?
C7 C12 1.408(5) . ?
C8 C9 1.390(5) . ?
C9 C10 1.389(6) . ?
C10 C11 1.374(5) . ?
C11 C12 1.393(5) . ?
C13 C14 1.429(5) . ?
C14 C19 1.420(5) . ?
C14 C15 1.423(5) . ?
C15 C16 1.351(6) . ?
C16 C17 1.404(6) . ?
C17 C18 1.384(5) . ?
C18 C19 1.437(5) . ?
C18 C28 1.540(5) . ?
C20 C23 1.529(4) . ?
C20 C22 1.530(5) . ?
C20 C21 1.538(4) . ?
C24 C27 1.527(6) . ?
C24 C25 1.530(7) . ?
C24 C26 1.534(7) . ?
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C28 C30 1.533(6) . ?
C28 C29 1.536(6) . ?
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C32 C33 1.448(5) . ?
C33 C34 1.368(5) . ?
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C34 C35 1.411(5) . ?
C35 C36 1.369(5) . ?
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C39 C44 1.414(5) . ?
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C42 C43 1.376(6) . ?
C43 C44 1.396(5) . ?
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C52 C53 1.538(6) . ?

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C56 C58 1.522(6) . ?
C56 C59 1.527(6) . ?
C56 C57 1.546(6) . ?
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C60 C61 1.538(6) . ?
C60 C63 1.539(6) . ?
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P1 C69 1.851(4) . ?
N5 C67 1.477(4) . ?
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N5 C66 1.481(4) . ?
N6 C64 1.480(4) . ?
N6 C68 1.481(5) . ?
N6 C65 1.486(5) . ?
N7 C69 1.467(4) . ?
N7 C66 1.485(4) . ?
N7 C65 1.498(5) . ?
P1' C69' 1.844(5) . ?
P1' C68' 1.850(5) . ?
P1' C67' 1.866(5) . ?
N5' C64' 1.480(5) . ?
N5' C66' 1.484(5) . ?
N5' C67' 1.490(5) . ?
N6' C68' 1.480(5) . ?
N6' C64' 1.480(5) . ?
N6' C65' 1.481(5) . ?
N7' C66' 1.474(5) . ?
N7' C65' 1.476(5) . ?
N7' C69' 1.486(5) . ?
C1X Cl1X 1.782(9) . ?
C1X Cl2X 1.794(9) . ?
C1Z Cl1Z 1.777(9) . ?
C1Z Cl2Z 1.794(10) . ?
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O1 Zn1 N2 149.29(11) . . ?
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O1 Zn1 N1 89.19(10) . . ?
O2 Zn1 N1 166.69(10) . . ?
N2 Zn1 N1 79.14(11) . . ?
O1 Zn1 N6' 102.4(4) . . ?
O2 Zn1 N6' 93.4(3) . . ?
N2 Zn1 N6' 107.0(4) . . ?
N1 Zn1 N6' 96.3(3) . . ?
O1 Zn1 N5 102.1(3) . . ?

O2 Zn1 N5 92.7(2) . . ?
N2 Zn1 N5 107.4(3) . . ?
N1 Zn1 N5 97.1(2) . . ?
N6' Zn1 N5 0.8(4) . . ?
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O4 Zn2 N3 152.37(11) . . ?
O3 Zn2 N3 90.69(10) . . ?
O4 Zn2 N4 88.78(12) . . ?
O3 Zn2 N4 165.13(11) . . ?
N3 Zn2 N4 79.97(12) . . ?
O4 Zn2 N6 102.8(3) . . ?
O3 Zn2 N6 93.9(2) . . ?
N3 Zn2 N6 103.9(2) . . ?
N4 Zn2 N6 99.5(2) . . ?
O4 Zn2 N5' 101.7(4) . . ?
O3 Zn2 N5' 93.3(4) . . ?
N3 Zn2 N5' 105.1(4) . . ?
N4 Zn2 N5' 100.3(3) . . ?
N6 Zn2 N5' 1.4(4) . . ?
C6 N1 C7 122.4(3) . . ?
C6 N1 Zn1 124.4(2) . . ?
C7 N1 Zn1 113.2(2) . . ?
C13 N2 C12 121.3(3) . . ?
C13 N2 Zn1 124.4(2) . . ?
C12 N2 Zn1 113.8(2) . . ?
