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Jacobs, I.; van Duin, A.C.T.; Kleij, A.W.; Kuil, M.; Tooke, D.M.; Spek, A.L.; Reek, J.N.H.

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D.M.Tooke & A.L.Spek
Crystal & Structural Chemistry
Padualaan 8, 3584CH Utrecht, The Netherlands

Note: The dataset has only limited resolution, related to the
high disordered solvent volume (4203 out of 19962 cubic Angstrom)
The disordered solvent contribution to the structure factors was taken
into account with the SQUEEZE procedure (see data at the end of this CIF)

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C11 C 0.2976(2) 0.2574(3) 0.12430(9) 0.0507(12) Uani 1 1 d . . .
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H12 H 0.2452 0.1177 0.1320 0.062 Uiso 1 1 calc R . .
C13 C 0.2283(3) 0.0240(3) 0.11338(9) 0.0527(13) Uani 1 1 d . . .
C14 C 0.1809(3) -0.0213(3) 0.13291(10) 0.0733(16) Uani 1 1 d . . .
H14 H 0.1704 0.0006 0.1469 0.088 Uiso 1 1 calc R . .
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C17 C 0.2126(3) -0.0880(3) 0.09190(10) 0.0606(14) Uani 1 1 d . . .
C18 C 0.2456(3) -0.0078(3) 0.09268(9) 0.0538(13) Uani 1 1 d . . .
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C23 C 0.5114(3) 0.2207(3) -0.01391(9) 0.0543(13) Uani 1 1 d . . .
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H24 H 0.5761 0.3330 -0.0187 0.069 Uiso 1 1 calc R . .
C25 C 0.5090(2) 0.3140(2) 0.01127(9) 0.0502(12) Uani 1 1 d . . .
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C26 C 0.2290(4) -0.1248(3) 0.06976(10) 0.0730(17) Uani 1 1 d . . .
C27 C 0.3109(4) -0.0996(3) 0.06839(11) 0.0825(18) Uani 1 1 d . . .
H27A H 0.3394 -0.0457 0.0665 0.124 Uiso 1 1 calc R . .
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H28C H 0.2077 -0.1345 0.0308 0.134 Uiso 1 1 calc R . .
C29 C 0.1853(4) -0.2104(3) 0.07271(11) 0.107(2) Uani 1 1 d . . .
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H29B H 0.1330 -0.2271 0.0757 0.160 Uiso 1 1 calc R . .
H29C H 0.2053 -0.2247 0.0870 0.160 Uiso 1 1 calc R . .
C30 C 0.4296(2) 0.0825(2) -0.00686(9) 0.0486(12) Uani 1 1 d . . .
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H32B H 0.4227 -0.0090 0.0118 0.082 Uiso 1 1 calc R . .

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 H33C H 0.3391 0.0662 -0.0281 0.089 Uiso 1 1 calc R . .
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 C39 C 0.5496(2) 0.3804(2) 0.10981(7) 0.0301(9) Uani 1 1 d . . .
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 H40 H 0.5539 0.2976 0.0908 0.047 Uiso 1 1 calc R . .
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 H66B H 0.2950 0.4448 0.2066 0.097 Uiso 1 1 calc R . .
 H66C H 0.3406 0.4390 0.1832 0.097 Uiso 1 1 calc R . .

loop_

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 _atom_site_aniso_U_13
 _atom_site_aniso_U_12