C38 N3 C39 122.0(3) . . ?
C38 N3 Zn2 123.9(2) . . ?
C39 N3 Zn2 113.9(2) . . ?
C45 N4 C44 123.4(3) . . ?
C45 N4 Zn2 123.1(3) . . ?
C44 N4 Zn2 113.1(2) . . ?
C1 O1 Zn1 129.7(2) . . ?
C19 O2 Zn1 130.5(2) . . ?
C32 O3 Zn2 129.6(2) . . ?
C47 O4 Zn2 129.1(3) . . ?
O1 C1 C5 123.5(3) . . ?
O1 C1 C2 119.6(3) . . ?
C5 C1 C2 117.0(3) . . ?
C3 C2 C1 119.0(3) . . ?
C3 C2 C20 121.2(3) . . ?
C1 C2 C20 119.8(3) . . ?
C2 C3 C4 124.9(3) . . ?
C70 C4 C3 116.4(3) . . ?
C70 C4 C24 120.8(3) . . ?
C3 C4 C24 122.7(3) . . ?
C70 C5 C1 120.6(3) . . ?
C70 C5 C6 115.5(3) . . ?
C1 C5 C6 123.7(3) . . ?
N1 C6 C5 126.1(3) . . ?
C8 C7 C12 119.7(3) . . ?
C8 C7 N1 125.0(3) . . ?
C12 C7 N1 115.3(3) . . ?
C7 C8 C9 120.4(3) . . ?
C10 C9 C8 119.9(3) . . ?

C11 C10 C9 119.9(3) . . ?
C10 C11 C12 121.2(3) . . ?
C11 C12 C7 118.9(3) . . ?
C11 C12 N2 125.0(3) . . ?
C7 C12 N2 116.1(3) . . ?
N2 C13 C14 126.6(3) . . ?
C19 C14 C15 119.7(3) . . ?
C19 C14 C13 124.9(3) . . ?
C15 C14 C13 115.4(3) . . ?
C16 C15 C14 121.4(4) . . ?
C15 C16 C17 119.2(4) . . ?
C18 C17 C16 122.7(4) . . ?
C17 C18 C19 118.7(4) . . ?
C17 C18 C28 121.2(3) . . ?
C19 C18 C28 120.1(3) . . ?
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O2 C19 C18 119.3(3) . . ?
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C23 C20 C22 106.8(3) . . ?
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C25 C24 C4 109.3(5) . . ?
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C31 C28 C18 110.1(3) . . ?
C30 C28 C18 110.2(3) . . ?
C29 C28 C18 111.1(3) . . ?
O3 C32 C37 123.0(3) . . ?
O3 C32 C33 119.2(3) . . ?
C37 C32 C33 117.8(3) . . ?
C34 C33 C32 118.1(3) . . ?
C34 C33 C52 121.5(3) . . ?
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C33 C34 C35 124.9(3) . . ?
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C36 C35 C56 124.3(3) . . ?
C34 C35 C56 119.1(3) . . ?
C35 C36 C37 122.5(3) . . ?
C36 C37 C32 120.1(3) . . ?
C36 C37 C38 115.4(3) . . ?
C32 C37 C38 124.0(3) . . ?
N3 C38 C37 127.4(3) . . ?
C40 C39 C44 119.2(3) . . ?
C40 C39 N3 124.9(3) . . ?
C44 C39 N3 115.9(3) . . ?

C41 C40 C39 121.1(4) . . ?
C40 C41 C42 119.8(4) . . ?
C43 C42 C41 120.0(4) . . ?
C42 C43 C44 120.8(4) . . ?
C43 C44 C39 119.1(4) . . ?
C43 C44 N4 125.2(3) . . ?
C39 C44 N4 115.7(3) . . ?
N4 C45 C46 125.9(4) . . ?
C51 C46 C45 115.9(4) . . ?
C51 C46 C47 119.5(4) . . ?
C45 C46 C47 124.4(3) . . ?
O4 C47 C46 122.6(4) . . ?
O4 C47 C48 118.5(4) . . ?
C46 C47 C48 118.9(3) . . ?
C49 C48 C47 117.7(4) . . ?
C49 C48 C60 122.4(4) . . ?
C47 C48 C60 119.9(3) . . ?
C50 C49 C48 123.7(4) . . ?
C49 C50 C51 119.4(4) . . ?
C50 C51 C46 120.7(4) . . ?
C55 C52 C33 112.0(3) . . ?
C55 C52 C53 108.0(4) . . ?
C33 C52 C53 109.7(3) . . ?
C55 C52 C54 107.4(3) . . ?
C33 C52 C54 109.6(3) . . ?
C53 C52 C54 110.1(3) . . ?
C58 C56 C59 107.7(4) . . ?
C58 C56 C35 111.5(3) . . ?
C59 C56 C35 111.0(3) . . ?
C58 C56 C57 109.2(3) . . ?
C59 C56 C57 109.5(4) . . ?
C35 C56 C57 108.0(3) . . ?
C62 C60 C48 109.7(3) . . ?
C62 C60 C61 109.0(3) . . ?
C48 C60 C61 111.9(3) . . ?
C62 C60 C63 107.5(3) . . ?
C48 C60 C63 112.0(4) . . ?
C61 C60 C63 106.5(4) . . ?
C68 P1 C67 95.4(3) . . ?
C68 P1 C69 95.3(3) . . ?
C67 P1 C69 95.9(3) . . ?
C67 N5 C64 115.4(9) . . ?
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C64 N5 C66 104.5(9) . . ?
C67 N5 Zn1 115.3(5) . . ?
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C66 N5 Zn1 106.3(4) . . ?
C64 N6 C68 117.0(9) . . ?
C64 N6 C65 112.2(10) . . ?
C68 N6 C65 101.4(7) . . ?
C64 N6 Zn2 106.6(5) . . ?
C68 N6 Zn2 105.5(4) . . ?
C65 N6 Zn2 114.3(5) . . ?
C69 N7 C66 108.5(5) . . ?

C69 N7 C65 102.2(5) . . ?
C66 N7 C65 116.5(5) . . ?
N6 C64 N5 112.7(10) . . ?
N6 C65 N7 111.8(5) . . ?
N5 C66 N7 114.2(5) . . ?
N5 C67 P1 115.6(4) . . ?
N6 C68 P1 115.0(4) . . ?
N7 C69 P1 116.0(4) . . ?
C69' P1' C68' 93.8(5) . . ?
C69' P1' C67' 103.6(4) . . ?
C68' P1' C67' 88.0(5) . . ?
C64' N5' C66' 98.4(14) . . ?
C64' N5' C67' 102.4(15) . . ?
C66' N5' C67' 125.3(8) . . ?
C64' N5' Zn2 106.0(8) . . ?
C66' N5' Zn2 107.0(5) . . ?
C67' N5' Zn2 114.6(7) . . ?
C68' N6' C64' 118.3(14) . . ?
C68' N6' C65' 111.2(10) . . ?
C64' N6' C65' 100.6(14) . . ?
C68' N6' Zn1 106.4(6) . . ?
C64' N6' Zn1 107.6(9) . . ?
C65' N6' Zn1 112.7(6) . . ?
C66' N7' C65' 107.4(8) . . ?
C66' N7' C69' 111.1(7) . . ?
C65' N7' C69' 114.0(7) . . ?
N5' C64' N6' 115.7(15) . . ?
N7' C65' N6' 111.0(8) . . ?
N7' C66' N5' 113.7(8) . . ?
N5' C67' P1' 112.9(5) . . ?
N6' C68' P1' 114.8(5) . . ?
N7' C69' P1' 115.0(4) . . ?
C4 C70 C5 122.2(3) . . ?
Cl1X C1X Cl2X 111.1(10) . . ?
Cl1Z C1Z Cl2Z 112.2(10) . . ?
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O2 Zn1 N1 C6 -136.5(4) . . . . ?
N2 Zn1 N1 C6 -167.0(3) . . . . ?
N6' Zn1 N1 C6 86.8(5) . . . . ?
N5 Zn1 N1 C6 86.5(4) . . . . ?
O1 Zn1 N1 C7 165.4(2) . . . . ?
O2 Zn1 N1 C7 44.5(5) . . . . ?
N2 Zn1 N1 C7 14.0(2) . . . . ?

N6' Zn1 N1 C7 -92.2(4) . . . . ?
N5 Zn1 N1 C7 -92.5(3) . . . . ?
O1 Zn1 N2 C13 91.3(3) . . . . ?