Zn1 0.0411(3) 0.0319(3) 0.0487(3) -0.0026(2) -0.0127(2) 0.0159(2)
 P1 0.0439(8) 0.0439(8) 0.0392(11) 0.000 0.000 0.0219(4)
 O1 0.071(2) 0.0351(18) 0.058(2) 0.0058(16) -0.0005(18) 0.0210(17)
 O2 0.0446(19) 0.0322(17) 0.060(2) -0.0052(15) -0.0054(16) 0.0180(16)
 N1 0.037(2) 0.036(2) 0.043(2) -0.0043(18) -0.0083(17) 0.0162(19)
 N2 0.045(2) 0.038(2) 0.047(2) -0.0032(19) -0.0138(19) 0.0178(19)
 N3 0.038(2) 0.032(2) 0.044(2) -0.0035(18) -0.0128(18) 0.0186(18)
 C1 0.039(3) 0.041(3) 0.036(2) -0.006(2) -0.007(2) 0.021(2)
 C2 0.042(3) 0.052(3) 0.045(3) -0.004(2) -0.010(2) 0.023(2)
 C3 0.042(3) 0.049(3) 0.038(3) 0.003(2) -0.004(2) 0.018(2)
 C4 0.035(3) 0.040(3) 0.039(3) -0.007(2) -0.008(2) 0.013(2)
 C5 0.049(3) 0.034(3) 0.035(2) -0.003(2) -0.009(2) 0.016(2)
 C6 0.043(3) 0.048(3) 0.041(3) -0.011(2) -0.016(2) 0.025(2)
 C7 0.039(3) 0.042(3) 0.042(3) -0.009(2) -0.016(2) 0.024(2)
 C8 0.051(3) 0.043(3) 0.046(3) -0.007(2) -0.016(2) 0.028(2)
 C9 0.054(3) 0.048(3) 0.055(3) -0.015(3) -0.021(3) 0.031(3)
 C10 0.052(3) 0.065(4) 0.050(3) -0.017(3) -0.015(3) 0.037(3)
 C11 0.046(3) 0.056(3) 0.049(3) 0.000(2) -0.009(2) 0.024(3)
 C12 0.049(3) 0.055(3) 0.046(3) -0.002(3) -0.013(2) 0.023(3)
 C13 0.047(3) 0.043(3) 0.053(3) 0.013(3) -0.010(2) 0.011(2)