O2 Zn1 N2 C13 -12.6(3) . . . . ?
N1 Zn1 N2 C13 160.7(3) . . . . ?
N6' Zn1 N2 C13 -106.0(4) . . . . ?
N5 Zn1 N2 C13 -105.2(3) . . . . ?
O1 Zn1 N2 C12 -81.1(3) . . . . ?
O2 Zn1 N2 C12 175.1(2) . . . . ?
N1 Zn1 N2 C12 -11.7(2) . . . . ?
N6' Zn1 N2 C12 81.7(4) . . . . ?
N5 Zn1 N2 C12 82.5(3) . . . . ?
O4 Zn2 N3 C38 97.9(3) . . . . ?
O3 Zn2 N3 C38 -3.1(3) . . . . ?
N4 Zn2 N3 C38 165.3(3) . . . . ?
N6 Zn2 N3 C38 -97.3(4) . . . . ?
N5' Zn2 N3 C38 -96.7(5) . . . . ?
O4 Zn2 N3 C39 -77.4(3) . . . . ?
O3 Zn2 N3 C39 -178.4(2) . . . . ?
N4 Zn2 N3 C39 -10.1(2) . . . . ?
N6 Zn2 N3 C39 87.4(3) . . . . ?
N5' Zn2 N3 C39 88.0(4) . . . . ?
O4 Zn2 N4 C45 -21.3(3) . . . . ?
O3 Zn2 N4 C45 -124.1(4) . . . . ?
N3 Zn2 N4 C45 -175.9(3) . . . . ?
N6 Zn2 N4 C45 81.5(4) . . . . ?
N5' Zn2 N4 C45 80.4(5) . . . . ?
O4 Zn2 N4 C44 165.3(2) . . . . ?
O3 Zn2 N4 C44 62.5(5) . . . . ?
N3 Zn2 N4 C44 10.7(2) . . . . ?
N6 Zn2 N4 C44 -91.9(3) . . . . ?
N5' Zn2 N4 C44 -93.0(5) . . . . ?
O2 Zn1 O1 C1 -171.5(3) . . . . ?
N2 Zn1 O1 C1 86.9(3) . . . . ?
N1 Zn1 O1 C1 20.0(3) . . . . ?
N6' Zn1 O1 C1 -76.3(4) . . . . ?
N5 Zn1 O1 C1 -77.1(3) . . . . ?
O1 Zn1 O2 C19 -134.6(3) . . . . ?
N2 Zn1 O2 C19 15.4(3) . . . . ?
N1 Zn1 O2 C19 -14.6(6) . . . . ?
N6' Zn1 O2 C19 122.4(4) . . . . ?
N5 Zn1 O2 C19 122.8(4) . . . . ?
O4 Zn2 O3 C32 -141.1(3) . . . . ?
N3 Zn2 O3 C32 11.7(3) . . . . ?
N4 Zn2 O3 C32 -38.9(6) . . . . ?
N6 Zn2 O3 C32 115.7(4) . . . . ?
N5' Zn2 O3 C32 116.9(5) . . . . ?
O3 Zn2 O4 C47 -168.3(3) . . . . ?
N3 Zn2 O4 C47 91.6(4) . . . . ?
N4 Zn2 O4 C47 26.2(3) . . . . ?
N6 Zn2 O4 C47 -73.2(4) . . . . ?
N5' Zn2 O4 C47 -74.0(5) . . . . ?
Zn1 O1 C1 C5 -13.9(5) . . . . ?
Zn1 O1 C1 C2 167.6(2) . . . . ?

O1 C1 C2 C3 179.4(3) . . . . ?
C5 C1 C2 C3 0.8(4) . . . . ?
O1 C1 C2 C20 1.9(4) . . . . ?
C5 C1 C2 C20 -176.7(3) . . . . ?
C1 C2 C3 C4 -0.5(5) . . . . ?
C20 C2 C3 C4 176.9(3) . . . . ?
C2 C3 C4 C70 0.0(5) . . . . ?
C2 C3 C4 C24 -176.6(3) . . . . ?
O1 C1 C5 C70 -179.0(3) . . . . ?
C2 C1 C5 C70 -0.5(5) . . . . ?
O1 C1 C5 C6 -4.2(5) . . . . ?
C2 C1 C5 C6 174.3(3) . . . . ?
C7 N1 C6 C5 -175.2(3) . . . . ?