C14 0.064(4) 0.066(4) 0.069(4) 0.006(3) -0.004(3) 0.017(3)
 C15 0.078(4) 0.057(4) 0.077(4) 0.019(3) 0.008(3) 0.011(3)
 C16 0.079(4) 0.043(3) 0.078(4) 0.002(3) -0.018(3) 0.007(3)
 C17 0.066(3) 0.036(3) 0.059(3) 0.007(3) -0.021(3) 0.010(3)
 C18 0.052(3) 0.051(3) 0.048(3) -0.001(3) -0.019(3) 0.018(3)
 C19 0.039(3) 0.032(2) 0.052(3) -0.004(2) -0.016(2) 0.019(2)
 C20 0.042(3) 0.034(3) 0.041(3) -0.003(2) -0.009(2) 0.021(2)
 C21 0.033(3) 0.031(3) 0.053(3) -0.004(2) -0.016(2) 0.016(2)
 C22 0.042(3) 0.044(3) 0.053(3) -0.010(2) -0.013(2) 0.027(2)
 C23 0.049(3) 0.057(3) 0.058(3) -0.012(3) -0.002(3) 0.027(3)
 C24 0.056(3) 0.042(3) 0.063(3) -0.006(3) 0.002(3) 0.016(3)
 C25 0.054(3) 0.032(3) 0.059(3) -0.006(2) -0.005(3) 0.018(2)
 C26 0.110(5) 0.034(3) 0.054(3) -0.001(2) -0.016(3) 0.020(3)
 C27 0.115(5) 0.061(4) 0.074(4) -0.001(3) -0.007(4) 0.045(4)
 C28 0.126(5) 0.056(4) 0.061(4) -0.008(3) -0.033(4) 0.026(4)
 C29 0.166(7) 0.037(3) 0.087(4) 0.000(3) -0.007(4) 0.028(4)
 C30 0.054(3) 0.044(3) 0.057(3) -0.011(2) -0.020(2) 0.030(2)
 C31 0.069(3) 0.056(3) 0.065(3) -0.017(3) -0.016(3) 0.041(3)
 C32 0.061(3) 0.040(3) 0.072(3) -0.013(2) -0.017(3) 0.032(3)
 C33 0.060(3) 0.048(3) 0.074(3) -0.020(3) -0.029(3) 0.030(3)
 Zn2 0.0345(3) 0.0331(3) 0.0271(3) -0.0024(2) 0.0000(2) 0.0195(2)
 P2 0.0326(6) 0.0326(6) 0.0258(10) 0.000 0.000 0.0163(3)
 O3 0.0417(17) 0.0347(17) 0.0359(16) -0.0033(13) 0.0065(13) 0.0191(14)
 O4 0.0419(17) 0.0381(18) 0.0405(17) -0.0014(13) 0.0032(13) 0.0249(15)
 N4 0.0332(19) 0.030(2) 0.0293(18) -0.0043(16) -0.0007(15) 0.0164(17)
 N5 0.0295(19) 0.033(2) 0.0280(18) -0.0034(15) -0.0006(15) 0.0173(16)
 N6 0.039(2) 0.034(2) 0.0286(18) -0.0002(15) -0.0027(15) 0.0215(17)
 C34 0.031(2) 0.033(2) 0.021(2) 0.0001(17) 0.0038(18) 0.0168(19)
 C35 0.033(2) 0.029(2) 0.028(2) -0.0038(18) 0.0017(19) 0.016(2)
 C36 0.040(3) 0.034(3) 0.038(2) 0.004(2) 0.005(2) 0.021(2)
 C37 0.048(3) 0.032(2) 0.038(3) -0.006(2) -0.010(2) 0.016(2)
 C38 0.036(2) 0.036(3) 0.029(2) -0.0041(19) -0.0113(19) 0.015(2)
 C39 0.026(2) 0.044(3) 0.024(2) -0.0036(19) -0.0044(18) 0.020(2)
 C40 0.038(3) 0.045(3) 0.034(2) -0.007(2) 0.002(2) 0.021(2)
 C41 0.037(3) 0.065(3) 0.030(2) -0.009(2) 0.002(2) 0.029(2)
 C42 0.038(3) 0.062(3) 0.032(2) 0.011(2) 0.005(2) 0.027(2)
 C43 0.043(3) 0.047(3) 0.037(3) 0.004(2) 0.005(2) 0.027(2)
 C44 0.030(2) 0.042(3) 0.025(2) -0.0034(19) -0.0047(18) 0.021(2)
 C45 0.035(2) 0.041(3) 0.034(2) -0.012(2) -0.008(2) 0.024(2)
 C46 0.032(2) 0.037(3) 0.029(2) -0.0020(19) -0.0023(19) 0.019(2)
 C47 0.030(2) 0.037(3) 0.032(2) -0.004(2) -0.0051(19) 0.018(2)
 C48 0.034(2) 0.036(3) 0.036(2) 0.002(2) 0.000(2) 0.016(2)
 C49 0.039(3) 0.044(3) 0.043(3) 0.007(2) 0.003(2) 0.013(2)
 C50 0.057(3) 0.027(2) 0.046(3) -0.002(2) -0.005(2) 0.018(2)
 C51 0.051(3) 0.041(3) 0.036(2) -0.005(2) -0.003(2) 0.028(2)
 C52 0.050(3) 0.040(3) 0.032(2) 0.005(2) 0.001(2) 0.023(2)
 C53 0.053(3) 0.038(3) 0.040(3) -0.004(2) 0.001(2) 0.027(2)
 C54 0.084(4) 0.048(3) 0.055(3) 0.003(3) 0.017(3) 0.035(3)
 C55 0.116(5) 0.041(3) 0.079(4) -0.002(3) 0.028(4) 0.042(3)
 C56 0.089(4) 0.050(3) 0.069(4) -0.005(3) 0.020(3) 0.043(3)
 C57 0.059(3) 0.039(3) 0.043(3) -0.006(2) -0.001(2) 0.032(2)
 C58 0.043(3) 0.038(3) 0.038(2) -0.006(2) -0.004(2) 0.026(2)
 C59 0.046(3) 0.050(3) 0.040(3) 0.004(2) 0.012(2) 0.023(2)
 C60 0.067(3) 0.070(3) 0.038(3) -0.010(2) 0.004(2) 0.037(3)

C61 0.068(4) 0.066(3) 0.057(3) 0.013(3) 0.030(3) 0.028(3)
 C62 0.049(3) 0.074(4) 0.063(3) 0.007(3) 0.017(2) 0.038(3)
 C63 0.053(3) 0.048(3) 0.052(3) -0.012(2) 0.008(2) 0.028(3)
 C64 0.084(4) 0.068(4) 0.076(4) -0.017(3) 0.021(3) 0.042(3)
 C65 0.067(3) 0.076(4) 0.041(3) 0.008(3) 0.012(3) 0.035(3)
 C66 0.045(3) 0.063(3) 0.088(4) -0.013(3) 0.010(3) 0.029(3)

_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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loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

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Zn1 O1 1.947(3) . ?

Zn1 O2 1.960(3) . ?

Zn1 N3 2.074(3) . ?

Zn1 N2 2.092(4) . ?

Zn1 N1 2.131(3) . ?

P1 C1 1.847(4) 2 ?

P1 C1 1.847(4) . ?

P1 C1 1.847(4) 3 ?

O1 C18 1.291(5) . ?

O2 C21 1.291(5) . ?

N1 C5 1.335(5) . ?

N1 C4 1.339(5) . ?

N2 C12 1.298(5) . ?

N2 C6 1.415(5) . ?

N3 C19 1.293(5) . ?

N3 C7 1.413(5) . ?

C1 C2 1.380(6) . ?

C1 C5 1.386(5) . ?

C2 C3 1.380(6) . ?

C2 H2 0.9500 . ?

C3 C4 1.380(6) . ?

C3 H3 0.9500 . ?

C4 H4 0.9500 . ?

C5 H5 0.9500 . ?

C6 C11 1.397(6) . ?

C6 C7 1.404(6) . ?

C7 C8 1.398(6) . ?

C8 C9 1.382(6) . ?

C8 H8 0.9500 . ?

C9 C10 1.385(6) . ?

C9 H9 0.9500 . ?

C10 C11 1.373(6) . ?
C10 H10 0.9500 . ?
C11 H11 0.9500 . ?
C12 C13 1.442(6) . ?
C12 H12 0.9500 . ?
C13 C14 1.417(7) . ?
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C14 H14 0.9500 . ?
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C16 C17 1.368(7) . ?
C16 H16 0.9500 . ?
C17 C18 1.456(6) . ?
C17 C26 1.531(7) . ?
C19 C20 1.440(6) . ?
C19 H19 0.9500 . ?
C20 C25 1.417(6) . ?
C20 C21 1.440(5) . ?
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C22 C23 1.370(6) . ?
C22 C30 1.537(6) . ?
C23 C24 1.400(6) . ?
C23 H23 0.9500 . ?
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C24 H24 0.9500 . ?
C25 H25 0.9500 . ?
C26 C27 1.519(8) . ?
C26 C29 1.555(7) . ?
C26 C28 1.558(7) . ?
C27 H27A 0.9800 . ?
C27 H27B 0.9800 . ?
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C28 H28A 0.9800 . ?
C28 H28B 0.9800 . ?
C28 H28C 0.9800 . ?
C29 H29A 0.9800 . ?
C29 H29B 0.9800 . ?
C29 H29C 0.9800 . ?
C30 C33 1.533(6) . ?
C30 C31 1.541(6) . ?
C30 C32 1.545(6) . ?
C31 H31A 0.9800 . ?
C31 H31B 0.9800 . ?
C31 H31C 0.9800 . ?
C32 H32A 0.9800 . ?
C32 H32B 0.9800 . ?
C32 H32C 0.9800 . ?
C33 H33A 0.9800 . ?
C33 H33B 0.9800 . ?
C33 H33C 0.9800 . ?
Zn2 O4 1.959(3) . ?
Zn2 O3 1.971(3) . ?
Zn2 N5 2.071(3) . ?