Zn1 N1 C6 C5 5.9(5) . . . . ?
C70 C5 C6 N1 -177.3(3) . . . . ?
C1 C5 C6 N1 7.6(5) . . . . ?
C6 N1 C7 C8 -12.8(5) . . . . ?
Zn1 N1 C7 C8 166.3(3) . . . . ?
C6 N1 C7 C12 166.7(3) . . . . ?
Zn1 N1 C7 C12 -14.2(3) . . . . ?
C12 C7 C8 C9 -4.0(5) . . . . ?
N1 C7 C8 C9 175.5(3) . . . . ?
C7 C8 C9 C10 2.5(6) . . . . ?
C8 C9 C10 C11 0.6(6) . . . . ?
C9 C10 C11 C12 -2.2(6) . . . . ?
C10 C11 C12 C7 0.7(5) . . . . ?
C10 C11 C12 N2 179.0(3) . . . . ?
C8 C7 C12 C11 2.4(5) . . . . ?
N1 C7 C12 C11 -177.1(3) . . . . ?
C8 C7 C12 N2 -176.0(3) . . . . ?
N1 C7 C12 N2 4.4(4) . . . . ?
C13 N2 C12 C11 16.7(5) . . . . ?
Zn1 N2 C12 C11 -170.7(3) . . . . ?
C13 N2 C12 C7 -165.0(3) . . . . ?
Zn1 N2 C12 C7 7.6(4) . . . . ?
C12 N2 C13 C14 -179.3(3) . . . . ?
Zn1 N2 C13 C14 8.9(5) . . . . ?
N2 C13 C14 C19 -1.4(6) . . . . ?
N2 C13 C14 C15 -178.9(3) . . . . ?
C19 C14 C15 C16 -0.9(6) . . . . ?
C13 C14 C15 C16 176.7(4) . . . . ?
C14 C15 C16 C17 -0.1(6) . . . . ?
C15 C16 C17 C18 0.0(6) . . . . ?
C16 C17 C18 C19 1.1(6) . . . . ?
C16 C17 C18 C28 -179.9(4) . . . . ?
Zn1 O2 C19 C14 -13.1(5) . . . . ?
Zn1 O2 C19 C18 165.3(2) . . . . ?
C15 C14 C19 O2 -179.6(3) . . . . ?
C13 C14 C19 O2 2.9(5) . . . . ?
C15 C14 C19 C18 1.9(5) . . . . ?
C13 C14 C19 C18 -175.5(3) . . . . ?
C17 C18 C19 O2 179.5(3) . . . . ?
C28 C18 C19 O2 0.5(5) . . . . ?
C17 C18 C19 C14 -2.0(5) . . . . ?

C28 C18 C19 C14 179.0(3) . . . . ?
C3 C2 C20 C23 6.3(4) . . . . ?
C1 C2 C20 C23 -176.2(3) . . . . ?
C3 C2 C20 C22 126.0(3) . . . . ?
C1 C2 C20 C22 -56.6(4) . . . . ?
C3 C2 C20 C21 -112.3(3) . . . . ?
C1 C2 C20 C21 65.2(4) . . . . ?
C70 C4 C24 C27 174.9(4) . . . . ?
C3 C4 C24 C27 -8.6(6) . . . . ?
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C3 C4 C24 C25 -130.4(5) . . . . ?
C70 C4 C24 C26 -64.9(6) . . . . ?
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C19 C18 C28 C31 63.2(5) . . . . ?
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C19 C18 C28 C29 -178.1(4) . . . . ?
Zn2 O3 C32 C37 -16.1(5) . . . . ?
Zn2 O3 C32 C33 163.1(2) . . . . ?
O3 C32 C33 C34 -178.7(3) . . . . ?
C37 C32 C33 C34 0.5(5) . . . . ?
O3 C32 C33 C52 0.3(5) . . . . ?
C37 C32 C33 C52 179.5(3) . . . . ?
C32 C33 C34 C35 -2.7(5) . . . . ?
C52 C33 C34 C35 178.3(3) . . . . ?
C33 C34 C35 C36 2.4(5) . . . . ?
C33 C34 C35 C56 178.6(3) . . . . ?
C34 C35 C36 C37 0.2(5) . . . . ?
C56 C35 C36 C37 -175.8(3) . . . . ?