Zn2 N6 2.105(3) . ?
Zn2 N4 2.114(3) . ?
P2 C34 1.826(4) . ?
P2 C34 1.827(4) 3_665 ?
P2 C34 1.827(4) 2_655 ?
O3 C47 1.298(4) . ?
O4 C58 1.300(5) . ?
N4 C36 1.335(5) . ?
N4 C35 1.344(5) . ?
N5 C45 1.297(5) . ?
N5 C39 1.423(5) . ?
N6 C52 1.286(5) . ?
N6 C44 1.417(5) . ?
C34 C35 1.384(5) . ?
C34 C38 1.393(5) . ?
C35 H35 0.9500 . ?
C36 C37 1.386(5) . ?
C36 H36 0.9500 . ?
C37 C38 1.369(5) . ?
C37 H37 0.9500 . ?
C38 H38 0.9500 . ?
C39 C40 1.392(5) . ?
C39 C44 1.410(5) . ?
C40 C41 1.381(6) . ?
C40 H40 0.9500 . ?
C41 C42 1.377(6) . ?
C41 H41 0.9500 . ?
C42 C43 1.368(6) . ?
C42 H42 0.9500 . ?
C43 C44 1.395(5) . ?
C43 H43 0.9500 . ?
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C45 H45 0.9500 . ?
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C46 C47 1.422(5) . ?
C47 C48 1.443(5) . ?
C48 C49 1.375(6) . ?
C48 C59 1.534(6) . ?
C49 C50 1.398(6) . ?
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C50 C51 1.361(6) . ?
C50 H50 0.9500 . ?
C51 H51 0.9500 . ?
C52 C53 1.432(6) . ?
C52 H52 0.9500 . ?
C53 C54 1.424(6) . ?
C53 C58 1.429(6) . ?
C54 C55 1.359(6) . ?
C54 H54 0.9500 . ?
C55 C56 1.401(7) . ?
C55 H55 0.9500 . ?
C56 C57 1.381(6) . ?
C56 H56 0.9500 . ?
C57 C58 1.435(5) . ?

C57 C63 1.541(6) . ?
 C59 C61 1.533(6) . ?
 C59 C62 1.539(6) . ?
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 C60 H60B 0.9800 . ?
 C60 H60C 0.9800 . ?
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 C61 H61B 0.9800 . ?
 C61 H61C 0.9800 . ?
 C62 H62A 0.9800 . ?
 C62 H62B 0.9800 . ?
 C62 H62C 0.9800 . ?
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 C63 C64 1.528(6) . ?
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 C64 H64C 0.9800 . ?
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 C65 H65B 0.9800 . ?
 C65 H65C 0.9800 . ?
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 C66 H66C 0.9800 . ?

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 O1 Zn1 N3 155.18(13) . . ?
 O2 Zn1 N3 89.92(13) . . ?
 O1 Zn1 N2 89.41(14) . . ?
 O2 Zn1 N2 163.05(13) . . ?
 N3 Zn1 N2 78.87(14) . . ?
 O1 Zn1 N1 103.42(13) . . ?
 O2 Zn1 N1 99.85(12) . . ?
 N3 Zn1 N1 99.29(13) . . ?
 N2 Zn1 N1 94.53(13) . . ?
 C1 P1 C1 100.69(16) 2 . ?
 C1 P1 C1 100.69(16) 2 3 ?
 C1 P1 C1 100.70(16) . 3 ?
 C18 O1 Zn1 128.7(3) . . ?
 C21 O2 Zn1 132.3(3) . . ?
 C5 N1 C4 117.7(4) . . ?
 C5 N1 Zn1 122.0(3) . . ?
 C4 N1 Zn1 119.7(3) . . ?
 C12 N2 C6 123.2(4) . . ?
 C12 N2 Zn1 123.4(3) . . ?

C6 N2 Zn1 113.3(3) . . ?
 C19 N3 C7 122.0(4) . . ?
 C19 N3 Zn1 124.0(3) . . ?
 C7 N3 Zn1 114.0(3) . . ?
 C2 C1 C5 117.1(4) . . ?
 C2 C1 P1 125.2(3) . . ?
 C5 C1 P1 117.7(3) . . ?
 C3 C2 C1 119.4(4) . . ?
 C3 C2 H2 120.3 . . ?
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 N1 C5 C1 124.3(4) . . ?
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 C7 C6 N2 116.1(4) . . ?
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 C7 C8 H8 119.4 . . ?
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 C14 C13 C18 120.5(5) . . ?
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 C17 C16 C15 124.5(5) . . ?
 C17 C16 H16 117.8 . . ?
 C15 C16 H16 117.8 . . ?
 C16 C17 C18 117.2(5) . . ?
 C16 C17 C26 122.7(5) . . ?

C18 C17 C26 120.2(5) . . ?
O1 C18 C13 122.9(4) . . ?
O1 C18 C17 118.7(5) . . ?
C13 C18 C17 118.4(5) . . ?
N3 C19 C20 127.6(4) . . ?
N3 C19 H19 116.2 . . ?
C20 C19 H19 116.2 . . ?
C25 C20 C21 119.9(4) . . ?
C25 C20 C19 116.0(4) . . ?
C21 C20 C19 124.0(4) . . ?
O2 C21 C20 122.0(4) . . ?
O2 C21 C22 120.0(4) . . ?
C20 C21 C22 117.9(4) . . ?
C23 C22 C21 118.5(4) . . ?
C23 C22 C30 121.7(4) . . ?
C21 C22 C30 119.9(4) . . ?
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C24 C23 H23 118.1 . . ?
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C23 C24 H24 120.6 . . ?
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C20 C25 H25 119.5 . . ?
C27 C26 C17 111.0(4) . . ?
C27 C26 C29 108.3(5) . . ?
C17 C26 C29 110.5(5) . . ?
C27 C26 C28 110.4(5) . . ?
C17 C26 C28 109.5(5) . . ?
C29 C26 C28 107.1(4) . . ?
C26 C27 H27A 109.5 . . ?
C26 C27 H27B 109.5 . . ?
H27A C27 H27B 109.5 . . ?
C26 C27 H27C 109.5 . . ?
H27A C27 H27C 109.5 . . ?
H27B C27 H27C 109.5 . . ?
C26 C28 H28A 109.5 . . ?
C26 C28 H28B 109.5 . . ?
H28A C28 H28B 109.5 . . ?
C26 C28 H28C 109.5 . . ?
H28A C28 H28C 109.5 . . ?
H28B C28 H28C 109.5 . . ?
C26 C29 H29A 109.5 . . ?
C26 C29 H29B 109.5 . . ?
H29A C29 H29B 109.5 . . ?
C26 C29 H29C 109.5 . . ?
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H29B C29 H29C 109.5 . . ?
C33 C30 C22 110.6(3) . . ?
C33 C30 C31 107.8(4) . . ?
C22 C30 C31 111.7(4) . . ?
C33 C30 C32 108.4(4) . . ?
C22 C30 C32 110.4(3) . . ?

C31 C30 C32 107.7(4) . . ?
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 H31A C31 H31B 109.5 . . ?
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 H31A C31 H31C 109.5 . . ?
 H31B C31 H31C 109.5 . . ?
 C30 C32 H32A 109.5 . . ?
 C30 C32 H32B 109.5 . . ?
 H32A C32 H32B 109.5 . . ?
 C30 C32 H32C 109.5 . . ?
 H32A C32 H32C 109.5 . . ?
 H32B C32 H32C 109.5 . . ?
 C30 C33 H33A 109.5 . . ?
 C30 C33 H33B 109.5 . . ?
 H33A C33 H33B 109.5 . . ?
 C30 C33 H33C 109.5 . . ?
 H33A C33 H33C 109.5 . . ?
 H33B C33 H33C 109.5 . . ?
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 O4 Zn2 N5 153.37(11) . . ?
 O3 Zn2 N5 89.81(11) . . ?
 O4 Zn2 N6 87.49(12) . . ?
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 C34 P2 C34 103.31(14) . 2_655 ?
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C44 C39 N5 116.7(3) . . ?
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C40 C41 H41 119.8 . . ?
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C39 C44 N6 115.3(3) . . ?
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N5 C45 H45 116.4 . . ?
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C51 C46 C45 115.5(3) . . ?
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O3 C47 C48 119.0(3) . . ?
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O4 C58 C53 122.4(3) . . ?
O4 C58 C57 118.8(4) . . ?
C53 C58 C57 118.7(4) . . ?
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C48 C59 C62 110.1(3) . . ?
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C62 C59 C60 110.3(4) . . ?
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H60B C60 H60C 109.5 . . ?
C59 C61 H61A 109.5 . . ?
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H61A C61 H61B 109.5 . . ?
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H61A C61 H61C 109.5 . . ?
H61B C61 H61C 109.5 . . ?
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H62A C62 H62B 109.5 . . ?
C59 C62 H62C 109.5 . . ?
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H62B C62 H62C 109.5 . . ?
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C64 C63 C65 108.1(4) . . ?
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C65 C63 C57 109.7(4) . . ?
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O1 Zn1 N2 C6 169.2(3) ?
O2 Zn1 N2 C6 60.7(6) ?
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O1 Zn1 N3 C19 104.8(4) ?
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 C2 C3 C4 N1 -2.1(6) ?
 C4 N1 C5 C1 0.6(6) ?
 Zn1 N1 C5 C1 171.9(3) ?
 C2 C1 C5 N1 -1.3(6) ?
 P1 C1 C5 N1 178.7(3) ?
 C12 N2 C6 C11 -6.1(6) ?
 Zn1 N2 C6 C11 170.1(3) ?
 C12 N2 C6 C7 174.5(4) ?
 Zn1 N2 C6 C7 -9.3(4) ?
 C11 C6 C7 C8 -0.3(6) ?
 N2 C6 C7 C8 179.2(3) ?
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 N2 C6 C7 N3 -0.5(5) ?
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 Zn1 N3 C7 C6 10.2(4) ?
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 C7 C8 C9 C10 -1.3(6) ?
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 C7 C6 C11 C10 -1.2(6) ?
 N2 C6 C11 C10 179.4(4) ?
 C6 N2 C12 C13 178.4(4) ?
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 C25 C20 C21 O2 -179.3(4) ?