C35 C36 C37 C32 -2.3(5) . . . . ?
C35 C36 C37 C38 170.2(3) . . . . ?
O3 C32 C37 C36 -179.0(3) . . . . ?
C33 C32 C37 C36 1.9(5) . . . . ?
O3 C32 C37 C38 9.2(5) . . . . ?
C33 C32 C37 C38 -170.0(3) . . . . ?
C39 N3 C38 C37 174.0(3) . . . . ?
Zn2 N3 C38 C37 -1.0(5) . . . . ?
C36 C37 C38 N3 -172.7(3) . . . . ?
C32 C37 C38 N3 -0.5(5) . . . . ?
C38 N3 C39 C40 12.2(5) . . . . ?
Zn2 N3 C39 C40 -172.3(3) . . . . ?
C38 N3 C39 C44 -167.6(3) . . . . ?
Zn2 N3 C39 C44 7.8(4) . . . . ?
C44 C39 C40 C41 0.9(5) . . . . ?
N3 C39 C40 C41 -178.9(3) . . . . ?
C39 C40 C41 C42 -0.8(6) . . . . ?
C40 C41 C42 C43 -0.4(6) . . . . ?
C41 C42 C43 C44 1.6(6) . . . . ?
C42 C43 C44 C39 -1.4(6) . . . . ?
C42 C43 C44 N4 177.1(4) . . . . ?
C40 C39 C44 C43 0.2(5) . . . . ?
N3 C39 C44 C43 -180.0(3) . . . . ?

C40 C39 C44 N4 -178.5(3) . . . . ?
N3 C39 C44 N4 1.4(4) . . . . ?
C45 N4 C44 C43 -1.8(6) . . . . ?
Zn2 N4 C44 C43 171.6(3) . . . . ?
C45 N4 C44 C39 176.8(3) . . . . ?
Zn2 N4 C44 C39 -9.8(4) . . . . ?
C44 N4 C45 C46 -177.8(3) . . . . ?
Zn2 N4 C45 C46 9.5(5) . . . . ?
N4 C45 C46 C51 -176.6(4) . . . . ?
N4 C45 C46 C47 8.6(6) . . . . ?
Zn2 O4 C47 C46 -17.7(5) . . . . ?
Zn2 O4 C47 C48 164.4(2) . . . . ?
C51 C46 C47 O4 -180.0(3) . . . . ?
C45 C46 C47 O4 -5.3(6) . . . . ?
C51 C46 C47 C48 -2.1(5) . . . . ?
C45 C46 C47 C48 172.5(3) . . . . ?
O4 C47 C48 C49 -179.1(3) . . . . ?
C46 C47 C48 C49 2.9(5) . . . . ?
O4 C47 C48 C60 1.6(5) . . . . ?
C46 C47 C48 C60 -176.3(3) . . . . ?
C47 C48 C49 C50 -0.9(6) . . . . ?
C60 C48 C49 C50 178.3(4) . . . . ?
C48 C49 C50 C51 -2.0(6) . . . . ?
C49 C50 C51 C46 2.8(6) . . . . ?
C45 C46 C51 C50 -175.9(4) . . . . ?
C47 C46 C51 C50 -0.8(6) . . . . ?
C34 C33 C52 C55 -0.1(5) . . . . ?
C32 C33 C52 C55 -179.1(3) . . . . ?
C34 C33 C52 C53 -120.0(4) . . . . ?
C32 C33 C52 C53 61.0(4) . . . . ?
C34 C33 C52 C54 119.0(4) . . . . ?
C32 C33 C52 C54 -60.0(4) . . . . ?
C36 C35 C56 C58 -132.1(4) . . . . ?
C34 C35 C56 C58 52.0(5) . . . . ?
C36 C35 C56 C59 -12.1(6) . . . . ?
C34 C35 C56 C59 172.0(4) . . . . ?
C36 C35 C56 C57 108.0(4) . . . . ?
C34 C35 C56 C57 -67.9(4) . . . . ?
C49 C48 C60 C62 -116.4(4) . . . . ?
C47 C48 C60 C62 62.8(4) . . . . ?
C49 C48 C60 C61 122.4(4) . . . . ?
C47 C48 C60 C61 -58.4(4) . . . . ?
C49 C48 C60 C63 2.9(5) . . . . ?
C47 C48 C60 C63 -177.9(3) . . . . ?
O1 Zn1 N5 C67 78.3(6) . . . . ?
O2 Zn1 N5 C67 176.6(6) . . . . ?
N2 Zn1 N5 C67 -93.2(6) . . . . ?
N1 Zn1 N5 C67 -12.4(6) . . . . ?
N6' Zn1 N5 C67 -30(47) . . . . ?
O1 Zn1 N5 C64 -154.0(8) . . . . ?
O2 Zn1 N5 C64 -55.7(8) . . . . ?
N2 Zn1 N5 C64 34.5(8) . . . . ?
N1 Zn1 N5 C64 115.3(8) . . . . ?
N6' Zn1 N5 C64 98(47) . . . . ?

O1 Zn1 N5 C66 -43.8(6) . . . . ?
O2 Zn1 N5 C66 54.5(6) . . . . ?
N2 Zn1 N5 C66 144.7(5) . . . . ?
N1 Zn1 N5 C66 -134.5(5) . . . . ?
N6' Zn1 N5 C66 -152(48) . . . . ?
O4 Zn2 N6 C64 -151.8(8) . . . . ?
O3 Zn2 N6 C64 -56.3(8) . . . . ?
N3 Zn2 N6 C64 35.4(8) . . . . ?
N4 Zn2 N6 C64 117.3(8) . . . . ?
N5' Zn2 N6 C64 -118(31) . . . . ?
O4 Zn2 N6 C68 -26.8(6) . . . . ?
O3 Zn2 N6 C68 68.7(6) . . . . ?
N3 Zn2 N6 C68 160.4(6) . . . . ?
N4 Zn2 N6 C68 -117.7(6) . . . . ?
N5' Zn2 N6 C68 6(31) . . . . ?
O4 Zn2 N6 C65 83.7(6) . . . . ?
O3 Zn2 N6 C65 179.2(6) . . . . ?
N3 Zn2 N6 C65 -89.1(7) . . . . ?
N4 Zn2 N6 C65 -7.2(7) . . . . ?
N5' Zn2 N6 C65 117(32) . . . . ?
C68 N6 C64 N5 55.7(14) . . . . ?
C65 N6 C64 N5 -60.9(13) . . . . ?
Zn2 N6 C64 N5 173.3(9) . . . . ?
C67 N5 C64 N6 -56.1(14) . . . . ?
C66 N5 C64 N6 64.8(13) . . . . ?
Zn1 N5 C64 N6 176.3(10) . . . . ?
C64 N6 C65 N7 43.6(9) . . . . ?
C68 N6 C65 N7 -82.0(9) . . . . ?
Zn2 N6 C65 N7 165.0(5) . . . . ?
C69 N7 C65 N6 80.6(7) . . . . ?
C66 N7 C65 N6 -37.5(9) . . . . ?
C67 N5 C66 N7 67.7(8) . . . . ?
C64 N5 C66 N7 -56.7(8) . . . . ?
Zn1 N5 C66 N7 -166.9(5) . . . . ?
C69 N7 C66 N5 -68.3(7) . . . . ?
C65 N7 C66 N5 46.4(8) . . . . ?
C64 N5 C67 P1 58.7(9) . . . . ?
C66 N5 C67 P1 -59.1(8) . . . . ?
Zn1 N5 C67 P1 -179.2(3) . . . . ?
C68 P1 C67 N5 -49.2(6) . . . . ?
C69 P1 C67 N5 46.7(6) . . . . ?
C64 N6 C68 P1 -56.8(9) . . . . ?
C65 N6 C68 P1 65.5(8) . . . . ?
Zn2 N6 C68 P1 -175.0(4) . . . . ?
C67 P1 C68 N6 47.6(7) . . . . ?
C69 P1 C68 N6 -48.8(7) . . . . ?
C66 N7 C69 P1 61.0(6) . . . . ?
C65 N7 C69 P1 -62.7(6) . . . . ?
C68 P1 C69 N7 47.7(5) . . . . ?
C67 P1 C69 N7 -48.3(5) . . . . ?
O4 Zn2 N5' C64' -148.8(13) . . . . ?
O3 Zn2 N5' C64' -53.6(13) . . . . ?
N3 Zn2 N5' C64' 38.0(13) . . . . ?
N4 Zn2 N5' C64' 120.3(12) . . . . ?