C19 C20 C21 O2 4.5(6) ?
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 O2 C21 C22 C23 179.4(4) ?
 C20 C21 C22 C23 -1.2(6) ?
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 C20 C21 C22 C30 178.0(3) ?
 C21 C22 C23 C24 0.1(7) ?
 C30 C22 C23 C24 -179.1(4) ?
 C22 C23 C24 C25 1.0(7) ?
 C23 C24 C25 C20 -0.9(7) ?
 C21 C20 C25 C24 -0.2(7) ?
 C19 C20 C25 C24 176.3(4) ?
 C16 C17 C26 C27 -119.4(5) ?
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 C16 C17 C26 C29 0.7(8) ?
 C18 C17 C26 C29 -177.9(5) ?
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 C21 C22 C30 C33 60.9(5) ?
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 C21 C22 C30 C31 -179.0(4) ?
 C23 C22 C30 C32 120.2(5) ?
 C21 C22 C30 C32 -59.1(5) ?
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 O3 Zn2 N4 C36 -125.0(3) ?
 N5 Zn2 N4 C36 143.6(3) ?
 N6 Zn2 N4 C36 61.9(3) ?
 O4 Zn2 N4 C35 145.6(3) ?
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 N6 Zn2 N5 C45 -170.0(3) ?
 N4 Zn2 N5 C45 90.7(3) ?
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 N6 Zn2 N5 C39 6.2(2) ?
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 O3 Zn2 N6 C52 123.0(4) ?
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 O4 Zn2 N6 C44 -164.2(2) ?

O3 Zn2 N6 C44 -61.2(5) ?
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N4 Zn2 N6 C44 96.7(2) ?
C34 P2 C34 C35 102.4(2) 3_665 . . . ?
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Zn2 N4 C35 C34 -173.2(3) ?
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P2 C34 C35 N4 172.9(3) ?
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C40 C39 C44 C43 -0.5(5) ?
N5 C39 C44 C43 -179.0(3) ?
C40 C39 C44 N6 176.6(3) ?
N5 C39 C44 N6 -1.9(5) ?
C52 N6 C44 C43 -0.1(6) ?
Zn2 N6 C44 C43 -176.0(3) ?
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Zn2 N6 C44 C39 7.1(4) ?
C39 N5 C45 C46 -174.3(3) ?
Zn2 N5 C45 C46 1.6(5) ?
N5 C45 C46 C51 -179.9(4) ?
N5 C45 C46 C47 4.8(6) ?
Zn2 O3 C47 C46 -0.2(5) ?
Zn2 O3 C47 C48 -178.6(3) ?
C51 C46 C47 O3 179.2(3) ?
C45 C46 C47 O3 -5.6(6) ?
C51 C46 C47 C48 -2.3(5) ?
C45 C46 C47 C48 172.8(3) ?
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C46 C47 C48 C59 -179.0(4) ?
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 4 0.333 0.667 0.604 342.1 51.2
 5 0.333 0.667 0.358 31.5 2.2

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