N6 Zn2 N5' C64' 64(31) . . . . ?
O4 Zn2 N5' C66' -44.6(10) . . . . ?
O3 Zn2 N5' C66' 50.7(10) . . . . ?
N3 Zn2 N5' C66' 142.3(9) . . . . ?
N4 Zn2 N5' C66' -135.5(9) . . . . ?
N6 Zn2 N5' C66' 169(32) . . . . ?
O4 Zn2 N5' C67' 99.0(10) . . . . ?
O3 Zn2 N5' C67' -165.8(10) . . . . ?
N3 Zn2 N5' C67' -74.2(11) . . . . ?
N4 Zn2 N5' C67' 8.1(11) . . . . ?
N6 Zn2 N5' C67' -48(30) . . . . ?
O1 Zn1 N6' C68' -29.7(9) . . . . ?
O2 Zn1 N6' C68' 68.8(9) . . . . ?
N2 Zn1 N6' C68' 159.2(8) . . . . ?
N1 Zn1 N6' C68' -120.3(9) . . . . ?
N5 Zn1 N6' C68' 42(47) . . . . ?
O1 Zn1 N6' C64' -157.5(13) . . . . ?
O2 Zn1 N6' C64' -58.9(13) . . . . ?
N2 Zn1 N6' C64' 31.4(13) . . . . ?
N1 Zn1 N6' C64' 112.0(13) . . . . ?
N5 Zn1 N6' C64' -86(47) . . . . ?
O1 Zn1 N6' C65' 92.5(8) . . . . ?
O2 Zn1 N6' C65' -169.0(9) . . . . ?
N2 Zn1 N6' C65' -78.6(9) . . . . ?
N1 Zn1 N6' C65' 1.9(9) . . . . ?
N5 Zn1 N6' C65' 164(48) . . . . ?
C66' N5' C64' N6' 69(2) . . . . ?
C67' N5' C64' N6' -60(2) . . . . ?
Zn2 N5' C64' N6' 179.1(16) . . . . ?
C68' N6' C64' N5' 51(2) . . . . ?
C65' N6' C64' N5' -70(2) . . . . ?
Zn1 N6' C64' N5' 171.4(15) . . . . ?
C66' N7' C65' N6' -60.7(11) . . . . ?
C69' N7' C65' N6' 62.9(10) . . . . ?
C68' N6' C65' N7' -64.8(12) . . . . ?
C64' N6' C65' N7' 61.4(12) . . . . ?
Zn1 N6' C65' N7' 175.8(7) . . . . ?
C65' N7' C66' N5' 61.9(12) . . . . ?
C69' N7' C66' N5' -63.4(11) . . . . ?
C64' N5' C66' N7' -61.2(11) . . . . ?
C67' N5' C66' N7' 50.6(19) . . . . ?
Zn2 N5' C66' N7' -170.8(7) . . . . ?
C64' N5' C67' P1' 78.6(11) . . . . ?
C66' N5' C67' P1' -31.2(19) . . . . ?
Zn2 N5' C67' P1' -167.1(6) . . . . ?
C69' P1' C67' N5' 23.1(11) . . . . ?
C68' P1' C67' N5' -70.2(10) . . . . ?
C64' N6' C68' P1' -50.6(15) . . . . ?
C65' N6' C68' P1' 65.2(13) . . . . ?
Zn1 N6' C68' P1' -171.7(6) . . . . ?
C69' P1' C68' N6' -52.1(10) . . . . ?
C67' P1' C68' N6' 51.4(10) . . . . ?
C66' N7' C69' P1' 61.5(9) . . . . ?
C65' N7' C69' P1' -60.0(10) . . . . ?

C68' P1' C69' N7' 48.8(8) . . . . ?
C67' P1' C69' N7' -40.1(8) . . . . ?
C3 C4 C70 C5 0.3(5) . . . . ?
C24 C4 C70 C5 177.0(3) . . . . ?
C1 C5 C70 C4 0.0(5) . . . . ?
C6 C5 C70 C4 -175.3(3) . . . . ?
_diffrn_measured_fraction_theta_max 0.980
_diffrn_reflns_theta_full 25.00
_diffrn_measured_fraction_theta_full 0.991
_refine_diff_density_max 2.016
_refine_diff_density_min -0.437
_refine_diff_density_rms 0.097